



Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 01:49 PM EDT

PDB ID : 9O4R / pdb_00009o4r
EMDB ID : EMD-70112
Title : Phosphonull (S56A) 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 : 3.76 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

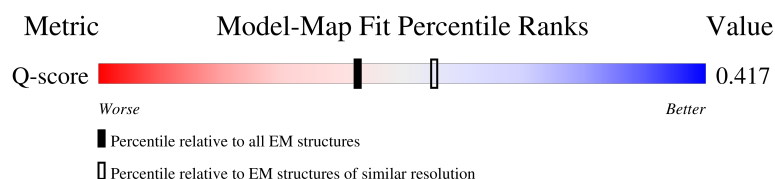
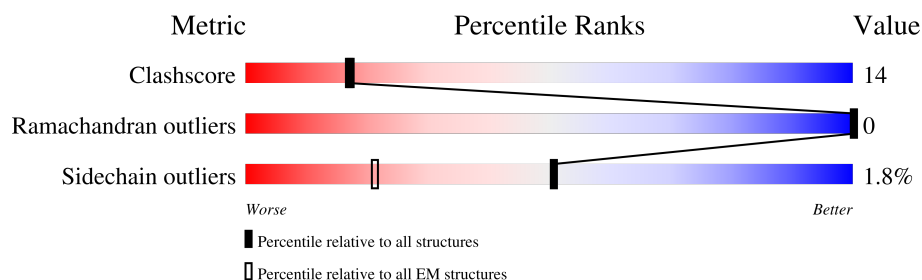
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.76 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.





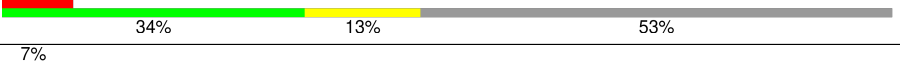



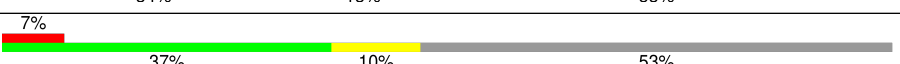
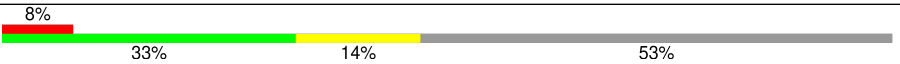

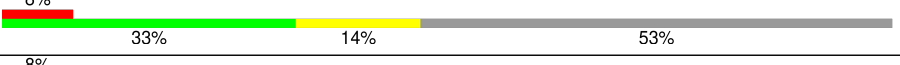




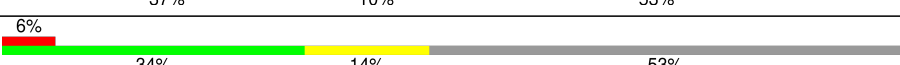
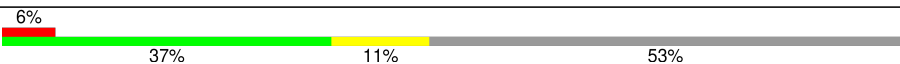









Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10214 (3.26 - 4.26)

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

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








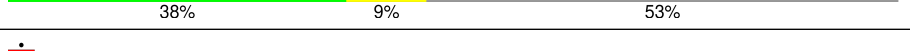
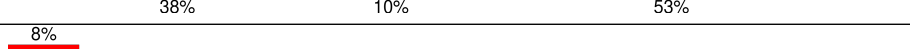
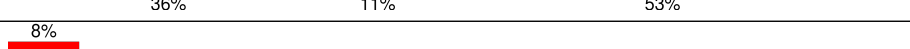
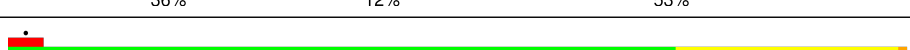

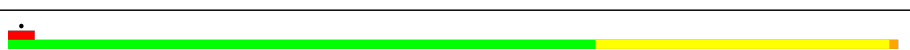

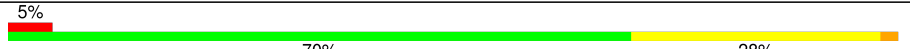





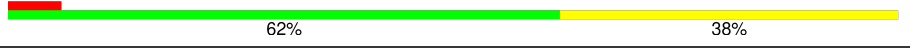
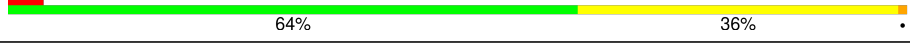



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Mol	Chain	Length	Quality of chain
1	C	278	
1	CB	278	
1	D	278	
1	DB	278	
1	E	278	
1	EB	278	
1	F	278	
1	FB	278	
1	G	278	
1	GB	278	
1	H	278	
1	HB	278	
1	I	278	
1	IB	278	
1	J	278	
1	JB	278	
1	K	278	
1	KB	278	
1	L	278	
1	LB	278	
1	M	278	
1	MB	278	
1	N	278	
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	
2	a	118	
2	ab	118	
2	b	118	
2	bb	118	
2	c	118	
2	cb	118	
2	d	118	
2	db	118	
2	e	118	
2	eb	118	
2	f	118	
2	fb	118	
2	g	118	
2	gb	118	

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Mol	Chain	Length	Quality of chain
2	h	118	 69%31%
2	hb	118	 64%36%
2	i	118	 5%65%34%
2	ib	118	 5%75%24%
2	j	118	 69%31%
2	jb	118	 81%19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 57760 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
			1004	638	171	189	6		
1	AB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	B	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	BB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	C	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	CB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	D	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	DB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	E	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	EB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	F	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	FB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	G	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	GB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	H	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	HB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	I	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	J	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	JB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	K	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	KB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	L	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	LB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	M	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	MB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	N	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	NB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	O	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	OB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	P	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	PB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	Q	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	QB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	R	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	RB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	S	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	SB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		
1	TB	132	Total	C	N	O	S	0	0
			1004	638	171	189	6		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ASP	ASN	conflict	UNP Q8GD19
AB	19	ASP	ASN	conflict	UNP Q8GD19
B	19	ASP	ASN	conflict	UNP Q8GD19
BB	19	ASP	ASN	conflict	UNP Q8GD19
C	19	ASP	ASN	conflict	UNP Q8GD19
CB	19	ASP	ASN	conflict	UNP Q8GD19
D	19	ASP	ASN	conflict	UNP Q8GD19
DB	19	ASP	ASN	conflict	UNP Q8GD19
E	19	ASP	ASN	conflict	UNP Q8GD19
EB	19	ASP	ASN	conflict	UNP Q8GD19
F	19	ASP	ASN	conflict	UNP Q8GD19
FB	19	ASP	ASN	conflict	UNP Q8GD19
G	19	ASP	ASN	conflict	UNP Q8GD19
GB	19	ASP	ASN	conflict	UNP Q8GD19
H	19	ASP	ASN	conflict	UNP Q8GD19
HB	19	ASP	ASN	conflict	UNP Q8GD19
I	19	ASP	ASN	conflict	UNP Q8GD19
IB	19	ASP	ASN	conflict	UNP Q8GD19
J	19	ASP	ASN	conflict	UNP Q8GD19
JB	19	ASP	ASN	conflict	UNP Q8GD19
K	19	ASP	ASN	conflict	UNP Q8GD19
KB	19	ASP	ASN	conflict	UNP Q8GD19
L	19	ASP	ASN	conflict	UNP Q8GD19
LB	19	ASP	ASN	conflict	UNP Q8GD19
M	19	ASP	ASN	conflict	UNP Q8GD19
MB	19	ASP	ASN	conflict	UNP Q8GD19
N	19	ASP	ASN	conflict	UNP Q8GD19
NB	19	ASP	ASN	conflict	UNP Q8GD19
O	19	ASP	ASN	conflict	UNP Q8GD19
OB	19	ASP	ASN	conflict	UNP Q8GD19
P	19	ASP	ASN	conflict	UNP Q8GD19
PB	19	ASP	ASN	conflict	UNP Q8GD19
Q	19	ASP	ASN	conflict	UNP Q8GD19
QB	19	ASP	ASN	conflict	UNP Q8GD19

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Chain	Residue	Modelled	Actual	Comment	Reference
R	19	ASP	ASN	conflict	UNP Q8GD19
RB	19	ASP	ASN	conflict	UNP Q8GD19
S	19	ASP	ASN	conflict	UNP Q8GD19
SB	19	ASP	ASN	conflict	UNP Q8GD19
T	19	ASP	ASN	conflict	UNP Q8GD19
TB	19	ASP	ASN	conflict	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
			880	565	136	174	5		
2	ab	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	b	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	bb	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	c	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	cb	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	d	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	db	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	e	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	eb	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	f	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	fb	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	g	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	gb	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	h	118	Total	C	N	O	S	0	0
			880	565	136	174	5		
2	hb	118	Total	C	N	O	S	0	0
			880	565	136	174	5		

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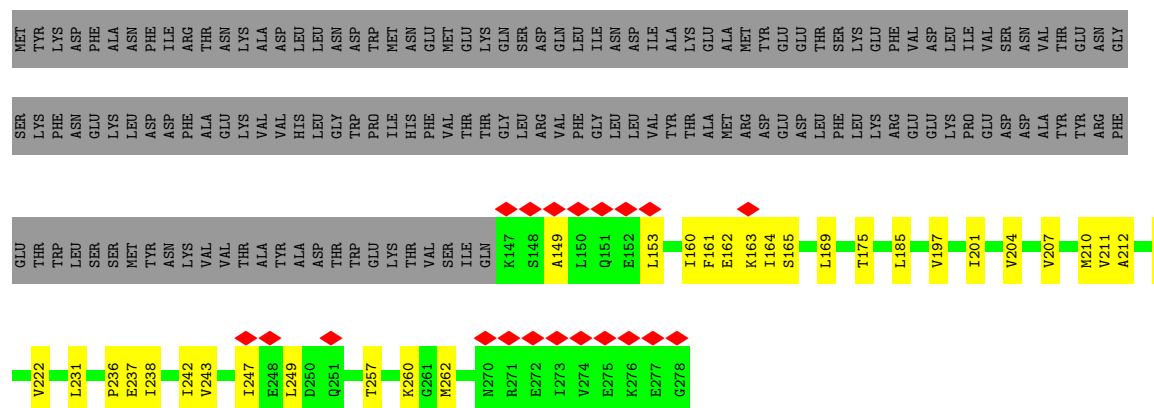
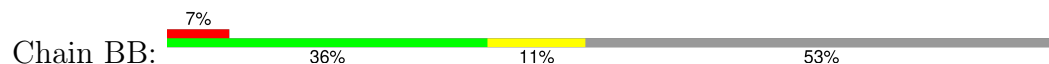
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	i	118	Total 880	C 565	N 136	O 174	S 5	0	0
2	ib	118	Total 880	C 565	N 136	O 174	S 5	0	0
2	j	118	Total 880	C 565	N 136	O 174	S 5	0	0
2	jb	118	Total 880	C 565	N 136	O 174	S 5	0	0

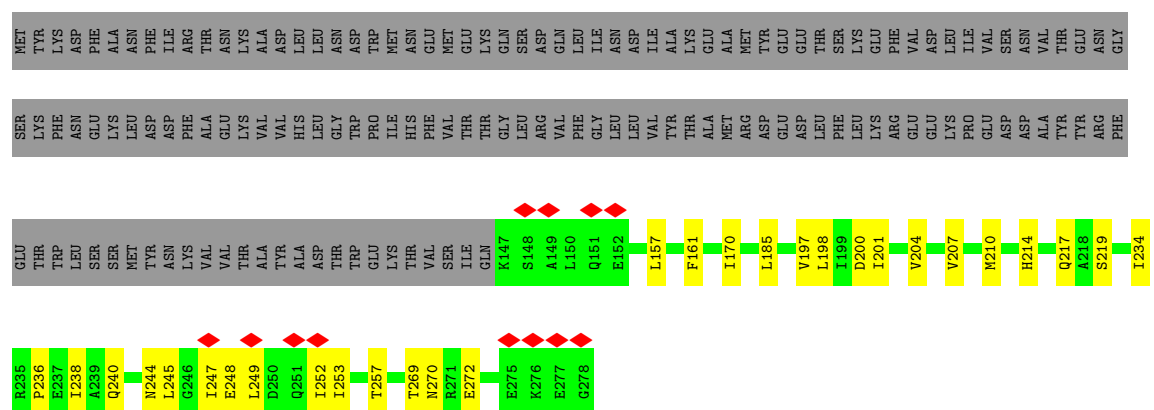
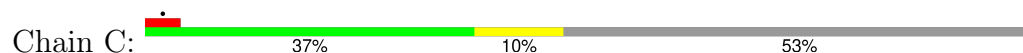
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	56	ALA	SER	conflict	UNP A0A0D8X5U2
ab	56	ALA	SER	conflict	UNP A0A0D8X5U2
b	56	ALA	SER	conflict	UNP A0A0D8X5U2
bb	56	ALA	SER	conflict	UNP A0A0D8X5U2
c	56	ALA	SER	conflict	UNP A0A0D8X5U2
cb	56	ALA	SER	conflict	UNP A0A0D8X5U2
d	56	ALA	SER	conflict	UNP A0A0D8X5U2
db	56	ALA	SER	conflict	UNP A0A0D8X5U2
e	56	ALA	SER	conflict	UNP A0A0D8X5U2
eb	56	ALA	SER	conflict	UNP A0A0D8X5U2
f	56	ALA	SER	conflict	UNP A0A0D8X5U2
fb	56	ALA	SER	conflict	UNP A0A0D8X5U2
g	56	ALA	SER	conflict	UNP A0A0D8X5U2
gb	56	ALA	SER	conflict	UNP A0A0D8X5U2
h	56	ALA	SER	conflict	UNP A0A0D8X5U2
hb	56	ALA	SER	conflict	UNP A0A0D8X5U2
i	56	ALA	SER	conflict	UNP A0A0D8X5U2
ib	56	ALA	SER	conflict	UNP A0A0D8X5U2
j	56	ALA	SER	conflict	UNP A0A0D8X5U2
jb	56	ALA	SER	conflict	UNP A0A0D8X5U2

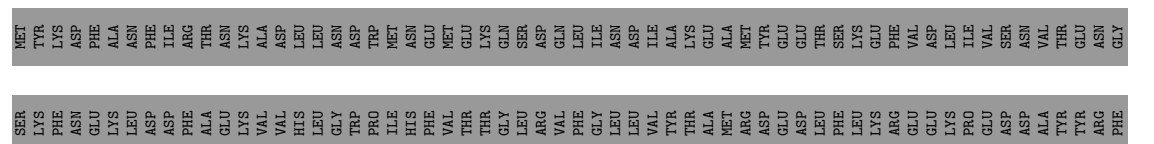
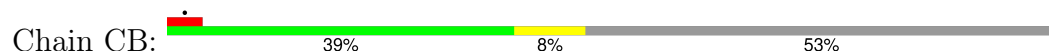
- Molecule 1: RsbR

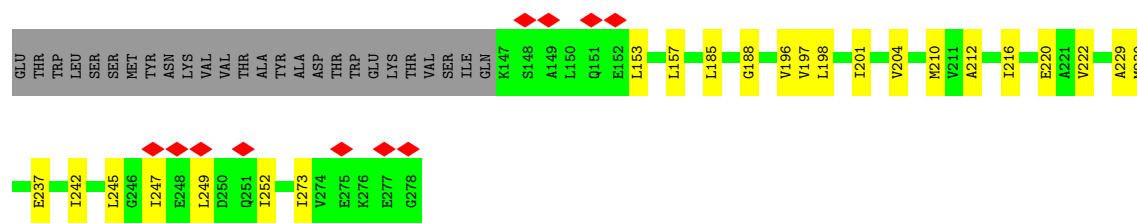


- Molecule 1: RsbR

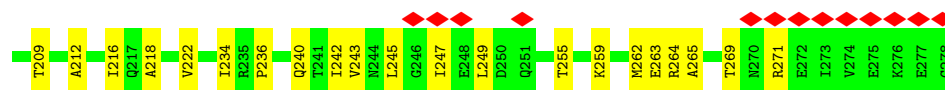
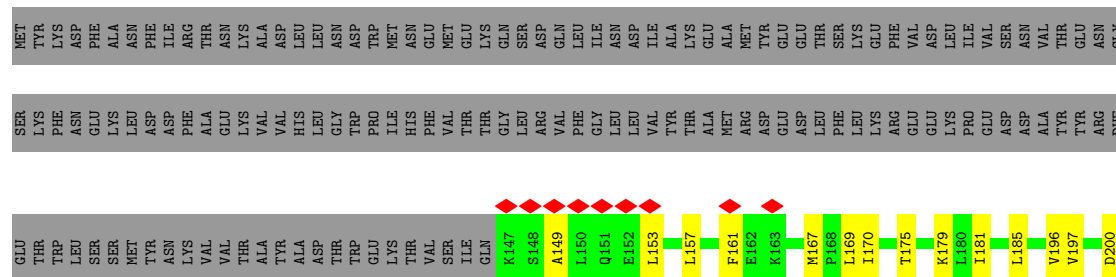
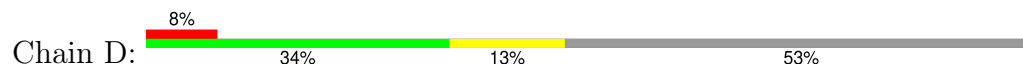


- Molecule 1: RsbR

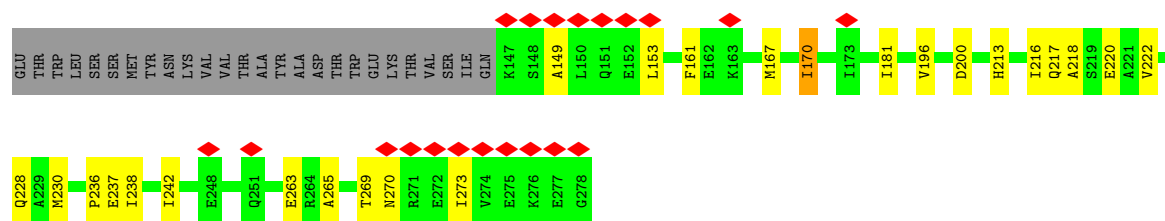
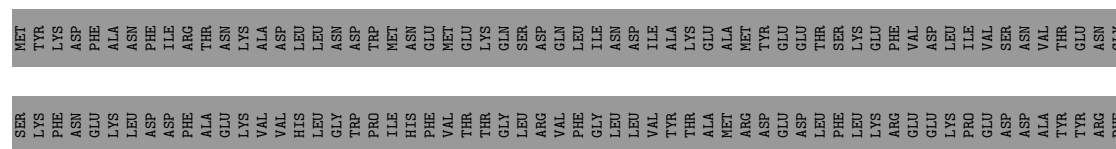
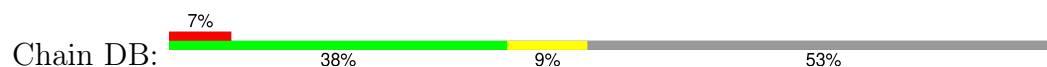




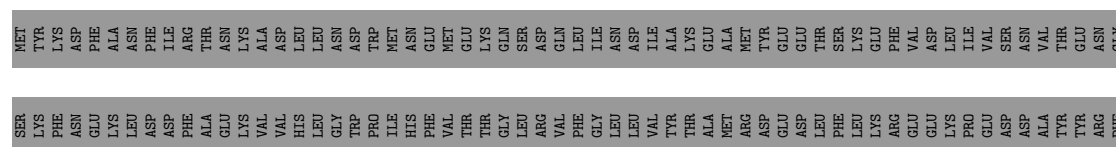
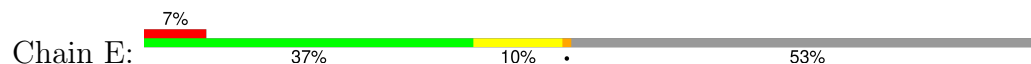
• Molecule 1: RsbR

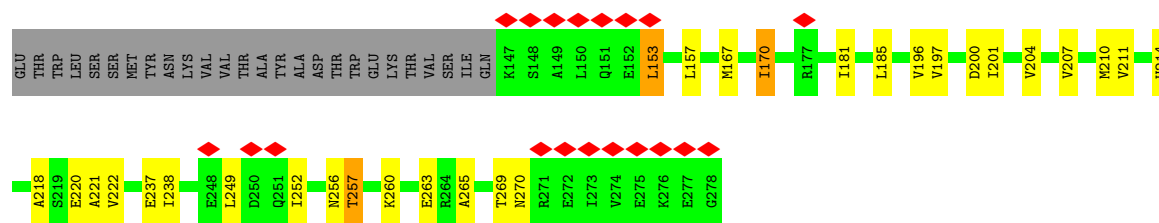


• Molecule 1: RsbR

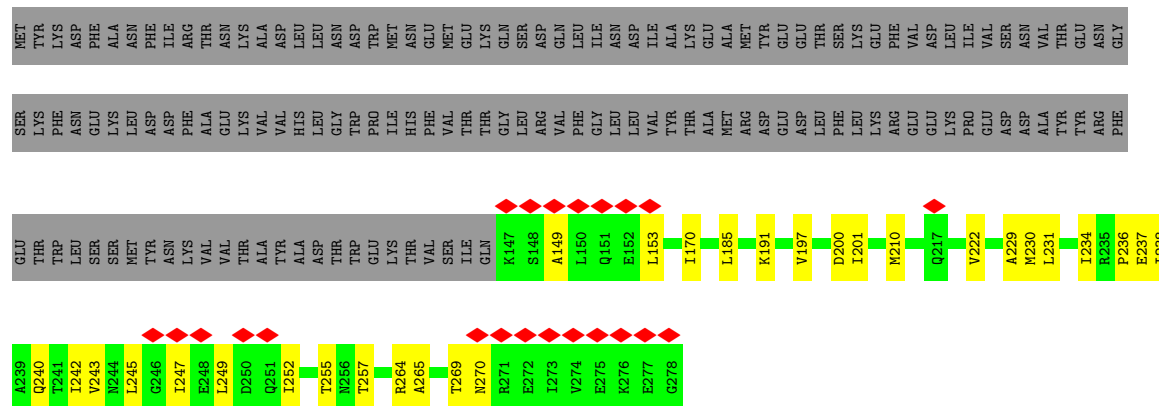
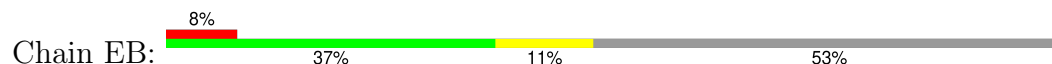


• Molecule 1: RsbR

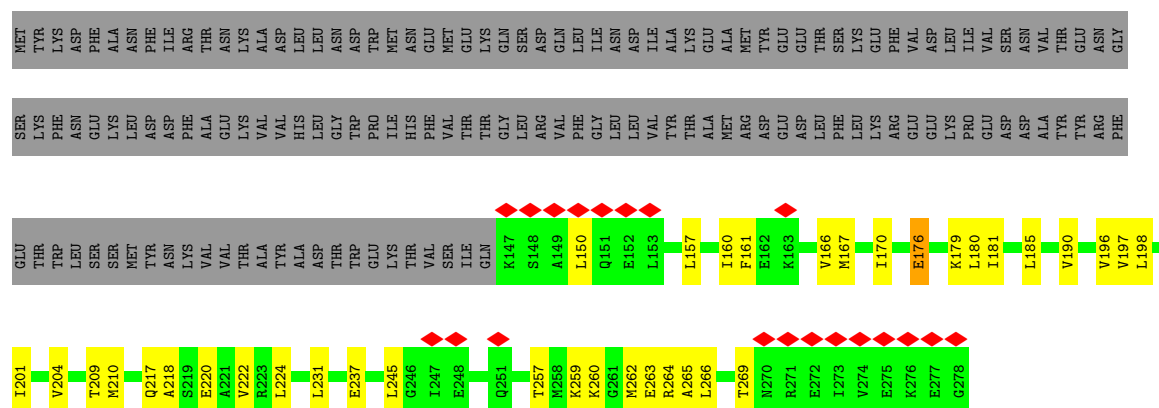
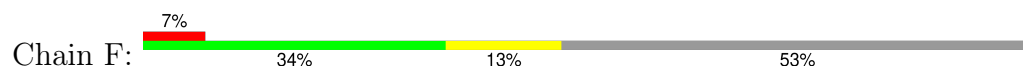




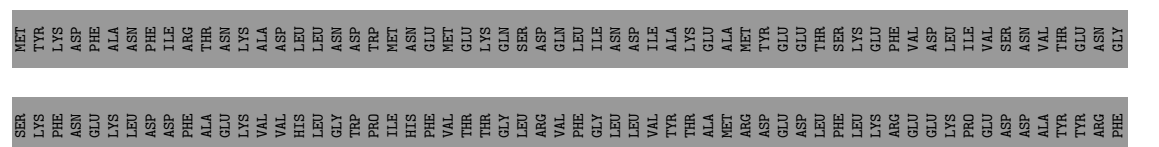
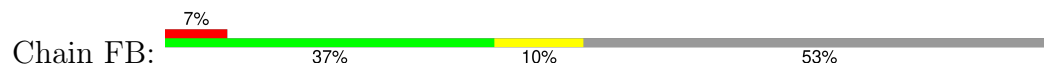
• Molecule 1: RsbR

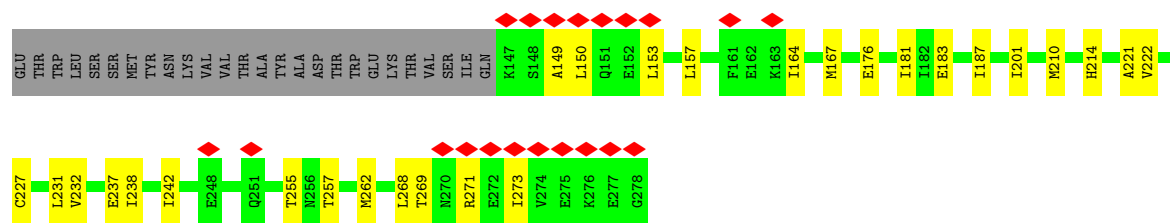


• Molecule 1: RsbR

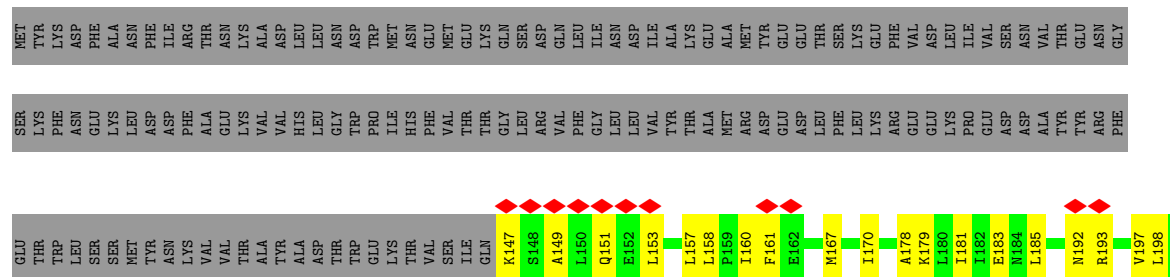
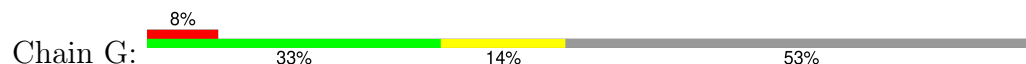


• Molecule 1: RsbR

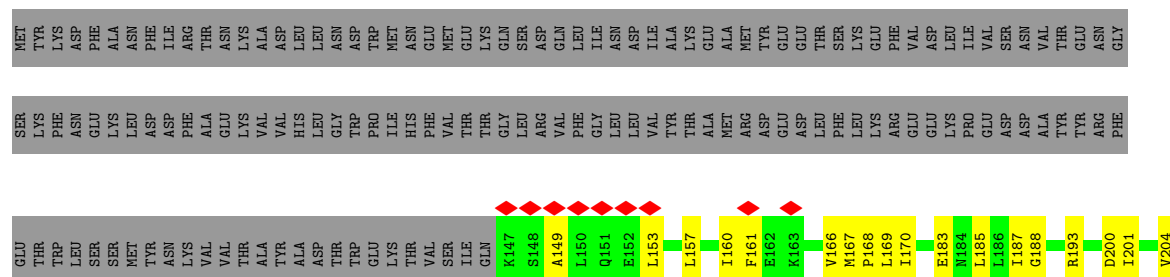
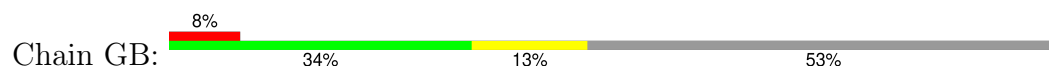




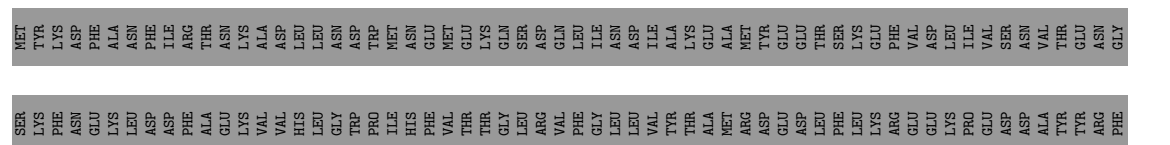
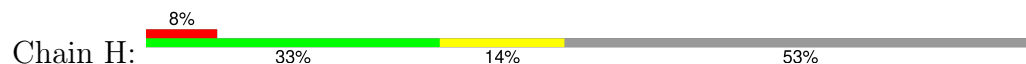
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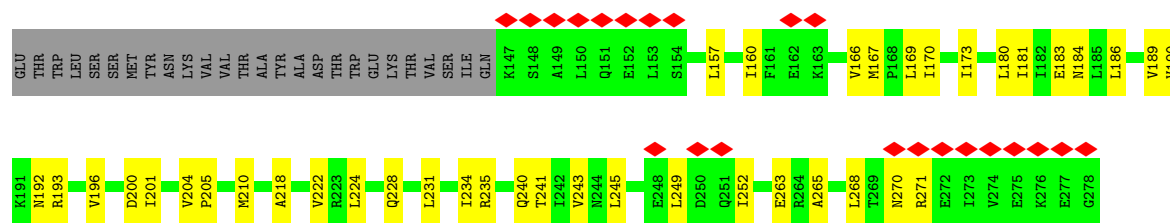


• Molecule 1: RsbR

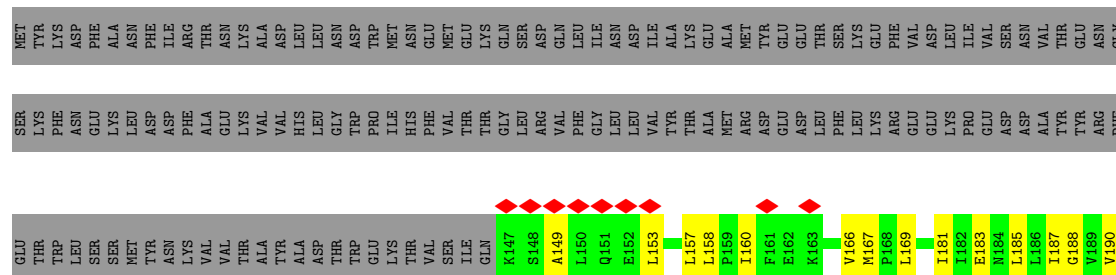
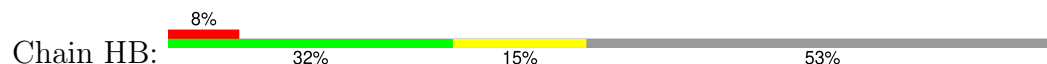


• Molecule 1: RsbR

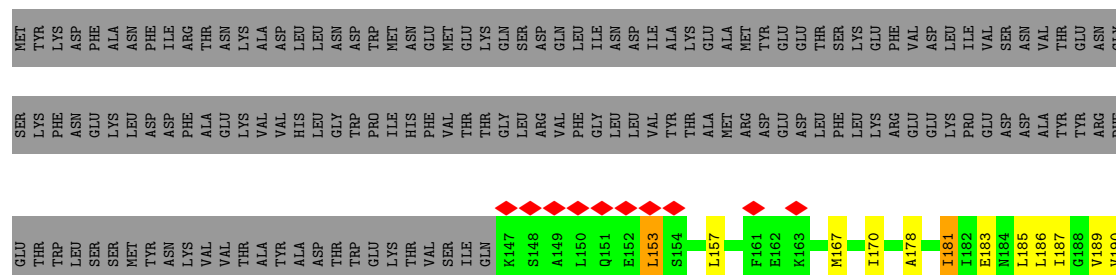
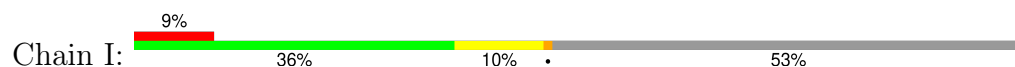




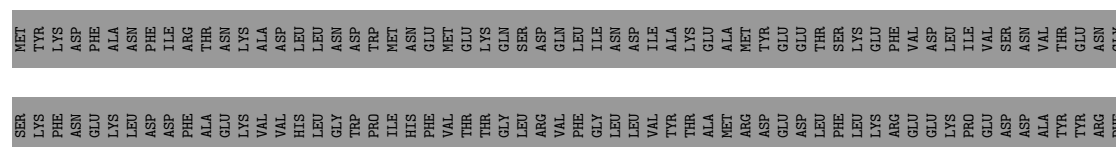
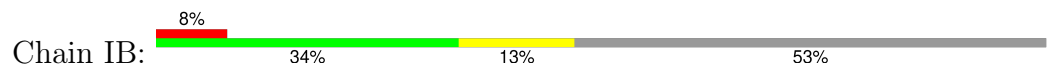
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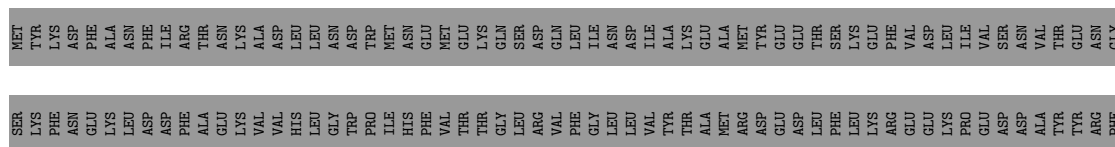


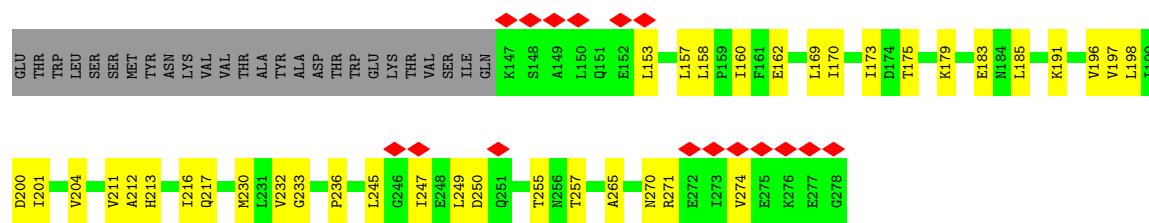
• Molecule 1: RsbR



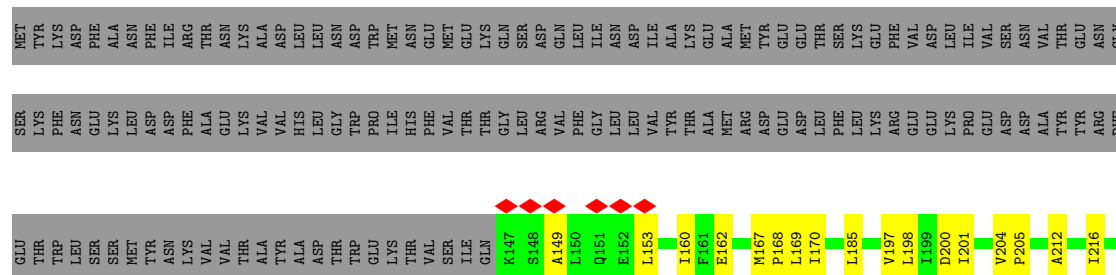
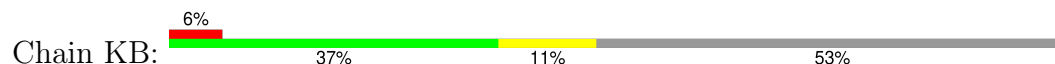
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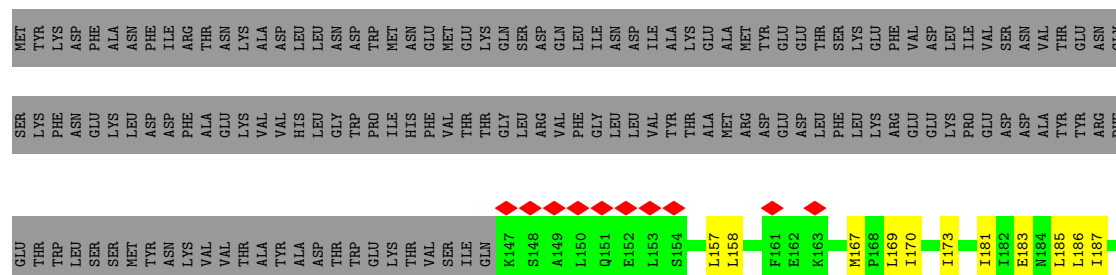
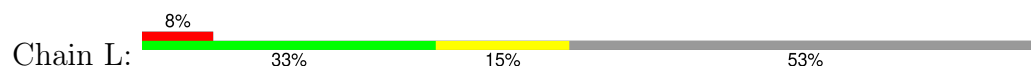




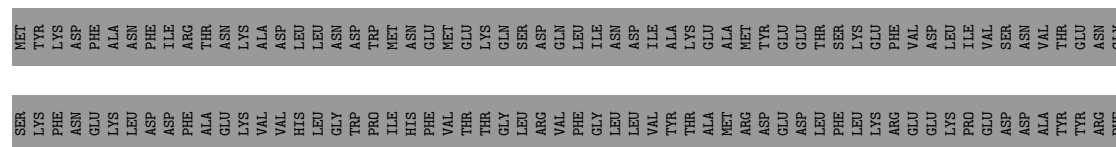
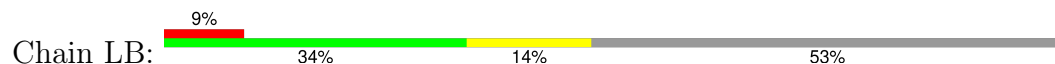
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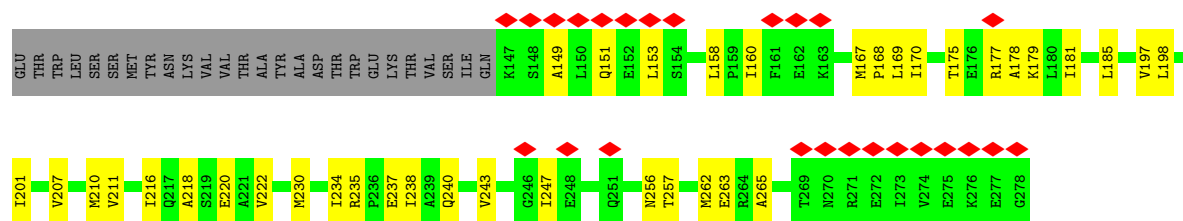


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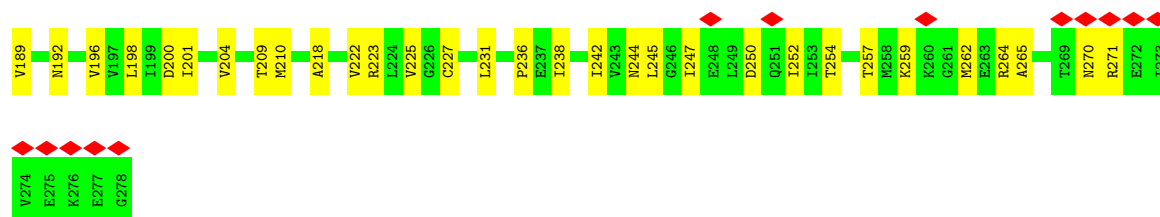
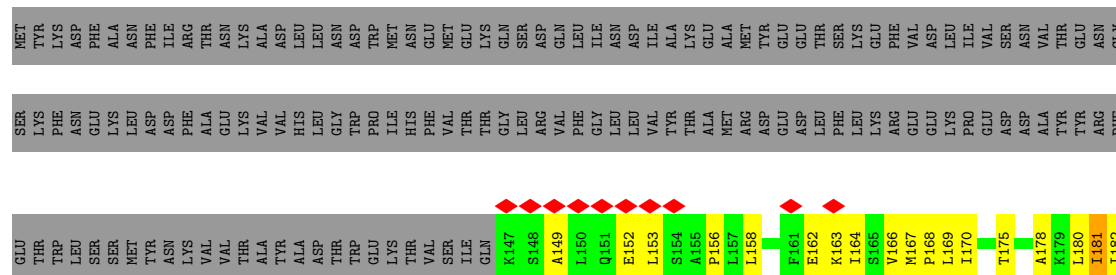
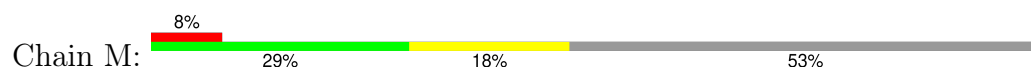


• Molecule 1: RsbR

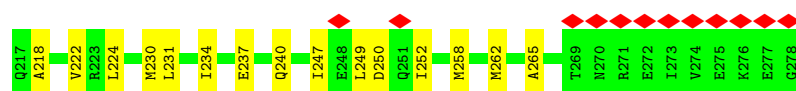
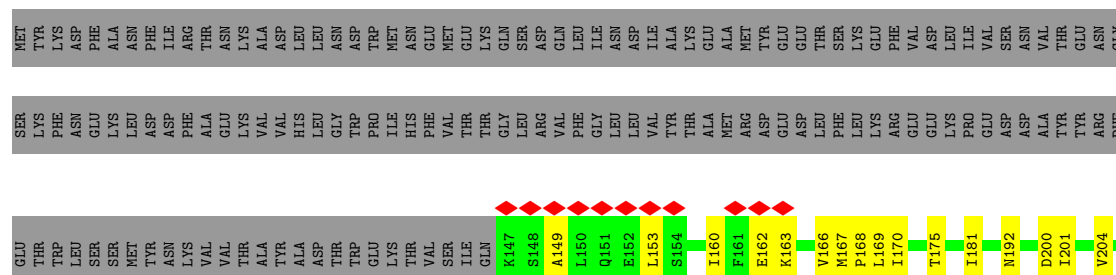
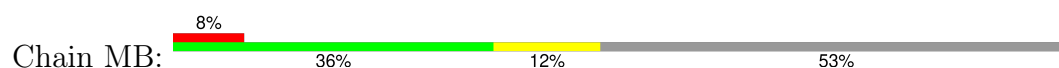




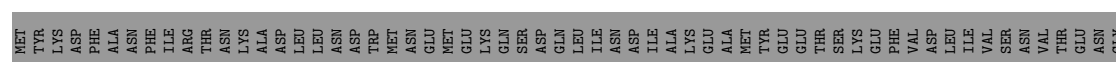
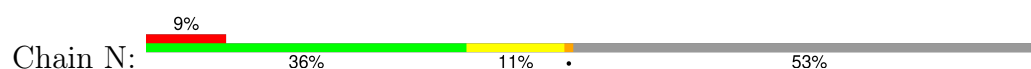
• Molecule 1: RsbR



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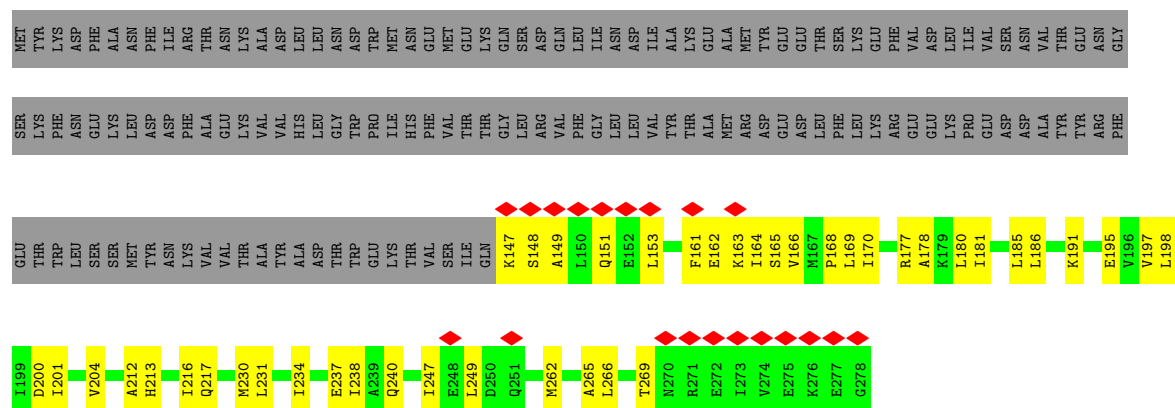
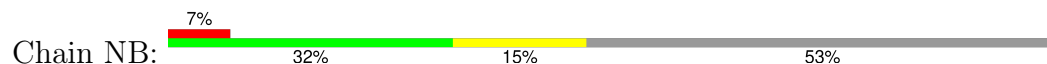


• Molecule 1: RsbR

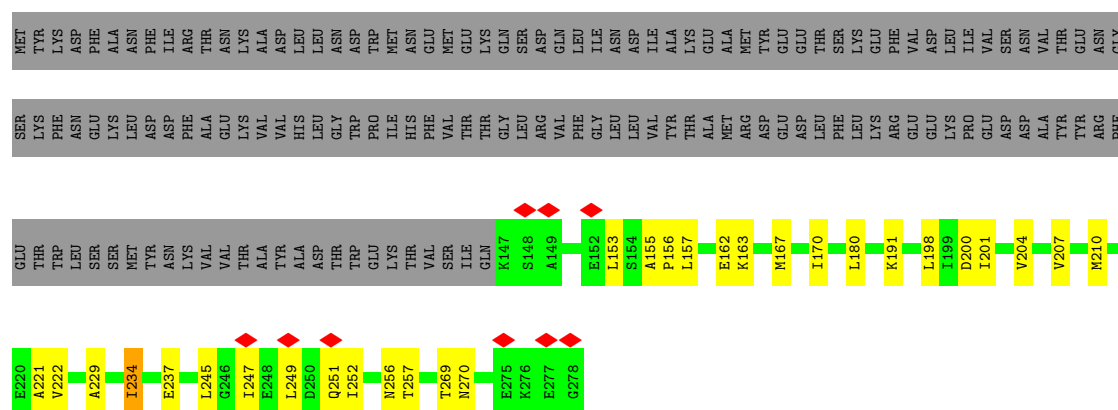
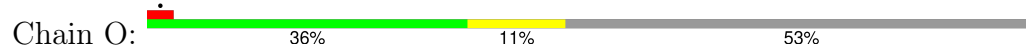




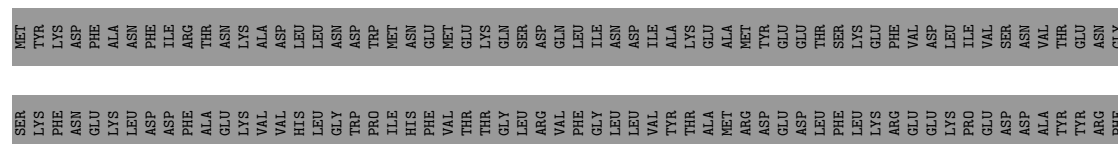
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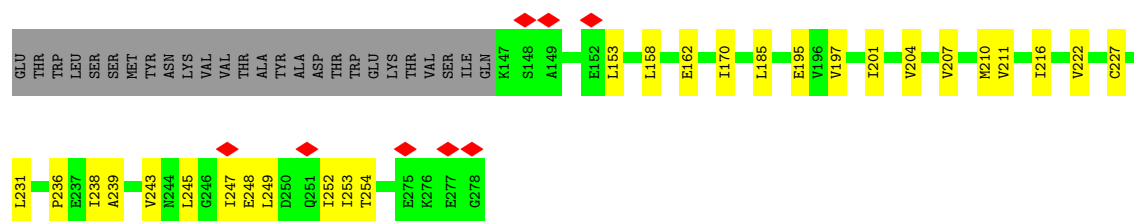


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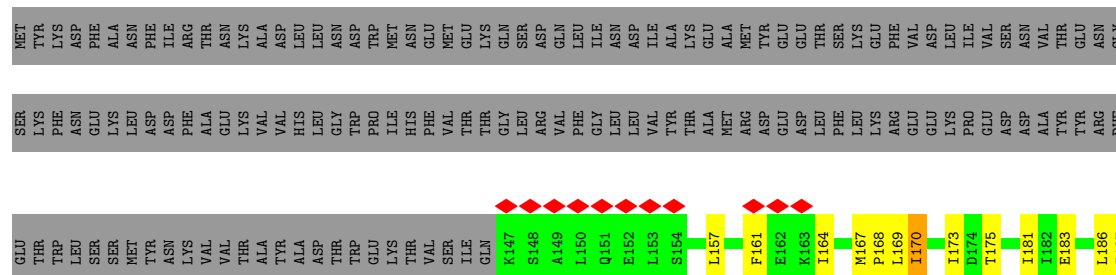
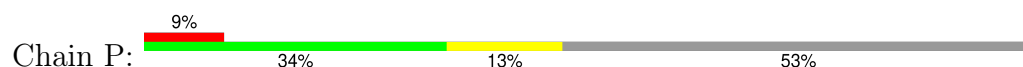


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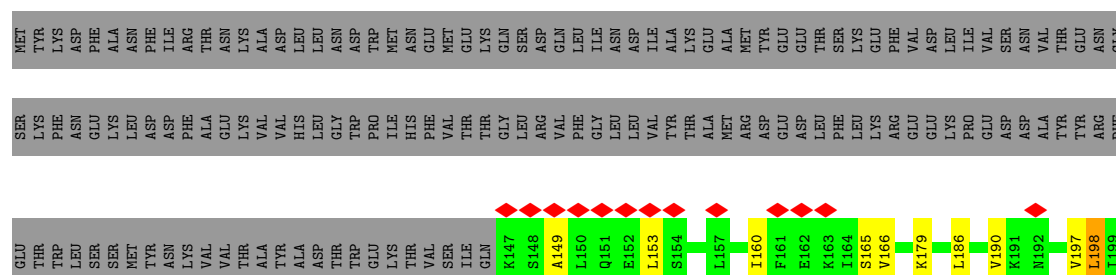
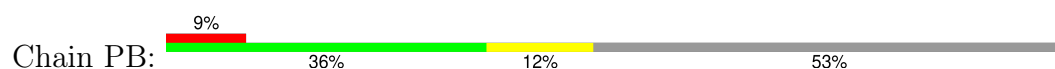




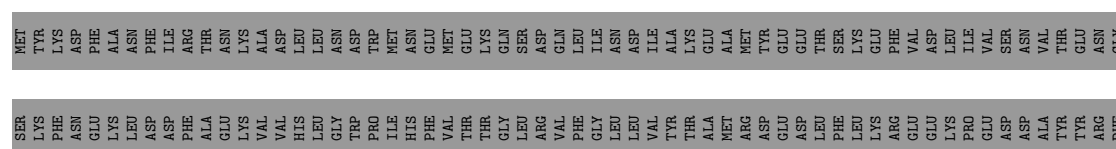
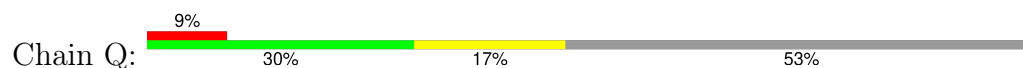
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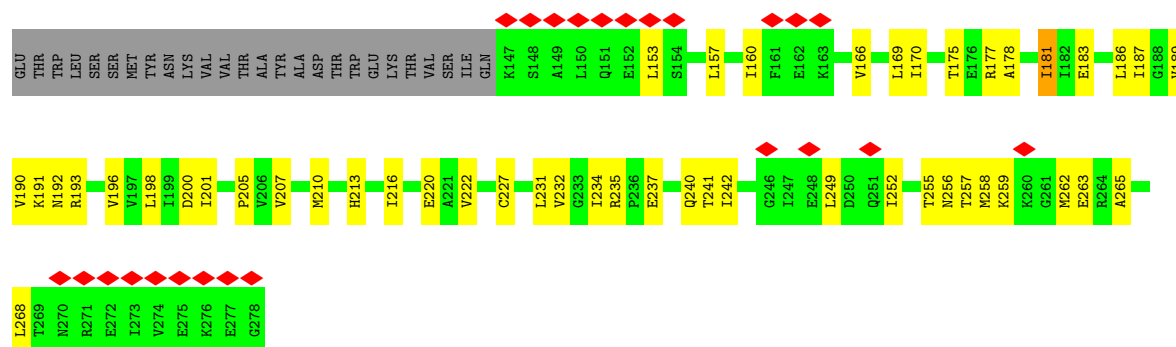


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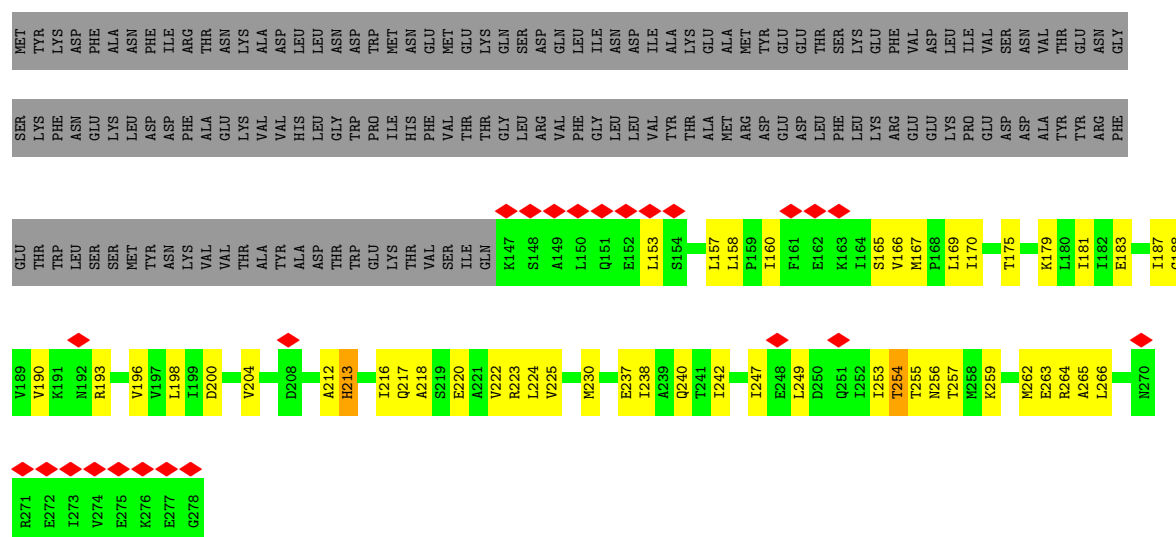
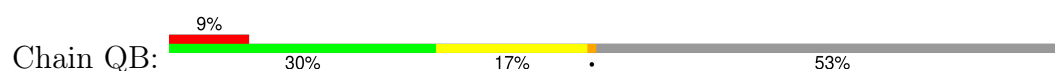


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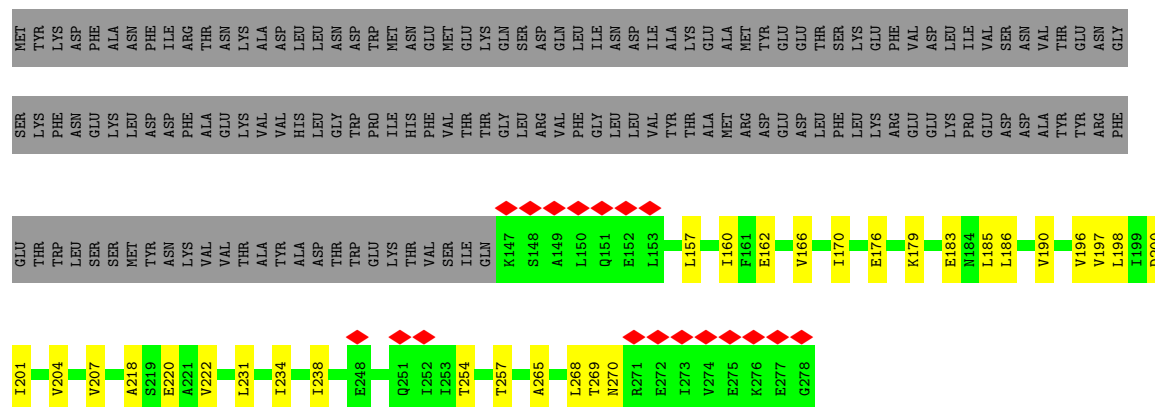
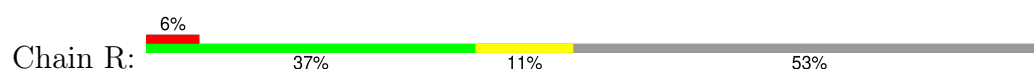




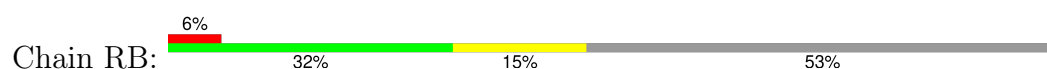
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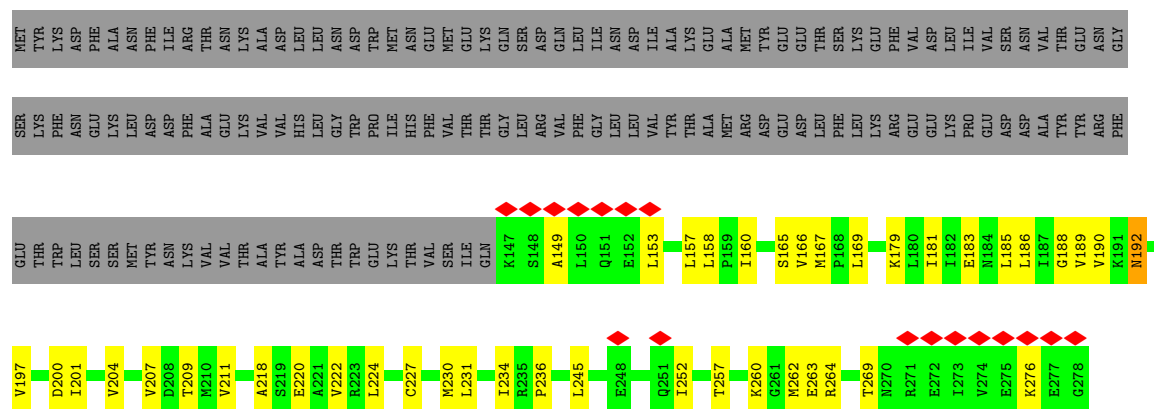


• Molecule 1: RsbR

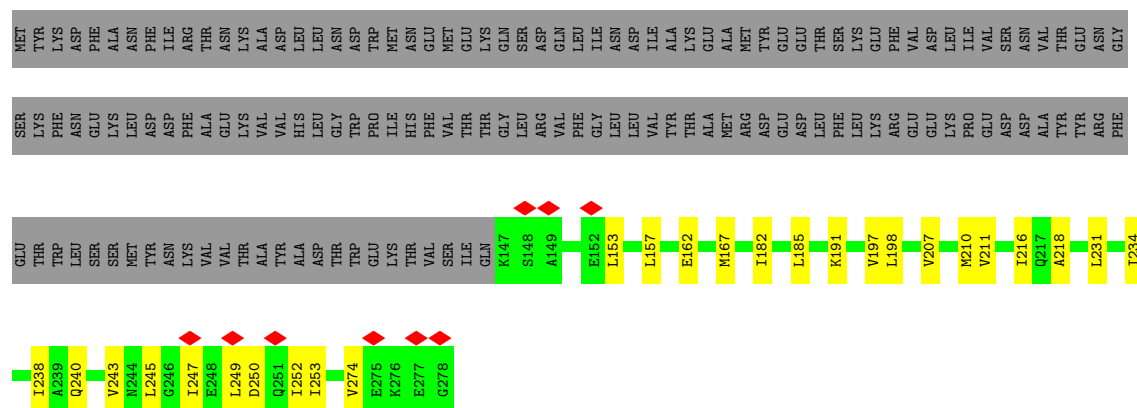
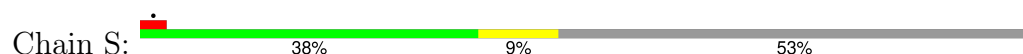


• Molecule 1: RsbR

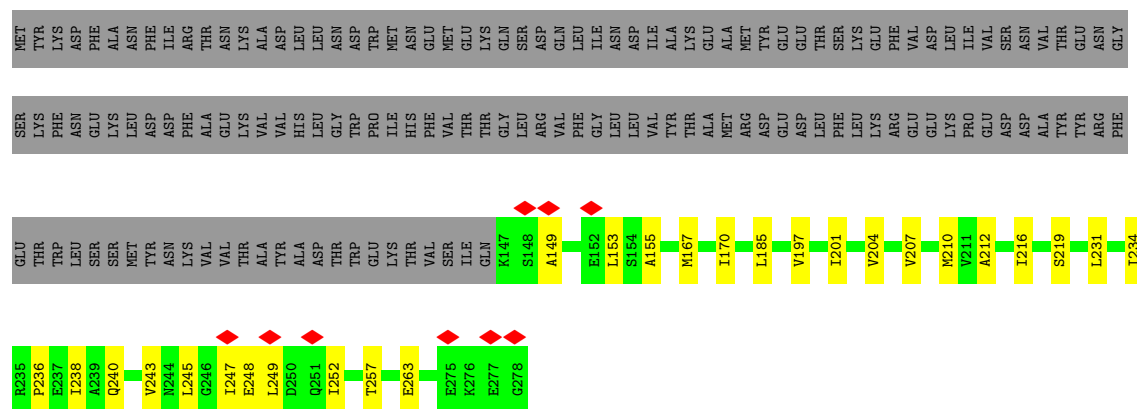
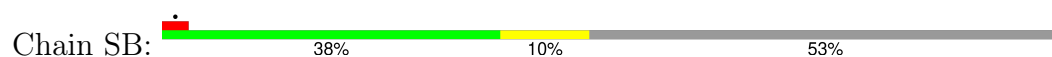




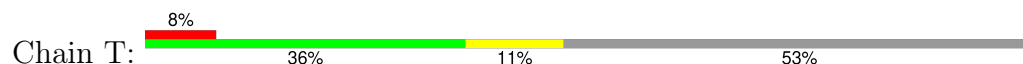
- Molecule 1: RsbR

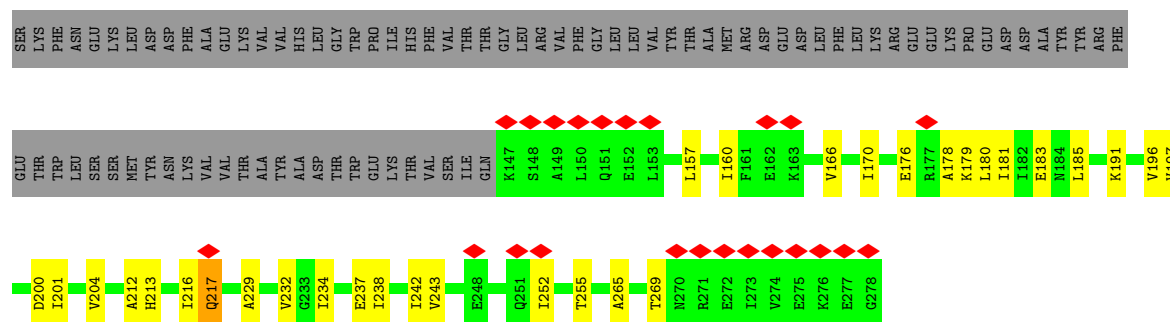


- Molecule 1: RsbR

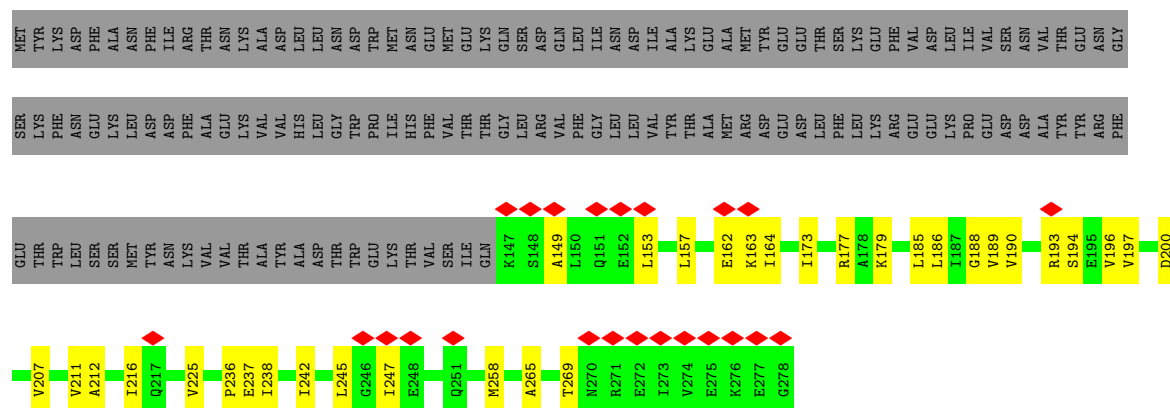
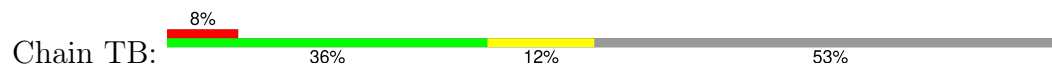


- Molecule 1: RsbR

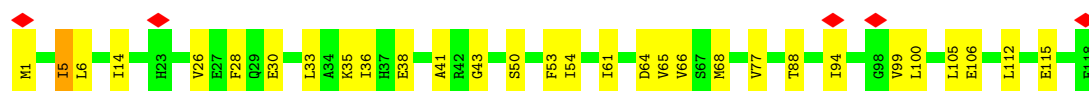




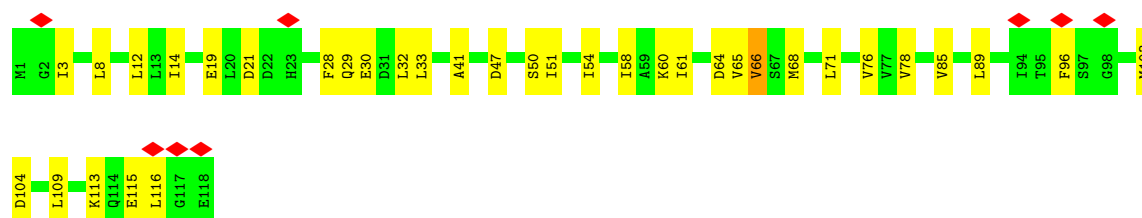
• Molecule 1: RsbR



• Molecule 2: RsbT antagonist protein RsbS

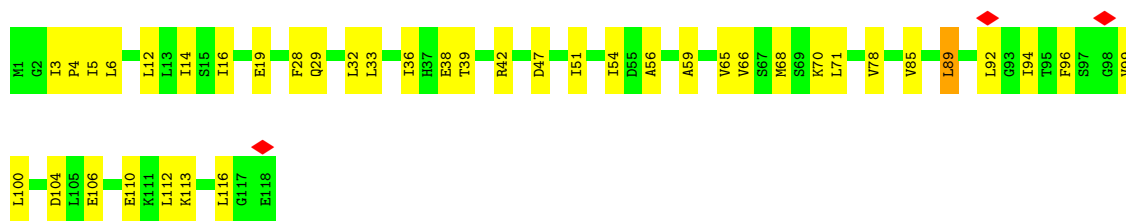


• Molecule 2: RsbT antagonist protein RsbS

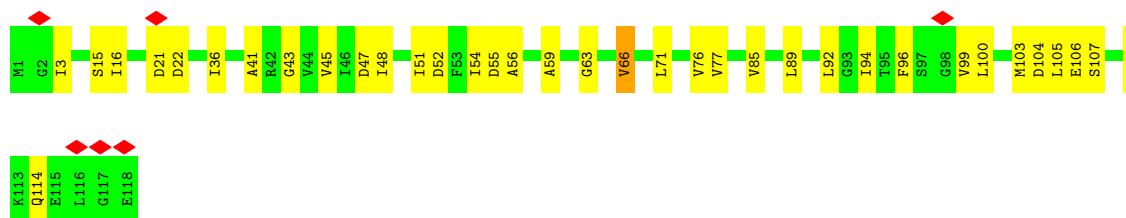


• Molecule 2: RsbT antagonist protein RsbS

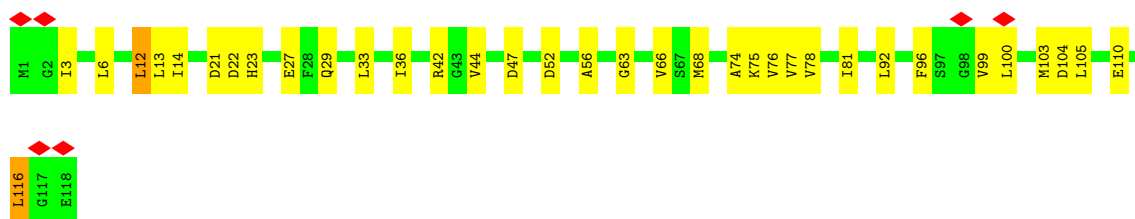




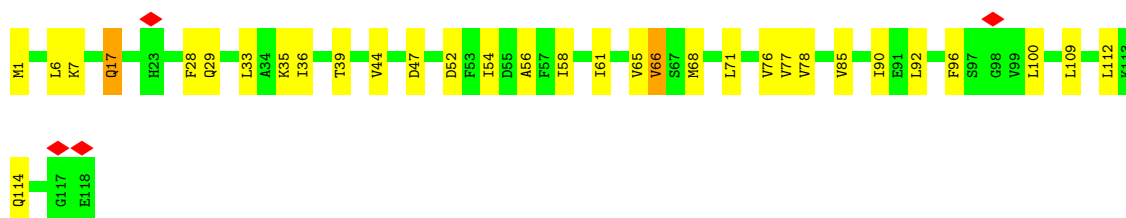
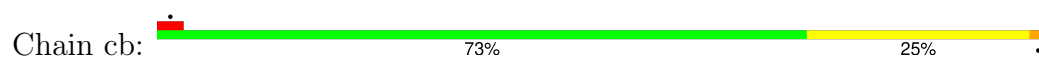
- Molecule 2: RsbT antagonist protein RsbS



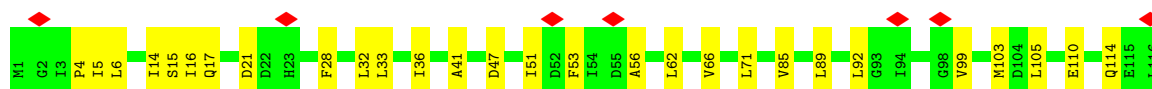
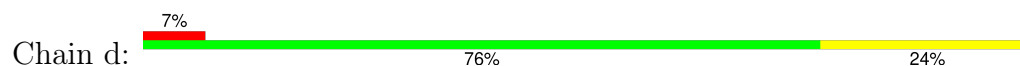
- Molecule 2: RsbT antagonist protein RsbS



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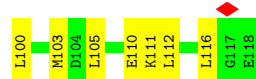


- Molecule 2: RsbT antagonist protein RsbS

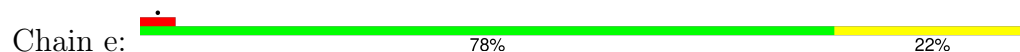




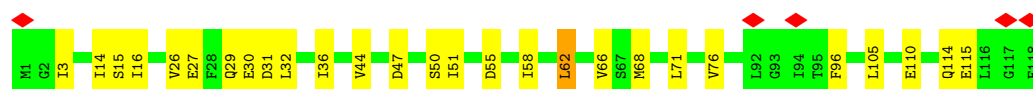
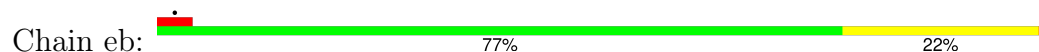
- Molecule 2: RsbT antagonist protein RsbS



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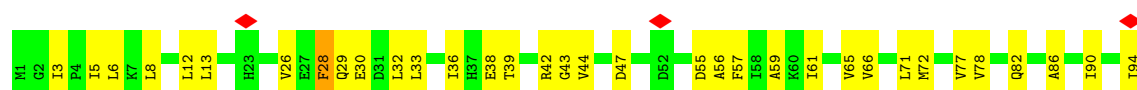
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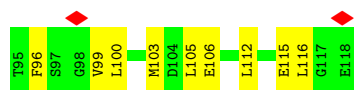


- Molecule 2: RsbT antagonist protein RsbS



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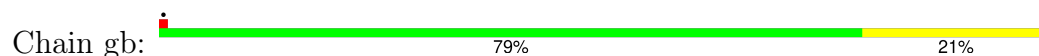




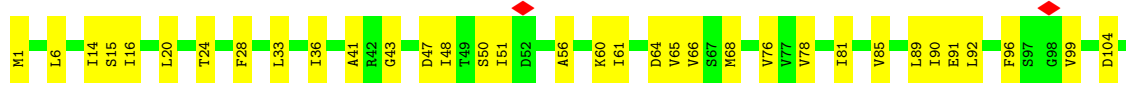
- Molecule 2: RsbT antagonist protein RsbS



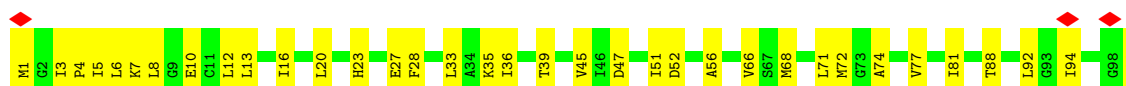
- Molecule 2: RsbT antagonist protein RsbS



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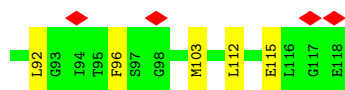


- Molecule 2: RsbT antagonist protein RsbS

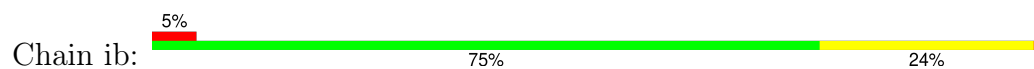


- Molecule 2: RsbT antagonist protein RsbS

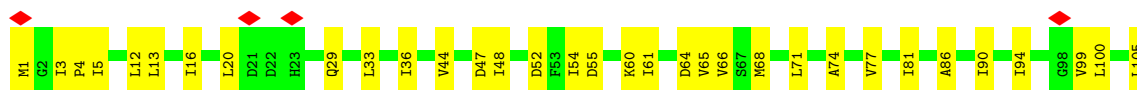




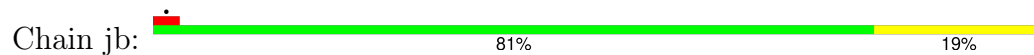
- Molecule 2: RsbT antagonist protein RsbS



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- 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	117803	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	1.446	Depositor
Minimum map value	-0.674	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	501.0, 501.0, 501.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.835, 0.835, 0.835	Depositor

5 Model quality [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	0.19	0/1011	0.46	2/1368 (0.1%)
1	AB	0.17	0/1011	0.36	0/1368
1	B	0.20	0/1011	0.51	3/1368 (0.2%)
1	BB	0.18	0/1011	0.38	0/1368
1	C	0.19	0/1011	0.46	2/1368 (0.1%)
1	CB	0.19	0/1011	0.38	0/1368
1	D	0.19	0/1011	0.49	2/1368 (0.1%)
1	DB	0.18	0/1011	0.41	0/1368
1	E	0.19	0/1011	0.48	2/1368 (0.1%)
1	EB	0.18	0/1011	0.39	0/1368
1	F	0.19	0/1011	0.50	2/1368 (0.1%)
1	FB	0.19	0/1011	0.43	0/1368
1	G	0.18	0/1011	0.51	1/1368 (0.1%)
1	GB	0.18	0/1011	0.40	0/1368
1	H	0.20	0/1011	0.49	3/1368 (0.2%)
1	HB	0.17	0/1011	0.39	0/1368
1	I	0.19	0/1011	0.47	3/1368 (0.2%)
1	IB	0.17	0/1011	0.39	0/1368
1	J	0.19	0/1011	0.49	2/1368 (0.1%)
1	JB	0.18	0/1011	0.40	0/1368
1	K	0.20	0/1011	0.47	2/1368 (0.1%)
1	KB	0.19	0/1011	0.40	0/1368
1	L	0.20	0/1011	0.51	3/1368 (0.2%)
1	LB	0.18	0/1011	0.41	0/1368
1	M	0.20	0/1011	0.48	0/1368
1	MB	0.18	0/1011	0.41	0/1368
1	N	0.20	0/1011	0.49	1/1368 (0.1%)
1	NB	0.17	0/1011	0.40	0/1368
1	O	0.22	0/1011	0.51	2/1368 (0.1%)
1	OB	0.19	0/1011	0.41	0/1368
1	P	0.20	0/1011	0.50	2/1368 (0.1%)
1	PB	0.18	0/1011	0.44	0/1368
1	Q	0.24	0/1011	0.56	3/1368 (0.2%)
1	QB	0.18	0/1011	0.41	0/1368

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	R	0.19	0/1011	0.46	3/1368 (0.2%)
1	RB	0.19	0/1011	0.42	0/1368
1	S	0.20	0/1011	0.47	2/1368 (0.1%)
1	SB	0.19	0/1011	0.39	0/1368
1	T	0.18	0/1011	0.47	2/1368 (0.1%)
1	TB	0.18	0/1011	0.38	0/1368
2	a	0.19	0/887	0.41	0/1196
2	ab	0.20	0/887	0.46	0/1196
2	b	0.19	0/887	0.41	0/1196
2	bb	0.19	0/887	0.42	0/1196
2	c	0.19	0/887	0.41	0/1196
2	cb	0.19	0/887	0.41	0/1196
2	d	0.19	0/887	0.41	0/1196
2	db	0.19	0/887	0.43	0/1196
2	e	0.19	0/887	0.39	0/1196
2	eb	0.19	0/887	0.39	0/1196
2	f	0.21	0/887	0.47	0/1196
2	fb	0.18	0/887	0.39	0/1196
2	g	0.19	0/887	0.39	0/1196
2	gb	0.19	0/887	0.40	0/1196
2	h	0.19	0/887	0.42	0/1196
2	hb	0.19	0/887	0.42	0/1196
2	i	0.18	0/887	0.38	0/1196
2	ib	0.18	0/887	0.41	0/1196
2	j	0.20	0/887	0.41	0/1196
2	jb	0.19	0/887	0.39	0/1196
All	All	0.19	0/58180	0.44	42/78640 (0.1%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	157	LEU	N-CA-CB	5.73	118.55	110.24
1	L	157	LEU	CB-CA-C	5.71	120.01	110.88
1	E	157	LEU	N-CA-CB	5.69	118.54	110.46
1	K	157	LEU	N-CA-CB	5.66	118.50	110.46
1	Q	157	LEU	CB-CA-C	5.64	119.90	110.88
1	T	157	LEU	N-CA-CB	5.63	118.45	110.46
1	F	157	LEU	N-CA-CB	5.58	118.34	110.24
1	I	157	LEU	N-CA-CB	5.56	118.66	109.88
1	Q	157	LEU	N-CA-CB	5.53	118.62	109.88
1	D	157	LEU	N-CA-CB	5.52	118.30	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	157	LEU	CB-CA-C	5.51	119.70	110.88
1	H	157	LEU	N-CA-CB	5.50	118.22	110.24
1	P	157	LEU	CB-CA-C	5.46	120.28	111.05
1	R	157	LEU	N-CA-CB	5.45	118.14	110.24
1	O	157	LEU	N-CA-C	5.43	117.56	107.99
1	J	157	LEU	CB-CA-C	5.40	120.45	112.03
1	A	157	LEU	N-CA-CB	5.40	118.39	110.35
1	B	157	LEU	N-CA-CB	5.38	118.04	110.24
1	F	157	LEU	CB-CA-C	5.36	120.10	111.05
1	N	157	LEU	N-CA-CB	5.32	118.37	110.49
1	S	157	LEU	N-CA-C	5.31	117.34	107.99
1	B	157	LEU	N-CA-C	5.26	117.27	108.23
1	R	157	LEU	CB-CA-C	5.24	119.91	111.05
1	H	157	LEU	CB-CA-C	5.24	119.90	111.05
1	E	157	LEU	CB-CA-C	5.21	120.01	111.41
1	G	157	LEU	N-CA-CB	5.18	118.16	110.49
1	A	157	LEU	CB-CA-C	5.16	120.08	111.30
1	B	157	LEU	CB-CA-C	5.16	119.77	111.05
1	D	157	LEU	CB-CA-C	5.16	119.92	111.41
1	L	157	LEU	N-CA-CB	5.13	117.99	109.88
1	O	157	LEU	CB-CA-C	5.13	120.03	111.30
1	T	157	LEU	CB-CA-C	5.12	119.85	111.41
1	R	157	LEU	N-CA-C	5.10	117.01	108.23
1	L	157	LEU	N-CA-C	5.09	116.77	108.63
1	H	157	LEU	N-CA-C	5.08	116.97	108.23
1	C	157	LEU	N-CA-CB	5.08	118.01	110.49
1	Q	157	LEU	N-CA-C	5.08	116.76	108.63
1	C	157	LEU	N-CA-C	5.04	117.46	107.98
1	K	157	LEU	CB-CA-C	5.04	119.72	111.41
1	I	157	LEU	N-CA-C	5.03	116.68	108.63
1	S	157	LEU	CB-CA-C	5.02	119.83	111.30
1	J	157	LEU	N-CA-CB	5.00	117.33	110.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1004	0	1085	33	0
1	AB	1004	0	1085	29	0
1	B	1004	0	1085	27	0
1	BB	1004	0	1085	27	0
1	C	1004	0	1085	25	0
1	CB	1004	0	1085	20	0
1	D	1004	0	1085	36	0
1	DB	1004	0	1085	23	0
1	E	1004	0	1085	25	0
1	EB	1004	0	1085	29	0
1	F	1004	0	1085	34	0
1	FB	1004	0	1085	24	0
1	G	1004	0	1085	35	0
1	GB	1004	0	1085	34	0
1	H	1004	0	1085	35	0
1	HB	1004	0	1085	36	0
1	I	1004	0	1085	25	0
1	IB	1004	0	1085	34	0
1	J	1004	0	1085	32	0
1	JB	1004	0	1085	25	0
1	K	1004	0	1085	30	0
1	KB	1004	0	1085	23	0
1	L	1004	0	1085	36	0
1	LB	1004	0	1085	35	0
1	M	1004	0	1085	39	0
1	MB	1004	0	1085	31	0
1	N	1004	0	1085	31	0
1	NB	1004	0	1085	41	0
1	O	1004	0	1085	20	0
1	OB	1004	0	1085	26	0
1	P	1004	0	1085	30	0
1	PB	1004	0	1085	27	0
1	Q	1004	0	1085	42	0
1	QB	1004	0	1085	41	0
1	R	1004	0	1085	25	0
1	RB	1004	0	1085	36	0
1	S	1004	0	1085	27	0
1	SB	1004	0	1085	21	0
1	T	1004	0	1085	25	0
1	TB	1004	0	1085	32	0
2	a	880	0	928	25	0
2	ab	880	0	928	28	0
2	b	880	0	928	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	bb	880	0	928	30	0
2	c	880	0	928	30	0
2	cb	880	0	928	31	0
2	d	880	0	928	26	0
2	db	880	0	928	31	0
2	e	880	0	928	26	0
2	eb	880	0	928	24	0
2	f	880	0	928	45	0
2	fb	880	0	928	35	0
2	g	880	0	928	26	0
2	gb	880	0	928	20	0
2	h	880	0	928	29	0
2	hb	880	0	928	41	0
2	i	880	0	928	38	0
2	ib	880	0	928	23	0
2	j	880	0	928	28	0
2	jb	880	0	928	21	0
All	All	57760	0	61960	1649	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1649) 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:S:249:LEU:HD22	1:S:252:ILE:HD11	1.41	1.01
1:G:167:MET:HE1	1:G:181:ILE:HG23	1.42	1.01
1:S:245:LEU:HD23	1:S:247:ILE:HD11	1.44	0.97
1:J:164:ILE:HG21	1:J:262:MET:HE1	1.48	0.96
1:OB:245:LEU:HD23	1:OB:247:ILE:HD11	1.52	0.92
1:GB:232:VAL:HG23	1:GB:255:THR:HG23	1.50	0.92
2:gb:36:ILE:HD11	2:gb:44:VAL:HG21	1.51	0.91
1:A:207:VAL:HG13	1:A:211:VAL:HG23	1.55	0.88
1:B:210:MET:HA	1:B:210:MET:HE2	1.57	0.84
1:LB:167:MET:HE1	1:LB:181:ILE:HD11	1.59	0.84
1:M:262:MET:HE2	1:M:262:MET:HA	1.60	0.83
2:c:56:ALA:HA	2:c:92:LEU:HD21	1.61	0.82
1:H:210:MET:HE2	1:H:210:MET:HA	1.62	0.82
2:fb:61:ILE:O	2:fb:65:VAL:HG23	1.79	0.82
1:TB:245:LEU:HD23	1:TB:247:ILE:HD11	1.60	0.81
1:J:170:ILE:HG22	1:JB:153:LEU:HD22	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LEU:HD23	1:D:247:ILE:HD11	1.61	0.80
1:CB:245:LEU:HD23	1:CB:247:ILE:HD11	1.64	0.80
2:cb:56:ALA:HA	2:cb:92:LEU:HD21	1.63	0.80
1:SB:210:MET:HA	1:SB:210:MET:HE3	1.65	0.79
1:G:262:MET:O	1:G:266:LEU:HD22	1.83	0.78
1:Q:175:THR:HG23	1:Q:210:MET:HE1	1.62	0.78
1:J:210:MET:HA	1:J:210:MET:HE2	1.66	0.78
1:MB:160:ILE:HD12	1:MB:166:VAL:HG21	1.66	0.78
1:EB:245:LEU:HD23	1:EB:247:ILE:HD11	1.64	0.78
2:fb:103:MET:HA	2:fb:103:MET:HE3	1.66	0.78
1:T:176:GLU:O	1:T:180:LEU:HD22	1.83	0.77
1:QB:175:THR:HG22	1:QB:179:LYS:NZ	1.99	0.77
1:G:201:ILE:HD11	1:G:234:ILE:HD13	1.65	0.77
1:MB:262:MET:HE2	1:MB:262:MET:HA	1.67	0.76
1:B:232:VAL:HG23	1:B:255:THR:HG23	1.68	0.76
1:QB:167:MET:HE1	1:QB:181:ILE:HD11	1.68	0.75
2:a:1:MET:HE3	2:a:1:MET:O	1.87	0.75
2:db:61:ILE:O	2:db:65:VAL:HG23	1.85	0.75
2:ib:103:MET:HA	2:ib:103:MET:HE3	1.67	0.74
2:hb:1:MET:HE2	2:hb:1:MET:HA	1.69	0.74
2:cb:58:ILE:HD12	2:cb:58:ILE:H	1.52	0.74
1:RB:209:THR:HG23	1:RB:245:LEU:HD21	1.69	0.74
1:GB:269:THR:O	1:GB:269:THR:HG22	1.87	0.74
2:db:26:VAL:HG12	2:db:30:GLU:OE2	1.88	0.74
2:jb:33:LEU:HD11	2:jb:68:MET:CE	2.17	0.74
2:e:103:MET:HA	2:e:103:MET:HE3	1.69	0.74
1:L:167:MET:HE1	1:L:181:ILE:HD11	1.71	0.73
1:A:269:THR:O	1:A:269:THR:HG22	1.87	0.73
1:K:245:LEU:HD23	1:K:247:ILE:HD11	1.69	0.73
1:Q:258:MET:C	1:Q:258:MET:HE3	2.13	0.73
1:PB:179:LYS:HA	1:PB:179:LYS:HE3	1.71	0.72
2:e:33:LEU:HD11	2:e:68:MET:CE	2.19	0.72
2:g:1:MET:HE2	2:g:1:MET:HA	1.71	0.72
1:B:170:ILE:CG2	1:BB:153:LEU:HD22	2.19	0.72
2:fb:29:GLN:HG3	2:fb:65:VAL:HG22	1.70	0.72
1:L:170:ILE:CG2	1:LB:153:LEU:HD22	2.20	0.71
2:d:56:ALA:HA	2:d:92:LEU:CD1	2.21	0.71
2:e:6:LEU:HD21	2:eb:15:SER:OG	1.91	0.70
2:fb:36:ILE:HD11	2:fb:44:VAL:HG21	1.71	0.70
1:I:170:ILE:CG2	1:IB:153:LEU:HD22	2.22	0.70
2:cb:61:ILE:O	2:cb:65:VAL:HG23	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:db:43:GLY:HA3	2:db:112:LEU:HD21	1.73	0.70
1:PB:166:VAL:HG22	1:PB:198:LEU:HD13	1.71	0.70
2:ab:33:LEU:HD11	2:ab:68:MET:CE	2.20	0.70
2:c:33:LEU:HD11	2:c:68:MET:CE	2.21	0.69
2:gb:33:LEU:HD11	2:gb:68:MET:HE3	1.74	0.69
2:hb:33:LEU:HD11	2:hb:68:MET:CE	2.21	0.69
1:IB:269:THR:O	1:IB:269:THR:HG22	1.92	0.69
2:ib:33:LEU:HD11	2:ib:68:MET:SD	2.32	0.69
1:G:216:ILE:HD11	1:G:247:ILE:HG23	1.74	0.69
1:M:164:ILE:HG21	1:M:262:MET:HE1	1.75	0.69
1:T:201:ILE:HD11	1:T:234:ILE:HG12	1.75	0.69
2:gb:33:LEU:HD11	2:gb:68:MET:CE	2.23	0.69
2:h:16:ILE:HG21	2:h:51:ILE:HD11	1.75	0.69
1:A:245:LEU:HD12	1:A:245:LEU:O	1.93	0.69
1:JB:269:THR:HG22	1:JB:269:THR:O	1.93	0.69
2:jb:33:LEU:HD11	2:jb:68:MET:HE2	1.74	0.68
1:C:170:ILE:CG2	1:CB:153:LEU:HD22	2.23	0.68
1:E:207:VAL:HG13	1:E:211:VAL:HG23	1.73	0.68
2:cb:66:VAL:HG23	2:cb:76:VAL:HG11	1.76	0.68
1:NB:262:MET:O	1:NB:266:LEU:HD22	1.94	0.68
2:ab:61:ILE:O	2:ab:65:VAL:HG23	1.93	0.68
1:O:219:SER:HB2	1:O:252:ILE:HD12	1.75	0.68
2:gb:1:MET:HA	2:gb:1:MET:HE2	1.75	0.68
1:QB:175:THR:HG22	1:QB:179:LYS:HZ1	1.57	0.68
1:Q:193:ARG:HD2	1:Q:193:ARG:O	1.94	0.68
2:cb:54:ILE:HD12	2:cb:85:VAL:CG1	2.24	0.68
1:E:170:ILE:CG2	1:EB:153:LEU:HD22	2.24	0.68
1:NB:185:LEU:HD11	1:NB:197:VAL:HG21	1.76	0.68
2:b:51:ILE:HG21	2:b:54:ILE:HD11	1.76	0.67
1:G:237:GLU:OE1	1:G:238:ILE:HD13	1.95	0.67
1:GB:210:MET:HE2	1:GB:210:MET:HA	1.75	0.67
2:i:61:ILE:O	2:i:65:VAL:HG23	1.94	0.67
2:i:29:GLN:HG3	2:i:65:VAL:HG22	1.77	0.67
1:D:175:THR:HG22	1:D:179:LYS:HZ3	1.59	0.67
1:F:209:THR:HG22	1:F:245:LEU:HD21	1.76	0.66
1:S:249:LEU:HD22	1:S:252:ILE:CD1	2.21	0.66
2:bb:103:MET:HE3	2:bb:103:MET:HA	1.76	0.66
2:hb:45:VAL:HG13	2:hb:77:VAL:HG23	1.78	0.66
1:H:160:ILE:HD12	1:H:166:VAL:CG2	2.26	0.66
2:f:33:LEU:HD11	2:f:68:MET:CE	2.25	0.66
1:DB:269:THR:O	1:DB:269:THR:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:ILE:CG2	1:FB:153:LEU:HD22	2.26	0.66
1:F:170:ILE:HG22	1:FB:153:LEU:HD22	1.76	0.66
1:PB:230:MET:HE1	1:PB:265:ALA:HA	1.78	0.66
2:ib:29:GLN:HG3	2:ib:65:VAL:HG22	1.77	0.65
2:ab:33:LEU:HD11	2:ab:68:MET:HE1	1.78	0.65
1:I:269:THR:O	1:I:269:THR:HG22	1.96	0.65
2:c:66:VAL:HG23	2:c:76:VAL:HG11	1.78	0.65
2:hb:12:LEU:C	2:hb:13:LEU:HD12	2.21	0.65
1:IB:207:VAL:HG13	1:IB:211:VAL:HG23	1.76	0.65
2:h:33:LEU:HD11	2:h:68:MET:SD	2.35	0.65
1:E:269:THR:HG22	1:E:269:THR:O	1.96	0.65
1:G:269:THR:O	1:G:269:THR:HG22	1.96	0.65
1:MB:160:ILE:HD12	1:MB:166:VAL:CG2	2.26	0.65
2:db:56:ALA:HA	2:db:92:LEU:CD1	2.27	0.65
2:eb:66:VAL:HG13	2:eb:76:VAL:HG11	1.78	0.65
1:F:269:THR:O	1:F:269:THR:HG22	1.97	0.65
1:L:269:THR:O	1:L:269:THR:HG22	1.97	0.65
2:cb:56:ALA:HA	2:cb:92:LEU:CD2	2.26	0.65
2:f:6:LEU:HD22	2:fb:105:LEU:HD13	1.78	0.65
1:H:249:LEU:HD23	1:H:252:ILE:HD11	1.78	0.65
1:L:170:ILE:HG21	1:LB:153:LEU:HD22	1.78	0.65
1:N:201:ILE:HD11	1:N:234:ILE:HD13	1.76	0.65
1:AB:201:ILE:HD11	1:AB:234:ILE:HD13	1.79	0.64
1:T:213:HIS:O	1:T:217:GLN:NE2	2.30	0.64
2:hb:56:ALA:HA	2:hb:92:LEU:CD1	2.28	0.64
1:A:231:LEU:HD22	1:A:234:ILE:HD11	1.80	0.64
1:B:245:LEU:HD23	1:B:247:ILE:HD11	1.78	0.64
2:db:66:VAL:HG21	2:db:99:VAL:HG21	1.80	0.64
1:AB:224:LEU:HD12	1:G:243:VAL:HG13	1.79	0.64
1:HB:230:MET:HE1	1:HB:265:ALA:HA	1.79	0.64
1:S:216:ILE:HD11	1:S:247:ILE:HD13	1.80	0.64
2:b:33:LEU:HD11	2:b:68:MET:HE2	1.79	0.64
1:FB:269:THR:O	1:FB:269:THR:HG22	1.98	0.64
1:GB:160:ILE:HG22	1:GB:161:PHE:CD2	2.32	0.64
1:EB:201:ILE:HD11	1:EB:234:ILE:HD13	1.78	0.64
1:RB:269:THR:HG22	1:RB:269:THR:O	1.97	0.64
1:RB:188:GLY:O	1:RB:192:ASN:ND2	2.29	0.63
1:P:170:ILE:CG2	1:PB:153:LEU:HD22	2.28	0.63
2:d:15:SER:HB3	2:db:6:LEU:HD21	1.80	0.63
1:R:170:ILE:CG2	1:RB:153:LEU:HD22	2.28	0.63
2:f:71:LEU:O	2:f:71:LEU:HD23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JB:185:LEU:HD11	1:JB:197:VAL:HG21	1.81	0.63
1:P:173:ILE:HG21	1:P:211:VAL:HG13	1.79	0.63
1:TB:269:THR:O	1:TB:269:THR:HG22	1.97	0.63
1:M:170:ILE:CG2	1:MB:153:LEU:HD22	2.28	0.63
2:a:61:ILE:O	2:a:65:VAL:HG23	1.99	0.63
1:L:169:LEU:HD22	1:L:173:ILE:HD11	1.80	0.63
1:RB:260:LYS:HA	1:RB:260:LYS:HE3	1.81	0.63
2:f:78:VAL:HG21	2:f:96:PHE:HE2	1.63	0.63
2:f:100:LEU:HD13	2:f:111:LYS:HE2	1.81	0.63
1:D:170:ILE:HG21	1:DB:153:LEU:HD22	1.80	0.62
2:eb:62:LEU:HD21	2:eb:96:PHE:CZ	2.34	0.62
2:ib:56:ALA:HA	2:ib:92:LEU:CD1	2.29	0.62
1:B:169:LEU:HD21	1:B:181:ILE:HD13	1.81	0.62
1:D:170:ILE:CG2	1:DB:153:LEU:HD22	2.28	0.62
1:HB:201:ILE:HD11	1:HB:234:ILE:HD13	1.80	0.62
2:b:3:ILE:HD12	2:b:3:ILE:H	1.62	0.62
2:b:85:VAL:O	2:b:89:LEU:HD12	1.98	0.62
2:cb:54:ILE:HD12	2:cb:85:VAL:HG13	1.80	0.62
2:db:5:ILE:HG21	2:db:35:LYS:HG2	1.81	0.62
2:h:56:ALA:HA	2:h:92:LEU:CD2	2.28	0.62
1:KB:269:THR:O	1:KB:269:THR:HG22	2.00	0.62
1:PB:220:GLU:HB3	1:SB:243:VAL:HG21	1.81	0.62
2:e:6:LEU:HD22	2:eb:105:LEU:HD13	1.82	0.62
2:a:26:VAL:HG12	2:a:30:GLU:OE2	1.99	0.62
1:GB:169:LEU:O	1:GB:170:ILE:HD13	1.99	0.62
2:f:78:VAL:HG21	2:f:96:PHE:CE2	2.35	0.62
1:H:218:ALA:O	1:H:222:VAL:HG12	1.99	0.62
1:LB:262:MET:HE2	1:LB:262:MET:HA	1.81	0.62
2:b:56:ALA:HA	2:b:92:LEU:HD11	1.82	0.62
2:g:4:PRO:C	2:g:5:ILE:HD12	2.24	0.62
1:G:170:ILE:CG2	1:GB:153:LEU:HD22	2.29	0.62
1:J:153:LEU:HD13	1:JB:170:ILE:HG22	1.81	0.62
1:RB:222:VAL:HG22	1:RB:227:CYS:HB3	1.82	0.62
2:db:29:GLN:CD	2:db:65:VAL:HG22	2.25	0.62
1:N:170:ILE:CG2	1:NB:153:LEU:HD22	2.30	0.62
1:R:196:VAL:HG11	1:R:265:ALA:HB1	1.82	0.62
2:c:56:ALA:HA	2:c:92:LEU:CD2	2.27	0.62
2:b:59:ALA:HB1	2:b:94:ILE:HD12	1.80	0.61
1:IB:245:LEU:HD23	1:IB:247:ILE:HD11	1.81	0.61
1:O:245:LEU:HD23	1:O:247:ILE:HD11	1.82	0.61
2:b:100:LEU:H	2:b:100:LEU:HD12	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:170:ILE:HG22	1:RB:153:LEU:HD22	1.82	0.61
2:i:66:VAL:HG23	2:i:76:VAL:HG11	1.82	0.61
1:OB:231:LEU:HB2	1:OB:252:ILE:HD11	1.82	0.61
1:Q:268:LEU:HD23	1:Q:268:LEU:O	2.00	0.61
1:R:196:VAL:HG11	1:R:265:ALA:CB	2.30	0.61
2:cb:77:VAL:CG2	2:cb:112:LEU:HD13	2.30	0.61
1:N:158:LEU:HD21	1:NB:168:PRO:HB3	1.82	0.61
2:f:36:ILE:HD11	2:f:44:VAL:HG22	1.81	0.61
1:D:243:VAL:HG21	1:R:220:GLU:HB3	1.82	0.61
1:G:170:ILE:HG21	1:GB:153:LEU:HD22	1.81	0.61
1:L:196:VAL:HG11	1:L:265:ALA:CB	2.31	0.61
1:E:218:ALA:O	1:E:222:VAL:HG13	2.01	0.61
1:A:166:VAL:HG22	1:A:198:LEU:HD13	1.83	0.60
1:Q:153:LEU:HD13	1:QB:170:ILE:HG22	1.82	0.60
2:cb:36:ILE:HD11	2:cb:44:VAL:HG21	1.83	0.60
1:S:185:LEU:HD11	1:S:197:VAL:HG21	1.82	0.60
2:hb:77:VAL:HG12	2:hb:100:LEU:HB2	1.83	0.60
1:E:210:MET:HE3	1:E:210:MET:HA	1.82	0.60
1:R:201:ILE:HD11	1:R:234:ILE:HD13	1.84	0.60
1:H:160:ILE:HD12	1:H:166:VAL:HG21	1.83	0.60
2:d:66:VAL:HG21	2:d:99:VAL:HG21	1.82	0.60
1:H:170:ILE:HG12	1:HB:153:LEU:HD22	1.84	0.60
1:HB:169:LEU:HD12	1:HB:201:ILE:HG22	1.83	0.60
1:LB:201:ILE:HD11	1:LB:234:ILE:HD13	1.84	0.60
1:SB:231:LEU:HB2	1:SB:252:ILE:HD11	1.84	0.60
2:fb:100:LEU:H	2:fb:100:LEU:HD12	1.67	0.60
1:K:170:ILE:CG2	1:KB:153:LEU:HD22	2.31	0.59
1:OB:185:LEU:HD11	1:OB:197:VAL:HG21	1.84	0.59
1:P:269:THR:HG22	1:P:269:THR:O	2.02	0.59
2:h:16:ILE:CG2	2:h:51:ILE:HD11	2.32	0.59
2:h:56:ALA:HA	2:h:92:LEU:HD21	1.84	0.59
1:QB:196:VAL:HG13	1:QB:230:MET:HE3	1.85	0.59
2:cb:33:LEU:HD11	2:cb:68:MET:CE	2.32	0.59
2:a:5:ILE:HD13	2:a:14:ILE:HD11	1.84	0.59
2:h:78:VAL:HG21	2:h:96:PHE:CE1	2.37	0.59
2:i:54:ILE:HG21	2:i:85:VAL:HG13	1.85	0.59
1:M:231:LEU:HB2	1:M:252:ILE:HD11	1.83	0.59
1:O:251:GLN:CD	1:O:251:GLN:H	2.11	0.59
1:PB:240:GLN:HA	2:g:68:MET:HE3	1.84	0.59
2:i:71:LEU:HD23	2:i:71:LEU:O	2.03	0.59
1:I:218:ALA:O	1:I:222:VAL:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:167:MET:CE	1:LB:181:ILE:HD11	2.31	0.59
1:S:231:LEU:HD22	1:S:234:ILE:HD11	1.83	0.59
2:fb:78:VAL:HG21	2:fb:96:PHE:CE1	2.37	0.59
1:TB:196:VAL:HG11	1:TB:265:ALA:HB1	1.83	0.59
2:jb:1:MET:HA	2:jb:1:MET:HE2	1.84	0.59
1:QB:256:ASN:OD1	1:QB:257:THR:HG23	2.02	0.59
2:db:4:PRO:C	2:db:5:ILE:HD12	2.28	0.59
2:f:36:ILE:HD11	2:f:44:VAL:CG2	2.33	0.59
2:f:77:VAL:HG21	2:f:112:LEU:HD13	1.83	0.59
2:jb:59:ALA:HB1	2:jb:94:ILE:HD12	1.83	0.59
1:L:225:VAL:O	1:L:225:VAL:HG12	2.02	0.58
1:TB:207:VAL:HB	1:TB:238:ILE:HG23	1.85	0.58
2:bb:66:VAL:HG23	2:bb:76:VAL:HG11	1.83	0.58
1:QB:196:VAL:HG11	1:QB:265:ALA:HB1	1.85	0.58
2:i:36:ILE:HD12	2:i:44:VAL:HG21	1.86	0.58
2:i:77:VAL:CG2	2:i:112:LEU:HD13	2.32	0.58
1:CB:212:ALA:HB1	1:CB:242:ILE:HD13	1.85	0.58
1:N:218:ALA:O	1:N:222:VAL:HG12	2.02	0.58
2:d:56:ALA:HA	2:d:92:LEU:HD11	1.85	0.58
2:ab:71:LEU:O	2:ab:71:LEU:HD23	2.02	0.58
1:C:269:THR:HG22	1:C:269:THR:O	2.03	0.58
2:b:71:LEU:HD23	2:b:71:LEU:O	2.04	0.58
2:f:77:VAL:CG2	2:f:112:LEU:HD13	2.33	0.58
2:gb:26:VAL:HG12	2:gb:30:GLU:OE2	2.03	0.58
1:B:169:LEU:HD21	1:B:181:ILE:CD1	2.33	0.58
1:C:253:ILE:H	1:C:253:ILE:HD12	1.68	0.58
1:GB:218:ALA:O	1:GB:222:VAL:HG13	2.03	0.58
1:L:201:ILE:O	1:L:204:VAL:HG12	2.04	0.58
2:i:12:LEU:HD13	2:i:41:ALA:HB2	1.84	0.58
1:NB:162:GLU:O	1:NB:164:ILE:HD12	2.04	0.58
1:B:236:PRO:HG3	1:F:190:VAL:HG21	1.86	0.58
1:K:175:THR:HG22	1:K:179:LYS:NZ	2.18	0.58
1:RB:207:VAL:HG13	1:RB:211:VAL:HG23	1.85	0.58
1:T:269:THR:O	1:T:269:THR:HG22	2.03	0.58
2:db:103:MET:O	2:db:103:MET:HE3	2.04	0.58
2:e:105:LEU:HD23	2:e:105:LEU:C	2.29	0.58
2:b:32:LEU:O	2:b:36:ILE:HG13	2.03	0.58
2:h:6:LEU:HD22	2:hb:105:LEU:HD13	1.86	0.58
1:J:170:ILE:CG2	1:JB:153:LEU:HD22	2.32	0.57
2:ab:78:VAL:HG21	2:ab:96:PHE:CE1	2.39	0.57
1:E:170:ILE:HG22	1:EB:153:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:196:VAL:HG11	1:T:265:ALA:CB	2.35	0.57
1:L:247:ILE:HG22	1:L:249:LEU:CD2	2.34	0.57
1:A:167:MET:HE1	1:A:169:LEU:HD21	1.86	0.57
1:K:196:VAL:HG11	1:K:265:ALA:CB	2.35	0.57
1:K:245:LEU:CD2	1:K:247:ILE:HD11	2.34	0.57
1:OB:249:LEU:HD12	1:QB:224:LEU:CD2	2.35	0.57
2:ab:33:LEU:HD11	2:ab:68:MET:HE3	1.87	0.57
1:EB:269:THR:C	1:EB:270:ASN:OD1	2.48	0.57
1:F:218:ALA:O	1:F:222:VAL:HG12	2.05	0.57
1:MB:216:ILE:HD11	1:MB:247:ILE:CG2	2.34	0.57
2:eb:62:LEU:HD21	2:eb:96:PHE:HZ	1.68	0.57
1:HB:231:LEU:HD21	1:HB:234:ILE:HD11	1.86	0.57
1:QB:262:MET:HE2	1:QB:262:MET:HA	1.87	0.57
2:cb:109:LEU:O	2:cb:109:LEU:HD23	2.05	0.57
1:M:259:LYS:HA	1:M:259:LYS:HE2	1.85	0.57
1:DB:167:MET:HE1	1:DB:181:ILE:HG23	1.86	0.56
1:E:270:ASN:OD1	1:E:270:ASN:O	2.22	0.56
1:I:236:PRO:HG3	1:TB:190:VAL:HG21	1.87	0.56
1:O:210:MET:HA	1:O:210:MET:HE3	1.86	0.56
2:g:48:ILE:HD11	2:g:81:ILE:HG12	1.86	0.56
1:AB:224:LEU:O	1:G:254:THR:HG21	2.05	0.56
2:ab:29:GLN:HG3	2:ab:65:VAL:HG22	1.88	0.56
1:EB:185:LEU:HD11	1:EB:197:VAL:HG21	1.87	0.56
2:b:66:VAL:CG1	2:b:99:VAL:HG21	2.35	0.56
2:c:77:VAL:HG22	2:c:100:LEU:HB2	1.86	0.56
1:F:262:MET:HA	1:F:262:MET:HE2	1.87	0.56
2:hb:66:VAL:HG21	2:hb:99:VAL:HG21	1.87	0.56
1:C:219:SER:HB2	1:C:252:ILE:HD12	1.87	0.56
1:HB:218:ALA:O	1:HB:222:VAL:HG13	2.06	0.56
1:JB:245:LEU:HG	1:JB:247:ILE:HD11	1.88	0.56
2:cb:78:VAL:HG21	2:cb:96:PHE:CE1	2.41	0.56
2:hb:23:HIS:O	2:hb:27:GLU:HG3	2.05	0.56
2:ab:60:LYS:O	2:ab:64:ASP:OD1	2.24	0.56
1:K:216:ILE:HD11	1:K:247:ILE:HD13	1.87	0.56
1:RB:231:LEU:HB3	1:RB:252:ILE:HD11	1.85	0.56
2:eb:36:ILE:HD11	2:eb:44:VAL:HG21	1.87	0.56
2:f:105:LEU:HD13	2:fb:6:LEU:HD22	1.87	0.56
1:D:245:LEU:CD2	1:D:247:ILE:HD11	2.35	0.56
2:hb:33:LEU:HD22	2:hb:72:MET:HE1	1.87	0.56
1:L:169:LEU:HD21	1:L:181:ILE:HD12	1.87	0.56
1:SB:245:LEU:HD23	1:SB:247:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RB:218:ALA:O	1:RB:222:VAL:HG12	2.06	0.55
2:fb:47:ASP:HB2	2:fb:105:LEU:HD12	1.87	0.55
2:a:94:ILE:H	2:a:94:ILE:HD12	1.72	0.55
1:N:173:ILE:HG21	1:N:211:VAL:HG13	1.88	0.55
2:hb:81:ILE:H	2:hb:81:ILE:HD12	1.71	0.55
1:E:185:LEU:HD11	1:E:197:VAL:HG21	1.87	0.55
1:R:270:ASN:O	1:R:270:ASN:OD1	2.24	0.55
2:c:12:LEU:C	2:c:13:LEU:HD12	2.30	0.55
1:C:201:ILE:HD11	1:C:234:ILE:HG12	1.88	0.55
2:ib:60:LYS:HE2	2:ib:60:LYS:HA	1.89	0.55
2:jb:77:VAL:HG12	2:jb:100:LEU:HB2	1.87	0.55
1:AB:200:ASP:OD1	1:AB:258:MET:HE2	2.07	0.55
1:AB:201:ILE:HD11	1:AB:234:ILE:CD1	2.36	0.55
1:G:269:THR:O	1:G:269:THR:CG2	2.54	0.55
1:H:160:ILE:HA	1:HB:258:MET:HE2	1.88	0.55
1:KB:269:THR:HG21	1:KB:271:ARG:NH2	2.22	0.55
1:N:170:ILE:HG21	1:NB:153:LEU:HD22	1.88	0.55
1:OB:236:PRO:HG3	1:QB:190:VAL:HG21	1.88	0.55
2:hb:71:LEU:HD23	2:hb:71:LEU:O	2.06	0.55
2:j:1:MET:O	2:j:1:MET:HE3	2.07	0.55
1:HB:258:MET:HE3	1:HB:258:MET:C	2.31	0.55
1:J:169:LEU:HD23	1:J:169:LEU:C	2.31	0.55
1:PB:224:LEU:CD2	1:SB:249:LEU:HD12	2.37	0.55
1:R:269:THR:O	1:R:269:THR:HG22	2.06	0.55
2:fb:55:ASP:OD1	2:fb:56:ALA:N	2.39	0.55
2:j:77:VAL:HG22	2:j:100:LEU:HB2	1.89	0.55
1:IB:185:LEU:HD11	1:IB:197:VAL:HG21	1.89	0.55
1:IB:218:ALA:O	1:IB:222:VAL:HG13	2.06	0.55
2:c:78:VAL:HG21	2:c:96:PHE:CE2	2.42	0.55
2:cb:52:ASP:C	2:cb:52:ASP:OD2	2.49	0.55
2:g:56:ALA:HA	2:g:92:LEU:CD2	2.37	0.55
2:h:78:VAL:HG21	2:h:96:PHE:HE1	1.70	0.55
2:jb:56:ALA:HA	2:jb:92:LEU:CD1	2.37	0.55
1:K:185:LEU:HD11	1:K:197:VAL:HG21	1.88	0.55
1:MB:230:MET:HE1	1:MB:265:ALA:CA	2.36	0.55
1:T:185:LEU:HD11	1:T:197:VAL:HG21	1.87	0.55
2:i:56:ALA:HA	2:i:92:LEU:CD1	2.37	0.55
1:EB:243:VAL:HG21	1:RB:220:GLU:HB2	1.88	0.55
1:C:161:PHE:CZ	1:CB:273:ILE:HD11	2.41	0.54
1:F:185:LEU:HD11	1:F:197:VAL:HG21	1.89	0.54
1:FB:262:MET:HE2	1:FB:262:MET:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:LYS:O	1:G:151:GLN:NE2	2.27	0.54
2:d:4:PRO:O	2:d:5:ILE:HD13	2.06	0.54
2:eb:26:VAL:HG12	2:eb:30:GLU:OE1	2.08	0.54
2:hb:4:PRO:C	2:hb:5:ILE:HD12	2.32	0.54
2:hb:94:ILE:H	2:hb:94:ILE:HD12	1.71	0.54
1:N:245:LEU:HD23	1:N:247:ILE:HD11	1.88	0.54
1:P:230:MET:HE1	1:P:261:GLY:O	2.07	0.54
1:CB:249:LEU:HD12	2:cb:71:LEU:CD1	2.37	0.54
1:F:237:GLU:C	1:F:237:GLU:OE1	2.49	0.54
1:LB:207:VAL:HG13	1:LB:211:VAL:HG23	1.89	0.54
1:M:175:THR:HG23	1:M:210:MET:SD	2.47	0.54
2:db:19:GLU:OE1	2:db:19:GLU:N	2.40	0.54
2:db:71:LEU:O	2:db:71:LEU:HD23	2.08	0.54
1:JB:245:LEU:HD12	1:JB:245:LEU:O	2.07	0.54
1:OB:216:ILE:HD11	1:OB:247:ILE:HD13	1.88	0.54
1:OB:210:MET:HA	1:OB:210:MET:HE2	1.89	0.54
1:PB:190:VAL:HG21	1:SB:236:PRO:HG3	1.89	0.54
2:gb:105:LEU:HD23	2:gb:105:LEU:C	2.33	0.54
1:K:153:LEU:HD22	1:KB:170:ILE:CG2	2.38	0.54
2:eb:55:ASP:C	2:eb:55:ASP:OD1	2.51	0.54
1:A:269:THR:O	1:A:269:THR:CG2	2.56	0.54
1:HB:207:VAL:HB	1:HB:238:ILE:HG23	1.89	0.54
1:D:269:THR:O	1:D:269:THR:HG22	2.07	0.54
1:GB:160:ILE:HG22	1:GB:161:PHE:CE2	2.43	0.54
2:gb:64:ASP:O	2:gb:68:MET:HG3	2.08	0.54
2:i:54:ILE:CG2	2:i:85:VAL:HG13	2.37	0.54
1:A:245:LEU:HD23	1:A:247:ILE:HD11	1.89	0.54
1:F:176:GLU:O	1:F:180:LEU:HD22	2.08	0.54
2:db:56:ALA:HA	2:db:92:LEU:HD11	1.89	0.54
2:jb:56:ALA:HA	2:jb:92:LEU:HD11	1.90	0.54
1:M:254:THR:HG21	2:e:71:LEU:O	2.08	0.53
1:P:269:THR:O	1:P:269:THR:CG2	2.56	0.53
2:hb:10:GLU:OE1	2:hb:10:GLU:N	2.41	0.53
1:CB:216:ILE:HD11	1:CB:247:ILE:HD13	1.90	0.53
1:H:268:LEU:C	1:H:268:LEU:HD23	2.33	0.53
1:K:170:ILE:HG22	1:KB:153:LEU:HD22	1.89	0.53
1:JB:207:VAL:HG13	1:JB:211:VAL:HG23	1.90	0.53
1:Q:170:ILE:HG12	1:QB:153:LEU:HD22	1.90	0.53
1:Q:222:VAL:HG22	1:Q:227:CYS:HB3	1.90	0.53
1:SB:185:LEU:HD11	1:SB:197:VAL:HG21	1.90	0.53
2:db:21:ASP:OD2	2:db:24:THR:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:db:66:VAL:CG2	2:db:99:VAL:HG21	2.38	0.53
1:LB:235:ARG:HG3	1:LB:238:ILE:HG12	1.90	0.53
1:NB:230:MET:HE1	1:NB:265:ALA:HA	1.89	0.53
1:RB:231:LEU:CB	1:RB:252:ILE:HD11	2.38	0.53
2:b:38:GLU:OE1	2:b:39:THR:HG23	2.09	0.53
2:eb:105:LEU:C	2:eb:105:LEU:HD23	2.33	0.53
1:TB:189:VAL:HG23	1:TB:194:SER:OG	2.08	0.53
2:eb:29:GLN:HE21	2:eb:68:MET:HE1	1.72	0.53
2:jb:64:ASP:O	2:jb:68:MET:HG3	2.08	0.53
2:jb:66:VAL:HG21	2:jb:99:VAL:HG21	1.91	0.53
1:LB:263:GLU:HA	1:LB:263:GLU:OE2	2.08	0.53
1:E:210:MET:HE2	1:E:214:HIS:CE1	2.43	0.53
1:P:170:ILE:HG22	1:PB:153:LEU:HD22	1.89	0.53
2:g:56:ALA:HA	2:g:92:LEU:HD23	1.90	0.53
1:EB:245:LEU:HD23	1:EB:247:ILE:CD1	2.37	0.53
1:GB:193:ARG:HG3	1:GB:193:ARG:O	2.08	0.53
1:L:196:VAL:HG11	1:L:265:ALA:HB1	1.91	0.53
2:fb:5:ILE:CG2	2:fb:12:LEU:HD12	2.39	0.53
1:F:179:LYS:HE2	1:F:179:LYS:HA	1.90	0.53
1:M:245:LEU:HD23	1:M:247:ILE:HD11	1.90	0.53
1:P:220:GLU:HA	1:P:220:GLU:OE1	2.09	0.53
2:d:21:ASP:OD2	2:d:21:ASP:C	2.52	0.53
2:ab:21:ASP:C	2:ab:21:ASP:OD2	2.52	0.53
1:G:192:ASN:C	1:G:193:ARG:HE	2.17	0.53
1:P:167:MET:HE3	1:P:181:ILE:HD12	1.91	0.53
1:P:201:ILE:HG12	1:P:231:LEU:HD11	1.91	0.53
1:S:245:LEU:HD23	1:S:247:ILE:CD1	2.29	0.53
1:SB:219:SER:HB2	1:SB:252:ILE:HD12	1.91	0.53
2:jb:36:ILE:HD11	2:jb:44:VAL:CG2	2.39	0.53
1:HB:158:LEU:HD12	1:HB:158:LEU:N	2.24	0.52
1:JB:207:VAL:HB	1:JB:238:ILE:HG23	1.91	0.52
2:eb:55:ASP:OD1	2:eb:58:ILE:HD12	2.09	0.52
1:CB:249:LEU:HD12	2:cb:71:LEU:HD11	1.89	0.52
1:O:222:VAL:HG21	1:O:229:ALA:HB2	1.90	0.52
1:H:169:LEU:HD22	1:H:173:ILE:HD11	1.91	0.52
1:NB:237:GLU:OE2	1:NB:238:ILE:HD13	2.08	0.52
1:QB:196:VAL:HG11	1:QB:265:ALA:CB	2.39	0.52
1:QB:220:GLU:OE1	1:QB:220:GLU:HA	2.10	0.52
2:e:66:VAL:HG21	2:e:99:VAL:HG21	1.91	0.52
1:A:196:VAL:HG11	1:A:265:ALA:HB1	1.91	0.52
1:BB:237:GLU:C	1:BB:237:GLU:OE1	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:LEU:HD23	1:I:231:LEU:C	2.33	0.52
1:B:179:LYS:HA	1:B:179:LYS:HE2	1.91	0.52
1:HB:166:VAL:HG22	1:HB:198:LEU:HD12	1.91	0.52
1:HB:231:LEU:HB2	1:HB:252:ILE:HD11	1.92	0.52
1:I:200:ASP:OD2	1:I:258:MET:HE2	2.09	0.52
1:IB:178:ALA:O	1:IB:182:ILE:HG13	2.09	0.52
1:LB:185:LEU:HD11	1:LB:197:VAL:HG21	1.91	0.52
2:bb:55:ASP:OD2	2:bb:56:ALA:N	2.42	0.52
2:bb:59:ALA:HB1	2:bb:94:ILE:HD13	1.92	0.52
2:f:16:ILE:HG21	2:f:20:LEU:HD21	1.92	0.52
1:I:256:ASN:C	1:I:256:ASN:OD1	2.53	0.52
1:MB:230:MET:HE1	1:MB:265:ALA:HA	1.91	0.52
1:O:200:ASP:OD1	1:O:200:ASP:C	2.53	0.52
1:E:170:ILE:HG21	1:EB:153:LEU:HD22	1.90	0.52
1:E:201:ILE:O	1:E:204:VAL:HG12	2.09	0.52
1:E:257:THR:HG23	1:E:260:LYS:HG2	1.90	0.52
1:EB:231:LEU:CB	1:EB:252:ILE:HD11	2.39	0.52
1:J:236:PRO:HB3	1:N:186:LEU:HB3	1.91	0.52
1:Q:169:LEU:HD12	1:Q:201:ILE:HG22	1.91	0.52
2:f:51:ILE:HG21	2:f:54:ILE:HD11	1.91	0.52
2:i:6:LEU:N	2:i:6:LEU:HD12	2.25	0.52
1:B:237:GLU:OE2	1:B:238:ILE:HD13	2.10	0.52
1:B:269:THR:O	1:B:269:THR:HG22	2.08	0.52
1:FB:210:MET:O	1:FB:210:MET:HE3	2.09	0.52
1:IB:158:LEU:N	1:IB:158:LEU:HD12	2.23	0.52
1:IB:186:LEU:O	1:IB:190:VAL:HG23	2.09	0.52
1:PB:165:SER:O	1:PB:198:LEU:HD12	2.10	0.52
2:hb:36:ILE:HD11	2:hb:74:ALA:CB	2.40	0.52
1:AB:269:THR:O	1:AB:269:THR:HG22	2.08	0.52
1:D:262:MET:HE2	1:D:262:MET:HA	1.91	0.52
1:LB:158:LEU:N	1:LB:158:LEU:HD12	2.24	0.52
1:M:196:VAL:HG21	1:M:265:ALA:HB1	1.90	0.52
2:b:16:ILE:HG21	2:b:51:ILE:HD11	1.92	0.52
1:B:195:GLU:OE2	1:B:195:GLU:N	2.43	0.51
1:M:196:VAL:HG21	1:M:265:ALA:CB	2.40	0.51
1:Q:196:VAL:HG11	1:Q:265:ALA:HB1	1.92	0.51
1:TB:186:LEU:O	1:TB:189:VAL:HG12	2.10	0.51
2:i:64:ASP:O	2:i:68:MET:HG3	2.10	0.51
1:E:221:ALA:HA	2:cb:90:ILE:HD11	1.91	0.51
1:GB:237:GLU:OE2	1:GB:237:GLU:C	2.53	0.51
1:NB:200:ASP:C	1:NB:200:ASP:OD2	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ab:115:GLU:OE1	2:ab:116:LEU:HD12	2.10	0.51
1:G:185:LEU:HD11	1:G:197:VAL:HG21	1.91	0.51
1:Q:198:LEU:N	1:Q:198:LEU:HD12	2.25	0.51
1:T:216:ILE:HG23	1:T:217:GLN:NE2	2.26	0.51
1:TB:237:GLU:N	1:TB:237:GLU:OE2	2.44	0.51
2:f:88:THR:O	2:f:92:LEU:HD22	2.10	0.51
2:hb:112:LEU:HD23	2:hb:116:LEU:HD13	1.92	0.51
2:a:64:ASP:O	2:a:68:MET:HG3	2.10	0.51
1:J:216:ILE:HD11	1:J:247:ILE:HD13	1.92	0.51
1:PB:255:THR:HG22	1:PB:264:ARG:NH1	2.24	0.51
1:Q:160:ILE:HD11	1:Q:166:VAL:HB	1.91	0.51
1:T:269:THR:O	1:T:269:THR:CG2	2.58	0.51
2:b:66:VAL:HG11	2:b:99:VAL:HG21	1.91	0.51
2:eb:47:ASP:C	2:eb:47:ASP:OD2	2.54	0.51
2:f:57:PHE:HE1	2:f:61:ILE:HD11	1.73	0.51
2:h:109:LEU:HD23	2:hb:8:LEU:HD11	1.91	0.51
2:ab:66:VAL:HG23	2:ab:76:VAL:HG11	1.91	0.51
1:D:269:THR:O	1:D:269:THR:CG2	2.59	0.51
1:K:160:ILE:HG21	1:KB:160:ILE:HD12	1.92	0.51
1:KB:237:GLU:OE1	1:KB:237:GLU:C	2.54	0.51
1:TB:245:LEU:HD23	1:TB:247:ILE:CD1	2.37	0.51
2:bb:103:MET:HE3	2:bb:103:MET:CA	2.40	0.51
1:B:170:ILE:HG22	1:BB:153:LEU:HD22	1.93	0.51
1:FB:238:ILE:O	1:FB:242:ILE:HG12	2.10	0.51
1:PB:218:ALA:O	1:PB:222:VAL:HG22	2.11	0.51
1:AB:204:VAL:HG11	1:AB:207:VAL:HG23	1.93	0.51
1:AB:212:ALA:O	1:AB:216:ILE:HD12	2.11	0.51
1:E:153:LEU:HD22	1:EB:170:ILE:HG22	1.91	0.51
2:b:78:VAL:HG21	2:b:96:PHE:CE1	2.46	0.51
1:BB:185:LEU:HD11	1:BB:197:VAL:HG21	1.93	0.51
1:EB:200:ASP:C	1:EB:200:ASP:OD1	2.53	0.51
1:K:247:ILE:HG22	1:K:249:LEU:HD12	1.92	0.51
1:KB:222:VAL:HG11	1:KB:229:ALA:HB2	1.92	0.51
2:f:53:PHE:O	2:f:54:ILE:HD13	2.10	0.51
2:fb:3:ILE:HD12	2:fb:28:PHE:HB2	1.93	0.51
2:hb:109:LEU:HD23	2:hb:109:LEU:C	2.36	0.51
1:A:170:ILE:HG12	1:AB:153:LEU:HD22	1.92	0.51
1:B:200:ASP:OD2	1:B:200:ASP:C	2.54	0.51
1:FB:167:MET:HE2	1:FB:181:ILE:HD12	1.93	0.51
1:L:269:THR:O	1:L:269:THR:CG2	2.58	0.51
1:N:237:GLU:OE1	1:N:237:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PB:230:MET:HE1	1:PB:265:ALA:CA	2.41	0.51
1:Q:200:ASP:C	1:Q:200:ASP:OD1	2.54	0.51
1:T:170:ILE:HG12	1:TB:153:LEU:HD22	1.93	0.51
2:bb:104:ASP:OD2	2:bb:104:ASP:C	2.54	0.51
2:g:104:ASP:C	2:g:104:ASP:OD1	2.53	0.51
2:ib:77:VAL:CG2	2:ib:112:LEU:HD13	2.40	0.51
2:j:47:ASP:OD2	2:j:47:ASP:C	2.54	0.51
1:EB:231:LEU:HB3	1:EB:252:ILE:HD11	1.93	0.51
1:H:231:LEU:CD2	1:H:234:ILE:HD11	2.41	0.51
1:R:270:ASN:O	1:RB:276:LYS:HB3	2.10	0.51
2:bb:36:ILE:HD11	2:bb:41:ALA:O	2.09	0.51
2:g:106:GLU:C	2:g:106:GLU:OE1	2.54	0.51
2:h:15:SER:HB3	2:hb:6:LEU:HD21	1.93	0.51
2:i:12:LEU:HD13	2:i:41:ALA:CB	2.40	0.51
2:a:54:ILE:O	2:a:88:THR:HG21	2.11	0.50
2:ab:19:GLU:N	2:ab:19:GLU:OE2	2.44	0.50
1:E:220:GLU:OE1	1:E:220:GLU:HA	2.11	0.50
1:HB:185:LEU:HD11	1:HB:197:VAL:HG21	1.93	0.50
1:NB:231:LEU:HD23	1:NB:231:LEU:C	2.36	0.50
1:RB:157:LEU:HD11	1:RB:165:SER:HB3	1.92	0.50
2:e:33:LEU:HD11	2:e:68:MET:HE1	1.92	0.50
2:e:103:MET:HE3	2:e:103:MET:CA	2.40	0.50
2:ib:13:LEU:HD11	2:ib:105:LEU:HD21	1.93	0.50
1:F:220:GLU:OE2	1:F:220:GLU:HA	2.11	0.50
1:FB:237:GLU:OE2	1:FB:237:GLU:C	2.55	0.50
1:G:160:ILE:HG22	1:G:161:PHE:CE2	2.46	0.50
1:MB:168:PRO:C	1:MB:169:LEU:HD12	2.37	0.50
1:NB:231:LEU:HD22	1:NB:234:ILE:HD11	1.92	0.50
1:O:237:GLU:C	1:O:237:GLU:OE1	2.53	0.50
1:R:160:ILE:HD12	1:R:166:VAL:CG2	2.42	0.50
2:h:60:LYS:O	2:h:64:ASP:OD1	2.29	0.50
1:DB:217:GLN:OE1	1:DB:217:GLN:HA	2.11	0.50
1:I:245:LEU:HD23	1:I:247:ILE:HD11	1.93	0.50
1:J:238:ILE:O	1:J:242:ILE:HG12	2.11	0.50
1:NB:166:VAL:HG12	1:NB:198:LEU:HD13	1.93	0.50
1:T:200:ASP:C	1:T:200:ASP:OD2	2.54	0.50
1:AB:269:THR:O	1:AB:269:THR:CG2	2.59	0.50
1:C:210:MET:HE2	1:C:214:HIS:CE1	2.47	0.50
1:IB:175:THR:HG23	1:IB:176:GLU:N	2.26	0.50
1:IB:217:GLN:OE1	1:IB:217:GLN:HA	2.12	0.50
1:M:200:ASP:C	1:M:200:ASP:OD1	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RB:200:ASP:OD2	1:RB:200:ASP:C	2.55	0.50
2:c:29:GLN:HE21	2:c:68:MET:HE1	1.75	0.50
2:d:47:ASP:C	2:d:47:ASP:OD1	2.54	0.50
2:i:48:ILE:HD11	2:i:81:ILE:CD1	2.41	0.50
1:B:269:THR:O	1:B:269:THR:CG2	2.59	0.50
1:I:170:ILE:HG22	1:IB:153:LEU:HD22	1.92	0.50
1:IB:245:LEU:CD2	1:IB:247:ILE:HD11	2.42	0.50
1:MB:218:ALA:O	1:MB:222:VAL:HG13	2.12	0.50
2:ib:16:ILE:CG2	2:ib:20:LEU:HD21	2.41	0.50
1:F:160:ILE:HD12	1:F:166:VAL:CG1	2.41	0.50
1:H:180:LEU:O	1:H:181:ILE:C	2.55	0.50
1:HB:157:LEU:HD22	1:HB:188:GLY:HA3	1.94	0.50
1:LB:220:GLU:HA	1:LB:220:GLU:OE2	2.11	0.50
1:OB:195:GLU:OE1	1:OB:195:GLU:N	2.44	0.50
1:P:216:ILE:HD11	1:P:247:ILE:HG21	1.94	0.50
1:PB:262:MET:HE2	1:PB:262:MET:HA	1.94	0.50
1:S:207:VAL:HB	1:S:238:ILE:HG23	1.92	0.50
2:d:5:ILE:HD12	2:d:14:ILE:HD11	1.93	0.50
2:d:110:GLU:C	2:d:110:GLU:OE1	2.55	0.50
2:e:16:ILE:HD12	2:e:48:ILE:HG22	1.94	0.50
2:f:66:VAL:HG21	2:f:99:VAL:HG21	1.92	0.50
1:D:247:ILE:HG22	1:D:249:LEU:HD22	1.93	0.50
1:J:201:ILE:HD11	1:J:234:ILE:CD1	2.41	0.50
1:J:269:THR:O	1:J:269:THR:HG22	2.11	0.50
1:PB:205:PRO:HA	1:PB:235:ARG:HH12	1.77	0.50
2:hb:5:ILE:HG21	2:hb:35:LYS:HG2	1.93	0.50
1:A:196:VAL:HG11	1:A:265:ALA:CB	2.42	0.50
2:ab:68:MET:SD	1:H:240:GLN:HA	2.52	0.50
2:ab:115:GLU:OE1	2:ab:115:GLU:C	2.55	0.50
1:J:201:ILE:HD11	1:J:234:ILE:HD13	1.94	0.50
1:JB:248:GLU:N	1:JB:248:GLU:OE2	2.44	0.50
1:S:210:MET:HE2	1:S:210:MET:N	2.26	0.50
2:bb:45:VAL:HG13	2:bb:77:VAL:HG23	1.94	0.50
2:d:71:LEU:HD23	2:d:71:LEU:O	2.12	0.50
2:j:3:ILE:O	2:j:5:ILE:HD12	2.11	0.50
1:FB:157:LEU:N	1:FB:157:LEU:HD12	2.27	0.50
1:K:196:VAL:HG11	1:K:265:ALA:HB1	1.94	0.50
1:L:185:LEU:HD11	1:L:197:VAL:HG21	1.93	0.50
1:MB:175:THR:HG23	1:MB:210:MET:HE1	1.94	0.50
1:N:170:ILE:HG22	1:NB:153:LEU:HD13	1.94	0.50
1:O:153:LEU:HD13	1:OB:170:ILE:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:256:ASN:OD1	1:O:257:THR:HG23	2.12	0.50
2:b:42:ARG:NH2	2:b:116:LEU:HD22	2.26	0.50
2:h:66:VAL:HG23	2:h:76:VAL:HG11	1.93	0.50
2:jb:109:LEU:HD23	2:jb:109:LEU:C	2.37	0.50
2:c:36:ILE:HD12	2:c:44:VAL:HG21	1.93	0.49
2:f:16:ILE:HG22	2:f:51:ILE:HD11	1.94	0.49
1:EB:255:THR:HG22	1:EB:264:ARG:NH2	2.27	0.49
1:H:228:GLN:OE1	1:H:228:GLN:N	2.45	0.49
1:HB:207:VAL:HG13	1:HB:211:VAL:HG23	1.94	0.49
1:J:157:LEU:HD23	1:J:188:GLY:HA3	1.94	0.49
1:J:212:ALA:HB1	1:J:242:ILE:HD12	1.94	0.49
1:L:216:ILE:O	1:L:220:GLU:HG3	2.11	0.49
1:L:238:ILE:O	1:L:242:ILE:HG12	2.11	0.49
1:MB:167:MET:HE1	1:MB:181:ILE:HG23	1.93	0.49
1:NB:231:LEU:HD23	1:NB:231:LEU:O	2.12	0.49
1:TB:225:VAL:O	1:TB:225:VAL:HG12	2.11	0.49
2:b:104:ASP:C	2:b:104:ASP:OD1	2.55	0.49
2:cb:29:GLN:HG3	2:cb:65:VAL:HG22	1.93	0.49
2:fb:42:ARG:NH2	2:fb:116:LEU:HD12	2.27	0.49
1:A:228:GLN:N	1:A:228:GLN:OE1	2.46	0.49
1:AB:190:VAL:HG21	1:G:236:PRO:HG3	1.94	0.49
1:J:207:VAL:HB	1:J:238:ILE:HG23	1.94	0.49
1:KB:160:ILE:HD11	1:KB:262:MET:CE	2.41	0.49
1:L:217:GLN:HA	1:L:217:GLN:OE1	2.11	0.49
1:LB:240:GLN:HA	2:b:68:MET:HE3	1.93	0.49
1:M:201:ILE:O	1:M:204:VAL:HG12	2.12	0.49
1:QB:200:ASP:C	1:QB:200:ASP:OD1	2.56	0.49
1:CB:237:GLU:OE1	1:CB:237:GLU:C	2.54	0.49
1:D:201:ILE:HD11	1:D:234:ILE:CD1	2.42	0.49
1:HB:200:ASP:C	1:HB:200:ASP:OD2	2.55	0.49
1:MB:200:ASP:C	1:MB:200:ASP:OD1	2.54	0.49
2:c:104:ASP:C	2:c:104:ASP:OD2	2.55	0.49
2:cb:78:VAL:HG11	2:cb:96:PHE:HE1	1.76	0.49
2:ib:104:ASP:C	2:ib:104:ASP:OD2	2.54	0.49
2:j:16:ILE:HG23	2:j:20:LEU:HD21	1.93	0.49
1:BB:175:THR:CA	1:BB:210:MET:HE1	2.42	0.49
1:IB:234:ILE:HD12	2:bb:71:LEU:HD21	1.94	0.49
1:S:253:ILE:H	1:S:253:ILE:HD12	1.76	0.49
2:b:71:LEU:HD23	2:b:71:LEU:C	2.37	0.49
2:b:85:VAL:HG12	2:b:89:LEU:CD1	2.42	0.49
2:db:103:MET:HE3	2:db:103:MET:CA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:207:VAL:HG13	1:BB:211:VAL:HG23	1.94	0.49
1:LB:218:ALA:O	1:LB:222:VAL:HG13	2.12	0.49
2:c:78:VAL:HG12	2:c:81:ILE:HD11	1.95	0.49
2:f:33:LEU:HD11	2:f:68:MET:HE3	1.93	0.49
2:ab:103:MET:HA	2:ab:103:MET:HE3	1.95	0.49
1:EB:230:MET:HE1	1:EB:265:ALA:CA	2.43	0.49
1:M:166:VAL:HG22	1:M:198:LEU:HD13	1.95	0.49
2:c:66:VAL:HG23	2:c:76:VAL:CG1	2.43	0.49
2:db:78:VAL:HG21	2:db:96:PHE:CZ	2.48	0.49
2:g:47:ASP:C	2:g:47:ASP:OD1	2.55	0.49
2:h:36:ILE:HD11	2:h:41:ALA:O	2.12	0.49
2:ib:66:VAL:HG21	2:ib:99:VAL:HG21	1.93	0.49
2:a:66:VAL:HG21	2:a:99:VAL:HG21	1.94	0.49
1:C:185:LEU:HD11	1:C:197:VAL:HG21	1.95	0.49
1:GB:183:GLU:O	1:GB:187:ILE:HG12	2.13	0.49
1:PB:200:ASP:OD2	1:PB:200:ASP:C	2.55	0.49
1:RB:201:ILE:HD11	1:RB:234:ILE:HG12	1.93	0.49
2:d:36:ILE:HD11	2:d:41:ALA:O	2.13	0.49
2:fb:8:LEU:HD22	2:fb:13:LEU:HD11	1.94	0.49
2:hb:104:ASP:C	2:hb:104:ASP:OD1	2.55	0.49
2:i:47:ASP:C	2:i:47:ASP:OD2	2.54	0.49
1:DB:230:MET:HE1	1:DB:265:ALA:CA	2.41	0.49
1:E:200:ASP:OD2	1:E:200:ASP:C	2.56	0.49
1:N:201:ILE:HD11	1:N:234:ILE:CD1	2.41	0.49
1:OB:210:MET:HE2	1:OB:210:MET:CA	2.43	0.49
1:Q:177:ARG:O	1:Q:181:ILE:HG22	2.13	0.49
1:S:245:LEU:HD12	1:S:245:LEU:O	2.13	0.49
2:b:56:ALA:HA	2:b:92:LEU:CD1	2.41	0.49
2:i:103:MET:CA	2:i:103:MET:HE3	2.43	0.49
2:jb:70:LYS:C	2:jb:70:LYS:HD3	2.38	0.49
2:a:94:ILE:HD12	2:a:94:ILE:N	2.28	0.49
1:C:210:MET:HA	1:C:210:MET:HE3	1.94	0.49
1:DB:269:THR:C	1:DB:270:ASN:OD1	2.56	0.49
1:RB:230:MET:HE1	1:RB:264:ARG:HB3	1.95	0.49
1:SB:263:GLU:O	1:SB:263:GLU:OE2	2.31	0.49
1:T:232:VAL:HG23	1:T:255:THR:OG1	2.13	0.49
2:bb:100:LEU:HD12	2:bb:100:LEU:N	2.27	0.49
1:C:244:ASN:O	1:C:244:ASN:OD1	2.31	0.48
1:G:158:LEU:N	1:G:158:LEU:HD12	2.28	0.48
1:LB:179:LYS:HA	1:LB:179:LYS:HE2	1.95	0.48
1:NB:169:LEU:HD23	1:NB:169:LEU:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bb:47:ASP:C	2:bb:47:ASP:OD2	2.55	0.48
2:cb:77:VAL:HG23	2:cb:112:LEU:HD13	1.93	0.48
2:i:33:LEU:O	2:i:36:ILE:HG22	2.13	0.48
2:ib:13:LEU:CD1	2:ib:105:LEU:HD21	2.42	0.48
1:A:273:ILE:HD11	1:AB:161:PHE:CE1	2.48	0.48
1:BB:237:GLU:OE1	1:BB:238:ILE:HD13	2.13	0.48
1:IB:230:MET:HE1	1:IB:265:ALA:HA	1.95	0.48
2:d:14:ILE:HD12	2:d:32:LEU:HD12	1.94	0.48
2:d:105:LEU:C	2:d:105:LEU:HD23	2.39	0.48
2:f:104:ASP:OD2	2:f:104:ASP:C	2.56	0.48
2:j:52:ASP:C	2:j:52:ASP:OD2	2.56	0.48
1:B:170:ILE:HG21	1:BB:153:LEU:HD22	1.96	0.48
1:H:180:LEU:O	1:H:184:ASN:OD1	2.30	0.48
1:QB:166:VAL:CG2	1:QB:198:LEU:HD13	2.44	0.48
1:S:210:MET:HE2	1:S:210:MET:HA	1.95	0.48
2:e:71:LEU:O	2:e:71:LEU:HD23	2.13	0.48
2:h:104:ASP:N	2:h:104:ASP:OD1	2.47	0.48
2:j:13:LEU:HD21	2:j:109:LEU:HD22	1.94	0.48
1:A:210:MET:HE2	1:A:210:MET:HA	1.95	0.48
1:A:216:ILE:HD11	1:A:247:ILE:HD13	1.94	0.48
1:BB:175:THR:HA	1:BB:210:MET:HE1	1.96	0.48
1:EB:249:LEU:HD12	1:RB:224:LEU:CD2	2.43	0.48
1:H:263:GLU:OE2	1:H:263:GLU:HA	2.13	0.48
1:QB:179:LYS:HD3	1:QB:179:LYS:N	2.27	0.48
1:R:207:VAL:HB	1:R:238:ILE:HG23	1.95	0.48
2:f:47:ASP:C	2:f:47:ASP:OD2	2.55	0.48
2:h:47:ASP:C	2:h:47:ASP:OD1	2.56	0.48
2:i:3:ILE:O	2:i:5:ILE:HD12	2.13	0.48
1:B:193:ARG:N	1:B:193:ARG:HD2	2.28	0.48
1:CB:210:MET:HE2	1:CB:210:MET:HA	1.95	0.48
1:FB:269:THR:HG21	1:FB:271:ARG:NH2	2.29	0.48
1:NB:237:GLU:OE2	1:NB:237:GLU:C	2.56	0.48
1:Q:187:ILE:HG23	1:Q:191:LYS:NZ	2.28	0.48
2:i:56:ALA:HA	2:i:92:LEU:HD11	1.95	0.48
2:j:33:LEU:HD11	2:j:68:MET:CE	2.43	0.48
1:H:186:LEU:HB3	1:JB:236:PRO:HB3	1.95	0.48
1:H:231:LEU:O	1:H:231:LEU:HD23	2.14	0.48
1:L:232:VAL:HG13	1:L:255:THR:OG1	2.13	0.48
1:NB:240:GLN:HA	2:i:68:MET:SD	2.54	0.48
1:Q:196:VAL:HG11	1:Q:265:ALA:CB	2.43	0.48
2:j:33:LEU:O	2:j:36:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:210:MET:HE3	1:FB:210:MET:CA	2.44	0.48
1:GB:269:THR:O	1:GB:269:THR:CG2	2.58	0.48
1:L:198:LEU:HD11	1:L:262:MET:HE2	1.95	0.48
1:O:170:ILE:HG12	1:OB:153:LEU:HD22	1.96	0.48
2:f:23:HIS:CE1	2:f:24:THR:HG23	2.49	0.48
2:a:36:ILE:HD11	2:a:41:ALA:O	2.14	0.48
1:DB:200:ASP:C	1:DB:200:ASP:OD1	2.57	0.48
1:F:150:LEU:HD21	1:FB:150:LEU:HD13	1.95	0.48
1:F:262:MET:O	1:F:266:LEU:HD23	2.13	0.48
1:L:204:VAL:HG13	1:L:204:VAL:O	2.13	0.48
1:NB:147:LYS:HE2	1:NB:147:LYS:HA	1.95	0.48
1:O:201:ILE:HD11	1:O:234:ILE:HD13	1.95	0.48
1:P:193:ARG:HB3	1:P:193:ARG:NH1	2.28	0.48
2:c:63:GLY:O	2:c:66:VAL:HG12	2.14	0.48
2:j:33:LEU:HD11	2:j:68:MET:HE3	1.95	0.48
2:j:36:ILE:HD11	2:j:74:ALA:HB3	1.96	0.48
2:jb:47:ASP:C	2:jb:47:ASP:OD1	2.56	0.48
1:G:253:ILE:HG21	1:G:264:ARG:HD2	1.95	0.48
1:HB:231:LEU:CB	1:HB:252:ILE:HD11	2.44	0.48
1:J:157:LEU:HD11	1:J:165:SER:HB3	1.96	0.48
1:OB:207:VAL:HG13	1:OB:211:VAL:HB	1.96	0.48
1:RB:263:GLU:HA	1:RB:263:GLU:OE2	2.13	0.48
2:d:16:ILE:HG21	2:d:51:ILE:HD11	1.96	0.48
1:D:196:VAL:HG11	1:D:265:ALA:HB1	1.96	0.48
1:D:269:THR:HG21	1:D:271:ARG:NH2	2.28	0.48
1:E:256:ASN:OD1	1:E:257:THR:HG22	2.14	0.48
1:F:210:MET:HA	1:F:210:MET:HE3	1.96	0.48
1:GB:219:SER:OG	1:GB:252:ILE:HD12	2.14	0.48
1:M:152:GLU:OE2	1:M:153:LEU:HD23	2.14	0.48
1:N:196:VAL:HG11	1:N:265:ALA:CB	2.44	0.48
1:P:212:ALA:O	1:P:216:ILE:HD12	2.14	0.48
1:Q:175:THR:CG2	1:Q:210:MET:HE1	2.38	0.48
1:Q:262:MET:HA	1:Q:262:MET:HE2	1.95	0.48
2:i:115:GLU:OE1	2:i:115:GLU:O	2.31	0.48
2:a:1:MET:HE3	2:a:1:MET:C	2.39	0.47
1:C:245:LEU:HD23	1:C:247:ILE:HD11	1.95	0.47
1:GB:247:ILE:HG22	1:GB:249:LEU:CD2	2.44	0.47
1:IB:256:ASN:C	1:IB:256:ASN:OD1	2.57	0.47
1:K:200:ASP:OD2	1:K:200:ASP:C	2.57	0.47
1:Q:175:THR:HG23	1:Q:210:MET:CE	2.38	0.47
2:b:51:ILE:HG21	2:b:54:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bb:3:ILE:HD13	2:bb:3:ILE:N	2.29	0.47
2:c:103:MET:HA	2:c:103:MET:HE3	1.95	0.47
2:e:43:GLY:HA3	2:e:112:LEU:HD21	1.95	0.47
1:JB:230:MET:HE1	1:JB:265:ALA:HB2	1.96	0.47
1:K:236:PRO:HB3	1:NB:186:LEU:HB3	1.96	0.47
1:M:166:VAL:HG12	1:M:168:PRO:HD3	1.96	0.47
1:NB:269:THR:O	1:NB:269:THR:HG22	2.14	0.47
1:Q:232:VAL:HG13	1:Q:255:THR:OG1	2.13	0.47
1:RB:192:ASN:HD22	1:RB:192:ASN:H	1.62	0.47
1:S:207:VAL:HG13	1:S:211:VAL:HG23	1.97	0.47
1:TB:212:ALA:HB1	1:TB:242:ILE:HD12	1.96	0.47
2:g:94:ILE:H	2:g:94:ILE:HD12	1.79	0.47
1:BB:238:ILE:O	1:BB:242:ILE:HG12	2.14	0.47
1:EB:249:LEU:HB3	1:EB:252:ILE:HG23	1.96	0.47
1:K:216:ILE:CD1	1:K:247:ILE:HD13	2.44	0.47
1:L:196:VAL:HG11	1:L:265:ALA:HB2	1.95	0.47
1:R:185:LEU:HD11	1:R:197:VAL:HG21	1.96	0.47
2:db:100:LEU:HD12	2:db:100:LEU:N	2.28	0.47
2:g:105:LEU:C	2:g:105:LEU:HD23	2.39	0.47
2:j:48:ILE:HD11	2:j:81:ILE:HG12	1.96	0.47
1:A:170:ILE:HD11	1:AB:153:LEU:HD22	1.95	0.47
2:ab:51:ILE:HG21	2:ab:54:ILE:HD11	1.95	0.47
1:C:207:VAL:HB	1:C:238:ILE:HG23	1.96	0.47
1:H:170:ILE:CG1	1:HB:153:LEU:HD22	2.44	0.47
1:J:162:GLU:N	1:J:162:GLU:OE2	2.47	0.47
1:R:160:ILE:HD12	1:R:166:VAL:HG21	1.95	0.47
1:RB:262:MET:HE2	1:RB:262:MET:HA	1.97	0.47
1:SB:149:ALA:O	1:SB:153:LEU:HG	2.14	0.47
2:fb:43:GLY:HA3	2:fb:112:LEU:HD21	1.96	0.47
2:i:62:LEU:HD22	2:i:96:PHE:HZ	1.79	0.47
2:i:78:VAL:HG21	2:i:96:PHE:CE1	2.50	0.47
1:BB:243:VAL:HG21	1:HB:220:GLU:HB3	1.97	0.47
1:D:216:ILE:HD11	1:D:249:LEU:HD21	1.97	0.47
1:HB:265:ALA:O	1:HB:269:THR:HG22	2.14	0.47
1:I:185:LEU:HD11	1:I:197:VAL:HG21	1.96	0.47
1:N:240:GLN:HA	2:jb:68:MET:HE3	1.95	0.47
1:R:176:GLU:H	1:R:176:GLU:CD	2.23	0.47
1:S:243:VAL:HG23	2:hb:71:LEU:HD12	1.96	0.47
1:SB:201:ILE:HD11	1:SB:234:ILE:HG12	1.96	0.47
2:e:56:ALA:HA	2:e:92:LEU:CD1	2.44	0.47
2:f:78:VAL:HG12	2:f:81:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:55:ASP:OD1	2:g:56:ALA:N	2.48	0.47
2:j:36:ILE:HD11	2:j:74:ALA:CB	2.45	0.47
1:BB:236:PRO:HG3	1:HB:190:VAL:HG21	1.95	0.47
1:BB:247:ILE:HG22	1:BB:249:LEU:HD22	1.97	0.47
1:IB:149:ALA:O	1:IB:153:LEU:HG	2.14	0.47
1:J:196:VAL:HG11	1:J:265:ALA:HB1	1.95	0.47
1:MB:175:THR:HG23	1:MB:210:MET:CE	2.44	0.47
1:NB:247:ILE:HG22	1:NB:249:LEU:CD2	2.45	0.47
1:OB:158:LEU:N	1:OB:158:LEU:HD12	2.30	0.47
1:QB:218:ALA:O	1:QB:222:VAL:HG13	2.14	0.47
1:S:182:ILE:HG12	1:S:218:ALA:HB2	1.94	0.47
2:i:33:LEU:HD22	2:i:72:MET:HE1	1.97	0.47
2:i:48:ILE:HD11	2:i:81:ILE:HD13	1.97	0.47
2:i:85:VAL:O	2:i:89:LEU:HG	2.14	0.47
2:i:103:MET:HE3	2:i:103:MET:HA	1.95	0.47
1:A:176:GLU:O	1:A:180:LEU:HD22	2.15	0.47
2:a:53:PHE:CD1	2:a:53:PHE:C	2.93	0.47
1:D:167:MET:CE	1:D:181:ILE:HG23	2.45	0.47
1:F:196:VAL:HG11	1:F:265:ALA:HB1	1.96	0.47
1:H:190:VAL:HG21	1:JB:236:PRO:HG3	1.97	0.47
1:HB:216:ILE:HD11	1:HB:247:ILE:HG21	1.97	0.47
1:HB:247:ILE:HG22	1:HB:249:LEU:CD2	2.44	0.47
1:J:238:ILE:H	1:J:238:ILE:HD12	1.80	0.47
1:L:158:LEU:HD21	1:LB:168:PRO:HB3	1.97	0.47
1:LB:256:ASN:OD1	1:LB:257:THR:HG23	2.15	0.47
1:M:166:VAL:CG2	1:M:198:LEU:HD13	2.44	0.47
1:OB:249:LEU:HD12	1:QB:224:LEU:HD21	1.95	0.47
1:PB:236:PRO:HB3	2:g:33:LEU:HB3	1.97	0.47
1:QB:240:GLN:C	1:QB:240:GLN:CD	2.83	0.47
1:R:218:ALA:O	1:R:222:VAL:HG13	2.15	0.47
1:T:196:VAL:HG11	1:T:265:ALA:HB1	1.97	0.47
1:TB:185:LEU:HD11	1:TB:197:VAL:HG21	1.97	0.47
2:db:42:ARG:HD3	2:db:116:LEU:HD22	1.97	0.47
2:fb:6:LEU:O	2:fb:12:LEU:HD13	2.15	0.47
2:g:3:ILE:HD13	2:g:3:ILE:N	2.29	0.47
2:j:29:GLN:OE1	2:j:68:MET:HE1	2.15	0.47
1:C:240:GLN:C	1:C:240:GLN:CD	2.82	0.47
1:FB:232:VAL:HG23	1:FB:255:THR:OG1	2.13	0.47
1:R:162:GLU:N	1:R:162:GLU:OE1	2.48	0.47
2:b:4:PRO:O	2:b:5:ILE:HD13	2.15	0.47
2:b:5:ILE:HD12	2:b:14:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:103:MET:HA	2:d:103:MET:HE3	1.97	0.47
2:ib:12:LEU:HD23	2:ib:41:ALA:CB	2.45	0.47
1:AB:217:GLN:OE1	1:AB:217:GLN:HA	2.15	0.47
1:C:236:PRO:HB3	1:P:186:LEU:HB3	1.95	0.47
1:D:169:LEU:HD23	1:D:169:LEU:C	2.39	0.47
1:IB:201:ILE:HD11	1:IB:234:ILE:HG12	1.96	0.47
1:IB:237:GLU:OE2	1:IB:237:GLU:C	2.58	0.47
1:J:200:ASP:C	1:J:200:ASP:OD2	2.58	0.47
1:K:169:LEU:C	1:K:169:LEU:HD23	2.40	0.47
1:K:232:VAL:HG23	1:K:255:THR:OG1	2.13	0.47
1:RB:149:ALA:O	1:RB:153:LEU:HG	2.15	0.47
1:S:210:MET:HE2	1:S:210:MET:CA	2.45	0.47
2:f:29:GLN:HG3	2:f:65:VAL:HG22	1.97	0.47
2:ib:16:ILE:HG23	2:ib:20:LEU:HD21	1.97	0.47
1:FB:269:THR:O	1:FB:269:THR:CG2	2.63	0.47
1:I:153:LEU:HD22	1:IB:170:ILE:CG2	2.45	0.47
1:K:173:ILE:HG21	1:K:211:VAL:HG13	1.97	0.47
1:L:218:ALA:O	1:L:222:VAL:HG12	2.15	0.47
1:Q:186:LEU:O	1:Q:190:VAL:HG12	2.15	0.47
1:Q:240:GLN:C	1:Q:240:GLN:CD	2.83	0.47
2:e:47:ASP:C	2:e:47:ASP:OD1	2.57	0.47
2:ab:3:ILE:HD13	2:ab:3:ILE:N	2.29	0.46
2:ab:85:VAL:HG12	2:ab:89:LEU:HD13	1.97	0.46
1:D:175:THR:HG22	1:D:179:LYS:NZ	2.28	0.46
1:GB:207:VAL:HB	1:GB:238:ILE:HG23	1.97	0.46
1:H:180:LEU:O	1:H:183:GLU:HG2	2.14	0.46
1:JB:152:GLU:OE2	1:JB:153:LEU:HD23	2.15	0.46
1:JB:158:LEU:HD12	1:JB:158:LEU:N	2.30	0.46
1:N:210:MET:HE2	1:N:210:MET:HA	1.95	0.46
2:gb:25:ALA:HB1	2:gb:61:ILE:HG21	1.97	0.46
2:i:57:PHE:CE2	2:i:61:ILE:HD11	2.50	0.46
1:A:170:ILE:CG1	1:AB:153:LEU:HD22	2.45	0.46
2:ab:71:LEU:HD12	1:H:243:VAL:HG23	1.96	0.46
1:BB:149:ALA:O	1:BB:153:LEU:HG	2.15	0.46
1:NB:163:LYS:C	1:NB:164:ILE:HD12	2.40	0.46
1:RB:167:MET:HE2	1:RB:181:ILE:HG23	1.98	0.46
2:eb:71:LEU:HD23	2:eb:71:LEU:C	2.40	0.46
2:fb:103:MET:HE3	2:fb:103:MET:CA	2.43	0.46
2:g:71:LEU:O	2:g:71:LEU:HD12	2.15	0.46
2:hb:66:VAL:CG2	2:hb:99:VAL:HG21	2.45	0.46
1:A:152:GLU:HG3	1:A:153:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ab:109:LEU:HD21	2:ab:113:LYS:HE3	1.95	0.46
1:FB:164:ILE:HG21	1:FB:262:MET:HE1	1.97	0.46
1:IB:198:LEU:HD12	1:IB:198:LEU:N	2.30	0.46
1:MB:216:ILE:HD11	1:MB:247:ILE:HG21	1.97	0.46
1:Q:249:LEU:O	1:Q:252:ILE:HG23	2.15	0.46
1:T:243:VAL:HG11	2:ib:68:MET:HE2	1.96	0.46
2:bb:85:VAL:O	2:bb:89:LEU:HG	2.15	0.46
2:cb:56:ALA:CA	2:cb:92:LEU:HD21	2.40	0.46
2:jb:105:LEU:HD23	2:jb:105:LEU:C	2.41	0.46
1:C:257:THR:HG21	1:P:193:ARG:HH21	1.80	0.46
1:N:236:PRO:HA	2:jb:72:MET:HE1	1.98	0.46
1:NB:162:GLU:O	1:NB:163:LYS:HB2	2.15	0.46
1:P:198:LEU:HD12	1:P:198:LEU:N	2.29	0.46
1:Q:201:ILE:HG12	1:Q:231:LEU:HD11	1.97	0.46
2:bb:71:LEU:HD23	2:bb:71:LEU:C	2.41	0.46
1:DB:230:MET:HE1	1:DB:265:ALA:HA	1.97	0.46
1:GB:185:LEU:HD21	1:GB:222:VAL:HG11	1.97	0.46
1:H:196:VAL:HG11	1:H:265:ALA:HB1	1.97	0.46
1:LB:216:ILE:HD11	1:LB:247:ILE:HD13	1.97	0.46
1:M:244:ASN:C	1:M:244:ASN:OD1	2.58	0.46
1:OB:162:GLU:N	1:OB:162:GLU:OE1	2.49	0.46
2:b:4:PRO:C	2:b:5:ILE:HD13	2.40	0.46
2:a:77:VAL:HG22	2:a:100:LEU:HB2	1.97	0.46
2:ab:58:ILE:H	2:ab:58:ILE:HD12	1.81	0.46
1:GB:201:ILE:O	1:GB:204:VAL:HG12	2.16	0.46
1:H:205:PRO:HA	1:H:235:ARG:HH12	1.80	0.46
1:JB:257:THR:HG23	1:JB:260:LYS:H	1.81	0.46
1:L:231:LEU:CB	1:L:252:ILE:HD11	2.45	0.46
1:L:231:LEU:HB2	1:L:252:ILE:HD11	1.98	0.46
1:O:269:THR:O	1:O:270:ASN:OD1	2.34	0.46
1:Q:237:GLU:OE2	1:Q:237:GLU:C	2.59	0.46
1:QB:259:LYS:O	1:QB:263:GLU:OE1	2.33	0.46
1:TB:207:VAL:HG13	1:TB:211:VAL:HG23	1.97	0.46
2:f:110:GLU:OE1	2:f:110:GLU:C	2.59	0.46
2:fb:38:GLU:OE1	2:fb:39:THR:HG23	2.16	0.46
2:h:1:MET:HE2	2:h:1:MET:HA	1.97	0.46
2:i:103:MET:HE3	2:i:103:MET:O	2.15	0.46
2:a:5:ILE:HG12	2:a:35:LYS:HG2	1.98	0.46
1:B:243:VAL:HG13	1:F:224:LEU:HD12	1.98	0.46
1:BB:218:ALA:O	1:BB:222:VAL:HG12	2.15	0.46
1:HB:160:ILE:HD13	1:HB:160:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:250:ASP:C	1:N:250:ASP:OD1	2.58	0.46
1:OB:222:VAL:HG22	1:OB:227:CYS:HB3	1.98	0.46
1:P:186:LEU:O	1:P:189:VAL:HG12	2.16	0.46
1:Q:249:LEU:HD13	1:Q:252:ILE:HG21	1.98	0.46
1:R:179:LYS:O	1:R:183:GLU:HG2	2.15	0.46
2:gb:54:ILE:HD11	2:gb:89:LEU:CD2	2.46	0.46
2:gb:109:LEU:HD23	2:gb:109:LEU:O	2.15	0.46
1:B:185:LEU:HD11	1:B:197:VAL:HG21	1.97	0.46
1:BB:210:MET:HE2	1:BB:211:VAL:HG13	1.96	0.46
1:D:201:ILE:HD11	1:D:234:ILE:HD13	1.96	0.46
1:D:247:ILE:HG22	1:D:249:LEU:CD2	2.45	0.46
1:FB:222:VAL:HG22	1:FB:227:CYS:HB3	1.98	0.46
1:G:179:LYS:O	1:G:183:GLU:HG3	2.16	0.46
1:L:262:MET:HE2	1:L:262:MET:HA	1.98	0.46
2:b:5:ILE:HG22	2:b:12:LEU:HD12	1.98	0.46
2:d:85:VAL:O	2:d:89:LEU:HG	2.16	0.46
2:h:48:ILE:HD11	2:h:81:ILE:HD13	1.98	0.46
2:h:85:VAL:O	2:h:89:LEU:HG	2.15	0.46
2:jb:36:ILE:HD11	2:jb:44:VAL:HG22	1.97	0.46
1:E:207:VAL:HG13	1:E:211:VAL:CG2	2.42	0.46
1:R:231:LEU:C	1:R:231:LEU:HD23	2.41	0.46
1:RB:185:LEU:HD11	1:RB:197:VAL:HG21	1.98	0.46
2:bb:56:ALA:HA	2:bb:92:LEU:CD1	2.45	0.46
2:c:81:ILE:N	2:c:81:ILE:HD12	2.31	0.46
1:B:204:VAL:HG11	1:B:207:VAL:HG23	1.98	0.46
1:C:210:MET:HE3	1:C:210:MET:CA	2.45	0.46
1:F:269:THR:O	1:F:269:THR:CG2	2.62	0.46
1:FB:183:GLU:O	1:FB:187:ILE:HG12	2.16	0.46
1:IB:249:LEU:HD12	1:IB:252:ILE:CG2	2.46	0.46
1:QB:157:LEU:C	1:QB:158:LEU:HD12	2.41	0.46
2:g:64:ASP:O	2:g:68:MET:HG3	2.16	0.46
2:h:90:ILE:HG13	2:h:91:GLU:N	2.30	0.46
2:hb:36:ILE:HD11	2:hb:74:ALA:HB3	1.97	0.46
1:D:200:ASP:C	1:D:200:ASP:OD2	2.59	0.45
1:OB:210:MET:HE2	1:OB:210:MET:N	2.32	0.45
1:Q:178:ALA:O	1:Q:181:ILE:HG23	2.16	0.45
2:c:21:ASP:OD1	2:c:22:ASP:N	2.49	0.45
2:fb:57:PHE:CZ	2:fb:61:ILE:HD11	2.51	0.45
2:g:33:LEU:O	2:g:36:ILE:HG22	2.16	0.45
1:BB:212:ALA:HB1	1:BB:242:ILE:HD12	1.97	0.45
1:EB:210:MET:HE2	1:EB:210:MET:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:186:LEU:O	1:I:189:VAL:HG12	2.16	0.45
1:LB:230:MET:HE1	1:LB:265:ALA:CA	2.47	0.45
1:MB:231:LEU:HB2	1:MB:252:ILE:HD11	1.98	0.45
1:QB:237:GLU:OE2	1:QB:237:GLU:C	2.59	0.45
2:bb:51:ILE:HG21	2:bb:54:ILE:CD1	2.46	0.45
2:e:66:VAL:CG2	2:e:99:VAL:HG21	2.46	0.45
2:f:81:ILE:H	2:f:81:ILE:HD12	1.80	0.45
2:fb:66:VAL:HG21	2:fb:99:VAL:HG21	1.97	0.45
2:i:32:LEU:HD12	2:i:32:LEU:O	2.16	0.45
1:AB:198:LEU:HD12	1:AB:198:LEU:N	2.31	0.45
1:B:207:VAL:HB	1:B:238:ILE:HG23	1.98	0.45
1:M:169:LEU:HD23	1:M:169:LEU:C	2.42	0.45
1:M:231:LEU:C	1:M:231:LEU:HD23	2.42	0.45
1:MB:237:GLU:C	1:MB:237:GLU:OE2	2.60	0.45
1:Q:178:ALA:HA	1:Q:181:ILE:HG22	1.99	0.45
2:bb:96:PHE:HB3	2:bb:99:VAL:HB	1.98	0.45
2:d:17:GLN:OE1	2:d:17:GLN:N	2.48	0.45
2:eb:71:LEU:HD23	2:eb:71:LEU:O	2.16	0.45
2:ab:109:LEU:HD23	2:ab:109:LEU:C	2.42	0.45
1:BB:169:LEU:HD23	1:BB:201:ILE:HG22	1.99	0.45
1:DB:237:GLU:OE1	1:DB:237:GLU:HA	2.15	0.45
1:LB:237:GLU:OE2	1:LB:238:ILE:HD13	2.16	0.45
1:TB:163:LYS:C	1:TB:164:ILE:HD12	2.42	0.45
2:hb:3:ILE:HD13	2:hb:3:ILE:N	2.32	0.45
1:AB:209:THR:HG23	1:AB:210:MET:N	2.31	0.45
1:DB:149:ALA:O	1:DB:153:LEU:HG	2.16	0.45
1:EB:236:PRO:HG3	1:RB:190:VAL:HG21	1.97	0.45
1:MB:200:ASP:OD2	1:MB:258:MET:HE2	2.17	0.45
1:NB:161:PHE:HB2	1:NB:164:ILE:HD13	1.98	0.45
1:QB:196:VAL:CG1	1:QB:230:MET:HE3	2.46	0.45
1:T:238:ILE:O	1:T:242:ILE:HG12	2.15	0.45
2:c:6:LEU:HD12	2:c:6:LEU:N	2.32	0.45
2:c:47:ASP:OD1	2:c:47:ASP:C	2.59	0.45
2:fb:26:VAL:HG12	2:fb:30:GLU:OE2	2.17	0.45
2:i:77:VAL:HG21	2:i:112:LEU:HD13	1.98	0.45
1:AB:155:ALA:HB1	1:AB:167:MET:HE3	1.99	0.45
1:CB:212:ALA:HB1	1:CB:242:ILE:CD1	2.45	0.45
1:G:232:VAL:HG23	1:G:255:THR:OG1	2.17	0.45
1:K:170:ILE:HG21	1:KB:153:LEU:HD22	1.97	0.45
1:P:168:PRO:O	1:P:169:LEU:HD22	2.16	0.45
1:QB:255:THR:HG22	1:QB:264:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TB:200:ASP:OD2	1:TB:258:MET:HE2	2.17	0.45
2:ib:66:VAL:CG2	2:ib:99:VAL:HG21	2.46	0.45
2:ab:104:ASP:OD2	2:ab:104:ASP:N	2.48	0.45
1:E:237:GLU:OE2	1:E:238:ILE:HD13	2.17	0.45
1:J:262:MET:HA	1:J:262:MET:HE3	1.98	0.45
1:M:162:GLU:O	1:M:163:LYS:HB2	2.17	0.45
1:P:243:VAL:HG11	2:j:68:MET:HG3	1.97	0.45
2:cb:109:LEU:HD23	2:cb:109:LEU:C	2.42	0.45
2:cb:114:GLN:CD	2:cb:114:GLN:C	2.85	0.45
2:d:6:LEU:N	2:d:6:LEU:HD12	2.32	0.45
2:hb:7:LYS:HZ1	2:hb:39:THR:HG21	1.81	0.45
2:ab:12:LEU:HD13	2:ab:41:ALA:HB2	1.99	0.45
1:E:249:LEU:HD12	1:E:252:ILE:HG23	1.99	0.45
1:K:212:ALA:O	1:K:216:ILE:HD12	2.17	0.45
1:M:270:ASN:O	1:M:271:ARG:HG3	2.17	0.45
1:TB:157:LEU:HD22	1:TB:188:GLY:HA3	1.98	0.45
2:db:4:PRO:O	2:db:5:ILE:HD12	2.17	0.45
2:f:85:VAL:O	2:f:89:LEU:HD13	2.17	0.45
1:L:167:MET:HE1	1:L:181:ILE:CD1	2.42	0.45
1:LB:198:LEU:HD12	1:LB:198:LEU:N	2.31	0.45
1:M:170:ILE:HG21	1:MB:153:LEU:HD22	1.96	0.45
1:MB:162:GLU:O	1:MB:163:LYS:HB2	2.17	0.45
1:N:179:LYS:HD2	1:N:179:LYS:N	2.32	0.45
1:O:251:GLN:CD	1:O:251:GLN:N	2.75	0.45
2:h:43:GLY:HA3	2:h:112:LEU:HD21	1.99	0.45
1:GB:263:GLU:HA	1:GB:263:GLU:OE2	2.16	0.45
1:K:158:LEU:HD11	1:KB:168:PRO:HG3	1.98	0.45
1:L:247:ILE:HG22	1:L:249:LEU:HD22	1.99	0.45
1:LB:177:ARG:O	1:LB:181:ILE:HG22	2.17	0.45
1:MB:201:ILE:O	1:MB:204:VAL:HG12	2.17	0.45
1:NB:147:LYS:O	1:NB:147:LYS:HD3	2.16	0.45
1:NB:178:ALA:O	1:NB:181:ILE:HG22	2.17	0.45
1:OB:239:ALA:O	1:OB:243:VAL:HG12	2.16	0.45
2:eb:3:ILE:HD13	2:eb:3:ILE:N	2.32	0.45
2:hb:103:MET:HA	2:hb:103:MET:HE3	1.98	0.45
2:a:6:LEU:N	2:a:6:LEU:HD12	2.32	0.44
2:ab:78:VAL:HG11	2:ab:96:PHE:HE1	1.82	0.44
1:BB:262:MET:O	1:BB:262:MET:HE3	2.17	0.44
1:EB:238:ILE:O	1:EB:242:ILE:HG12	2.18	0.44
1:FB:210:MET:CE	1:FB:214:HIS:CE1	2.99	0.44
1:GB:245:LEU:O	1:GB:245:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:LEU:HD23	1:K:230:MET:HB3	1.99	0.44
1:P:196:VAL:HG11	1:P:265:ALA:CB	2.46	0.44
2:bb:56:ALA:HA	2:bb:92:LEU:HD11	1.99	0.44
1:AB:240:GLN:HA	2:a:68:MET:HE2	2.00	0.44
2:a:66:VAL:CG2	2:a:99:VAL:HG21	2.48	0.44
1:GB:247:ILE:HG22	1:GB:249:LEU:HD22	1.99	0.44
1:J:245:LEU:HD23	1:J:247:ILE:HD11	1.99	0.44
1:Q:268:LEU:HD23	1:Q:268:LEU:C	2.41	0.44
1:R:170:ILE:HG21	1:RB:153:LEU:HD22	1.98	0.44
1:TB:200:ASP:C	1:TB:200:ASP:OD1	2.60	0.44
2:e:103:MET:HA	2:e:103:MET:CE	2.45	0.44
2:f:58:ILE:H	2:f:58:ILE:HD12	1.83	0.44
2:ib:56:ALA:HA	2:ib:92:LEU:HD12	1.98	0.44
2:ab:47:ASP:C	2:ab:47:ASP:OD1	2.59	0.44
1:B:210:MET:HA	1:B:210:MET:CE	2.38	0.44
1:GB:149:ALA:O	1:GB:153:LEU:HG	2.18	0.44
1:HB:210:MET:SD	1:HB:214:HIS:NE2	2.91	0.44
1:J:222:VAL:HG21	1:J:229:ALA:HB2	1.99	0.44
1:JB:149:ALA:O	1:JB:153:LEU:HG	2.17	0.44
1:M:153:LEU:HD22	1:MB:170:ILE:HG22	1.99	0.44
1:M:192:ASN:OD1	1:M:192:ASN:O	2.34	0.44
1:O:198:LEU:HD12	1:O:198:LEU:N	2.32	0.44
1:RB:179:LYS:O	1:RB:183:GLU:OE1	2.36	0.44
1:S:162:GLU:CD	1:S:162:GLU:H	2.26	0.44
1:TB:173:ILE:HD13	1:TB:177:ARG:NH2	2.32	0.44
2:b:47:ASP:OD2	2:b:47:ASP:C	2.60	0.44
2:bb:71:LEU:HD23	2:bb:71:LEU:O	2.18	0.44
1:A:187:ILE:O	1:A:191:LYS:HG2	2.18	0.44
1:D:170:ILE:HG22	1:DB:153:LEU:HD22	2.00	0.44
1:G:253:ILE:HG21	1:G:264:ARG:CD	2.47	0.44
1:GB:169:LEU:C	1:GB:170:ILE:HD13	2.41	0.44
1:LB:207:VAL:HB	1:LB:238:ILE:HG23	1.99	0.44
1:LB:238:ILE:HD13	1:LB:238:ILE:N	2.32	0.44
1:M:149:ALA:O	1:M:153:LEU:HD11	2.17	0.44
1:M:162:GLU:O	1:M:164:ILE:HD12	2.18	0.44
1:M:238:ILE:O	1:M:242:ILE:HG13	2.18	0.44
1:MB:250:ASP:OD2	1:MB:250:ASP:N	2.50	0.44
1:P:170:ILE:HG21	1:PB:153:LEU:HD22	1.95	0.44
1:Q:232:VAL:HG11	1:Q:258:MET:HA	2.00	0.44
1:S:249:LEU:CD2	1:S:252:ILE:HD11	2.29	0.44
2:bb:106:GLU:OE2	2:bb:107:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:57:PHE:CE1	2:f:61:ILE:HD11	2.52	0.44
1:A:170:ILE:CD1	1:AB:153:LEU:HD22	2.48	0.44
1:BB:201:ILE:O	1:BB:204:VAL:HG12	2.18	0.44
1:D:209:THR:HG23	1:D:245:LEU:HD22	1.99	0.44
1:D:218:ALA:O	1:D:222:VAL:HG13	2.17	0.44
1:DB:218:ALA:O	1:DB:222:VAL:HG12	2.16	0.44
1:HB:238:ILE:O	1:HB:242:ILE:HG12	2.16	0.44
1:NB:201:ILE:O	1:NB:204:VAL:HG12	2.18	0.44
1:T:170:ILE:CG1	1:TB:153:LEU:HD22	2.48	0.44
1:TB:216:ILE:HG13	1:TB:247:ILE:HG21	1.99	0.44
2:cb:66:VAL:HG23	2:cb:76:VAL:CG1	2.45	0.44
2:f:16:ILE:CG2	2:f:20:LEU:HD21	2.47	0.44
2:fb:77:VAL:HG13	2:fb:100:LEU:HB2	1.99	0.44
1:IB:160:ILE:HD12	1:IB:166:VAL:HG11	2.00	0.44
1:M:222:VAL:HG22	1:M:227:CYS:HB3	1.99	0.44
1:NB:177:ARG:HE	1:NB:180:LEU:HD12	1.83	0.44
1:PB:206:VAL:HA	1:PB:238:ILE:HD11	2.00	0.44
1:QB:169:LEU:HD23	1:QB:169:LEU:C	2.42	0.44
1:R:198:LEU:HD12	1:R:198:LEU:N	2.32	0.44
1:S:153:LEU:HD13	1:SB:170:ILE:HG22	1.98	0.44
1:S:253:ILE:HD12	1:S:253:ILE:N	2.32	0.44
2:c:13:LEU:HD12	2:c:13:LEU:N	2.33	0.44
2:db:103:MET:HE3	2:db:103:MET:HA	2.00	0.44
2:f:66:VAL:CG2	2:f:99:VAL:HG21	2.48	0.44
2:h:61:ILE:O	2:h:65:VAL:HG23	2.18	0.44
2:hb:13:LEU:HD12	2:hb:13:LEU:N	2.32	0.44
1:AB:232:VAL:HG23	1:AB:255:THR:OG1	2.18	0.44
1:G:160:ILE:HG22	1:G:161:PHE:CD2	2.52	0.44
1:G:231:LEU:HD12	1:G:232:VAL:N	2.33	0.44
1:J:198:LEU:HD12	1:J:198:LEU:N	2.32	0.44
1:KB:149:ALA:O	1:KB:153:LEU:HG	2.18	0.44
1:LB:207:VAL:H	1:LB:238:ILE:HD12	1.83	0.44
2:bb:16:ILE:HD12	2:bb:48:ILE:HG22	1.98	0.44
2:e:38:GLU:OE2	2:e:39:THR:HG22	2.17	0.44
2:e:71:LEU:HD23	2:e:71:LEU:C	2.43	0.44
2:f:1:MET:O	2:f:1:MET:HE3	2.17	0.44
1:FB:201:ILE:HG12	1:FB:231:LEU:HD11	2.00	0.44
1:S:198:LEU:N	1:S:198:LEU:HD12	2.33	0.44
2:gb:109:LEU:HD23	2:gb:109:LEU:C	2.43	0.44
2:a:105:LEU:CD2	2:ab:8:LEU:HD13	2.48	0.44
1:BB:231:LEU:HD23	1:BB:231:LEU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:THR:HG22	1:D:264:ARG:NH2	2.33	0.44
1:DB:220:GLU:OE1	1:DB:220:GLU:HA	2.16	0.44
1:JB:198:LEU:HD12	1:JB:198:LEU:N	2.32	0.44
1:T:212:ALA:HB1	1:T:242:ILE:HD12	1.99	0.44
2:hb:52:ASP:OD2	2:hb:52:ASP:N	2.51	0.44
2:jb:104:ASP:OD2	2:jb:104:ASP:C	2.61	0.44
1:A:222:VAL:HG22	1:A:227:CYS:HB3	2.00	0.43
1:CB:222:VAL:HG21	1:CB:229:ALA:HB2	1.98	0.43
1:EB:149:ALA:O	1:EB:153:LEU:HG	2.18	0.43
1:H:210:MET:HA	1:H:210:MET:CE	2.41	0.43
1:LB:178:ALA:HA	1:LB:181:ILE:HG22	2.00	0.43
1:N:170:ILE:HG22	1:NB:153:LEU:HD22	1.98	0.43
1:QB:157:LEU:HD11	1:QB:165:SER:CB	2.48	0.43
2:db:12:LEU:HD13	2:db:41:ALA:CB	2.48	0.43
1:A:243:VAL:HG11	2:f:68:MET:HG3	1.99	0.43
1:H:196:VAL:HG11	1:H:265:ALA:CB	2.49	0.43
1:JB:160:ILE:HD12	1:JB:166:VAL:CG2	2.48	0.43
1:K:179:LYS:O	1:K:183:GLU:HG2	2.18	0.43
1:KB:228:GLN:OE1	1:KB:228:GLN:C	2.61	0.43
1:L:183:GLU:O	1:L:187:ILE:HD12	2.18	0.43
1:NB:231:LEU:CD2	1:NB:234:ILE:HD11	2.49	0.43
1:QB:157:LEU:HD22	1:QB:188:GLY:HA3	1.99	0.43
1:QB:204:VAL:HG13	1:QB:204:VAL:O	2.18	0.43
1:QB:262:MET:O	1:QB:266:LEU:HD23	2.18	0.43
2:b:110:GLU:C	2:b:110:GLU:OE1	2.61	0.43
2:g:51:ILE:HG21	2:g:54:ILE:HD13	1.99	0.43
1:AB:236:PRO:HB3	2:a:33:LEU:HB3	1.99	0.43
1:C:248:GLU:CD	1:C:248:GLU:N	2.76	0.43
1:J:196:VAL:HG11	1:J:265:ALA:CB	2.48	0.43
1:MB:224:LEU:CD2	1:O:249:LEU:HD12	2.48	0.43
1:P:231:LEU:HB2	1:P:252:ILE:HD11	2.00	0.43
1:P:269:THR:HG21	1:P:271:ARG:HH21	1.83	0.43
1:QB:167:MET:HE1	1:QB:181:ILE:CD1	2.44	0.43
1:QB:183:GLU:O	1:QB:187:ILE:HG12	2.19	0.43
2:c:42:ARG:HB2	2:c:116:LEU:HD21	2.00	0.43
2:eb:14:ILE:HD11	2:eb:32:LEU:HD13	2.00	0.43
2:f:89:LEU:HD23	2:f:96:PHE:CE1	2.54	0.43
2:g:43:GLY:HA3	2:g:112:LEU:HD21	2.00	0.43
2:gb:94:ILE:HG22	2:gb:96:PHE:CE2	2.53	0.43
1:A:240:GLN:CD	1:A:240:GLN:C	2.87	0.43
1:H:268:LEU:HD23	1:H:268:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:262:MET:HE2	1:LB:262:MET:CA	2.47	0.43
1:NB:149:ALA:O	1:NB:153:LEU:HG	2.18	0.43
1:PB:216:ILE:HD11	1:PB:249:LEU:HD11	1.99	0.43
2:fb:32:LEU:HD23	2:fb:65:VAL:CG1	2.49	0.43
2:j:61:ILE:O	2:j:65:VAL:HG23	2.19	0.43
1:A:243:VAL:HG23	2:f:71:LEU:HD12	2.00	0.43
1:F:160:ILE:HG22	1:F:161:PHE:CD2	2.53	0.43
1:I:167:MET:HE1	1:I:181:ILE:HD11	2.00	0.43
1:KB:205:PRO:HA	1:KB:235:ARG:HH22	1.82	0.43
1:L:263:GLU:OE1	1:L:264:ARG:N	2.52	0.43
1:NB:212:ALA:O	1:NB:216:ILE:HD12	2.18	0.43
1:S:231:LEU:CD2	1:S:234:ILE:HD11	2.47	0.43
1:T:178:ALA:O	1:T:181:ILE:HG22	2.18	0.43
1:TB:162:GLU:O	1:TB:163:LYS:HB2	2.19	0.43
2:b:6:LEU:HD22	2:bb:105:LEU:HD13	2.01	0.43
2:db:38:GLU:OE1	2:db:39:THR:HG23	2.18	0.43
2:fb:42:ARG:HH21	2:fb:116:LEU:HD12	1.83	0.43
1:B:229:ALA:HB3	1:B:252:ILE:HD12	2.01	0.43
1:DB:236:PRO:HB3	1:I:186:LEU:HB3	2.01	0.43
1:E:196:VAL:HG11	1:E:265:ALA:HB1	2.01	0.43
1:G:201:ILE:O	1:G:204:VAL:HG12	2.19	0.43
1:GB:216:ILE:HG13	1:GB:247:ILE:HG21	2.00	0.43
1:H:193:ARG:NH2	1:JB:257:THR:HG21	2.34	0.43
1:HB:167:MET:HE1	1:HB:181:ILE:HG23	2.01	0.43
1:IB:231:LEU:O	1:IB:231:LEU:HD23	2.19	0.43
1:IB:240:GLN:C	1:IB:240:GLN:CD	2.87	0.43
1:K:270:ASN:O	1:K:271:ARG:HG2	2.18	0.43
1:LB:243:VAL:HG11	2:b:68:MET:HG3	2.01	0.43
1:NB:216:ILE:HD11	1:NB:247:ILE:HG21	2.01	0.43
1:R:200:ASP:C	1:R:200:ASP:OD1	2.62	0.43
1:S:216:ILE:CD1	1:S:247:ILE:HD13	2.47	0.43
1:T:204:VAL:O	1:T:204:VAL:HG13	2.18	0.43
2:d:114:GLN:C	2:d:114:GLN:CD	2.85	0.43
2:e:35:LYS:O	2:e:39:THR:HG23	2.19	0.43
2:fb:78:VAL:HG11	2:fb:96:PHE:HE1	1.83	0.43
2:g:6:LEU:N	2:g:6:LEU:HD12	2.34	0.43
1:C:249:LEU:HD12	1:P:224:LEU:CD2	2.49	0.43
1:DB:213:HIS:O	1:DB:216:ILE:HG22	2.18	0.43
1:E:263:GLU:HA	1:E:263:GLU:OE1	2.19	0.43
1:GB:200:ASP:OD1	1:GB:200:ASP:C	2.62	0.43
1:JB:201:ILE:O	1:JB:204:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:230:MET:HE1	1:LB:265:ALA:HA	2.01	0.43
1:NB:230:MET:HE1	1:NB:265:ALA:CA	2.48	0.43
1:OB:201:ILE:HD13	1:OB:231:LEU:HD11	2.01	0.43
2:b:112:LEU:HD23	2:b:112:LEU:C	2.43	0.43
2:c:33:LEU:O	2:c:36:ILE:HG22	2.18	0.43
2:c:36:ILE:HD11	2:c:74:ALA:HB3	2.01	0.43
2:hb:47:ASP:HB2	2:hb:105:LEU:HD12	1.99	0.43
2:j:105:LEU:HD23	2:j:105:LEU:C	2.44	0.43
1:A:230:MET:HE1	1:A:265:ALA:HB2	2.01	0.43
1:CB:157:LEU:HD22	1:CB:188:GLY:HA3	2.00	0.43
1:F:198:LEU:N	1:F:198:LEU:HD12	2.34	0.43
1:IB:234:ILE:CD1	2:bb:71:LEU:HD21	2.49	0.43
1:L:225:VAL:O	1:L:225:VAL:CG1	2.67	0.43
1:M:250:ASP:OD2	1:M:250:ASP:N	2.52	0.43
1:O:162:GLU:O	1:O:163:LYS:HB2	2.19	0.43
1:Q:256:ASN:OD1	1:Q:257:THR:HG23	2.18	0.43
2:b:113:LYS:HD3	2:b:113:LYS:HA	1.88	0.43
2:hb:33:LEU:HD11	2:hb:68:MET:HE2	2.00	0.43
2:j:71:LEU:HD12	2:j:71:LEU:O	2.19	0.43
1:CB:198:LEU:N	1:CB:198:LEU:HD12	2.34	0.43
1:DB:236:PRO:HG3	1:I:190:VAL:HG21	2.00	0.43
1:HB:212:ALA:O	1:HB:216:ILE:HD12	2.19	0.43
1:I:209:THR:HG22	1:I:245:LEU:HD13	2.01	0.43
1:J:231:LEU:HD13	1:J:252:ILE:CD1	2.49	0.43
1:J:270:ASN:O	1:J:271:ARG:HG3	2.18	0.43
1:K:175:THR:HG22	1:K:179:LYS:HZ3	1.81	0.43
1:S:274:VAL:O	1:S:274:VAL:HG23	2.19	0.43
2:b:112:LEU:HD23	2:b:112:LEU:O	2.19	0.43
2:f:62:LEU:C	2:f:62:LEU:HD23	2.44	0.43
2:fb:82:GLN:OE1	2:fb:82:GLN:HA	2.19	0.43
2:fb:106:GLU:OE1	2:fb:106:GLU:C	2.62	0.43
2:i:16:ILE:HG22	2:i:51:ILE:HD11	2.00	0.43
1:D:263:GLU:C	1:D:263:GLU:OE1	2.62	0.43
1:F:160:ILE:HD12	1:F:166:VAL:HG13	2.00	0.43
1:G:198:LEU:HD12	1:G:198:LEU:N	2.34	0.43
1:KB:185:LEU:HD11	1:KB:197:VAL:HG21	2.01	0.43
1:LB:169:LEU:HD23	1:LB:169:LEU:C	2.44	0.43
1:M:236:PRO:HG3	2:e:37:HIS:HB2	2.00	0.43
1:N:269:THR:HG21	1:N:271:ARG:HH21	1.84	0.43
1:RB:201:ILE:O	1:RB:204:VAL:HG12	2.19	0.43
2:b:38:GLU:CD	2:b:38:GLU:C	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:hb:56:ALA:HA	2:hb:92:LEU:HD12	1.98	0.43
2:hb:103:MET:HE3	2:hb:103:MET:CA	2.49	0.43
2:j:66:VAL:HG11	2:j:99:VAL:HG21	2.00	0.43
1:A:151:GLN:OE1	1:A:180:LEU:HD23	2.19	0.42
1:D:259:LYS:HE2	1:DB:161:PHE:HA	2.01	0.42
1:GB:169:LEU:C	1:GB:169:LEU:HD23	2.44	0.42
1:GB:238:ILE:O	1:GB:242:ILE:HG12	2.19	0.42
1:M:178:ALA:O	1:M:182:ILE:HG13	2.19	0.42
1:M:225:VAL:O	1:M:225:VAL:HG12	2.19	0.42
1:MB:231:LEU:HD22	1:MB:234:ILE:HD11	2.01	0.42
1:NB:148:SER:O	1:NB:151:GLN:HG2	2.19	0.42
1:OB:248:GLU:N	1:OB:248:GLU:CD	2.76	0.42
1:PB:197:VAL:HG13	1:PB:227:CYS:SG	2.59	0.42
1:PB:224:LEU:HD21	1:SB:249:LEU:HD12	2.01	0.42
1:Q:169:LEU:HD21	1:Q:181:ILE:HD12	2.00	0.42
1:RB:167:MET:CE	1:RB:181:ILE:HG23	2.49	0.42
1:T:196:VAL:HG11	1:T:265:ALA:HB2	2.00	0.42
2:bb:51:ILE:HG21	2:bb:54:ILE:HD13	2.01	0.42
2:fb:59:ALA:HB1	2:fb:94:ILE:HD13	2.00	0.42
2:j:4:PRO:C	2:j:5:ILE:HD12	2.43	0.42
2:j:106:GLU:OE1	2:j:107:SER:N	2.52	0.42
1:C:244:ASN:OD1	1:C:244:ASN:C	2.62	0.42
1:D:216:ILE:HG13	1:D:247:ILE:HG21	2.01	0.42
1:E:201:ILE:O	1:E:201:ILE:HG13	2.19	0.42
1:F:210:MET:HE3	1:F:210:MET:CA	2.49	0.42
1:FB:176:GLU:N	1:FB:176:GLU:OE2	2.52	0.42
1:HB:169:LEU:HD12	1:HB:201:ILE:CG2	2.48	0.42
1:I:237:GLU:OE1	1:I:237:GLU:C	2.62	0.42
1:K:213:HIS:O	1:K:217:GLN:HG2	2.19	0.42
1:N:232:VAL:HG23	1:N:255:THR:OG1	2.20	0.42
1:P:167:MET:O	1:P:167:MET:HG2	2.19	0.42
1:PB:160:ILE:HD11	1:PB:166:VAL:HB	2.01	0.42
1:SB:207:VAL:HB	1:SB:238:ILE:HG23	2.00	0.42
1:T:201:ILE:O	1:T:204:VAL:HG12	2.20	0.42
1:TB:149:ALA:O	1:TB:153:LEU:HG	2.19	0.42
2:e:59:ALA:HB1	2:e:94:ILE:CD1	2.50	0.42
2:eb:27:GLU:OE1	2:eb:27:GLU:HA	2.19	0.42
2:eb:27:GLU:O	2:eb:31:ASP:OD2	2.38	0.42
2:f:100:LEU:N	2:f:100:LEU:HD23	2.34	0.42
2:i:23:HIS:CD2	2:i:23:HIS:N	2.86	0.42
1:D:236:PRO:HG3	1:R:190:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:263:GLU:OE1	1:DB:263:GLU:C	2.63	0.42
1:EB:240:GLN:CD	1:EB:240:GLN:C	2.87	0.42
1:HB:236:PRO:HB3	2:h:33:LEU:HB3	2.00	0.42
1:I:220:GLU:O	1:I:220:GLU:OE2	2.36	0.42
1:J:212:ALA:CB	1:J:242:ILE:HD12	2.49	0.42
1:KB:201:ILE:O	1:KB:204:VAL:HG12	2.19	0.42
1:L:237:GLU:OE1	1:L:237:GLU:C	2.61	0.42
1:OB:201:ILE:O	1:OB:204:VAL:HG12	2.19	0.42
1:Q:207:VAL:HG11	1:Q:242:ILE:HD11	2.00	0.42
1:R:270:ASN:OD1	1:R:270:ASN:C	2.62	0.42
1:SB:216:ILE:HD11	1:SB:247:ILE:HD13	2.02	0.42
1:T:160:ILE:HD12	1:T:166:VAL:CG2	2.50	0.42
1:T:229:ALA:HB3	1:T:252:ILE:HD12	2.01	0.42
1:TB:245:LEU:CD2	1:TB:247:ILE:HD11	2.42	0.42
2:b:5:ILE:CG2	2:b:12:LEU:HD12	2.49	0.42
2:e:109:LEU:HD12	2:e:109:LEU:O	2.18	0.42
2:eb:62:LEU:HD23	2:eb:62:LEU:C	2.45	0.42
2:h:115:GLU:C	2:h:115:GLU:OE1	2.63	0.42
2:a:43:GLY:CA	2:a:112:LEU:HD21	2.49	0.42
1:C:200:ASP:C	1:C:200:ASP:OD1	2.62	0.42
1:D:201:ILE:O	1:D:204:VAL:HG12	2.19	0.42
1:G:178:ALA:HA	1:G:181:ILE:HD12	2.01	0.42
1:N:240:GLN:CD	1:N:240:GLN:C	2.87	0.42
1:Q:186:LEU:O	1:Q:189:VAL:HG12	2.18	0.42
1:RB:236:PRO:HB3	2:fb:33:LEU:HB3	2.00	0.42
2:cb:77:VAL:HG13	2:cb:100:LEU:HB2	2.02	0.42
2:i:66:VAL:HG23	2:i:76:VAL:CG1	2.49	0.42
2:ib:1:MET:O	2:ib:1:MET:HE3	2.20	0.42
1:A:212:ALA:O	1:A:216:ILE:HD12	2.20	0.42
2:ab:14:ILE:HD11	2:ab:32:LEU:HD13	2.00	0.42
1:C:198:LEU:N	1:C:198:LEU:HD12	2.34	0.42
1:EB:230:MET:HE1	1:EB:265:ALA:HA	2.00	0.42
1:H:201:ILE:O	1:H:204:VAL:HG12	2.18	0.42
1:J:209:THR:HG23	1:J:245:LEU:HD21	2.02	0.42
1:JB:263:GLU:C	1:JB:263:GLU:OE1	2.63	0.42
1:LB:160:ILE:HD13	1:LB:160:ILE:N	2.34	0.42
1:LB:240:GLN:C	1:LB:240:GLN:CD	2.88	0.42
1:QB:193:ARG:N	1:QB:193:ARG:HD2	2.34	0.42
1:TB:193:ARG:N	1:TB:193:ARG:HD2	2.34	0.42
2:gb:47:ASP:OD1	2:gb:47:ASP:C	2.63	0.42
2:gb:110:GLU:C	2:gb:110:GLU:CD	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:33:LEU:O	2:h:36:ILE:HG22	2.19	0.42
2:h:96:PHE:HB3	2:h:99:VAL:HB	2.01	0.42
2:a:115:GLU:HA	2:a:115:GLU:OE2	2.19	0.42
1:BB:164:ILE:HG22	1:BB:165:SER:N	2.35	0.42
1:F:201:ILE:O	1:F:204:VAL:HG12	2.20	0.42
1:FB:269:THR:HG21	1:FB:271:ARG:HH21	1.83	0.42
1:LB:149:ALA:O	1:LB:153:LEU:HG	2.19	0.42
1:LB:207:VAL:O	1:LB:207:VAL:HG12	2.20	0.42
1:M:264:ARG:NH1	1:M:264:ARG:HG3	2.34	0.42
1:MB:204:VAL:O	1:MB:204:VAL:HG13	2.20	0.42
1:P:161:PHE:HB2	1:P:164:ILE:HD12	2.01	0.42
1:PB:231:LEU:HD22	1:PB:234:ILE:HD11	2.02	0.42
1:Q:160:ILE:HD11	1:Q:166:VAL:CG2	2.50	0.42
1:QB:213:HIS:CE1	1:QB:217:GLN:CG	3.03	0.42
1:RB:160:ILE:HD11	1:RB:166:VAL:CG1	2.49	0.42
2:c:110:GLU:C	2:c:110:GLU:CD	2.88	0.42
2:d:105:LEU:HD13	2:db:6:LEU:HD22	2.02	0.42
2:db:105:LEU:HD23	2:db:105:LEU:C	2.45	0.42
2:h:48:ILE:HB	2:h:51:ILE:HD12	2.02	0.42
2:ib:72:MET:HE3	2:ib:72:MET:O	2.20	0.42
2:j:60:LYS:O	2:j:64:ASP:OD2	2.37	0.42
1:G:149:ALA:O	1:G:153:LEU:HG	2.19	0.42
1:HB:149:ALA:O	1:HB:153:LEU:HG	2.19	0.42
1:M:186:LEU:O	1:M:189:VAL:HG12	2.20	0.42
1:NB:195:GLU:N	1:NB:195:GLU:OE2	2.52	0.42
1:P:175:THR:HG23	1:P:210:MET:SD	2.60	0.42
1:S:240:GLN:CD	1:S:240:GLN:C	2.87	0.42
1:SB:204:VAL:O	1:SB:204:VAL:HG13	2.20	0.42
1:T:191:LYS:HE2	1:T:191:LYS:HB3	1.89	0.42
1:TB:238:ILE:O	1:TB:242:ILE:HG12	2.19	0.42
2:c:78:VAL:HG21	2:c:96:PHE:HE2	1.85	0.42
2:eb:16:ILE:HG22	2:eb:51:ILE:HD11	2.00	0.42
2:f:81:ILE:HD12	2:f:81:ILE:N	2.34	0.42
2:fb:66:VAL:CG2	2:fb:99:VAL:HG21	2.49	0.42
2:fb:72:MET:O	2:fb:72:MET:HE3	2.19	0.42
2:ib:48:ILE:HD11	2:ib:81:ILE:HG12	2.02	0.42
1:B:212:ALA:HB1	1:B:242:ILE:HD12	2.01	0.42
1:C:204:VAL:HG11	1:C:207:VAL:HG23	2.01	0.42
1:CB:220:GLU:OE1	1:CB:220:GLU:HA	2.19	0.42
1:F:161:PHE:CE1	1:FB:273:ILE:CD1	3.02	0.42
1:G:170:ILE:HG22	1:GB:153:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:167:MET:O	1:GB:167:MET:HG3	2.19	0.42
1:H:200:ASP:OD1	1:H:200:ASP:C	2.62	0.42
1:IB:222:VAL:HG21	1:IB:229:ALA:HB2	2.02	0.42
1:IB:230:MET:HE1	1:IB:265:ALA:CA	2.50	0.42
1:M:262:MET:HA	1:M:262:MET:CE	2.40	0.42
2:bb:21:ASP:OD2	2:bb:22:ASP:N	2.52	0.42
2:e:6:LEU:HD22	2:eb:105:LEU:CD1	2.49	0.42
2:f:54:ILE:HG22	2:f:55:ASP:O	2.20	0.42
2:gb:59:ALA:HB1	2:gb:94:ILE:HD12	2.02	0.42
2:a:43:GLY:HA3	2:a:112:LEU:HD21	2.01	0.42
1:DB:238:ILE:O	1:DB:242:ILE:HG12	2.19	0.42
1:E:167:MET:CE	1:E:181:ILE:HG23	2.50	0.42
1:G:237:GLU:C	1:G:237:GLU:CD	2.88	0.42
1:IB:204:VAL:HG13	1:IB:204:VAL:O	2.20	0.42
1:J:201:ILE:O	1:J:204:VAL:HG12	2.20	0.42
1:N:178:ALA:O	1:N:181:ILE:HG22	2.20	0.42
1:N:201:ILE:O	1:N:204:VAL:HG12	2.20	0.42
1:PB:230:MET:HB3	1:PB:253:ILE:O	2.20	0.42
1:Q:263:GLU:CD	1:Q:263:GLU:C	2.88	0.42
1:RB:186:LEU:O	1:RB:189:VAL:HG12	2.20	0.42
1:SB:155:ALA:HB1	1:SB:167:MET:HE2	2.00	0.42
2:d:33:LEU:O	2:d:36:ILE:HG22	2.18	0.42
2:g:53:PHE:CD1	2:g:53:PHE:C	2.97	0.42
2:hb:33:LEU:O	2:hb:36:ILE:HG22	2.20	0.42
2:j:110:GLU:CD	2:j:110:GLU:C	2.87	0.42
2:jb:82:GLN:OE1	2:jb:82:GLN:HA	2.20	0.42
1:A:186:LEU:HB3	1:TB:236:PRO:HB3	2.01	0.42
1:AB:255:THR:HG22	1:AB:264:ARG:NH2	2.35	0.42
1:C:269:THR:C	1:C:270:ASN:OD1	2.63	0.42
1:HB:188:GLY:O	1:HB:192:ASN:OD1	2.38	0.42
1:P:183:GLU:O	1:P:187:ILE:HD12	2.20	0.42
2:g:57:PHE:O	2:g:61:ILE:HG12	2.19	0.42
1:A:255:THR:HG22	1:A:264:ARG:CZ	2.50	0.41
1:BB:207:VAL:CG1	1:BB:211:VAL:HG23	2.50	0.41
1:CB:196:VAL:HG21	1:CB:230:MET:HE3	2.02	0.41
1:EB:237:GLU:C	1:EB:237:GLU:CD	2.87	0.41
1:FB:149:ALA:O	1:FB:153:LEU:HG	2.19	0.41
1:FB:221:ALA:HA	2:db:90:ILE:HD11	2.02	0.41
1:GB:157:LEU:HD22	1:GB:188:GLY:HA3	2.01	0.41
1:IB:200:ASP:OD2	1:IB:200:ASP:C	2.63	0.41
1:P:201:ILE:HD11	1:P:234:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:204:VAL:HG13	1:R:204:VAL:O	2.19	0.41
1:S:167:MET:O	1:S:167:MET:HG3	2.19	0.41
1:SB:240:GLN:C	1:SB:240:GLN:CD	2.87	0.41
1:T:179:LYS:O	1:T:183:GLU:OE2	2.37	0.41
1:T:237:GLU:OE2	1:T:238:ILE:HD13	2.19	0.41
2:c:52:ASP:OD2	2:c:52:ASP:N	2.52	0.41
2:e:43:GLY:CA	2:e:112:LEU:HD21	2.50	0.41
2:g:94:ILE:HD12	2:g:94:ILE:N	2.35	0.41
2:gb:85:VAL:O	2:gb:89:LEU:HG	2.20	0.41
1:B:245:LEU:HG	1:B:245:LEU:O	2.19	0.41
1:D:236:PRO:HB3	1:R:186:LEU:HB3	2.02	0.41
1:F:209:THR:CG2	1:F:245:LEU:HD21	2.49	0.41
1:G:263:GLU:OE2	1:G:264:ARG:N	2.53	0.41
1:GB:210:MET:HE2	1:GB:210:MET:CA	2.46	0.41
1:HB:216:ILE:CD1	1:HB:247:ILE:HG21	2.50	0.41
1:L:237:GLU:OE1	1:L:238:ILE:N	2.54	0.41
1:LB:175:THR:HG23	1:LB:210:MET:SD	2.60	0.41
1:M:156:PRO:HB3	1:MB:170:ILE:HD12	2.02	0.41
1:N:273:ILE:HD11	1:NB:161:PHE:CE1	2.55	0.41
1:TB:162:GLU:OE2	1:TB:162:GLU:HA	2.20	0.41
2:d:32:LEU:C	2:d:32:LEU:HD23	2.45	0.41
2:fb:100:LEU:HD12	2:fb:100:LEU:N	2.33	0.41
2:g:29:GLN:HG3	2:g:65:VAL:HG22	2.01	0.41
1:A:207:VAL:HG13	1:A:211:VAL:CG2	2.38	0.41
2:a:38:GLU:OE2	2:a:38:GLU:C	2.63	0.41
1:B:264:ARG:HH11	1:B:264:ARG:HG3	1.85	0.41
1:F:259:LYS:HD3	1:F:259:LYS:C	2.45	0.41
1:F:260:LYS:HE3	1:F:260:LYS:HA	2.03	0.41
1:F:263:GLU:OE1	1:F:264:ARG:N	2.53	0.41
1:I:248:GLU:CD	1:I:248:GLU:N	2.78	0.41
1:K:245:LEU:HD23	1:K:247:ILE:CD1	2.44	0.41
1:NB:164:ILE:HG22	1:NB:165:SER:N	2.35	0.41
1:QB:253:ILE:HG22	1:QB:254:THR:N	2.36	0.41
2:bb:52:ASP:OD2	2:bb:52:ASP:C	2.63	0.41
2:c:23:HIS:O	2:c:27:GLU:HG2	2.19	0.41
2:cb:1:MET:SD	2:cb:1:MET:C	3.03	0.41
2:cb:35:LYS:O	2:cb:39:THR:HG23	2.21	0.41
2:db:110:GLU:OE1	2:db:111:LYS:N	2.53	0.41
2:fb:71:LEU:O	2:fb:71:LEU:HD12	2.20	0.41
2:ib:14:ILE:CG2	2:ib:15:SER:N	2.83	0.41
1:AB:216:ILE:HD11	1:AB:247:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:162:GLU:O	1:BB:163:LYS:HB2	2.21	0.41
1:D:212:ALA:HB1	1:D:242:ILE:HD13	2.02	0.41
1:EB:237:GLU:C	1:EB:237:GLU:OE2	2.63	0.41
1:G:158:LEU:HD21	1:GB:168:PRO:HB3	2.03	0.41
1:GB:160:ILE:HD11	1:GB:166:VAL:HB	2.01	0.41
1:HB:212:ALA:HB1	1:HB:242:ILE:CD1	2.50	0.41
1:IB:186:LEU:HD21	1:IB:221:ALA:HB1	2.02	0.41
1:J:273:ILE:HD11	1:JB:161:PHE:CZ	2.56	0.41
1:L:270:ASN:O	1:L:271:ARG:HG3	2.20	0.41
1:MB:168:PRO:O	1:MB:169:LEU:HD12	2.21	0.41
1:OB:207:VAL:HB	1:OB:238:ILE:HG23	2.03	0.41
2:c:96:PHE:HB3	2:c:99:VAL:HB	2.02	0.41
2:e:29:GLN:HG3	2:e:65:VAL:HG22	2.02	0.41
2:fb:86:ALA:O	2:fb:90:ILE:HG22	2.21	0.41
2:ib:42:ARG:NH2	2:ib:116:LEU:HD22	2.36	0.41
1:A:190:VAL:HG21	1:TB:236:PRO:HG3	2.02	0.41
1:B:218:ALA:O	1:B:222:VAL:HG13	2.21	0.41
1:CB:201:ILE:O	1:CB:204:VAL:HG12	2.20	0.41
1:EB:231:LEU:HB2	1:EB:252:ILE:HD11	2.02	0.41
1:H:186:LEU:O	1:H:189:VAL:HG12	2.21	0.41
1:I:178:ALA:HA	1:I:181:ILE:HG22	2.03	0.41
1:Q:205:PRO:HA	1:Q:235:ARG:HH21	1.86	0.41
1:Q:213:HIS:O	1:Q:216:ILE:HG22	2.21	0.41
1:Q:258:MET:HE3	1:Q:259:LYS:N	2.36	0.41
1:QB:165:SER:O	1:QB:198:LEU:HD12	2.20	0.41
1:RB:157:LEU:HD22	1:RB:188:GLY:HA3	2.02	0.41
2:bb:63:GLY:O	2:bb:66:VAL:HG12	2.20	0.41
2:db:77:VAL:HG23	2:db:112:LEU:HD13	2.01	0.41
1:BB:257:THR:HG23	1:BB:260:LYS:HG2	2.03	0.41
1:F:263:GLU:CD	1:F:263:GLU:C	2.89	0.41
1:HB:240:GLN:C	1:HB:240:GLN:CD	2.88	0.41
1:I:183:GLU:O	1:I:187:ILE:HD12	2.21	0.41
1:IB:229:ALA:O	1:IB:252:ILE:HG13	2.20	0.41
1:K:201:ILE:O	1:K:204:VAL:HG12	2.20	0.41
1:KB:220:GLU:OE1	1:KB:220:GLU:HA	2.20	0.41
1:N:167:MET:HE1	1:N:181:ILE:HD11	2.01	0.41
1:N:207:VAL:O	1:N:207:VAL:HG12	2.20	0.41
1:O:156:PRO:HB3	1:OB:170:ILE:HD12	2.03	0.41
1:Q:183:GLU:O	1:Q:187:ILE:HG12	2.21	0.41
1:Q:207:VAL:O	1:Q:241:THR:HG21	2.20	0.41
1:QB:160:ILE:HD12	1:QB:166:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QB:212:ALA:O	1:QB:216:ILE:HG12	2.21	0.41
2:bb:94:ILE:HG22	2:bb:96:PHE:CE2	2.56	0.41
2:c:3:ILE:HD13	2:c:3:ILE:N	2.35	0.41
2:db:32:LEU:O	2:db:36:ILE:HG22	2.21	0.41
2:f:23:HIS:ND1	2:f:24:THR:N	2.69	0.41
2:g:70:LYS:HD2	2:g:70:LYS:C	2.46	0.41
2:hb:16:ILE:HG22	2:hb:51:ILE:HD11	2.02	0.41
2:hb:92:LEU:N	2:hb:92:LEU:HD23	2.36	0.41
2:i:77:VAL:HG23	2:i:112:LEU:HD13	2.02	0.41
1:AB:168:PRO:O	1:AB:169:LEU:HD22	2.21	0.41
1:C:170:ILE:HG22	1:CB:153:LEU:HD22	1.99	0.41
1:F:160:ILE:HD12	1:F:166:VAL:HG11	2.02	0.41
1:F:217:GLN:HA	1:F:217:GLN:OE1	2.21	0.41
1:G:200:ASP:OD2	1:G:200:ASP:C	2.63	0.41
1:GB:220:GLU:HA	1:GB:220:GLU:OE2	2.21	0.41
1:H:167:MET:CE	1:H:181:ILE:HG23	2.50	0.41
1:HB:183:GLU:O	1:HB:187:ILE:HG12	2.20	0.41
1:I:178:ALA:O	1:I:181:ILE:HG22	2.21	0.41
1:JB:269:THR:O	1:JB:270:ASN:OD1	2.39	0.41
1:MB:216:ILE:HD11	1:MB:247:ILE:HG23	2.02	0.41
1:MB:230:MET:HE1	1:MB:265:ALA:N	2.35	0.41
1:O:204:VAL:HG11	1:O:207:VAL:CG2	2.51	0.41
1:QB:160:ILE:HD12	1:QB:166:VAL:CG2	2.51	0.41
1:SB:248:GLU:N	1:SB:248:GLU:CD	2.79	0.41
1:TB:179:LYS:N	1:TB:179:LYS:HD2	2.35	0.41
2:bb:45:VAL:HG13	2:bb:77:VAL:CG2	2.51	0.41
2:i:63:GLY:O	2:i:66:VAL:HG12	2.19	0.41
2:j:12:LEU:O	2:j:13:LEU:HD23	2.21	0.41
2:jb:71:LEU:HD12	2:jb:71:LEU:O	2.21	0.41
2:a:106:GLU:C	2:a:106:GLU:OE2	2.64	0.41
1:G:264:ARG:HG3	1:G:264:ARG:HH11	1.86	0.41
1:K:274:VAL:HG23	1:K:274:VAL:O	2.21	0.41
1:KB:200:ASP:OD2	1:KB:258:MET:HE2	2.20	0.41
1:KB:236:PRO:HB3	1:L:186:LEU:HB3	2.02	0.41
1:M:180:LEU:N	1:M:180:LEU:HD23	2.36	0.41
1:N:195:GLU:N	1:N:195:GLU:OE2	2.53	0.41
1:O:155:ALA:HB1	1:O:167:MET:HE2	2.03	0.41
1:RB:157:LEU:C	1:RB:158:LEU:HD12	2.46	0.41
2:eb:58:ILE:HD12	2:eb:58:ILE:H	1.85	0.41
1:A:247:ILE:HG22	1:A:249:LEU:CD2	2.50	0.41
1:AB:149:ALA:O	1:AB:153:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:GLN:OE1	1:C:217:GLN:HA	2.21	0.41
1:CB:185:LEU:HD11	1:CB:197:VAL:HG21	2.03	0.41
1:CB:249:LEU:HB3	1:CB:252:ILE:CG2	2.51	0.41
1:EB:191:LYS:HB3	1:EB:191:LYS:NZ	2.36	0.41
1:EB:222:VAL:HG21	1:EB:229:ALA:HB2	2.03	0.41
1:G:231:LEU:HD12	1:G:231:LEU:C	2.46	0.41
1:H:241:THR:O	1:H:245:LEU:HD23	2.21	0.41
1:H:270:ASN:O	1:H:271:ARG:HG3	2.21	0.41
1:I:204:VAL:HG13	1:I:238:ILE:HD11	2.02	0.41
1:KB:198:LEU:HD12	1:KB:198:LEU:N	2.36	0.41
1:KB:212:ALA:O	1:KB:216:ILE:HD12	2.20	0.41
1:KB:249:LEU:HD12	1:L:224:LEU:CD2	2.51	0.41
1:M:167:MET:HE1	1:M:181:ILE:HD12	2.03	0.41
1:N:153:LEU:HB3	1:NB:170:ILE:HG21	2.02	0.41
1:P:237:GLU:OE1	1:P:237:GLU:O	2.39	0.41
1:QB:238:ILE:O	1:QB:242:ILE:HG12	2.21	0.41
1:QB:247:ILE:HG22	1:QB:249:LEU:CD2	2.51	0.41
1:RB:169:LEU:HD12	1:RB:201:ILE:HG22	2.02	0.41
2:b:19:GLU:CD	2:b:19:GLU:C	2.89	0.41
2:db:43:GLY:CA	2:db:112:LEU:HD21	2.44	0.41
2:f:51:ILE:CG2	2:f:54:ILE:HD11	2.51	0.41
2:h:109:LEU:HD12	2:h:109:LEU:O	2.21	0.41
2:hb:71:LEU:HD23	2:hb:71:LEU:C	2.46	0.41
2:ib:12:LEU:O	2:ib:13:LEU:HD22	2.21	0.41
2:j:94:ILE:O	2:j:94:ILE:HG22	2.19	0.41
1:F:201:ILE:HG12	1:F:231:LEU:HD11	2.03	0.41
1:K:232:VAL:HG22	1:K:233:GLY:N	2.36	0.41
1:N:191:LYS:HA	1:N:191:LYS:HE3	2.03	0.41
1:OB:253:ILE:HG22	1:OB:254:THR:N	2.36	0.41
2:d:62:LEU:HD23	2:d:62:LEU:C	2.45	0.41
2:eb:114:GLN:OE1	2:eb:115:GLU:N	2.54	0.41
2:fb:115:GLU:OE2	2:fb:116:LEU:HD22	2.20	0.41
2:gb:103:MET:HA	2:gb:103:MET:HE3	2.03	0.41
2:h:20:LEU:HD13	2:h:24:THR:OG1	2.21	0.41
2:h:56:ALA:HA	2:h:92:LEU:HD23	2.03	0.41
2:i:14:ILE:HD13	2:i:28:PHE:HE1	1.86	0.41
2:ib:71:LEU:HD12	2:ib:71:LEU:O	2.22	0.41
1:D:161:PHE:CE2	1:DB:273:ILE:CD1	3.04	0.40
1:H:224:LEU:HD12	1:JB:243:VAL:HG23	2.03	0.40
1:KB:167:MET:SD	1:KB:169:LEU:HD21	2.61	0.40
1:N:196:VAL:HG11	1:N:265:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NB:213:HIS:O	1:NB:217:GLN:OE1	2.39	0.40
2:b:29:GLN:NE2	2:b:68:MET:HE1	2.36	0.40
2:cb:33:LEU:HD11	2:cb:68:MET:HE3	2.03	0.40
2:cb:58:ILE:HD12	2:cb:58:ILE:N	2.29	0.40
2:d:89:LEU:HD23	2:d:89:LEU:N	2.36	0.40
2:e:110:GLU:OE1	2:e:111:LYS:N	2.54	0.40
2:f:87:ILE:O	2:f:90:ILE:HG22	2.21	0.40
1:AB:238:ILE:O	1:AB:242:ILE:HG12	2.20	0.40
1:D:185:LEU:HD11	1:D:197:VAL:HG21	2.02	0.40
1:DB:228:GLN:C	1:DB:228:GLN:OE1	2.63	0.40
1:I:231:LEU:HD23	1:I:231:LEU:O	2.21	0.40
2:b:70:LYS:CD	2:b:70:LYS:C	2.94	0.40
2:db:110:GLU:C	2:db:110:GLU:CD	2.89	0.40
2:eb:110:GLU:CD	2:eb:110:GLU:C	2.89	0.40
2:f:85:VAL:HG12	2:f:89:LEU:HD13	2.03	0.40
2:a:33:LEU:O	2:a:36:ILE:HG22	2.22	0.40
1:D:153:LEU:HD22	1:DB:170:ILE:CG2	2.51	0.40
1:D:240:GLN:CD	1:D:240:GLN:C	2.90	0.40
1:I:204:VAL:HG13	1:I:204:VAL:O	2.21	0.40
1:QB:157:LEU:HD11	1:QB:165:SER:HB3	2.04	0.40
1:SB:210:MET:HE3	1:SB:210:MET:CA	2.43	0.40
1:TB:269:THR:O	1:TB:269:THR:CG2	2.66	0.40
2:c:75:LYS:HD2	2:c:75:LYS:N	2.35	0.40
2:f:62:LEU:HD22	2:f:96:PHE:CZ	2.57	0.40
2:gb:16:ILE:HD12	2:gb:48:ILE:HG22	2.03	0.40
2:gb:82:GLN:OE1	2:gb:82:GLN:HA	2.21	0.40
2:i:36:ILE:HD11	2:i:74:ALA:CB	2.51	0.40
2:j:36:ILE:HD12	2:j:44:VAL:HG21	2.03	0.40
2:jb:45:VAL:HG13	2:jb:77:VAL:HG23	2.03	0.40
1:AB:210:MET:SD	1:AB:210:MET:C	3.04	0.40
1:B:222:VAL:HG21	1:B:229:ALA:HB2	2.03	0.40
1:BB:160:ILE:HG22	1:BB:161:PHE:CD2	2.56	0.40
1:BB:204:VAL:O	1:BB:204:VAL:HG13	2.20	0.40
1:D:149:ALA:O	1:D:153:LEU:HD11	2.21	0.40
1:E:153:LEU:HD22	1:EB:170:ILE:CG2	2.51	0.40
1:G:242:ILE:HG23	1:G:247:ILE:HD13	2.02	0.40
1:J:147:LYS:O	1:J:151:GLN:HG2	2.22	0.40
1:N:178:ALA:HA	1:N:181:ILE:HG22	2.03	0.40
1:O:221:ALA:HA	2:g:90:ILE:HD11	2.04	0.40
1:OB:207:VAL:HG13	1:OB:211:VAL:CG1	2.51	0.40
1:OB:249:LEU:HB3	1:OB:252:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PB:149:ALA:O	1:PB:153:LEU:HG	2.21	0.40
1:PB:186:LEU:HD21	1:PB:221:ALA:HB1	2.03	0.40
1:Q:220:GLU:OE1	1:Q:220:GLU:HA	2.20	0.40
1:RB:222:VAL:CG2	1:RB:227:CYS:HB3	2.49	0.40
1:S:250:ASP:OD2	1:S:250:ASP:N	2.54	0.40
1:TB:164:ILE:HD12	1:TB:164:ILE:N	2.36	0.40
2:b:29:GLN:HG3	2:b:65:VAL:CG2	2.51	0.40
2:bb:43:GLY:HA3	2:bb:112:LEU:HD21	2.04	0.40
2:cb:47:ASP:OD2	2:cb:47:ASP:C	2.62	0.40
2:d:53:PHE:CD1	2:d:53:PHE:C	3.00	0.40
2:f:106:GLU:OE1	2:f:107:SER:N	2.54	0.40
2:gb:100:LEU:HD22	2:gb:100:LEU:H	1.86	0.40
2:hb:81:ILE:HD12	2:hb:81:ILE:N	2.35	0.40
2:hb:88:THR:O	2:hb:92:LEU:HG	2.22	0.40
1:AB:167:MET:HE1	1:AB:181:ILE:HG23	2.03	0.40
1:CB:212:ALA:O	1:CB:216:ILE:HD12	2.21	0.40
1:F:167:MET:CE	1:F:181:ILE:HG23	2.52	0.40
1:H:169:LEU:CD2	1:H:173:ILE:HD11	2.52	0.40
1:IB:197:VAL:C	1:IB:198:LEU:HD12	2.46	0.40
1:IB:247:ILE:HG22	1:IB:249:LEU:HD22	2.04	0.40
1:L:191:LYS:NZ	1:L:191:LYS:HB3	2.36	0.40
1:M:218:ALA:O	1:M:222:VAL:HG12	2.21	0.40
1:MB:149:ALA:O	1:MB:153:LEU:HG	2.21	0.40
1:MB:262:MET:HA	1:MB:262:MET:CE	2.43	0.40
1:NB:164:ILE:HD12	1:NB:164:ILE:N	2.36	0.40
1:P:269:THR:HG21	1:P:271:ARG:NH2	2.37	0.40
1:Q:178:ALA:O	1:Q:181:ILE:CG2	2.69	0.40
1:SB:212:ALA:O	1:SB:216:ILE:HD12	2.21	0.40
2:c:105:LEU:HD13	2:cb:6:LEU:HD22	2.02	0.40
2:cb:17:GLN:N	2:cb:17:GLN:OE1	2.55	0.40
2:d:66:VAL:CG2	2:d:99:VAL:HG21	2.49	0.40
2:hb:47:ASP:OD2	2:hb:47:ASP:C	2.64	0.40
2:j:54:ILE:HG22	2:j:55:ASP:O	2.22	0.40
2:j:86:ALA:O	2:j:90:ILE:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	AB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	B	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	BB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	C	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	CB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	D	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	DB	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
1	E	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	EB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	F	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	FB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	G	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	GB	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	H	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	HB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	I	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	IB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	J	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	JB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	K	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	KB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	L	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	LB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	M	130/278 (47%)	119 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	N	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
1	NB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	O	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	OB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	P	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	PB	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	Q	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	QB	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
1	R	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	RB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	S	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	SB	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	T	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	TB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
2	a	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	ab	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	b	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	bb	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	c	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	cb	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	d	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	db	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	e	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	eb	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	f	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	fb	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	g	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	gb	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	h	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	hb	116/118 (98%)	114 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	i	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	ib	116/118 (98%)	116 (100%)	0	0	100	100
2	j	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	jb	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
All	All	7520/13480 (56%)	7271 (97%)	249 (3%)	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	114/247 (46%)	112 (98%)	2 (2%)	51	66
1	AB	114/247 (46%)	111 (97%)	3 (3%)	40	59
1	B	114/247 (46%)	114 (100%)	0	100	100
1	BB	114/247 (46%)	114 (100%)	0	100	100
1	C	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	CB	114/247 (46%)	114 (100%)	0	100	100
1	D	114/247 (46%)	114 (100%)	0	100	100
1	DB	114/247 (46%)	112 (98%)	2 (2%)	51	66
1	E	114/247 (46%)	111 (97%)	3 (3%)	40	59
1	EB	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	F	114/247 (46%)	112 (98%)	2 (2%)	51	66
1	FB	114/247 (46%)	112 (98%)	2 (2%)	51	66
1	G	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	GB	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	H	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	HB	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	I	114/247 (46%)	110 (96%)	4 (4%)	32	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IB	114/247 (46%)	112 (98%)	2 (2%)	51	66
1	J	114/247 (46%)	109 (96%)	5 (4%)	25	48
1	JB	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	K	114/247 (46%)	110 (96%)	4 (4%)	32	53
1	KB	114/247 (46%)	112 (98%)	2 (2%)	51	66
1	L	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	LB	114/247 (46%)	112 (98%)	2 (2%)	51	66
1	M	114/247 (46%)	109 (96%)	5 (4%)	25	48
1	MB	114/247 (46%)	111 (97%)	3 (3%)	40	59
1	N	114/247 (46%)	112 (98%)	2 (2%)	51	66
1	NB	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	O	114/247 (46%)	111 (97%)	3 (3%)	40	59
1	OB	114/247 (46%)	114 (100%)	0	100	100
1	P	114/247 (46%)	110 (96%)	4 (4%)	32	53
1	PB	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	Q	114/247 (46%)	111 (97%)	3 (3%)	40	59
1	QB	114/247 (46%)	110 (96%)	4 (4%)	32	53
1	R	114/247 (46%)	111 (97%)	3 (3%)	40	59
1	RB	114/247 (46%)	112 (98%)	2 (2%)	51	66
1	S	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	SB	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	T	114/247 (46%)	113 (99%)	1 (1%)	70	74
1	TB	114/247 (46%)	114 (100%)	0	100	100
2	a	99/99 (100%)	96 (97%)	3 (3%)	36	56
2	ab	99/99 (100%)	95 (96%)	4 (4%)	28	51
2	b	99/99 (100%)	96 (97%)	3 (3%)	36	56
2	bb	99/99 (100%)	96 (97%)	3 (3%)	36	56
2	c	99/99 (100%)	96 (97%)	3 (3%)	36	56
2	cb	99/99 (100%)	95 (96%)	4 (4%)	28	51
2	d	99/99 (100%)	98 (99%)	1 (1%)	68	73
2	db	99/99 (100%)	97 (98%)	2 (2%)	48	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	e	99/99 (100%)	99 (100%)	0	100	100
2	eb	99/99 (100%)	97 (98%)	2 (2%)	48	64
2	f	99/99 (100%)	96 (97%)	3 (3%)	36	56
2	fb	99/99 (100%)	98 (99%)	1 (1%)	68	73
2	g	99/99 (100%)	96 (97%)	3 (3%)	36	56
2	gb	99/99 (100%)	99 (100%)	0	100	100
2	h	99/99 (100%)	96 (97%)	3 (3%)	36	56
2	hb	99/99 (100%)	97 (98%)	2 (2%)	48	64
2	i	99/99 (100%)	98 (99%)	1 (1%)	68	73
2	ib	99/99 (100%)	97 (98%)	2 (2%)	48	64
2	j	99/99 (100%)	99 (100%)	0	100	100
2	jb	99/99 (100%)	99 (100%)	0	100	100
All	All	6540/11860 (55%)	6425 (98%)	115 (2%)	51	66

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LEU
1	A	254	THR
1	AB	170	ILE
1	AB	234	ILE
1	AB	257	THR
2	a	5	ILE
2	a	28	PHE
2	a	50	SER
2	ab	28	PHE
2	ab	30	GLU
2	ab	50	SER
2	ab	66	VAL
1	C	272	GLU
1	DB	170	ILE
1	DB	196	VAL
1	E	153	LEU
1	E	170	ILE
1	E	257	THR
1	EB	257	THR
1	F	176	GLU
1	F	257	THR

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Mol	Chain	Res	Type
1	FB	257	THR
1	FB	268	LEU
1	G	266	LEU
1	GB	254	THR
1	H	192	ASN
1	HB	254	THR
1	I	153	LEU
1	I	181	ILE
1	I	252	ILE
1	I	268	LEU
1	IB	182	ILE
1	IB	232	VAL
1	J	153	LEU
1	J	191	LYS
1	J	220	GLU
1	J	224	LEU
1	J	234	ILE
1	JB	217	GLN
1	K	162	GLU
1	K	191	LYS
1	K	250	ASP
1	K	257	THR
1	KB	162	GLU
1	KB	243	VAL
1	L	259	LYS
1	LB	151	GLN
1	LB	170	ILE
1	M	158	LEU
1	M	181	ILE
1	M	209	THR
1	M	223	ARG
1	M	257	THR
1	MB	192	ASN
1	MB	240	GLN
1	MB	249	LEU
1	N	170	ILE
1	N	181	ILE
1	NB	191	LYS
1	O	180	LEU
1	O	191	LYS
1	O	234	ILE
1	P	170	ILE

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Mol	Chain	Res	Type
1	P	223	ARG
1	P	249	LEU
1	P	257	THR
1	PB	198	LEU
1	Q	181	ILE
1	Q	192	ASN
1	Q	234	ILE
1	QB	213	HIS
1	QB	223	ARG
1	QB	225	VAL
1	QB	254	THR
1	R	254	THR
1	R	257	THR
1	R	268	LEU
1	RB	192	ASN
1	RB	257	THR
1	S	191	LYS
1	SB	257	THR
1	T	217	GLN
2	b	28	PHE
2	b	89	LEU
2	b	106	GLU
2	bb	15	SER
2	bb	66	VAL
2	bb	114	GLN
2	c	12	LEU
2	c	14	ILE
2	c	116	LEU
2	cb	7	LYS
2	cb	17	GLN
2	cb	28	PHE
2	cb	66	VAL
2	d	28	PHE
2	db	17	GLN
2	db	28	PHE
2	eb	50	SER
2	eb	62	LEU
2	f	12	LEU
2	f	17	GLN
2	f	28	PHE
2	fb	28	PHE
2	g	28	PHE

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Mol	Chain	Res	Type
2	g	85	VAL
2	g	113	LYS
2	h	14	ILE
2	h	28	PHE
2	h	50	SER
2	hb	20	LEU
2	hb	28	PHE
2	i	66	VAL
2	ib	12	LEU
2	ib	23	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	37	HIS
1	BB	192	ASN
1	C	213	HIS
1	C	251	GLN
1	E	213	HIS
1	EB	214	HIS
1	FB	213	HIS
1	FB	214	HIS
1	G	214	HIS
1	GB	213	HIS
1	H	214	HIS
1	J	213	HIS
1	JB	251	GLN
1	K	214	HIS
1	K	251	GLN
1	L	192	ASN
1	L	214	HIS
1	L	240	GLN
1	L	251	GLN
1	LB	151	GLN
1	LB	214	HIS
1	MB	192	ASN
1	MB	240	GLN
1	MB	251	GLN
1	N	192	ASN
1	N	251	GLN
1	NB	213	HIS
1	NB	270	ASN

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Mol	Chain	Res	Type
1	O	151	GLN
1	O	192	ASN
1	O	251	GLN
1	P	214	HIS
1	QB	213	HIS
1	R	151	GLN
1	S	192	ASN
1	SB	192	ASN
1	T	214	HIS
1	T	217	GLN
1	TB	244	ASN
2	b	114	GLN
2	c	23	HIS
2	d	37	HIS
2	e	29	GLN
2	eb	29	GLN
2	eb	37	HIS
2	fb	37	HIS
2	fb	114	GLN
2	gb	29	GLN
2	h	23	HIS
2	h	114	GLN
2	hb	37	HIS
2	i	23	HIS
2	ib	114	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

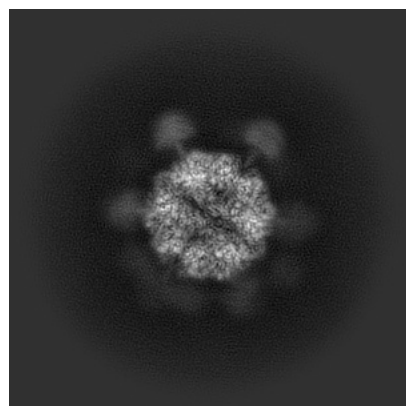
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70112. These allow visual inspection of the internal detail of the map and identification of artifacts.

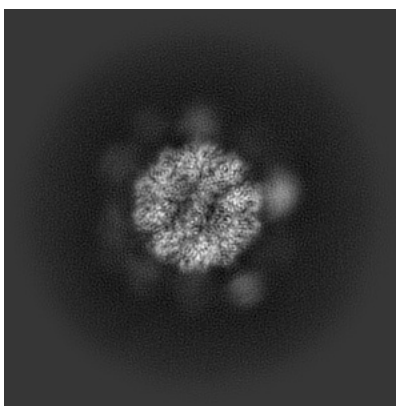
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

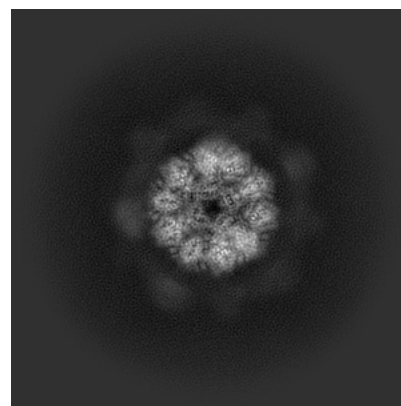
6.1.1 Primary map



X

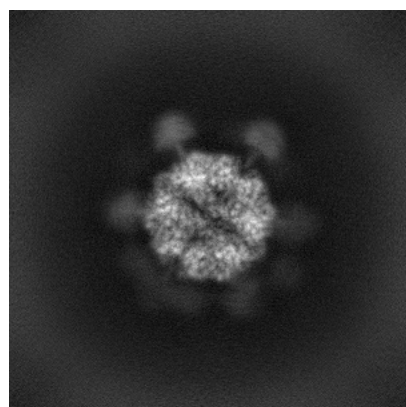


Y

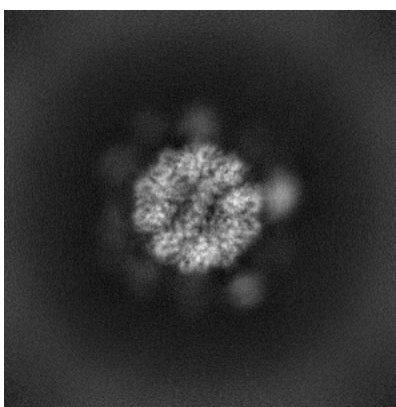


Z

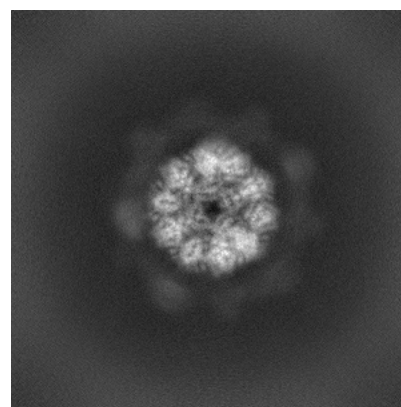
6.1.2 Raw map



X



Y

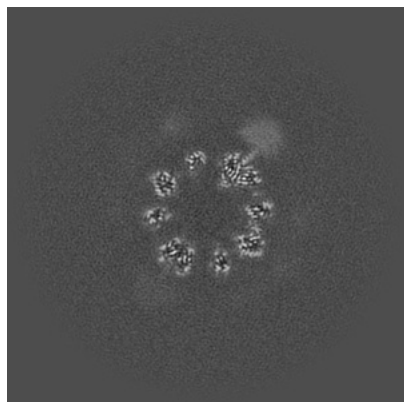


Z

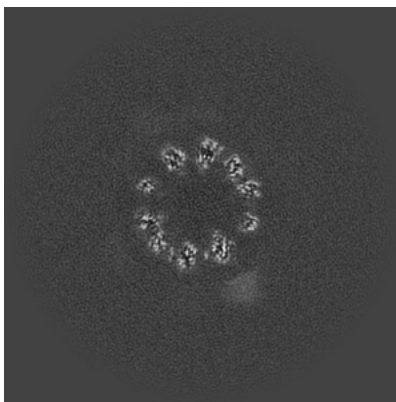
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

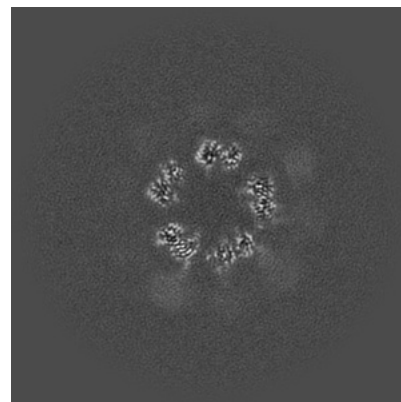
6.2.1 Primary map



X Index: 300

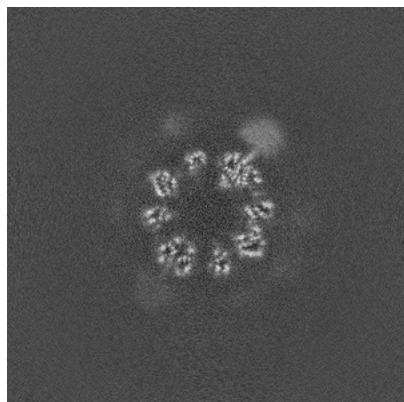


Y Index: 300

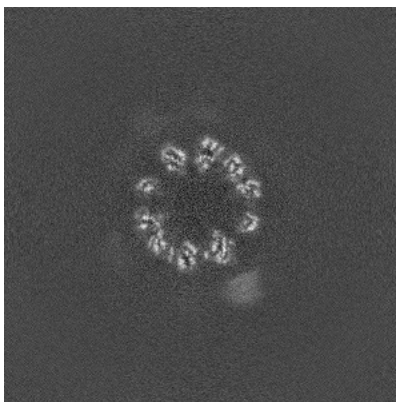


Z Index: 300

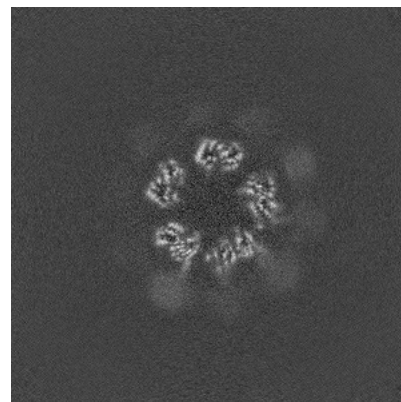
6.2.2 Raw map



X Index: 300



Y Index: 300

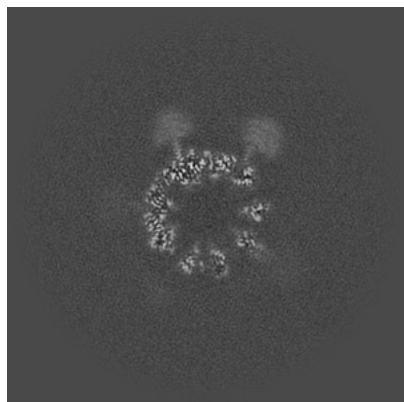


Z Index: 300

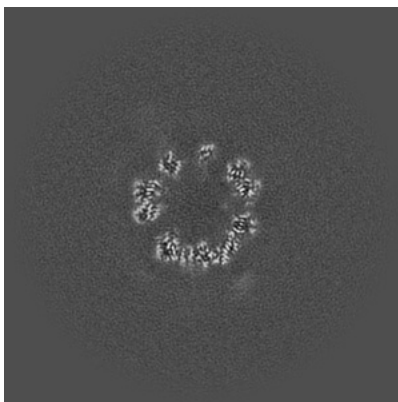
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

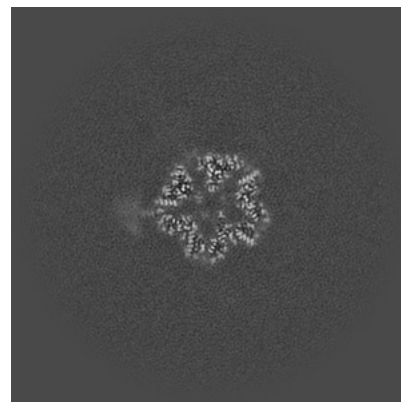
6.3.1 Primary map



X Index: 318

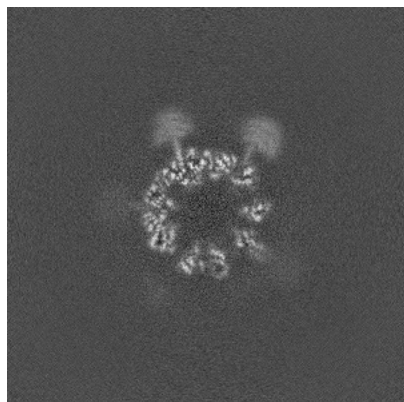


Y Index: 316

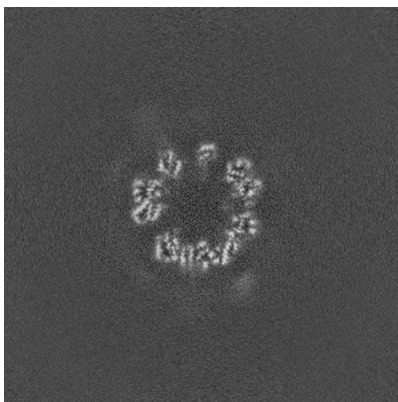


Z Index: 342

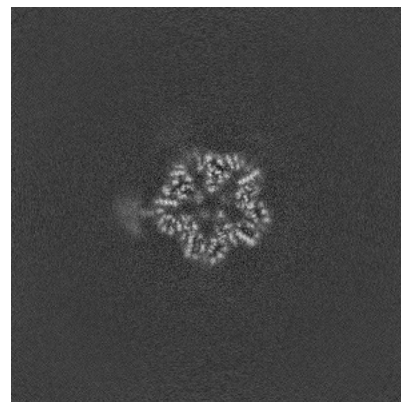
6.3.2 Raw map



X Index: 318



Y Index: 316

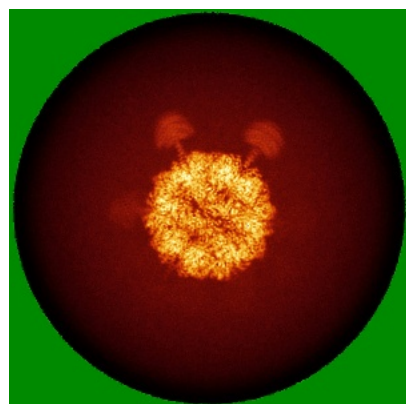


Z Index: 342

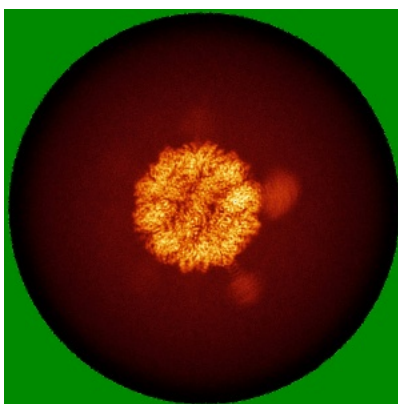
The images above show the largest variance slices of the map in three orthogonal directions.

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

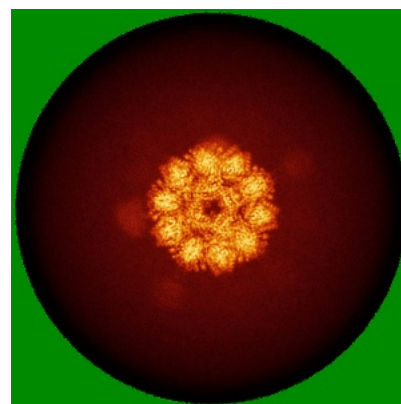
6.4.1 Primary map



X

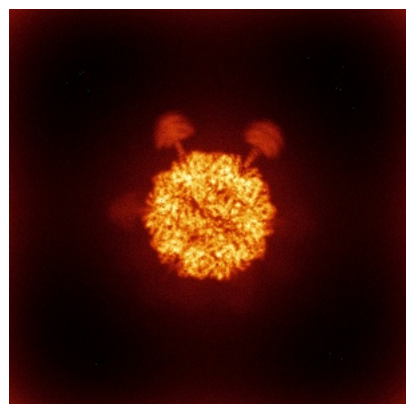


Y

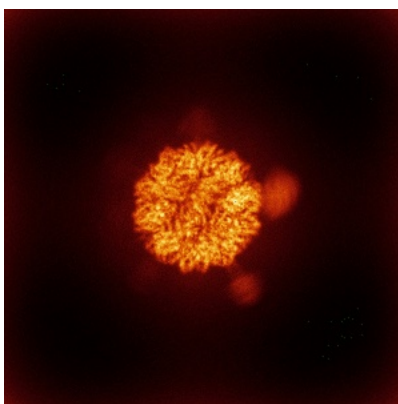


Z

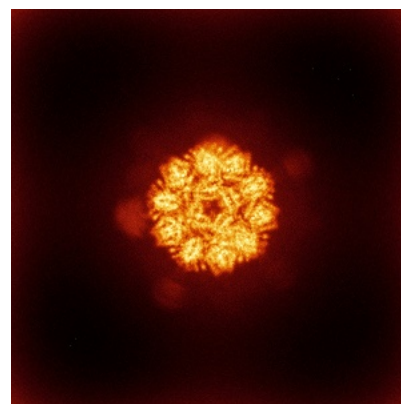
6.4.2 Raw map



X



Y

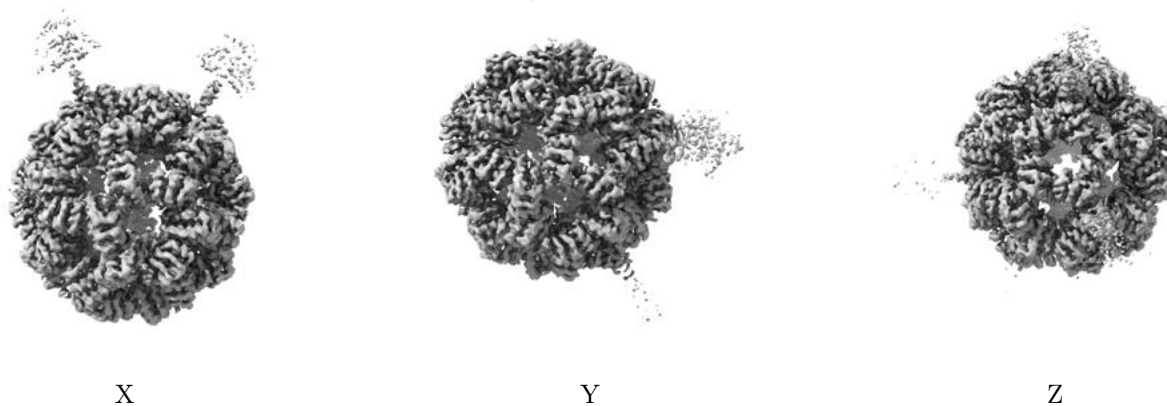


Z

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.

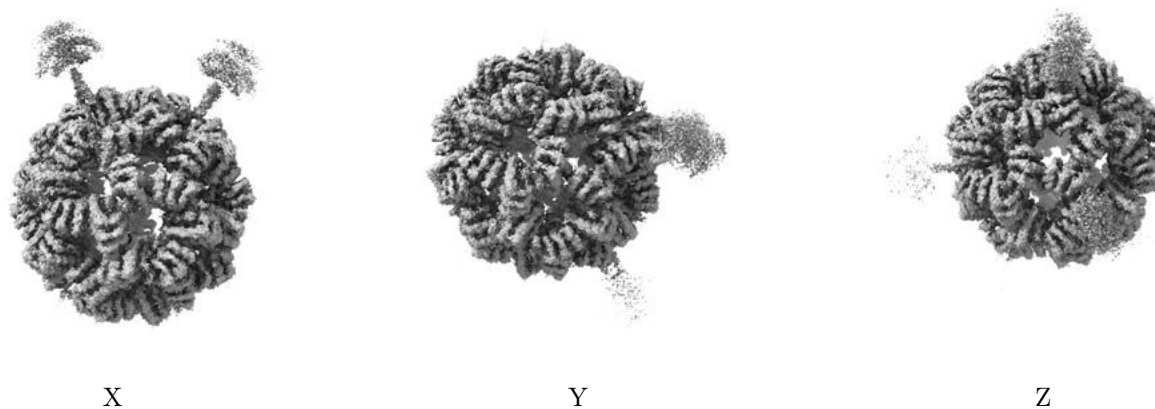
6.5 Orthogonal surface views [i](#)

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.

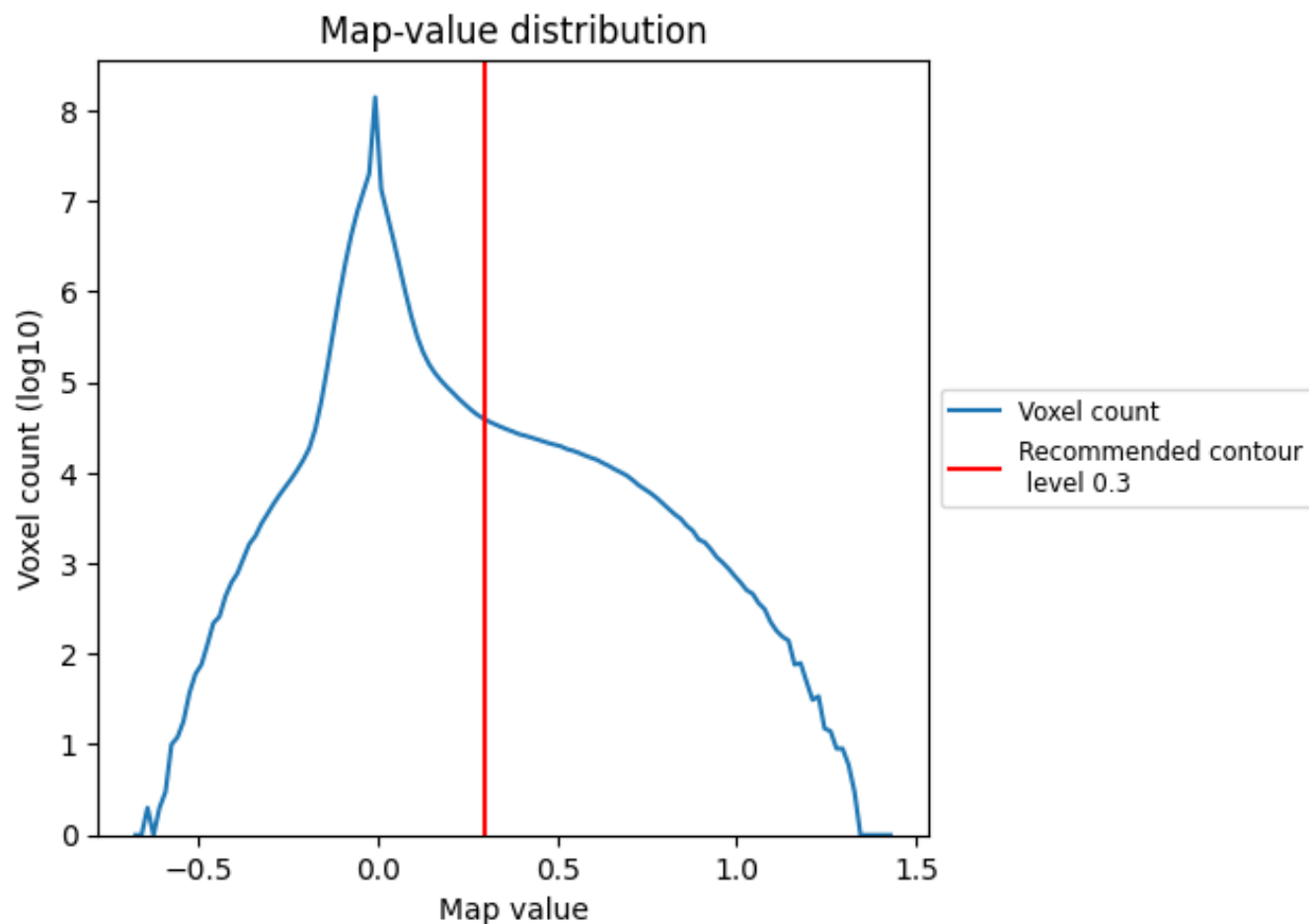
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

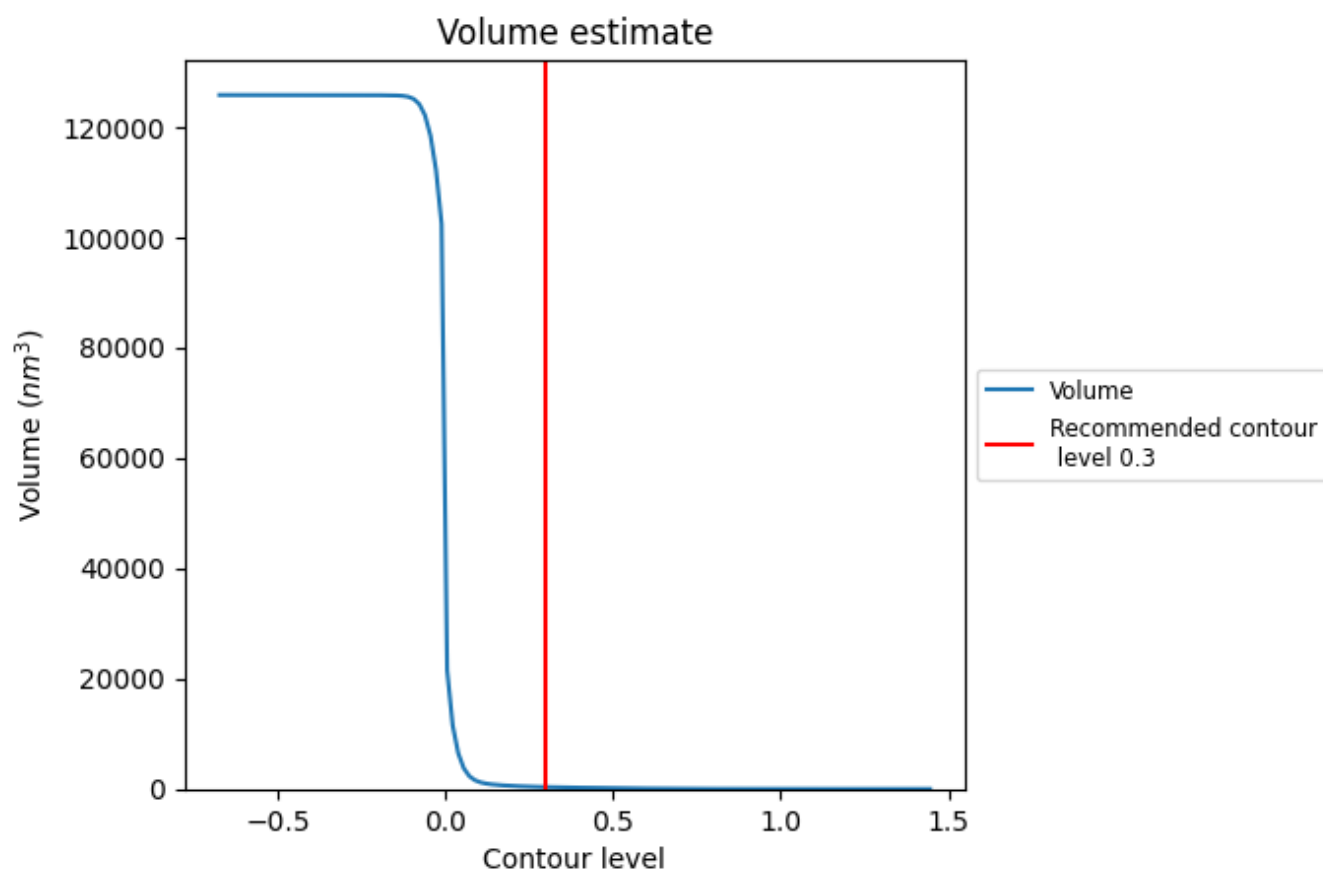
This section contains the results of statistical analysis of the map.

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.

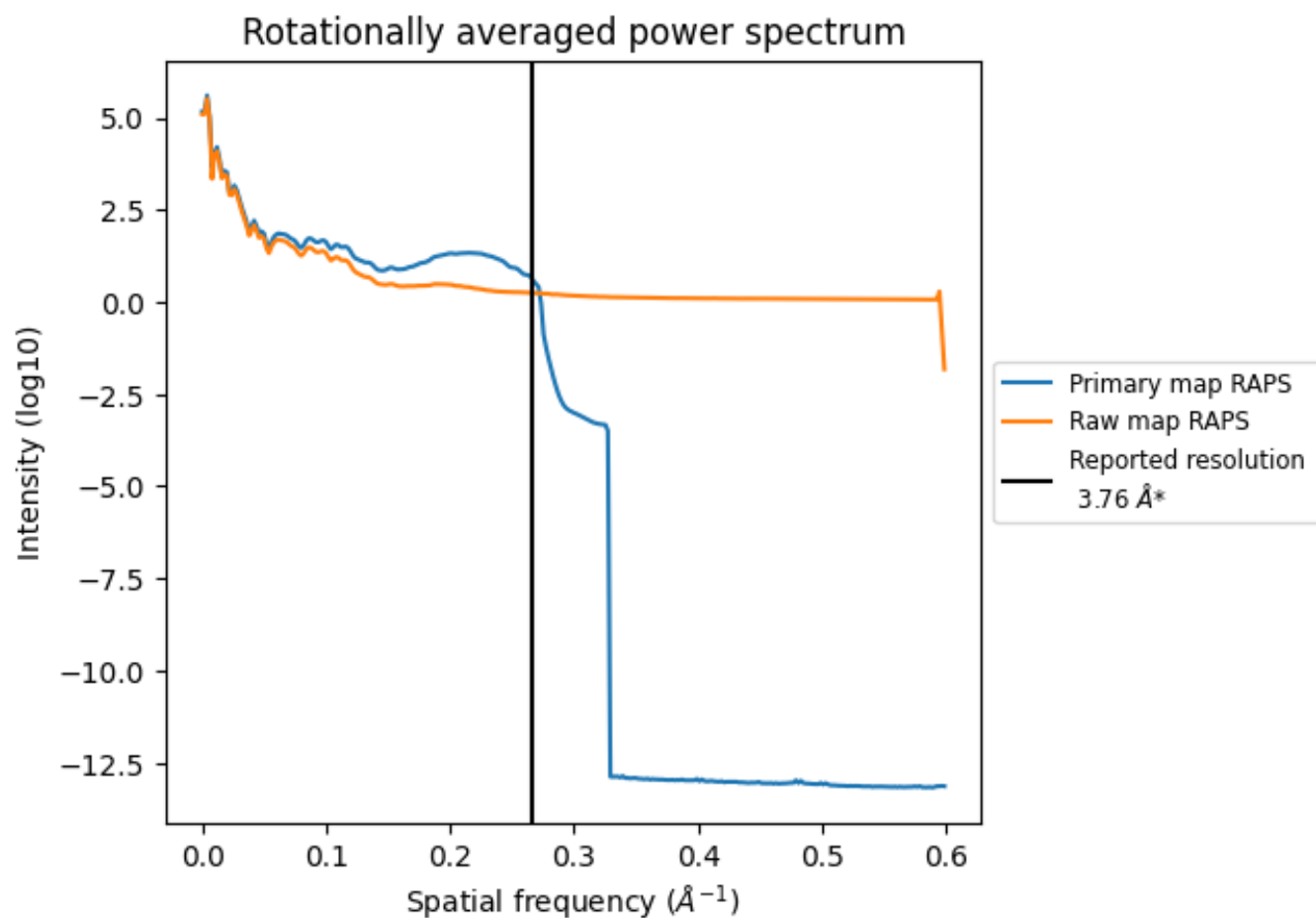
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 340 nm^3 ; this corresponds to an approximate mass of 307 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 ⓘ

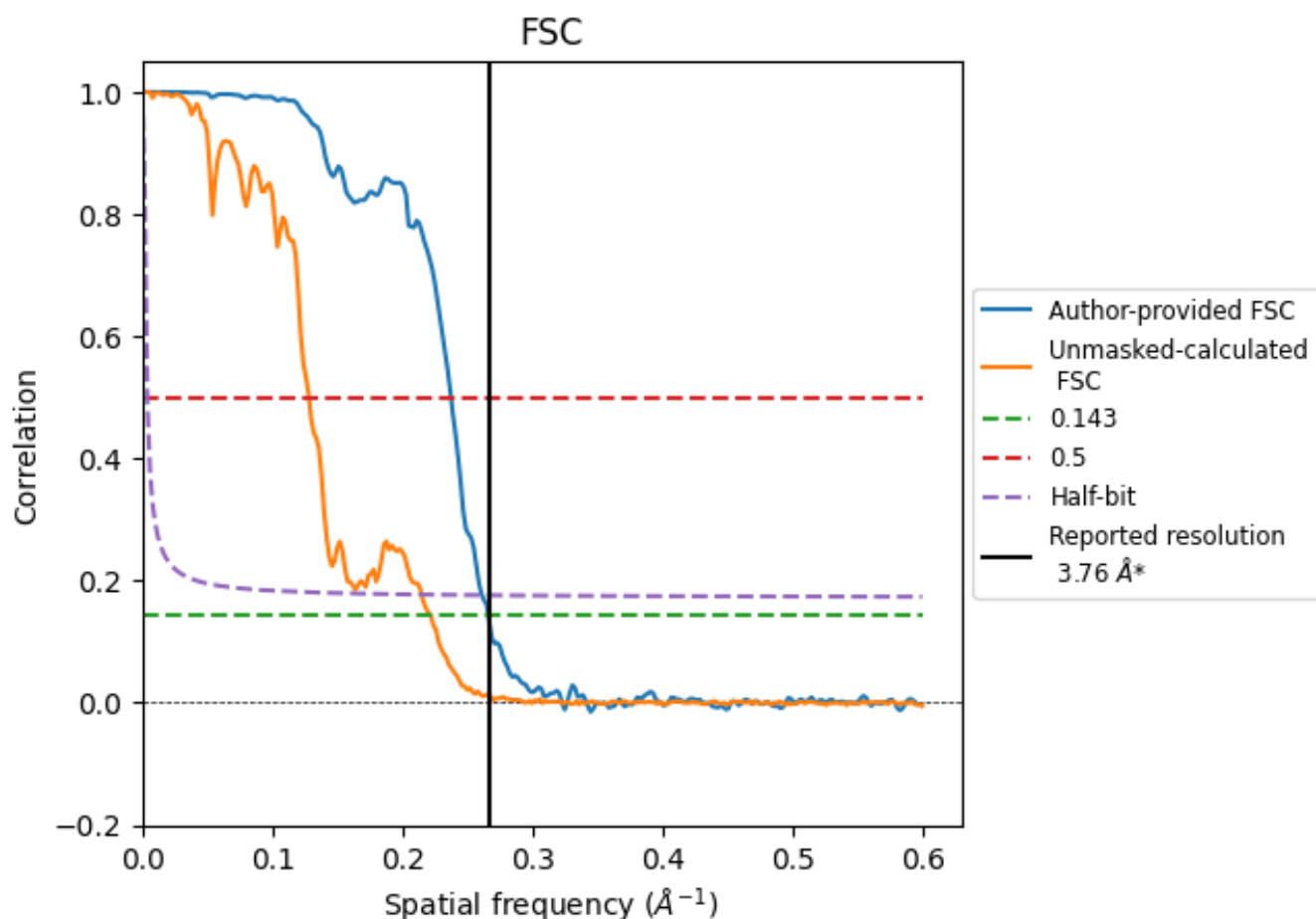


*Reported resolution corresponds to spatial frequency of 0.266 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.266 \AA^{-1}

8.2 Resolution estimates [i](#)

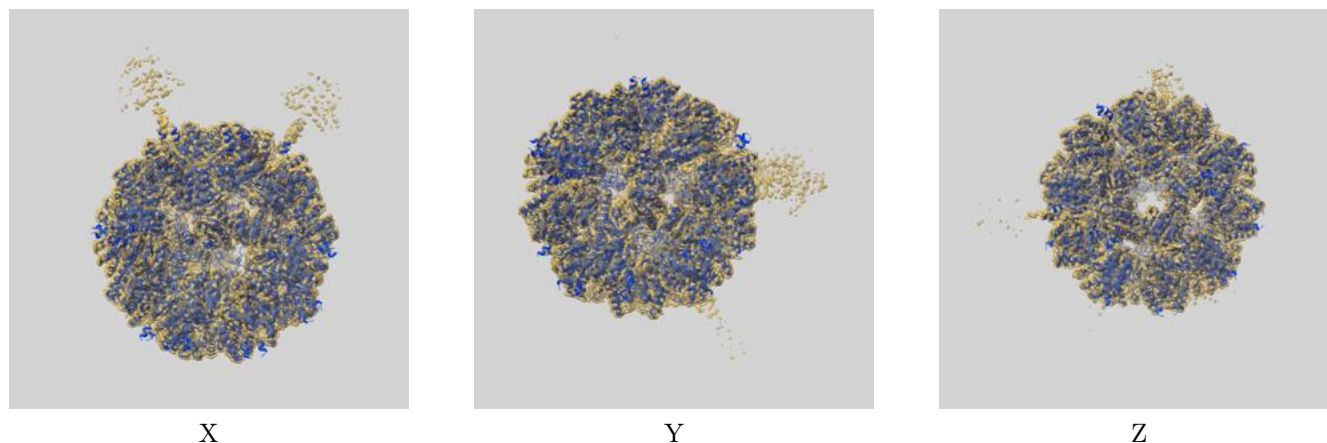
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.76	-	-
Author-provided FSC curve	3.77	4.22	3.83
Unmasked-calculated*	4.52	7.81	4.66

*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 4.52 differs from the reported value 3.76 by more than 10 %

9 Map-model fit [i](#)

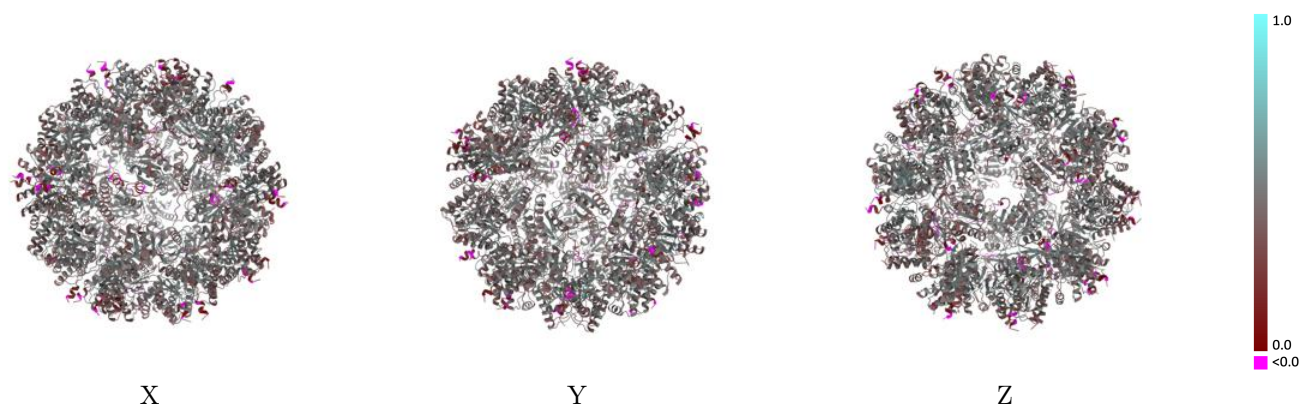
This section contains information regarding the fit between EMDB map EMD-70112 and PDB model 9O4R. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



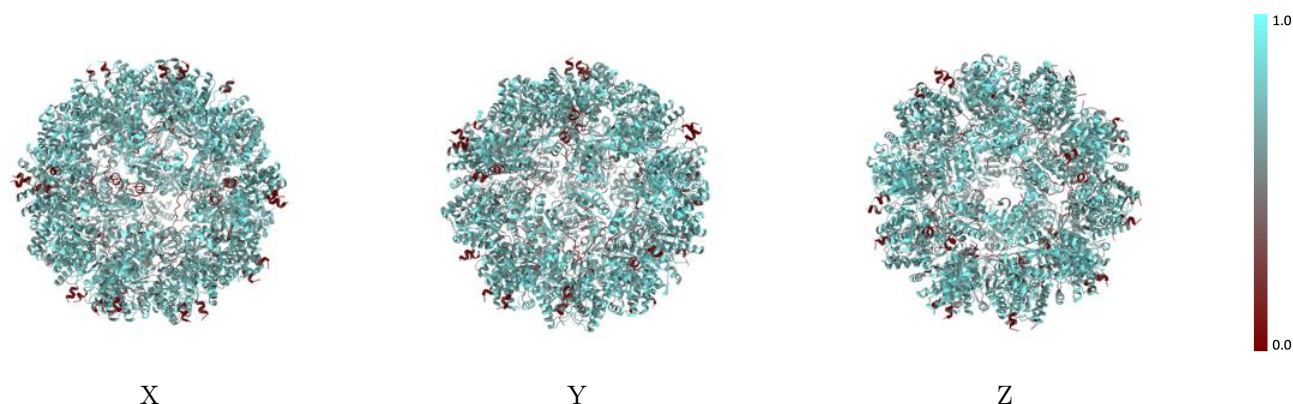
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



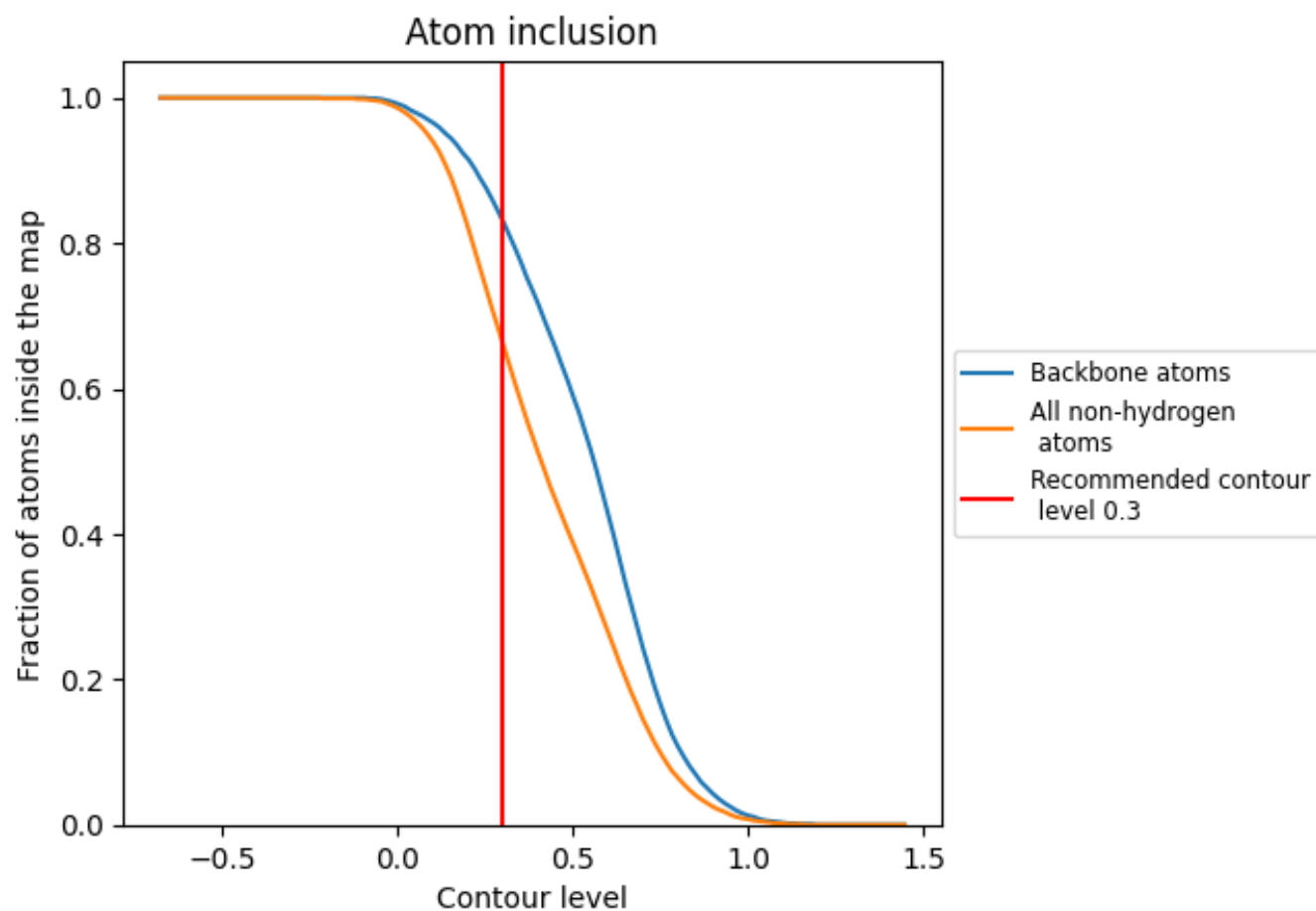
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.4170
A	 0.6120	 0.4040
AB	 0.6050	 0.4040
B	 0.6590	 0.4130
BB	 0.6550	 0.4220
C	 0.7380	 0.4310
CB	 0.7380	 0.4460
D	 0.6060	 0.3790
DB	 0.6060	 0.4070
E	 0.6270	 0.4030
EB	 0.6180	 0.3950
F	 0.6050	 0.3970
FB	 0.6240	 0.4060
G	 0.6000	 0.3800
GB	 0.6010	 0.4010
H	 0.6160	 0.4060
HB	 0.6110	 0.4010
I	 0.6010	 0.4050
IB	 0.6020	 0.4060
J	 0.6370	 0.4040
JB	 0.6310	 0.4040
K	 0.6630	 0.4250
KB	 0.6670	 0.4260
L	 0.6200	 0.3790
LB	 0.6060	 0.3850
M	 0.6040	 0.3690
MB	 0.6140	 0.3810
N	 0.6040	 0.3970
NB	 0.6170	 0.3880
O	 0.7660	 0.4460
OB	 0.7620	 0.4440
P	 0.6020	 0.3660
PB	 0.6150	 0.3760
Q	 0.6210	 0.3840
QB	 0.6230	 0.3810



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Chain	Atom inclusion	Q-score
R	 0.6390	 0.4150
RB	 0.6380	 0.4040
S	 0.7600	 0.4390
SB	 0.7520	 0.4430
T	 0.6200	 0.4180
TB	 0.6130	 0.3960
a	 0.6980	 0.4520
ab	 0.6990	 0.4370
b	 0.7040	 0.4440
bb	 0.7230	 0.4500
c	 0.6970	 0.4490
cb	 0.7320	 0.4440
d	 0.6860	 0.4340
db	 0.6930	 0.4330
e	 0.7360	 0.4650
eb	 0.7350	 0.4600
f	 0.6870	 0.4360
fb	 0.6810	 0.4350
g	 0.7540	 0.4630
gb	 0.7610	 0.4640
h	 0.6960	 0.4380
hb	 0.7160	 0.4520
i	 0.6860	 0.4400
ib	 0.7100	 0.4330
j	 0.7280	 0.4400
jb	 0.7520	 0.4570