



## Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 01:12 PM EDT

PDB ID : 9O3Z / pdb\_00009o3z  
EMDB ID : EMD-70087  
Title : Phosphonull (T209A) of stress-activating residues  
Authors : Martinez-Bond, E.A.; Lopez-Ayala, I.; Qiu, L.; Garda, V.; Yu, Z.; Williams, A.H.  
Deposited on : 2025-04-08  
Resolution : 3.42 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

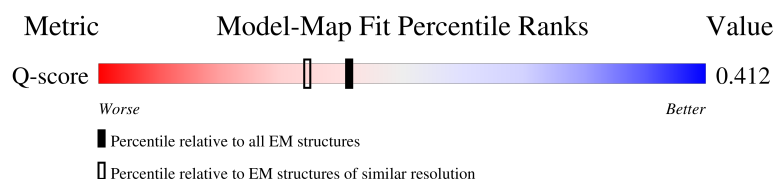
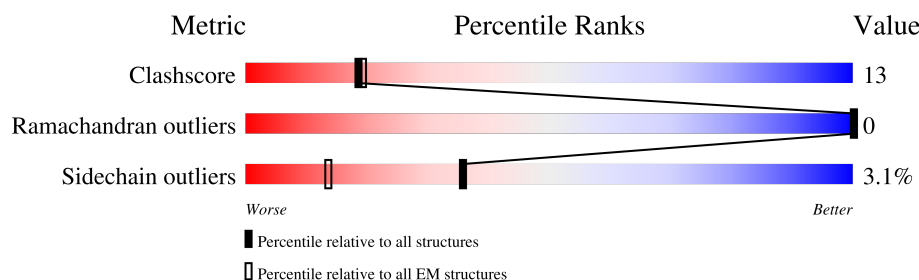
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.42 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	13959 ( 2.92 - 3.92 )

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

Mol	Chain	Length	Quality of chain
1	A	278	
1	AB	278	
1	B	278	
1	BB	278	

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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	






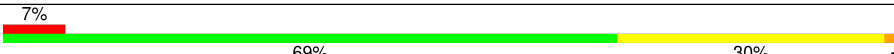
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Mol	Chain	Length	Quality of chain
1	OB	278	
1	P	278	
1	PB	278	
1	Q	278	
1	QB	278	
1	R	278	
1	RB	278	
1	S	278	
1	SB	278	
1	T	278	
1	TB	278	
1	U	278	
1	UB	278	
1	V	278	
1	VB	278	
1	W	278	
1	WB	278	
2	a	118	
2	ab	118	
2	b	118	
2	bb	118	
2	c	118	
2	cb	118	
2	d	118	
2	db	118	

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Mol	Chain	Length	Quality of chain
2	e	118	 8% 69% 31%
2	eb	118	 5% 70% 28% •
2	f	118	 8% 69% 30% •
2	fb	118	 5% 65% 34% •
2	g	118	 6% 64% 34% •
2	gb	118	 7% 69% 30% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 58426 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 RsbR.

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		
1	U	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	UB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	V	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	VB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	W	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	WB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ASP	ASN	conflict	UNP Q8GD19
A	209	ALA	THR	engineered mutation	UNP Q8GD19
AB	19	ASP	ASN	conflict	UNP Q8GD19
AB	209	ALA	THR	engineered mutation	UNP Q8GD19
B	19	ASP	ASN	conflict	UNP Q8GD19
B	209	ALA	THR	engineered mutation	UNP Q8GD19
BB	19	ASP	ASN	conflict	UNP Q8GD19
BB	209	ALA	THR	engineered mutation	UNP Q8GD19
C	19	ASP	ASN	conflict	UNP Q8GD19
C	209	ALA	THR	engineered mutation	UNP Q8GD19
CB	19	ASP	ASN	conflict	UNP Q8GD19
CB	209	ALA	THR	engineered mutation	UNP Q8GD19
D	19	ASP	ASN	conflict	UNP Q8GD19
D	209	ALA	THR	engineered mutation	UNP Q8GD19
DB	19	ASP	ASN	conflict	UNP Q8GD19
DB	209	ALA	THR	engineered mutation	UNP Q8GD19
E	19	ASP	ASN	conflict	UNP Q8GD19
E	209	ALA	THR	engineered mutation	UNP Q8GD19
EB	19	ASP	ASN	conflict	UNP Q8GD19
EB	209	ALA	THR	engineered mutation	UNP Q8GD19
F	19	ASP	ASN	conflict	UNP Q8GD19
F	209	ALA	THR	engineered mutation	UNP Q8GD19
FB	19	ASP	ASN	conflict	UNP Q8GD19

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Chain	Residue	Modelled	Actual	Comment	Reference
FB	209	ALA	THR	engineered mutation	UNP Q8GD19
G	19	ASP	ASN	conflict	UNP Q8GD19
G	209	ALA	THR	engineered mutation	UNP Q8GD19
GB	19	ASP	ASN	conflict	UNP Q8GD19
GB	209	ALA	THR	engineered mutation	UNP Q8GD19
H	19	ASP	ASN	conflict	UNP Q8GD19
H	209	ALA	THR	engineered mutation	UNP Q8GD19
HB	19	ASP	ASN	conflict	UNP Q8GD19
HB	209	ALA	THR	engineered mutation	UNP Q8GD19
I	19	ASP	ASN	conflict	UNP Q8GD19
I	209	ALA	THR	engineered mutation	UNP Q8GD19
IB	19	ASP	ASN	conflict	UNP Q8GD19
IB	209	ALA	THR	engineered mutation	UNP Q8GD19
J	19	ASP	ASN	conflict	UNP Q8GD19
J	209	ALA	THR	engineered mutation	UNP Q8GD19
JB	19	ASP	ASN	conflict	UNP Q8GD19
JB	209	ALA	THR	engineered mutation	UNP Q8GD19
K	19	ASP	ASN	conflict	UNP Q8GD19
K	209	ALA	THR	engineered mutation	UNP Q8GD19
KB	19	ASP	ASN	conflict	UNP Q8GD19
KB	209	ALA	THR	engineered mutation	UNP Q8GD19
L	19	ASP	ASN	conflict	UNP Q8GD19
L	209	ALA	THR	engineered mutation	UNP Q8GD19
LB	19	ASP	ASN	conflict	UNP Q8GD19
LB	209	ALA	THR	engineered mutation	UNP Q8GD19
M	19	ASP	ASN	conflict	UNP Q8GD19
M	209	ALA	THR	engineered mutation	UNP Q8GD19
MB	19	ASP	ASN	conflict	UNP Q8GD19
MB	209	ALA	THR	engineered mutation	UNP Q8GD19
N	19	ASP	ASN	conflict	UNP Q8GD19
N	209	ALA	THR	engineered mutation	UNP Q8GD19
NB	19	ASP	ASN	conflict	UNP Q8GD19
NB	209	ALA	THR	engineered mutation	UNP Q8GD19
O	19	ASP	ASN	conflict	UNP Q8GD19
O	209	ALA	THR	engineered mutation	UNP Q8GD19
OB	19	ASP	ASN	conflict	UNP Q8GD19
OB	209	ALA	THR	engineered mutation	UNP Q8GD19
P	19	ASP	ASN	conflict	UNP Q8GD19
P	209	ALA	THR	engineered mutation	UNP Q8GD19
PB	19	ASP	ASN	conflict	UNP Q8GD19
PB	209	ALA	THR	engineered mutation	UNP Q8GD19
Q	19	ASP	ASN	conflict	UNP Q8GD19

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	209	ALA	THR	engineered mutation	UNP Q8GD19
QB	19	ASP	ASN	conflict	UNP Q8GD19
QB	209	ALA	THR	engineered mutation	UNP Q8GD19
R	19	ASP	ASN	conflict	UNP Q8GD19
R	209	ALA	THR	engineered mutation	UNP Q8GD19
RB	19	ASP	ASN	conflict	UNP Q8GD19
RB	209	ALA	THR	engineered mutation	UNP Q8GD19
S	19	ASP	ASN	conflict	UNP Q8GD19
S	209	ALA	THR	engineered mutation	UNP Q8GD19
SB	19	ASP	ASN	conflict	UNP Q8GD19
SB	209	ALA	THR	engineered mutation	UNP Q8GD19
T	19	ASP	ASN	conflict	UNP Q8GD19
T	209	ALA	THR	engineered mutation	UNP Q8GD19
TB	19	ASP	ASN	conflict	UNP Q8GD19
TB	209	ALA	THR	engineered mutation	UNP Q8GD19
U	19	ASP	ASN	conflict	UNP Q8GD19
U	209	ALA	THR	engineered mutation	UNP Q8GD19
UB	19	ASP	ASN	conflict	UNP Q8GD19
UB	209	ALA	THR	engineered mutation	UNP Q8GD19
V	19	ASP	ASN	conflict	UNP Q8GD19
V	209	ALA	THR	engineered mutation	UNP Q8GD19
VB	19	ASP	ASN	conflict	UNP Q8GD19
VB	209	ALA	THR	engineered mutation	UNP Q8GD19
W	19	ASP	ASN	conflict	UNP Q8GD19
W	209	ALA	THR	engineered mutation	UNP Q8GD19
WB	19	ASP	ASN	conflict	UNP Q8GD19
WB	209	ALA	THR	engineered mutation	UNP Q8GD19

- 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		

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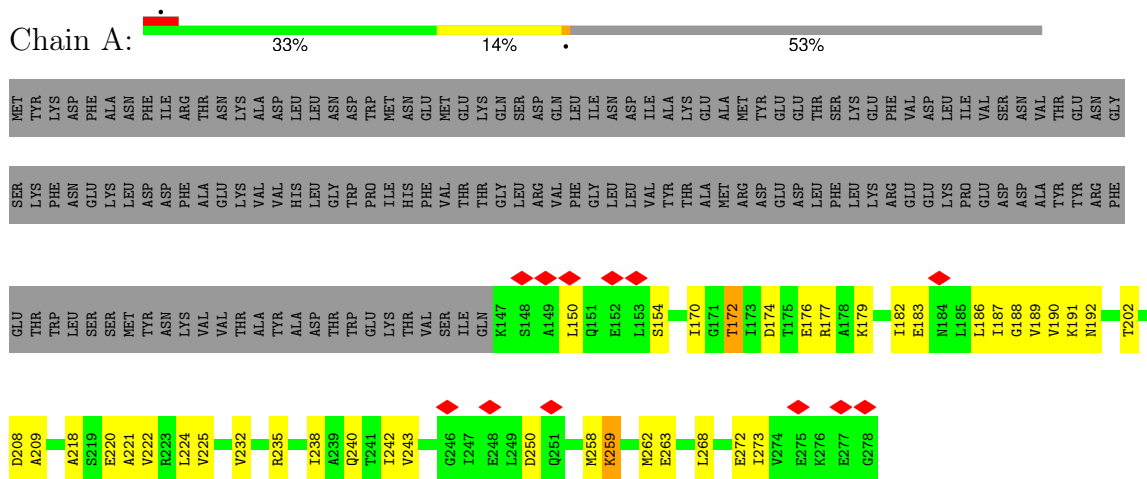
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	db	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	e	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	eb	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	f	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	fb	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	g	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	gb	118	Total 881	C 565	N 136	O 175	S 5	0	0

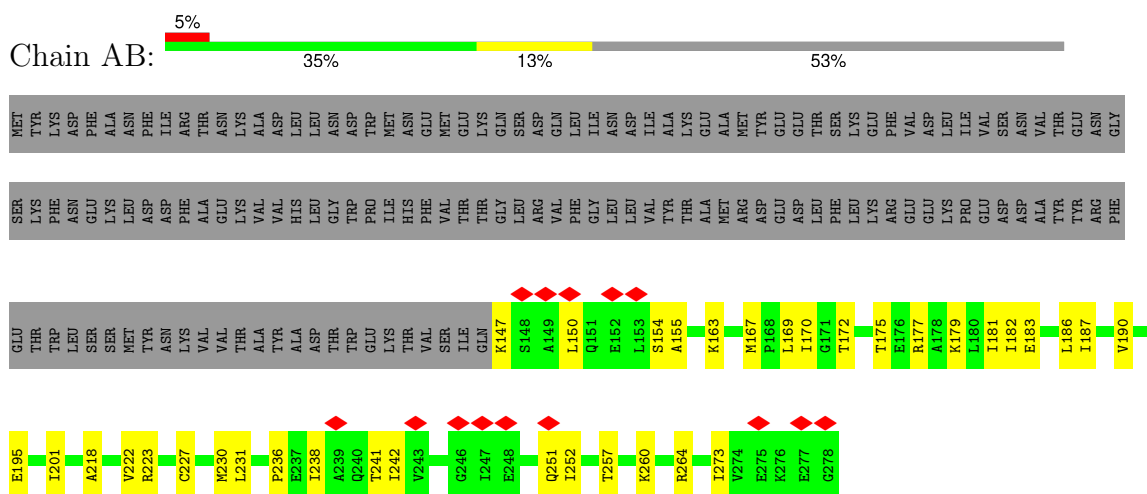
### 3 Residue-property plots

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

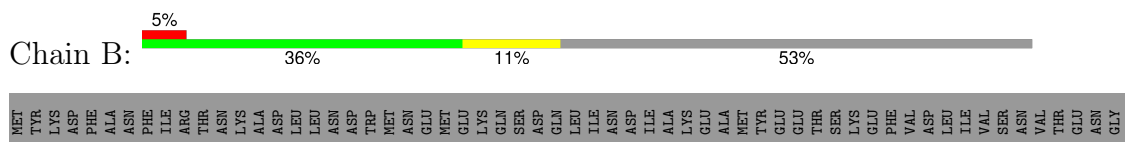
#### • Molecule 1: RsbR

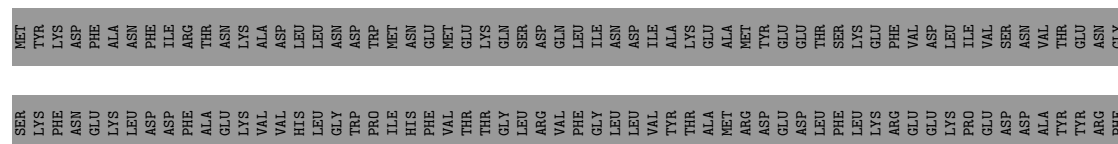


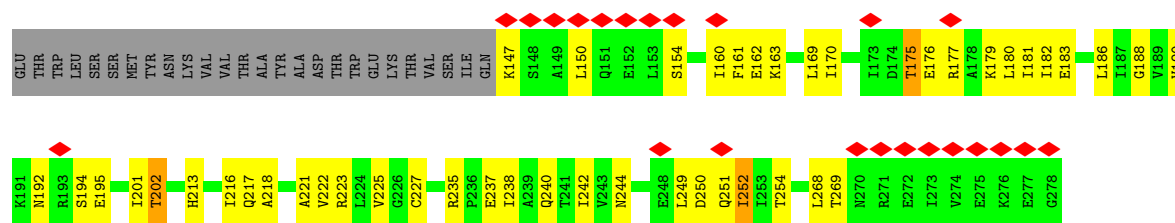
#### • Molecule 1: RsbR



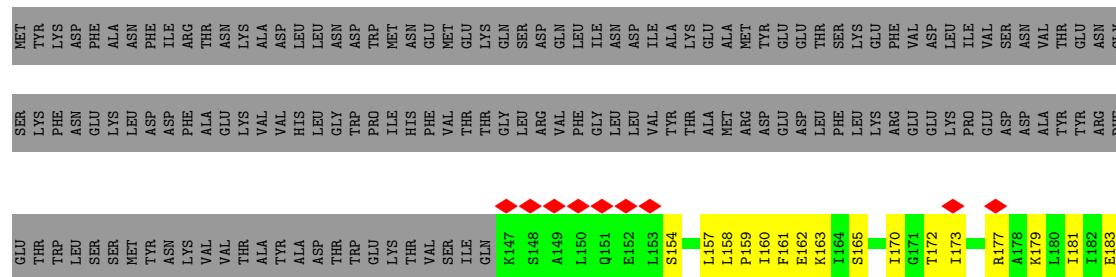
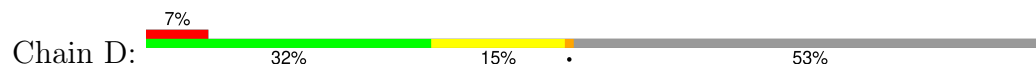
#### • Molecule 1: RsbR



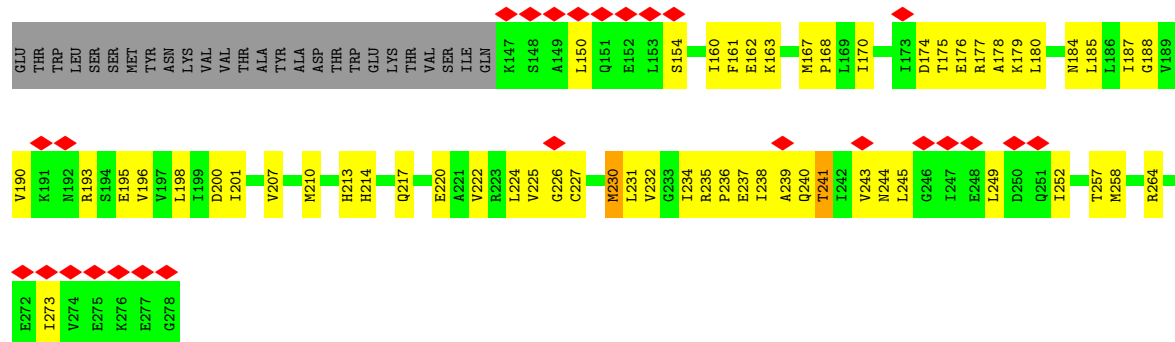
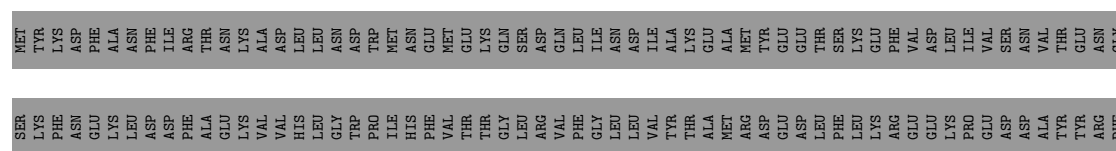
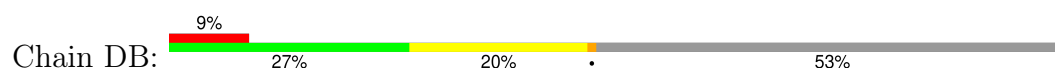




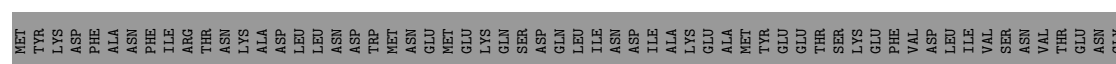
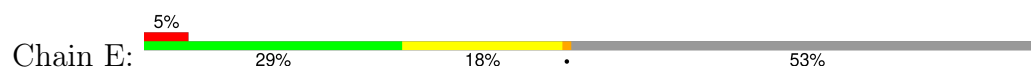
• Molecule 1: RsbR



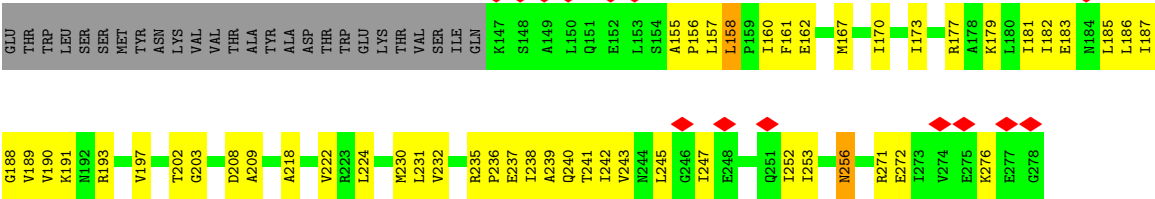
• Molecule 1: RsbR



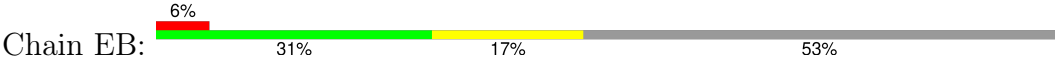
• Molecule 1: RsbR



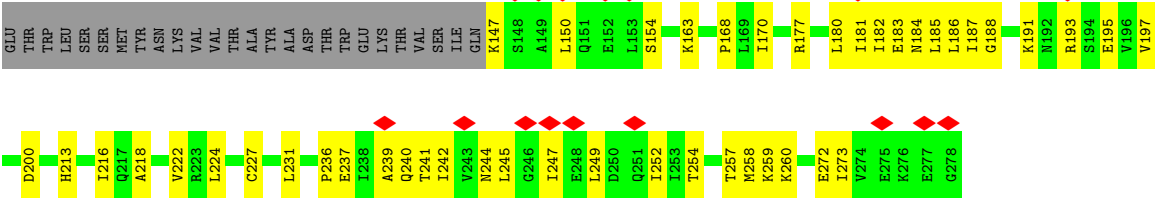
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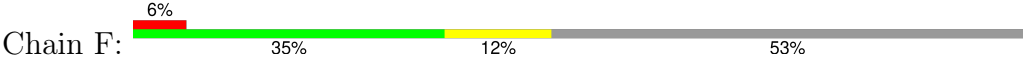
• Molecule 1: RsbR



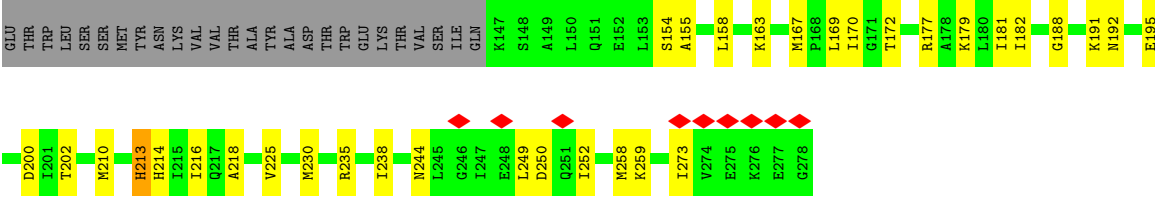
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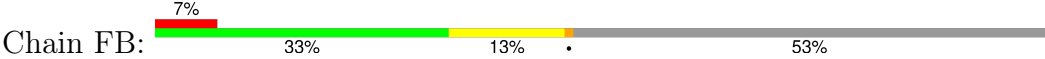
• Molecule 1: RsbR



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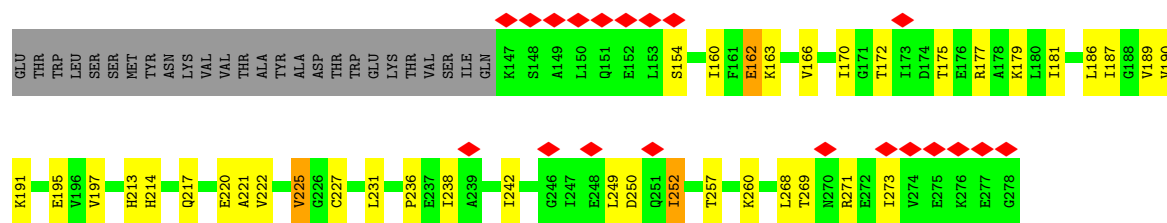


• Molecule 1: RsbR

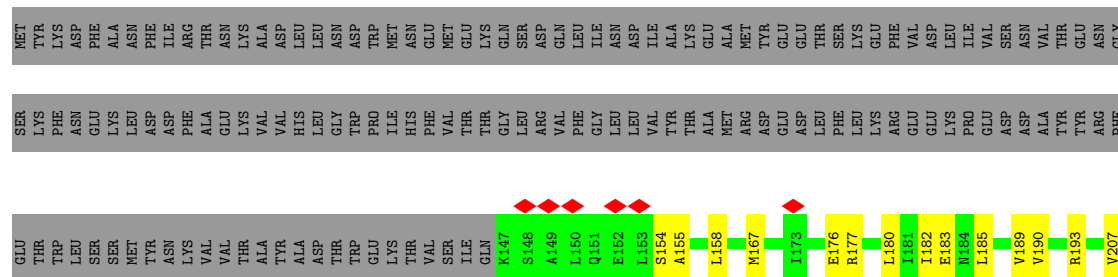
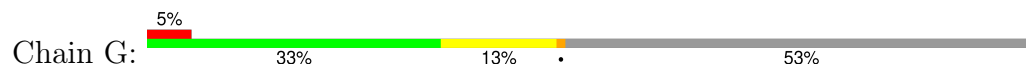


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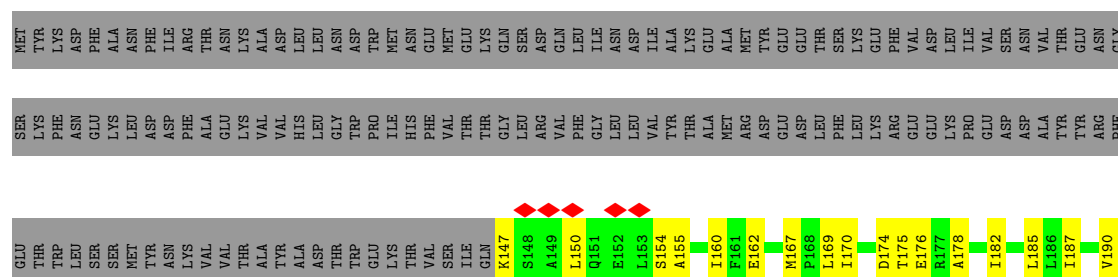
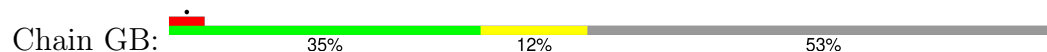
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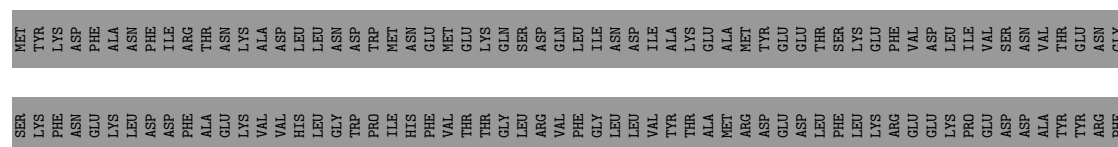
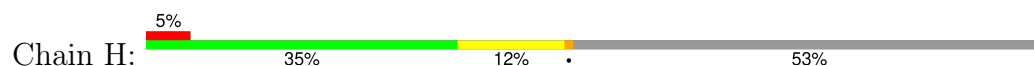
## • Molecule 1: RsbR



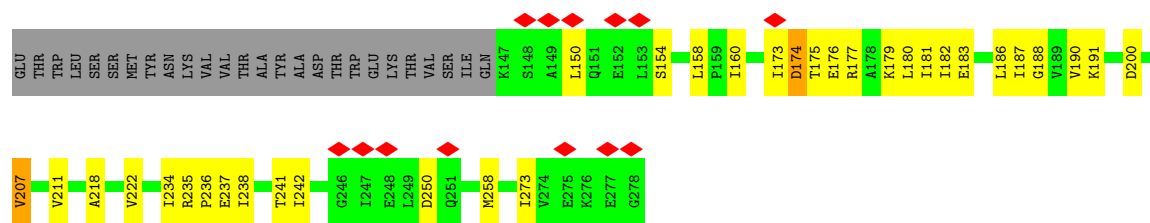
## • Molecule 1: RsbR



## • Molecule 1: RsbR

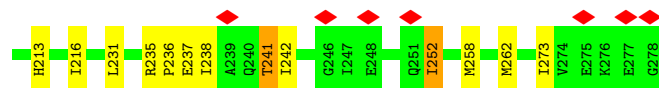
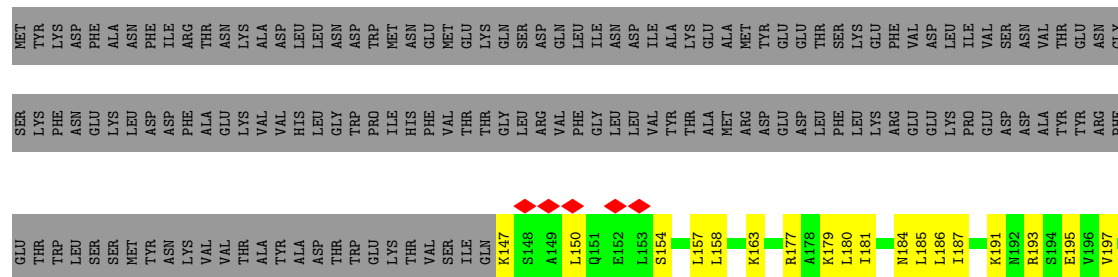






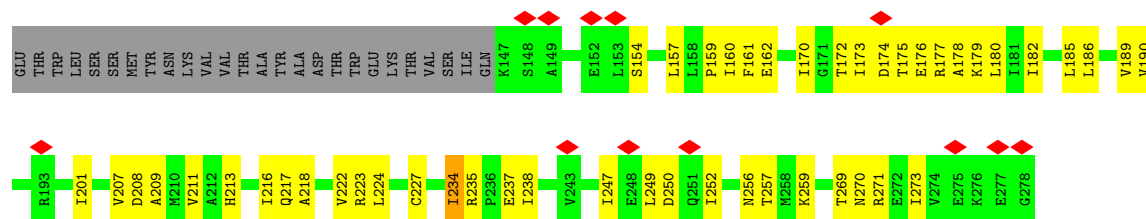
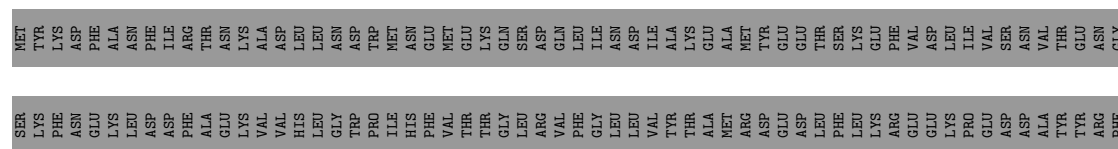
• Molecule 1: RsbR

Chain HB: 36% 11% 53%



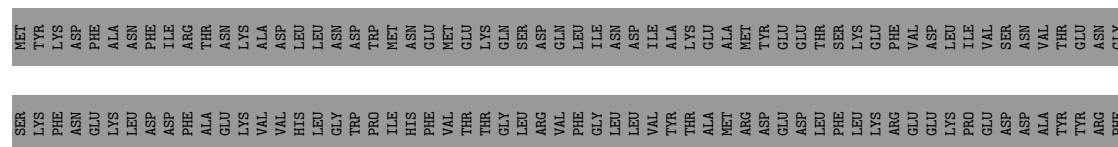
• Molecule 1: RsbR

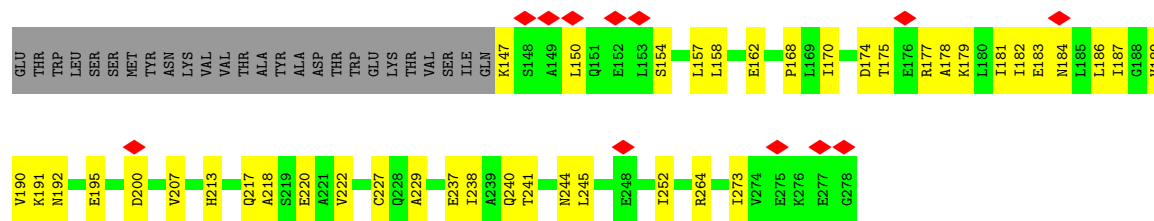
Chain I: 30% 17% 53%



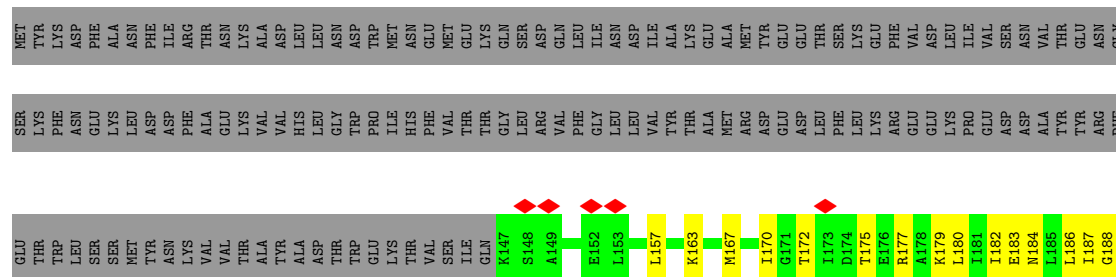
• Molecule 1: RsbR

Chain IB: 32% 15% 53%

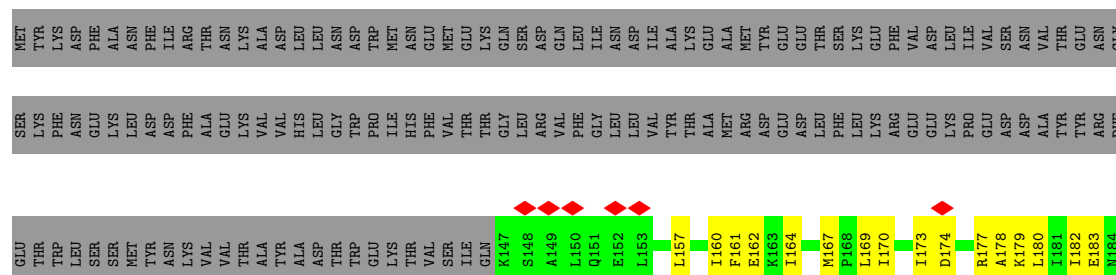
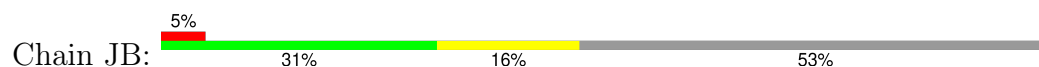




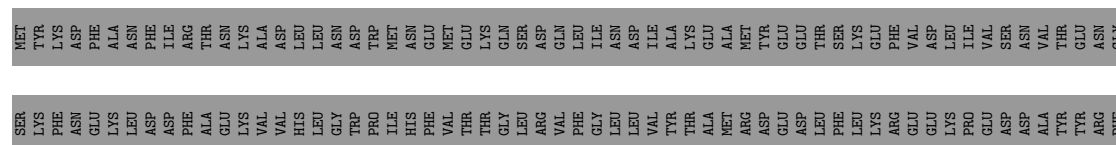
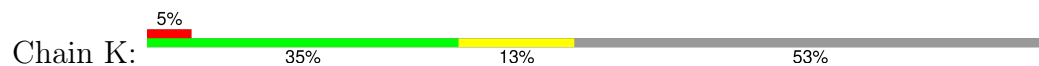
• Molecule 1: RsbR

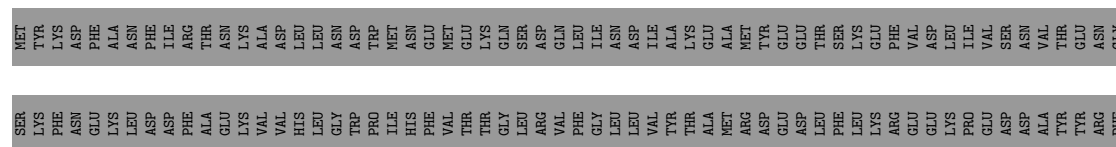


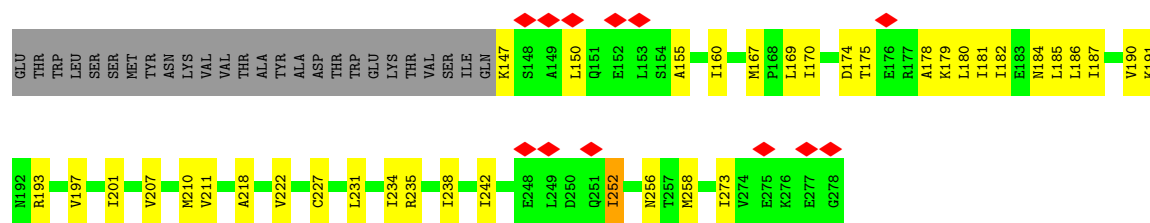
• Molecule 1: RsbR



• Molecule 1: RsbR

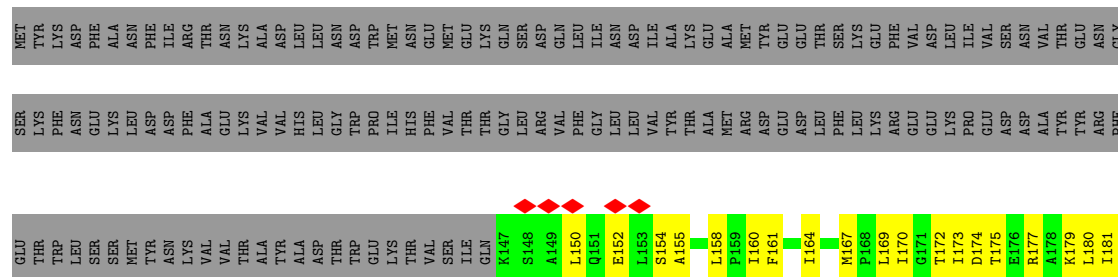






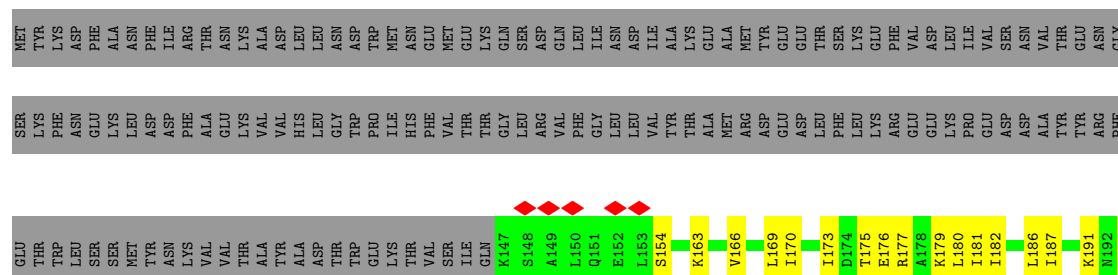
• Molecule 1: RsbR

Chain M: 29% 17% 53%



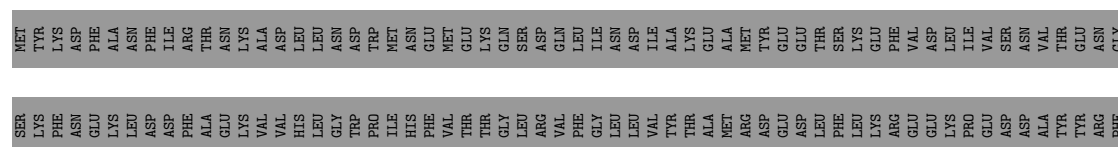
• Molecule 1: RsbR

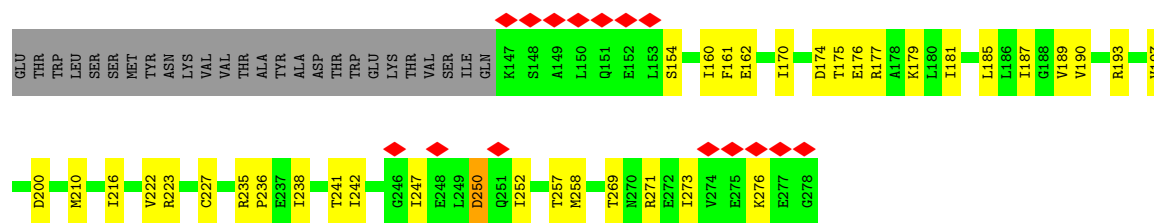
Chain MB: 6% 32% 14% 53%



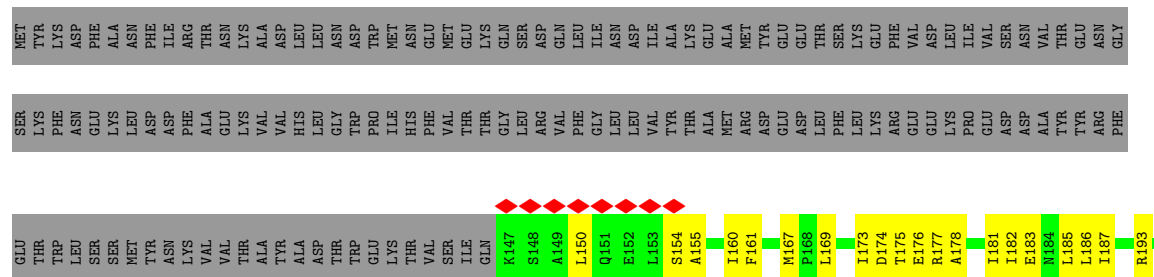
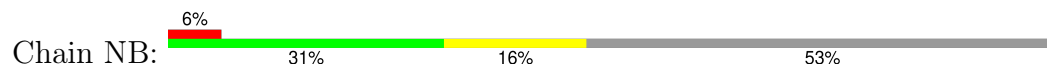
• Molecule 1: RsbR

Chain N: 5% 34% 13% 53%

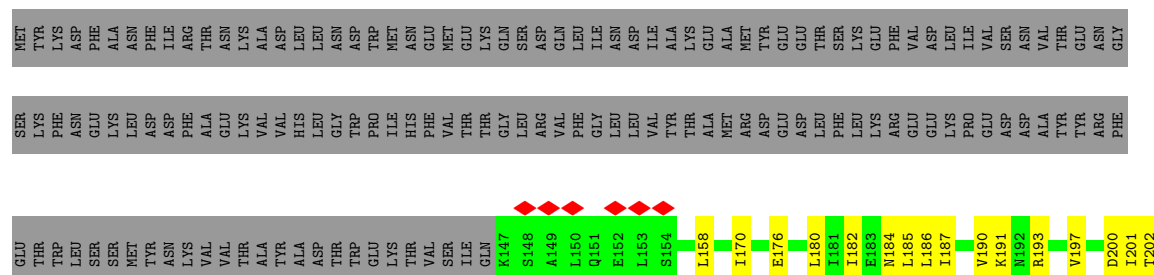
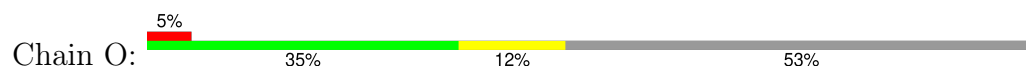




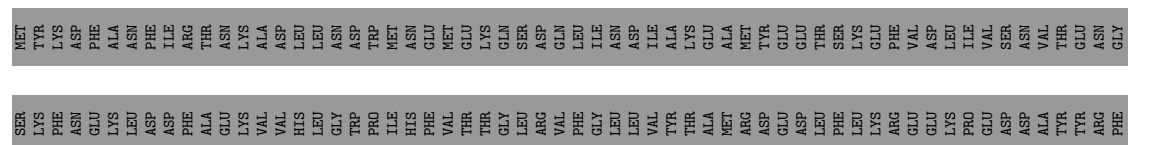
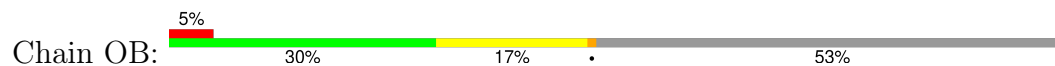
## ● Molecule 1: RsbR

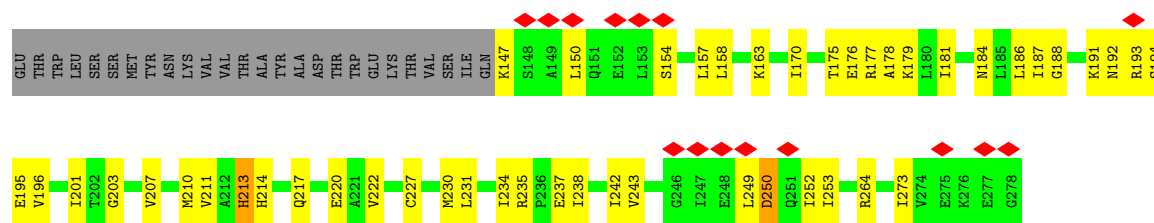


## ● Molecule 1: RsbR

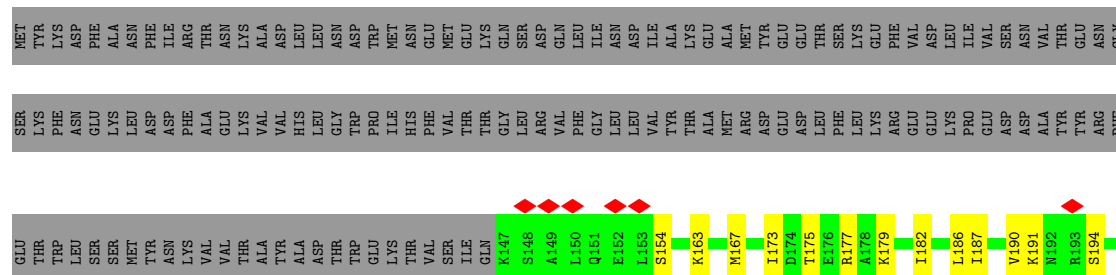
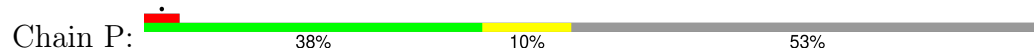


## ● Molecule 1: RsbR

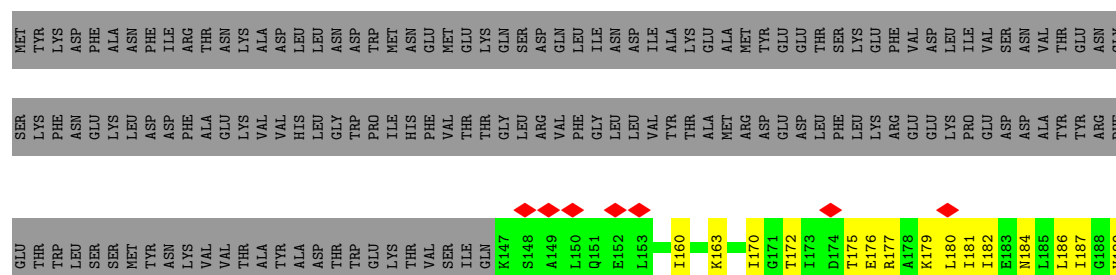
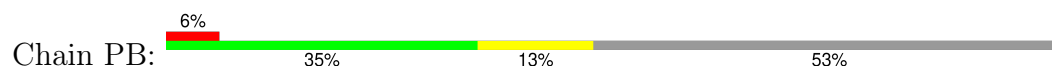




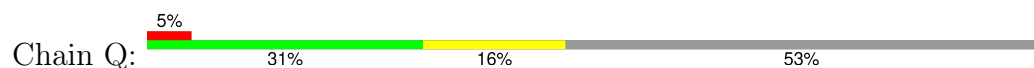
• Molecule 1: RsbR

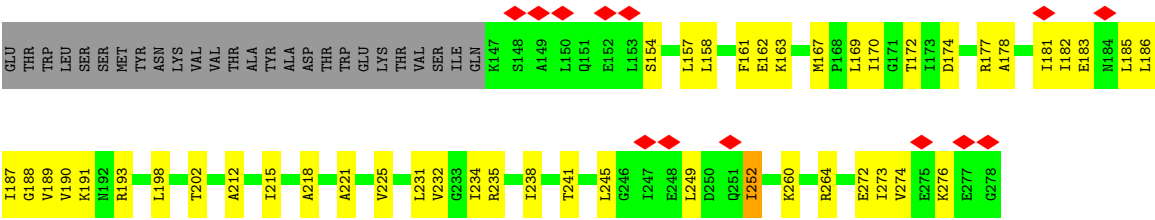


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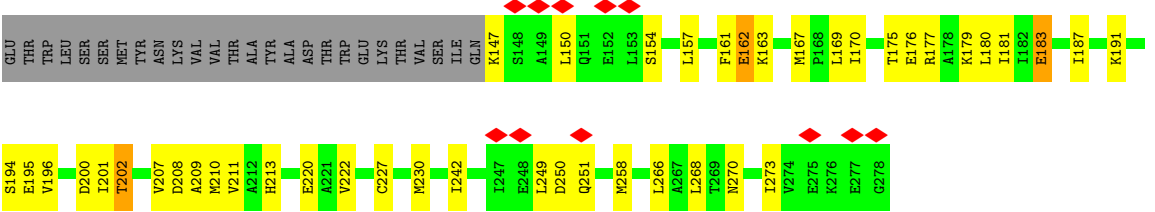
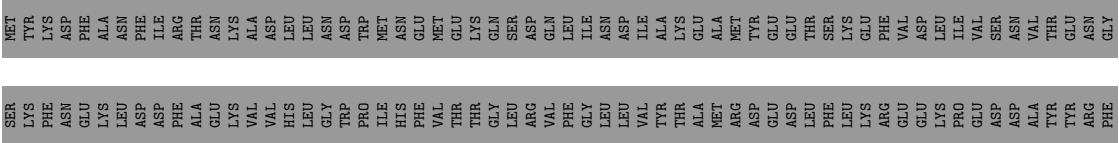
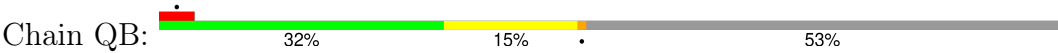


• Molecule 1: RsbR

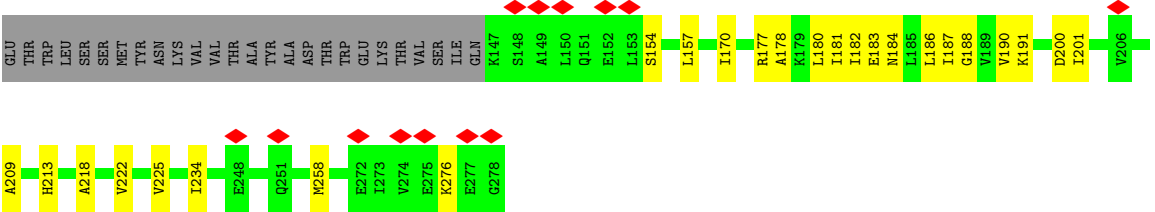
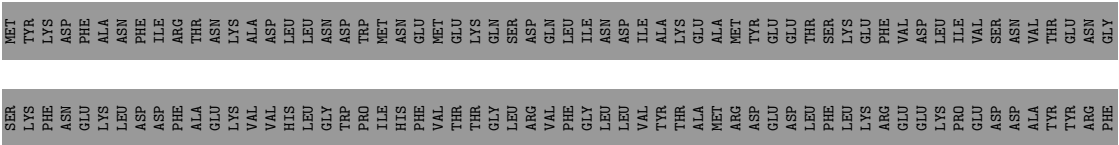
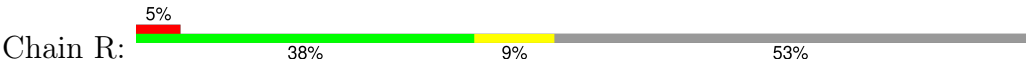




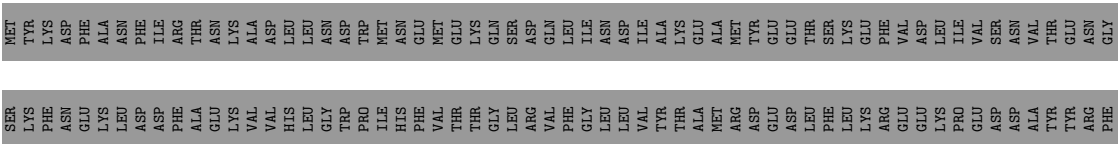
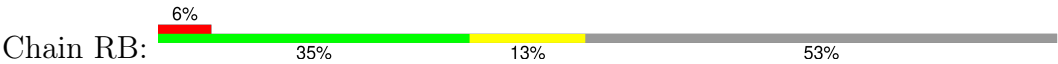
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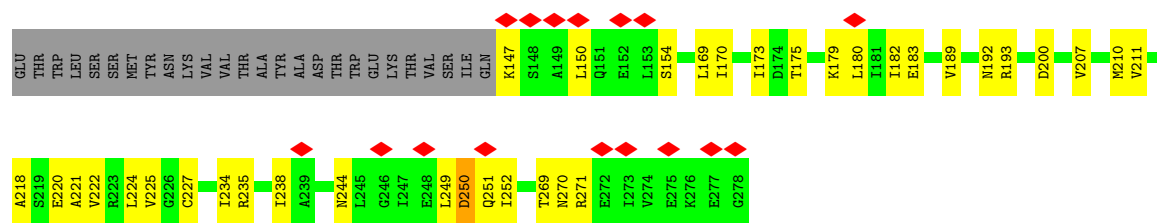


• Molecule 1: RsbR

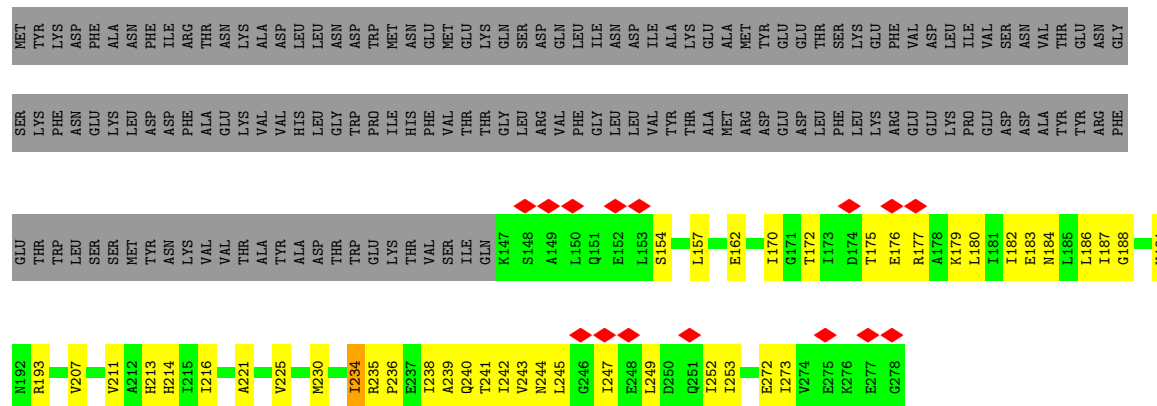
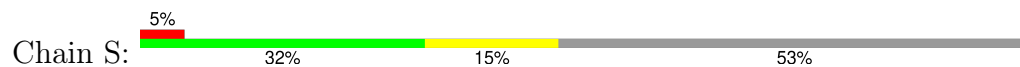


• Molecule 1: RsbR

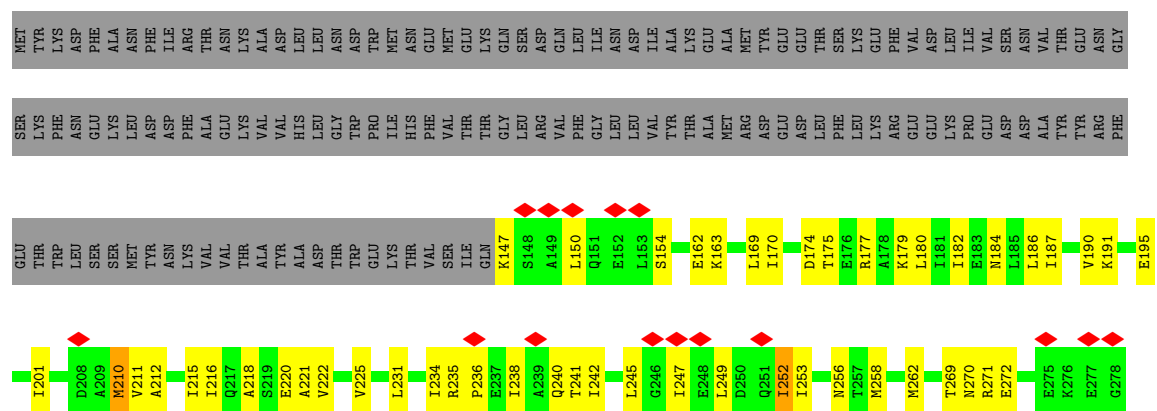
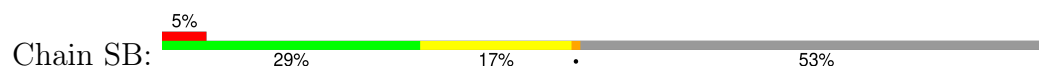




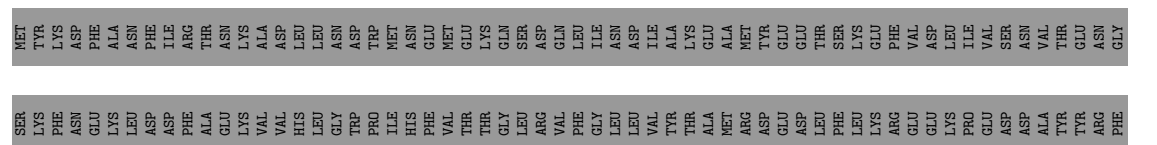
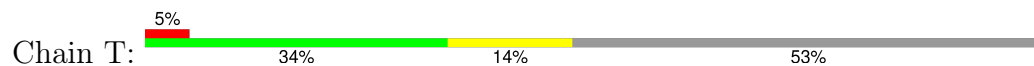
• Molecule 1: RsbR



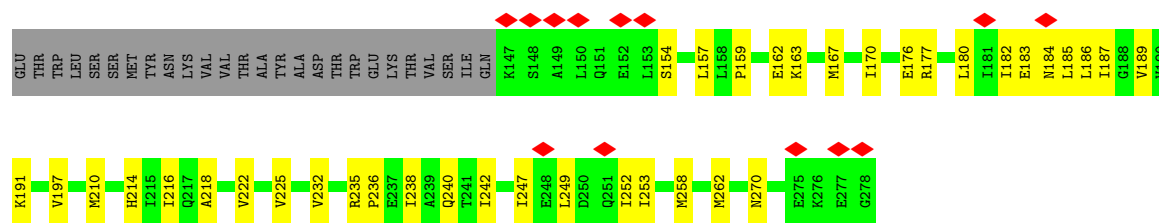
• Molecule 1: RsbR



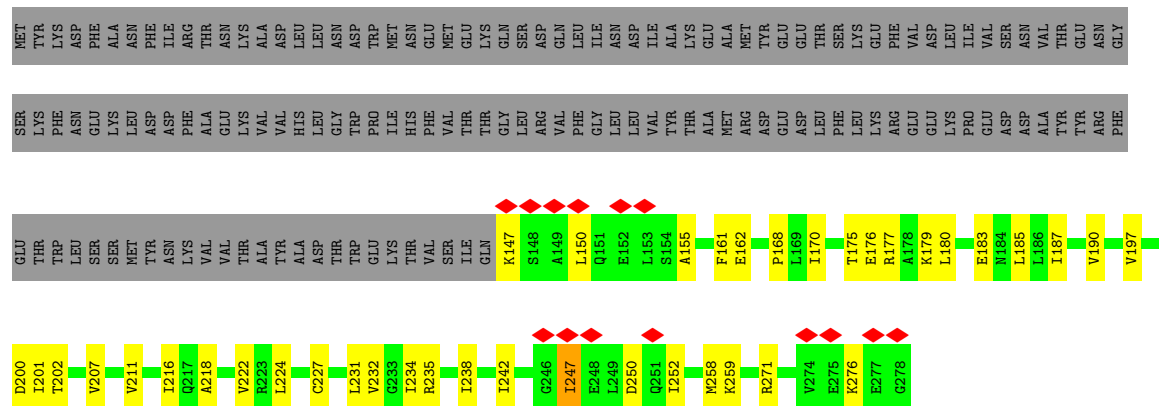
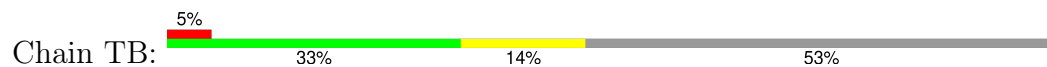
• Molecule 1: RsbR



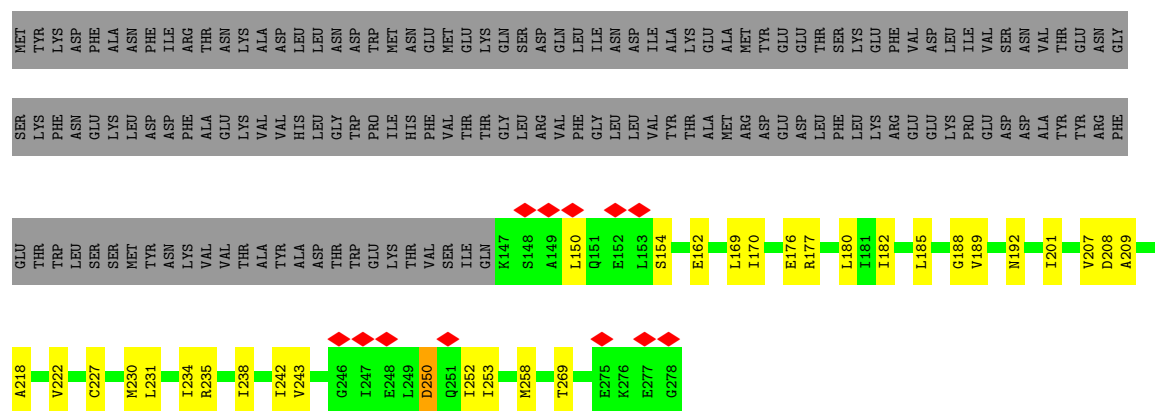
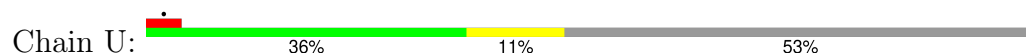




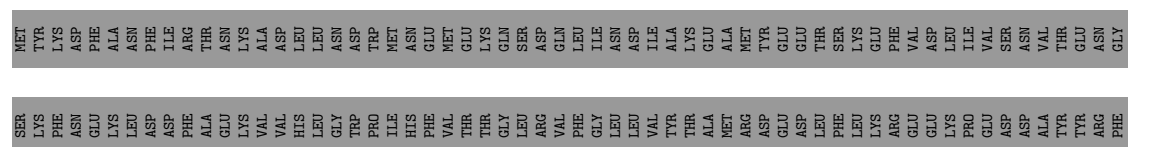
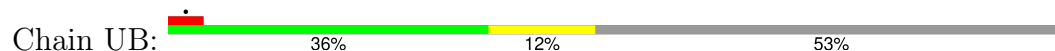
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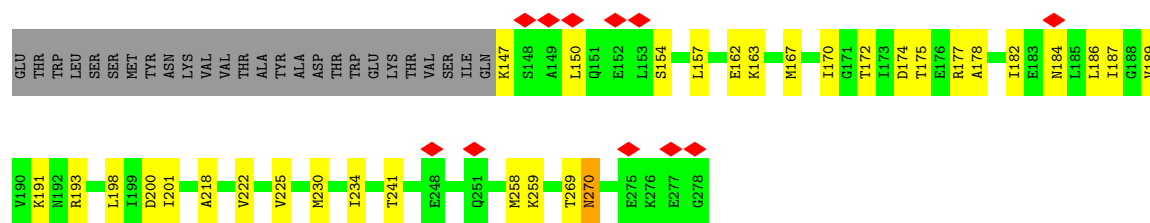


• Molecule 1: RsbR

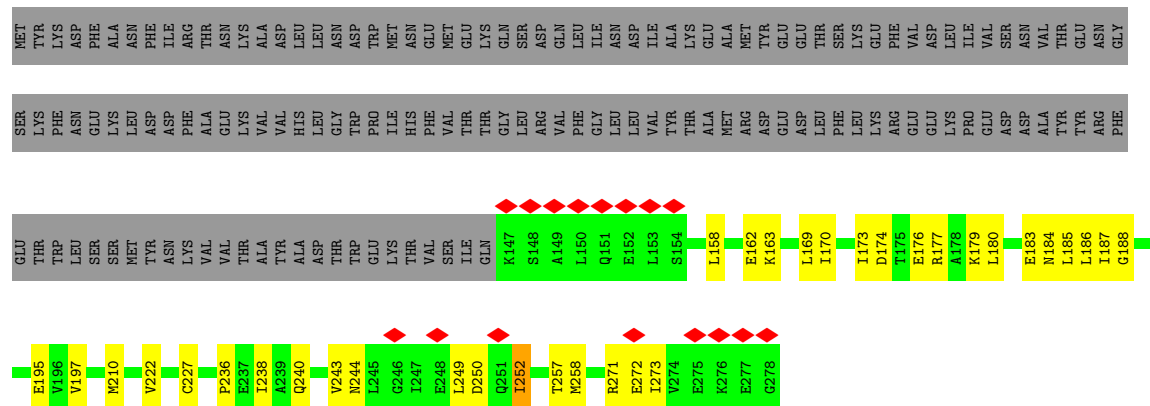
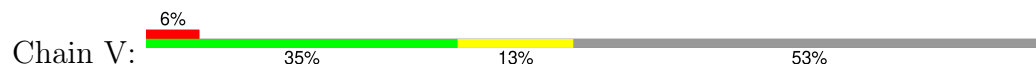


• Molecule 1: RsbR

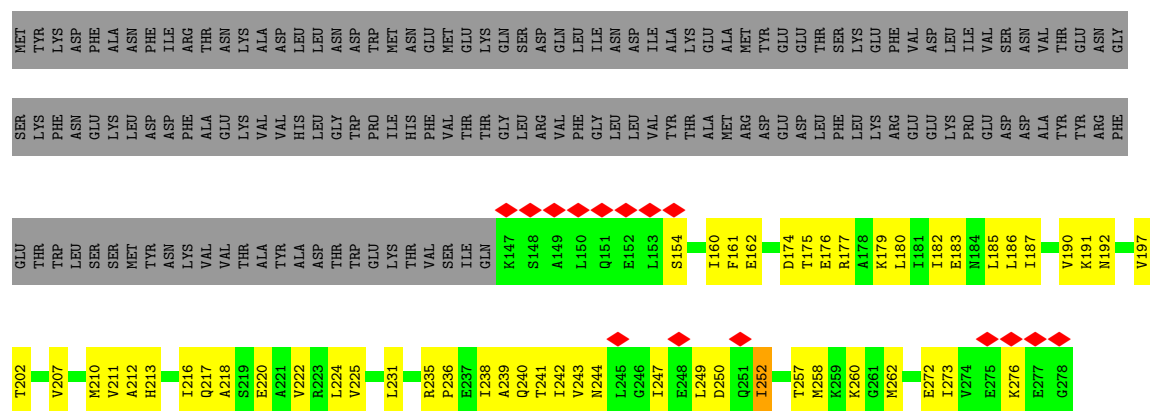
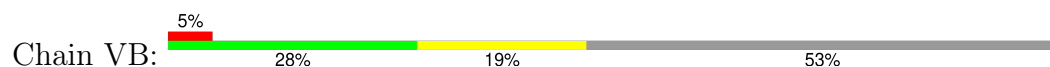




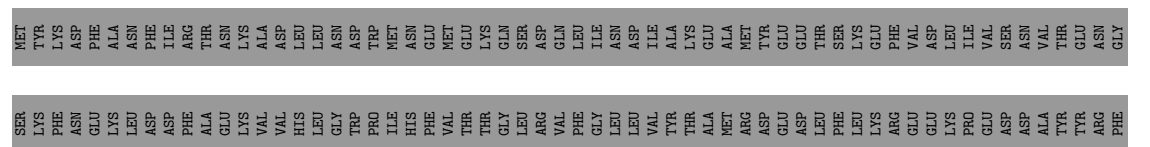
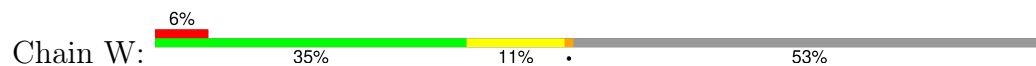
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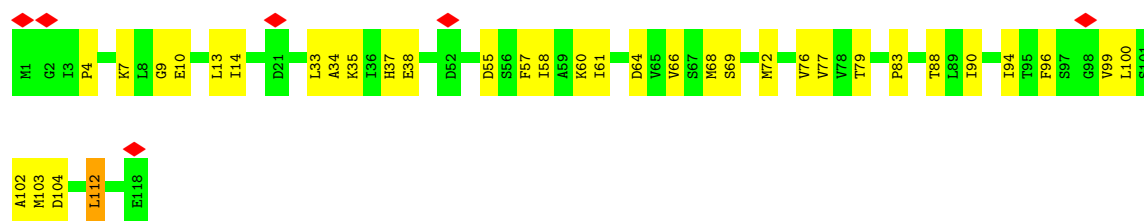
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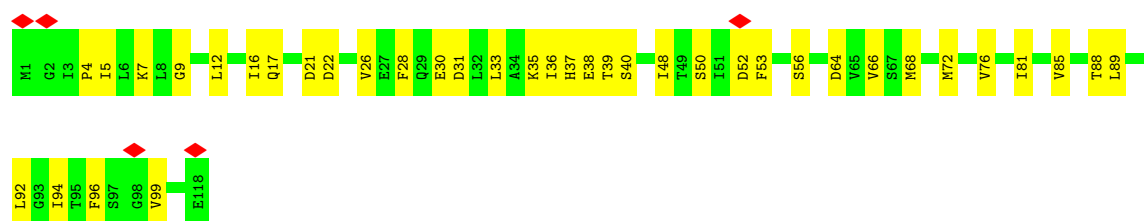
• Molecule 1: RsbR



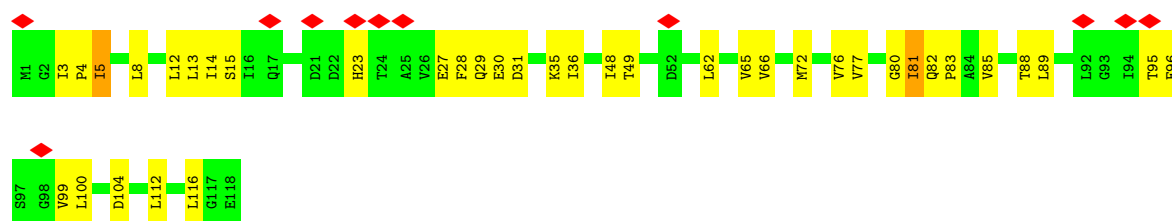




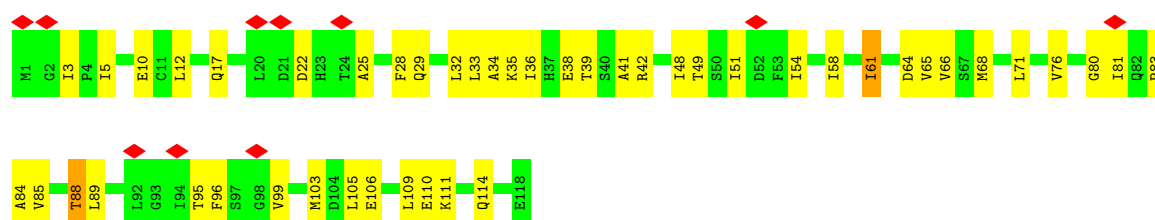
- Molecule 2: RsbT antagonist protein RsbS



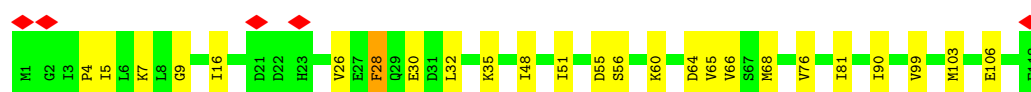
- Molecule 2: RsbT antagonist protein RsbS



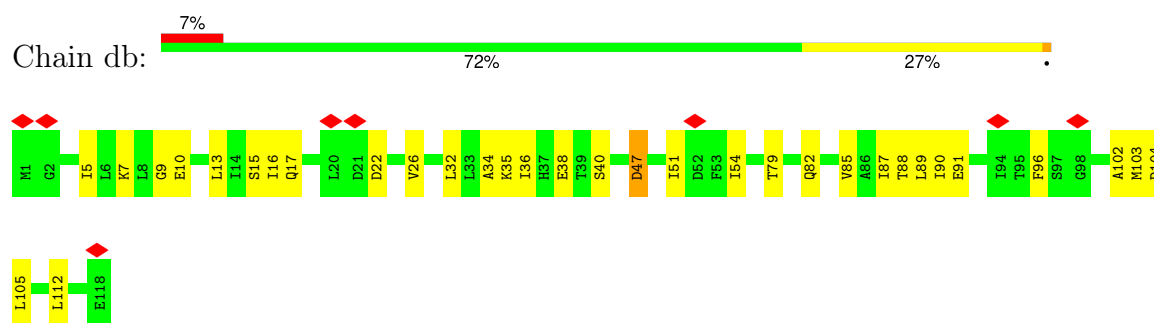
- Molecule 2: RsbT antagonist protein RsbS



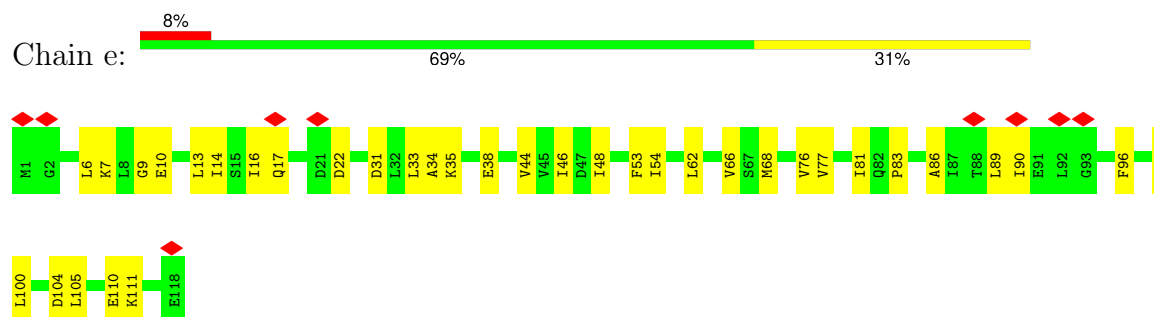
- Molecule 2: RsbT antagonist protein RsbS



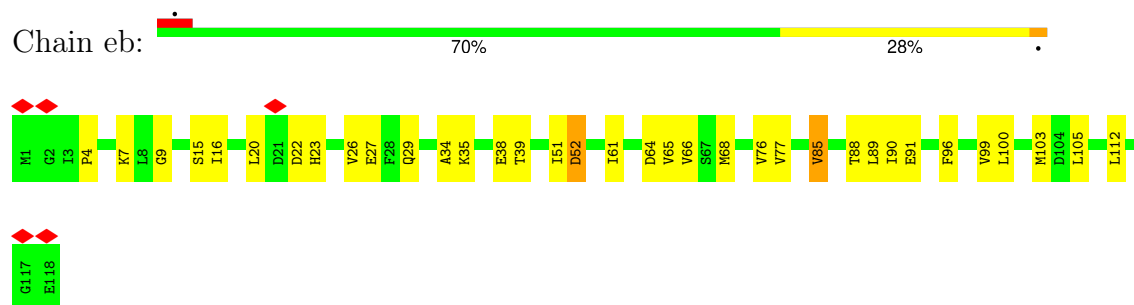
- Molecule 2: RsbT antagonist protein RsbS



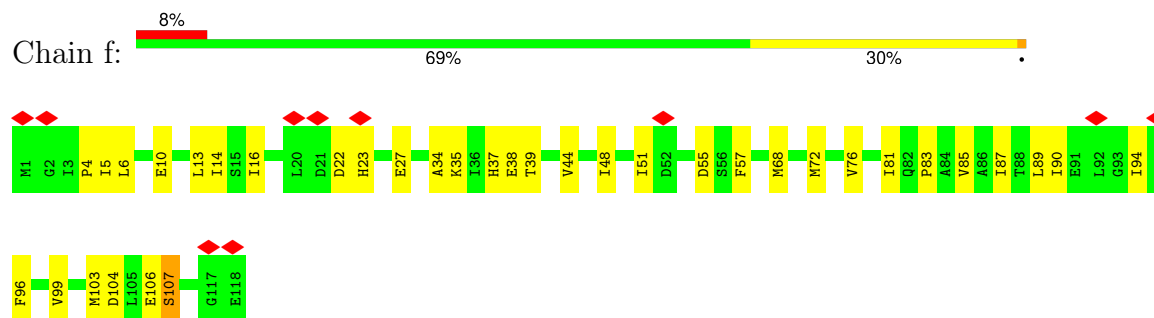
- Molecule 2: RsbT antagonist protein RsbS



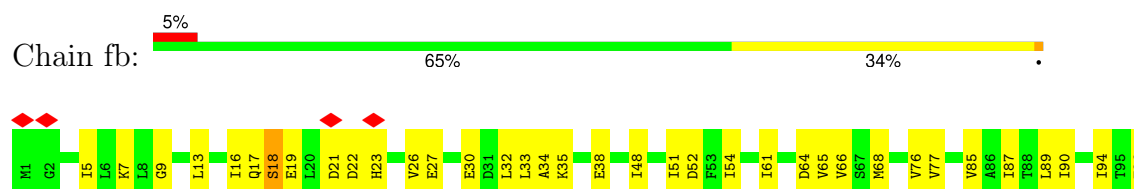
- Molecule 2: RsbT antagonist protein RsbS



- Molecule 2: RsbT antagonist protein RsbS

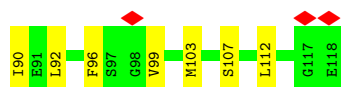


- Molecule 2: RsbT antagonist protein RsbS

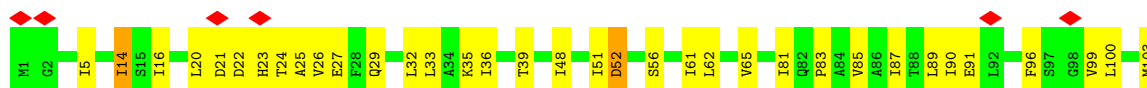




- Molecule 2: RsbT antagonist protein RsbS



- 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	233090	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	1.916	Depositor
Minimum map value	-0.848	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.3	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	0.835, 0.835, 0.835	Depositor

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.15	0/1009	0.37	0/1365
1	AB	0.15	0/1009	0.35	0/1365
1	B	0.16	0/1009	0.36	0/1365
1	BB	0.17	0/1009	0.39	0/1365
1	C	0.15	0/1009	0.41	0/1365
1	CB	0.17	0/1009	0.43	0/1365
1	D	0.21	0/1009	0.52	1/1365 (0.1%)
1	DB	0.19	0/1009	0.52	0/1365
1	E	0.18	0/1009	0.48	0/1365
1	EB	0.16	0/1009	0.38	0/1365
1	F	0.15	0/1009	0.37	0/1365
1	FB	0.15	0/1009	0.35	0/1365
1	G	0.17	0/1009	0.37	0/1365
1	GB	0.14	0/1009	0.30	0/1365
1	H	0.16	0/1009	0.39	0/1365
1	HB	0.14	0/1009	0.32	0/1365
1	I	0.17	0/1009	0.39	0/1365
1	IB	0.17	0/1009	0.41	0/1365
1	J	0.25	0/1009	0.55	0/1365
1	JB	0.18	0/1009	0.46	0/1365
1	K	0.15	0/1009	0.34	0/1365
1	KB	0.16	0/1009	0.36	0/1365
1	L	0.15	0/1009	0.35	0/1365
1	LB	0.17	0/1009	0.35	0/1365
1	M	0.17	0/1009	0.45	0/1365
1	MB	0.18	0/1009	0.45	0/1365
1	N	0.16	0/1009	0.42	0/1365
1	NB	0.18	0/1009	0.41	0/1365
1	O	0.16	0/1009	0.46	1/1365 (0.1%)
1	OB	0.15	0/1009	0.37	0/1365
1	P	0.14	0/1009	0.33	0/1365
1	PB	0.16	0/1009	0.41	0/1365
1	Q	0.17	0/1009	0.42	0/1365
1	QB	0.16	0/1009	0.42	0/1365



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	R	0.15	0/1009	0.38	0/1365
1	RB	0.18	0/1009	0.40	0/1365
1	S	0.18	0/1009	0.46	0/1365
1	SB	0.17	0/1009	0.41	0/1365
1	T	0.17	0/1009	0.40	0/1365
1	TB	0.18	0/1009	0.48	0/1365
1	U	0.17	0/1009	0.41	0/1365
1	UB	0.16	0/1009	0.36	0/1365
1	V	0.14	0/1009	0.39	0/1365
1	VB	0.17	0/1009	0.42	0/1365
1	W	0.13	0/1009	0.31	0/1365
1	WB	0.14	0/1009	0.33	0/1365
2	a	0.17	0/888	0.37	0/1197
2	ab	0.16	0/888	0.37	0/1197
2	b	0.15	0/888	0.35	0/1197
2	bb	0.17	0/888	0.37	0/1197
2	c	0.17	0/888	0.41	0/1197
2	cb	0.18	0/888	0.46	0/1197
2	d	0.15	0/888	0.33	0/1197
2	db	0.15	0/888	0.39	0/1197
2	e	0.16	0/888	0.40	0/1197
2	eb	0.15	0/888	0.33	0/1197
2	f	0.18	0/888	0.51	0/1197
2	fb	0.16	0/888	0.39	0/1197
2	g	0.15	0/888	0.39	0/1197
2	gb	0.16	0/888	0.37	0/1197
All	All	0.17	0/58846	0.40	2/79548 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	DB	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	ARG	CB-CG-CD	7.58	128.74	111.30
1	O	235	ARG	CB-CG-CD	5.15	123.14	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DB	226	GLY	Peptide

## 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	33	0
1	AB	1002	0	1083	27	0
1	B	1002	0	1083	21	0
1	BB	1002	0	1083	33	0
1	C	1002	0	1083	27	0
1	CB	1002	0	1083	39	0
1	D	1002	0	1083	33	0
1	DB	1002	0	1083	44	0
1	E	1002	0	1083	47	0
1	EB	1002	0	1083	33	0
1	F	1002	0	1083	24	0
1	FB	1002	0	1083	32	0
1	G	1002	0	1083	29	0
1	GB	1002	0	1083	20	0
1	H	1002	0	1083	24	0
1	HB	1002	0	1083	22	0
1	I	1002	0	1083	39	0
1	IB	1002	0	1083	34	0
1	J	1002	0	1083	38	0
1	JB	1002	0	1083	37	0
1	K	1002	0	1083	24	0
1	KB	1002	0	1083	32	0
1	L	1002	0	1083	25	0
1	LB	1002	0	1083	23	0
1	M	1002	0	1083	33	0
1	MB	1002	0	1083	31	0
1	N	1002	0	1083	31	0
1	NB	1002	0	1083	34	0
1	O	1002	0	1083	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	OB	1002	0	1083	36	0
1	P	1002	0	1083	19	0
1	PB	1002	0	1083	23	0
1	Q	1002	0	1083	33	0
1	QB	1002	0	1083	28	0
1	R	1002	0	1083	22	0
1	RB	1002	0	1083	30	0
1	S	1002	0	1083	39	0
1	SB	1002	0	1083	38	0
1	T	1002	0	1083	36	0
1	TB	1002	0	1083	33	0
1	U	1002	0	1083	23	0
1	UB	1002	0	1083	22	0
1	V	1002	0	1083	23	0
1	VB	1002	0	1083	43	0
1	W	1002	0	1083	23	0
1	WB	1002	0	1083	31	0
2	a	881	0	928	25	0
2	ab	881	0	928	26	0
2	b	881	0	928	25	0
2	bb	881	0	928	23	0
2	c	881	0	928	28	0
2	cb	881	0	928	38	0
2	d	881	0	928	18	0
2	db	881	0	928	22	0
2	e	881	0	928	29	0
2	eb	881	0	928	24	0
2	f	881	0	928	31	0
2	fb	881	0	928	26	0
2	g	881	0	928	35	0
2	gb	881	0	928	25	0
All	All	58426	0	62810	1577	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 (1577) 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:NB:167:MET:HE2	1:NB:185:LEU:HD12	1.59	0.85
1:H:177:ARG:HA	1:H:180:LEU:HD12	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:208:ASP:OD1	1:U:209:ALA:N	2.12	0.83
2:g:5:ILE:HG21	2:g:35:LYS:HG2	1.61	0.82
1:LB:207:VAL:HG23	1:LB:211:VAL:HB	1.63	0.81
2:f:87:ILE:HA	2:f:90:ILE:HD12	1.63	0.80
1:B:190:VAL:HG21	1:HB:235:ARG:HH12	1.46	0.79
1:C:259:LYS:NZ	1:CB:162:GLU:OE2	2.15	0.79
1:C:249:LEU:HD12	1:C:252:ILE:HD11	1.66	0.78
1:W:273:ILE:HG12	1:WB:273:ILE:HG12	1.65	0.78
1:VB:236:PRO:O	1:VB:240:GLN:HB2	1.84	0.78
1:U:188:GLY:O	1:U:192:ASN:ND2	2.17	0.77
1:UB:182:ILE:HD12	1:UB:218:ALA:HB2	1.66	0.77
1:A:188:GLY:O	1:A:192:ASN:ND2	2.18	0.77
1:EB:249:LEU:HD22	1:MB:224:LEU:HD22	1.65	0.77
1:NB:173:ILE:HD12	1:NB:177:ARG:HD3	1.66	0.76
2:gb:29:GLN:HG3	2:gb:65:VAL:HG22	1.66	0.76
1:QB:163:LYS:HB3	1:QB:195:GLU:HG3	1.68	0.76
1:VB:177:ARG:HA	1:VB:180:LEU:HD12	1.68	0.76
1:N:175:THR:HG22	1:N:210:MET:HE1	1.67	0.75
1:I:249:LEU:HD22	1:I:252:ILE:HD11	1.66	0.75
1:V:273:ILE:HG12	1:VB:273:ILE:HG12	1.68	0.75
1:K:170:ILE:HG22	1:K:203:GLY:HA3	1.67	0.75
2:cb:96:PHE:HB3	2:cb:99:VAL:HB	1.69	0.75
2:fb:21:ASP:OD2	2:fb:22:ASP:N	2.20	0.74
1:OB:187:ILE:HG13	1:OB:191:LYS:HE2	1.69	0.74
1:T:249:LEU:HD22	1:T:252:ILE:HD11	1.69	0.74
1:J:188:GLY:O	1:J:192:ASN:ND2	2.20	0.74
1:QB:208:ASP:OD2	1:QB:209:ALA:N	2.20	0.74
1:B:187:ILE:O	1:B:191:LYS:HG2	1.87	0.74
1:IB:187:ILE:O	1:IB:191:LYS:HG2	1.86	0.73
1:P:273:ILE:HG12	1:PB:273:ILE:HG12	1.69	0.73
1:D:160:ILE:HD13	1:DB:258:MET:HG2	1.70	0.73
1:V:188:GLY:O	1:V:192:ASN:ND2	2.21	0.73
1:VB:187:ILE:O	1:VB:191:LYS:HG2	1.88	0.73
2:a:4:PRO:HB3	2:ab:17:GLN:HG3	1.71	0.73
1:DB:154:SER:HB2	1:DB:177:ARG:HH12	1.54	0.73
1:E:161:PHE:HE1	1:EB:273:ILE:HG13	1.54	0.73
1:S:245:LEU:HD23	1:S:247:ILE:HD11	1.71	0.72
1:UB:187:ILE:O	1:UB:191:LYS:HG2	1.88	0.72
1:GB:231:LEU:HB2	1:GB:252:ILE:HD11	1.71	0.72
1:NB:249:LEU:HD22	1:NB:252:ILE:HD11	1.70	0.72
2:cb:85:VAL:O	2:cb:89:LEU:HD12	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JB:170:ILE:O	1:JB:177:ARG:NH2	2.22	0.72
1:BB:177:ARG:O	1:BB:181:ILE:HG13	1.90	0.72
2:f:85:VAL:O	2:f:89:LEU:HD12	1.90	0.72
1:VB:240:GLN:HA	2:cb:68:MET:HE1	1.70	0.72
1:H:238:ILE:O	1:H:242:ILE:HG13	1.90	0.71
1:D:170:ILE:HD13	1:DB:154:SER:HA	1.73	0.71
1:E:157:LEU:HD21	1:E:188:GLY:HA3	1.72	0.71
1:F:163:LYS:HB3	1:F:195:GLU:HG3	1.72	0.71
1:E:224:LEU:HB3	2:f:81:ILE:HD11	1.72	0.71
1:L:273:ILE:HG12	1:LB:273:ILE:HG12	1.72	0.71
1:MB:235:ARG:HD3	1:MB:236:PRO:HD2	1.73	0.71
1:S:235:ARG:HB3	1:S:238:ILE:HD13	1.73	0.71
1:AB:238:ILE:O	1:AB:242:ILE:HG13	1.91	0.71
1:V:249:LEU:HD22	1:V:252:ILE:HD11	1.71	0.71
1:CB:177:ARG:HD2	1:CB:180:LEU:HD11	1.73	0.70
1:G:177:ARG:HA	1:G:180:LEU:HD12	1.73	0.70
1:HB:231:LEU:HB2	1:HB:252:ILE:HD11	1.72	0.70
2:d:5:ILE:HG21	2:d:35:LYS:HG2	1.72	0.70
1:V:177:ARG:HA	1:V:180:LEU:HD12	1.73	0.70
1:O:187:ILE:O	1:O:191:LYS:HG3	1.90	0.70
1:E:202:THR:HA	1:E:235:ARG:HH22	1.57	0.69
2:cb:61:ILE:O	2:cb:65:VAL:HG23	1.92	0.69
1:JB:190:VAL:HG23	1:JB:191:LYS:HD3	1.73	0.69
1:EB:249:LEU:HG	1:EB:252:ILE:HD11	1.73	0.69
1:G:255:THR:HG21	1:G:260:LYS:HG2	1.73	0.69
1:JB:157:LEU:HG	1:JB:188:GLY:HA3	1.74	0.69
1:K:273:ILE:HG12	1:KB:273:ILE:HG12	1.73	0.69
1:H:273:ILE:HG12	1:HB:273:ILE:HG12	1.73	0.69
1:PB:180:LEU:O	1:PB:184:ASN:ND2	2.26	0.69
1:E:179:LYS:HE2	1:E:179:LYS:HA	1.74	0.69
1:J:236:PRO:HB3	2:b:33:LEU:HD23	1.75	0.69
1:FB:172:THR:O	1:FB:177:ARG:NH1	2.26	0.69
1:N:177:ARG:O	1:N:181:ILE:HG13	1.93	0.69
1:I:222:VAL:HG22	1:I:227:CYS:HB3	1.75	0.68
1:D:207:VAL:HB	1:D:238:ILE:HG23	1.74	0.68
1:J:235:ARG:HG2	1:J:238:ILE:HD12	1.76	0.68
1:VB:238:ILE:HD12	1:VB:238:ILE:H	1.58	0.68
1:RB:175:THR:HG22	1:RB:210:MET:HE1	1.74	0.68
1:MB:222:VAL:HG22	1:MB:227:CYS:HB3	1.75	0.68
1:C:187:ILE:O	1:C:191:LYS:HG3	1.94	0.68
1:G:212:ALA:HB1	1:G:242:ILE:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:187:ILE:HG22	1:KB:191:LYS:NZ	2.08	0.68
1:T:183:GLU:O	1:T:187:ILE:HG13	1.94	0.68
1:E:157:LEU:HB3	1:E:167:MET:HE3	1.76	0.68
2:gb:61:ILE:O	2:gb:65:VAL:HG23	1.94	0.68
1:F:188:GLY:O	1:F:192:ASN:ND2	2.25	0.68
1:KB:163:LYS:HB3	1:KB:195:GLU:HG3	1.74	0.68
1:O:273:ILE:HG12	1:OB:273:ILE:HG12	1.76	0.68
2:e:16:ILE:HD12	2:e:48:ILE:HG22	1.76	0.68
1:FB:187:ILE:O	1:FB:191:LYS:HG3	1.93	0.68
1:M:154:SER:HB3	1:M:177:ARG:HH21	1.59	0.68
1:M:238:ILE:O	1:M:242:ILE:HG13	1.94	0.68
2:b:33:LEU:HG	2:b:72:MET:HE1	1.76	0.68
1:O:222:VAL:HG22	1:O:227:CYS:HB3	1.76	0.67
1:LB:155:ALA:HB1	1:LB:167:MET:HE2	1.75	0.67
1:NB:173:ILE:HD11	1:NB:181:ILE:HD13	1.75	0.67
1:NB:238:ILE:H	1:NB:238:ILE:HD12	1.58	0.67
1:QB:187:ILE:O	1:QB:191:LYS:HG3	1.93	0.67
1:U:170:ILE:HD12	1:UB:170:ILE:HD11	1.77	0.67
1:U:222:VAL:HG22	1:U:227:CYS:HB3	1.75	0.67
1:B:202:THR:O	1:B:235:ARG:NH2	2.28	0.67
1:PB:176:GLU:OE1	1:PB:176:GLU:N	2.27	0.67
1:N:154:SER:HB2	1:N:177:ARG:HH12	1.59	0.67
1:VB:231:LEU:HB2	1:VB:252:ILE:HD11	1.74	0.67
1:T:170:ILE:HD11	1:TB:170:ILE:HD12	1.77	0.67
1:Q:172:THR:O	1:Q:177:ARG:NH1	2.27	0.67
1:QB:222:VAL:HG22	1:QB:227:CYS:HB3	1.76	0.67
2:fb:96:PHE:HB3	2:fb:99:VAL:HB	1.76	0.67
1:F:177:ARG:O	1:F:181:ILE:HG13	1.94	0.66
1:SB:231:LEU:HB2	1:SB:252:ILE:HD11	1.75	0.66
1:PB:182:ILE:O	1:PB:186:LEU:HD12	1.94	0.66
2:g:16:ILE:HD13	2:g:20:LEU:HD11	1.75	0.66
1:Q:185:LEU:O	1:Q:189:VAL:HG23	1.95	0.66
1:E:238:ILE:HD12	1:E:238:ILE:H	1.60	0.66
1:Q:154:SER:HA	1:QB:170:ILE:HG21	1.78	0.66
1:Q:273:ILE:HG12	1:QB:273:ILE:HG12	1.76	0.66
1:FB:177:ARG:O	1:FB:181:ILE:HG13	1.95	0.66
1:I:173:ILE:HA	1:I:177:ARG:HD3	1.77	0.66
1:DB:257:THR:OG1	1:NB:193:ARG:NH2	2.29	0.66
1:FB:231:LEU:HB2	1:FB:252:ILE:HD11	1.77	0.66
1:IB:189:VAL:HG12	2:b:103:MET:HE1	1.77	0.66
2:cb:51:ILE:HG21	2:cb:54:ILE:HD13	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ILE:O	1:E:242:ILE:HG13	1.96	0.66
2:b:4:PRO:HB3	2:bb:17:GLN:HG3	1.77	0.66
2:e:7:LYS:NZ	2:e:9:GLY:O	2.28	0.66
1:F:170:ILE:HD12	1:FB:170:ILE:HD12	1.78	0.66
1:Q:190:VAL:HG13	1:Q:191:LYS:HD3	1.78	0.66
1:E:239:ALA:O	1:E:243:VAL:HG23	1.96	0.65
1:JB:162:GLU:OE2	1:JB:162:GLU:N	2.21	0.65
1:N:238:ILE:HD12	1:N:238:ILE:H	1.60	0.65
1:J:231:LEU:HB2	1:J:252:ILE:HD11	1.79	0.65
1:N:238:ILE:O	1:N:242:ILE:HG12	1.96	0.65
1:R:154:SER:HA	1:RB:170:ILE:HG21	1.79	0.65
1:U:162:GLU:N	1:U:162:GLU:OE2	2.27	0.65
1:EB:222:VAL:HG22	1:EB:227:CYS:HB3	1.76	0.65
1:TB:177:ARG:HA	1:TB:180:LEU:HD12	1.78	0.65
1:T:182:ILE:HG12	1:T:218:ALA:HB2	1.78	0.65
2:d:7:LYS:NZ	2:d:9:GLY:O	2.29	0.65
1:M:223:ARG:O	1:M:223:ARG:NH1	2.29	0.65
1:WB:186:LEU:HD13	2:c:83:PRO:HB3	1.77	0.65
1:VB:162:GLU:OE2	1:VB:162:GLU:N	2.29	0.65
1:D:235:ARG:H	1:D:238:ILE:HD12	1.60	0.65
1:IB:240:GLN:O	1:IB:244:ASN:ND2	2.30	0.65
2:g:23:HIS:O	2:g:27:GLU:HG2	1.96	0.65
1:B:154:SER:HA	1:BB:170:ILE:HD12	1.78	0.65
1:D:170:ILE:O	1:D:177:ARG:NH2	2.29	0.65
1:P:154:SER:HB2	1:P:177:ARG:HH12	1.62	0.65
1:AB:163:LYS:HB3	1:AB:195:GLU:HG3	1.79	0.64
1:S:176:GLU:O	1:S:180:LEU:HG	1.98	0.64
1:VB:175:THR:OG1	1:VB:210:MET:SD	2.52	0.64
2:c:35:LYS:HD3	2:c:35:LYS:N	2.12	0.64
1:A:258:MET:HE3	1:A:262:MET:HG2	1.79	0.64
1:RB:222:VAL:HG12	1:RB:227:CYS:HB3	1.80	0.64
1:TB:179:LYS:O	1:TB:183:GLU:HG3	1.98	0.64
1:AB:222:VAL:HG22	1:AB:227:CYS:HB3	1.78	0.64
1:DB:176:GLU:O	1:DB:180:LEU:HG	1.98	0.64
1:GB:185:LEU:HD11	1:GB:197:VAL:HG21	1.80	0.64
1:HB:147:LYS:HA	1:HB:150:LEU:HD12	1.79	0.64
1:N:170:ILE:HG21	1:NB:154:SER:HA	1.78	0.64
1:WB:193:ARG:NH2	2:c:104:ASP:OD2	2.30	0.64
2:f:23:HIS:O	2:f:27:GLU:HG2	1.96	0.64
2:fb:54:ILE:HD11	2:fb:89:LEU:HD11	1.80	0.64
1:F:238:ILE:HD12	1:F:238:ILE:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:240:GLN:O	1:M:244:ASN:ND2	2.31	0.64
1:EB:163:LYS:HB3	1:EB:195:GLU:HG3	1.80	0.64
1:H:238:ILE:HD12	1:H:238:ILE:H	1.63	0.64
1:F:154:SER:HB3	1:F:177:ARG:HH21	1.63	0.64
2:b:77:VAL:HG22	2:b:100:LEU:HB2	1.80	0.64
1:CB:160:ILE:HG22	1:CB:161:PHE:CD1	2.33	0.64
1:GB:187:ILE:O	1:GB:191:LYS:HG3	1.97	0.64
1:V:222:VAL:HG22	1:V:227:CYS:HB3	1.78	0.64
2:e:34:ALA:HB3	2:e:35:LYS:HZ2	1.63	0.64
1:G:231:LEU:HB3	1:G:254:THR:HG22	1.80	0.64
1:I:162:GLU:N	1:I:162:GLU:OE2	2.25	0.64
1:Q:249:LEU:HD22	1:Q:252:ILE:HD11	1.79	0.64
1:DB:224:LEU:HD11	1:V:243:VAL:HG23	1.80	0.63
1:J:191:LYS:O	1:J:193:ARG:NH2	2.31	0.63
1:FB:238:ILE:HD12	1:FB:238:ILE:H	1.63	0.63
1:G:189:VAL:HG21	1:G:222:VAL:HG23	1.79	0.63
2:bb:21:ASP:OD1	2:bb:22:ASP:N	2.31	0.63
2:eb:35:LYS:O	2:eb:39:THR:OG1	2.12	0.63
1:OB:176:GLU:OE2	1:OB:176:GLU:N	2.31	0.63
1:SB:186:LEU:O	1:SB:190:VAL:HG23	1.98	0.63
1:TB:222:VAL:HG22	1:TB:227:CYS:HB3	1.80	0.63
1:DB:240:GLN:O	1:DB:244:ASN:ND2	2.31	0.63
1:S:238:ILE:HD12	1:S:238:ILE:H	1.64	0.63
2:fb:16:ILE:HD12	2:fb:48:ILE:HG22	1.80	0.63
1:U:177:ARG:HA	1:U:180:LEU:HD12	1.80	0.63
1:EB:240:GLN:O	1:EB:244:ASN:ND2	2.31	0.63
1:I:170:ILE:HG21	1:IB:154:SER:HA	1.81	0.63
1:L:182:ILE:HG12	1:L:218:ALA:HB2	1.80	0.63
1:S:187:ILE:HG23	1:S:191:LYS:HZ3	1.64	0.63
1:E:208:ASP:OD1	1:E:209:ALA:N	2.30	0.62
1:FB:222:VAL:HG22	1:FB:227:CYS:HB3	1.81	0.62
1:GB:231:LEU:HB3	1:GB:254:THR:HG22	1.81	0.62
1:A:186:LEU:HD22	2:a:83:PRO:HG3	1.81	0.62
1:E:177:ARG:O	1:E:181:ILE:HG12	1.98	0.62
1:J:222:VAL:HG22	1:J:227:CYS:HB3	1.82	0.62
1:R:187:ILE:O	1:R:191:LYS:HG2	1.99	0.62
1:WB:187:ILE:HG22	1:WB:191:LYS:HE2	1.82	0.62
1:A:220:GLU:HG2	2:a:90:ILE:HD11	1.79	0.62
1:D:260:LYS:HE3	1:D:260:LYS:HA	1.81	0.62
1:Q:174:ASP:O	1:Q:178:ALA:N	2.28	0.62
2:b:10:GLU:OE2	2:b:10:GLU:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ILE:HG21	1:CB:154:SER:HA	1.82	0.62
2:bb:35:LYS:N	2:bb:35:LYS:HD3	2.14	0.62
1:A:273:ILE:HG12	1:AB:273:ILE:HG12	1.82	0.62
1:CB:182:ILE:HG12	1:CB:218:ALA:HB2	1.81	0.62
1:FB:269:THR:HG21	1:FB:271:ARG:HH21	1.65	0.62
1:JB:201:ILE:HD11	1:JB:234:ILE:HG12	1.81	0.62
1:M:155:ALA:HB1	1:M:167:MET:HE1	1.79	0.62
1:JB:210:MET:HE3	1:JB:210:MET:HA	1.82	0.62
1:OB:177:ARG:O	1:OB:181:ILE:HG23	2.00	0.62
1:RB:220:GLU:OE2	1:RB:251:GLN:NE2	2.32	0.62
2:c:3:ILE:HD12	2:c:28:PHE:HB2	1.82	0.62
1:FB:213:HIS:HD2	1:FB:214:HIS:HD2	1.47	0.61
1:R:182:ILE:HG12	1:R:218:ALA:HB2	1.82	0.61
1:S:172:THR:O	1:S:177:ARG:NH1	2.33	0.61
1:CB:163:LYS:NZ	1:CB:195:GLU:OE2	2.29	0.61
1:Q:198:LEU:HD23	1:Q:232:VAL:HG21	1.82	0.61
1:VB:212:ALA:O	1:VB:216:ILE:HG12	2.00	0.61
2:a:6:LEU:HD22	2:ab:105:LEU:HD13	1.82	0.61
1:F:155:ALA:HB1	1:F:167:MET:HE1	1.83	0.61
1:A:186:LEU:O	1:A:190:VAL:HG23	2.01	0.61
1:B:157:LEU:HD13	1:B:188:GLY:HA3	1.82	0.61
1:JB:169:LEU:HD12	1:JB:201:ILE:HG22	1.81	0.61
1:W:187:ILE:HG22	1:W:191:LYS:HE3	1.83	0.61
1:WB:238:ILE:HD12	1:WB:238:ILE:H	1.65	0.61
1:A:170:ILE:O	1:A:177:ARG:NH2	2.27	0.61
1:G:231:LEU:HB2	1:G:252:ILE:HD11	1.83	0.61
1:T:182:ILE:O	1:T:186:LEU:HG	2.01	0.61
2:cb:66:VAL:HG23	2:cb:76:VAL:HB	1.83	0.61
1:G:207:VAL:HB	1:G:238:ILE:HG23	1.81	0.61
1:OB:249:LEU:HD12	1:VB:224:LEU:HD22	1.81	0.61
1:SB:162:GLU:OE1	1:SB:162:GLU:N	2.29	0.61
2:c:23:HIS:O	2:c:27:GLU:HG2	2.00	0.61
2:cb:32:LEU:HD23	2:cb:65:VAL:HG11	1.81	0.61
2:d:26:VAL:O	2:d:30:GLU:HG2	2.01	0.61
1:K:256:ASN:HD21	2:ab:40:SER:HB2	1.65	0.61
2:b:7:LYS:NZ	2:b:9:GLY:O	2.34	0.61
1:BB:202:THR:O	1:BB:235:ARG:NH2	2.34	0.61
1:E:170:ILE:HG22	1:E:203:GLY:HA3	1.82	0.61
1:H:188:GLY:HA2	1:H:191:LYS:HG3	1.83	0.61
1:S:238:ILE:O	1:S:242:ILE:HG13	2.00	0.61
1:UB:193:ARG:NH2	2:g:107:SER:OG	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:64:ASP:O	2:d:68:MET:HG3	2.00	0.61
1:A:202:THR:O	1:A:235:ARG:NH2	2.34	0.61
1:DB:201:ILE:HD11	1:DB:234:ILE:HA	1.83	0.61
2:ab:96:PHE:HB3	2:ab:99:VAL:HB	1.81	0.61
2:cb:10:GLU:OE2	2:cb:42:ARG:NH2	2.34	0.61
2:eb:64:ASP:O	2:eb:68:MET:HG3	2.01	0.60
1:R:186:LEU:HD13	2:cb:83:PRO:HB3	1.82	0.60
1:W:187:ILE:O	1:W:191:LYS:HG2	2.01	0.60
2:cb:49:THR:HG22	2:cb:80:GLY:HA3	1.82	0.60
2:fb:26:VAL:O	2:fb:30:GLU:HG2	2.01	0.60
1:N:235:ARG:CZ	1:N:236:PRO:HD2	2.31	0.60
1:NB:183:GLU:O	1:NB:187:ILE:HG22	2.01	0.60
1:W:202:THR:O	1:W:235:ARG:NH2	2.33	0.60
1:E:186:LEU:O	1:E:190:VAL:HG23	2.00	0.60
1:SB:187:ILE:O	1:SB:191:LYS:HG2	2.01	0.60
1:TB:238:ILE:HD12	1:TB:238:ILE:H	1.66	0.60
1:CB:218:ALA:O	1:CB:222:VAL:HG12	2.02	0.60
1:LB:169:LEU:HD12	1:LB:201:ILE:HG22	1.84	0.60
1:IB:241:THR:HA	1:IB:244:ASN:HD21	1.64	0.60
1:M:211:VAL:O	1:M:215:ILE:HG12	2.02	0.60
1:D:193:ARG:HH12	1:E:256:ASN:HB3	1.66	0.60
2:a:64:ASP:O	2:a:68:MET:HG3	2.01	0.60
2:a:77:VAL:HG22	2:a:100:LEU:HB2	1.83	0.60
1:GB:222:VAL:HG22	1:GB:227:CYS:HB3	1.83	0.60
1:HB:193:ARG:NH1	2:ab:104:ASP:OD2	2.34	0.60
1:JB:182:ILE:HD11	1:JB:214:HIS:HB3	1.84	0.60
2:db:10:GLU:OE2	2:db:10:GLU:N	2.35	0.60
1:OB:193:ARG:HA	2:gb:103:MET:HE1	1.83	0.60
1:V:170:ILE:HG21	1:VB:154:SER:HA	1.82	0.60
2:eb:85:VAL:O	2:eb:89:LEU:HG	2.00	0.60
1:I:273:ILE:HG12	1:IB:273:ILE:HG12	1.83	0.59
1:WB:238:ILE:HG22	1:WB:242:ILE:HD11	1.83	0.59
1:E:162:GLU:OE2	1:EB:259:LYS:NZ	2.35	0.59
1:G:190:VAL:HA	2:d:103:MET:HE1	1.84	0.59
1:JB:179:LYS:O	1:JB:183:GLU:HG3	2.02	0.59
1:KB:186:LEU:O	1:KB:190:VAL:HG23	2.01	0.59
1:NB:238:ILE:O	1:NB:242:ILE:HG13	2.03	0.59
1:WB:187:ILE:O	1:WB:191:LYS:HG2	2.03	0.59
1:AB:238:ILE:HD12	1:AB:238:ILE:H	1.67	0.59
1:H:218:ALA:O	1:H:222:VAL:HG12	2.02	0.59
1:MB:176:GLU:O	1:MB:180:LEU:HG	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WB:188:GLY:O	1:WB:192:ASN:ND2	2.30	0.59
1:B:222:VAL:HG22	1:B:227:CYS:HB3	1.84	0.59
1:J:216:ILE:HD13	1:J:247:ILE:HG21	1.83	0.59
1:Q:182:ILE:HG12	1:Q:218:ALA:HB2	1.84	0.59
1:QB:154:SER:O	1:QB:177:ARG:NH2	2.34	0.59
1:TB:231:LEU:HB2	1:TB:252:ILE:HD11	1.84	0.59
2:db:85:VAL:O	2:db:89:LEU:HD22	2.02	0.59
2:g:61:ILE:O	2:g:65:VAL:HG12	2.02	0.59
1:CB:213:HIS:O	1:CB:217:GLN:HG2	2.01	0.59
1:F:170:ILE:HG21	1:FB:154:SER:HA	1.83	0.59
1:IB:150:LEU:O	1:IB:154:SER:OG	2.13	0.59
1:PB:163:LYS:NZ	1:PB:195:GLU:OE2	2.30	0.59
2:a:34:ALA:O	2:a:38:GLU:HG3	2.03	0.59
1:GB:182:ILE:HG12	1:GB:218:ALA:HB2	1.84	0.59
1:NB:222:VAL:HG22	1:NB:227:CYS:HB3	1.84	0.59
1:R:180:LEU:O	1:R:184:ASN:ND2	2.36	0.59
1:SB:235:ARG:HG2	1:SB:238:ILE:HG13	1.85	0.59
1:TB:179:LYS:HD3	1:TB:179:LYS:N	2.18	0.59
2:a:96:PHE:HB3	2:a:99:VAL:HB	1.83	0.59
2:cb:29:GLN:OE1	2:cb:61:ILE:HG23	2.02	0.59
1:CB:222:VAL:HG22	1:CB:227:CYS:HB3	1.84	0.59
1:G:222:VAL:HG22	1:G:227:CYS:HB3	1.84	0.59
1:H:186:LEU:O	1:H:190:VAL:HG23	2.02	0.59
1:I:259:LYS:NZ	1:IB:162:GLU:OE2	2.35	0.59
1:P:202:THR:O	1:P:235:ARG:NH2	2.35	0.59
2:ab:34:ALA:O	2:ab:38:GLU:HG3	2.03	0.59
1:LB:201:ILE:HD11	1:LB:234:ILE:HG12	1.83	0.59
1:OB:222:VAL:HG22	1:OB:227:CYS:HB3	1.85	0.59
1:CB:240:GLN:O	1:CB:244:ASN:ND2	2.36	0.59
1:I:162:GLU:HG2	1:I:271:ARG:HH12	1.68	0.59
1:L:238:ILE:HD12	1:L:238:ILE:H	1.66	0.59
1:TB:201:ILE:HD11	1:TB:234:ILE:HD12	1.85	0.59
2:b:96:PHE:HB3	2:b:99:VAL:HB	1.84	0.59
2:bb:26:VAL:O	2:bb:30:GLU:HG2	2.03	0.59
2:fb:16:ILE:HG21	2:fb:51:ILE:HD11	1.85	0.59
1:B:185:LEU:HD11	1:B:197:VAL:HG21	1.85	0.59
1:HB:186:LEU:HD13	2:ab:83:PRO:HB3	1.85	0.58
1:KB:187:ILE:HG22	1:KB:191:LYS:HZ1	1.67	0.58
2:g:6:LEU:HD22	2:gb:105:LEU:HD13	1.85	0.58
1:HB:163:LYS:HB3	1:HB:195:GLU:HG3	1.84	0.58
1:K:172:THR:O	1:K:177:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:ALA:HB2	1:M:181:ILE:HG12	1.85	0.58
2:e:44:VAL:HB	2:e:76:VAL:HG22	1.85	0.58
1:CB:176:GLU:HA	1:CB:179:LYS:HG2	1.85	0.58
1:L:222:VAL:HG22	1:L:227:CYS:HB3	1.84	0.58
1:RB:218:ALA:O	1:RB:222:VAL:HG23	2.03	0.58
1:S:186:LEU:HD11	1:S:225:VAL:HG21	1.85	0.58
1:VB:240:GLN:OE1	1:VB:244:ASN:ND2	2.30	0.58
2:c:8:LEU:HD11	2:cb:109:LEU:HD13	1.85	0.58
1:AB:154:SER:HB3	1:AB:177:ARG:HH21	1.68	0.58
1:G:207:VAL:HG13	1:G:211:VAL:HB	1.85	0.58
1:I:238:ILE:HD12	1:I:238:ILE:H	1.69	0.58
1:NB:202:THR:O	1:NB:235:ARG:NH2	2.35	0.58
1:S:235:ARG:HD3	1:S:236:PRO:HD2	1.84	0.58
2:c:85:VAL:O	2:c:89:LEU:HG	2.03	0.58
1:M:160:ILE:HG22	1:M:161:PHE:HD2	1.68	0.58
1:S:249:LEU:HD22	1:S:252:ILE:HD11	1.84	0.58
2:cb:48:ILE:HD11	2:cb:81:ILE:HG13	1.85	0.58
1:H:182:ILE:HG12	1:H:218:ALA:HB2	1.84	0.58
1:PB:249:LEU:HD22	2:a:71:LEU:HD22	1.85	0.58
2:e:96:PHE:HB3	2:e:99:VAL:HB	1.85	0.58
1:G:193:ARG:HA	2:d:103:MET:HE2	1.84	0.58
2:ab:22:ASP:O	2:ab:26:VAL:HG23	2.04	0.58
1:J:179:LYS:HA	1:J:182:ILE:HD12	1.85	0.58
1:Q:272:GLU:N	1:Q:272:GLU:OE2	2.37	0.58
1:RB:175:THR:HB	1:RB:179:LYS:HZ1	1.68	0.58
1:U:231:LEU:HB2	1:U:252:ILE:HD11	1.86	0.58
1:CB:249:LEU:HD22	1:CB:252:ILE:HD12	1.85	0.58
1:AB:183:GLU:O	1:AB:187:ILE:HG12	2.03	0.58
1:BB:182:ILE:O	1:BB:186:LEU:HD12	2.04	0.58
1:EB:236:PRO:HB3	1:MB:186:LEU:HB3	1.85	0.58
1:UB:172:THR:O	1:UB:177:ARG:NH1	2.35	0.58
1:S:187:ILE:HG23	1:S:191:LYS:NZ	2.18	0.57
1:S:230:MET:HG3	1:S:253:ILE:HB	1.86	0.57
1:SB:154:SER:HB3	1:SB:177:ARG:HH21	1.68	0.57
1:JB:222:VAL:HG22	1:JB:227:CYS:HB3	1.85	0.57
1:L:249:LEU:HD22	1:L:252:ILE:HD11	1.86	0.57
1:N:189:VAL:HG11	1:N:222:VAL:HG23	1.85	0.57
1:T:222:VAL:HA	1:T:225:VAL:HG22	1.86	0.57
1:VB:218:ALA:O	1:VB:222:VAL:HG22	2.05	0.57
1:NB:155:ALA:HB1	1:NB:167:MET:HE3	1.86	0.57
1:P:173:ILE:HA	1:P:177:ARG:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cb:35:LYS:HD3	2:cb:35:LYS:N	2.19	0.57
2:e:34:ALA:O	2:e:38:GLU:HG3	2.04	0.57
2:fb:34:ALA:O	2:fb:38:GLU:HG3	2.04	0.57
1:D:218:ALA:O	1:D:222:VAL:HG12	2.04	0.57
1:G:176:GLU:OE1	1:G:176:GLU:N	2.26	0.57
1:JB:186:LEU:O	1:JB:190:VAL:HG22	2.04	0.57
1:LB:185:LEU:HD11	1:LB:197:VAL:HG21	1.87	0.57
1:LB:186:LEU:O	1:LB:190:VAL:HG22	2.04	0.57
1:LB:235:ARG:HG2	1:LB:238:ILE:HD12	1.86	0.57
1:T:253:ILE:HD12	1:T:253:ILE:H	1.68	0.57
1:S:207:VAL:HG13	1:S:211:VAL:HB	1.86	0.57
1:E:189:VAL:HG12	2:f:103:MET:HE1	1.86	0.57
1:FB:186:LEU:O	1:FB:190:VAL:HG23	2.05	0.57
1:I:235:ARG:HG2	1:I:238:ILE:CD1	2.34	0.57
1:KB:179:LYS:HD3	1:KB:179:LYS:N	2.19	0.57
1:T:218:ALA:O	1:T:222:VAL:HG22	2.04	0.57
1:A:183:GLU:O	1:A:187:ILE:HG22	2.05	0.57
1:AB:231:LEU:HB2	1:AB:252:ILE:HD11	1.85	0.57
2:ab:35:LYS:NZ	2:ab:39:THR:OG1	2.36	0.57
1:K:170:ILE:HD11	1:KB:170:ILE:HG12	1.87	0.57
1:FB:160:ILE:HD12	1:FB:166:VAL:HB	1.86	0.57
2:b:34:ALA:O	2:b:38:GLU:HG3	2.05	0.57
1:A:182:ILE:HG12	1:A:218:ALA:HB2	1.85	0.57
1:T:187:ILE:O	1:T:191:LYS:HG2	2.05	0.57
1:UB:186:LEU:HB3	2:g:83:PRO:HG3	1.87	0.57
1:DB:222:VAL:O	1:DB:227:CYS:N	2.32	0.56
1:IB:177:ARG:HE	1:IB:181:ILE:HD11	1.70	0.56
1:QB:163:LYS:HA	1:QB:194:SER:HA	1.85	0.56
2:c:5:ILE:HD11	2:c:12:LEU:HD13	1.87	0.56
2:gb:85:VAL:O	2:gb:89:LEU:HD23	2.05	0.56
1:A:250:ASP:OD1	1:A:250:ASP:N	2.38	0.56
1:JB:187:ILE:HG23	1:JB:191:LYS:NZ	2.20	0.56
1:T:176:GLU:CD	1:T:176:GLU:H	2.13	0.56
2:a:23:HIS:O	2:a:27:GLU:HG2	2.04	0.56
1:L:239:ALA:O	1:L:243:VAL:HG23	2.05	0.56
2:a:17:GLN:HA	2:a:50:SER:HB2	1.87	0.56
2:ab:36:ILE:HD11	2:ab:44:VAL:HG21	1.87	0.56
1:E:247:ILE:HD12	1:E:247:ILE:H	1.69	0.56
1:E:276:LYS:NZ	1:EB:272:GLU:OE2	2.31	0.56
1:Q:183:GLU:O	1:Q:187:ILE:HG12	2.05	0.56
2:ab:26:VAL:HG12	2:ab:30:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JB:240:GLN:HA	2:e:68:MET:HE2	1.88	0.56
1:T:189:VAL:HG21	1:T:222:VAL:HG12	1.87	0.56
2:b:104:ASP:OD2	2:b:104:ASP:N	2.36	0.56
1:A:221:ALA:O	1:A:225:VAL:HG23	2.05	0.56
1:G:182:ILE:HG12	1:G:218:ALA:HB2	1.87	0.56
1:EB:177:ARG:O	1:EB:181:ILE:HG12	2.05	0.56
1:Q:187:ILE:HA	1:Q:190:VAL:HG12	1.88	0.56
1:RB:179:LYS:HD3	1:RB:179:LYS:N	2.21	0.56
1:S:221:ALA:O	1:S:225:VAL:HG23	2.05	0.56
2:db:7:LYS:NZ	2:db:9:GLY:O	2.37	0.56
2:e:34:ALA:HB3	2:e:35:LYS:NZ	2.21	0.56
1:AB:179:LYS:HD3	1:AB:179:LYS:N	2.19	0.56
1:R:218:ALA:O	1:R:222:VAL:HG12	2.06	0.56
1:S:240:GLN:O	1:S:244:ASN:ND2	2.39	0.56
2:eb:29:GLN:HG3	2:eb:65:VAL:HG22	1.88	0.56
1:N:269:THR:O	1:N:269:THR:HG22	2.06	0.56
1:O:182:ILE:HG12	1:O:218:ALA:HB2	1.88	0.56
1:IB:182:ILE:HG12	1:IB:218:ALA:HB2	1.88	0.56
1:LB:231:LEU:HB2	1:LB:252:ILE:HD11	1.88	0.56
2:eb:34:ALA:O	2:eb:38:GLU:HG3	2.05	0.56
1:OB:231:LEU:HB2	1:OB:252:ILE:HD11	1.87	0.55
1:SB:218:ALA:O	1:SB:222:VAL:HG22	2.05	0.55
1:U:207:VAL:HG21	1:U:238:ILE:HG23	1.87	0.55
1:U:238:ILE:O	1:U:242:ILE:HG13	2.07	0.55
1:A:170:ILE:HD12	1:AB:170:ILE:HD12	1.87	0.55
1:BB:186:LEU:HD21	1:BB:221:ALA:HB1	1.88	0.55
1:D:222:VAL:HG22	1:D:227:CYS:HB3	1.88	0.55
1:O:239:ALA:HA	1:O:242:ILE:HD12	1.88	0.55
2:eb:16:ILE:HG21	2:eb:51:ILE:HD11	1.87	0.55
1:U:150:LEU:O	1:U:154:SER:OG	2.19	0.55
1:B:186:LEU:HD13	1:HB:236:PRO:HB3	1.86	0.55
1:E:245:LEU:HB2	1:E:247:ILE:HD11	1.87	0.55
1:JB:191:LYS:HD3	1:JB:191:LYS:N	2.21	0.55
1:U:169:LEU:HD12	1:U:201:ILE:HG22	1.88	0.55
1:VB:240:GLN:HA	2:cb:68:MET:CE	2.35	0.55
2:bb:12:LEU:HD21	2:bb:39:THR:HG21	1.88	0.55
2:f:104:ASP:OD2	2:f:104:ASP:N	2.37	0.55
1:BB:154:SER:HB3	1:BB:177:ARG:HH21	1.71	0.55
1:E:161:PHE:CE1	1:EB:273:ILE:HG13	2.38	0.55
1:E:193:ARG:NH2	2:f:104:ASP:OD1	2.40	0.55
1:HB:213:HIS:HA	1:HB:216:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:208:ASP:OD1	1:I:209:ALA:N	2.37	0.55
1:M:186:LEU:HD23	2:e:83:PRO:HG3	1.86	0.55
1:M:197:VAL:HG12	1:M:229:ALA:HA	1.88	0.55
1:J:172:THR:O	1:J:177:ARG:NH1	2.39	0.55
1:R:181:ILE:HA	1:R:184:ASN:HD22	1.72	0.55
2:e:77:VAL:HG22	2:e:100:LEU:HB2	1.89	0.55
1:C:170:ILE:HD12	1:CB:170:ILE:HD12	1.89	0.55
1:C:222:VAL:HG22	1:C:227:CYS:HB3	1.89	0.55
1:N:222:VAL:HG22	1:N:227:CYS:HB3	1.87	0.55
1:PB:187:ILE:O	1:PB:191:LYS:HG3	2.07	0.55
1:PB:238:ILE:O	1:PB:242:ILE:HG13	2.07	0.55
1:RB:150:LEU:O	1:RB:154:SER:OG	2.21	0.55
2:f:16:ILE:HD12	2:f:48:ILE:HG22	1.89	0.55
1:C:258:MET:HG2	1:CB:160:ILE:HD13	1.88	0.55
1:W:218:ALA:O	1:W:222:VAL:HG22	2.07	0.55
1:EB:187:ILE:HG22	1:EB:191:LYS:HE2	1.89	0.55
1:NB:208:ASP:OD2	1:NB:209:ALA:N	2.32	0.55
1:VB:239:ALA:O	1:VB:243:VAL:HG23	2.07	0.55
2:f:6:LEU:HD22	2:fb:105:LEU:HD13	1.87	0.55
1:C:154:SER:HA	1:CB:170:ILE:HG21	1.89	0.55
1:CB:186:LEU:O	1:CB:190:VAL:HG12	2.07	0.55
1:L:235:ARG:HG2	1:L:236:PRO:HD2	1.89	0.55
1:OB:188:GLY:HA2	1:OB:191:LYS:HG3	1.88	0.55
1:UB:218:ALA:O	1:UB:222:VAL:HG22	2.07	0.55
1:V:162:GLU:H	1:V:162:GLU:CD	2.14	0.55
1:VB:160:ILE:HG22	1:VB:161:PHE:CD2	2.42	0.55
1:DB:177:ARG:HA	1:DB:180:LEU:HD12	1.88	0.54
1:NB:231:LEU:HB3	1:NB:254:THR:HG22	1.89	0.54
1:S:170:ILE:HG21	1:SB:154:SER:HA	1.89	0.54
1:U:238:ILE:HD12	1:U:238:ILE:H	1.72	0.54
2:cb:33:LEU:HD21	2:cb:68:MET:HB3	1.89	0.54
2:d:106:GLU:N	2:d:106:GLU:OE1	2.35	0.54
2:g:29:GLN:HG3	2:g:65:VAL:HB	1.89	0.54
1:I:170:ILE:O	1:I:177:ARG:NH2	2.27	0.54
1:P:218:ALA:O	1:P:222:VAL:HG22	2.06	0.54
1:S:235:ARG:CD	1:S:236:PRO:HD2	2.37	0.54
2:g:96:PHE:HB3	2:g:99:VAL:HB	1.89	0.54
1:LB:193:ARG:NH1	2:fb:104:ASP:OD2	2.41	0.54
1:TB:155:ALA:HB2	1:TB:177:ARG:HH21	1.72	0.54
1:E:218:ALA:O	1:E:222:VAL:HG22	2.07	0.54
1:E:256:ASN:C	1:E:256:ASN:ND2	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:235:ARG:HG3	1:I:237:GLU:OE1	2.08	0.54
1:L:175:THR:HG23	1:L:179:LYS:HE3	1.88	0.54
1:M:186:LEU:O	1:M:190:VAL:HG12	2.06	0.54
2:gb:32:LEU:HD23	2:gb:65:VAL:HG11	1.89	0.54
1:BB:236:PRO:HB3	1:C:186:LEU:HB3	1.89	0.54
1:DB:195:GLU:N	1:DB:195:GLU:OE2	2.41	0.54
1:EB:213:HIS:HA	1:EB:216:ILE:HD12	1.88	0.54
1:F:210:MET:HE3	1:F:214:HIS:CE1	2.43	0.54
1:HB:238:ILE:O	1:HB:242:ILE:HG13	2.08	0.54
1:UB:157:LEU:HD12	1:UB:167:MET:HE1	1.88	0.54
2:ab:14:ILE:HD11	2:ab:32:LEU:HD13	1.90	0.54
2:bb:7:LYS:NZ	2:bb:9:GLY:O	2.41	0.54
1:P:276:LYS:O	1:PB:270:ASN:ND2	2.40	0.54
1:PB:186:LEU:O	1:PB:190:VAL:HG22	2.07	0.54
1:Q:221:ALA:O	1:Q:225:VAL:HG23	2.07	0.54
1:T:154:SER:HB3	1:T:177:ARG:HH21	1.73	0.54
1:W:185:LEU:HD21	1:W:197:VAL:HG21	1.90	0.54
2:c:31:ASP:HB3	2:c:35:LYS:HE2	1.89	0.54
2:g:33:LEU:HD21	2:g:68:MET:HB3	1.90	0.54
1:O:258:MET:HE3	1:OB:158:LEU:HD23	1.89	0.54
1:U:170:ILE:HG21	1:UB:154:SER:HA	1.90	0.54
1:V:184:ASN:HA	1:V:187:ILE:HD12	1.90	0.54
1:J:269:THR:HG21	1:J:271:ARG:HH21	1.71	0.54
1:QB:180:LEU:HA	1:QB:183:GLU:OE2	2.08	0.54
1:QB:207:VAL:HG13	1:QB:211:VAL:HB	1.89	0.54
1:SB:211:VAL:O	1:SB:215:ILE:HD12	2.08	0.54
2:eb:89:LEU:HD13	2:eb:96:PHE:HE2	1.73	0.54
2:fb:85:VAL:O	2:fb:89:LEU:HD13	2.07	0.54
1:AB:236:PRO:HB3	1:KB:186:LEU:HD13	1.90	0.54
1:DB:179:LYS:HD2	1:DB:179:LYS:C	2.32	0.54
1:J:175:THR:HG22	1:J:179:LYS:HE3	1.90	0.54
1:J:201:ILE:HD11	1:J:234:ILE:HG12	1.90	0.54
1:M:170:ILE:HG21	1:MB:154:SER:HA	1.90	0.54
1:PB:186:LEU:HD21	1:PB:221:ALA:HB1	1.90	0.54
1:TB:242:ILE:HG23	1:TB:247:ILE:HD12	1.90	0.54
1:DB:175:THR:HG22	1:DB:210:MET:HE1	1.90	0.54
1:EB:249:LEU:HD23	1:EB:254:THR:HG21	1.90	0.54
1:G:245:LEU:HB2	1:G:247:ILE:HD11	1.89	0.54
1:HB:185:LEU:HD11	1:HB:197:VAL:HG21	1.89	0.54
1:JB:241:THR:HA	1:JB:244:ASN:HD21	1.72	0.54
1:FB:163:LYS:NZ	1:FB:195:GLU:OE2	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:182:ILE:HG12	1:K:218:ALA:HB2	1.90	0.53
1:NB:250:ASP:OD1	1:NB:251:GLN:N	2.40	0.53
1:W:201:ILE:HD11	1:W:234:ILE:HD12	1.90	0.53
1:W:212:ALA:O	1:W:216:ILE:HG12	2.08	0.53
1:BB:186:LEU:HD23	1:BB:225:VAL:HG21	1.89	0.53
1:E:173:ILE:HA	1:E:177:ARG:HG2	1.90	0.53
2:fb:23:HIS:O	2:fb:27:GLU:HG2	2.07	0.53
1:I:160:ILE:HG22	1:I:161:PHE:HD2	1.72	0.53
1:TB:168:PRO:HA	1:TB:200:ASP:HB2	1.91	0.53
2:g:10:GLU:OE2	2:g:42:ARG:NH1	2.41	0.53
1:F:182:ILE:HG12	1:F:218:ALA:HB2	1.90	0.53
1:N:185:LEU:HD11	1:N:197:VAL:HG21	1.90	0.53
1:SB:150:LEU:O	1:SB:154:SER:OG	2.19	0.53
2:gb:48:ILE:HD11	2:gb:81:ILE:HG12	1.90	0.53
1:D:249:LEU:HD22	1:D:252:ILE:HD11	1.90	0.53
1:EB:237:GLU:H	1:EB:237:GLU:CD	2.17	0.53
1:F:191:LYS:HB2	1:F:191:LYS:NZ	2.23	0.53
1:MB:231:LEU:HB2	1:MB:252:ILE:HD11	1.91	0.53
1:Q:182:ILE:O	1:Q:186:LEU:HG	2.08	0.53
2:a:7:LYS:NZ	2:a:9:GLY:O	2.41	0.53
1:D:154:SER:HA	1:DB:170:ILE:HG21	1.89	0.53
1:J:180:LEU:HA	1:J:183:GLU:OE1	2.08	0.53
1:P:186:LEU:O	1:P:190:VAL:HG22	2.09	0.53
1:S:157:LEU:HD13	1:S:188:GLY:HA3	1.90	0.53
2:d:66:VAL:HG22	2:d:76:VAL:HG11	1.91	0.53
2:gb:96:PHE:HB3	2:gb:99:VAL:HB	1.91	0.53
1:A:170:ILE:HG21	1:AB:154:SER:HA	1.91	0.53
1:MB:241:THR:O	1:MB:245:LEU:HG	2.09	0.53
1:N:179:LYS:HD3	1:N:179:LYS:N	2.23	0.53
1:NB:218:ALA:O	1:NB:222:VAL:HG12	2.09	0.53
1:OB:220:GLU:HB3	2:gb:90:ILE:HD11	1.91	0.53
1:RB:249:LEU:HD13	1:TB:224:LEU:HD21	1.91	0.53
1:UB:269:THR:C	1:UB:270:ASN:HD22	2.15	0.53
1:A:232:VAL:HG11	1:A:258:MET:HA	1.91	0.53
1:EB:185:LEU:HD11	1:EB:197:VAL:HG21	1.91	0.53
1:H:207:VAL:HB	1:H:211:VAL:HB	1.90	0.53
1:R:201:ILE:HD11	1:R:234:ILE:HD13	1.89	0.53
1:UB:186:LEU:HD13	2:g:83:PRO:HB3	1.90	0.53
1:WB:207:VAL:HG13	1:WB:211:VAL:HB	1.91	0.53
1:EB:245:LEU:HD23	1:EB:247:ILE:HD11	1.91	0.53
1:OB:147:LYS:HA	1:OB:150:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:160:ILE:HG22	1:I:161:PHE:CD2	2.44	0.53
1:MB:223:ARG:HE	1:MB:224:LEU:HD23	1.73	0.53
2:c:49:THR:HG22	2:c:80:GLY:HA3	1.91	0.53
1:J:177:ARG:HA	1:J:180:LEU:HD12	1.90	0.52
1:U:176:GLU:O	1:U:180:LEU:HG	2.09	0.52
1:F:202:THR:O	1:F:235:ARG:NH2	2.43	0.52
1:J:218:ALA:O	1:J:222:VAL:HG12	2.08	0.52
1:NB:182:ILE:HG12	1:NB:218:ALA:HB2	1.91	0.52
1:O:170:ILE:HD12	1:OB:154:SER:HA	1.91	0.52
1:O:238:ILE:HG22	1:O:242:ILE:HD11	1.92	0.52
1:S:272:GLU:OE2	1:S:272:GLU:N	2.42	0.52
1:TB:200:ASP:OD2	1:TB:258:MET:HE1	2.09	0.52
1:UB:147:LYS:HA	1:UB:150:LEU:HD12	1.92	0.52
2:c:77:VAL:HG22	2:c:100:LEU:HB2	1.89	0.52
2:cb:34:ALA:O	2:cb:38:GLU:HG2	2.09	0.52
1:CB:147:LYS:HA	1:CB:150:LEU:HD12	1.92	0.52
1:D:236:PRO:HB3	1:O:186:LEU:HD13	1.91	0.52
1:JB:218:ALA:O	1:JB:222:VAL:HG12	2.09	0.52
1:JB:253:ILE:HD12	1:JB:253:ILE:H	1.74	0.52
1:KB:178:ALA:O	1:KB:181:ILE:HG13	2.09	0.52
2:d:55:ASP:OD2	2:d:55:ASP:N	2.42	0.52
2:g:66:VAL:HG22	2:g:76:VAL:HG11	1.91	0.52
1:G:262:MET:HE3	1:GB:160:ILE:HG23	1.90	0.52
1:J:170:ILE:O	1:J:177:ARG:NH2	2.40	0.52
1:J:235:ARG:HG3	1:J:237:GLU:H	1.74	0.52
1:SB:242:ILE:HG21	1:SB:249:LEU:HD21	1.91	0.52
2:cb:64:ASP:OD2	2:cb:68:MET:HE2	2.10	0.52
2:g:57:PHE:O	2:g:61:ILE:HG12	2.10	0.52
1:E:237:GLU:O	1:E:241:THR:OG1	2.24	0.52
1:G:243:VAL:HG11	1:J:220:GLU:CD	2.35	0.52
1:IB:168:PRO:HA	1:IB:200:ASP:HB2	1.90	0.52
1:V:258:MET:HG2	1:VB:160:ILE:HD13	1.91	0.52
1:J:235:ARG:HG2	1:J:238:ILE:CD1	2.38	0.52
1:JB:185:LEU:O	1:JB:189:VAL:HG23	2.10	0.52
1:S:241:THR:HA	1:S:244:ASN:HD21	1.75	0.52
1:T:167:MET:HE3	1:T:185:LEU:HG	1.91	0.52
1:V:169:LEU:HD21	1:V:173:ILE:HD11	1.91	0.52
1:W:258:MET:HE3	1:WB:158:LEU:HD23	1.90	0.52
2:bb:68:MET:O	2:bb:72:MET:HE3	2.09	0.52
1:AB:186:LEU:HB3	1:MB:236:PRO:HB3	1.92	0.52
1:C:185:LEU:HD11	1:C:197:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:223:ARG:NH1	1:CB:251:GLN:HB3	2.25	0.52
1:IB:175:THR:HG22	1:IB:179:LYS:HE3	1.90	0.52
1:J:184:ASN:HA	1:J:187:ILE:HD12	1.91	0.52
1:J:207:VAL:HB	1:J:238:ILE:HG12	1.92	0.52
1:K:238:ILE:O	1:K:242:ILE:HG13	2.10	0.52
1:S:235:ARG:HB3	1:S:238:ILE:CD1	2.38	0.52
1:UB:174:ASP:O	1:UB:178:ALA:N	2.41	0.52
2:fb:66:VAL:HG23	2:fb:76:VAL:HB	1.92	0.52
1:KB:174:ASP:O	1:KB:178:ALA:N	2.43	0.52
1:DB:184:ASN:HA	1:DB:187:ILE:HG12	1.91	0.52
1:GB:174:ASP:O	1:GB:178:ALA:N	2.40	0.52
2:f:22:ASP:HA	2:f:57:PHE:CE2	2.45	0.52
2:gb:5:ILE:O	2:gb:35:LYS:NZ	2.42	0.52
1:AB:175:THR:HG23	1:AB:179:LYS:HE3	1.91	0.51
1:DB:241:THR:O	1:DB:245:LEU:HG	2.10	0.51
1:I:161:PHE:HE1	1:IB:273:ILE:HD12	1.76	0.51
1:IB:222:VAL:HG22	1:IB:227:CYS:SG	2.49	0.51
1:O:185:LEU:HD11	1:O:197:VAL:HG21	1.92	0.51
1:SB:236:PRO:HD2	2:f:37:HIS:ND1	2.24	0.51
1:TB:179:LYS:HD3	1:TB:179:LYS:H	1.75	0.51
1:BB:190:VAL:HG11	1:WB:235:ARG:HH22	1.73	0.51
1:DB:168:PRO:HA	1:DB:200:ASP:HB2	1.92	0.51
1:FB:154:SER:HB3	1:FB:177:ARG:HH21	1.76	0.51
1:GB:175:THR:HG23	1:GB:214:HIS:HE1	1.74	0.51
1:OB:213:HIS:O	1:OB:217:GLN:HG2	2.10	0.51
1:VB:191:LYS:HG3	1:VB:192:ASN:ND2	2.24	0.51
1:WB:240:GLN:O	1:WB:244:ASN:ND2	2.44	0.51
2:gb:20:LEU:HD11	2:gb:25:ALA:HA	1.91	0.51
2:gb:23:HIS:O	2:gb:27:GLU:HG2	2.10	0.51
1:BB:257:THR:HG21	1:C:193:ARG:HH11	1.75	0.51
1:E:170:ILE:HD11	1:EB:170:ILE:HD12	1.92	0.51
1:HB:200:ASP:HB2	1:HB:258:MET:HE1	1.91	0.51
1:O:180:LEU:HD23	1:O:184:ASN:OD1	2.10	0.51
1:RB:221:ALA:O	1:RB:225:VAL:HG23	2.10	0.51
1:V:272:GLU:OE1	1:VB:276:LYS:NZ	2.37	0.51
2:c:66:VAL:HG23	2:c:76:VAL:HB	1.93	0.51
2:db:13:LEU:HD22	2:db:105:LEU:HD11	1.93	0.51
1:B:236:PRO:HB3	1:FB:186:LEU:HB3	1.92	0.51
1:NB:174:ASP:OD1	1:NB:177:ARG:HB2	2.10	0.51
1:Q:193:ARG:NH2	2:db:104:ASP:OD1	2.43	0.51
1:TB:147:LYS:HA	1:TB:150:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TB:187:ILE:HA	1:TB:190:VAL:HG22	1.91	0.51
1:JB:193:ARG:O	1:JB:193:ARG:HG2	2.11	0.51
1:M:216:ILE:HD13	1:M:247:ILE:HD13	1.91	0.51
1:OB:237:GLU:H	1:OB:237:GLU:CD	2.18	0.51
2:cb:106:GLU:O	2:cb:110:GLU:HG2	2.10	0.51
1:GB:176:GLU:H	1:GB:176:GLU:CD	2.17	0.51
1:K:218:ALA:O	1:K:222:VAL:HG22	2.10	0.51
1:WB:182:ILE:HG12	1:WB:218:ALA:HB2	1.92	0.51
2:b:64:ASP:O	2:b:68:MET:HE3	2.11	0.51
1:EB:180:LEU:O	1:EB:184:ASN:ND2	2.44	0.51
1:JB:177:ARG:HA	1:JB:180:LEU:HG	1.93	0.51
1:QB:147:LYS:HA	1:QB:150:LEU:HD12	1.93	0.51
1:QB:176:GLU:O	1:QB:180:LEU:HG	2.10	0.51
1:T:232:VAL:HG11	1:T:258:MET:HA	1.93	0.51
2:eb:61:ILE:O	2:eb:65:VAL:HG23	2.10	0.51
1:DB:207:VAL:HB	1:DB:238:ILE:HD12	1.93	0.51
1:G:154:SER:HB3	1:G:177:ARG:HH21	1.76	0.51
1:HB:177:ARG:O	1:HB:181:ILE:HG13	2.10	0.51
1:T:177:ARG:HA	1:T:180:LEU:HD12	1.92	0.51
1:TB:162:GLU:O	1:TB:271:ARG:NH2	2.44	0.51
2:d:60:LYS:NZ	2:d:64:ASP:OD2	2.43	0.51
1:G:193:ARG:HG3	1:G:193:ARG:HH11	1.76	0.51
1:P:187:ILE:O	1:P:191:LYS:HG2	2.11	0.51
2:cb:12:LEU:HD13	2:cb:41:ALA:HB2	1.93	0.51
1:HB:186:LEU:HB3	2:ab:83:PRO:HG3	1.93	0.50
1:KB:213:HIS:O	1:KB:217:GLN:HG2	2.11	0.50
1:LB:147:LYS:HA	1:LB:150:LEU:HD12	1.92	0.50
1:E:187:ILE:HG12	1:E:191:LYS:HE2	1.93	0.50
1:G:176:GLU:O	1:G:180:LEU:HG	2.11	0.50
1:P:163:LYS:HA	1:P:194:SER:HA	1.93	0.50
1:SB:253:ILE:HD12	1:SB:253:ILE:H	1.77	0.50
1:T:157:LEU:HD12	1:T:167:MET:HE1	1.92	0.50
2:db:82:GLN:HB2	2:db:85:VAL:HG23	1.92	0.50
2:gb:52:ASP:OD1	2:gb:52:ASP:N	2.29	0.50
1:FB:162:GLU:O	1:FB:271:ARG:NH2	2.29	0.50
1:IB:220:GLU:HB2	2:b:90:ILE:HD12	1.93	0.50
1:K:178:ALA:O	1:K:181:ILE:HG12	2.11	0.50
2:a:81:ILE:HD12	2:a:81:ILE:H	1.76	0.50
2:db:54:ILE:HG13	2:db:88:THR:HG21	1.93	0.50
1:JB:157:LEU:HD22	1:JB:167:MET:HG3	1.93	0.50
1:KB:238:ILE:HG22	1:KB:242:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:201:ILE:HD11	1:O:234:ILE:HG12	1.93	0.50
1:OB:186:LEU:HD13	2:gb:83:PRO:HB3	1.92	0.50
1:SB:201:ILE:HD11	1:SB:234:ILE:HG12	1.93	0.50
1:TB:202:THR:O	1:TB:235:ARG:NH2	2.42	0.50
2:fb:13:LEU:HD22	2:fb:105:LEU:HD11	1.93	0.50
1:K:177:ARG:O	1:K:181:ILE:HG23	2.12	0.50
1:M:172:THR:O	1:M:177:ARG:NH1	2.42	0.50
1:N:162:GLU:O	1:N:271:ARG:NH2	2.44	0.50
1:RB:169:LEU:HD12	1:RB:173:ILE:HD11	1.92	0.50
1:SB:162:GLU:HG2	1:SB:271:ARG:HH12	1.75	0.50
1:V:179:LYS:O	1:V:183:GLU:HG2	2.12	0.50
1:W:237:GLU:HG2	1:W:238:ILE:HD12	1.93	0.50
1:KB:147:LYS:HA	1:KB:150:LEU:HD12	1.92	0.50
1:M:265:ALA:O	1:M:269:THR:HG22	2.12	0.50
1:T:186:LEU:HA	1:T:189:VAL:HG22	1.94	0.50
1:VB:207:VAL:HB	1:VB:238:ILE:HG23	1.93	0.50
1:WB:186:LEU:HD21	1:WB:221:ALA:HB1	1.93	0.50
2:ab:16:ILE:HG22	2:ab:51:ILE:HD11	1.93	0.50
2:c:5:ILE:HD13	2:c:35:LYS:HB2	1.93	0.50
2:cb:54:ILE:HD11	2:cb:58:ILE:HG21	1.94	0.50
2:db:22:ASP:O	2:db:26:VAL:HG23	2.11	0.50
2:e:10:GLU:OE1	2:e:10:GLU:N	2.45	0.50
1:D:255:THR:HG22	1:D:257:THR:H	1.77	0.50
1:H:173:ILE:HG23	1:H:177:ARG:HG3	1.94	0.50
1:Q:202:THR:O	1:Q:235:ARG:NH2	2.45	0.50
1:T:176:GLU:O	1:T:180:LEU:HG	2.12	0.50
1:CB:223:ARG:NH2	1:CB:251:GLN:O	2.45	0.50
1:PB:213:HIS:HA	1:PB:216:ILE:HD12	1.94	0.50
1:Q:231:LEU:HD21	1:Q:234:ILE:HD11	1.94	0.50
1:D:157:LEU:HD22	1:D:188:GLY:HA3	1.93	0.50
1:E:182:ILE:HG12	1:E:218:ALA:HB2	1.94	0.50
1:EB:241:THR:HA	1:EB:244:ASN:HD21	1.76	0.50
1:H:234:ILE:HD11	1:H:238:ILE:HB	1.93	0.50
1:A:224:LEU:O	2:a:81:ILE:HD13	2.11	0.49
1:D:160:ILE:HG22	1:D:161:PHE:CD2	2.47	0.49
1:O:235:ARG:CZ	1:O:236:PRO:HD3	2.42	0.49
1:M:213:HIS:O	1:M:217:GLN:HG2	2.12	0.49
1:MB:177:ARG:HA	1:MB:180:LEU:HD12	1.93	0.49
1:SB:163:LYS:HB3	1:SB:195:GLU:HG3	1.92	0.49
2:e:13:LEU:C	2:e:14:ILE:HD13	2.38	0.49
2:f:5:ILE:HG23	2:f:14:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:LYS:HB2	1:F:191:LYS:HZ3	1.78	0.49
1:LB:256:ASN:OD1	1:LB:256:ASN:N	2.43	0.49
1:MB:175:THR:O	1:MB:179:LYS:HG2	2.12	0.49
1:OB:154:SER:HB3	1:OB:177:ARG:HH21	1.76	0.49
2:d:32:LEU:HD13	2:d:65:VAL:HG11	1.94	0.49
2:fb:64:ASP:O	2:fb:68:MET:HG2	2.11	0.49
1:G:236:PRO:HB3	1:J:186:LEU:HD22	1.94	0.49
1:I:216:ILE:HD11	1:I:247:ILE:HG23	1.93	0.49
1:M:160:ILE:HG22	1:M:161:PHE:CD2	2.45	0.49
1:T:270:ASN:OD1	1:TB:276:LYS:HB3	2.13	0.49
1:TB:216:ILE:HD13	1:TB:247:ILE:HG21	1.94	0.49
1:A:238:ILE:O	1:A:242:ILE:HG13	2.13	0.49
1:AB:230:MET:HE1	1:AB:264:ARG:HB3	1.94	0.49
1:N:269:THR:HG21	1:N:271:ARG:HH21	1.77	0.49
2:fb:18:SER:OG	2:fb:19:GLU:N	2.44	0.49
2:gb:21:ASP:O	2:gb:25:ALA:N	2.41	0.49
1:C:189:VAL:HG11	1:C:222:VAL:HG23	1.93	0.49
1:L:231:LEU:HB3	1:L:254:THR:HG22	1.95	0.49
1:OB:207:VAL:HG13	1:OB:211:VAL:HB	1.94	0.49
1:R:178:ALA:O	1:R:181:ILE:HG12	2.12	0.49
1:TB:185:LEU:HD11	1:TB:197:VAL:HG21	1.94	0.49
1:VB:175:THR:HG22	1:VB:179:LYS:HE2	1.95	0.49
1:IB:186:LEU:HD13	2:b:83:PRO:HB3	1.94	0.49
2:e:104:ASP:OD1	2:e:105:LEU:N	2.45	0.49
1:D:170:ILE:HG21	1:DB:154:SER:HA	1.95	0.49
1:FB:221:ALA:O	1:FB:225:VAL:HG23	2.12	0.49
1:M:150:LEU:O	1:M:154:SER:OG	2.24	0.49
1:S:243:VAL:HG11	2:g:68:MET:HG3	1.94	0.49
1:SB:175:THR:HG22	1:SB:179:LYS:HE3	1.93	0.49
1:VB:257:THR:HG23	1:VB:260:LYS:H	1.76	0.49
2:e:14:ILE:HB	2:e:46:ILE:HA	1.94	0.49
2:eb:96:PHE:HB3	2:eb:99:VAL:HB	1.94	0.49
2:fb:52:ASP:OD1	2:fb:52:ASP:N	2.37	0.49
1:AB:150:LEU:O	1:AB:154:SER:OG	2.18	0.49
1:CB:188:GLY:O	1:CB:192:ASN:ND2	2.36	0.49
1:D:163:LYS:HB3	1:D:195:GLU:HB2	1.93	0.49
1:F:249:LEU:HG	1:F:252:ILE:HD11	1.94	0.49
1:HB:154:SER:HB3	1:HB:177:ARG:HH21	1.77	0.49
1:I:161:PHE:CE1	1:IB:273:ILE:HD12	2.48	0.49
1:OB:235:ARG:HH12	1:VB:190:VAL:HG21	1.76	0.49
1:PB:221:ALA:O	1:PB:225:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QB:200:ASP:OD2	1:QB:258:MET:HE1	2.12	0.49
1:S:182:ILE:HD11	1:S:214:HIS:HB3	1.95	0.49
1:W:221:ALA:O	1:W:225:VAL:HG23	2.13	0.49
1:E:170:ILE:O	1:E:177:ARG:NH2	2.46	0.48
1:EB:186:LEU:HD13	1:N:236:PRO:HB3	1.95	0.48
1:H:250:ASP:OD1	1:H:250:ASP:N	2.46	0.48
1:L:205:PRO:O	1:L:235:ARG:NH2	2.46	0.48
1:NB:175:THR:OG1	1:NB:176:GLU:N	2.46	0.48
1:Q:161:PHE:HZ	1:QB:161:PHE:HZ	1.61	0.48
1:UB:178:ALA:O	1:UB:182:ILE:HG12	2.12	0.48
2:bb:52:ASP:OD1	2:bb:53:PHE:N	2.46	0.48
2:cb:25:ALA:HB1	2:cb:61:ILE:HG21	1.95	0.48
2:g:88:THR:O	2:g:92:LEU:HG	2.13	0.48
1:A:188:GLY:HA2	1:A:191:LYS:HE2	1.94	0.48
1:B:182:ILE:HG12	1:B:218:ALA:HB2	1.94	0.48
1:D:219:SER:OG	1:D:220:GLU:OE1	2.31	0.48
1:GB:169:LEU:HD12	1:GB:201:ILE:HG22	1.95	0.48
1:NB:260:LYS:HA	1:NB:263:GLU:HG2	1.95	0.48
1:OB:253:ILE:HG21	1:OB:264:ARG:HH22	1.77	0.48
2:ab:7:LYS:NZ	2:ab:9:GLY:O	2.38	0.48
2:ab:77:VAL:HG22	2:ab:100:LEU:HB2	1.95	0.48
2:b:66:VAL:HG22	2:b:76:VAL:HG11	1.95	0.48
1:B:184:ASN:HA	1:B:187:ILE:HG22	1.95	0.48
1:BB:221:ALA:O	1:BB:225:VAL:HG23	2.13	0.48
1:E:230:MET:HG2	1:E:253:ILE:HB	1.94	0.48
1:G:242:ILE:HD11	1:G:249:LEU:HD11	1.95	0.48
1:L:242:ILE:HD11	1:L:249:LEU:HD21	1.95	0.48
1:LB:174:ASP:O	1:LB:178:ALA:N	2.42	0.48
1:N:276:LYS:NZ	1:NB:272:GLU:OE2	2.41	0.48
1:OB:250:ASP:OD1	1:OB:250:ASP:N	2.46	0.48
1:U:230:MET:HG2	1:U:253:ILE:HB	1.95	0.48
1:W:175:THR:HG23	1:W:214:HIS:HE1	1.78	0.48
2:e:86:ALA:O	2:e:90:ILE:HG23	2.13	0.48
2:f:106:GLU:HG2	2:f:107:SER:N	2.27	0.48
2:g:64:ASP:O	2:g:68:MET:HE3	2.14	0.48
2:gb:14:ILE:HD11	2:gb:32:LEU:HD13	1.95	0.48
1:BB:147:LYS:HA	1:BB:150:LEU:HD12	1.95	0.48
1:D:236:PRO:HG3	1:O:186:LEU:HB3	1.95	0.48
1:EB:154:SER:HB3	1:EB:177:ARG:HH22	1.77	0.48
1:VB:250:ASP:OD1	1:VB:250:ASP:N	2.47	0.48
2:g:29:GLN:OE1	2:g:61:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:238:ILE:O	1:CB:242:ILE:HG13	2.13	0.48
1:M:237:GLU:O	1:M:241:THR:OG1	2.29	0.48
1:NB:186:LEU:HD11	1:NB:225:VAL:HG21	1.95	0.48
2:eb:7:LYS:NZ	2:eb:9:GLY:O	2.46	0.48
1:F:179:LYS:HD2	1:F:179:LYS:O	2.14	0.48
1:HB:179:LYS:HZ2	1:HB:179:LYS:C	2.21	0.48
1:JB:178:ALA:O	1:JB:182:ILE:HG13	2.13	0.48
1:L:238:ILE:O	1:L:242:ILE:HG22	2.14	0.48
1:Q:235:ARG:HB2	1:Q:238:ILE:HD12	1.94	0.48
1:QB:242:ILE:HG21	1:QB:249:LEU:HD21	1.95	0.48
2:bb:37:HIS:HB3	2:bb:38:GLU:OE2	2.14	0.48
2:bb:66:VAL:HG22	2:bb:76:VAL:HG11	1.96	0.48
1:A:240:GLN:O	1:A:240:GLN:NE2	2.38	0.48
1:E:188:GLY:HA2	1:E:191:LYS:HG2	1.96	0.48
1:EB:147:LYS:HA	1:EB:150:LEU:HD12	1.96	0.48
1:F:172:THR:O	1:F:177:ARG:NH1	2.43	0.48
1:JB:187:ILE:HG23	1:JB:191:LYS:HZ3	1.79	0.48
1:K:167:MET:HE3	1:K:185:LEU:HD13	1.96	0.48
1:P:175:THR:O	1:P:179:LYS:NZ	2.39	0.48
1:RB:235:ARG:NH2	1:TB:190:VAL:HG21	2.28	0.48
2:c:5:ILE:HD12	2:c:14:ILE:HD11	1.95	0.48
2:eb:52:ASP:OD1	2:eb:52:ASP:N	2.33	0.48
2:gb:22:ASP:O	2:gb:26:VAL:HG23	2.12	0.48
1:B:150:LEU:O	1:B:154:SER:OG	2.21	0.48
1:K:202:THR:O	1:K:235:ARG:NH2	2.46	0.48
1:KB:218:ALA:O	1:KB:222:VAL:HG22	2.13	0.48
1:M:170:ILE:HD12	1:MB:170:ILE:HD12	1.94	0.48
1:N:216:ILE:HD13	1:N:247:ILE:HG21	1.96	0.48
1:Q:276:LYS:HB3	1:QB:270:ASN:OD1	2.13	0.48
1:UB:184:ASN:HA	1:UB:187:ILE:HG22	1.96	0.48
2:e:89:LEU:HD22	2:e:96:PHE:HE1	1.79	0.48
1:D:162:GLU:O	1:D:271:ARG:NH2	2.38	0.48
1:GB:220:GLU:OE2	1:GB:251:GLN:NE2	2.47	0.48
1:J:207:VAL:HG13	1:J:211:VAL:HB	1.96	0.48
1:RB:250:ASP:N	1:RB:250:ASP:OD1	2.47	0.48
1:S:183:GLU:O	1:S:187:ILE:HD12	2.14	0.48
1:V:174:ASP:OD1	1:V:176:GLU:N	2.43	0.48
2:ab:96:PHE:HD2	2:ab:99:VAL:HG11	1.77	0.48
2:b:55:ASP:OD1	2:b:58:ILE:HG12	2.14	0.48
2:cb:32:LEU:O	2:cb:36:ILE:HG12	2.12	0.48
2:d:66:VAL:HG11	2:d:99:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:213:HIS:CD2	1:FB:214:HIS:HD2	2.28	0.48
1:I:201:ILE:HD11	1:I:234:ILE:HG12	1.95	0.48
1:J:157:LEU:HD22	1:J:188:GLY:HA3	1.96	0.48
1:M:169:LEU:HD12	1:M:173:ILE:HD11	1.96	0.48
1:PB:177:ARG:O	1:PB:181:ILE:HG13	2.14	0.48
1:S:184:ASN:HA	1:S:187:ILE:HD12	1.95	0.48
1:E:183:GLU:O	1:E:187:ILE:HG22	2.14	0.47
1:I:235:ARG:HG2	1:I:238:ILE:HD12	1.96	0.47
1:JB:173:ILE:HG23	1:JB:177:ARG:HB3	1.96	0.47
1:K:186:LEU:O	1:K:190:VAL:HG12	2.13	0.47
1:QB:169:LEU:HD12	1:QB:201:ILE:HG22	1.95	0.47
1:QB:210:MET:N	1:QB:210:MET:HE2	2.29	0.47
1:SB:240:GLN:HB2	2:f:68:MET:SD	2.54	0.47
1:T:210:MET:HG3	1:T:214:HIS:NE2	2.29	0.47
2:db:15:SER:HA	2:db:47:ASP:OD1	2.14	0.47
1:NB:154:SER:HB3	1:NB:177:ARG:HH22	1.78	0.47
1:O:249:LEU:HD13	1:O:252:ILE:HD11	1.96	0.47
1:PB:213:HIS:O	1:PB:217:GLN:HG2	2.14	0.47
1:PB:216:ILE:HD11	1:PB:247:ILE:HG21	1.96	0.47
1:RB:249:LEU:HB3	1:RB:252:ILE:HD11	1.95	0.47
1:WB:160:ILE:HG22	1:WB:161:PHE:CD2	2.49	0.47
1:C:162:GLU:HB2	1:C:271:ARG:HH12	1.79	0.47
1:N:175:THR:OG1	1:N:176:GLU:N	2.46	0.47
1:O:245:LEU:O	1:O:245:LEU:HD23	2.13	0.47
2:f:16:ILE:HG22	2:f:51:ILE:HD11	1.96	0.47
2:g:40:SER:O	2:g:40:SER:OG	2.32	0.47
1:E:186:LEU:HG	2:f:83:PRO:HG3	1.96	0.47
1:I:179:LYS:HD3	1:I:179:LYS:N	2.29	0.47
1:J:238:ILE:HD12	1:J:238:ILE:H	1.79	0.47
1:L:179:LYS:HD3	1:L:179:LYS:N	2.29	0.47
1:S:239:ALA:O	1:S:243:VAL:HG12	2.14	0.47
1:W:207:VAL:HG13	1:W:211:VAL:HB	1.97	0.47
2:b:94:ILE:H	2:b:94:ILE:HD12	1.79	0.47
2:cb:103:MET:HE3	2:cb:103:MET:HA	1.96	0.47
1:C:213:HIS:O	1:C:217:GLN:HG2	2.14	0.47
1:K:241:THR:O	1:K:245:LEU:HD23	2.14	0.47
1:N:273:ILE:HD13	1:NB:161:PHE:HE1	1.78	0.47
1:R:170:ILE:HG21	1:RB:154:SER:HA	1.97	0.47
1:S:154:SER:HA	1:SB:170:ILE:HG21	1.97	0.47
1:U:176:GLU:OE2	1:U:176:GLU:N	2.30	0.47
1:D:201:ILE:HD11	1:D:234:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:ASN:ND2	1:E:256:ASN:O	2.47	0.47
1:SB:147:LYS:HA	1:SB:150:LEU:HD12	1.96	0.47
1:TB:207:VAL:HB	1:TB:211:VAL:HB	1.97	0.47
1:VB:249:LEU:HD12	2:cb:71:LEU:HD22	1.95	0.47
2:e:13:LEU:O	2:e:14:ILE:HD13	2.15	0.47
1:BB:237:GLU:O	1:BB:241:THR:OG1	2.30	0.47
1:DB:154:SER:HB3	1:DB:177:ARG:HH22	1.80	0.47
1:DB:190:VAL:HG21	1:V:236:PRO:HG3	1.97	0.47
1:DB:220:GLU:HA	1:DB:220:GLU:OE2	2.14	0.47
1:G:154:SER:HA	1:GB:170:ILE:HG21	1.97	0.47
1:H:174:ASP:OD1	1:H:176:GLU:N	2.48	0.47
1:H:187:ILE:HG22	1:H:191:LYS:HE2	1.95	0.47
1:IB:183:GLU:O	1:IB:187:ILE:HG22	2.15	0.47
1:M:258:MET:HE3	1:M:262:MET:HB2	1.96	0.47
1:NB:150:LEU:O	1:NB:154:SER:OG	2.26	0.47
1:RB:207:VAL:HG13	1:RB:211:VAL:HB	1.96	0.47
2:gb:14:ILE:HD12	2:gb:32:LEU:HD22	1.95	0.47
1:C:154:SER:HA	1:CB:170:ILE:HD13	1.97	0.47
1:G:208:ASP:OD1	1:G:210:MET:HB3	2.15	0.47
1:I:250:ASP:N	1:I:250:ASP:OD1	2.46	0.47
1:IB:157:LEU:HD23	1:IB:192:ASN:ND2	2.30	0.47
1:JB:160:ILE:HD11	1:JB:262:MET:SD	2.55	0.47
1:SB:221:ALA:O	1:SB:225:VAL:HG23	2.14	0.47
1:VB:207:VAL:HG13	1:VB:211:VAL:HB	1.96	0.47
2:ab:23:HIS:O	2:ab:27:GLU:HG2	2.15	0.47
2:f:6:LEU:HB2	2:f:13:LEU:HB2	1.97	0.47
2:g:26:VAL:HG23	2:g:27:GLU:OE1	2.15	0.47
1:C:187:ILE:HG22	1:C:191:LYS:HE2	1.95	0.47
1:E:208:ASP:CG	1:E:209:ALA:H	2.20	0.47
1:FB:213:HIS:O	1:FB:217:GLN:HG2	2.15	0.47
1:KB:231:LEU:HB2	1:KB:252:ILE:HD11	1.97	0.47
1:LB:180:LEU:O	1:LB:184:ASN:ND2	2.48	0.47
1:N:161:PHE:CE1	1:NB:273:ILE:HD12	2.50	0.47
1:W:242:ILE:HG21	1:W:249:LEU:HD21	1.96	0.47
1:WB:221:ALA:O	1:WB:225:VAL:HG23	2.14	0.47
1:G:235:ARG:HG3	1:G:236:PRO:HD2	1.95	0.47
1:H:236:PRO:HB3	1:P:186:LEU:HB3	1.97	0.47
1:TB:176:GLU:O	1:TB:180:LEU:HG	2.14	0.47
1:AB:163:LYS:HD3	1:AB:195:GLU:OE1	2.15	0.46
1:C:182:ILE:HG12	1:C:218:ALA:HB2	1.97	0.46
1:K:258:MET:HG2	1:KB:160:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MB:176:GLU:OE1	1:MB:176:GLU:N	2.29	0.46
1:MB:177:ARG:O	1:MB:181:ILE:HG23	2.15	0.46
1:MB:269:THR:HG21	1:MB:271:ARG:HH21	1.79	0.46
1:SB:238:ILE:O	1:SB:242:ILE:HD12	2.15	0.46
1:WB:163:LYS:HA	1:WB:194:SER:HA	1.97	0.46
2:c:27:GLU:HA	2:c:30:GLU:OE1	2.14	0.46
1:GB:147:LYS:HA	1:GB:150:LEU:HD12	1.96	0.46
1:JB:174:ASP:OD1	1:JB:177:ARG:N	2.37	0.46
1:KB:177:ARG:HA	1:KB:180:LEU:HD12	1.97	0.46
1:LB:182:ILE:HG12	1:LB:218:ALA:HB2	1.98	0.46
1:OB:196:VAL:HG11	1:OB:230:MET:HE3	1.97	0.46
1:S:273:ILE:HD12	1:S:273:ILE:HA	1.82	0.46
1:TB:175:THR:HG23	1:TB:176:GLU:H	1.79	0.46
2:g:65:VAL:O	2:g:69:SER:OG	2.30	0.46
1:AB:147:LYS:HA	1:AB:150:LEU:HD12	1.98	0.46
1:OB:243:VAL:HG21	1:VB:220:GLU:HB3	1.97	0.46
1:Q:162:GLU:HG2	1:Q:163:LYS:HG3	1.96	0.46
1:T:262:MET:HG2	1:TB:161:PHE:HE1	1.80	0.46
1:W:182:ILE:HG12	1:W:218:ALA:HB2	1.96	0.46
2:bb:17:GLN:HA	2:bb:50:SER:OG	2.15	0.46
2:eb:77:VAL:HG22	2:eb:100:LEU:HB2	1.97	0.46
1:BB:264:ARG:HE	1:BB:264:ARG:HB2	1.62	0.46
1:H:180:LEU:HA	1:H:183:GLU:OE2	2.15	0.46
1:RB:192:ASN:O	1:RB:193:ARG:HG2	2.15	0.46
1:SB:272:GLU:OE1	1:SB:272:GLU:N	2.49	0.46
2:d:16:ILE:HG22	2:d:51:ILE:HD11	1.98	0.46
2:f:5:ILE:O	2:f:35:LYS:NZ	2.48	0.46
1:A:172:THR:O	1:A:177:ARG:NH1	2.47	0.46
1:AB:155:ALA:HB2	1:AB:181:ILE:HG12	1.97	0.46
1:C:201:ILE:HD11	1:C:234:ILE:HA	1.96	0.46
1:E:155:ALA:N	1:E:156:PRO:HD3	2.30	0.46
1:H:258:MET:HE3	1:HB:158:LEU:HD23	1.97	0.46
1:KB:187:ILE:HG22	1:KB:191:LYS:HZ2	1.80	0.46
1:SB:262:MET:HE2	1:SB:262:MET:HB2	1.85	0.46
1:W:237:GLU:H	1:W:237:GLU:CD	2.22	0.46
2:bb:48:ILE:HD11	2:bb:81:ILE:HG12	1.98	0.46
2:cb:111:LYS:O	2:cb:114:GLN:HG3	2.14	0.46
2:fb:33:LEU:HD21	2:fb:68:MET:HG3	1.97	0.46
1:A:189:VAL:HG12	2:a:103:MET:HE1	1.97	0.46
1:BB:181:ILE:O	1:BB:185:LEU:HB2	2.15	0.46
1:BB:184:ASN:HA	1:BB:187:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ILE:O	1:C:190:VAL:HG12	2.14	0.46
1:LB:222:VAL:HG22	1:LB:227:CYS:HB3	1.97	0.46
1:NB:178:ALA:O	1:NB:181:ILE:HG12	2.16	0.46
1:OB:186:LEU:HB3	2:gb:83:PRO:HG3	1.98	0.46
1:EB:257:THR:HG23	1:EB:260:LYS:H	1.80	0.46
1:IB:147:LYS:HA	1:IB:150:LEU:HD12	1.97	0.46
1:U:182:ILE:HG12	1:U:218:ALA:HB2	1.98	0.46
2:e:48:ILE:HD11	2:e:81:ILE:HG23	1.98	0.46
2:fb:5:ILE:HG21	2:fb:35:LYS:HD3	1.97	0.46
1:A:150:LEU:HD21	1:AB:172:THR:HG23	1.97	0.46
1:G:234:ILE:HG23	1:J:225:VAL:HG12	1.98	0.46
1:MB:269:THR:O	1:MB:269:THR:HG22	2.15	0.46
1:RB:224:LEU:HD22	1:U:243:VAL:HG23	1.96	0.46
2:bb:16:ILE:O	2:bb:50:SER:OG	2.34	0.46
2:db:32:LEU:O	2:db:36:ILE:HG13	2.16	0.46
1:B:276:LYS:HB3	1:BB:270:ASN:OD1	2.16	0.46
1:B:276:LYS:NZ	1:BB:272:GLU:OE2	2.49	0.46
1:DB:235:ARG:HB2	1:DB:238:ILE:HG12	1.97	0.46
1:SB:256:ASN:HB3	2:f:72:MET:HE1	1.98	0.46
1:T:184:ASN:HA	1:T:187:ILE:HD12	1.97	0.46
1:TB:218:ALA:O	1:TB:222:VAL:HG12	2.15	0.46
2:ab:89:LEU:HD23	2:ab:96:PHE:CE1	2.51	0.46
2:d:90:ILE:HD13	2:d:90:ILE:HA	1.83	0.46
2:f:48:ILE:HD11	2:f:81:ILE:HG22	1.98	0.46
1:A:218:ALA:O	1:A:222:VAL:HG22	2.16	0.46
1:BB:269:THR:HG21	1:BB:271:ARG:HH21	1.81	0.46
1:D:179:LYS:O	1:D:183:GLU:HG2	2.15	0.46
1:E:160:ILE:HG22	1:E:161:PHE:CD2	2.51	0.46
1:MB:198:LEU:HD23	1:MB:232:VAL:HG11	1.98	0.46
1:R:186:LEU:HB3	2:cb:83:PRO:HG3	1.97	0.46
1:SB:256:ASN:HD22	2:f:72:MET:HE1	1.80	0.46
2:fb:32:LEU:HD23	2:fb:65:VAL:HG11	1.97	0.46
1:HB:258:MET:HE2	1:HB:258:MET:HB2	1.88	0.45
1:I:175:THR:HG22	1:I:179:LYS:CE	2.45	0.45
1:OB:238:ILE:O	1:OB:242:ILE:HG13	2.16	0.45
2:eb:66:VAL:HG23	2:eb:76:VAL:HB	1.98	0.45
1:AB:182:ILE:HG12	1:AB:218:ALA:HB2	1.99	0.45
1:E:237:GLU:HG2	1:E:238:ILE:HD12	1.98	0.45
1:FB:250:ASP:N	1:FB:250:ASP:OD1	2.49	0.45
1:I:176:GLU:OE1	1:I:180:LEU:HG	2.16	0.45
1:IB:229:ALA:O	1:IB:252:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:241:THR:HA	1:J:244:ASN:ND2	2.31	0.45
1:KB:221:ALA:O	1:KB:225:VAL:HG23	2.16	0.45
1:LB:238:ILE:HG22	1:LB:242:ILE:HD12	1.98	0.45
1:M:174:ASP:OD1	1:M:175:THR:N	2.49	0.45
1:MB:163:LYS:HA	1:MB:194:SER:HA	1.98	0.45
1:N:258:MET:HG2	1:NB:160:ILE:HD13	1.97	0.45
1:PB:186:LEU:HA	1:PB:189:VAL:HG22	1.98	0.45
1:AB:257:THR:HG23	1:AB:260:LYS:H	1.81	0.45
1:I:177:ARG:HA	1:I:180:LEU:HD12	1.97	0.45
1:N:273:ILE:HD12	1:NB:273:ILE:HG12	1.98	0.45
1:P:231:LEU:HB3	1:P:254:THR:HG22	1.97	0.45
1:WB:150:LEU:O	1:WB:154:SER:OG	2.20	0.45
2:db:79:THR:HG22	2:db:102:ALA:HB3	1.97	0.45
1:JB:182:ILE:HG12	1:JB:218:ALA:HB2	1.98	0.45
1:L:262:MET:HE2	1:L:262:MET:HB2	1.83	0.45
1:P:231:LEU:HB2	1:P:252:ILE:HD11	1.97	0.45
1:QB:162:GLU:H	1:QB:162:GLU:CD	2.23	0.45
1:T:210:MET:HG3	1:T:214:HIS:CE1	2.52	0.45
1:TB:258:MET:HE2	1:TB:258:MET:HA	1.99	0.45
1:VB:176:GLU:HA	1:VB:179:LYS:HD2	1.98	0.45
2:cb:17:GLN:N	2:cb:17:GLN:OE1	2.50	0.45
1:B:243:VAL:HG21	1:FB:220:GLU:HB3	1.99	0.45
1:BB:163:LYS:HB3	1:BB:195:GLU:HG3	1.99	0.45
1:CB:169:LEU:HD12	1:CB:201:ILE:HG22	1.96	0.45
1:CB:180:LEU:HA	1:CB:183:GLU:OE1	2.16	0.45
1:CB:235:ARG:HB2	1:CB:238:ILE:HD13	1.98	0.45
1:FB:236:PRO:HB3	1:K:186:LEU:HB3	1.99	0.45
1:K:249:LEU:HD12	1:K:252:ILE:HD11	1.98	0.45
1:V:240:GLN:O	1:V:244:ASN:HB2	2.17	0.45
1:AB:186:LEU:O	1:AB:190:VAL:HG12	2.17	0.45
1:FB:179:LYS:HD3	1:FB:179:LYS:N	2.31	0.45
1:K:221:ALA:O	1:K:225:VAL:HG23	2.16	0.45
1:L:154:SER:O	1:L:177:ARG:NH2	2.50	0.45
1:U:250:ASP:N	1:U:250:ASP:OD1	2.49	0.45
1:UB:230:MET:HE2	1:UB:230:MET:HB3	1.72	0.45
1:VB:262:MET:HE2	1:VB:262:MET:HB2	1.84	0.45
2:c:112:LEU:HD23	2:c:112:LEU:HA	1.78	0.45
2:f:96:PHE:HB3	2:f:99:VAL:HB	1.99	0.45
2:fb:77:VAL:HG22	2:fb:100:LEU:HB2	1.97	0.45
1:B:207:VAL:HG13	1:B:211:VAL:HB	1.98	0.45
1:L:154:SER:HA	1:LB:170:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:235:ARG:NE	1:S:236:PRO:HD2	2.32	0.45
1:T:240:GLN:O	1:T:240:GLN:NE2	2.48	0.45
2:g:112:LEU:HD23	2:g:112:LEU:HA	1.83	0.45
1:A:154:SER:HA	1:AB:170:ILE:HG21	1.97	0.45
1:CB:202:THR:O	1:CB:235:ARG:NH2	2.50	0.45
1:DB:213:HIS:O	1:DB:217:GLN:HG2	2.17	0.45
1:O:220:GLU:OE2	1:O:223:ARG:NH2	2.46	0.45
1:P:216:ILE:O	1:P:220:GLU:HG2	2.15	0.45
1:Q:154:SER:HB3	1:Q:177:ARG:HH21	1.82	0.45
1:SB:212:ALA:O	1:SB:216:ILE:HG13	2.15	0.45
2:bb:94:ILE:HD12	2:bb:94:ILE:H	1.81	0.45
1:BB:157:LEU:HG	1:BB:188:GLY:HA3	1.97	0.45
1:D:179:LYS:HD2	1:D:179:LYS:HA	1.79	0.45
1:DB:237:GLU:OE1	1:DB:241:THR:OG1	2.34	0.45
1:I:175:THR:HG22	1:I:179:LYS:HE2	1.99	0.45
1:UB:150:LEU:O	1:UB:154:SER:OG	2.25	0.45
1:VB:242:ILE:HG23	1:VB:247:ILE:HB	1.97	0.45
2:cb:71:LEU:HD23	2:cb:71:LEU:HA	1.85	0.45
1:C:157:LEU:HD22	1:C:188:GLY:HA3	1.99	0.45
1:IB:186:LEU:HB3	2:b:83:PRO:HG3	1.99	0.45
1:J:258:MET:HB2	1:J:258:MET:HE2	1.81	0.45
1:PB:231:LEU:HB2	1:PB:252:ILE:HD11	1.99	0.45
1:Q:189:VAL:HG12	2:db:103:MET:HE1	1.99	0.45
1:R:187:ILE:HA	1:R:190:VAL:HG12	1.99	0.45
2:d:4:PRO:HA	2:db:17:GLN:NE2	2.32	0.45
2:d:48:ILE:HD11	2:d:81:ILE:HG12	1.99	0.45
2:gb:24:THR:HA	2:gb:27:GLU:HG2	1.98	0.45
1:CB:163:LYS:HA	1:CB:194:SER:HA	1.99	0.44
1:CB:177:ARG:HA	1:CB:180:LEU:HG	1.99	0.44
1:D:257:THR:HG21	1:O:193:ARG:HH12	1.82	0.44
1:FB:238:ILE:HG22	1:FB:242:ILE:HD11	1.99	0.44
1:GB:201:ILE:HD11	1:GB:234:ILE:HG12	1.99	0.44
1:I:207:VAL:HG13	1:I:211:VAL:HB	1.99	0.44
1:RB:147:LYS:HD2	1:RB:150:LEU:HD12	1.99	0.44
1:SB:269:THR:O	1:SB:270:ASN:ND2	2.51	0.44
1:TB:259:LYS:HE3	1:TB:259:LYS:HB2	1.62	0.44
2:a:18:SER:OG	2:ab:1:MET:SD	2.62	0.44
1:H:160:ILE:HG23	1:HB:262:MET:HE3	1.98	0.44
1:MB:213:HIS:O	1:MB:217:GLN:HG3	2.18	0.44
1:WB:207:VAL:HB	1:WB:238:ILE:HG23	1.99	0.44
2:cb:3:ILE:HD12	2:cb:28:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:28:PHE:CE1	2:d:32:LEU:HD12	2.53	0.44
2:g:96:PHE:HD2	2:g:99:VAL:HG11	1.82	0.44
1:D:230:MET:HE2	1:D:230:MET:HB3	1.86	0.44
1:E:236:PRO:O	1:E:240:GLN:HG2	2.17	0.44
1:OB:163:LYS:NZ	1:OB:195:GLU:OE2	2.32	0.44
1:RB:269:THR:HG21	1:RB:271:ARG:NH2	2.32	0.44
1:S:191:LYS:O	1:S:193:ARG:NH2	2.50	0.44
1:SB:174:ASP:C	1:SB:174:ASP:OD1	2.60	0.44
1:U:185:LEU:O	1:U:189:VAL:HG23	2.18	0.44
1:VB:176:GLU:O	1:VB:180:LEU:HG	2.18	0.44
2:c:4:PRO:HG3	2:cb:17:GLN:HB3	2.00	0.44
2:db:87:ILE:HA	2:db:90:ILE:HG22	1.99	0.44
2:g:86:ALA:O	2:g:90:ILE:HG22	2.18	0.44
1:V:197:VAL:HG11	1:V:222:VAL:HG21	2.00	0.44
1:W:188:GLY:O	1:W:192:ASN:ND2	2.30	0.44
1:D:173:ILE:HA	1:D:177:ARG:HD3	2.00	0.44
1:GB:250:ASP:OD1	1:GB:250:ASP:N	2.49	0.44
1:HB:184:ASN:HA	1:HB:187:ILE:HG22	2.00	0.44
1:JB:240:GLN:OE1	1:JB:244:ASN:ND2	2.35	0.44
1:JB:240:GLN:O	1:JB:244:ASN:ND2	2.49	0.44
1:NB:181:ILE:O	1:NB:185:LEU:HD13	2.17	0.44
1:O:245:LEU:HD22	1:O:247:ILE:HG13	1.99	0.44
2:f:4:PRO:HG3	2:fb:17:GLN:OE1	2.17	0.44
1:H:200:ASP:OD1	1:H:200:ASP:C	2.60	0.44
1:I:157:LEU:O	1:I:159:PRO:HD3	2.17	0.44
1:L:174:ASP:O	1:L:178:ALA:N	2.44	0.44
1:L:231:LEU:HD12	1:L:231:LEU:HA	1.85	0.44
1:LB:175:THR:HG22	1:LB:210:MET:HE1	1.98	0.44
1:O:243:VAL:HG21	1:SB:220:GLU:HB3	2.00	0.44
1:V:162:GLU:OE1	1:V:271:ARG:NH1	2.50	0.44
1:VB:160:ILE:HG22	1:VB:161:PHE:CE2	2.53	0.44
1:VB:240:GLN:NE2	1:VB:244:ASN:OD1	2.51	0.44
2:cb:84:ALA:O	2:cb:88:THR:OG1	2.35	0.44
2:fb:64:ASP:HB3	2:fb:68:MET:HE3	2.00	0.44
1:DB:193:ARG:HD3	1:DB:193:ARG:N	2.33	0.44
1:G:155:ALA:HB1	1:G:167:MET:HE2	1.99	0.44
1:GB:237:GLU:CD	1:GB:237:GLU:H	2.26	0.44
1:I:186:LEU:O	1:I:190:VAL:HG12	2.18	0.44
1:J:201:ILE:O	1:J:204:VAL:HG22	2.18	0.44
1:MB:187:ILE:O	1:MB:191:LYS:HG2	2.17	0.44
1:NB:235:ARG:HB2	1:NB:238:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:182:ILE:HG12	1:P:218:ALA:HB2	1.99	0.44
1:PB:192:ASN:O	1:PB:193:ARG:HG2	2.18	0.44
1:RB:235:ARG:HB2	1:RB:238:ILE:CD1	2.47	0.44
1:WB:160:ILE:HG22	1:WB:161:PHE:CE2	2.52	0.44
2:fb:7:LYS:NZ	2:fb:9:GLY:O	2.41	0.44
2:g:12:LEU:HD21	2:g:39:THR:HG21	2.00	0.44
1:B:216:ILE:HD13	1:B:247:ILE:HG21	1.98	0.44
1:EB:231:LEU:HB3	1:EB:254:THR:HG22	2.00	0.44
1:OB:170:ILE:HG22	1:OB:203:GLY:HA3	1.99	0.44
1:OB:178:ALA:O	1:OB:181:ILE:HG12	2.18	0.44
1:QB:196:VAL:HG21	1:QB:230:MET:HE3	2.00	0.44
1:S:235:ARG:HE	1:S:236:PRO:HD2	1.82	0.44
1:S:241:THR:HA	1:S:244:ASN:ND2	2.33	0.44
1:U:269:THR:O	1:U:269:THR:HG22	2.18	0.44
1:UB:189:VAL:HG12	2:g:103:MET:HE1	1.99	0.44
1:VB:174:ASP:OD1	1:VB:174:ASP:C	2.60	0.44
2:c:82:GLN:OE1	2:c:83:PRO:HD3	2.18	0.44
2:e:89:LEU:HD22	2:e:96:PHE:CE1	2.53	0.44
1:DB:174:ASP:H	1:DB:177:ARG:HB3	1.83	0.44
1:G:180:LEU:HA	1:G:183:GLU:OE1	2.17	0.44
1:K:207:VAL:HG13	1:K:211:VAL:HB	2.00	0.44
1:MB:173:ILE:HG23	1:MB:177:ARG:HG3	1.99	0.44
1:RB:238:ILE:HD12	1:RB:238:ILE:H	1.83	0.44
1:S:234:ILE:HG22	2:g:72:MET:HG3	2.00	0.44
1:SB:241:THR:O	1:SB:245:LEU:HD23	2.17	0.44
1:T:187:ILE:HG13	1:T:187:ILE:H	1.70	0.44
1:VB:180:LEU:HA	1:VB:183:GLU:OE1	2.18	0.44
2:b:60:LYS:HD3	2:b:60:LYS:C	2.43	0.44
2:cb:29:GLN:OE1	2:cb:61:ILE:HD13	2.18	0.44
2:g:3:ILE:HD13	2:g:3:ILE:HA	1.88	0.44
1:DB:249:LEU:HG	1:DB:252:ILE:HD11	1.98	0.43
1:DB:273:ILE:HD12	1:DB:273:ILE:HA	1.82	0.43
1:HB:237:GLU:O	1:HB:241:THR:OG1	2.32	0.43
1:IB:207:VAL:HB	1:IB:238:ILE:HG23	2.00	0.43
1:JB:272:GLU:N	1:JB:272:GLU:OE1	2.51	0.43
1:OB:235:ARG:HB2	1:OB:238:ILE:HD12	1.99	0.43
1:Q:212:ALA:O	1:Q:215:ILE:HG12	2.18	0.43
1:R:209:ALA:HB1	1:R:213:HIS:CE1	2.53	0.43
1:SB:169:LEU:HD12	1:SB:201:ILE:HG22	2.00	0.43
1:T:159:PRO:O	1:TB:258:MET:HB3	2.18	0.43
1:UB:200:ASP:OD1	1:UB:200:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:100:LEU:HD22	2:b:100:LEU:H	1.83	0.43
2:bb:96:PHE:HB3	2:bb:99:VAL:HB	2.00	0.43
2:eb:22:ASP:O	2:eb:26:VAL:HG13	2.18	0.43
2:fb:61:ILE:O	2:fb:65:VAL:HG23	2.18	0.43
1:BB:186:LEU:HD22	1:WB:236:PRO:HB3	1.99	0.43
1:CB:235:ARG:HB3	1:CB:237:GLU:OE2	2.18	0.43
1:F:169:LEU:HD11	1:F:181:ILE:HD13	1.99	0.43
1:FB:236:PRO:HB2	1:K:186:LEU:HD13	1.99	0.43
1:IB:244:ASN:OD1	1:IB:245:LEU:HD22	2.18	0.43
1:J:163:LYS:HA	1:J:194:SER:HA	1.99	0.43
1:JB:162:GLU:HG2	1:JB:271:ARG:HH12	1.82	0.43
1:LB:175:THR:O	1:LB:179:LYS:HG2	2.18	0.43
1:MB:166:VAL:HG22	1:MB:198:LEU:HB2	2.00	0.43
1:O:238:ILE:H	1:O:238:ILE:HD12	1.84	0.43
2:e:31:ASP:O	2:e:35:LYS:NZ	2.42	0.43
2:g:32:LEU:HD23	2:g:65:VAL:HG21	2.00	0.43
1:A:179:LYS:HB2	1:A:179:LYS:HE3	1.72	0.43
1:CB:221:ALA:O	1:CB:225:VAL:HG23	2.18	0.43
1:EB:239:ALA:HA	1:EB:242:ILE:HD12	1.99	0.43
1:FB:213:HIS:HD2	1:FB:214:HIS:CD2	2.31	0.43
1:H:238:ILE:HG22	1:H:242:ILE:HD11	1.99	0.43
1:MB:182:ILE:HG12	1:MB:218:ALA:HB2	2.00	0.43
1:N:187:ILE:HA	1:N:190:VAL:HG12	2.00	0.43
1:Q:260:LYS:O	1:Q:264:ARG:HG3	2.18	0.43
2:b:13:LEU:C	2:b:14:ILE:HD12	2.43	0.43
2:bb:64:ASP:O	2:bb:68:MET:HG3	2.19	0.43
2:e:22:ASP:OD1	2:e:22:ASP:N	2.51	0.43
2:gb:33:LEU:HA	2:gb:36:ILE:HD12	2.00	0.43
1:CB:269:THR:O	1:CB:269:THR:HG22	2.18	0.43
1:D:157:LEU:O	1:D:159:PRO:HD3	2.18	0.43
1:D:225:VAL:HG12	1:E:256:ASN:HB2	2.01	0.43
1:EB:168:PRO:HA	1:EB:200:ASP:HB3	2.00	0.43
1:IB:174:ASP:OD2	1:IB:174:ASP:C	2.60	0.43
1:L:262:MET:HE3	1:LB:160:ILE:HG23	1.99	0.43
1:M:152:GLU:HG2	1:M:180:LEU:HD12	1.99	0.43
1:WB:162:GLU:HG3	1:WB:163:LYS:HG3	2.01	0.43
1:A:272:GLU:N	1:A:272:GLU:OE1	2.51	0.43
1:EB:193:ARG:NH2	1:N:257:THR:OG1	2.51	0.43
1:G:240:GLN:O	1:G:244:ASN:HB2	2.19	0.43
1:GB:150:LEU:O	1:GB:154:SER:OG	2.19	0.43
1:N:250:ASP:OD1	1:N:250:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RB:189:VAL:HG11	1:RB:222:VAL:HG13	1.99	0.43
1:VB:202:THR:O	1:VB:235:ARG:NH2	2.51	0.43
1:W:234:ILE:HG13	1:W:235:ARG:N	2.34	0.43
1:WB:174:ASP:H	1:WB:177:ARG:HB3	1.83	0.43
2:bb:66:VAL:HG11	2:bb:99:VAL:HG21	1.99	0.43
1:DB:150:LEU:O	1:DB:154:SER:OG	2.29	0.43
1:L:185:LEU:HD11	1:L:197:VAL:HG21	2.01	0.43
1:V:185:LEU:HD11	1:V:197:VAL:HG21	2.00	0.43
2:e:111:LYS:HB2	2:e:111:LYS:HE3	1.72	0.43
1:DB:160:ILE:HG22	1:DB:161:PHE:CE2	2.54	0.43
1:KB:208:ASP:CG	1:KB:209:ALA:H	2.27	0.43
1:M:237:GLU:OE2	1:M:237:GLU:N	2.28	0.43
1:O:200:ASP:HB2	1:O:258:MET:HE1	2.01	0.43
1:OB:157:LEU:HD23	1:OB:192:ASN:ND2	2.34	0.43
1:WB:235:ARG:HB3	1:WB:236:PRO:HD2	2.00	0.43
2:a:47:ASP:OD1	2:a:79:THR:OG1	2.33	0.43
2:cb:96:PHE:CD1	2:cb:96:PHE:N	2.87	0.43
2:gb:100:LEU:HD12	2:gb:100:LEU:H	1.83	0.43
1:BB:256:ASN:HB3	1:C:225:VAL:HG12	1.99	0.43
1:DB:231:LEU:HD12	1:DB:231:LEU:HA	1.76	0.43
1:I:172:THR:O	1:I:177:ARG:NH1	2.52	0.43
1:IB:213:HIS:O	1:IB:217:GLN:HG2	2.18	0.43
1:KB:174:ASP:C	1:KB:174:ASP:OD1	2.61	0.43
1:KB:186:LEU:HD21	1:KB:221:ALA:HB1	2.00	0.43
1:L:245:LEU:HB2	1:L:247:ILE:HD12	2.01	0.43
1:M:180:LEU:O	1:M:184:ASN:ND2	2.51	0.43
1:M:231:LEU:O	1:M:254:THR:HA	2.19	0.43
1:RB:224:LEU:O	1:U:234:ILE:HG21	2.19	0.43
2:f:10:GLU:N	2:f:10:GLU:CD	2.76	0.43
1:B:269:THR:O	1:B:269:THR:HG22	2.18	0.43
1:BB:273:ILE:HD12	1:BB:273:ILE:HA	1.81	0.43
1:GB:155:ALA:HB1	1:GB:167:MET:HE2	2.00	0.43
1:KB:185:LEU:HD11	1:KB:197:VAL:HG21	2.00	0.43
1:M:161:PHE:HB2	1:M:164:ILE:HB	2.01	0.43
1:Q:191:LYS:HD3	1:Q:191:LYS:N	2.33	0.43
1:S:235:ARG:NE	1:S:235:ARG:HA	2.33	0.43
2:c:62:LEU:HD23	2:c:62:LEU:HA	1.88	0.43
2:db:5:ILE:O	2:db:35:LYS:NZ	2.52	0.43
2:eb:22:ASP:OD1	2:eb:22:ASP:C	2.61	0.43
1:C:219:SER:HB2	1:C:252:ILE:HG21	2.00	0.43
1:F:273:ILE:HG12	1:FB:273:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:189:VAL:HG21	1:FB:222:VAL:HG23	2.01	0.43
1:NB:255:THR:OG1	1:NB:256:ASN:N	2.52	0.43
1:SB:180:LEU:O	1:SB:184:ASN:ND2	2.52	0.43
1:T:185:LEU:HD22	1:T:222:VAL:HG11	2.01	0.43
2:a:44:VAL:HB	2:a:76:VAL:HG22	2.00	0.43
1:CB:250:ASP:OD1	1:CB:250:ASP:N	2.52	0.42
1:JB:212:ALA:O	1:JB:216:ILE:HG12	2.19	0.42
1:KB:182:ILE:HG12	1:KB:218:ALA:HB2	2.01	0.42
1:S:207:VAL:HB	1:S:238:ILE:HG12	2.00	0.42
1:U:258:MET:HE3	1:U:258:MET:O	2.19	0.42
1:VB:186:LEU:O	1:VB:190:VAL:HG12	2.19	0.42
2:a:17:GLN:NE2	2:ab:4:PRO:HA	2.34	0.42
2:ab:66:VAL:HG23	2:ab:76:VAL:HB	2.00	0.42
2:eb:112:LEU:HD23	2:eb:112:LEU:HA	1.83	0.42
1:I:174:ASP:O	1:I:178:ALA:N	2.51	0.42
1:IB:264:ARG:HE	1:IB:264:ARG:HB2	1.70	0.42
1:KB:163:LYS:HA	1:KB:194:SER:HA	2.01	0.42
1:QB:200:ASP:OD1	1:QB:202:THR:N	2.31	0.42
1:RB:147:LYS:HA	1:RB:150:LEU:HD12	2.00	0.42
2:a:22:ASP:O	2:a:26:VAL:HG22	2.19	0.42
2:c:48:ILE:HD11	2:c:81:ILE:HG13	2.01	0.42
1:B:242:ILE:HG23	1:B:247:ILE:HD12	2.00	0.42
1:BB:190:VAL:HG21	1:WB:235:ARG:HH12	1.84	0.42
1:CB:175:THR:HG22	1:CB:179:LYS:HE2	2.02	0.42
1:D:181:ILE:O	1:D:185:LEU:HD13	2.19	0.42
1:EB:182:ILE:HG12	1:EB:218:ALA:HB2	2.00	0.42
1:F:167:MET:HE3	1:F:167:MET:HB3	1.92	0.42
1:L:150:LEU:O	1:L:154:SER:OG	2.24	0.42
1:NB:200:ASP:OD1	1:NB:202:THR:OG1	2.30	0.42
1:AB:223:ARG:NH1	1:AB:251:GLN:OE1	2.52	0.42
1:EB:188:GLY:HA2	1:EB:191:LYS:HG3	2.01	0.42
1:J:200:ASP:OD2	1:J:200:ASP:C	2.62	0.42
1:LB:258:MET:HE2	1:LB:258:MET:HB2	1.83	0.42
1:R:209:ALA:HB1	1:R:213:HIS:HE1	1.85	0.42
1:V:186:LEU:HB3	1:W:236:PRO:HB3	2.02	0.42
1:W:200:ASP:OD2	1:W:202:THR:OG1	2.28	0.42
2:b:79:THR:HG22	2:b:102:ALA:HB3	2.01	0.42
2:bb:85:VAL:O	2:bb:89:LEU:HG	2.19	0.42
2:f:55:ASP:OD2	2:f:55:ASP:C	2.62	0.42
1:BB:269:THR:HG21	1:BB:271:ARG:NH2	2.34	0.42
1:DB:240:GLN:H	1:DB:240:GLN:HG2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:239:ALA:HB1	1:MB:224:LEU:HB2	2.01	0.42
1:FB:257:THR:HG23	1:FB:260:LYS:H	1.83	0.42
1:IB:174:ASP:O	1:IB:178:ALA:N	2.46	0.42
1:JB:161:PHE:HB2	1:JB:164:ILE:HG12	2.00	0.42
1:MB:163:LYS:HB3	1:MB:195:GLU:HG3	2.00	0.42
1:MB:235:ARG:HB3	1:MB:238:ILE:HD12	2.01	0.42
1:R:187:ILE:C	1:R:191:LYS:HE2	2.44	0.42
1:S:162:GLU:OE2	1:S:162:GLU:N	2.45	0.42
1:VB:272:GLU:N	1:VB:272:GLU:OE1	2.52	0.42
2:b:35:LYS:HE2	2:b:35:LYS:HB3	1.88	0.42
1:E:158:LEU:HD13	1:EB:258:MET:HE3	2.02	0.42
1:Q:157:LEU:HD22	1:Q:188:GLY:HA3	2.02	0.42
1:R:276:LYS:HB3	1:RB:270:ASN:OD1	2.19	0.42
1:RB:180:LEU:HA	1:RB:183:GLU:OE1	2.19	0.42
1:UB:201:ILE:HD11	1:UB:234:ILE:HD13	2.02	0.42
2:a:104:ASP:OD1	2:a:104:ASP:N	2.52	0.42
2:ab:27:GLU:HA	2:ab:30:GLU:OE2	2.20	0.42
2:ab:47:ASP:C	2:ab:47:ASP:OD2	2.62	0.42
2:b:57:PHE:HD1	2:b:58:ILE:HD13	1.85	0.42
2:db:16:ILE:HG22	2:db:51:ILE:HD11	2.00	0.42
2:eb:90:ILE:HD13	2:eb:90:ILE:HA	1.83	0.42
1:A:208:ASP:CG	1:A:209:ALA:H	2.27	0.42
1:C:258:MET:HE2	1:C:258:MET:HB2	1.86	0.42
1:CB:179:LYS:HD3	1:CB:179:LYS:N	2.35	0.42
1:DB:264:ARG:HE	1:DB:264:ARG:HB2	1.51	0.42
1:K:222:VAL:HB	1:K:227:CYS:HB3	2.02	0.42
1:MB:193:ARG:O	1:MB:193:ARG:HG3	2.20	0.42
1:P:179:LYS:HA	1:P:179:LYS:HD3	1.86	0.42
1:VB:179:LYS:HA	1:VB:182:ILE:HD12	2.02	0.42
2:f:72:MET:HE3	2:f:72:MET:C	2.44	0.42
1:BB:180:LEU:HD23	1:BB:180:LEU:HA	1.86	0.42
1:BB:242:ILE:HG23	1:BB:247:ILE:HD12	2.02	0.42
1:DB:232:VAL:HG21	1:DB:258:MET:HA	2.01	0.42
1:H:150:LEU:O	1:H:154:SER:OG	2.17	0.42
1:HB:187:ILE:O	1:HB:191:LYS:HG3	2.19	0.42
1:I:154:SER:HA	1:IB:170:ILE:HG21	2.01	0.42
1:JB:160:ILE:HG13	1:JB:161:PHE:CD2	2.55	0.42
1:L:256:ASN:OD1	1:L:256:ASN:N	2.49	0.42
1:OB:175:THR:OG1	1:OB:210:MET:HE1	2.20	0.42
1:SB:236:PRO:HD2	2:f:37:HIS:CE1	2.54	0.42
1:TB:235:ARG:HB2	1:TB:238:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ab:103:MET:HE2	2:ab:103:MET:HB2	1.99	0.42
2:bb:4:PRO:C	2:bb:5:ILE:HD12	2.45	0.42
2:db:35:LYS:HE2	2:db:35:LYS:HB3	1.73	0.42
2:e:62:LEU:O	2:e:66:VAL:HG12	2.20	0.42
2:f:34:ALA:O	2:f:38:GLU:HG2	2.19	0.42
2:g:89:LEU:HD23	2:g:96:PHE:HE1	1.84	0.42
1:A:154:SER:HB3	1:A:177:ARG:NH2	2.35	0.42
1:D:157:LEU:HD11	1:D:165:SER:HB3	2.02	0.42
1:DB:198:LEU:HD13	1:DB:230:MET:HB3	2.02	0.42
1:DB:239:ALA:O	1:DB:243:VAL:HG23	2.18	0.42
1:G:167:MET:SD	1:G:185:LEU:HD13	2.60	0.42
1:J:236:PRO:HD3	2:b:37:HIS:ND1	2.35	0.42
1:J:242:ILE:HG23	1:J:247:ILE:HD12	2.02	0.42
1:T:167:MET:HE2	1:T:167:MET:HB2	1.95	0.42
1:WB:163:LYS:NZ	1:WB:195:GLU:OE1	2.34	0.42
2:gb:112:LEU:HD12	2:gb:112:LEU:HA	1.89	0.42
1:B:235:ARG:HB3	1:B:236:PRO:HD2	2.02	0.42
1:E:167:MET:SD	1:E:185:LEU:HG	2.60	0.42
1:E:235:ARG:HB2	1:E:238:ILE:CD1	2.50	0.42
1:F:202:THR:HA	1:F:235:ARG:HH22	1.84	0.42
1:I:223:ARG:HA	1:I:227:CYS:O	2.20	0.42
1:IB:218:ALA:O	1:IB:222:VAL:HG12	2.20	0.42
1:KB:216:ILE:HD11	1:KB:247:ILE:HG21	2.02	0.42
1:KB:237:GLU:CD	1:KB:237:GLU:H	2.28	0.42
1:LB:187:ILE:HG22	1:LB:191:LYS:HD3	2.02	0.42
1:N:174:ASP:OD2	1:N:174:ASP:C	2.63	0.42
1:QB:157:LEU:HD12	1:QB:167:MET:HB2	2.02	0.42
1:R:177:ARG:O	1:R:181:ILE:HG23	2.19	0.42
1:T:162:GLU:HG3	1:T:163:LYS:HG3	2.01	0.42
2:c:36:ILE:HG22	2:c:72:MET:HE2	2.01	0.42
2:cb:64:ASP:O	2:cb:68:MET:HG2	2.20	0.42
1:C:200:ASP:OD1	1:C:258:MET:HE1	2.20	0.41
1:C:207:VAL:HG22	1:C:238:ILE:HG23	2.00	0.41
1:DB:187:ILE:HG13	1:DB:188:GLY:N	2.35	0.41
1:DB:235:ARG:HB3	1:DB:236:PRO:HD2	2.01	0.41
1:GB:190:VAL:O	1:GB:193:ARG:NH1	2.53	0.41
1:H:175:THR:O	1:H:179:LYS:HG2	2.20	0.41
1:M:224:LEU:HD23	1:M:224:LEU:HA	1.88	0.41
1:M:270:ASN:OD1	1:M:270:ASN:O	2.38	0.41
1:SB:182:ILE:HG12	1:SB:218:ALA:HB2	2.02	0.41
2:e:110:GLU:OE1	2:e:111:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:MET:HE2	1:F:230:MET:HB2	1.93	0.41
1:F:258:MET:HG3	1:FB:160:ILE:HA	2.02	0.41
1:I:185:LEU:O	1:I:189:VAL:HG23	2.20	0.41
1:P:175:THR:O	1:P:179:LYS:HG2	2.20	0.41
1:P:258:MET:HG2	1:PB:160:ILE:HD13	2.02	0.41
1:R:186:LEU:CB	2:cb:83:PRO:HG3	2.50	0.41
1:SB:175:THR:OG1	1:SB:210:MET:HE1	2.20	0.41
1:T:154:SER:HB3	1:T:177:ARG:NH2	2.34	0.41
1:T:154:SER:HA	1:TB:170:ILE:HG21	2.02	0.41
1:V:238:ILE:HD12	1:V:238:ILE:H	1.85	0.41
2:c:13:LEU:C	2:c:14:ILE:HD12	2.45	0.41
2:cb:105:LEU:HD23	2:cb:105:LEU:O	2.21	0.41
2:db:96:PHE:N	2:db:96:PHE:CD2	2.87	0.41
1:A:174:ASP:OD2	1:A:176:GLU:N	2.53	0.41
1:BB:238:ILE:H	1:BB:238:ILE:HD12	1.84	0.41
1:IB:220:GLU:HA	1:IB:220:GLU:OE2	2.21	0.41
1:OB:179:LYS:HD2	1:OB:179:LYS:O	2.21	0.41
1:OB:184:ASN:HA	1:OB:187:ILE:HG22	2.02	0.41
1:V:250:ASP:OD1	1:V:250:ASP:N	2.53	0.41
2:c:5:ILE:HG21	2:c:35:LYS:HG3	2.02	0.41
2:gb:87:ILE:O	2:gb:91:GLU:HG3	2.21	0.41
1:BB:186:LEU:O	1:BB:190:VAL:HG12	2.19	0.41
1:H:237:GLU:O	1:H:241:THR:OG1	2.33	0.41
1:I:182:ILE:HG12	1:I:218:ALA:HB2	2.01	0.41
1:IB:184:ASN:HA	1:IB:187:ILE:HG22	2.03	0.41
1:OB:201:ILE:HD11	1:OB:234:ILE:HG12	2.02	0.41
1:QB:177:ARG:HA	1:QB:180:LEU:HG	2.02	0.41
1:T:235:ARG:HB3	1:T:236:PRO:HD2	2.02	0.41
1:WB:188:GLY:HA2	1:WB:191:LYS:HE3	2.00	0.41
2:f:44:VAL:HB	2:f:76:VAL:HG22	2.02	0.41
1:DB:162:GLU:HG2	1:DB:163:LYS:HG3	2.02	0.41
1:E:155:ALA:HB2	1:E:181:ILE:HD13	2.03	0.41
1:E:155:ALA:HB2	1:E:181:ILE:CD1	2.50	0.41
1:FB:249:LEU:HB3	1:FB:252:ILE:HG23	2.02	0.41
1:I:189:VAL:HG21	1:I:222:VAL:HG23	2.02	0.41
1:J:157:LEU:HB2	1:J:167:MET:HE2	2.02	0.41
1:J:266:LEU:HA	1:J:269:THR:HG22	2.03	0.41
1:K:262:MET:HE2	1:K:262:MET:HB2	1.86	0.41
1:L:163:LYS:HB3	1:L:195:GLU:HB2	2.02	0.41
1:PB:207:VAL:HB	1:PB:238:ILE:HG23	2.03	0.41
1:T:216:ILE:HD11	1:T:247:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:238:ILE:O	1:T:242:ILE:HG13	2.19	0.41
2:c:72:MET:HE3	2:c:72:MET:C	2.45	0.41
2:db:35:LYS:HA	2:db:38:GLU:HG2	2.02	0.41
2:e:100:LEU:H	2:e:100:LEU:HD22	1.86	0.41
2:eb:103:MET:HB2	2:eb:103:MET:HE3	1.82	0.41
1:DB:241:THR:HA	1:DB:244:ASN:HD21	1.86	0.41
1:KB:257:THR:HG21	1:N:193:ARG:NH1	2.35	0.41
1:RB:182:ILE:HG12	1:RB:218:ALA:HB2	2.03	0.41
1:S:216:ILE:HD11	1:S:247:ILE:HD13	2.02	0.41
1:S:235:ARG:HH21	2:g:37:HIS:CE1	2.39	0.41
1:UB:198:LEU:HD22	1:UB:258:MET:HE1	2.02	0.41
1:W:150:LEU:O	1:W:154:SER:OG	2.29	0.41
2:bb:33:LEU:HA	2:bb:36:ILE:HG22	2.02	0.41
2:d:103:MET:HE3	2:d:103:MET:HB3	1.81	0.41
2:g:22:ASP:OD1	2:g:22:ASP:N	2.52	0.41
1:A:243:VAL:HG11	2:eb:68:MET:HG2	2.03	0.41
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.82	0.41
1:DB:167:MET:SD	1:DB:185:LEU:HD13	2.61	0.41
1:I:213:HIS:O	1:I:217:GLN:HG2	2.20	0.41
1:L:249:LEU:HB3	1:L:252:ILE:HG13	2.02	0.41
1:MB:169:LEU:HD12	1:MB:173:ILE:HD11	2.02	0.41
1:Q:169:LEU:HD11	1:Q:181:ILE:HG21	2.01	0.41
1:RB:200:ASP:C	1:RB:200:ASP:OD1	2.64	0.41
1:VB:258:MET:HE2	1:VB:258:MET:HB2	1.94	0.41
2:a:35:LYS:O	2:a:35:LYS:HG2	2.19	0.41
2:db:87:ILE:HG22	2:db:91:GLU:OE1	2.20	0.41
2:gb:16:ILE:HG22	2:gb:51:ILE:HD11	2.02	0.41
1:B:250:ASP:N	1:B:250:ASP:OD1	2.54	0.41
1:CB:163:LYS:HB3	1:CB:195:GLU:HG3	2.03	0.41
1:N:258:MET:HE2	1:N:258:MET:HB2	1.76	0.41
1:QB:180:LEU:O	1:QB:181:ILE:C	2.64	0.41
1:T:157:LEU:HB2	1:T:167:MET:HE1	2.02	0.41
1:UB:162:GLU:HG2	1:UB:163:LYS:HD2	2.03	0.41
2:bb:31:ASP:OD1	2:bb:31:ASP:N	2.54	0.41
2:g:62:LEU:HD23	2:g:62:LEU:HA	1.94	0.41
1:AB:242:ILE:HG13	1:AB:242:ILE:H	1.68	0.41
1:BB:256:ASN:OD1	1:BB:257:THR:HG23	2.20	0.41
1:CB:160:ILE:HG22	1:CB:161:PHE:CE1	2.55	0.41
1:FB:197:VAL:HG11	1:FB:222:VAL:HG21	2.03	0.41
1:I:269:THR:C	1:I:270:ASN:OD1	2.64	0.41
1:JB:240:GLN:HA	2:e:68:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:272:GLU:OE1	1:K:272:GLU:N	2.54	0.41
1:KB:250:ASP:OD1	1:KB:250:ASP:N	2.53	0.41
1:M:164:ILE:HD11	1:M:269:THR:HG21	2.02	0.41
1:N:200:ASP:OD2	1:N:200:ASP:C	2.63	0.41
1:Q:170:ILE:HG21	1:QB:154:SER:HA	2.02	0.41
1:Q:241:THR:O	1:Q:245:LEU:HD22	2.21	0.41
1:SB:235:ARG:CG	1:SB:238:ILE:HG13	2.51	0.41
1:VB:185:LEU:HD11	1:VB:197:VAL:HG21	2.03	0.41
1:WB:147:LYS:HA	1:WB:150:LEU:HD12	2.02	0.41
1:WB:186:LEU:HB3	2:c:83:PRO:HG3	2.03	0.41
2:bb:31:ASP:HA	2:bb:35:LYS:NZ	2.35	0.41
2:bb:56:SER:HA	2:bb:92:LEU:HD13	2.03	0.41
2:cb:5:ILE:HD13	2:cb:35:LYS:HG2	2.03	0.41
2:db:34:ALA:O	2:db:38:GLU:HG2	2.20	0.41
2:e:6:LEU:HD22	2:eb:105:LEU:HD13	2.03	0.41
2:eb:88:THR:O	2:eb:91:GLU:HG3	2.21	0.41
2:f:89:LEU:HB3	2:f:94:ILE:HB	2.03	0.41
1:CB:213:HIS:O	1:CB:216:ILE:HG22	2.21	0.41
1:D:235:ARG:NH1	1:O:190:VAL:HG21	2.35	0.41
1:D:253:ILE:HD12	1:D:253:ILE:H	1.86	0.41
1:M:185:LEU:O	1:M:189:VAL:HG23	2.20	0.41
1:NB:169:LEU:HD13	1:NB:169:LEU:HA	1.90	0.41
1:S:175:THR:O	1:S:179:LYS:HG2	2.21	0.41
1:WB:170:ILE:O	1:WB:170:ILE:HG13	2.21	0.41
2:a:5:ILE:O	2:a:35:LYS:NZ	2.53	0.41
2:ab:100:LEU:HD12	2:ab:100:LEU:H	1.86	0.41
2:c:27:GLU:O	2:c:28:PHE:C	2.64	0.41
2:c:29:GLN:HG3	2:c:65:VAL:HG22	2.02	0.41
2:db:96:PHE:N	2:db:96:PHE:HD2	2.19	0.41
1:A:259:LYS:O	1:A:263:GLU:HG3	2.21	0.40
1:BB:169:LEU:HB2	1:BB:200:ASP:O	2.21	0.40
1:CB:175:THR:HG22	1:CB:179:LYS:CE	2.50	0.40
1:E:231:LEU:HD23	1:E:252:ILE:HD12	2.03	0.40
1:OB:163:LYS:HA	1:OB:194:SER:HA	2.03	0.40
1:OB:213:HIS:CD2	1:OB:214:HIS:HD2	2.39	0.40
1:R:183:GLU:HG2	1:R:187:ILE:HD11	2.02	0.40
1:R:209:ALA:O	1:R:213:HIS:ND1	2.54	0.40
1:SB:258:MET:HE3	1:SB:258:MET:HB3	1.87	0.40
1:W:179:LYS:C	1:W:179:LYS:HZ2	2.30	0.40
2:a:112:LEU:HD23	2:a:112:LEU:HA	1.77	0.40
2:c:96:PHE:HB3	2:c:99:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:eb:23:HIS:O	2:eb:27:GLU:HG2	2.20	0.40
2:fb:112:LEU:HD23	2:fb:112:LEU:HA	1.80	0.40
2:g:33:LEU:HD11	2:g:68:MET:SD	2.60	0.40
2:g:36:ILE:HD13	2:g:69:SER:HB3	2.02	0.40
1:A:154:SER:HB3	1:A:177:ARG:HH21	1.87	0.40
1:DB:258:MET:HE2	1:DB:258:MET:HB2	1.82	0.40
1:H:177:ARG:O	1:H:181:ILE:HG23	2.21	0.40
1:IB:187:ILE:HA	1:IB:190:VAL:HG12	2.02	0.40
1:M:179:LYS:O	1:M:182:ILE:HG12	2.20	0.40
1:O:158:LEU:H	1:O:158:LEU:HD12	1.86	0.40
1:Q:264:ARG:HE	1:Q:264:ARG:HB3	1.69	0.40
1:R:157:LEU:HD22	1:R:188:GLY:HA3	2.02	0.40
1:WB:213:HIS:HA	1:WB:216:ILE:HD12	2.04	0.40
2:e:17:GLN:NE2	2:eb:4:PRO:HA	2.36	0.40
2:eb:20:LEU:HD12	2:eb:20:LEU:HA	1.88	0.40
1:F:250:ASP:OD1	1:F:250:ASP:N	2.53	0.40
1:I:224:LEU:HD23	1:I:224:LEU:HA	1.95	0.40
1:IB:195:GLU:C	1:IB:227:CYS:HB2	2.47	0.40
1:J:170:ILE:HA	1:J:170:ILE:HD12	1.82	0.40
1:J:193:ARG:HH11	1:J:193:ARG:HG2	1.85	0.40
1:JB:231:LEU:HB2	1:JB:252:ILE:HD11	2.03	0.40
1:K:270:ASN:OD1	1:KB:276:LYS:HD3	2.21	0.40
1:KB:175:THR:O	1:KB:179:LYS:NZ	2.49	0.40
1:N:160:ILE:HG22	1:N:161:PHE:CD2	2.56	0.40
1:N:223:ARG:HA	1:N:227:CYS:O	2.22	0.40
1:Q:273:ILE:HD13	1:QB:266:LEU:HD21	2.03	0.40
1:R:200:ASP:OD2	1:R:258:MET:HE2	2.21	0.40
1:VB:213:HIS:O	1:VB:217:GLN:HG2	2.21	0.40
1:W:260:LYS:HB3	1:W:260:LYS:HE3	1.86	0.40
2:a:61:ILE:O	2:a:65:VAL:HG12	2.21	0.40
2:e:33:LEU:HD11	2:e:68:MET:SD	2.61	0.40
2:fb:87:ILE:HA	2:fb:90:ILE:HG12	2.03	0.40
1:BB:258:MET:HE3	1:BB:258:MET:HB3	1.78	0.40
1:C:256:ASN:OD1	1:C:257:THR:HG23	2.22	0.40
1:D:237:GLU:O	1:D:241:THR:OG1	2.36	0.40
1:DB:178:ALA:CB	1:DB:214:HIS:HD2	2.34	0.40
1:E:271:ARG:O	1:E:272:GLU:HG3	2.21	0.40
1:JB:258:MET:O	1:JB:258:MET:HG3	2.21	0.40
1:P:167:MET:HE2	1:P:167:MET:HB2	1.92	0.40
1:PB:258:MET:HE3	1:PB:258:MET:HB3	1.79	0.40
1:Q:167:MET:HE3	1:Q:167:MET:HB3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QB:175:THR:O	1:QB:179:LYS:HG2	2.22	0.40
2:b:112:LEU:HA	2:b:112:LEU:HD23	1.81	0.40
1:AB:169:LEU:HD12	1:AB:201:ILE:HG22	2.04	0.40
1:C:157:LEU:HD11	1:C:165:SER:HB3	2.04	0.40
1:CB:177:ARG:NH2	1:CB:181:ILE:HD11	2.37	0.40
1:EB:177:ARG:HG3	1:EB:177:ARG:HH11	1.87	0.40
1:F:213:HIS:O	1:F:216:ILE:HG22	2.22	0.40
1:J:231:LEU:HD12	1:J:231:LEU:HA	1.91	0.40
1:KB:170:ILE:HG22	1:KB:203:GLY:HA3	2.04	0.40
1:MB:212:ALA:O	1:MB:216:ILE:HG12	2.21	0.40
1:MB:257:THR:HG23	1:MB:260:LYS:H	1.86	0.40
1:PB:179:LYS:O	1:PB:182:ILE:HB	2.22	0.40
1:QB:220:GLU:OE1	1:QB:251:GLN:NE2	2.55	0.40
1:RB:234:ILE:HG21	1:TB:224:LEU:O	2.20	0.40
1:T:235:ARG:HB2	1:T:238:ILE:CD1	2.52	0.40
1:V:163:LYS:HB3	1:V:195:GLU:HG3	2.01	0.40
2:f:5:ILE:HB	2:f:35:LYS:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/278 (47%)	128 (98%)	2 (2%)	0	100	100
1	AB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	B	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	BB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	C	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	CB	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	D	130/278 (47%)	128 (98%)	2 (2%)	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%)	127 (98%)	3 (2%)	0	100	100
1	EB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	F	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	FB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	G	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	GB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	H	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	HB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	I	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	IB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	J	130/278 (47%)	121 (93%)	9 (7%)	0	100	100
1	JB	130/278 (47%)	128 (98%)	2 (2%)	0	100	100
1	K	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	KB	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
1	L	130/278 (47%)	128 (98%)	2 (2%)	0	100	100
1	LB	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	M	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	MB	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
1	N	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	NB	130/278 (47%)	128 (98%)	2 (2%)	0	100	100
1	O	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	OB	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	P	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	PB	130/278 (47%)	121 (93%)	9 (7%)	0	100	100
1	Q	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	QB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	R	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	RB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	S	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	SB	130/278 (47%)	127 (98%)	3 (2%)	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%)	122 (94%)	8 (6%)	0	100	100
1	U	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	UB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	V	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
1	VB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	W	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	WB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
2	a	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	ab	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	b	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	bb	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	c	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
2	cb	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	d	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	db	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
2	e	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	eb	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	f	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	fb	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	g	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	gb	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
All	All	7604/14440 (53%)	7340 (96%)	264 (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%)	111 (98%)	2 (2%)	51	66
1	AB	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	B	113/246 (46%)	108 (96%)	5 (4%)	25	50
1	BB	113/246 (46%)	109 (96%)	4 (4%)	32	55
1	C	113/246 (46%)	112 (99%)	1 (1%)	70	75
1	CB	113/246 (46%)	108 (96%)	5 (4%)	25	50
1	D	113/246 (46%)	109 (96%)	4 (4%)	32	55
1	DB	113/246 (46%)	109 (96%)	4 (4%)	32	55
1	E	113/246 (46%)	109 (96%)	4 (4%)	32	55
1	EB	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	F	113/246 (46%)	107 (95%)	6 (5%)	20	46
1	FB	113/246 (46%)	108 (96%)	5 (4%)	25	50
1	G	113/246 (46%)	109 (96%)	4 (4%)	32	55
1	GB	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	H	113/246 (46%)	109 (96%)	4 (4%)	32	55
1	HB	113/246 (46%)	109 (96%)	4 (4%)	32	55
1	I	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	IB	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	J	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	JB	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	K	113/246 (46%)	108 (96%)	5 (4%)	25	50
1	KB	113/246 (46%)	108 (96%)	5 (4%)	25	50
1	L	113/246 (46%)	107 (95%)	6 (5%)	20	46
1	LB	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	M	113/246 (46%)	108 (96%)	5 (4%)	25	50
1	MB	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	N	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	NB	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	O	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	OB	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	P	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	PB	113/246 (46%)	108 (96%)	5 (4%)	25	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	QB	113/246 (46%)	107 (95%)	6 (5%)	20	46
1	R	113/246 (46%)	112 (99%)	1 (1%)	70	75
1	RB	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	S	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	SB	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	T	113/246 (46%)	112 (99%)	1 (1%)	70	75
1	TB	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	U	113/246 (46%)	111 (98%)	2 (2%)	51	66
1	UB	113/246 (46%)	108 (96%)	5 (4%)	25	50
1	V	113/246 (46%)	109 (96%)	4 (4%)	32	55
1	VB	113/246 (46%)	110 (97%)	3 (3%)	39	60
1	W	113/246 (46%)	109 (96%)	4 (4%)	32	55
1	WB	113/246 (46%)	109 (96%)	4 (4%)	32	55
2	a	100/100 (100%)	95 (95%)	5 (5%)	22	48
2	ab	100/100 (100%)	95 (95%)	5 (5%)	22	48
2	b	100/100 (100%)	96 (96%)	4 (4%)	28	52
2	bb	100/100 (100%)	97 (97%)	3 (3%)	36	59
2	c	100/100 (100%)	94 (94%)	6 (6%)	17	42
2	cb	100/100 (100%)	95 (95%)	5 (5%)	22	48
2	d	100/100 (100%)	98 (98%)	2 (2%)	48	65
2	db	100/100 (100%)	97 (97%)	3 (3%)	36	59
2	e	100/100 (100%)	98 (98%)	2 (2%)	48	65
2	eb	100/100 (100%)	97 (97%)	3 (3%)	36	59
2	f	100/100 (100%)	98 (98%)	2 (2%)	48	65
2	fb	100/100 (100%)	98 (98%)	2 (2%)	48	65
2	g	100/100 (100%)	97 (97%)	3 (3%)	36	59
2	gb	100/100 (100%)	95 (95%)	5 (5%)	22	48
All	All	6598/12716 (52%)	6393 (97%)	205 (3%)	36	58

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	THR
1	A	259	LYS
1	AB	167	MET
1	AB	241	THR
1	B	157	LEU
1	B	158	LEU
1	B	200	ASP
1	B	234	ILE
1	B	252	ILE
1	BB	180	LEU
1	BB	202	THR
1	BB	241	THR
1	BB	247	ILE
1	C	207	VAL
1	CB	175	THR
1	CB	202	THR
1	CB	252	ILE
1	CB	254	THR
1	CB	268	LEU
1	D	158	LEU
1	D	172	THR
1	D	213	HIS
1	D	225	VAL
1	DB	196	VAL
1	DB	225	VAL
1	DB	230	MET
1	DB	241	THR
1	E	158	LEU
1	E	197	VAL
1	E	232	VAL
1	E	256	ASN
1	EB	183	GLU
1	EB	224	LEU
1	F	158	LEU
1	F	200	ASP
1	F	213	HIS
1	F	225	VAL
1	F	244	ASN
1	F	259	LYS
1	FB	162	GLU
1	FB	175	THR
1	FB	225	VAL
1	FB	252	ILE

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Mol	Chain	Res	Type
1	FB	268	LEU
1	G	158	LEU
1	G	213	HIS
1	G	247	ILE
1	G	252	ILE
1	GB	162	GLU
1	GB	249	LEU
1	GB	252	ILE
1	H	158	LEU
1	H	174	ASP
1	H	207	VAL
1	H	235	ARG
1	HB	157	LEU
1	HB	180	LEU
1	HB	241	THR
1	HB	252	ILE
1	I	234	ILE
1	I	256	ASN
1	I	257	THR
1	IB	158	LEU
1	IB	237	GLU
1	J	197	VAL
1	J	217	GLN
1	J	220	GLU
1	JB	219	SER
1	JB	245	LEU
1	K	158	LEU
1	K	165	SER
1	K	170	ILE
1	K	187	ILE
1	K	197	VAL
1	KB	173	ILE
1	KB	207	VAL
1	KB	213	HIS
1	KB	263	GLU
1	KB	272	GLU
1	L	202	THR
1	L	210	MET
1	L	213	HIS
1	L	232	VAL
1	L	234	ILE
1	L	252	ILE

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Mol	Chain	Res	Type
1	LB	181	ILE
1	LB	252	ILE
1	M	158	LEU
1	M	197	VAL
1	M	202	THR
1	M	214	HIS
1	M	241	THR
1	MB	213	HIS
1	MB	232	VAL
1	MB	255	THR
1	N	241	THR
1	N	250	ASP
1	N	252	ILE
1	NB	214	HIS
1	NB	268	LEU
1	O	176	GLU
1	O	202	THR
1	O	206	VAL
1	OB	213	HIS
1	OB	250	ASP
1	P	234	ILE
1	P	257	THR
1	PB	170	ILE
1	PB	172	THR
1	PB	175	THR
1	PB	213	HIS
1	PB	268	LEU
1	Q	158	LEU
1	Q	252	ILE
1	Q	274	VAL
1	QB	162	GLU
1	QB	183	GLU
1	QB	202	THR
1	QB	213	HIS
1	QB	250	ASP
1	QB	268	LEU
1	R	225	VAL
1	RB	244	ASN
1	RB	250	ASP
1	S	213	HIS
1	S	234	ILE
1	SB	210	MET

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Mol	Chain	Res	Type
1	SB	247	ILE
1	SB	252	ILE
1	T	197	VAL
1	TB	232	VAL
1	TB	247	ILE
1	TB	250	ASP
1	U	235	ARG
1	U	250	ASP
1	UB	175	THR
1	UB	225	VAL
1	UB	241	THR
1	UB	259	LYS
1	UB	270	ASN
1	V	158	LEU
1	V	210	MET
1	V	252	ILE
1	V	257	THR
1	VB	225	VAL
1	VB	241	THR
1	VB	252	ILE
1	W	173	ILE
1	W	185	LEU
1	W	197	VAL
1	W	225	VAL
1	WB	157	LEU
1	WB	200	ASP
1	WB	225	VAL
1	WB	240	GLN
2	a	39	THR
2	a	40	SER
2	a	56	SER
2	a	90	ILE
2	a	94	ILE
2	ab	5	ILE
2	ab	22	ASP
2	ab	33	LEU
2	ab	39	THR
2	ab	55	ASP
2	b	61	ILE
2	b	69	SER
2	b	88	THR
2	b	112	LEU

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Mol	Chain	Res	Type
2	bb	28	PHE
2	bb	40	SER
2	bb	88	THR
2	c	5	ILE
2	c	15	SER
2	c	81	ILE
2	c	88	THR
2	c	95	THR
2	c	116	LEU
2	cb	22	ASP
2	cb	39	THR
2	cb	61	ILE
2	cb	88	THR
2	cb	95	THR
2	d	28	PHE
2	d	56	SER
2	db	40	SER
2	db	47	ASP
2	db	112	LEU
2	e	53	PHE
2	e	54	ILE
2	eb	15	SER
2	eb	52	ASP
2	eb	85	VAL
2	f	39	THR
2	f	107	SER
2	fb	18	SER
2	fb	94	ILE
2	g	40	SER
2	g	54	ILE
2	g	69	SER
2	gb	14	ILE
2	gb	39	THR
2	gb	52	ASP
2	gb	56	SER
2	gb	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	240	GLN
1	B	251	GLN

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Mol	Chain	Res	Type
1	C	151	GLN
1	C	251	GLN
1	CB	151	GLN
1	CB	214	HIS
1	D	256	ASN
1	DB	240	GLN
1	E	151	GLN
1	E	251	GLN
1	EB	244	ASN
1	FB	213	HIS
1	FB	214	HIS
1	FB	228	GLN
1	GB	184	ASN
1	GB	213	HIS
1	IB	217	GLN
1	IB	244	ASN
1	K	251	GLN
1	KB	251	GLN
1	LB	184	ASN
1	LB	251	GLN
1	M	244	ASN
1	M	251	GLN
1	MB	240	GLN
1	N	151	GLN
1	N	217	GLN
1	NB	251	GLN
1	O	251	GLN
1	P	251	GLN
1	PB	184	ASN
1	PB	251	GLN
1	QB	240	GLN
1	QB	251	GLN
1	R	184	ASN
1	R	217	GLN
1	RB	244	ASN
1	S	244	ASN
1	S	251	GLN
1	SB	213	HIS
1	SB	214	HIS
1	SB	251	GLN
1	SB	270	ASN
1	T	228	GLN

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Mol	Chain	Res	Type
1	T	251	GLN
1	TB	251	GLN
1	U	151	GLN
1	U	251	GLN
1	UB	184	ASN
1	UB	251	GLN
1	UB	270	ASN
1	V	251	GLN
1	VB	151	GLN
1	VB	192	ASN
1	VB	240	GLN
1	VB	244	ASN
1	W	251	GLN
1	WB	184	ASN
1	WB	214	HIS
1	WB	217	GLN
1	WB	251	GLN
2	a	17	GLN
2	b	82	GLN
2	d	82	GLN
2	db	17	GLN
2	db	29	GLN
2	eb	29	GLN
2	g	23	HIS
2	gb	23	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

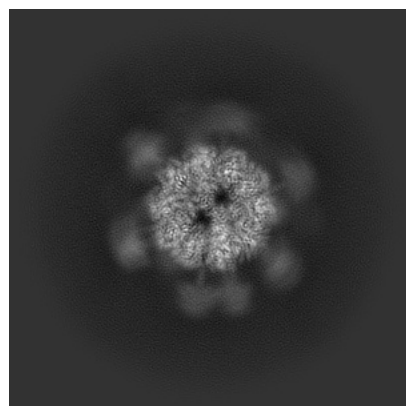
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70087. These allow visual inspection of the internal detail of the map and identification of artifacts.

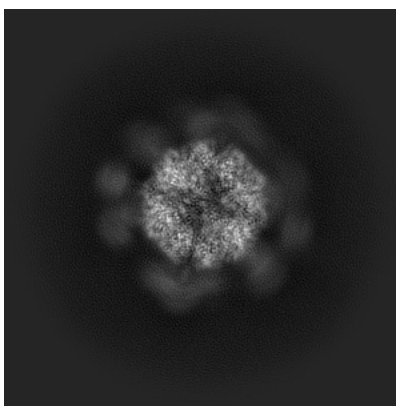
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

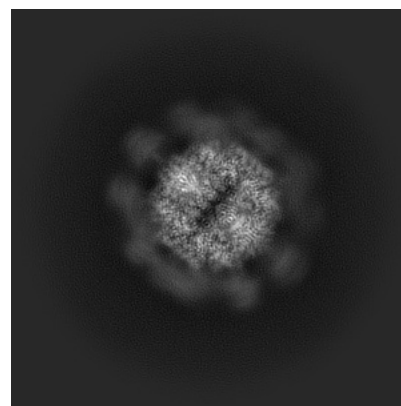
#### 6.1.1 Primary map



X

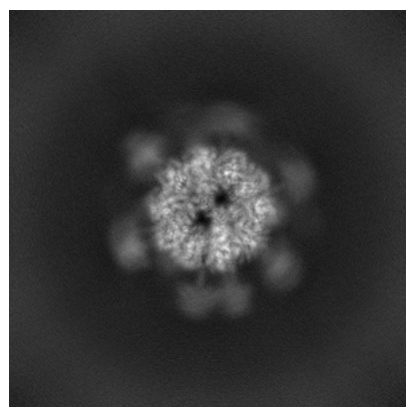


Y

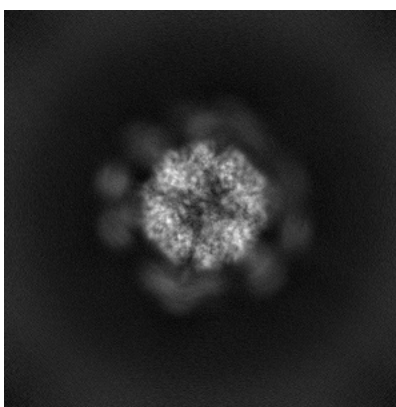


Z

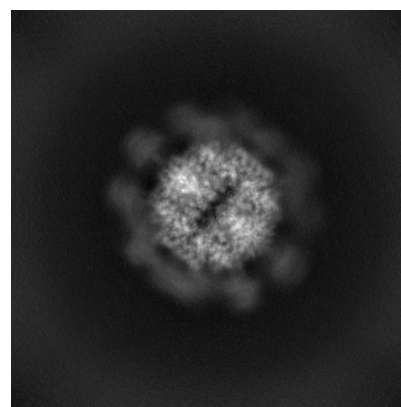
#### 6.1.2 Raw map



X



Y

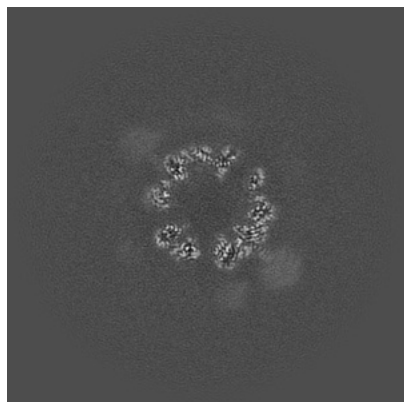


Z

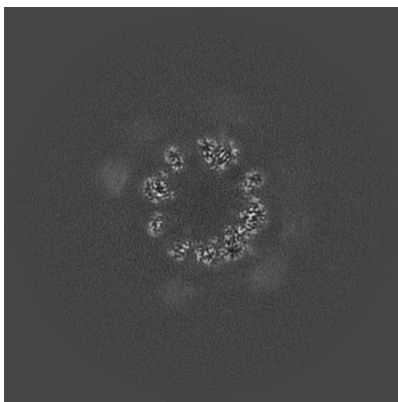
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

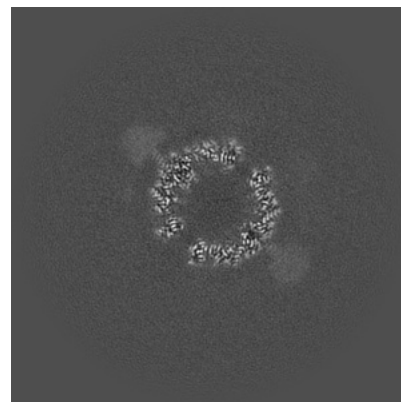
### 6.2.1 Primary map



X Index: 300

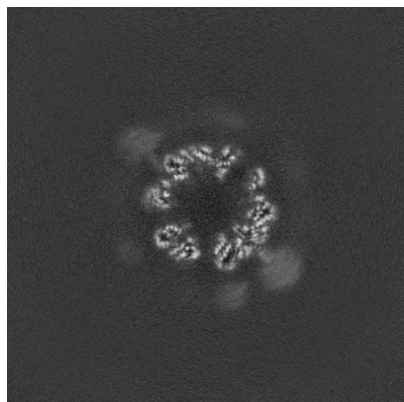


Y Index: 300

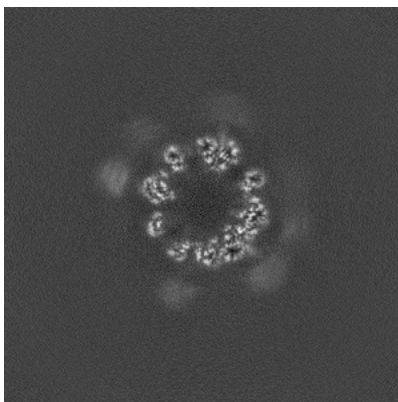


Z Index: 300

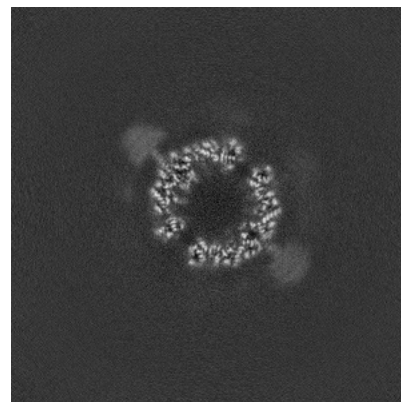
### 6.2.2 Raw map



X Index: 300



Y Index: 300



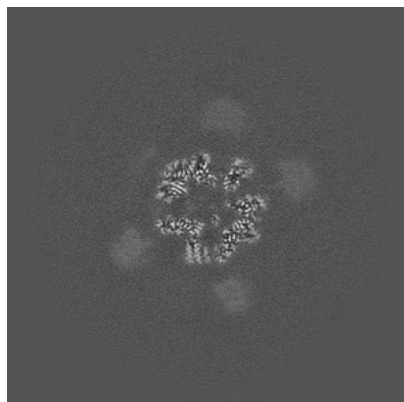
Z Index: 300

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

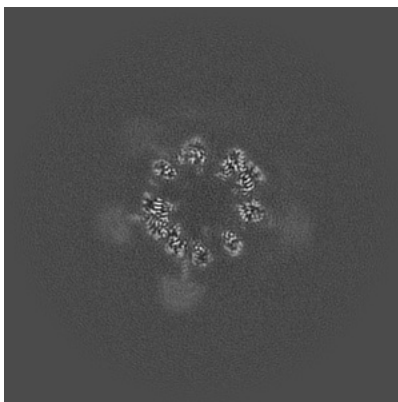


## 6.3 Largest variance slices [i](#)

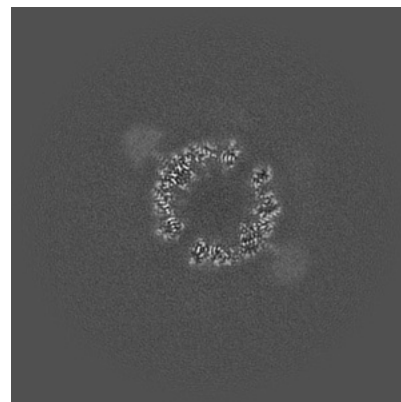
### 6.3.1 Primary map



X Index: 261



Y Index: 325

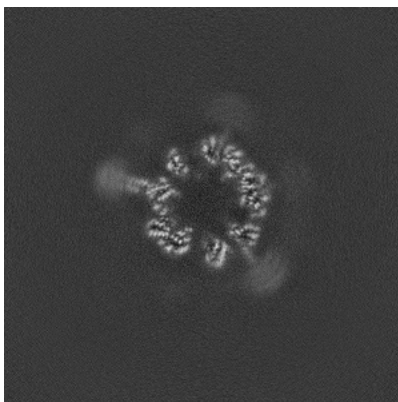


Z Index: 302

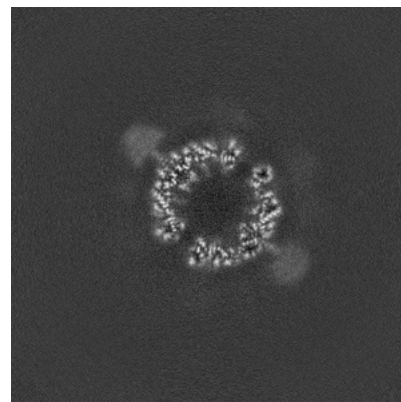
### 6.3.2 Raw map



X Index: 261



Y Index: 285

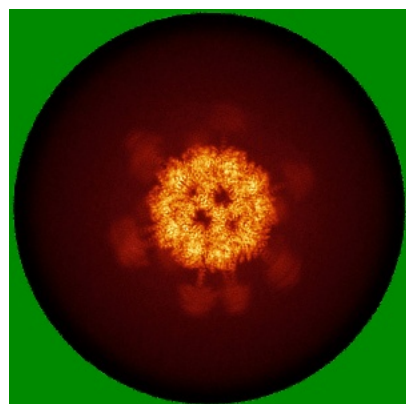


Z Index: 302

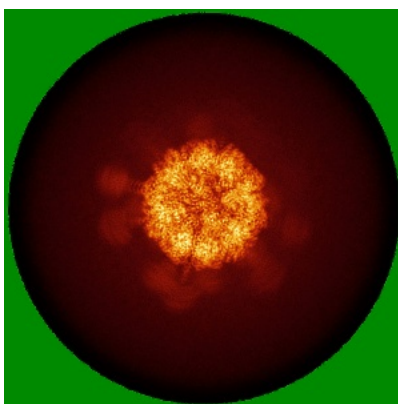
The images above show the largest variance slices of the map in three orthogonal directions.

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

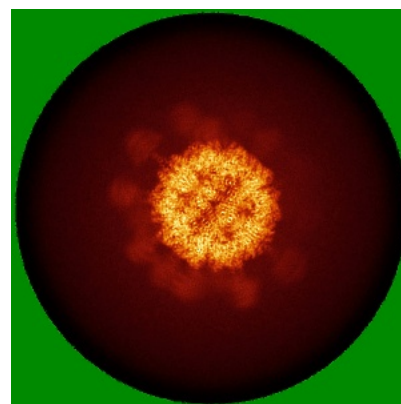
### 6.4.1 Primary map



X

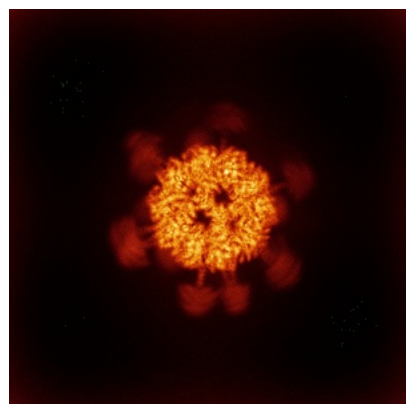


Y

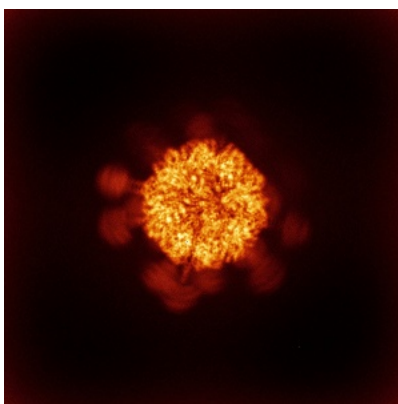


Z

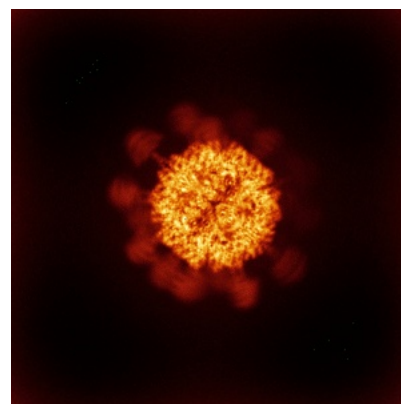
### 6.4.2 Raw map



X



Y

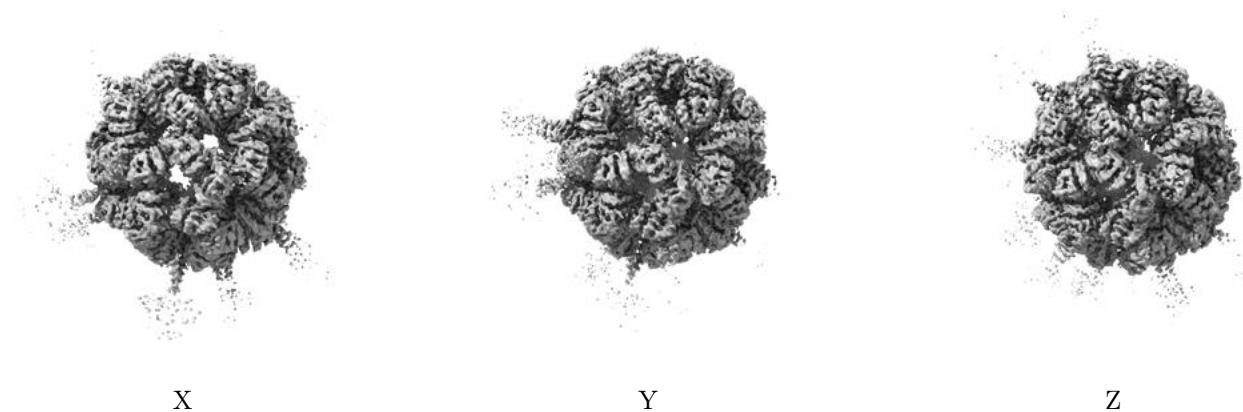


Z

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.

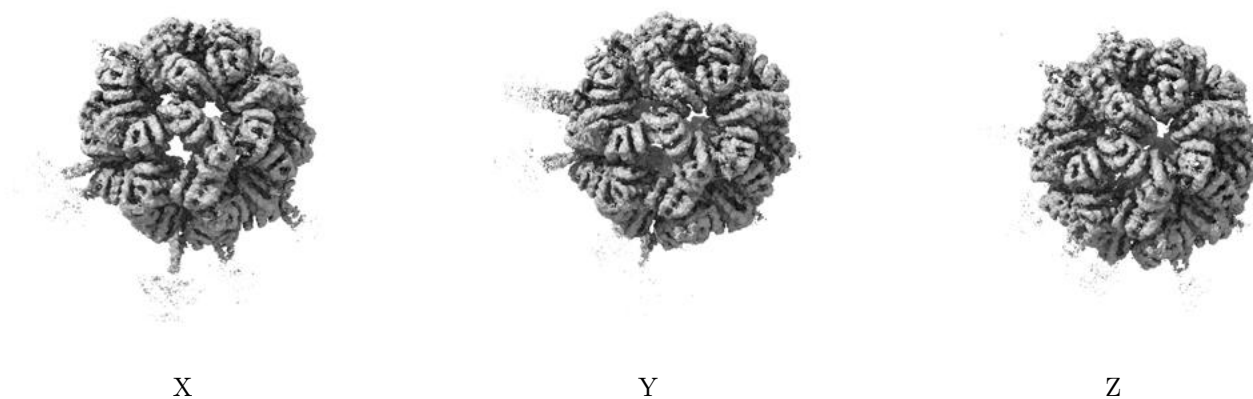
## 6.5 Orthogonal surface views [i](#)

### 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.

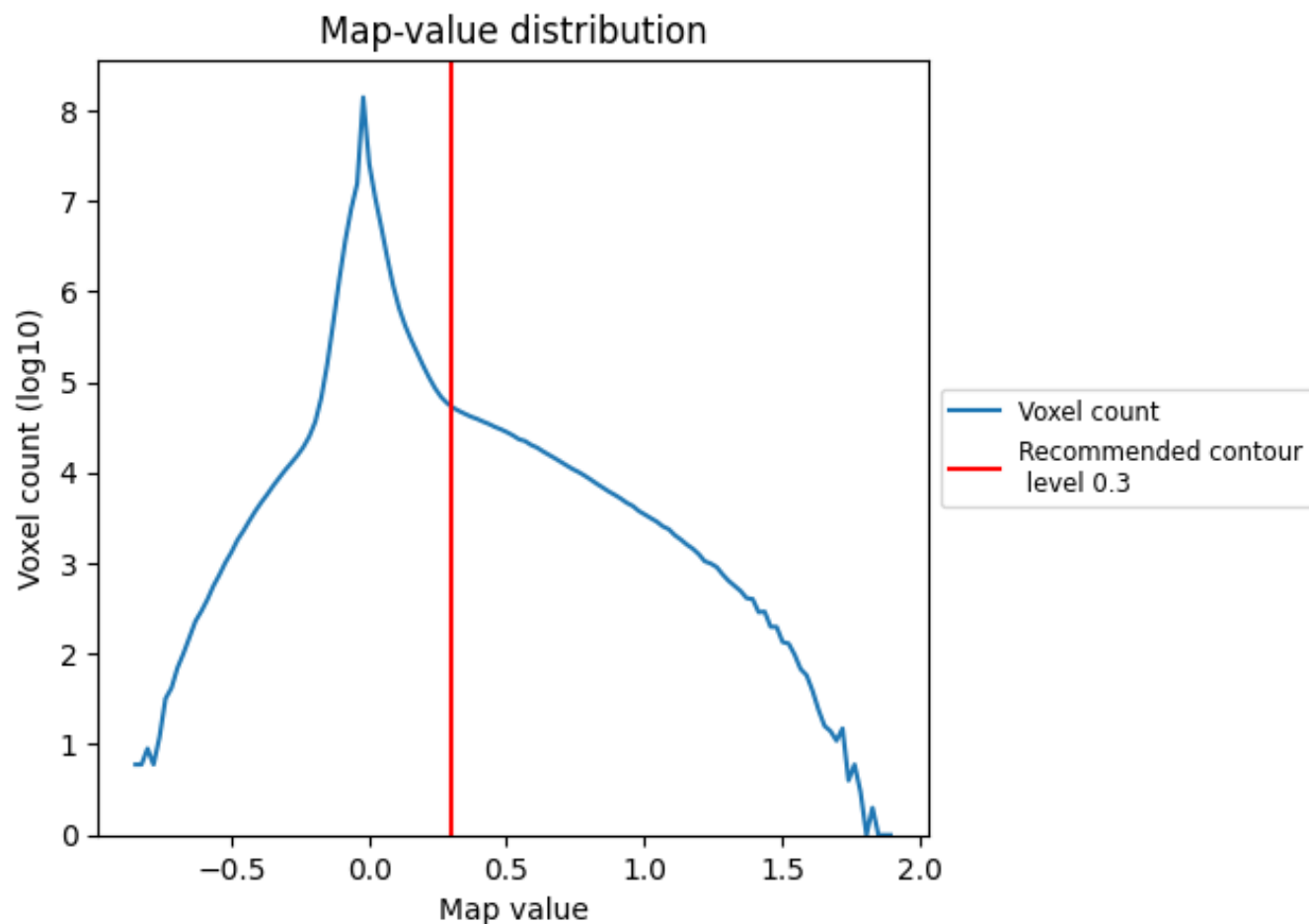
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

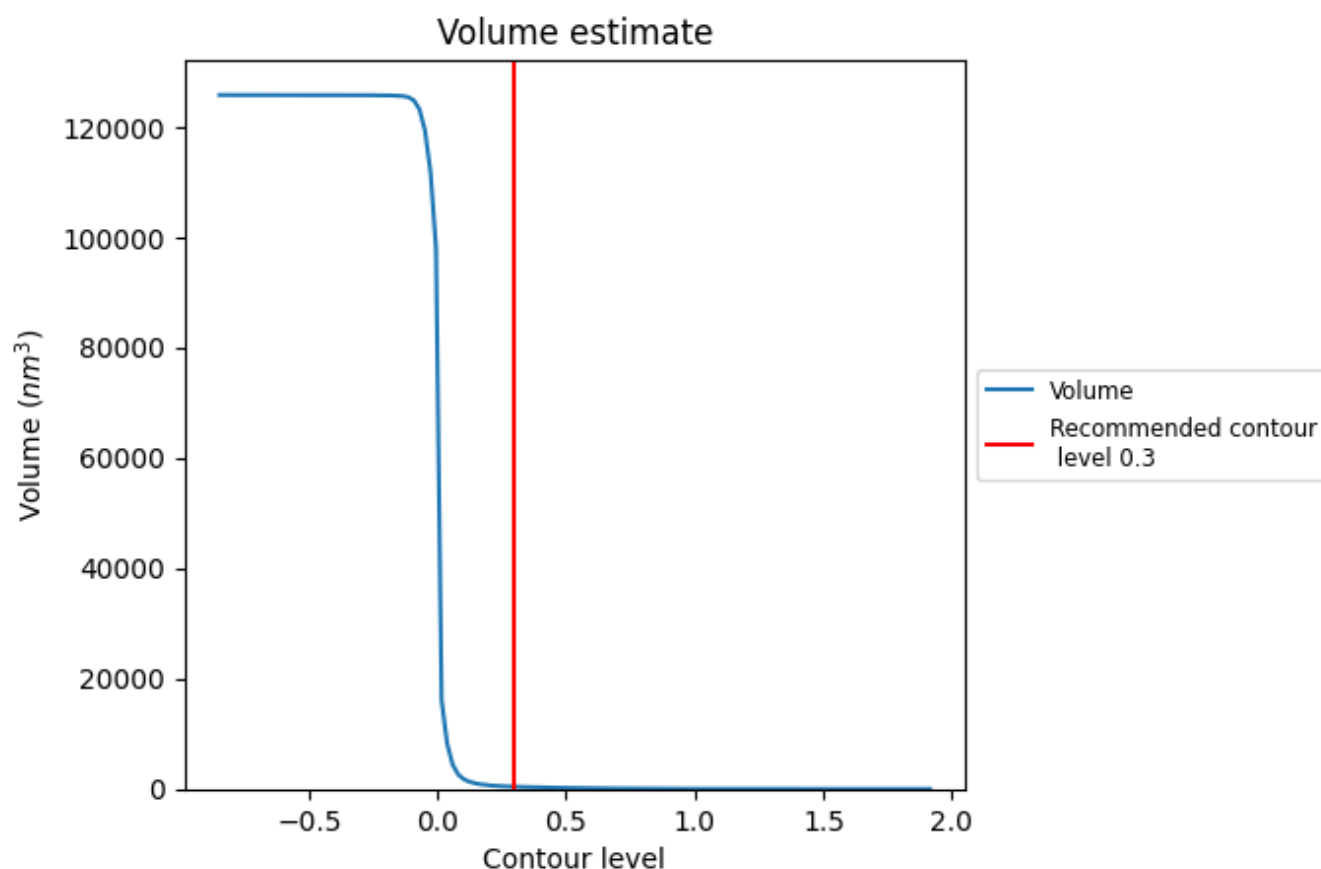
This section contains the results of statistical analysis of the map.

### 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.

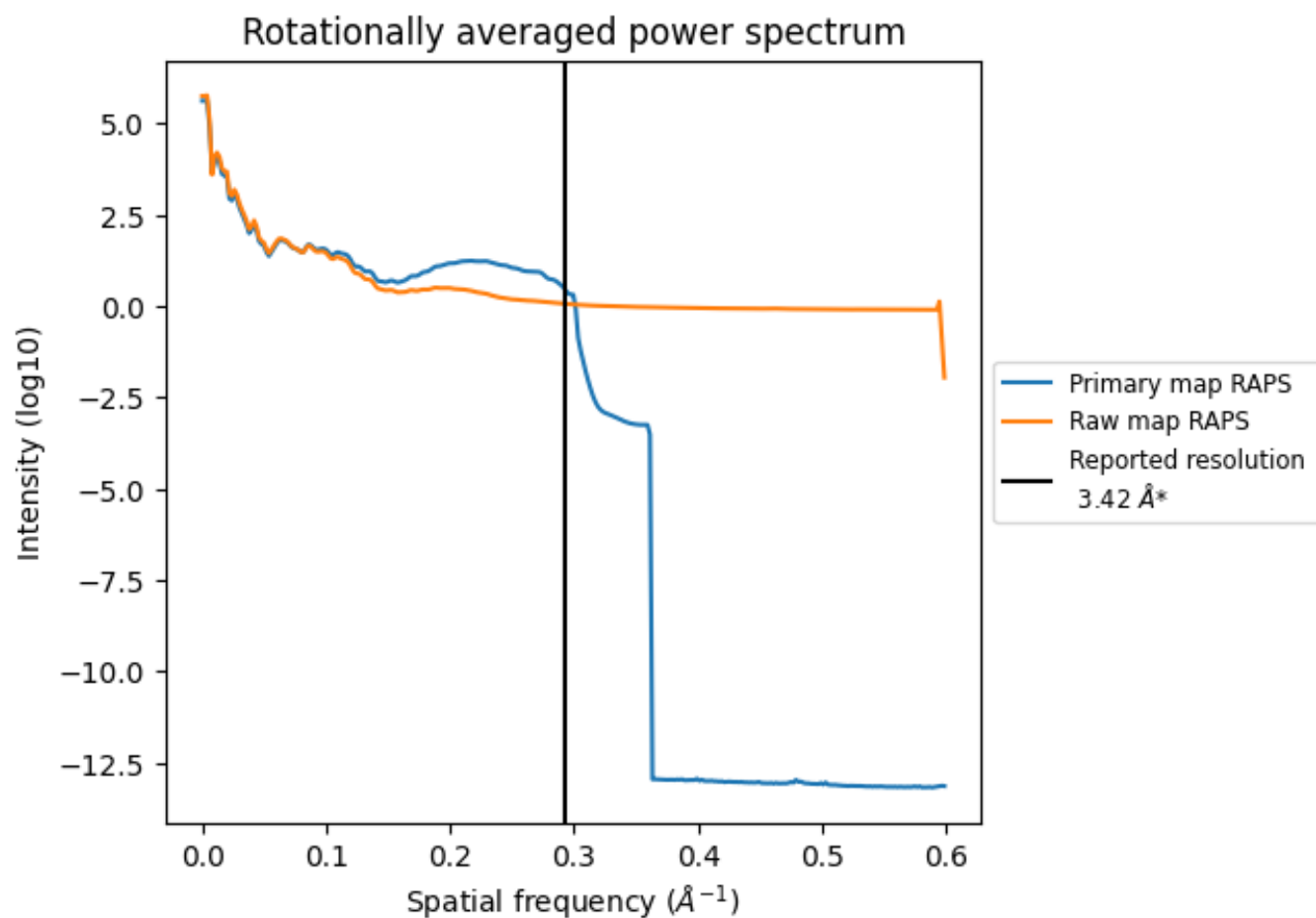
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 405 nm<sup>3</sup>; this corresponds to an approximate mass of 366 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 ⓘ

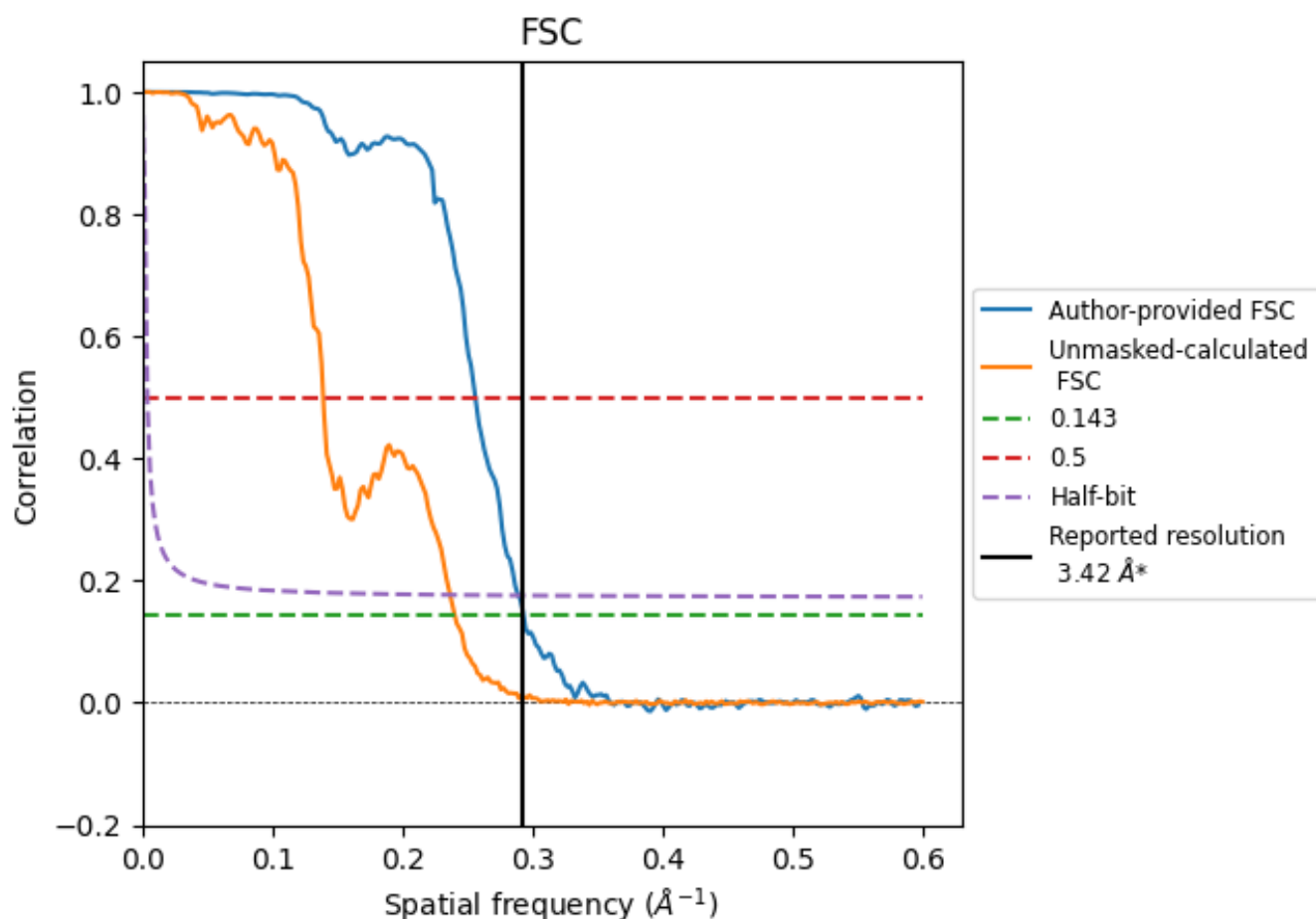


\*Reported resolution corresponds to spatial frequency of 0.292 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.292  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	3.91	3.46
Unmasked-calculated*	4.17	7.19	4.23

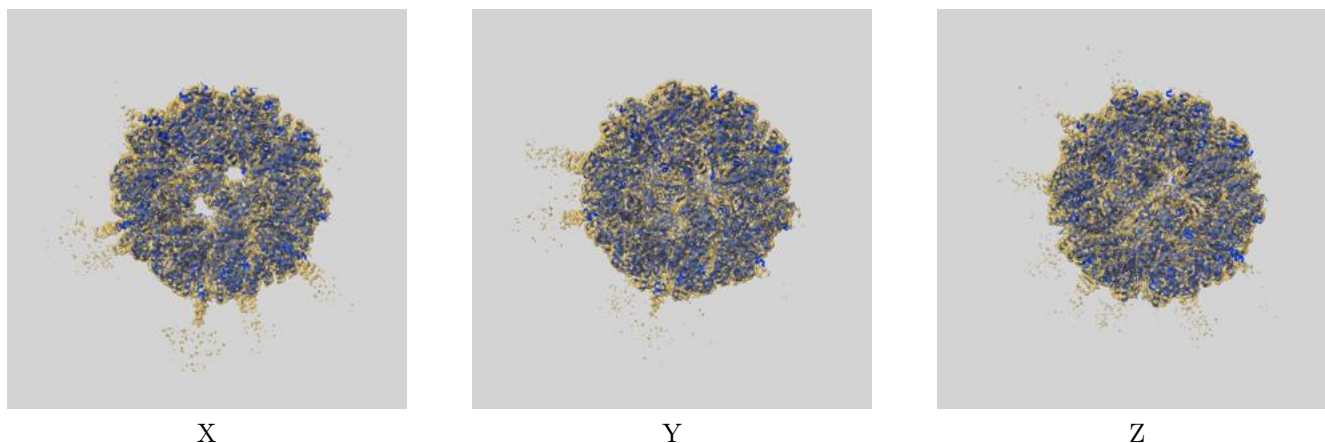
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.42 by more than 10 %



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

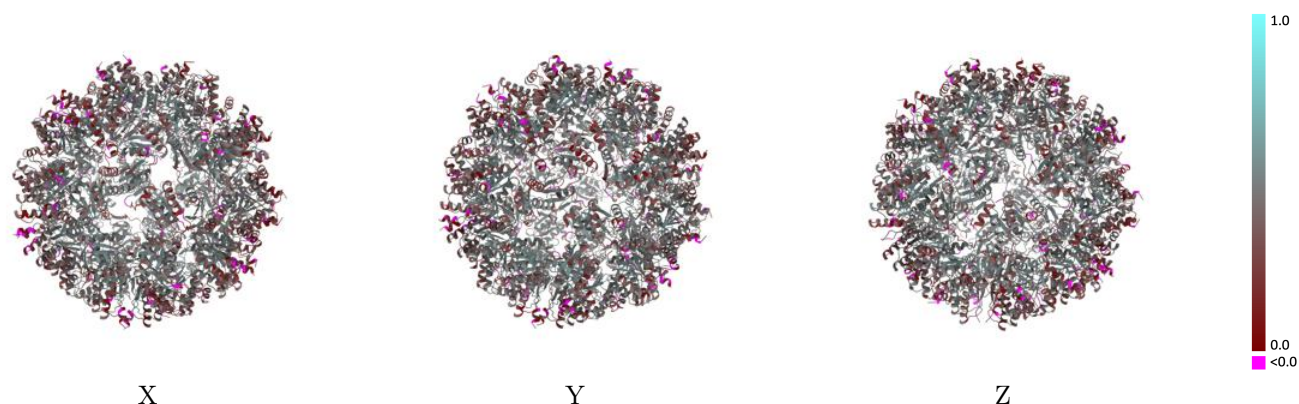
This section contains information regarding the fit between EMDB map EMD-70087 and PDB model 9O3Z. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



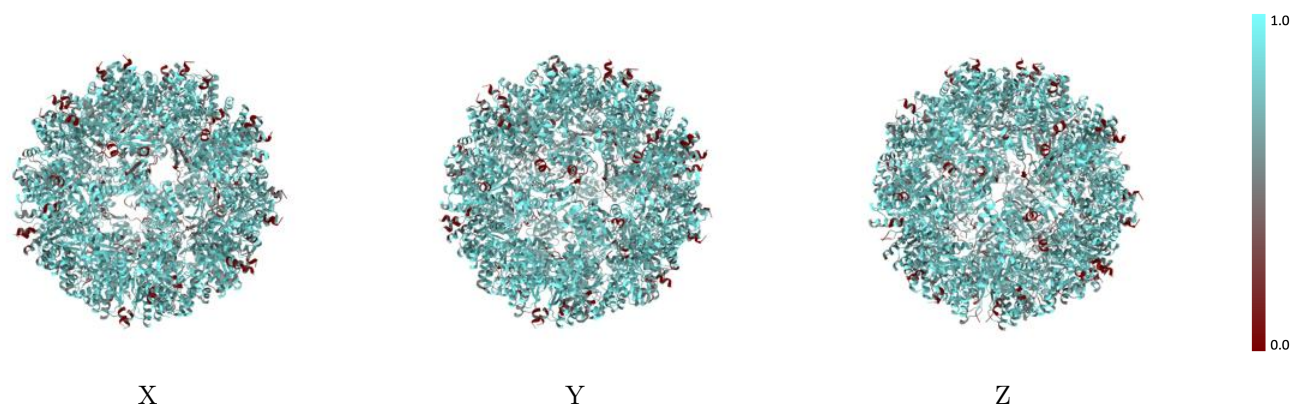
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



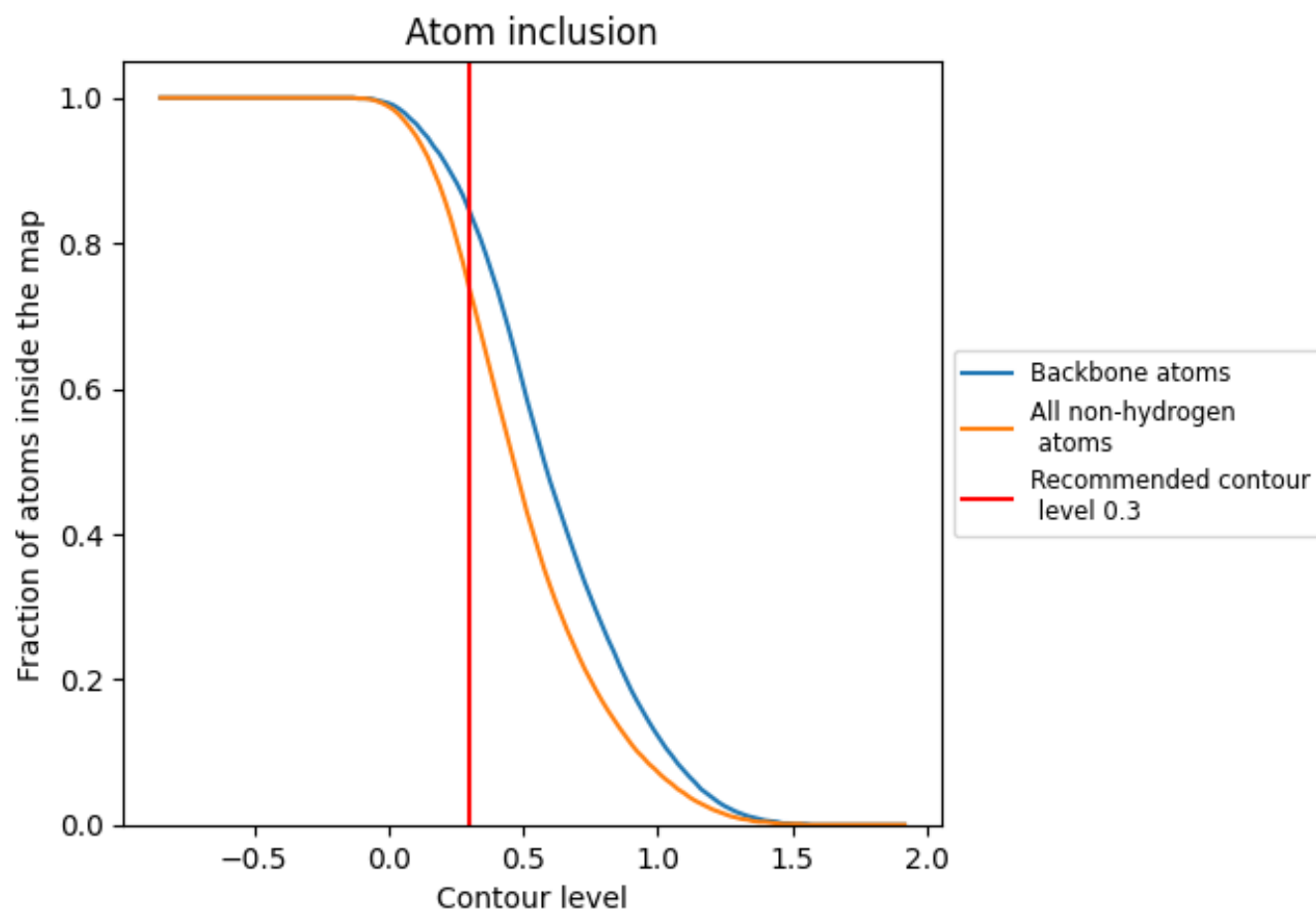
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 74% 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	 0.7370	 0.4120
A	 0.7380	 0.4290
AB	 0.7580	 0.4230
B	 0.7240	 0.4090
BB	 0.7290	 0.4140
C	 0.6450	 0.3680
CB	 0.6680	 0.3850
D	 0.6770	 0.3690
DB	 0.6430	 0.3450
E	 0.7220	 0.3880
EB	 0.7190	 0.3930
F	 0.7050	 0.4200
FB	 0.6890	 0.4140
G	 0.7590	 0.4120
GB	 0.7590	 0.4330
H	 0.7350	 0.4130
HB	 0.7720	 0.4310
I	 0.7600	 0.4150
IB	 0.7350	 0.3880
J	 0.7490	 0.3710
JB	 0.7730	 0.3990
K	 0.7420	 0.4360
KB	 0.7470	 0.4240
L	 0.7540	 0.4130
LB	 0.7610	 0.4320
M	 0.7230	 0.4110
MB	 0.7410	 0.3710
N	 0.7080	 0.4180
NB	 0.7090	 0.4280
O	 0.7240	 0.4280
OB	 0.7460	 0.4080
P	 0.7430	 0.4140
PB	 0.7460	 0.4120
Q	 0.7230	 0.3780
QB	 0.7400	 0.3970



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Chain	Atom inclusion	Q-score
R	 0.7280	 0.4090
RB	 0.7190	 0.4140
S	 0.7350	 0.3860
SB	 0.7240	 0.3760
T	 0.7010	 0.3880
TB	 0.6960	 0.4060
U	 0.7590	 0.4160
UB	 0.7460	 0.4000
V	 0.7140	 0.4140
VB	 0.7330	 0.4100
W	 0.7170	 0.4370
WB	 0.7060	 0.4110
a	 0.7510	 0.4160
ab	 0.7710	 0.4260
b	 0.8080	 0.4680
bb	 0.8020	 0.4680
c	 0.7520	 0.4180
cb	 0.7490	 0.3960
d	 0.7910	 0.4740
db	 0.7970	 0.4450
e	 0.7590	 0.4150
eb	 0.7820	 0.4480
f	 0.7550	 0.4120
fb	 0.7950	 0.4590
g	 0.7830	 0.4420
gb	 0.7690	 0.4450