



Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 01:49 PM EDT

PDB ID : 9O4H / pdb_00009o4h
EMDB ID : EMD-70101
Title : Phosphomimetic (T209E) 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 : 4.02 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

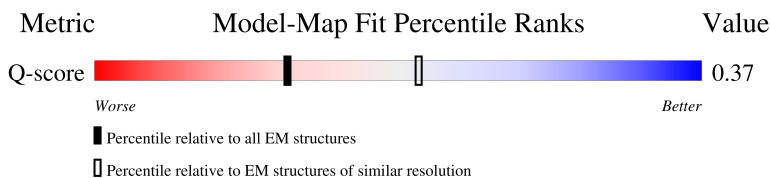
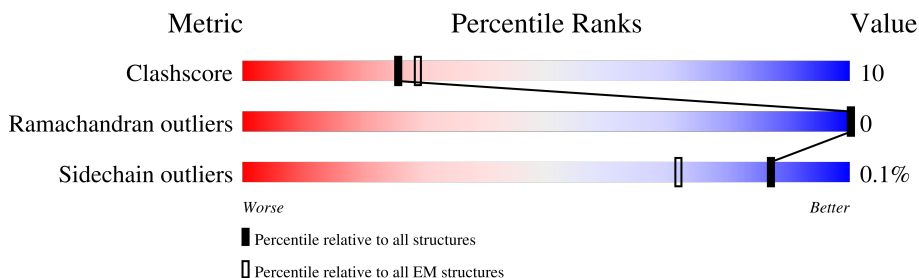
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.02 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.







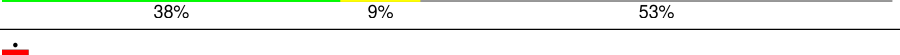
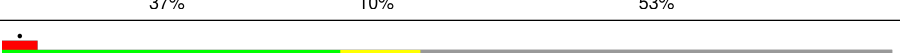

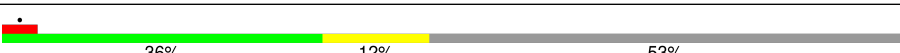







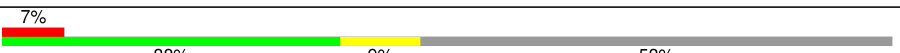





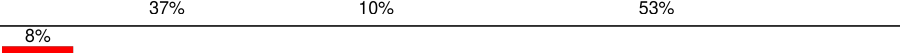



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6727 (3.52 - 4.52)

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

Mol	Chain	Length	Quality of chain
1	A	278	<div> <div>8%</div> <div>37%</div> <div>10%</div> <div>53%</div> </div>
1	AB	278	<div> <div>8%</div> <div>37%</div> <div>11%</div> <div>53%</div> </div>
1	B	278	<div> <div>7%</div> <div>35%</div> <div>13%</div> <div>53%</div> </div>
1	BB	278	<div> <div>8%</div> <div>35%</div> <div>13%</div> <div>53%</div> </div>

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



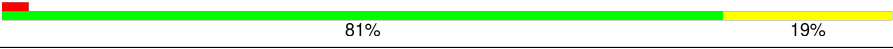



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Mol	Chain	Length	Quality of chain
1	OB	278	
2	a	118	
2	ab	118	
2	b	118	
2	bb	118	
2	c	118	
2	cb	118	
2	d	118	
2	db	118	
2	e	118	
2	eb	118	
2	f	118	
2	fb	118	
2	g	118	
2	gb	118	
2	h	118	
2	hb	118	
2	i	118	
2	ib	118	
2	j	118	
2	jb	118	
2	k	118	
2	kb	118	
2	l	118	
2	lb	118	

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Mol	Chain	Length	Quality of chain
2	m	118	 81%19%
2	mb	118	 80%20%
2	n	118	 81%19%
2	nb	118	 75%25%
2	o	118	 74%26%
2	ob	118	 76%24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 56610 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
			1006	639	171	190	6		
1	AB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	BB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	CB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	DB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	EB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	FB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	GB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	HB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	IB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	JB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	KB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	LB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	MB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	NB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	OB	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	B	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	D	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	E	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	F	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	G	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	H	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	I	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	J	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	K	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	L	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	M	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	N	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		
1	O	132	Total	C	N	O	S	0	0
			1006	639	171	190	6		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ASP	ASN	conflict	UNP Q8GD19
A	209	GLU	THR	engineered mutation	UNP Q8GD19
AB	19	ASP	ASN	conflict	UNP Q8GD19
AB	209	GLU	THR	engineered mutation	UNP Q8GD19
BB	19	ASP	ASN	conflict	UNP Q8GD19
BB	209	GLU	THR	engineered mutation	UNP Q8GD19
CB	19	ASP	ASN	conflict	UNP Q8GD19
CB	209	GLU	THR	engineered mutation	UNP Q8GD19
DB	19	ASP	ASN	conflict	UNP Q8GD19
DB	209	GLU	THR	engineered mutation	UNP Q8GD19
EB	19	ASP	ASN	conflict	UNP Q8GD19
EB	209	GLU	THR	engineered mutation	UNP Q8GD19
FB	19	ASP	ASN	conflict	UNP Q8GD19

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Chain	Residue	Modelled	Actual	Comment	Reference
FB	209	GLU	THR	engineered mutation	UNP Q8GD19
GB	19	ASP	ASN	conflict	UNP Q8GD19
GB	209	GLU	THR	engineered mutation	UNP Q8GD19
HB	19	ASP	ASN	conflict	UNP Q8GD19
HB	209	GLU	THR	engineered mutation	UNP Q8GD19
IB	19	ASP	ASN	conflict	UNP Q8GD19
IB	209	GLU	THR	engineered mutation	UNP Q8GD19
JB	19	ASP	ASN	conflict	UNP Q8GD19
JB	209	GLU	THR	engineered mutation	UNP Q8GD19
KB	19	ASP	ASN	conflict	UNP Q8GD19
KB	209	GLU	THR	engineered mutation	UNP Q8GD19
LB	19	ASP	ASN	conflict	UNP Q8GD19
LB	209	GLU	THR	engineered mutation	UNP Q8GD19
MB	19	ASP	ASN	conflict	UNP Q8GD19
MB	209	GLU	THR	engineered mutation	UNP Q8GD19
NB	19	ASP	ASN	conflict	UNP Q8GD19
NB	209	GLU	THR	engineered mutation	UNP Q8GD19
OB	19	ASP	ASN	conflict	UNP Q8GD19
OB	209	GLU	THR	engineered mutation	UNP Q8GD19
B	19	ASP	ASN	conflict	UNP Q8GD19
B	209	GLU	THR	engineered mutation	UNP Q8GD19
C	19	ASP	ASN	conflict	UNP Q8GD19
C	209	GLU	THR	engineered mutation	UNP Q8GD19
D	19	ASP	ASN	conflict	UNP Q8GD19
D	209	GLU	THR	engineered mutation	UNP Q8GD19
E	19	ASP	ASN	conflict	UNP Q8GD19
E	209	GLU	THR	engineered mutation	UNP Q8GD19
F	19	ASP	ASN	conflict	UNP Q8GD19
F	209	GLU	THR	engineered mutation	UNP Q8GD19
G	19	ASP	ASN	conflict	UNP Q8GD19
G	209	GLU	THR	engineered mutation	UNP Q8GD19
H	19	ASP	ASN	conflict	UNP Q8GD19
H	209	GLU	THR	engineered mutation	UNP Q8GD19
I	19	ASP	ASN	conflict	UNP Q8GD19
I	209	GLU	THR	engineered mutation	UNP Q8GD19
J	19	ASP	ASN	conflict	UNP Q8GD19
J	209	GLU	THR	engineered mutation	UNP Q8GD19
K	19	ASP	ASN	conflict	UNP Q8GD19
K	209	GLU	THR	engineered mutation	UNP Q8GD19
L	19	ASP	ASN	conflict	UNP Q8GD19
L	209	GLU	THR	engineered mutation	UNP Q8GD19
M	19	ASP	ASN	conflict	UNP Q8GD19

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Chain	Residue	Modelled	Actual	Comment	Reference
M	209	GLU	THR	engineered mutation	UNP Q8GD19
N	19	ASP	ASN	conflict	UNP Q8GD19
N	209	GLU	THR	engineered mutation	UNP Q8GD19
O	19	ASP	ASN	conflict	UNP Q8GD19
O	209	GLU	THR	engineered mutation	UNP Q8GD19

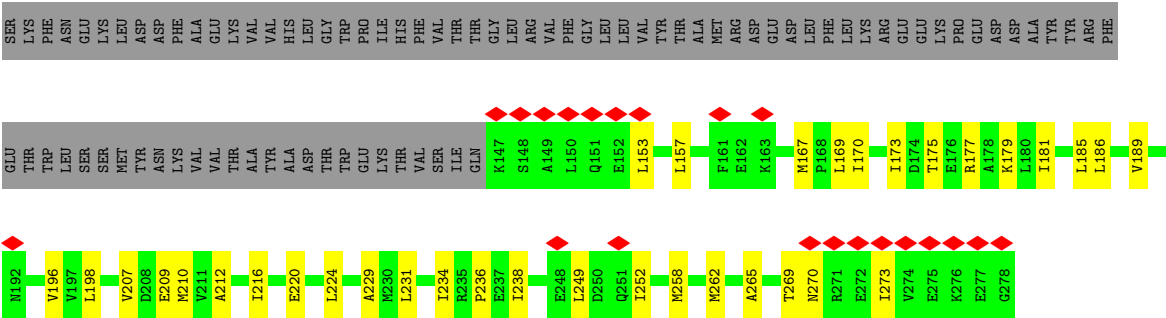
- Molecule 2 is a protein called RsbT antagonist protein RsbS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	ab	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	bb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	cb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	db	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	eb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	fb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	gb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	hb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	ib	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	jb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	kb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	lb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	mb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	nb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	ob	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	b	118	Total	C	N	O	S	0	0
			881	565	136	175	5		

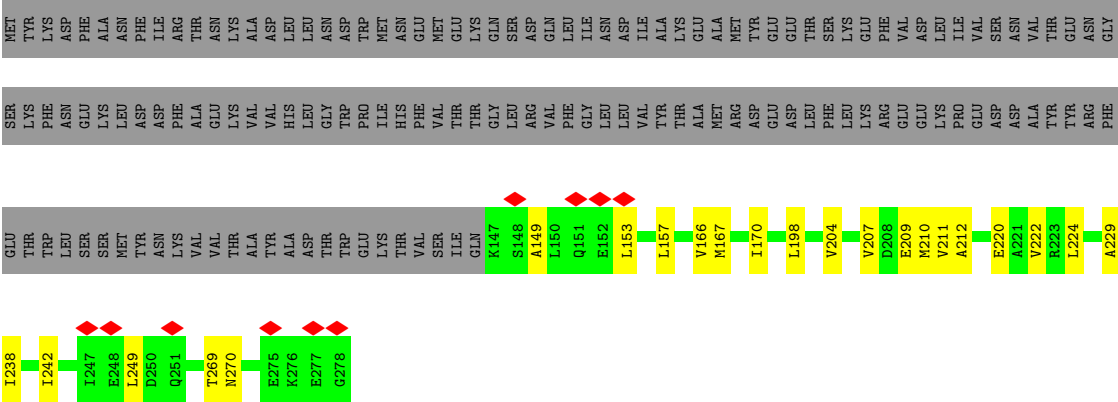
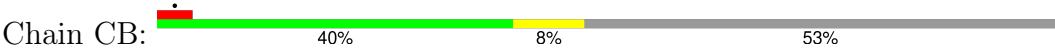
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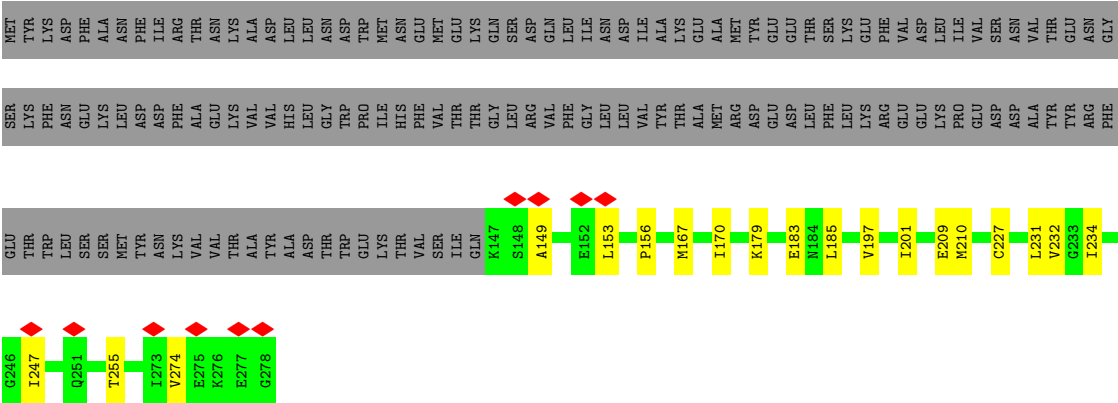
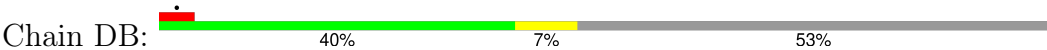
Mol	Chain	Residues	Atoms					AltConf	Trace
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2	d	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	e	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	f	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	g	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	h	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	i	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	j	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	k	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	l	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	m	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	n	118	Total 881	C 565	N 136	O 175	S 5	0	0
2	o	118	Total 881	C 565	N 136	O 175	S 5	0	0



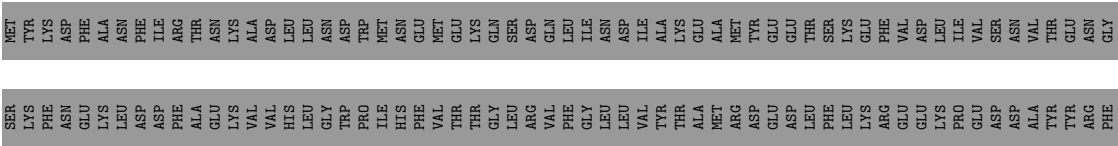
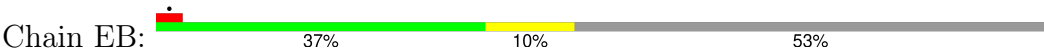
● Molecule 1: RsbR

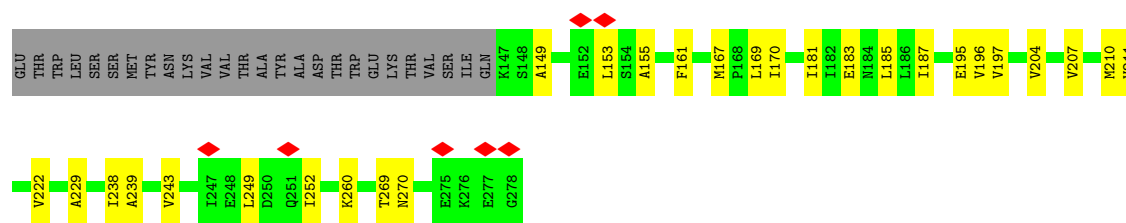


● Molecule 1: RsbR

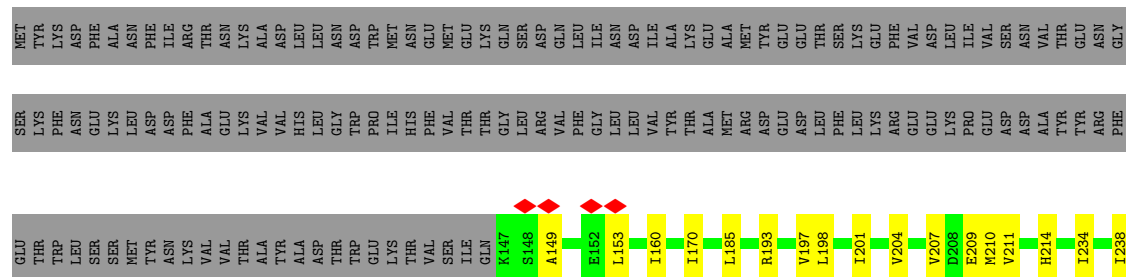
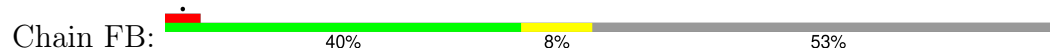


● Molecule 1: RsbR

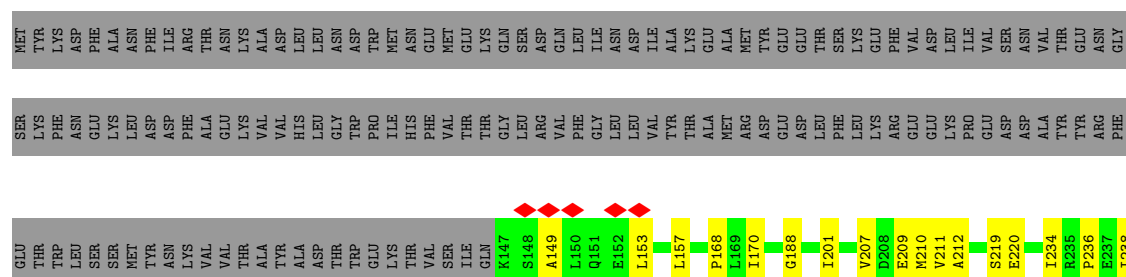
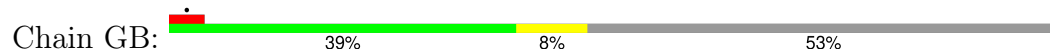




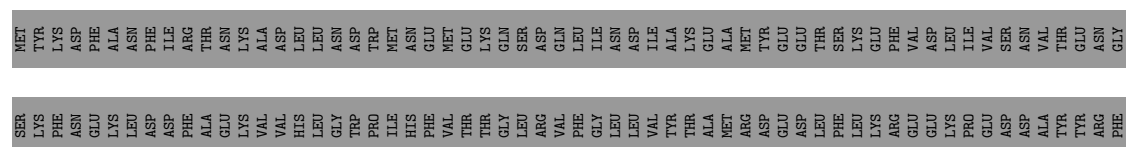
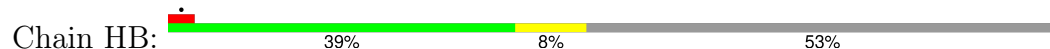
• Molecule 1: RsbR

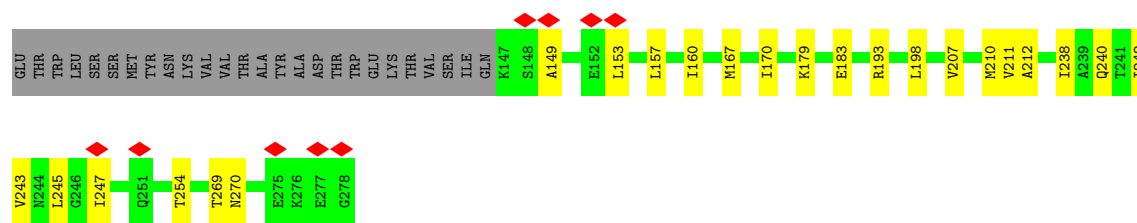


• Molecule 1: RsbR

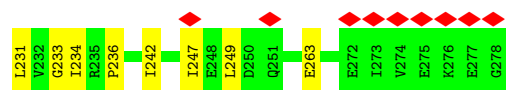
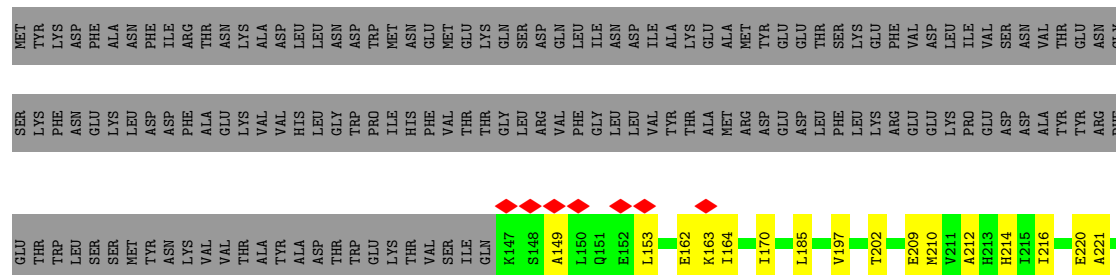
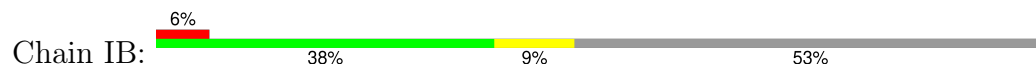


• Molecule 1: RsbR

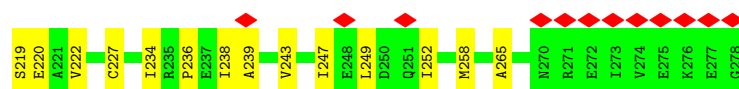
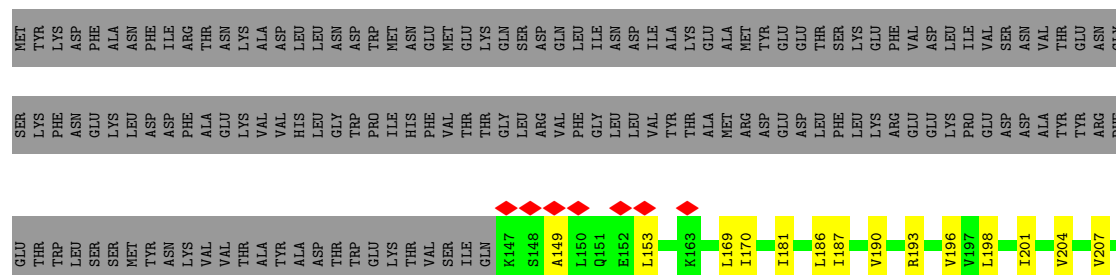
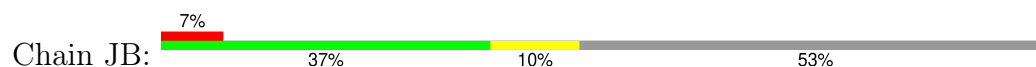




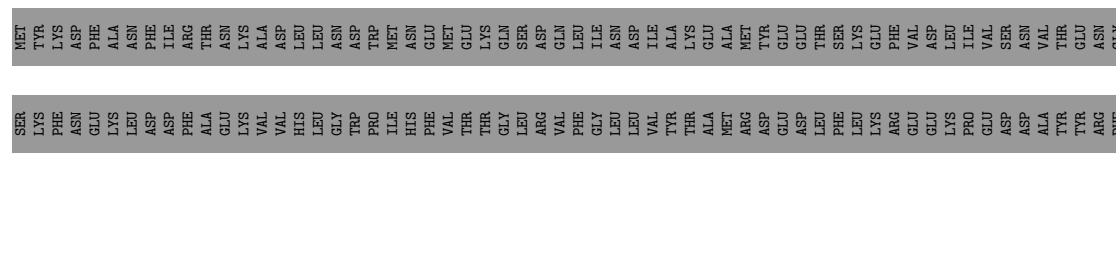
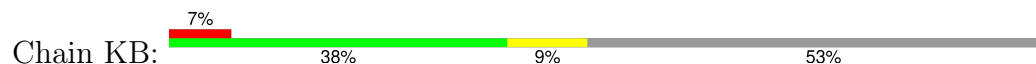
• Molecule 1: RsbR

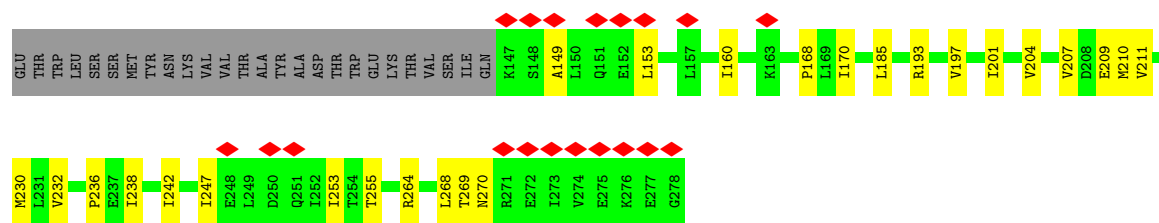


• Molecule 1: RsbR

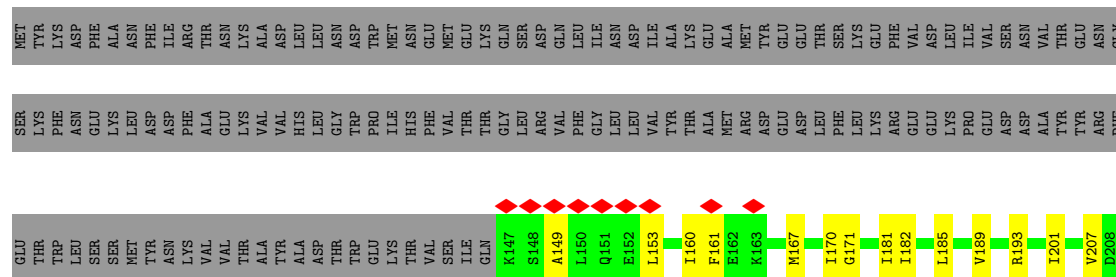
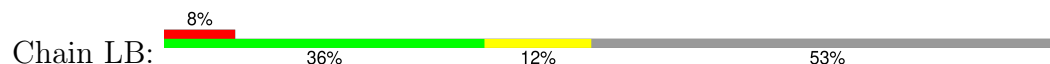


• Molecule 1: RsbR

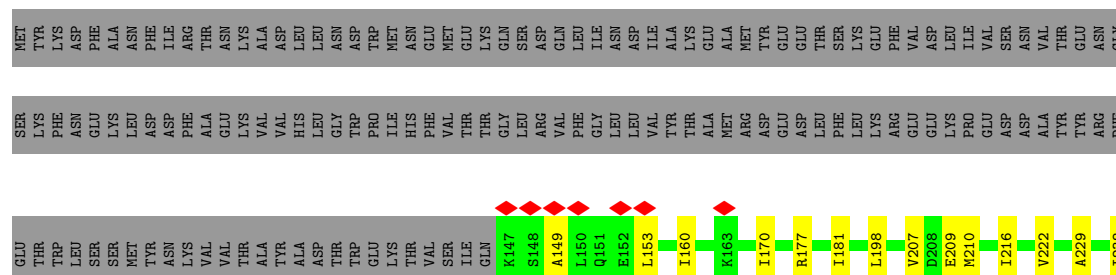
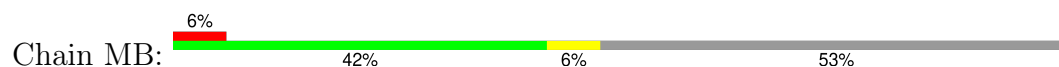




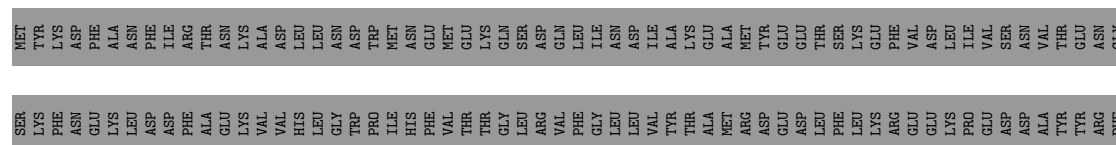
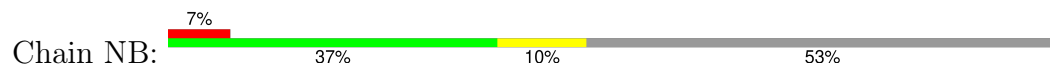
• Molecule 1: RsbR

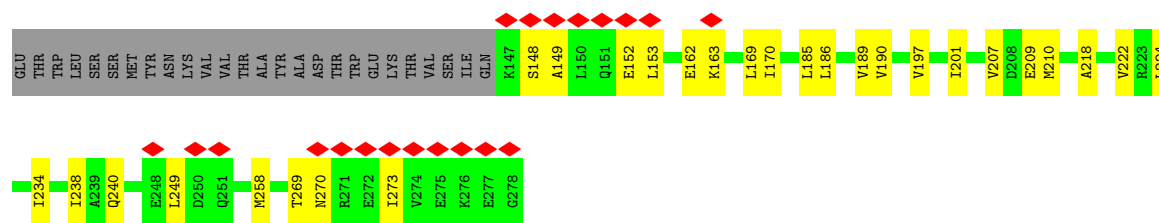


• Molecule 1: RsbR

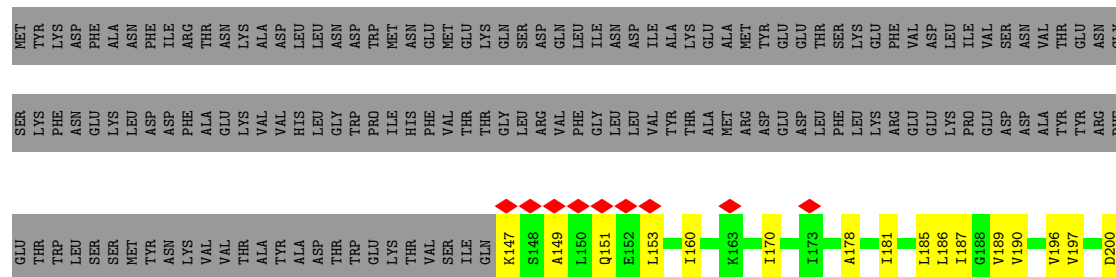
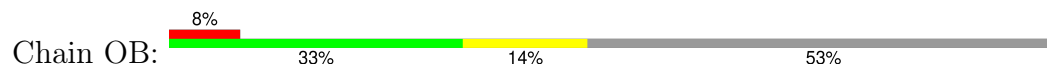


• Molecule 1: RsbR

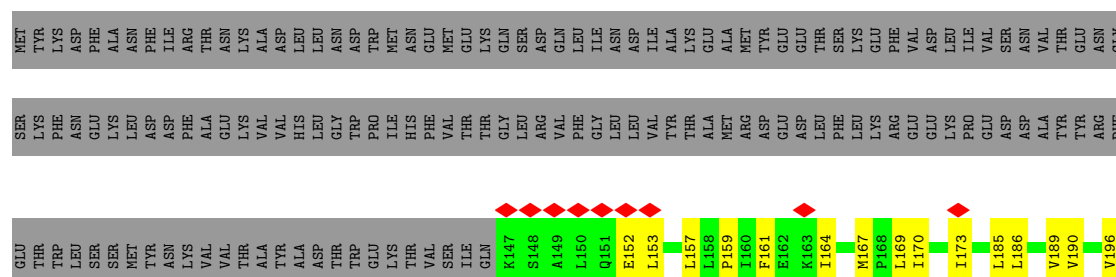
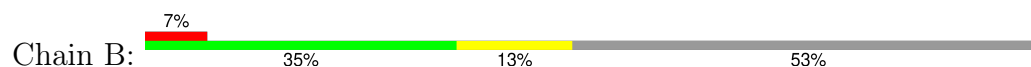




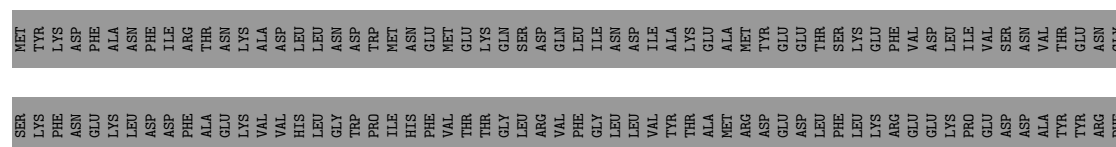
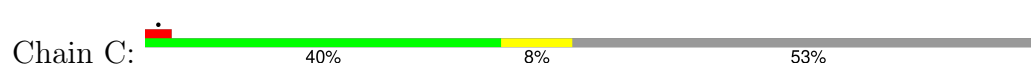
• Molecule 1: RsbR

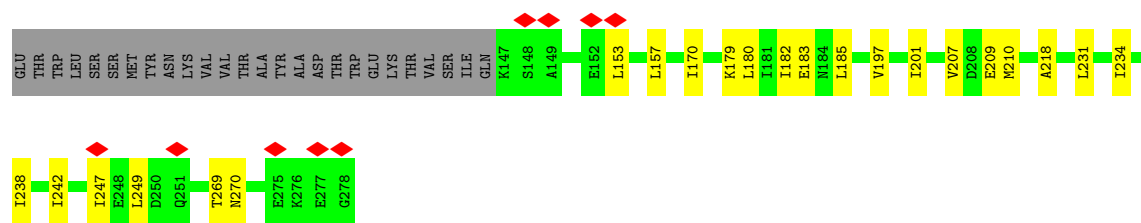


• Molecule 1: RsbR

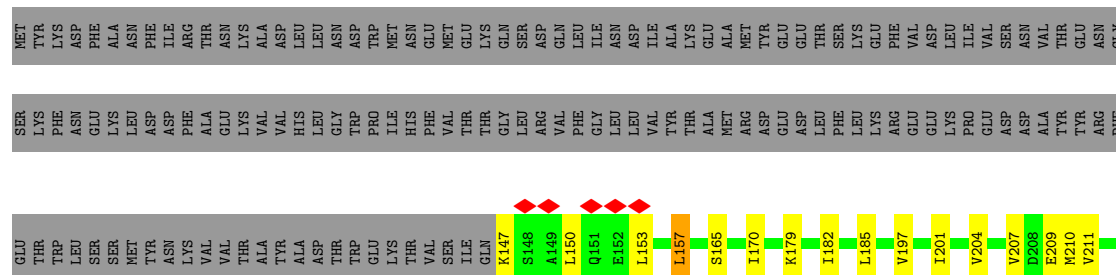
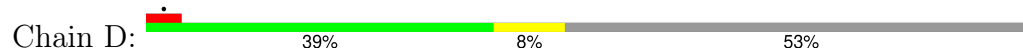


• Molecule 1: RsbR

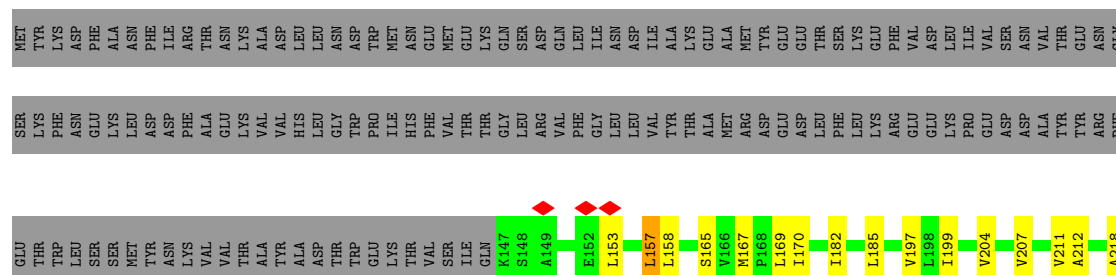
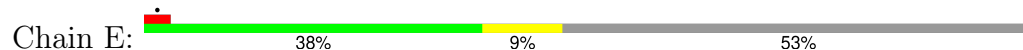




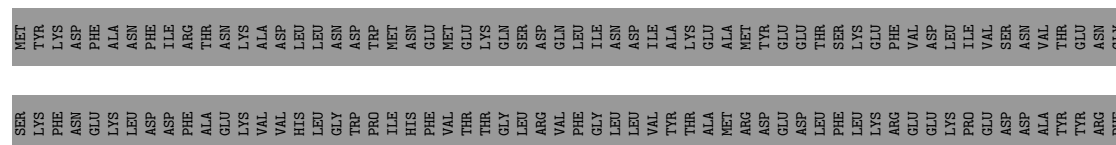
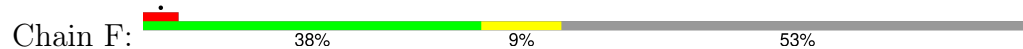
• Molecule 1: RsbR

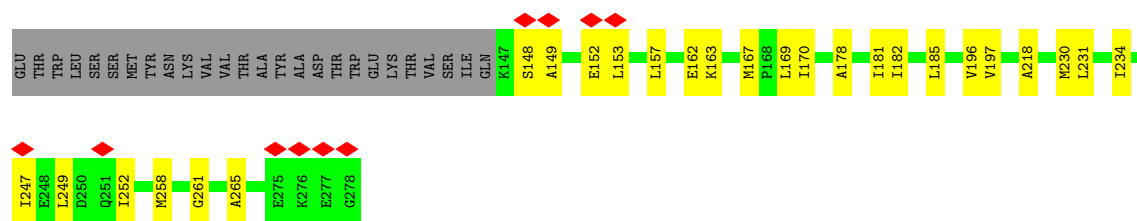


• Molecule 1: RsbR

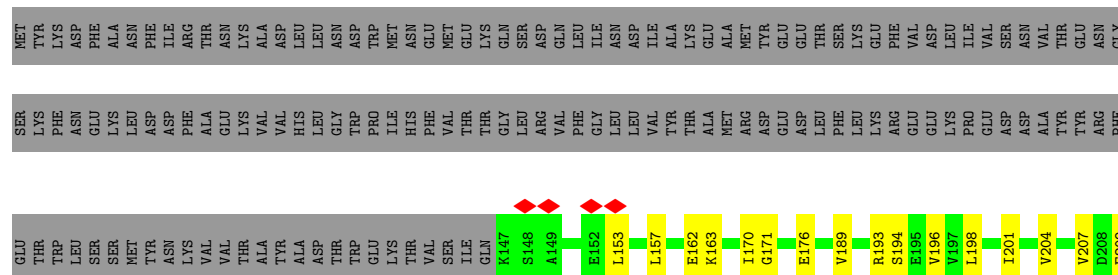
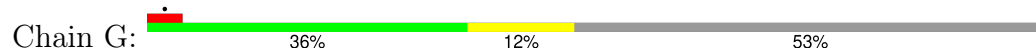


• Molecule 1: RsbR

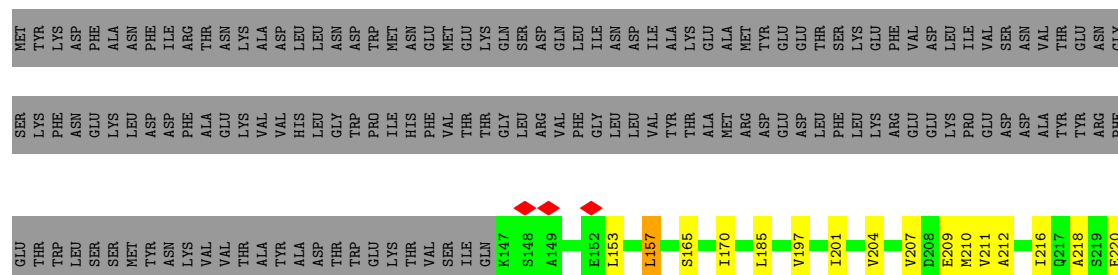
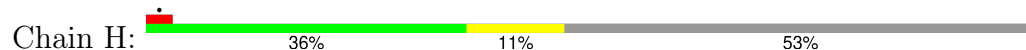




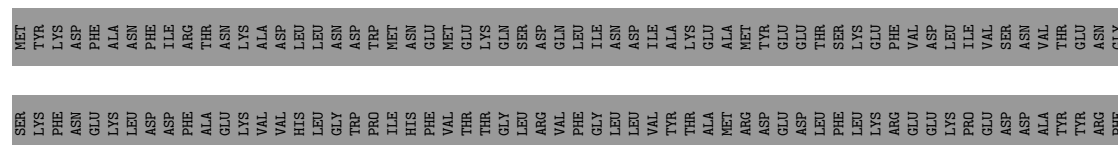
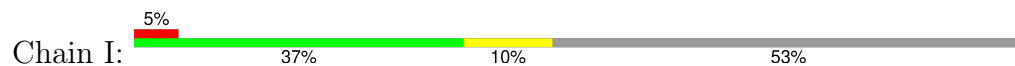
● Molecule 1: RsbR

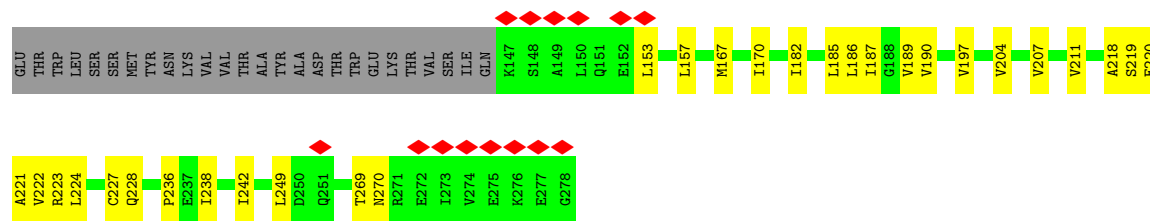


● Molecule 1: RsbR

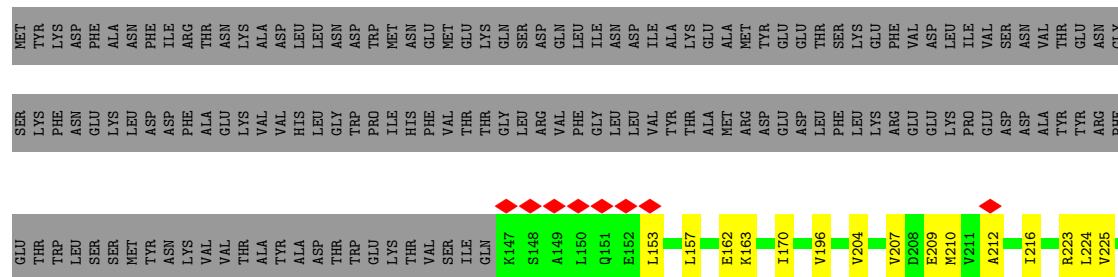
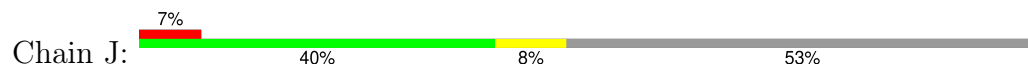


● Molecule 1: RsbR

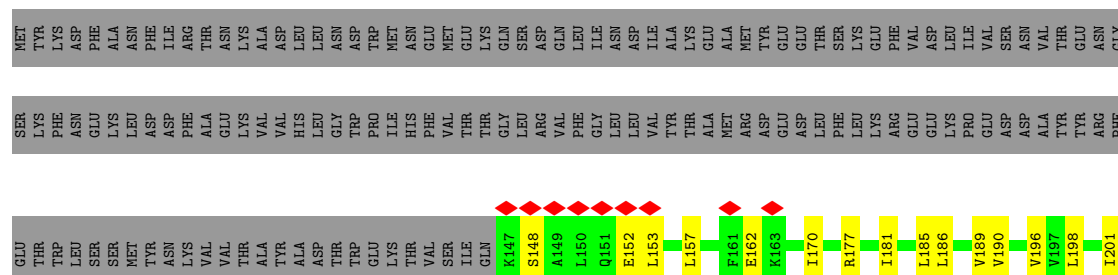
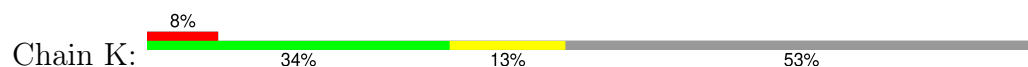




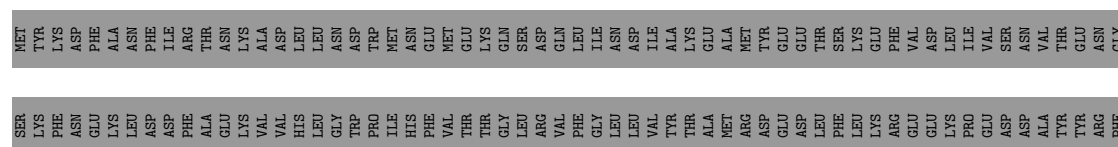
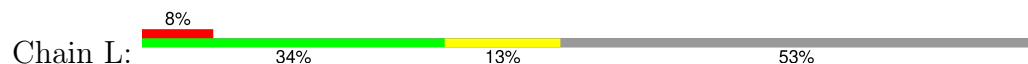
• Molecule 1: RsbR

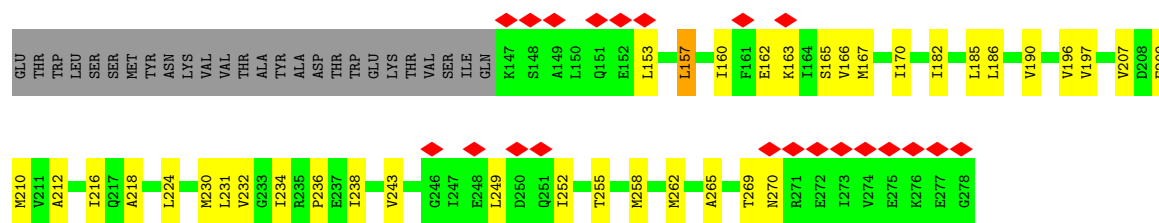


• Molecule 1: RsbR

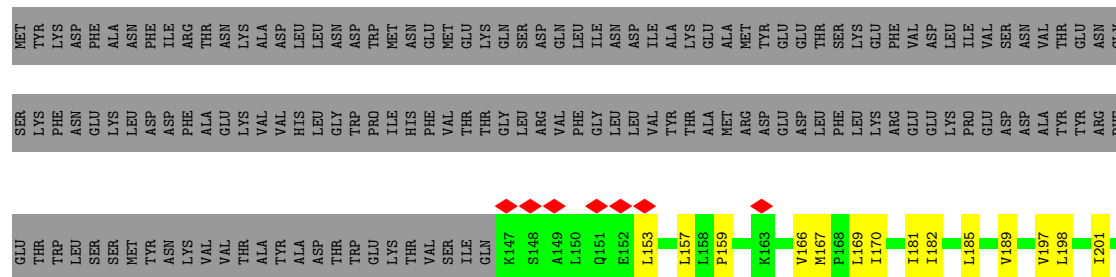
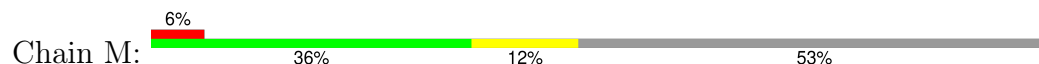


• Molecule 1: RsbR

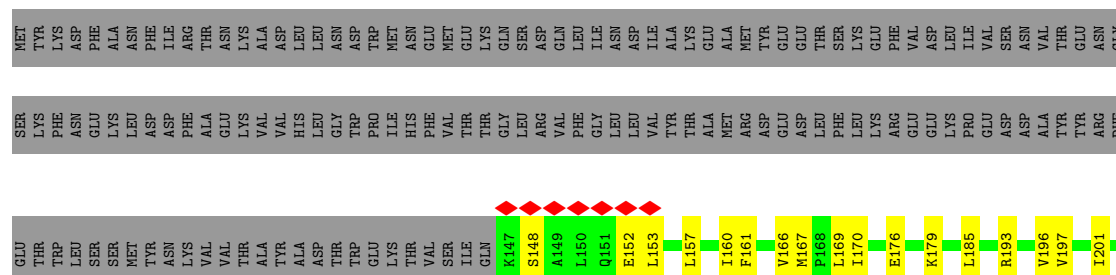
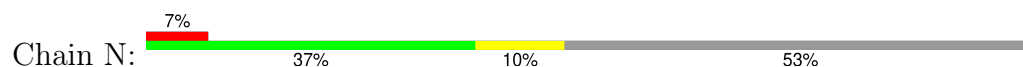




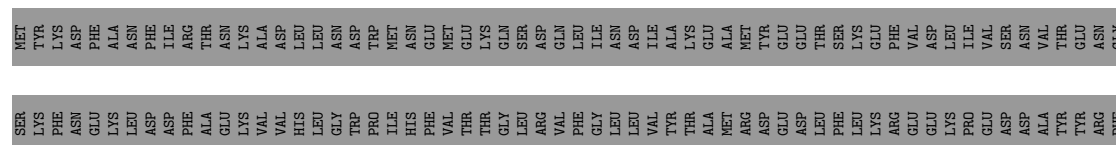
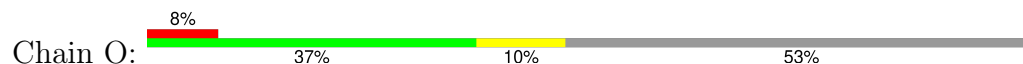
• Molecule 1: RsbR

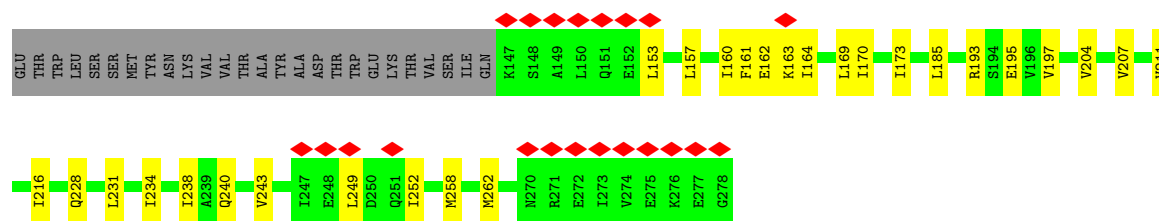


• Molecule 1: RsbR

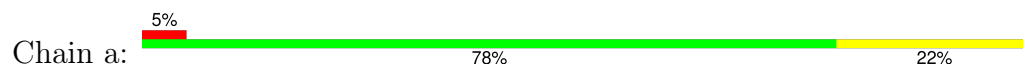


• Molecule 1: RsbR

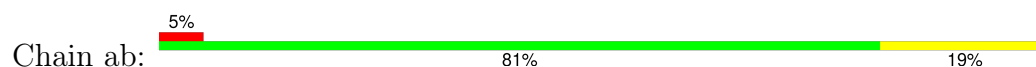




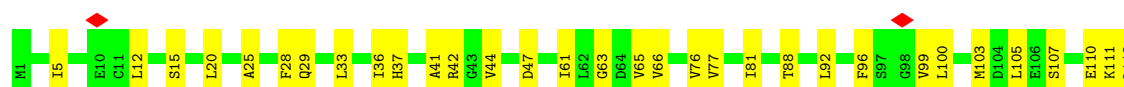
• Molecule 2: RsbT antagonist protein RsbS



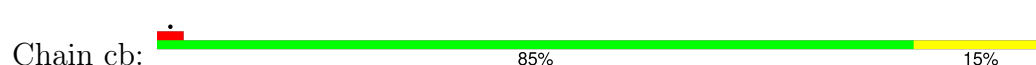
• Molecule 2: RsbT antagonist protein RsbS



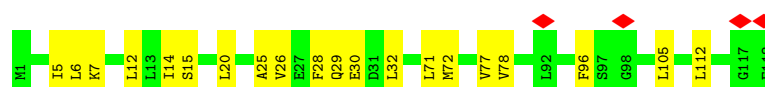
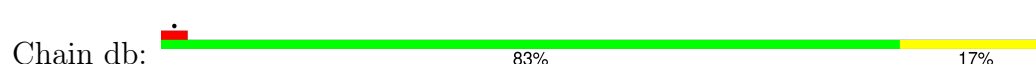
• Molecule 2: RsbT antagonist protein RsbS



• Molecule 2: RsbT antagonist protein RsbS



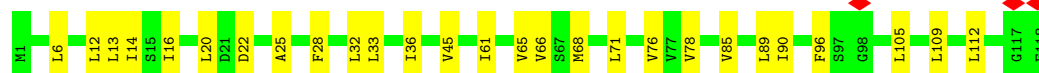
• Molecule 2: RsbT antagonist protein RsbS



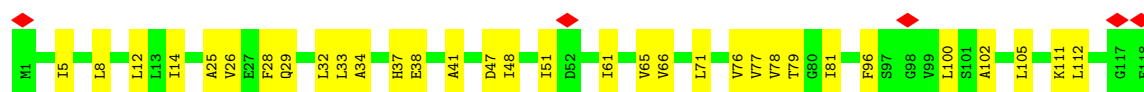
• Molecule 2: RsbT antagonist protein RsbS



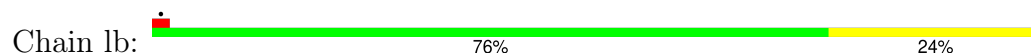
- [illegible]



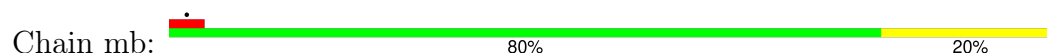
- Chain kb: 



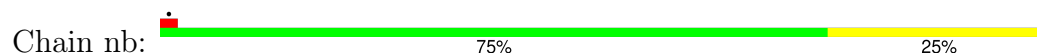
- Molecule 2: RsbT antagonist protein RsbS



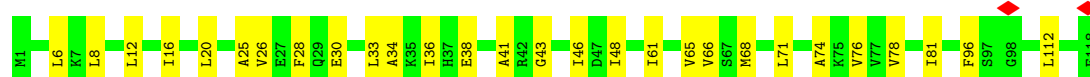
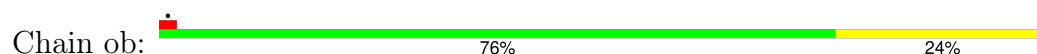
- Molecule 2: RsbT antagonist protein RsbS



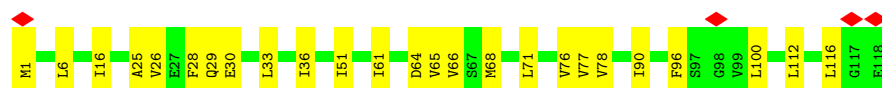
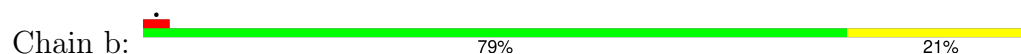
- Molecule 2: RsbT antagonist protein RsbS



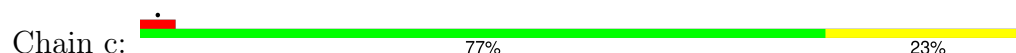
- Molecule 2: RsbT antagonist protein RsbS




- Molecule 2: RsbT antagonist protein RsbS



- Molecule 2: RsbT antagonist protein RsbS



- Molecule 2: RsbT antagonist protein RsbS

Chain d:  79% 21%




- Molecule 2: RsbT antagonist protein RsbS

Chain e:  76% 24%




- Molecule 2: RsbT antagonist protein RsbS

Chain f:  6% 79% 21%




- Molecule 2: RsbT antagonist protein RsbS

Chain g:  6% 80% 20%




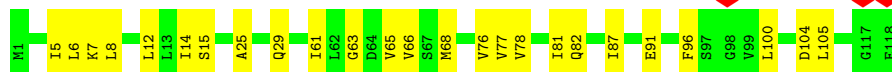
- Molecule 2: RsbT antagonist protein RsbS

Chain h:  81% 19%




- Molecule 2: RsbT antagonist protein RsbS

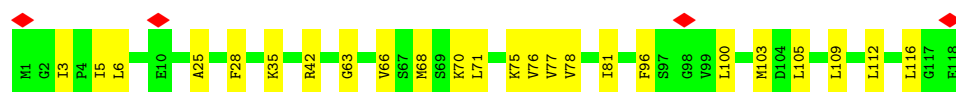
Chain i:  79% 21%



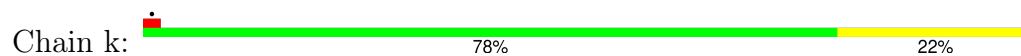
- Molecule 2: RsbT antagonist protein RsbS

Chain j:  80% 20%

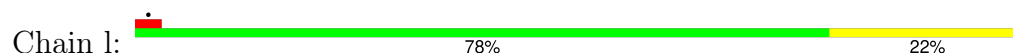




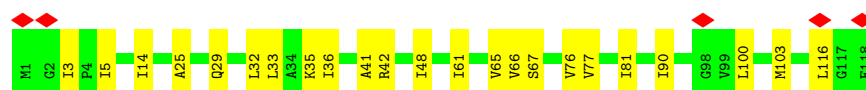
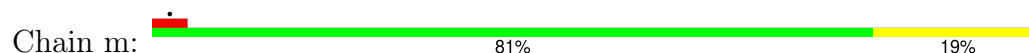
- Molecule 2: RsbT antagonist protein RsbS



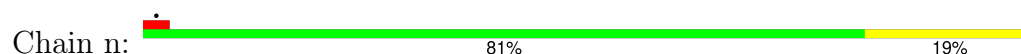
- Molecule 2: RsbT antagonist protein RsbS



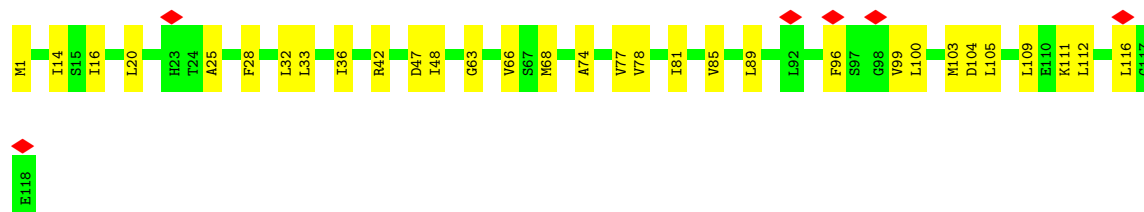
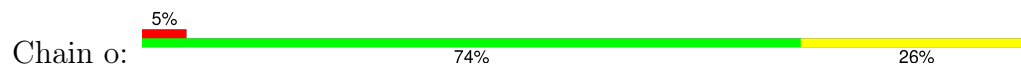
- Molecule 2: RsbT antagonist protein RsbS



- Molecule 2: RsbT antagonist protein RsbS



- Molecule 2: RsbT antagonist protein RsbS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31771	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	0.986	Depositor
Minimum map value	-0.355	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	501.0, 501.0, 501.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/1013	0.43	1/1370 (0.1%)
1	AB	0.15	0/1013	0.37	0/1370
1	B	0.15	0/1013	0.43	2/1370 (0.1%)
1	BB	0.13	0/1013	0.33	0/1370
1	C	0.14	0/1013	0.41	1/1370 (0.1%)
1	CB	0.15	0/1013	0.35	0/1370
1	D	0.15	0/1013	0.41	1/1370 (0.1%)
1	DB	0.14	0/1013	0.33	0/1370
1	E	0.15	0/1013	0.42	3/1370 (0.2%)
1	EB	0.14	0/1013	0.33	0/1370
1	F	0.15	0/1013	0.40	3/1370 (0.2%)
1	FB	0.13	0/1013	0.30	0/1370
1	G	0.15	0/1013	0.43	1/1370 (0.1%)
1	GB	0.14	0/1013	0.34	0/1370
1	H	0.15	0/1013	0.42	2/1370 (0.1%)
1	HB	0.15	0/1013	0.36	0/1370
1	I	0.14	0/1013	0.41	2/1370 (0.1%)
1	IB	0.14	0/1013	0.35	0/1370
1	J	0.14	0/1013	0.43	3/1370 (0.2%)
1	JB	0.15	0/1013	0.36	0/1370
1	K	0.15	0/1013	0.43	2/1370 (0.1%)
1	KB	0.14	0/1013	0.33	0/1370
1	L	0.15	0/1013	0.41	1/1370 (0.1%)
1	LB	0.17	0/1013	0.39	0/1370
1	M	0.14	0/1013	0.43	3/1370 (0.2%)
1	MB	0.12	0/1013	0.32	0/1370
1	N	0.15	0/1013	0.43	3/1370 (0.2%)
1	NB	0.15	0/1013	0.35	0/1370
1	O	0.14	0/1013	0.43	1/1370 (0.1%)
1	OB	0.15	0/1013	0.37	0/1370
2	a	0.14	0/888	0.34	0/1197
2	ab	0.14	0/888	0.34	0/1197
2	b	0.14	0/888	0.36	0/1197
2	bb	0.15	0/888	0.39	0/1197

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	c	0.13	0/888	0.34	0/1197
2	cb	0.12	0/888	0.31	0/1197
2	d	0.14	0/888	0.35	0/1197
2	db	0.13	0/888	0.34	0/1197
2	e	0.15	0/888	0.40	0/1197
2	eb	0.15	0/888	0.36	0/1197
2	f	0.15	0/888	0.39	0/1197
2	fb	0.14	0/888	0.35	0/1197
2	g	0.13	0/888	0.32	0/1197
2	gb	0.13	0/888	0.33	0/1197
2	h	0.14	0/888	0.34	0/1197
2	hb	0.14	0/888	0.36	0/1197
2	i	0.14	0/888	0.34	0/1197
2	ib	0.15	0/888	0.35	0/1197
2	j	0.12	0/888	0.32	0/1197
2	jb	0.14	0/888	0.34	0/1197
2	k	0.14	0/888	0.36	0/1197
2	kb	0.16	0/888	0.39	0/1197
2	l	0.16	0/888	0.39	0/1197
2	lb	0.14	0/888	0.33	0/1197
2	m	0.13	0/888	0.29	0/1197
2	mb	0.14	0/888	0.36	0/1197
2	n	0.14	0/888	0.41	0/1197
2	nb	0.13	0/888	0.37	0/1197
2	o	0.14	0/888	0.37	0/1197
2	ob	0.16	0/888	0.39	0/1197
All	All	0.14	0/57030	0.37	29/77010 (0.0%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	157	LEU	N-CA-CB	6.02	119.01	110.46
1	B	157	LEU	N-CA-CB	5.79	118.68	110.46
1	N	157	LEU	N-CA-CB	5.79	118.64	110.24
1	J	157	LEU	N-CA-CB	5.75	118.58	110.24
1	A	157	LEU	N-CA-CB	5.66	118.87	110.49
1	O	157	LEU	N-CA-CB	5.66	118.87	110.49
1	I	157	LEU	N-CA-CB	5.64	118.47	110.46
1	E	157	LEU	N-CA-CB	5.63	118.74	110.35
1	F	157	LEU	N-CA-CB	5.57	118.66	110.35
1	L	157	LEU	N-CA-CB	5.46	118.57	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	157	LEU	N-CA-CB	5.43	118.18	110.46
1	M	157	LEU	N-CA-C	5.38	117.46	107.99
1	M	157	LEU	N-CA-CB	5.36	118.33	110.35
1	K	157	LEU	CB-CA-C	5.33	120.20	111.41
1	G	157	LEU	N-CA-CB	5.31	118.36	110.49
1	C	157	LEU	N-CA-CB	5.23	118.15	110.35
1	I	157	LEU	CB-CA-C	5.23	120.04	111.41
1	B	157	LEU	CB-CA-C	5.23	120.04	111.41
1	N	157	LEU	CB-CA-C	5.23	119.89	111.05
1	N	157	LEU	N-CA-C	5.17	117.12	108.23
1	M	157	LEU	CB-CA-C	5.14	120.03	111.30
1	D	157	LEU	N-CA-CB	5.11	118.05	110.49
1	F	157	LEU	N-CA-C	5.08	116.92	107.99
1	J	157	LEU	N-CA-C	5.07	116.96	108.23
1	E	157	LEU	N-CA-C	5.07	116.91	107.99
1	H	157	LEU	CB-CA-C	5.06	119.76	111.41
1	F	157	LEU	CB-CA-C	5.06	119.90	111.30
1	E	157	LEU	CB-CA-C	5.03	119.86	111.30
1	J	157	LEU	CB-CA-C	5.01	119.51	111.05

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	1006	0	1084	28	0
1	AB	1006	0	1084	32	0
1	B	1006	0	1084	30	0
1	BB	1006	0	1084	35	0
1	C	1006	0	1084	20	0
1	CB	1006	0	1084	23	0
1	D	1006	0	1084	25	0
1	DB	1006	0	1084	17	0
1	E	1006	0	1084	26	0
1	EB	1006	0	1084	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1006	0	1084	21	0
1	FB	1006	0	1084	20	0
1	G	1006	0	1084	30	0
1	GB	1006	0	1084	26	0
1	H	1006	0	1084	31	0
1	HB	1006	0	1084	22	0
1	I	1006	0	1084	29	0
1	IB	1006	0	1084	22	0
1	J	1006	0	1084	24	0
1	JB	1006	0	1084	29	0
1	K	1006	0	1084	37	0
1	KB	1006	0	1084	23	0
1	L	1006	0	1084	36	0
1	LB	1006	0	1084	29	0
1	M	1006	0	1084	34	0
1	MB	1006	0	1084	15	0
1	N	1006	0	1084	27	0
1	NB	1006	0	1084	26	0
1	O	1006	0	1084	25	0
1	OB	1006	0	1084	42	0
2	a	881	0	928	17	0
2	ab	881	0	928	17	0
2	b	881	0	928	21	0
2	bb	881	0	928	27	0
2	c	881	0	928	20	0
2	cb	881	0	928	14	0
2	d	881	0	928	19	0
2	db	881	0	928	16	0
2	e	881	0	928	21	0
2	eb	881	0	928	23	0
2	f	881	0	928	20	0
2	fb	881	0	928	25	0
2	g	881	0	928	21	0
2	gb	881	0	928	23	0
2	h	881	0	928	20	0
2	hb	881	0	928	23	0
2	i	881	0	928	23	0
2	ib	881	0	928	27	0
2	j	881	0	928	19	0
2	jb	881	0	928	13	0
2	k	881	0	928	24	0
2	kb	881	0	928	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	l	881	0	928	18	0
2	lb	881	0	928	20	0
2	m	881	0	928	16	0
2	mb	881	0	928	20	0
2	n	881	0	928	20	0
2	nb	881	0	928	23	0
2	o	881	0	928	27	0
2	ob	881	0	928	28	0
All	All	56610	0	60360	1210	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 10.

All (1210) 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:A:201:ILE:HD11	1:A:234:ILE:HD13	1.55	0.89
1:JB:243:VAL:HG22	1:I:220:GLU:OE1	1.75	0.87
1:AB:249:LEU:HD13	1:OB:224:LEU:HD23	1.57	0.85
1:D:209:GLU:HG3	1:D:245:LEU:HD22	1.60	0.84
1:BB:224:LEU:HD23	1:M:249:LEU:HD13	1.59	0.83
1:G:201:ILE:HD11	1:G:234:ILE:HD13	1.60	0.82
1:EB:170:ILE:CG2	1:E:153:LEU:HD22	2.10	0.81
1:EB:170:ILE:HG21	1:E:153:LEU:HD22	1.63	0.79
1:LB:170:ILE:HG21	1:L:153:LEU:HD22	1.62	0.79
2:a:77:VAL:HG13	2:a:112:LEU:HD21	1.67	0.77
1:KB:170:ILE:HG21	1:K:153:LEU:HD22	1.65	0.77
1:LB:170:ILE:CG2	1:L:153:LEU:HD22	2.15	0.77
1:E:249:LEU:HD11	1:E:252:ILE:HD11	1.63	0.77
2:cb:48:ILE:HD11	2:cb:81:ILE:HD13	1.68	0.76
1:AB:224:LEU:HD22	1:BB:249:LEU:HD12	1.67	0.76
2:ob:33:LEU:HD11	2:ob:68:MET:CE	2.17	0.75
1:B:231:LEU:HD13	1:B:252:ILE:HD12	1.69	0.75
1:JB:249:LEU:HD12	1:I:224:LEU:HD22	1.69	0.75
2:eb:61:ILE:O	2:eb:65:VAL:HG23	1.87	0.74
2:o:48:ILE:HD11	2:o:81:ILE:HG22	1.70	0.74
1:LB:258:MET:HE1	1:L:160:ILE:HA	1.69	0.74
1:F:149:ALA:O	1:F:153:LEU:HD13	1.88	0.73
2:bb:77:VAL:HG13	2:bb:112:LEU:HD21	1.69	0.73
1:KB:170:ILE:CG2	1:K:153:LEU:HD22	2.18	0.73
1:LB:153:LEU:HD22	1:L:170:ILE:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:249:LEU:HD12	1:L:224:LEU:HD22	1.70	0.72
1:JB:153:LEU:HD22	1:J:170:ILE:CG2	2.19	0.72
1:A:149:ALA:O	1:A:153:LEU:HD13	1.90	0.72
1:OB:160:ILE:HA	1:O:258:MET:HE1	1.72	0.71
1:GB:170:ILE:CG2	1:G:153:LEU:HD22	2.19	0.71
1:HB:170:ILE:CG2	1:H:153:LEU:HD22	2.18	0.71
1:D:249:LEU:HD23	1:D:252:ILE:HD11	1.72	0.71
2:db:77:VAL:HG23	2:db:112:LEU:HD21	1.72	0.71
1:C:210:MET:N	1:C:210:MET:HE2	2.04	0.71
1:JB:201:ILE:HD11	1:JB:234:ILE:HG12	1.72	0.71
1:M:167:MET:HE1	1:M:181:ILE:HG23	1.71	0.71
2:f:77:VAL:HG12	2:f:100:LEU:HB2	1.71	0.71
1:JB:170:ILE:CG2	1:J:153:LEU:HD22	2.21	0.70
1:DB:153:LEU:HD22	1:D:170:ILE:CG2	2.21	0.70
1:IB:153:LEU:HD22	1:I:170:ILE:CG2	2.21	0.70
2:d:35:LYS:HE2	2:d:39:THR:HG21	1.72	0.70
1:KB:153:LEU:HD22	1:K:170:ILE:CG2	2.21	0.70
1:OB:153:LEU:HD22	1:O:170:ILE:CG2	2.22	0.70
1:CB:170:ILE:CG2	1:C:153:LEU:HD22	2.21	0.69
1:H:245:LEU:HD23	1:H:245:LEU:O	1.91	0.69
2:jb:77:VAL:HG23	2:jb:112:LEU:HD21	1.74	0.69
2:o:100:LEU:HD23	2:o:111:LYS:HE2	1.75	0.69
2:cb:14:ILE:HD11	2:cb:32:LEU:HD13	1.75	0.69
1:NB:170:ILE:CG2	1:N:153:LEU:HD22	2.23	0.69
1:M:167:MET:CE	1:M:181:ILE:HG23	2.23	0.69
2:l:77:VAL:HG12	2:l:100:LEU:HB2	1.75	0.69
2:g:77:VAL:HG12	2:g:100:LEU:HB2	1.74	0.69
1:CB:153:LEU:HD22	1:C:170:ILE:CG2	2.23	0.68
1:HB:153:LEU:HD22	1:H:170:ILE:CG2	2.24	0.68
1:IB:170:ILE:CG2	1:I:153:LEU:HD22	2.22	0.68
2:ob:46:ILE:HG22	2:ob:48:ILE:HD11	1.75	0.68
1:FB:153:LEU:HD22	1:F:170:ILE:CG2	2.24	0.68
2:ib:77:VAL:HG23	2:ib:112:LEU:HD21	1.76	0.68
1:HB:170:ILE:HG21	1:H:153:LEU:HD22	1.75	0.68
1:BB:153:LEU:HD22	1:B:170:ILE:CG2	2.24	0.68
1:DB:170:ILE:CG2	1:D:153:LEU:HD22	2.24	0.68
1:D:157:LEU:HD11	1:D:165:SER:HB3	1.76	0.68
1:A:170:ILE:CG2	1:AB:153:LEU:HD22	2.24	0.68
1:MB:170:ILE:CG2	1:M:153:LEU:HD22	2.24	0.68
1:A:153:LEU:HD23	1:AB:170:ILE:HG22	1.77	0.68
1:MB:153:LEU:HD22	1:M:170:ILE:CG2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:LEU:HD11	1:E:165:SER:HB3	1.77	0.67
1:JB:170:ILE:HG21	1:J:153:LEU:HD22	1.75	0.67
2:b:77:VAL:HG23	2:b:112:LEU:HD21	1.76	0.66
2:f:26:VAL:O	2:f:30:GLU:OE1	2.13	0.66
1:C:201:ILE:HD11	1:C:234:ILE:HD13	1.77	0.66
1:OB:170:ILE:HG22	1:O:153:LEU:HD22	1.77	0.66
1:EB:153:LEU:HD23	1:E:170:ILE:HG22	1.75	0.66
1:M:167:MET:HE2	1:M:169:LEU:HD21	1.77	0.66
2:bb:25:ALA:HA	2:bb:28:PHE:CE1	2.30	0.66
1:K:209:GLU:HG2	1:K:210:MET:N	2.10	0.66
2:e:77:VAL:HG22	2:e:100:LEU:HB2	1.79	0.65
1:EB:260:LYS:HE3	1:EB:260:LYS:HA	1.78	0.65
1:C:185:LEU:HD11	1:C:197:VAL:HG21	1.78	0.65
1:H:207:VAL:HG13	1:H:211:VAL:HG23	1.79	0.65
1:NB:209:GLU:HG2	1:NB:210:MET:N	2.11	0.65
1:B:232:VAL:HG21	1:B:258:MET:HA	1.78	0.65
2:nb:6:LEU:HD22	2:n:105:LEU:HD13	1.79	0.65
1:AB:224:LEU:CD2	1:BB:249:LEU:HD12	2.27	0.65
1:E:219:SER:HB2	1:E:252:ILE:HG21	1.79	0.65
1:D:231:LEU:HD23	1:D:234:ILE:HD11	1.78	0.65
1:OB:170:ILE:CG2	1:O:153:LEU:HD22	2.26	0.65
1:F:249:LEU:HD22	2:k:71:LEU:HD22	1.78	0.65
2:gb:109:LEU:HD21	2:gb:113:LYS:HE2	1.79	0.65
1:KB:185:LEU:HD11	1:KB:197:VAL:HG21	1.79	0.64
2:ib:6:LEU:HD21	2:i:15:SER:OG	1.97	0.64
2:lb:61:ILE:O	2:lb:65:VAL:HG23	1.97	0.64
2:fb:14:ILE:HD11	2:fb:32:LEU:HD13	1.78	0.64
2:b:61:ILE:O	2:b:65:VAL:HG23	1.97	0.64
1:N:209:GLU:HG2	1:N:210:MET:N	2.12	0.64
2:eb:25:ALA:HA	2:eb:28:PHE:CE1	2.32	0.64
1:F:249:LEU:HD23	1:F:252:ILE:HD11	1.78	0.64
2:b:26:VAL:O	2:b:30:GLU:OE1	2.16	0.64
2:j:77:VAL:HG22	2:j:100:LEU:HB2	1.79	0.64
1:NB:153:LEU:HD22	1:N:170:ILE:CG2	2.27	0.64
2:eb:36:ILE:HD11	2:eb:74:ALA:CB	2.28	0.63
2:mb:78:VAL:HG21	2:mb:96:PHE:HE2	1.62	0.63
2:h:77:VAL:HG13	2:h:112:LEU:HD21	1.80	0.63
2:n:23:HIS:O	2:n:27:GLU:OE1	2.15	0.63
1:LB:209:GLU:HG2	1:LB:245:LEU:HD13	1.78	0.63
2:bb:61:ILE:O	2:bb:65:VAL:HG23	1.99	0.63
2:m:61:ILE:O	2:m:65:VAL:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:269:THR:HG22	1:K:269:THR:O	1.98	0.63
2:ib:6:LEU:HD22	2:i:105:LEU:HD13	1.81	0.63
2:ib:48:ILE:HD11	2:ib:81:ILE:CD1	2.29	0.63
2:nb:109:LEU:HD23	2:n:8:LEU:HD11	1.80	0.63
2:d:77:VAL:HG22	2:d:100:LEU:HB2	1.80	0.63
2:j:78:VAL:HG21	2:j:96:PHE:HE2	1.61	0.63
2:ib:34:ALA:O	2:ib:38:GLU:OE1	2.16	0.62
1:IB:162:GLU:O	1:IB:164:ILE:HD12	1.99	0.62
2:ib:48:ILE:HD11	2:ib:81:ILE:HD13	1.81	0.62
1:OB:185:LEU:HD11	1:OB:197:VAL:HG21	1.81	0.62
1:G:201:ILE:HD11	1:G:234:ILE:CD1	2.27	0.62
1:LB:160:ILE:HG22	1:LB:161:PHE:CD1	2.34	0.62
1:L:157:LEU:HD11	1:L:165:SER:HB3	1.80	0.62
2:d:77:VAL:HG23	2:d:112:LEU:HD21	1.81	0.62
2:m:77:VAL:HG22	2:m:100:LEU:HB2	1.80	0.62
2:e:71:LEU:O	2:e:71:LEU:HD23	2.00	0.62
1:NB:185:LEU:HD11	1:NB:197:VAL:HG21	1.81	0.61
2:eb:36:ILE:HD11	2:eb:74:ALA:HB3	1.80	0.61
2:kb:77:VAL:HG12	2:kb:100:LEU:HB2	1.81	0.61
1:DB:170:ILE:HG21	1:D:153:LEU:HD22	1.81	0.61
1:MB:170:ILE:HG21	1:M:153:LEU:HD22	1.81	0.61
1:CB:153:LEU:HD22	1:C:170:ILE:HG22	1.82	0.61
1:A:231:LEU:HG	1:A:234:ILE:HD11	1.82	0.61
1:AB:243:VAL:HG22	1:OB:220:GLU:HG3	1.82	0.61
2:bb:66:VAL:HG23	2:bb:76:VAL:HG11	1.81	0.61
2:db:71:LEU:O	2:db:71:LEU:HD23	2.01	0.61
2:nb:64:ASP:O	2:nb:68:MET:HE3	2.00	0.61
2:fb:66:VAL:HG23	2:fb:76:VAL:HG11	1.82	0.61
1:GB:153:LEU:HD22	1:G:170:ILE:CG2	2.30	0.61
2:mb:77:VAL:HG12	2:mb:100:LEU:HB2	1.82	0.61
2:mb:103:MET:HE3	2:mb:103:MET:HA	1.83	0.61
2:g:78:VAL:HG21	2:g:96:PHE:CE2	2.35	0.61
2:k:64:ASP:O	2:k:68:MET:HG3	2.01	0.61
2:o:78:VAL:HG21	2:o:96:PHE:CE1	2.35	0.61
1:NB:224:LEU:HD22	1:OB:249:LEU:HD12	1.83	0.61
2:n:25:ALA:HA	2:n:28:PHE:CE1	2.36	0.61
1:JB:249:LEU:HD12	1:I:224:LEU:CD2	2.30	0.61
2:m:14:ILE:HD11	2:m:32:LEU:HD13	1.83	0.61
1:FB:209:GLU:HG2	1:FB:210:MET:N	2.16	0.61
2:kb:14:ILE:HD11	2:kb:32:LEU:HD13	1.82	0.61
1:NB:224:LEU:CD2	1:OB:249:LEU:HD12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HD11	1:D:197:VAL:HG21	1.82	0.61
1:DB:209:GLU:HG2	1:DB:210:MET:N	2.15	0.60
2:kb:34:ALA:O	2:kb:38:GLU:OE1	2.18	0.60
1:BB:209:GLU:HG2	1:BB:210:MET:N	2.16	0.60
1:G:243:VAL:HG11	2:m:67:SER:OG	2.00	0.60
2:h:77:VAL:HG12	2:h:100:LEU:HB2	1.82	0.60
1:AB:185:LEU:O	1:AB:189:VAL:HG23	2.02	0.60
1:EB:155:ALA:HB1	1:EB:167:MET:HE1	1.83	0.60
1:FB:210:MET:HE3	1:FB:214:HIS:CE1	2.37	0.60
2:o:1:MET:HE2	2:o:1:MET:N	2.16	0.60
2:ob:25:ALA:HA	2:ob:28:PHE:CE1	2.37	0.60
2:ab:77:VAL:HG13	2:ab:112:LEU:HD21	1.83	0.60
2:e:77:VAL:HG23	2:e:112:LEU:HD21	1.82	0.60
2:o:78:VAL:HG21	2:o:96:PHE:CZ	2.36	0.60
1:M:201:ILE:HD11	1:M:234:ILE:HG13	1.83	0.60
2:ob:48:ILE:O	2:ob:48:ILE:HG22	2.01	0.60
2:kb:77:VAL:HG13	2:kb:112:LEU:HD21	1.83	0.60
2:lb:66:VAL:HG23	2:lb:76:VAL:HG11	1.84	0.60
2:i:78:VAL:HG21	2:i:96:PHE:HE1	1.66	0.60
1:N:193:ARG:HA	2:g:103:MET:HE2	1.82	0.60
2:mb:66:VAL:HG23	2:mb:76:VAL:HG11	1.84	0.60
1:EB:149:ALA:O	1:EB:153:LEU:HD13	2.01	0.60
1:IB:170:ILE:HG21	1:I:153:LEU:HD22	1.82	0.60
2:c:77:VAL:HG22	2:c:100:LEU:HB2	1.83	0.60
2:d:100:LEU:HD12	2:d:111:LYS:HE2	1.84	0.60
1:J:196:VAL:HG11	1:J:265:ALA:CB	2.32	0.60
2:d:78:VAL:HG21	2:d:96:PHE:HE1	1.67	0.60
1:GB:170:ILE:HG21	1:G:153:LEU:HD22	1.82	0.59
1:LB:160:ILE:HG22	1:LB:161:PHE:HD1	1.66	0.59
1:OB:269:THR:O	1:OB:269:THR:HG22	2.02	0.59
2:e:34:ALA:O	2:e:38:GLU:OE1	2.19	0.59
2:kb:105:LEU:HD13	2:k:6:LEU:HD22	1.84	0.59
2:ob:33:LEU:HD11	2:ob:68:MET:HE2	1.84	0.59
1:AB:269:THR:O	1:AB:269:THR:HG22	2.03	0.59
1:CB:157:LEU:HD13	1:CB:167:MET:HE2	1.84	0.59
1:CB:170:ILE:HG22	1:C:153:LEU:HD22	1.84	0.59
1:H:209:GLU:HG2	1:H:210:MET:N	2.17	0.59
1:EB:207:VAL:HG13	1:EB:211:VAL:HG23	1.83	0.59
1:GB:153:LEU:HD22	1:G:170:ILE:HG22	1.84	0.59
1:HB:240:GLN:HB2	2:ob:68:MET:HE3	1.85	0.59
1:LB:249:LEU:HD13	1:LB:252:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:103:MET:N	2:m:103:MET:HE2	2.18	0.59
1:D:147:LYS:HA	1:D:150:LEU:HD13	1.85	0.59
1:D:249:LEU:HD22	2:h:71:LEU:HD13	1.83	0.59
1:J:196:VAL:HG11	1:J:265:ALA:HB1	1.84	0.59
2:bb:29:GLN:O	2:bb:33:LEU:HD23	2.03	0.59
2:kb:8:LEU:HD11	2:k:109:LEU:HD13	1.85	0.59
2:kb:71:LEU:O	2:kb:71:LEU:HD23	2.03	0.59
1:M:234:ILE:HD12	1:M:234:ILE:H	1.67	0.59
2:ib:105:LEU:HD13	2:i:6:LEU:HD22	1.84	0.59
2:b:77:VAL:HG22	2:b:100:LEU:HB2	1.85	0.59
1:HB:243:VAL:HG11	2:ob:68:MET:CG	2.33	0.58
2:a:78:VAL:HG21	2:a:96:PHE:CE2	2.38	0.58
2:jb:14:ILE:HD11	2:jb:32:LEU:HD13	1.84	0.58
2:f:14:ILE:HD11	2:f:32:LEU:HD13	1.85	0.58
1:DB:179:LYS:O	1:DB:183:GLU:OE1	2.21	0.58
1:DB:185:LEU:HD11	1:DB:197:VAL:HG21	1.85	0.58
2:gb:8:LEU:HD11	2:g:109:LEU:HD23	1.84	0.58
1:IB:216:ILE:O	1:IB:220:GLU:OE1	2.22	0.58
1:N:201:ILE:O	1:N:204:VAL:HG12	2.04	0.58
2:j:66:VAL:HG23	2:j:76:VAL:HG11	1.85	0.58
2:n:29:GLN:HG3	2:n:65:VAL:HG22	1.84	0.58
1:A:190:VAL:HG21	1:L:236:PRO:HG3	1.85	0.58
1:AB:190:VAL:HG21	1:BB:236:PRO:HG3	1.85	0.58
1:CB:207:VAL:HG13	1:CB:211:VAL:HG23	1.85	0.58
2:ob:34:ALA:O	2:ob:38:GLU:OE1	2.21	0.58
1:BB:196:VAL:HG11	1:BB:265:ALA:HB1	1.85	0.58
2:eb:29:GLN:HG3	2:eb:65:VAL:HG22	1.85	0.58
1:G:210:MET:HA	1:G:210:MET:HE3	1.83	0.58
2:d:78:VAL:HG21	2:d:96:PHE:CE1	2.38	0.58
1:IB:153:LEU:HD22	1:I:170:ILE:HG22	1.86	0.58
1:G:189:VAL:HG23	1:G:194:SER:OG	2.03	0.58
1:G:196:VAL:HG11	1:G:265:ALA:CB	2.34	0.58
2:cb:48:ILE:HD11	2:cb:81:ILE:CD1	2.33	0.58
2:eb:109:LEU:HD23	2:e:8:LEU:HD11	1.85	0.58
2:jb:29:GLN:HG3	2:jb:65:VAL:HG22	1.86	0.58
1:NB:170:ILE:HG21	1:N:153:LEU:HD22	1.86	0.58
1:L:249:LEU:HD22	1:L:252:ILE:HD11	1.86	0.58
2:hb:66:VAL:HG23	2:hb:76:VAL:HG11	1.86	0.58
2:l:85:VAL:O	2:l:89:LEU:HD23	2.04	0.58
2:m:29:GLN:HG3	2:m:65:VAL:HG22	1.86	0.58
1:FB:240:GLN:OE1	2:hb:33:LEU:HD11	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:VAL:HG13	1:E:211:VAL:HG23	1.86	0.57
1:H:157:LEU:HD11	1:H:165:SER:HB3	1.86	0.57
2:cb:6:LEU:HD22	2:c:105:LEU:HD13	1.85	0.57
1:C:201:ILE:HD11	1:C:234:ILE:CD1	2.34	0.57
1:AB:243:VAL:HG23	1:OB:224:LEU:HD11	1.86	0.57
2:k:14:ILE:HD11	2:k:32:LEU:HD13	1.85	0.57
2:a:14:ILE:HD11	2:a:32:LEU:HD13	1.86	0.57
2:n:81:ILE:HD12	2:n:81:ILE:H	1.69	0.57
1:G:209:GLU:HG2	1:G:210:MET:N	2.20	0.57
1:G:213:HIS:O	1:G:217:GLN:OE1	2.23	0.57
2:lb:45:VAL:HG13	2:lb:77:VAL:HG23	1.87	0.57
1:HB:179:LYS:O	1:HB:183:GLU:OE1	2.22	0.57
1:N:167:MET:HE3	1:N:167:MET:O	2.05	0.57
2:hb:105:LEU:HD13	2:h:6:LEU:HD22	1.86	0.57
2:mb:64:ASP:O	2:mb:68:MET:HG3	2.04	0.57
2:k:61:ILE:O	2:k:65:VAL:HG23	2.04	0.57
2:k:72:MET:HE3	2:k:72:MET:O	2.05	0.57
2:n:78:VAL:HG21	2:n:96:PHE:HE2	1.70	0.57
2:o:20:LEU:HD13	2:o:28:PHE:CE1	2.40	0.57
1:D:249:LEU:HD22	2:h:71:LEU:CD1	2.34	0.57
1:B:186:LEU:HB3	1:J:236:PRO:HB3	1.87	0.57
1:B:196:VAL:HG11	1:B:265:ALA:HB1	1.87	0.57
1:E:251:GLN:HG2	1:E:252:ILE:HG23	1.87	0.57
2:a:48:ILE:HD11	2:a:81:ILE:HG12	1.86	0.57
1:FB:160:ILE:HA	1:F:258:MET:HE1	1.87	0.56
1:B:232:VAL:HG23	1:B:255:THR:OG1	2.04	0.56
1:L:262:MET:HE2	1:L:262:MET:HA	1.87	0.56
1:N:196:VAL:HG11	1:N:265:ALA:HB1	1.87	0.56
2:bb:5:ILE:CG2	2:bb:12:LEU:HD12	2.35	0.56
2:f:25:ALA:HA	2:f:28:PHE:CE1	2.40	0.56
1:A:160:ILE:HD12	1:A:166:VAL:CG2	2.36	0.56
1:CB:209:GLU:HG2	1:CB:210:MET:N	2.19	0.56
1:K:231:LEU:HG	1:K:234:ILE:HD11	1.86	0.56
2:lb:34:ALA:O	2:lb:38:GLU:OE1	2.22	0.56
2:ob:36:ILE:HD11	2:ob:74:ALA:HB3	1.87	0.56
2:e:25:ALA:HA	2:e:28:PHE:CE1	2.40	0.56
1:O:249:LEU:HD22	1:O:252:ILE:HD11	1.87	0.56
2:nb:105:LEU:HD13	2:n:6:LEU:HD22	1.87	0.56
2:ob:78:VAL:HG21	2:ob:96:PHE:CE2	2.41	0.56
2:db:25:ALA:HA	2:db:28:PHE:CE1	2.40	0.56
2:jb:103:MET:HE3	2:jb:103:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:23:HIS:O	2:l:27:GLU:OE1	2.23	0.56
2:n:78:VAL:HG21	2:n:96:PHE:CE2	2.41	0.56
2:hb:90:ILE:HD11	2:ib:71:LEU:HD12	1.88	0.56
2:e:78:VAL:HG21	2:e:96:PHE:CE1	2.40	0.56
2:j:78:VAL:HG21	2:j:96:PHE:CE2	2.40	0.56
1:KB:232:VAL:HG12	1:KB:255:THR:OG1	2.04	0.56
2:nb:14:ILE:HD11	2:nb:32:LEU:HD13	1.88	0.56
2:o:25:ALA:HA	2:o:28:PHE:CE1	2.41	0.56
2:kb:111:LYS:HE2	2:kb:111:LYS:HA	1.88	0.56
1:A:153:LEU:CD2	1:AB:170:ILE:HG22	2.35	0.56
1:IB:209:GLU:HG2	1:IB:210:MET:N	2.20	0.56
1:F:249:LEU:CD2	1:F:252:ILE:HD11	2.36	0.56
1:H:243:VAL:HG11	2:b:68:MET:HG3	1.87	0.56
2:l:16:ILE:HG22	2:l:51:ILE:HD11	1.87	0.56
1:DB:153:LEU:HD22	1:D:170:ILE:HG21	1.87	0.56
1:EB:167:MET:HE2	1:EB:181:ILE:HG23	1.88	0.56
1:AB:186:LEU:HB3	1:BB:236:PRO:HB3	1.87	0.56
1:CB:209:GLU:HG2	1:CB:210:MET:HE2	1.87	0.56
1:M:210:MET:N	1:M:210:MET:HE2	2.20	0.56
2:kb:51:ILE:HG23	2:kb:51:ILE:O	2.05	0.56
2:h:26:VAL:O	2:h:30:GLU:OE1	2.24	0.56
1:K:249:LEU:HD12	1:L:224:LEU:CD2	2.36	0.55
1:K:249:LEU:HD13	1:K:252:ILE:HD11	1.87	0.55
2:cb:61:ILE:O	2:cb:65:VAL:HG23	2.06	0.55
1:IB:210:MET:HA	1:IB:210:MET:HE2	1.88	0.55
2:ab:66:VAL:HG23	2:ab:76:VAL:HG11	1.88	0.55
2:o:16:ILE:HG21	2:o:20:LEU:HD11	1.89	0.55
2:hb:25:ALA:HA	2:hb:28:PHE:CE1	2.42	0.55
2:i:77:VAL:HG22	2:i:100:LEU:HB2	1.88	0.55
1:K:185:LEU:O	1:K:189:VAL:HG23	2.05	0.55
2:n:61:ILE:O	2:n:65:VAL:HG23	2.05	0.55
2:n:103:MET:HE3	2:n:103:MET:HA	1.88	0.55
1:E:207:VAL:HB	1:E:238:ILE:HG23	1.89	0.55
2:db:5:ILE:HG22	2:db:12:LEU:HD12	1.88	0.55
2:c:25:ALA:HA	2:c:28:PHE:CE1	2.41	0.55
2:g:78:VAL:HG21	2:g:96:PHE:HE2	1.72	0.55
1:GB:170:ILE:HG22	1:G:153:LEU:HD22	1.88	0.55
1:NB:249:LEU:HD22	1:M:224:LEU:CD2	2.36	0.55
1:OB:209:GLU:HG2	1:OB:210:MET:N	2.21	0.55
2:jb:60:LYS:HE2	2:jb:60:LYS:HA	1.88	0.55
1:FB:239:ALA:CB	2:hb:71:LEU:HD22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NB:186:LEU:HB3	1:OB:236:PRO:HB3	1.89	0.55
1:DB:210:MET:HE3	1:DB:210:MET:HA	1.89	0.54
1:GB:254:THR:HG21	2:kb:71:LEU:O	2.07	0.54
1:K:234:ILE:HD12	1:K:234:ILE:H	1.73	0.54
1:LB:153:LEU:HD22	1:L:170:ILE:HG22	1.87	0.54
1:DB:231:LEU:HD23	1:DB:234:ILE:HD11	1.89	0.54
1:N:148:SER:O	1:N:152:GLU:OE1	2.25	0.54
2:mb:36:ILE:HD11	2:mb:74:ALA:HB3	1.90	0.54
2:j:71:LEU:HD23	2:j:71:LEU:O	2.08	0.54
1:A:224:LEU:HD22	1:L:249:LEU:HD12	1.90	0.54
1:NB:269:THR:O	1:NB:270:ASN:OD1	2.25	0.54
2:m:48:ILE:HD11	2:m:81:ILE:HG12	1.89	0.54
2:db:26:VAL:O	2:db:30:GLU:OE1	2.26	0.54
2:bb:20:LEU:HD13	2:bb:28:PHE:CE1	2.43	0.54
2:ib:103:MET:HE3	2:ib:103:MET:HA	1.88	0.54
1:B:196:VAL:HG11	1:B:265:ALA:CB	2.38	0.54
2:h:48:ILE:HD11	2:h:81:ILE:HG13	1.89	0.54
1:AB:196:VAL:HG11	1:AB:265:ALA:HB1	1.89	0.54
1:E:243:VAL:HG11	2:j:68:MET:HG3	1.90	0.54
2:db:20:LEU:HD13	2:db:28:PHE:CE1	2.42	0.54
1:FB:170:ILE:HG22	1:F:153:LEU:HD23	1.89	0.53
1:G:196:VAL:HG11	1:G:265:ALA:HB1	1.90	0.53
1:L:232:VAL:HG21	1:L:258:MET:HA	1.90	0.53
2:db:15:SER:HB2	2:d:6:LEU:HD21	1.89	0.53
2:gb:71:LEU:HD23	2:gb:71:LEU:O	2.09	0.53
1:FB:170:ILE:HG22	1:F:153:LEU:CD2	2.38	0.53
2:kb:78:VAL:HG21	2:kb:96:PHE:HE2	1.72	0.53
1:FB:207:VAL:HB	1:FB:238:ILE:HG23	1.89	0.53
1:HB:157:LEU:HD13	1:HB:167:MET:HE2	1.89	0.53
1:F:247:ILE:HG22	1:F:249:LEU:HD12	1.90	0.53
2:cb:6:LEU:HD21	2:c:15:SER:HB2	1.89	0.53
2:fb:6:LEU:O	2:fb:12:LEU:HD13	2.09	0.53
1:K:236:PRO:HB3	1:L:186:LEU:HB3	1.91	0.53
2:a:77:VAL:HG12	2:a:100:LEU:HB2	1.91	0.53
2:ib:14:ILE:HD11	2:ib:32:LEU:HD13	1.89	0.53
2:kb:25:ALA:HA	2:kb:28:PHE:CE1	2.44	0.53
2:e:16:ILE:HG21	2:e:20:LEU:HD11	1.90	0.53
2:n:14:ILE:HD11	2:n:32:LEU:HD13	1.90	0.53
1:CB:269:THR:O	1:CB:269:THR:HG22	2.08	0.53
1:N:196:VAL:HG11	1:N:265:ALA:CB	2.38	0.53
1:AB:231:LEU:HD23	1:AB:234:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NB:153:LEU:HD22	1:N:170:ILE:HG22	1.89	0.53
1:N:210:MET:HE2	1:N:210:MET:HA	1.91	0.53
2:nb:25:ALA:HA	2:nb:28:PHE:CE1	2.44	0.53
2:e:26:VAL:O	2:e:30:GLU:OE1	2.27	0.53
2:o:42:ARG:CZ	2:o:116:LEU:HD12	2.38	0.53
1:D:209:GLU:HG3	1:D:245:LEU:CD2	2.33	0.53
1:EB:167:MET:HE3	1:EB:169:LEU:HD21	1.89	0.53
2:a:105:LEU:HD13	2:ab:6:LEU:HD22	1.91	0.53
2:lb:33:LEU:O	2:lb:36:ILE:HG22	2.09	0.53
2:k:1:MET:HA	2:k:1:MET:HE2	1.89	0.53
1:KB:209:GLU:HG2	1:KB:210:MET:N	2.22	0.52
2:g:5:ILE:HG22	2:g:12:LEU:HD12	1.91	0.52
1:NB:169:LEU:HD23	1:NB:201:ILE:HG22	1.90	0.52
1:J:209:GLU:HG2	1:J:210:MET:N	2.24	0.52
2:c:5:ILE:CG2	2:c:12:LEU:HD12	2.39	0.52
1:JB:153:LEU:HD22	1:J:170:ILE:HG22	1.90	0.52
2:fb:105:LEU:CD1	2:f:6:LEU:HD22	2.40	0.52
1:EB:170:ILE:HG22	1:E:153:LEU:HD22	1.89	0.52
1:JB:201:ILE:O	1:JB:204:VAL:HG12	2.10	0.52
1:LB:249:LEU:HD12	2:eb:71:LEU:HD22	1.92	0.52
1:H:245:LEU:HD22	1:H:247:ILE:HD11	1.90	0.52
1:K:216:ILE:O	1:K:220:GLU:OE1	2.27	0.52
2:bb:81:ILE:H	2:bb:81:ILE:HD12	1.75	0.52
2:fb:15:SER:HB3	2:f:6:LEU:HD21	1.91	0.52
1:M:209:GLU:HG3	1:M:245:LEU:HD13	1.91	0.52
1:B:167:MET:HE3	1:B:167:MET:O	2.10	0.52
1:D:157:LEU:HD11	1:D:165:SER:CB	2.38	0.52
2:hb:90:ILE:HD12	2:ib:68:MET:HG2	1.92	0.52
1:KB:153:LEU:HD22	1:K:170:ILE:HG22	1.92	0.52
2:i:66:VAL:HG23	2:i:76:VAL:HG11	1.92	0.52
2:l:3:ILE:O	2:l:5:ILE:HD12	2.10	0.52
1:BB:196:VAL:HG11	1:BB:265:ALA:CB	2.40	0.52
1:BB:207:VAL:HB	1:BB:238:ILE:HG23	1.91	0.52
2:ib:15:SER:HB2	2:i:6:LEU:HD21	1.92	0.52
2:k:78:VAL:HG21	2:k:96:PHE:HE2	1.75	0.52
1:CB:212:ALA:HB1	1:CB:242:ILE:CD1	2.40	0.52
1:HB:207:VAL:HB	1:HB:238:ILE:HG23	1.92	0.52
1:A:185:LEU:O	1:A:189:VAL:HG23	2.10	0.52
1:IB:170:ILE:HG22	1:I:153:LEU:HD22	1.91	0.52
1:H:201:ILE:O	1:H:204:VAL:HG12	2.10	0.52
2:h:78:VAL:HG21	2:h:96:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:198:LEU:HD22	1:BB:262:MET:HE2	1.91	0.51
1:LB:220:GLU:HG3	1:O:243:VAL:HG22	1.92	0.51
1:J:216:ILE:HG12	1:J:249:LEU:HD21	1.91	0.51
2:eb:75:LYS:HE3	2:eb:116:LEU:HD23	1.91	0.51
1:E:249:LEU:CD1	1:E:252:ILE:HD11	2.37	0.51
1:M:249:LEU:H	1:M:249:LEU:HD23	1.75	0.51
2:eb:20:LEU:HD13	2:eb:28:PHE:CE1	2.45	0.51
2:j:81:ILE:HD12	2:j:81:ILE:H	1.74	0.51
2:cb:26:VAL:O	2:cb:30:GLU:OE1	2.29	0.51
2:ib:62:LEU:HD22	2:ib:96:PHE:HZ	1.74	0.51
2:f:16:ILE:HG21	2:f:20:LEU:HD11	1.92	0.51
1:BB:157:LEU:HD13	1:BB:167:MET:HE2	1.93	0.51
1:GB:209:GLU:HG2	1:GB:210:MET:CE	2.41	0.51
1:MB:153:LEU:HD22	1:M:170:ILE:HG21	1.92	0.51
1:HB:153:LEU:HD22	1:H:170:ILE:HG22	1.91	0.51
1:LB:207:VAL:HG13	1:LB:211:VAL:HG23	1.92	0.51
1:J:249:LEU:HD22	1:J:252:ILE:CD1	2.41	0.51
2:g:14:ILE:HG21	2:g:28:PHE:HE1	1.75	0.51
2:fb:25:ALA:HA	2:fb:28:PHE:CE1	2.45	0.51
2:ob:26:VAL:O	2:ob:30:GLU:OE1	2.28	0.51
1:LB:185:LEU:O	1:LB:189:VAL:HG23	2.10	0.51
1:J:225:VAL:O	2:m:103:MET:HE1	2.11	0.51
1:O:207:VAL:HG13	1:O:211:VAL:HG23	1.91	0.51
2:bb:42:ARG:CZ	2:bb:116:LEU:HD12	2.41	0.51
2:gb:51:ILE:HG23	2:gb:51:ILE:O	2.11	0.51
2:hb:14:ILE:HD11	2:hb:32:LEU:HD13	1.93	0.51
2:l:103:MET:HE2	2:l:103:MET:HA	1.93	0.51
1:OB:153:LEU:HD22	1:O:170:ILE:HG22	1.93	0.51
1:J:262:MET:HE2	1:J:262:MET:HA	1.93	0.51
1:O:164:ILE:HG21	1:O:262:MET:HE1	1.93	0.51
2:ab:26:VAL:O	2:ab:30:GLU:OE1	2.29	0.51
2:db:5:ILE:CG2	2:db:12:LEU:HD12	2.40	0.51
2:h:14:ILE:HG21	2:h:28:PHE:CE1	2.46	0.51
1:FB:239:ALA:HB2	2:hb:71:LEU:HD22	1.93	0.51
2:bb:88:THR:O	2:bb:92:LEU:HD23	2.11	0.51
2:db:78:VAL:HG21	2:db:96:PHE:CE1	2.46	0.51
2:b:78:VAL:HG21	2:b:96:PHE:CE1	2.46	0.51
2:o:112:LEU:O	2:o:116:LEU:HD23	2.11	0.51
1:A:160:ILE:HA	1:AB:258:MET:HE2	1.93	0.51
1:AB:196:VAL:HG11	1:AB:265:ALA:CB	2.41	0.51
1:FB:207:VAL:HG13	1:FB:211:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:207:VAL:HB	1:GB:238:ILE:HG23	1.93	0.51
1:GB:212:ALA:HB1	1:GB:242:ILE:CD1	2.41	0.51
2:ob:6:LEU:HD22	2:o:105:LEU:HD13	1.93	0.51
2:j:109:LEU:C	2:j:109:LEU:HD23	2.36	0.51
1:HB:212:ALA:HB1	1:HB:242:ILE:CD1	2.41	0.50
1:H:207:VAL:HB	1:H:238:ILE:HG23	1.93	0.50
1:J:249:LEU:HD22	1:J:252:ILE:HD11	1.93	0.50
2:a:16:ILE:HG21	2:a:51:ILE:HD11	1.92	0.50
2:bb:103:MET:HE3	2:bb:103:MET:HA	1.92	0.50
2:nb:26:VAL:O	2:nb:30:GLU:OE1	2.29	0.50
2:c:5:ILE:HG22	2:c:12:LEU:HD12	1.93	0.50
2:d:25:ALA:HA	2:d:28:PHE:CE1	2.46	0.50
2:o:1:MET:HE2	2:o:1:MET:H2	1.76	0.50
1:JB:239:ALA:O	1:JB:243:VAL:HG23	2.11	0.50
2:ab:12:LEU:C	2:ab:13:LEU:HD12	2.36	0.50
2:gb:36:ILE:HD11	2:gb:41:ALA:O	2.11	0.50
2:jb:66:VAL:HG23	2:jb:76:VAL:HG11	1.92	0.50
2:bb:15:SER:HB2	2:b:6:LEU:HD21	1.94	0.50
2:ob:36:ILE:HD11	2:ob:74:ALA:CB	2.40	0.50
2:kb:48:ILE:O	2:kb:51:ILE:HG22	2.12	0.50
2:i:5:ILE:HG22	2:i:12:LEU:HD12	1.94	0.50
1:AB:236:PRO:HB3	1:OB:186:LEU:HB3	1.93	0.50
1:LB:201:ILE:HD11	1:LB:234:ILE:HD13	1.93	0.50
1:NB:190:VAL:HG21	1:OB:236:PRO:HG3	1.92	0.50
1:B:236:PRO:HB3	2:lb:33:LEU:HB3	1.94	0.50
1:I:204:VAL:HG11	1:I:207:VAL:HG22	1.93	0.50
2:d:61:ILE:O	2:d:65:VAL:HG23	2.11	0.50
2:e:85:VAL:O	2:e:89:LEU:HD13	2.12	0.50
2:i:5:ILE:CG2	2:i:12:LEU:HD12	2.42	0.50
1:GB:209:GLU:HG2	1:GB:210:MET:N	2.26	0.50
1:G:193:ARG:HA	2:lb:103:MET:HE2	1.94	0.50
2:ob:43:GLY:HA3	2:ob:112:LEU:HD21	1.92	0.50
1:C:180:LEU:HA	1:C:183:GLU:OE1	2.12	0.50
2:a:12:LEU:C	2:a:13:LEU:HD22	2.37	0.50
2:jb:78:VAL:HG21	2:jb:96:PHE:CE1	2.46	0.50
1:I:249:LEU:HD12	1:K:224:LEU:CD2	2.41	0.50
2:ob:81:ILE:HD12	2:ob:81:ILE:H	1.76	0.50
1:OB:185:LEU:O	1:OB:189:VAL:HG23	2.11	0.50
1:D:201:ILE:HD11	1:D:234:ILE:HG12	1.93	0.50
1:H:185:LEU:HD11	1:H:197:VAL:HG21	1.93	0.50
2:fb:5:ILE:CG2	2:fb:12:LEU:HD12	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:201:ILE:HD11	1:LB:234:ILE:CD1	2.42	0.49
1:MB:170:ILE:HG22	1:M:153:LEU:HD22	1.94	0.49
1:C:247:ILE:HG22	1:C:249:LEU:HD12	1.93	0.49
1:I:236:PRO:HB3	1:K:186:LEU:HB3	1.93	0.49
1:N:185:LEU:HD11	1:N:197:VAL:HG21	1.93	0.49
2:eb:103:MET:HA	2:eb:103:MET:HE2	1.94	0.49
2:f:12:LEU:HD13	2:f:41:ALA:CB	2.42	0.49
1:BB:175:THR:HG22	1:BB:179:LYS:HE3	1.93	0.49
1:NB:148:SER:O	1:NB:152:GLU:OE1	2.30	0.49
1:A:236:PRO:HB3	1:JB:186:LEU:HB3	1.94	0.49
1:CB:207:VAL:HB	1:CB:238:ILE:HG23	1.93	0.49
1:KB:153:LEU:HD22	1:K:170:ILE:HG21	1.94	0.49
1:C:231:LEU:HB3	1:C:234:ILE:HD11	1.94	0.49
2:hb:61:ILE:O	2:hb:65:VAL:HG23	2.12	0.49
2:jb:77:VAL:HG22	2:jb:100:LEU:HB2	1.93	0.49
2:c:3:ILE:O	2:c:5:ILE:HD12	2.12	0.49
2:n:72:MET:O	2:o:103:MET:HE1	2.12	0.49
1:BB:220:GLU:HB2	1:M:243:VAL:HG21	1.94	0.49
1:GB:209:GLU:HG2	1:GB:210:MET:HE2	1.94	0.49
2:ab:77:VAL:HG12	2:ab:100:LEU:HB2	1.93	0.49
2:fb:7:LYS:C	2:fb:8:LEU:HD22	2.37	0.49
2:fb:111:LYS:O	2:fb:115:GLU:OE1	2.29	0.49
1:I:185:LEU:HD11	1:I:197:VAL:HG21	1.93	0.49
1:I:269:THR:O	1:I:270:ASN:OD1	2.31	0.49
2:hb:90:ILE:HD12	2:ib:68:MET:CG	2.43	0.49
2:d:81:ILE:HD12	2:d:81:ILE:H	1.77	0.49
2:g:14:ILE:HG21	2:g:28:PHE:CE1	2.47	0.49
1:EB:222:VAL:HG21	1:EB:229:ALA:HB2	1.93	0.49
1:MB:207:VAL:HB	1:MB:238:ILE:HG23	1.94	0.49
1:C:242:ILE:HG21	1:C:249:LEU:HD11	1.94	0.49
1:G:245:LEU:HB2	1:G:247:ILE:HD12	1.94	0.49
1:L:157:LEU:HD13	1:L:167:MET:HB2	1.94	0.49
1:HB:170:ILE:HG22	1:H:153:LEU:HD22	1.93	0.49
1:KB:201:ILE:O	1:KB:204:VAL:HG12	2.12	0.49
1:B:164:ILE:HG21	1:B:262:MET:HE1	1.95	0.49
2:kb:61:ILE:O	2:kb:65:VAL:HG23	2.13	0.49
2:k:42:ARG:CZ	2:k:116:LEU:HD12	2.42	0.49
1:AB:167:MET:HG2	1:AB:185:LEU:HD13	1.94	0.49
1:I:207:VAL:HG13	1:I:211:VAL:HG23	1.95	0.49
1:M:248:GLU:O	1:M:248:GLU:HG2	2.13	0.49
2:a:84:ALA:O	2:a:88:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:gb:103:MET:HE3	2:gb:103:MET:HA	1.94	0.49
2:e:33:LEU:O	2:e:36:ILE:HG22	2.13	0.49
1:BB:185:LEU:O	1:BB:189:VAL:HG23	2.12	0.49
1:M:185:LEU:HD11	1:M:197:VAL:HG21	1.94	0.49
1:O:185:LEU:HD11	1:O:197:VAL:HG21	1.95	0.49
2:a:106:GLU:OE2	2:a:110:GLU:OE2	2.30	0.49
2:gb:105:LEU:HD23	2:gb:105:LEU:C	2.38	0.49
2:mb:85:VAL:O	2:mb:89:LEU:HD13	2.13	0.49
2:ob:16:ILE:HG21	2:ob:20:LEU:HD11	1.95	0.49
2:i:104:ASP:OD2	2:i:104:ASP:C	2.55	0.49
1:EB:183:GLU:OE2	1:EB:187:ILE:HD12	2.12	0.48
1:MB:160:ILE:HA	1:M:258:MET:HE1	1.95	0.48
1:G:209:GLU:HG2	1:G:210:MET:SD	2.53	0.48
2:gb:15:SER:HB2	2:g:6:LEU:HD21	1.95	0.48
2:o:104:ASP:OD1	2:o:104:ASP:C	2.56	0.48
1:LB:222:VAL:HG22	1:LB:227:CYS:HB3	1.95	0.48
2:fb:69:SER:OG	2:fb:76:VAL:HG21	2.12	0.48
2:gb:109:LEU:HD21	2:gb:113:LYS:CE	2.43	0.48
2:e:3:ILE:O	2:e:5:ILE:HD12	2.13	0.48
2:h:42:ARG:CZ	2:h:116:LEU:HD12	2.44	0.48
2:i:7:LYS:HD3	2:i:7:LYS:C	2.38	0.48
1:HB:193:ARG:HA	2:c:103:MET:HE2	1.95	0.48
1:D:201:ILE:O	1:D:204:VAL:HG12	2.13	0.48
1:D:207:VAL:HG13	1:D:211:VAL:HG23	1.96	0.48
1:F:231:LEU:HD23	1:F:234:ILE:HD11	1.95	0.48
1:L:212:ALA:O	1:L:216:ILE:HD12	2.13	0.48
2:hb:85:VAL:O	2:hb:89:LEU:HD13	2.13	0.48
2:ib:29:GLN:HG3	2:ib:65:VAL:HG22	1.95	0.48
2:nb:48:ILE:HD11	2:nb:81:ILE:HG12	1.94	0.48
2:nb:71:LEU:O	2:nb:71:LEU:HD23	2.14	0.48
2:ob:48:ILE:HD13	2:ob:78:VAL:HG13	1.95	0.48
1:B:152:GLU:HG3	1:B:153:LEU:HD23	1.94	0.48
1:F:178:ALA:O	1:F:181:ILE:HG22	2.13	0.48
1:B:169:LEU:HD11	1:B:173:ILE:CD1	2.44	0.48
2:mb:3:ILE:O	2:mb:5:ILE:HD12	2.13	0.48
2:g:71:LEU:HD12	2:h:90:ILE:HD11	1.94	0.48
2:g:104:ASP:OD1	2:g:104:ASP:C	2.57	0.48
1:KB:269:THR:O	1:KB:270:ASN:OD1	2.30	0.48
2:gb:6:LEU:HD22	2:g:105:LEU:HD13	1.96	0.48
2:f:69:SER:OG	2:f:76:VAL:HG21	2.12	0.48
2:m:42:ARG:NH1	2:m:116:LEU:HD22	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JB:243:VAL:HG21	1:I:221:ALA:HB2	1.95	0.48
1:E:238:ILE:O	1:E:242:ILE:HG12	2.14	0.48
1:J:223:ARG:O	1:J:223:ARG:HD3	2.14	0.48
1:O:249:LEU:HD22	1:O:252:ILE:CD1	2.43	0.48
2:gb:48:ILE:O	2:gb:51:ILE:HG22	2.14	0.48
2:hb:12:LEU:C	2:hb:13:LEU:HD22	2.39	0.48
2:mb:110:GLU:HA	2:mb:110:GLU:OE1	2.13	0.48
1:BB:224:LEU:CD2	1:M:249:LEU:HD13	2.37	0.48
1:JB:236:PRO:HB3	1:I:186:LEU:HB3	1.96	0.48
2:eb:6:LEU:HD22	2:e:105:LEU:HD13	1.96	0.48
2:eb:105:LEU:HD13	2:e:6:LEU:HD22	1.94	0.48
2:b:16:ILE:HG21	2:b:51:ILE:HD11	1.94	0.48
2:j:3:ILE:O	2:j:5:ILE:HD12	2.14	0.48
2:n:20:LEU:HD13	2:n:28:PHE:CZ	2.49	0.48
2:kb:5:ILE:HD11	2:kb:12:LEU:HD23	1.95	0.48
2:c:79:THR:HG22	2:c:102:ALA:HB3	1.95	0.48
2:j:25:ALA:HA	2:j:28:PHE:CE1	2.48	0.48
1:EB:185:LEU:HD11	1:EB:197:VAL:HG21	1.96	0.48
1:GB:201:ILE:HD11	1:GB:234:ILE:HG12	1.96	0.48
1:JB:207:VAL:HB	1:JB:238:ILE:HG23	1.94	0.48
1:I:167:MET:SD	1:I:185:LEU:HD13	2.53	0.48
1:K:196:VAL:HG11	1:K:265:ALA:CB	2.43	0.48
2:f:104:ASP:C	2:f:104:ASP:OD1	2.57	0.48
2:k:104:ASP:OD2	2:k:104:ASP:C	2.57	0.48
2:bb:77:VAL:HG12	2:bb:100:LEU:HB2	1.96	0.47
2:fb:6:LEU:HD22	2:f:105:LEU:HD13	1.95	0.47
2:fb:78:VAL:HG21	2:fb:96:PHE:CE1	2.49	0.47
2:gb:14:ILE:HD11	2:gb:32:LEU:HD13	1.96	0.47
2:nb:59:ALA:HB1	2:nb:94:ILE:HD12	1.96	0.47
2:d:5:ILE:HG21	2:d:35:LYS:HG2	1.95	0.47
1:KB:236:PRO:HB3	2:bb:33:LEU:HB3	1.95	0.47
2:ob:61:ILE:O	2:ob:65:VAL:HG23	2.15	0.47
1:AB:243:VAL:HG23	1:OB:224:LEU:CD1	2.44	0.47
1:B:190:VAL:HG21	1:J:236:PRO:HG3	1.96	0.47
2:k:81:ILE:HD12	2:k:81:ILE:H	1.78	0.47
2:l:109:LEU:C	2:l:109:LEU:HD23	2.39	0.47
1:AB:249:LEU:HD13	1:OB:224:LEU:CD2	2.38	0.47
1:IB:236:PRO:HB3	2:mb:33:LEU:HB3	1.96	0.47
1:E:204:VAL:HG11	1:E:207:VAL:HG22	1.96	0.47
2:i:81:ILE:HD12	2:i:81:ILE:H	1.78	0.47
1:AB:212:ALA:O	1:AB:216:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:236:PRO:HB3	2:kb:33:LEU:HB3	1.97	0.47
1:H:238:ILE:O	1:H:242:ILE:HG12	2.15	0.47
1:O:228:GLN:C	1:O:228:GLN:OE1	2.57	0.47
2:a:3:ILE:O	2:a:5:ILE:HD12	2.15	0.47
2:e:78:VAL:HG21	2:e:96:PHE:HE1	1.79	0.47
1:BB:153:LEU:HD22	1:B:170:ILE:HG22	1.96	0.47
1:GB:149:ALA:O	1:GB:153:LEU:HG	2.15	0.47
1:HB:243:VAL:HG11	2:ob:68:MET:HG3	1.97	0.47
1:JB:220:GLU:OE2	1:JB:220:GLU:HA	2.14	0.47
1:G:207:VAL:HB	1:G:238:ILE:HG23	1.96	0.47
2:eb:36:ILE:HD12	2:eb:44:VAL:HG21	1.97	0.47
2:c:81:ILE:HD12	2:c:81:ILE:H	1.79	0.47
1:BB:212:ALA:O	1:BB:216:ILE:HD12	2.14	0.47
1:CB:157:LEU:HD12	1:CB:166:VAL:O	2.15	0.47
1:FB:153:LEU:HD22	1:F:170:ILE:HG21	1.93	0.47
1:NB:218:ALA:O	1:NB:222:VAL:HG22	2.14	0.47
1:O:207:VAL:HB	1:O:238:ILE:HG23	1.96	0.47
2:ab:72:MET:HE2	2:ab:72:MET:HA	1.97	0.47
2:ib:33:LEU:O	2:ib:36:ILE:HG22	2.14	0.47
2:kb:66:VAL:HG23	2:kb:76:VAL:HG11	1.96	0.47
1:JB:196:VAL:HG11	1:JB:265:ALA:CB	2.45	0.47
1:KB:236:PRO:HG3	2:bb:37:HIS:HB2	1.97	0.47
1:MB:258:MET:HE1	1:M:159:PRO:O	2.15	0.47
1:NB:170:ILE:HG22	1:N:153:LEU:HD22	1.95	0.47
2:hb:6:LEU:HD22	2:h:105:LEU:HD13	1.97	0.47
2:ob:20:LEU:HD13	2:ob:28:PHE:CE1	2.50	0.47
2:i:87:ILE:O	2:i:91:GLU:OE1	2.32	0.47
2:k:16:ILE:HG21	2:k:20:LEU:HD11	1.97	0.47
1:GB:207:VAL:HG13	1:GB:211:VAL:HG23	1.97	0.47
1:E:185:LEU:HD11	1:E:197:VAL:HG21	1.96	0.47
2:bb:36:ILE:HD11	2:bb:44:VAL:HG22	1.96	0.47
2:bb:105:LEU:HD13	2:b:6:LEU:HD22	1.97	0.47
2:db:14:ILE:HD11	2:db:32:LEU:HD13	1.96	0.47
2:d:12:LEU:HD13	2:d:41:ALA:CB	2.45	0.47
2:g:6:LEU:O	2:g:12:LEU:HD13	2.15	0.47
2:m:36:ILE:HD11	2:m:41:ALA:O	2.15	0.47
1:A:170:ILE:HG22	1:AB:153:LEU:HD22	1.96	0.47
1:L:269:THR:O	1:L:270:ASN:OD1	2.33	0.47
2:kb:105:LEU:CD2	2:k:8:LEU:HD13	2.45	0.47
2:lb:12:LEU:HD23	2:lb:41:ALA:CB	2.45	0.47
1:A:160:ILE:HD12	1:A:166:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:207:VAL:HG13	1:KB:211:VAL:HG23	1.97	0.46
1:J:230:MET:HE1	1:J:265:ALA:HB2	1.96	0.46
2:o:103:MET:HA	2:o:103:MET:HE2	1.96	0.46
1:IB:231:LEU:HD23	1:IB:234:ILE:HD11	1.96	0.46
1:E:249:LEU:HG	1:E:249:LEU:O	2.16	0.46
1:G:219:SER:HB2	1:G:252:ILE:HD12	1.98	0.46
2:cb:29:GLN:HG3	2:cb:65:VAL:HG22	1.96	0.46
2:g:5:ILE:CG2	2:g:12:LEU:HD12	2.45	0.46
1:CB:249:LEU:HD12	2:ab:71:LEU:HD22	1.97	0.46
1:IB:221:ALA:HA	2:b:90:ILE:HD11	1.97	0.46
1:JB:216:ILE:HD11	1:JB:247:ILE:CG2	2.45	0.46
1:E:169:LEU:HD13	1:E:199:ILE:HG23	1.97	0.46
1:I:238:ILE:O	1:I:242:ILE:HG12	2.15	0.46
1:O:204:VAL:HG11	1:O:207:VAL:HG22	1.97	0.46
2:bb:110:GLU:OE2	2:bb:111:LYS:HE3	2.15	0.46
2:lb:1:MET:HE3	2:lb:1:MET:O	2.16	0.46
2:c:5:ILE:HG21	2:c:35:LYS:HG2	1.97	0.46
1:EB:239:ALA:HB2	2:a:71:LEU:HD22	1.98	0.46
1:MB:209:GLU:HG2	1:MB:210:MET:N	2.30	0.46
1:NB:201:ILE:HD11	1:NB:234:ILE:HG12	1.96	0.46
1:B:185:LEU:O	1:B:189:VAL:HG23	2.15	0.46
1:I:187:ILE:O	1:I:190:VAL:HG12	2.16	0.46
2:l:78:VAL:HG21	2:l:96:PHE:CE2	2.51	0.46
1:AB:201:ILE:O	1:AB:204:VAL:HG12	2.15	0.46
1:CB:238:ILE:O	1:CB:242:ILE:HG12	2.16	0.46
1:G:162:GLU:HB3	1:G:163:LYS:HD2	1.98	0.46
1:O:216:ILE:HG12	1:O:249:LEU:HD21	1.97	0.46
2:g:29:GLN:HG3	2:g:65:VAL:HG22	1.98	0.46
1:BB:186:LEU:HD22	1:M:236:PRO:HB3	1.96	0.46
1:BB:273:ILE:HD13	1:B:161:PHE:CE1	2.50	0.46
1:GB:219:SER:OG	1:GB:252:ILE:HD12	2.16	0.46
1:I:249:LEU:HD12	1:K:224:LEU:HD22	1.98	0.46
1:M:185:LEU:O	1:M:189:VAL:HG23	2.14	0.46
2:fb:12:LEU:C	2:fb:13:LEU:HD22	2.40	0.46
2:gb:33:LEU:HA	2:gb:36:ILE:HG22	1.96	0.46
2:h:114:GLN:C	2:h:114:GLN:OE1	2.59	0.46
2:l:70:LYS:HD3	2:l:70:LYS:C	2.41	0.46
1:BB:231:LEU:HD23	1:BB:234:ILE:HD11	1.97	0.46
1:FB:269:THR:O	1:FB:270:ASN:OD1	2.33	0.46
1:OB:220:GLU:OE1	1:OB:220:GLU:HA	2.15	0.46
1:G:176:GLU:N	1:G:176:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:33:LEU:O	2:a:36:ILE:HG22	2.16	0.46
2:ab:16:ILE:HG21	2:ab:20:LEU:HD11	1.98	0.46
2:fb:29:GLN:HG3	2:fb:65:VAL:HG22	1.97	0.46
2:gb:61:ILE:O	2:gb:65:VAL:HG23	2.15	0.46
2:ib:6:LEU:O	2:ib:12:LEU:HD13	2.15	0.46
2:kb:8:LEU:HD13	2:k:105:LEU:HD22	1.97	0.46
2:b:33:LEU:O	2:b:36:ILE:HG22	2.16	0.46
1:CB:220:GLU:OE1	1:CB:220:GLU:HA	2.14	0.46
1:H:212:ALA:HB1	1:H:242:ILE:HD12	1.98	0.46
1:M:240:GLN:HA	1:M:243:VAL:HG12	1.98	0.46
2:eb:59:ALA:HB1	2:eb:94:ILE:HD13	1.96	0.46
2:nb:36:ILE:HD11	2:nb:41:ALA:O	2.16	0.46
1:A:177:ARG:O	1:A:181:ILE:HG13	2.15	0.46
1:KB:160:ILE:HA	1:K:258:MET:HE1	1.98	0.46
1:OB:238:ILE:O	1:OB:242:ILE:HG12	2.16	0.46
2:gb:64:ASP:C	2:gb:68:MET:HE3	2.40	0.46
2:ib:109:LEU:HD23	2:i:8:LEU:HD11	1.97	0.46
2:g:12:LEU:C	2:g:13:LEU:HD22	2.41	0.46
1:EB:239:ALA:CB	2:a:71:LEU:HD22	2.46	0.46
1:B:269:THR:C	1:B:270:ASN:OD1	2.59	0.46
1:L:157:LEU:HD12	1:L:166:VAL:O	2.16	0.46
2:ib:62:LEU:HD23	2:ib:62:LEU:O	2.15	0.46
2:ib:87:ILE:HG22	2:ib:91:GLU:OE2	2.16	0.46
2:lb:78:VAL:HG12	2:lb:81:ILE:HD11	1.98	0.46
2:n:5:ILE:HG21	2:n:35:LYS:HG2	1.97	0.46
2:o:33:LEU:HD11	2:o:68:MET:SD	2.56	0.46
2:o:36:ILE:HD11	2:o:74:ALA:HB3	1.98	0.46
1:MB:216:ILE:HD11	1:MB:247:ILE:CG2	2.46	0.45
2:kb:8:LEU:HD13	2:k:105:LEU:CD2	2.45	0.45
2:b:1:MET:HE3	2:b:1:MET:O	2.16	0.45
2:l:25:ALA:HA	2:l:28:PHE:CE1	2.51	0.45
2:o:47:ASP:OD1	2:o:47:ASP:C	2.59	0.45
1:AB:238:ILE:O	1:AB:242:ILE:HG12	2.17	0.45
1:BB:269:THR:O	1:BB:270:ASN:OD1	2.35	0.45
1:JB:170:ILE:HG22	1:J:153:LEU:HD22	1.96	0.45
1:KB:207:VAL:HB	1:KB:238:ILE:HG23	1.98	0.45
1:OB:207:VAL:HB	1:OB:238:ILE:HG23	1.98	0.45
2:lb:5:ILE:CG2	2:lb:12:LEU:HD12	2.46	0.45
2:nb:33:LEU:O	2:nb:36:ILE:HG22	2.16	0.45
1:AB:222:VAL:HG22	1:AB:227:CYS:HB3	1.98	0.45
1:EB:269:THR:O	1:EB:270:ASN:OD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HB:245:LEU:HB2	1:HB:247:ILE:HD12	1.96	0.45
1:IB:247:ILE:HG22	1:IB:249:LEU:HD12	1.99	0.45
1:B:231:LEU:HD12	1:B:231:LEU:N	2.31	0.45
2:db:7:LYS:HD2	2:db:7:LYS:C	2.42	0.45
2:hb:109:LEU:HD23	2:h:8:LEU:HD11	1.98	0.45
2:mb:81:ILE:HD12	2:mb:81:ILE:H	1.80	0.45
2:c:62:LEU:O	2:c:65:VAL:HG12	2.16	0.45
1:A:220:GLU:HB2	1:L:243:VAL:HG21	1.97	0.45
1:OB:153:LEU:HD22	1:O:170:ILE:HG21	1.96	0.45
2:ab:3:ILE:O	2:ab:5:ILE:HD12	2.16	0.45
2:d:118:GLU:N	2:d:118:GLU:OE2	2.49	0.45
2:o:14:ILE:HD11	2:o:32:LEU:HD13	1.97	0.45
1:AB:157:LEU:HD11	1:AB:165:SER:CB	2.47	0.45
1:LB:153:LEU:HD22	1:L:170:ILE:HG21	1.97	0.45
1:NB:258:MET:SD	1:NB:258:MET:C	3.00	0.45
1:O:162:GLU:CD	1:O:163:LYS:HG3	2.42	0.45
2:d:29:GLN:HG3	2:d:65:VAL:HG22	1.98	0.45
2:g:5:ILE:HG21	2:g:35:LYS:HG2	1.97	0.45
2:o:77:VAL:HG12	2:o:100:LEU:HB2	1.97	0.45
1:BB:186:LEU:HB3	1:M:236:PRO:HB3	1.98	0.45
1:DB:156:PRO:O	1:DB:167:MET:SD	2.75	0.45
1:FB:185:LEU:HD11	1:FB:197:VAL:HG11	1.98	0.45
2:gb:64:ASP:O	2:gb:68:MET:HE3	2.17	0.45
2:jb:70:LYS:HD3	2:jb:70:LYS:O	2.17	0.45
2:nb:15:SER:HB2	2:n:6:LEU:HD21	1.98	0.45
1:A:186:LEU:HB3	1:L:236:PRO:HB3	1.98	0.45
1:EB:153:LEU:CD2	1:E:170:ILE:HG22	2.43	0.45
1:MB:149:ALA:O	1:MB:153:LEU:HG	2.16	0.45
1:G:238:ILE:O	1:G:242:ILE:HG12	2.16	0.45
2:gb:3:ILE:O	2:gb:5:ILE:HD12	2.16	0.45
2:hb:78:VAL:HG21	2:hb:96:PHE:CE1	2.52	0.45
2:ob:12:LEU:HD13	2:ob:41:ALA:CB	2.46	0.45
2:f:35:LYS:NZ	2:f:39:THR:HG21	2.32	0.45
2:f:81:ILE:HD12	2:f:81:ILE:H	1.81	0.45
2:h:115:GLU:OE2	2:h:115:GLU:HA	2.17	0.45
1:GB:269:THR:O	1:GB:270:ASN:OD1	2.34	0.45
1:B:263:GLU:O	1:B:263:GLU:OE1	2.35	0.45
1:C:209:GLU:HB3	1:C:210:MET:CE	2.47	0.45
1:D:182:ILE:HG12	1:D:218:ALA:HB2	1.99	0.45
1:F:230:MET:HE1	1:F:261:GLY:O	2.17	0.45
1:G:236:PRO:HB2	2:m:33:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:LEU:HD11	1:H:165:SER:CB	2.47	0.45
1:H:210:MET:HE2	1:H:210:MET:HA	1.97	0.45
1:I:207:VAL:HB	1:I:238:ILE:HG23	1.97	0.45
1:M:166:VAL:HG22	1:M:198:LEU:HB2	1.99	0.45
2:gb:22:ASP:OD1	2:gb:23:HIS:N	2.50	0.45
2:e:24:THR:O	2:e:28:PHE:CD1	2.70	0.45
2:e:70:LYS:HD3	2:e:70:LYS:C	2.42	0.45
1:NB:210:MET:HA	1:NB:210:MET:HE2	1.98	0.45
1:OB:219:SER:O	1:OB:222:VAL:HG12	2.17	0.45
2:jb:63:GLY:O	2:jb:66:VAL:HG12	2.16	0.45
2:lb:25:ALA:O	2:lb:28:PHE:CD1	2.70	0.45
2:f:47:ASP:OD1	2:f:47:ASP:C	2.60	0.45
2:j:75:LYS:HB2	2:j:112:LEU:HD11	1.98	0.45
1:BB:210:MET:HA	1:BB:210:MET:HE2	1.98	0.45
1:HB:269:THR:O	1:HB:270:ASN:OD1	2.34	0.45
1:NB:162:GLU:O	1:NB:163:LYS:HG2	2.16	0.45
1:L:162:GLU:O	1:L:163:LYS:HB2	2.17	0.45
1:L:182:ILE:HG12	1:L:218:ALA:HB2	1.99	0.45
2:cb:23:HIS:O	2:cb:27:GLU:HG3	2.17	0.45
2:cb:75:LYS:HE2	2:cb:75:LYS:HA	1.98	0.45
2:ib:5:ILE:CG2	2:ib:12:LEU:HD12	2.47	0.45
2:nb:3:ILE:O	2:nb:5:ILE:HD12	2.17	0.45
1:BB:153:LEU:HD22	1:B:170:ILE:HG21	1.99	0.44
1:CB:209:GLU:HG2	1:CB:210:MET:CE	2.47	0.44
1:LB:167:MET:HE2	1:LB:181:ILE:HG23	1.99	0.44
1:C:179:LYS:O	1:C:183:GLU:OE1	2.35	0.44
1:E:269:THR:O	1:E:270:ASN:OD1	2.34	0.44
1:I:189:VAL:CG2	1:I:227:CYS:SG	3.05	0.44
2:eb:16:ILE:CG2	2:eb:20:LEU:HD11	2.46	0.44
2:mb:29:GLN:HG3	2:mb:65:VAL:HG22	1.98	0.44
1:LB:182:ILE:HG12	1:LB:218:ALA:HB2	1.99	0.44
1:K:201:ILE:HD11	1:K:234:ILE:HG13	1.99	0.44
2:jb:105:LEU:CD1	2:j:6:LEU:HD23	2.47	0.44
2:mb:36:ILE:HD11	2:mb:74:ALA:CB	2.46	0.44
2:k:78:VAL:HG12	2:k:81:ILE:HD11	1.99	0.44
1:OB:231:LEU:C	1:OB:231:LEU:HD23	2.42	0.44
1:C:207:VAL:HB	1:C:238:ILE:HG23	1.99	0.44
1:E:182:ILE:HG12	1:E:218:ALA:HB2	1.99	0.44
1:I:189:VAL:HG21	1:I:227:CYS:SG	2.57	0.44
2:ab:5:ILE:HG21	2:ab:35:LYS:HG2	2.00	0.44
2:fb:112:LEU:O	2:fb:116:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:kb:81:ILE:HD12	2:kb:81:ILE:H	1.81	0.44
2:c:66:VAL:HG23	2:c:76:VAL:HG11	1.99	0.44
2:l:48:ILE:HD11	2:l:81:ILE:HG13	2.00	0.44
1:DB:153:LEU:HD22	1:D:170:ILE:HG22	1.99	0.44
1:DB:232:VAL:HG23	1:DB:255:THR:OG1	2.16	0.44
1:GB:157:LEU:HD22	1:GB:188:GLY:HA3	2.00	0.44
1:JB:198:LEU:HD12	1:JB:198:LEU:N	2.32	0.44
1:LB:193:ARG:HD3	1:LB:193:ARG:N	2.33	0.44
1:MB:177:ARG:O	1:MB:181:ILE:HG12	2.17	0.44
1:G:216:ILE:HD11	1:G:247:ILE:HG21	1.99	0.44
1:G:247:ILE:HG22	1:G:249:LEU:HD12	1.99	0.44
1:H:269:THR:O	1:H:270:ASN:OD1	2.36	0.44
1:I:236:PRO:CG	1:K:190:VAL:HG21	2.47	0.44
1:L:185:LEU:HD11	1:L:197:VAL:HG21	1.99	0.44
2:a:27:GLU:OE2	2:a:31:ASP:OD2	2.35	0.44
2:db:77:VAL:CG2	2:db:112:LEU:HD21	2.45	0.44
2:l:69:SER:OG	2:l:76:VAL:HG21	2.18	0.44
1:G:207:VAL:HG13	1:G:211:VAL:HG23	1.99	0.44
1:H:216:ILE:HD13	1:H:247:ILE:HG21	2.00	0.44
2:f:64:ASP:HB3	2:f:68:MET:HE3	1.99	0.44
1:CB:170:ILE:HG21	1:C:153:LEU:HD22	1.99	0.44
1:FB:201:ILE:HD11	1:FB:234:ILE:HD12	1.99	0.44
1:HB:240:GLN:CB	2:ob:68:MET:HE3	2.47	0.44
1:C:269:THR:O	1:C:270:ASN:OD1	2.36	0.44
1:K:269:THR:O	1:K:270:ASN:OD1	2.36	0.44
1:L:196:VAL:HG11	1:L:265:ALA:HB1	1.99	0.44
1:O:231:LEU:HD23	1:O:234:ILE:HD11	1.99	0.44
2:eb:81:ILE:HD12	2:eb:81:ILE:H	1.81	0.44
2:ib:25:ALA:HB1	2:ib:61:ILE:HG21	1.99	0.44
2:kb:47:ASP:HB2	2:kb:105:LEU:HD12	2.00	0.44
2:mb:47:ASP:OD1	2:mb:47:ASP:C	2.60	0.44
1:FB:243:VAL:HB	2:hb:68:MET:HE2	1.99	0.44
1:HB:207:VAL:HG13	1:HB:211:VAL:HG23	2.00	0.44
1:F:169:LEU:HD21	1:F:181:ILE:HD11	1.98	0.44
2:o:1:MET:HE2	2:o:1:MET:CA	2.48	0.44
1:DB:245:LEU:HB2	1:DB:247:ILE:HD12	2.00	0.44
1:NB:207:VAL:HB	1:NB:238:ILE:HG23	2.00	0.44
1:NB:273:ILE:HD11	1:N:161:PHE:CZ	2.53	0.44
1:E:212:ALA:HB1	1:E:242:ILE:CD1	2.48	0.44
1:H:243:VAL:HG11	2:b:68:MET:CG	2.47	0.44
1:K:177:ARG:O	1:K:181:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:lb:105:LEU:HD22	2:l:6:LEU:HD22	2.00	0.44
2:h:81:ILE:HD12	2:h:81:ILE:H	1.83	0.44
1:A:161:PHE:HB2	1:A:164:ILE:HB	2.00	0.44
1:EB:243:VAL:HG11	2:a:68:MET:CG	2.48	0.44
1:KB:242:ILE:HG23	1:KB:247:ILE:HG21	2.00	0.44
1:OB:223:ARG:HD3	1:OB:223:ARG:C	2.43	0.44
1:B:236:PRO:HG3	2:lb:37:HIS:HB2	1.99	0.44
1:C:209:GLU:HB3	1:C:210:MET:HE2	2.00	0.44
1:G:198:LEU:N	1:G:198:LEU:HD12	2.33	0.44
2:m:3:ILE:O	2:m:5:ILE:HD12	2.17	0.44
1:A:212:ALA:O	1:A:216:ILE:HD12	2.18	0.43
1:JB:153:LEU:HD22	1:J:170:ILE:HG21	1.98	0.43
1:JB:219:SER:OG	1:JB:252:ILE:HD12	2.18	0.43
1:D:210:MET:HE3	1:D:210:MET:HA	2.00	0.43
1:L:209:GLU:HG2	1:L:210:MET:HE2	1.98	0.43
2:bb:47:ASP:OD2	2:bb:47:ASP:C	2.61	0.43
2:i:78:VAL:HG21	2:i:96:PHE:CE1	2.49	0.43
1:EB:207:VAL:CG1	1:EB:211:VAL:HG23	2.47	0.43
1:NB:249:LEU:HD22	1:M:224:LEU:HD22	2.00	0.43
1:NB:270:ASN:O	1:N:276:LYS:HB3	2.18	0.43
1:OB:149:ALA:O	1:OB:153:LEU:HG	2.18	0.43
1:B:238:ILE:O	1:B:242:ILE:HG12	2.18	0.43
2:mb:90:ILE:HD12	2:nb:68:MET:HG3	2.00	0.43
1:IB:185:LEU:HD11	1:IB:197:VAL:HG21	1.99	0.43
1:JB:169:LEU:HD11	1:JB:181:ILE:HD13	1.99	0.43
1:JB:258:MET:O	1:JB:258:MET:SD	2.76	0.43
1:LB:210:MET:HA	1:LB:210:MET:HE2	2.00	0.43
1:OB:147:LYS:O	1:OB:151:GLN:OE1	2.37	0.43
1:OB:200:ASP:OD2	1:OB:258:MET:HE1	2.18	0.43
1:F:153:LEU:N	1:F:153:LEU:HD12	2.33	0.43
1:F:182:ILE:HG12	1:F:218:ALA:HB2	2.00	0.43
1:M:182:ILE:HG12	1:M:218:ALA:HB2	2.00	0.43
2:bb:77:VAL:CG1	2:bb:112:LEU:HD21	2.45	0.43
2:fb:13:LEU:HD12	2:fb:105:LEU:HD11	2.00	0.43
2:hb:16:ILE:HG23	2:hb:20:LEU:HD21	1.99	0.43
2:d:16:ILE:HG22	2:d:51:ILE:HD11	1.98	0.43
2:f:20:LEU:HD13	2:f:28:PHE:CE1	2.52	0.43
2:i:6:LEU:O	2:i:12:LEU:HD13	2.18	0.43
2:k:33:LEU:O	2:k:36:ILE:HG22	2.18	0.43
1:BB:198:LEU:N	1:BB:198:LEU:HD12	2.34	0.43
1:M:269:THR:O	1:M:270:ASN:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:160:ILE:HD12	1:N:166:VAL:CG2	2.49	0.43
2:b:25:ALA:HA	2:b:28:PHE:CD1	2.54	0.43
2:k:112:LEU:O	2:k:116:LEU:HD23	2.19	0.43
1:JB:222:VAL:HG22	1:JB:227:CYS:HB3	2.01	0.43
1:KB:264:ARG:O	1:KB:268:LEU:HD23	2.19	0.43
1:LB:212:ALA:O	1:LB:216:ILE:HD12	2.18	0.43
1:LB:262:MET:HA	1:LB:262:MET:HE2	2.01	0.43
1:E:157:LEU:HD12	1:E:158:LEU:N	2.32	0.43
1:K:222:VAL:HG22	1:K:227:CYS:HB3	1.99	0.43
1:L:230:MET:HE1	1:L:265:ALA:HA	2.00	0.43
1:O:162:GLU:OE2	1:O:163:LYS:HG3	2.18	0.43
2:bb:29:GLN:HG2	2:bb:65:VAL:HG22	2.01	0.43
2:fb:3:ILE:O	2:fb:5:ILE:HD12	2.18	0.43
2:fb:16:ILE:HG22	2:fb:51:ILE:HD11	2.01	0.43
2:gb:66:VAL:HG23	2:gb:76:VAL:HG11	2.01	0.43
2:c:78:VAL:HG12	2:c:81:ILE:HD11	2.00	0.43
2:e:79:THR:HG22	2:e:102:ALA:HB3	2.01	0.43
2:j:70:LYS:C	2:j:70:LYS:HD3	2.44	0.43
1:OB:196:VAL:HG11	1:OB:265:ALA:HB1	1.99	0.43
1:OB:231:LEU:HD23	1:OB:232:VAL:N	2.33	0.43
2:ab:81:ILE:HD12	2:ab:81:ILE:H	1.84	0.43
2:bb:107:SER:O	2:bb:111:LYS:HG2	2.19	0.43
2:gb:33:LEU:O	2:gb:36:ILE:HG22	2.19	0.43
2:f:12:LEU:HD21	2:f:35:LYS:HG3	2.01	0.43
2:i:29:GLN:HG3	2:i:65:VAL:HG22	2.00	0.43
1:BB:198:LEU:HD13	1:BB:262:MET:HE1	2.01	0.43
1:EB:204:VAL:HG11	1:EB:207:VAL:HG22	2.00	0.43
1:EB:210:MET:HE2	1:EB:210:MET:HA	2.01	0.43
1:H:247:ILE:HG22	1:H:249:LEU:HD12	2.01	0.43
2:bb:5:ILE:HG22	2:bb:12:LEU:HD12	2.01	0.43
2:lb:63:GLY:O	2:lb:66:VAL:HG12	2.18	0.43
2:nb:24:THR:O	2:nb:28:PHE:CD1	2.72	0.43
2:g:25:ALA:HB1	2:g:61:ILE:HG21	2.00	0.43
2:i:63:GLY:O	2:i:66:VAL:HG12	2.18	0.43
2:k:29:GLN:HG3	2:k:65:VAL:HG22	2.00	0.43
1:A:204:VAL:HG11	1:A:207:VAL:CG2	2.49	0.43
1:LB:209:GLU:HG2	1:LB:245:LEU:CD1	2.46	0.43
1:NB:186:LEU:O	1:NB:189:VAL:HG12	2.18	0.43
1:L:207:VAL:HB	1:L:238:ILE:HG23	2.01	0.43
1:O:195:GLU:N	1:O:195:GLU:OE1	2.51	0.43
2:bb:63:GLY:O	2:bb:66:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:hb:33:LEU:O	2:hb:36:ILE:HG22	2.18	0.43
2:lb:81:ILE:HD12	2:lb:81:ILE:H	1.82	0.43
2:nb:60:LYS:O	2:nb:60:LYS:HD3	2.19	0.43
2:e:81:ILE:HD12	2:e:81:ILE:H	1.84	0.43
2:i:82:GLN:OE1	2:i:82:GLN:HA	2.17	0.43
2:l:25:ALA:HA	2:l:28:PHE:CD1	2.54	0.43
1:BB:169:LEU:HD12	1:BB:173:ILE:HD11	2.01	0.43
1:B:269:THR:O	1:B:270:ASN:OD1	2.36	0.43
1:G:204:VAL:HG11	1:G:207:VAL:HG22	2.01	0.43
1:L:209:GLU:HG2	1:L:210:MET:N	2.34	0.43
2:a:13:LEU:HD12	2:a:105:LEU:HD11	1.99	0.43
2:ib:104:ASP:OD1	2:ib:104:ASP:C	2.62	0.43
2:kb:78:VAL:HG21	2:kb:96:PHE:CE2	2.52	0.43
1:E:249:LEU:HD11	1:E:252:ILE:CD1	2.41	0.43
1:F:162:GLU:O	1:F:163:LYS:HB2	2.19	0.43
1:J:228:GLN:N	1:J:228:GLN:OE1	2.52	0.43
2:ab:58:ILE:HA	2:ab:61:ILE:HG22	2.01	0.43
2:ab:87:ILE:HG13	2:i:68:MET:CE	2.49	0.43
2:nb:8:LEU:HD11	2:n:109:LEU:CD2	2.49	0.43
2:ob:33:LEU:O	2:ob:36:ILE:HG22	2.18	0.43
2:i:14:ILE:HG22	2:i:15:SER:N	2.34	0.43
2:j:71:LEU:HD23	2:j:71:LEU:C	2.44	0.43
2:k:109:LEU:HD23	2:k:109:LEU:C	2.44	0.43
1:AB:235:ARG:HG2	1:AB:238:ILE:HD12	2.00	0.42
1:N:256:ASN:H	1:N:256:ASN:HD22	1.67	0.42
2:eb:3:ILE:O	2:eb:5:ILE:HD12	2.19	0.42
2:n:24:THR:O	2:n:28:PHE:CD1	2.72	0.42
1:A:187:ILE:O	1:A:191:LYS:HG2	2.19	0.42
1:EB:249:LEU:HD22	1:EB:252:ILE:HG21	2.00	0.42
1:FB:204:VAL:HG11	1:FB:207:VAL:HG22	2.01	0.42
1:IB:149:ALA:O	1:IB:153:LEU:HG	2.19	0.42
1:F:196:VAL:HG11	1:F:265:ALA:CB	2.49	0.42
1:H:204:VAL:HG13	1:H:204:VAL:O	2.20	0.42
1:H:218:ALA:O	1:H:222:VAL:HG12	2.19	0.42
1:I:228:GLN:N	1:I:228:GLN:OE1	2.52	0.42
2:eb:16:ILE:HG22	2:eb:51:ILE:HD11	2.00	0.42
2:b:112:LEU:O	2:b:116:LEU:HD23	2.18	0.42
2:d:66:VAL:HG23	2:d:76:VAL:HG11	2.01	0.42
2:h:14:ILE:HG21	2:h:28:PHE:CZ	2.54	0.42
2:k:31:ASP:OD2	2:k:31:ASP:C	2.62	0.42
2:m:66:VAL:HG23	2:m:76:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HG21	1:AB:153:LEU:HD22	1.99	0.42
1:A:231:LEU:CG	1:A:234:ILE:HD11	2.46	0.42
1:BB:224:LEU:HD23	1:M:249:LEU:CD1	2.39	0.42
1:DB:149:ALA:O	1:DB:153:LEU:HG	2.19	0.42
1:GB:220:GLU:HB2	2:n:90:ILE:HD12	2.00	0.42
1:KB:149:ALA:O	1:KB:153:LEU:HG	2.20	0.42
1:D:207:VAL:CG1	1:D:211:VAL:HG23	2.48	0.42
1:N:176:GLU:O	1:N:179:LYS:HG2	2.19	0.42
1:O:169:LEU:HD22	1:O:173:ILE:HD11	2.01	0.42
2:db:105:LEU:HD13	2:d:6:LEU:HD22	2.00	0.42
2:b:66:VAL:HG23	2:b:76:VAL:HG11	2.00	0.42
2:g:3:ILE:O	2:g:5:ILE:HD12	2.18	0.42
1:A:224:LEU:CD2	1:L:249:LEU:HD12	2.50	0.42
1:EB:207:VAL:HG13	1:EB:211:VAL:CG2	2.49	0.42
1:HB:210:MET:HE2	1:HB:210:MET:HA	2.00	0.42
1:K:198:LEU:HD12	1:K:198:LEU:N	2.34	0.42
2:gb:70:LYS:C	2:gb:70:LYS:HD3	2.44	0.42
2:hb:105:LEU:CD1	2:h:6:LEU:HD22	2.49	0.42
2:kb:71:LEU:HD23	2:kb:71:LEU:C	2.43	0.42
2:m:5:ILE:HG21	2:m:35:LYS:HG2	2.02	0.42
1:AB:157:LEU:HD11	1:AB:165:SER:HB2	2.02	0.42
1:KB:210:MET:HE2	1:KB:210:MET:HA	2.00	0.42
1:D:236:PRO:HB3	2:h:33:LEU:HB3	2.00	0.42
1:F:148:SER:O	1:F:152:GLU:OE1	2.37	0.42
1:H:209:GLU:HG2	1:H:210:MET:H	1.83	0.42
1:H:231:LEU:HB2	1:H:252:ILE:HD11	2.02	0.42
1:O:160:ILE:HG22	1:O:161:PHE:CD2	2.55	0.42
2:ib:36:ILE:HD11	2:ib:41:ALA:O	2.19	0.42
2:kb:105:LEU:HD23	2:k:8:LEU:HD13	2.01	0.42
2:nb:20:LEU:HD13	2:nb:28:PHE:CZ	2.55	0.42
2:ob:66:VAL:HG23	2:ob:76:VAL:HG11	2.01	0.42
2:c:24:THR:O	2:c:28:PHE:CD1	2.73	0.42
2:o:85:VAL:O	2:o:89:LEU:HD13	2.19	0.42
1:CB:269:THR:O	1:CB:270:ASN:OD1	2.38	0.42
1:K:236:PRO:CG	1:L:190:VAL:HG21	2.50	0.42
1:N:167:MET:SD	1:N:167:MET:C	3.03	0.42
1:N:207:VAL:HG13	1:N:211:VAL:HG23	2.00	0.42
2:ib:100:LEU:HD12	2:ib:100:LEU:N	2.35	0.42
2:d:16:ILE:HG21	2:d:20:LEU:HD11	2.01	0.42
2:k:109:LEU:HD23	2:k:109:LEU:O	2.19	0.42
1:DB:201:ILE:HD11	1:DB:234:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:236:PRO:HG3	2:kb:37:HIS:HB2	2.02	0.42
1:B:167:MET:SD	1:B:167:MET:C	3.03	0.42
1:D:245:LEU:O	1:D:245:LEU:HG	2.19	0.42
1:K:148:SER:O	1:K:152:GLU:OE1	2.38	0.42
1:N:204:VAL:O	1:N:204:VAL:HG13	2.19	0.42
2:bb:12:LEU:HD23	2:bb:41:ALA:CB	2.48	0.42
2:jb:6:LEU:HD22	2:j:105:LEU:HD13	2.02	0.42
2:kb:47:ASP:OD1	2:kb:47:ASP:C	2.63	0.42
2:mb:78:VAL:HG21	2:mb:96:PHE:CE2	2.48	0.42
1:BB:270:ASN:O	1:B:276:LYS:HB3	2.20	0.42
1:CB:149:ALA:O	1:CB:153:LEU:HG	2.19	0.42
1:CB:204:VAL:HG11	1:CB:207:VAL:HG22	2.01	0.42
1:IB:162:GLU:O	1:IB:163:LYS:HB2	2.20	0.42
1:E:157:LEU:HD13	1:E:167:MET:HB2	2.00	0.42
2:mb:63:GLY:O	2:mb:66:VAL:HG12	2.20	0.42
2:c:3:ILE:HG21	2:c:16:ILE:HD13	2.02	0.42
2:j:5:ILE:HG21	2:j:35:LYS:HG2	2.01	0.42
1:DB:197:VAL:HG12	1:DB:227:CYS:SG	2.59	0.42
1:OB:228:GLN:OE1	1:OB:228:GLN:N	2.53	0.42
1:OB:262:MET:HE2	1:OB:262:MET:HA	2.01	0.42
1:B:222:VAL:HG22	1:B:227:CYS:HB3	2.00	0.42
1:I:223:ARG:HA	1:I:227:CYS:O	2.19	0.42
1:J:212:ALA:O	1:J:216:ILE:HD12	2.19	0.42
2:gb:48:ILE:HD11	2:gb:81:ILE:HG12	2.02	0.42
2:e:20:LEU:HD13	2:e:28:PHE:CE1	2.55	0.42
2:i:25:ALA:HB1	2:i:61:ILE:HG21	2.02	0.42
2:j:42:ARG:NH2	2:j:116:LEU:HD22	2.34	0.42
2:l:77:VAL:HG13	2:l:112:LEU:HD21	2.01	0.42
1:A:202:THR:HG22	1:A:202:THR:O	2.20	0.42
1:JB:258:MET:SD	1:JB:258:MET:C	3.03	0.42
1:LB:149:ALA:O	1:LB:153:LEU:HG	2.20	0.42
1:NB:149:ALA:O	1:NB:153:LEU:HG	2.20	0.42
1:OB:178:ALA:O	1:OB:181:ILE:HG22	2.20	0.42
1:OB:216:ILE:HD13	1:OB:249:LEU:CD2	2.50	0.42
1:H:239:ALA:HB1	2:b:71:LEU:HD23	2.01	0.42
1:L:232:VAL:HG23	1:L:255:THR:OG1	2.19	0.42
1:N:207:VAL:HB	1:N:238:ILE:HG23	2.01	0.42
2:bb:81:ILE:O	2:cb:72:MET:HE3	2.19	0.42
1:GB:210:MET:HE2	1:GB:210:MET:HA	2.01	0.41
1:JB:187:ILE:O	1:JB:190:VAL:HG12	2.19	0.41
1:LB:160:ILE:O	1:L:258:MET:HE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:236:PRO:HB3	2:b:33:LEU:HB3	2.01	0.41
2:db:26:VAL:O	2:db:29:GLN:HB3	2.20	0.41
2:fb:8:LEU:HD11	2:f:105:LEU:CD2	2.50	0.41
2:l:29:GLN:HG3	2:l:65:VAL:HG22	2.02	0.41
1:GB:242:ILE:HG23	1:GB:247:ILE:HG21	2.02	0.41
1:OB:213:HIS:O	1:OB:216:ILE:HG22	2.19	0.41
1:K:207:VAL:HB	1:K:238:ILE:HG23	2.00	0.41
1:K:217:GLN:OE1	1:K:217:GLN:HA	2.20	0.41
2:db:6:LEU:O	2:db:12:LEU:HD13	2.19	0.41
2:lb:15:SER:HB2	2:l:6:LEU:HD21	2.02	0.41
2:o:20:LEU:HD13	2:o:28:PHE:CZ	2.55	0.41
1:EB:195:GLU:OE1	1:EB:196:VAL:HG23	2.20	0.41
1:HB:254:THR:HG21	2:ob:71:LEU:O	2.20	0.41
1:OB:187:ILE:O	1:OB:190:VAL:HG12	2.21	0.41
1:L:258:MET:SD	1:L:258:MET:C	3.03	0.41
2:kb:12:LEU:HD13	2:kb:41:ALA:CB	2.50	0.41
2:kb:26:VAL:O	2:kb:29:GLN:HG2	2.21	0.41
2:lb:6:LEU:O	2:lb:12:LEU:HD13	2.20	0.41
2:f:24:THR:O	2:f:28:PHE:CD1	2.73	0.41
1:CB:222:VAL:HG21	1:CB:229:ALA:HB2	2.01	0.41
1:HB:160:ILE:HG23	1:H:262:MET:HE2	2.02	0.41
1:LB:170:ILE:HG22	1:LB:171:GLY:N	2.36	0.41
1:LB:238:ILE:O	1:LB:242:ILE:HG12	2.20	0.41
1:I:219:SER:O	1:I:222:VAL:HG22	2.21	0.41
2:cb:64:ASP:HB3	2:cb:68:MET:HE3	2.03	0.41
2:fb:105:LEU:C	2:fb:105:LEU:HD23	2.45	0.41
2:hb:45:VAL:CG2	2:hb:112:LEU:HD12	2.51	0.41
2:kb:79:THR:HG22	2:kb:102:ALA:HB3	2.03	0.41
2:nb:61:ILE:O	2:nb:65:VAL:HG23	2.20	0.41
2:c:60:LYS:HD2	2:c:60:LYS:O	2.20	0.41
1:AB:258:MET:SD	1:AB:258:MET:C	3.03	0.41
1:IB:212:ALA:HB1	1:IB:242:ILE:CD1	2.50	0.41
1:KB:168:PRO:HB2	1:KB:170:ILE:HD11	2.02	0.41
1:H:216:ILE:HG22	1:H:220:GLU:OE1	2.19	0.41
1:J:162:GLU:O	1:J:163:LYS:HB2	2.19	0.41
1:N:220:GLU:HB2	2:g:90:ILE:CD1	2.50	0.41
1:N:230:MET:HE1	1:N:264:ARG:HG3	2.02	0.41
2:ab:109:LEU:HD23	2:ab:109:LEU:O	2.19	0.41
2:bb:96:PHE:HB3	2:bb:99:VAL:HB	2.02	0.41
2:eb:64:ASP:O	2:eb:68:MET:HG3	2.20	0.41
1:BB:258:MET:HE1	1:B:159:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:153:LEU:HD13	1:G:171:GLY:CA	2.50	0.41
1:GB:168:PRO:HB2	1:GB:170:ILE:HD11	2.03	0.41
1:GB:242:ILE:HG21	2:kb:71:LEU:HD11	2.03	0.41
1:IB:202:THR:HG23	1:IB:233:GLY:HA3	2.01	0.41
1:KB:193:ARG:N	1:KB:193:ARG:HD2	2.36	0.41
1:MB:160:ILE:HD13	1:M:258:MET:HE1	2.01	0.41
1:C:209:GLU:C	1:C:210:MET:HE2	2.46	0.41
2:cb:27:GLU:HA	2:cb:30:GLU:OE1	2.20	0.41
2:ib:6:LEU:HD22	2:i:105:LEU:CD1	2.47	0.41
2:mb:89:LEU:HD23	2:mb:96:PHE:HE1	1.85	0.41
2:b:29:GLN:HG3	2:b:65:VAL:HG22	2.03	0.41
2:c:16:ILE:HG22	2:c:51:ILE:HD11	2.02	0.41
1:AB:239:ALA:HB1	1:OB:224:LEU:HD12	2.03	0.41
1:EB:161:PHE:CE1	1:E:262:MET:HG2	2.55	0.41
1:HB:198:LEU:N	1:HB:198:LEU:HD12	2.36	0.41
1:KB:204:VAL:O	1:KB:204:VAL:HG13	2.21	0.41
1:OB:259:LYS:NZ	1:O:162:GLU:HB2	2.35	0.41
1:B:216:ILE:HD11	1:B:247:ILE:HG21	2.03	0.41
1:J:224:LEU:HD11	2:m:90:ILE:HG13	2.03	0.41
2:db:72:MET:O	2:eb:103:MET:HE1	2.21	0.41
2:fb:48:ILE:HD11	2:fb:81:ILE:HG12	2.03	0.41
2:fb:64:ASP:HB3	2:fb:68:MET:HE3	2.02	0.41
2:kb:51:ILE:O	2:kb:51:ILE:CG2	2.68	0.41
2:lb:48:ILE:HD11	2:lb:81:ILE:HG13	2.02	0.41
2:nb:20:LEU:HD13	2:nb:28:PHE:CE1	2.55	0.41
2:e:20:LEU:HD13	2:e:28:PHE:CZ	2.56	0.41
2:j:63:GLY:O	2:j:66:VAL:HG12	2.20	0.41
1:A:228:GLN:OE1	1:A:228:GLN:N	2.54	0.41
1:A:243:VAL:HG21	1:JB:220:GLU:HB2	2.03	0.41
1:FB:198:LEU:HD12	1:FB:198:LEU:N	2.36	0.41
1:JB:149:ALA:O	1:JB:153:LEU:HG	2.21	0.41
1:KB:230:MET:HG2	1:KB:253:ILE:HB	2.02	0.41
1:MB:222:VAL:HG21	1:MB:229:ALA:HB2	2.03	0.41
2:ib:12:LEU:HD23	2:ib:41:ALA:CB	2.51	0.41
2:n:20:LEU:HD13	2:n:28:PHE:CE1	2.55	0.41
1:IB:224:LEU:HD11	2:b:90:ILE:HG13	2.02	0.41
1:JB:193:ARG:HD3	1:JB:193:ARG:N	2.36	0.41
1:F:167:MET:SD	1:F:181:ILE:HD11	2.61	0.41
1:H:264:ARG:O	1:H:268:LEU:HD23	2.21	0.41
1:J:204:VAL:HG11	1:J:207:VAL:HG22	2.03	0.41
1:K:162:GLU:OE1	1:K:162:GLU:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:240:GLN:HA	1:K:243:VAL:HG12	2.01	0.41
1:L:258:MET:SD	1:L:258:MET:O	2.79	0.41
1:N:201:ILE:HD11	1:N:234:ILE:HD12	2.02	0.41
1:O:193:ARG:NH1	1:O:193:ARG:HB2	2.36	0.41
2:cb:45:VAL:CG2	2:cb:112:LEU:HD12	2.50	0.41
2:hb:22:ASP:O	2:hb:25:ALA:HB3	2.21	0.41
2:lb:112:LEU:O	2:lb:116:LEU:HD23	2.21	0.41
2:mb:66:VAL:HG23	2:mb:76:VAL:CG1	2.50	0.41
2:c:36:ILE:HD11	2:c:41:ALA:O	2.21	0.41
2:f:5:ILE:HG21	2:f:35:LYS:HG2	2.03	0.41
2:m:25:ALA:HB1	2:m:61:ILE:HG21	2.02	0.41
2:o:36:ILE:HD11	2:o:74:ALA:CB	2.51	0.41
1:EB:207:VAL:HB	1:EB:238:ILE:HG23	2.02	0.41
1:HB:149:ALA:O	1:HB:153:LEU:HG	2.21	0.41
1:B:205:PRO:HA	1:B:235:ARG:HH22	1.86	0.41
1:C:182:ILE:HG12	1:C:218:ALA:HB2	2.02	0.41
1:I:236:PRO:HB3	1:K:186:LEU:HD22	2.03	0.41
2:fb:32:LEU:O	2:fb:36:ILE:HG22	2.21	0.41
2:h:66:VAL:HG23	2:h:76:VAL:HG11	2.02	0.41
2:l:22:ASP:O	2:l:25:ALA:HB3	2.20	0.41
2:o:63:GLY:O	2:o:66:VAL:HG12	2.21	0.41
2:o:96:PHE:CD1	2:o:99:VAL:HG11	2.56	0.41
1:DB:274:VAL:HG13	1:DB:274:VAL:O	2.21	0.40
1:FB:149:ALA:O	1:FB:153:LEU:HG	2.21	0.40
1:OB:170:ILE:HG21	1:O:153:LEU:HD22	2.01	0.40
1:D:179:LYS:N	1:D:179:LYS:HD2	2.36	0.40
1:F:185:LEU:HD11	1:F:197:VAL:HG21	2.03	0.40
1:J:204:VAL:HG11	1:J:207:VAL:CG2	2.51	0.40
1:M:219:SER:O	1:M:222:VAL:HG12	2.21	0.40
1:M:231:LEU:HB3	1:M:234:ILE:HD11	2.03	0.40
2:eb:33:LEU:O	2:eb:36:ILE:HG22	2.21	0.40
2:eb:36:ILE:HD12	2:eb:44:VAL:CG2	2.51	0.40
2:nb:71:LEU:HD23	2:nb:71:LEU:C	2.46	0.40
2:g:64:ASP:HB3	2:g:68:MET:HE1	2.02	0.40
1:BB:177:ARG:O	1:BB:181:ILE:HG12	2.21	0.40
1:BB:229:ALA:HB3	1:BB:252:ILE:CD1	2.52	0.40
1:OB:200:ASP:C	1:OB:200:ASP:OD1	2.63	0.40
1:OB:264:ARG:CZ	1:OB:267:ALA:HB3	2.52	0.40
1:I:182:ILE:HG12	1:I:218:ALA:HB2	2.02	0.40
1:K:196:VAL:HG11	1:K:265:ALA:HB1	2.02	0.40
2:ab:72:MET:HE2	2:ab:72:MET:CA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:gb:78:VAL:HG21	2:gb:96:PHE:CE1	2.56	0.40
2:ob:78:VAL:HG12	2:ob:81:ILE:HD11	2.02	0.40
1:AB:198:LEU:HD12	1:AB:198:LEU:N	2.37	0.40
1:BB:170:ILE:CG2	1:B:153:LEU:HD22	2.52	0.40
1:CB:198:LEU:HD12	1:CB:198:LEU:N	2.36	0.40
1:L:231:LEU:HD23	1:L:234:ILE:HD11	2.04	0.40
2:ab:58:ILE:O	2:ab:61:ILE:HG22	2.21	0.40
2:fb:7:LYS:O	2:fb:8:LEU:HD22	2.21	0.40
2:hb:66:VAL:HG23	2:hb:76:VAL:CG1	2.51	0.40
2:nb:7:LYS:HD2	2:nb:7:LYS:C	2.45	0.40
2:b:64:ASP:O	2:b:68:MET:HE3	2.21	0.40
1:CB:224:LEU:HD11	2:d:90:ILE:HG13	2.03	0.40
1:GB:219:SER:CB	1:GB:252:ILE:HD12	2.52	0.40
1:IB:210:MET:SD	1:IB:214:HIS:CE1	3.15	0.40
1:IB:216:ILE:HD11	1:IB:247:ILE:HG21	2.03	0.40
1:IB:263:GLU:HA	1:IB:263:GLU:OE2	2.22	0.40
1:MB:198:LEU:HD12	1:MB:198:LEU:N	2.37	0.40
1:D:157:LEU:CD1	1:D:165:SER:HB3	2.48	0.40
1:M:222:VAL:HG22	1:M:227:CYS:HB3	2.04	0.40
1:N:169:LEU:C	1:N:169:LEU:HD23	2.47	0.40
2:fb:12:LEU:HD23	2:fb:41:ALA:CB	2.51	0.40
2:kb:111:LYS:HD3	2:kb:111:LYS:O	2.21	0.40
2:ob:8:LEU:HD11	2:o:109:LEU:HD23	2.04	0.40
2:c:42:ARG:CZ	2:c:116:LEU:HD12	2.52	0.40
1:A:201:ILE:HD11	1:A:234:ILE:CD1	2.37	0.40
1:BB:249:LEU:HB3	1:BB:252:ILE:CG2	2.52	0.40
1:EB:167:MET:HE3	1:EB:169:LEU:CD2	2.51	0.40
1:FB:193:ARG:HA	2:j:103:MET:SD	2.62	0.40
1:LB:240:GLN:HA	2:eb:68:MET:SD	2.62	0.40
1:E:157:LEU:HD12	1:E:158:LEU:H	1.87	0.40
1:G:212:ALA:HB1	1:G:242:ILE:HD12	2.03	0.40
1:K:204:VAL:HG11	1:K:207:VAL:HG22	2.03	0.40
1:K:258:MET:SD	1:K:258:MET:O	2.80	0.40
1:K:269:THR:O	1:K:269:THR:CG2	2.68	0.40
2:jb:81:ILE:HD12	2:jb:81:ILE:H	1.86	0.40
2:mb:19:GLU:OE2	2:mb:19:GLU:N	2.54	0.40
2:ob:46:ILE:HG22	2:ob:48:ILE:CD1	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/278 (47%)	128 (98%)	2 (2%)	0	100	100
1	AB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	B	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	BB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	C	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	CB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	D	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	DB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	E	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	EB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	F	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	FB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	G	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
1	GB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	H	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	HB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	I	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	IB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	J	130/278 (47%)	128 (98%)	2 (2%)	0	100	100
1	JB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	K	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
1	KB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	L	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	LB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	M	130/278 (47%)	126 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MB	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
1	N	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	NB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	O	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	OB	130/278 (47%)	127 (98%)	3 (2%)	0	100	100
2	a	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	ab	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	b	116/118 (98%)	116 (100%)	0	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%)	113 (97%)	3 (3%)	0	100	100
2	d	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	db	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	e	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	eb	116/118 (98%)	116 (100%)	0	0	100	100
2	f	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	fb	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	g	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	gb	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	h	116/118 (98%)	116 (100%)	0	0	100	100
2	hb	116/118 (98%)	116 (100%)	0	0	100	100
2	i	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	ib	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	j	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	jb	116/118 (98%)	116 (100%)	0	0	100	100
2	k	116/118 (98%)	116 (100%)	0	0	100	100
2	kb	116/118 (98%)	116 (100%)	0	0	100	100
2	l	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	lb	116/118 (98%)	116 (100%)	0	0	100	100
2	m	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	mb	116/118 (98%)	115 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	n	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
2	nb	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	o	116/118 (98%)	116 (100%)	0	0	100	100
2	ob	116/118 (98%)	116 (100%)	0	0	100	100
All	All	7380/11880 (62%)	7212 (98%)	168 (2%)	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%)	114 (100%)	0	100	100
1	AB	114/247 (46%)	114 (100%)	0	100	100
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%)	114 (100%)	0	100	100
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%)	114 (100%)	0	100	100
1	E	114/247 (46%)	114 (100%)	0	100	100
1	EB	114/247 (46%)	114 (100%)	0	100	100
1	F	114/247 (46%)	114 (100%)	0	100	100
1	FB	114/247 (46%)	114 (100%)	0	100	100
1	G	114/247 (46%)	114 (100%)	0	100	100
1	GB	114/247 (46%)	114 (100%)	0	100	100
1	H	114/247 (46%)	114 (100%)	0	100	100
1	HB	114/247 (46%)	114 (100%)	0	100	100
1	I	114/247 (46%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IB	114/247 (46%)	114 (100%)	0	100	100
1	J	114/247 (46%)	114 (100%)	0	100	100
1	JB	114/247 (46%)	114 (100%)	0	100	100
1	K	114/247 (46%)	114 (100%)	0	100	100
1	KB	114/247 (46%)	114 (100%)	0	100	100
1	L	114/247 (46%)	114 (100%)	0	100	100
1	LB	114/247 (46%)	114 (100%)	0	100	100
1	M	114/247 (46%)	114 (100%)	0	100	100
1	MB	114/247 (46%)	114 (100%)	0	100	100
1	N	114/247 (46%)	113 (99%)	1 (1%)	70	77
1	NB	114/247 (46%)	113 (99%)	1 (1%)	70	77
1	O	114/247 (46%)	113 (99%)	1 (1%)	70	77
1	OB	114/247 (46%)	114 (100%)	0	100	100
2	a	100/100 (100%)	100 (100%)	0	100	100
2	ab	100/100 (100%)	100 (100%)	0	100	100
2	b	100/100 (100%)	100 (100%)	0	100	100
2	bb	100/100 (100%)	100 (100%)	0	100	100
2	c	100/100 (100%)	100 (100%)	0	100	100
2	cb	100/100 (100%)	100 (100%)	0	100	100
2	d	100/100 (100%)	100 (100%)	0	100	100
2	db	100/100 (100%)	100 (100%)	0	100	100
2	e	100/100 (100%)	100 (100%)	0	100	100
2	eb	100/100 (100%)	100 (100%)	0	100	100
2	f	100/100 (100%)	100 (100%)	0	100	100
2	fb	100/100 (100%)	100 (100%)	0	100	100
2	g	100/100 (100%)	100 (100%)	0	100	100
2	gb	100/100 (100%)	100 (100%)	0	100	100
2	h	100/100 (100%)	100 (100%)	0	100	100
2	hb	100/100 (100%)	100 (100%)	0	100	100
2	i	100/100 (100%)	100 (100%)	0	100	100
2	ib	100/100 (100%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	j	100/100 (100%)	100 (100%)	0	100	100
2	jb	100/100 (100%)	100 (100%)	0	100	100
2	k	100/100 (100%)	100 (100%)	0	100	100
2	kb	100/100 (100%)	100 (100%)	0	100	100
2	l	100/100 (100%)	100 (100%)	0	100	100
2	lb	100/100 (100%)	99 (99%)	1 (1%)	68	76
2	m	100/100 (100%)	100 (100%)	0	100	100
2	mb	100/100 (100%)	100 (100%)	0	100	100
2	n	100/100 (100%)	100 (100%)	0	100	100
2	nb	100/100 (100%)	100 (100%)	0	100	100
2	o	100/100 (100%)	100 (100%)	0	100	100
2	ob	100/100 (100%)	100 (100%)	0	100	100
All	All	6420/10410 (62%)	6416 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	NB	240	GLN
1	N	256	ASN
1	O	240	GLN
2	lb	17	GLN

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

Mol	Chain	Res	Type
1	BB	217	GLN
1	BB	251	GLN
1	CB	228	GLN
1	DB	251	GLN
1	IB	213	HIS
1	IB	214	HIS
1	JB	214	HIS
1	JB	228	GLN
1	LB	213	HIS
1	MB	251	GLN
1	NB	228	GLN
1	B	192	ASN

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Mol	Chain	Res	Type
1	B	228	GLN
1	C	251	GLN
1	D	192	ASN
1	E	192	ASN
1	F	151	GLN
1	F	213	HIS
1	I	217	GLN
1	J	192	ASN
1	N	240	GLN
1	N	256	ASN
1	O	151	GLN
1	O	240	GLN
1	O	251	GLN
2	a	37	HIS
2	cb	29	GLN
2	cb	37	HIS
2	db	29	GLN
2	eb	37	HIS
2	fb	29	GLN
2	fb	114	GLN
2	gb	82	GLN
2	hb	37	HIS
2	lb	29	GLN
2	mb	29	GLN
2	mb	37	HIS
2	ob	29	GLN
2	ob	37	HIS
2	b	29	GLN
2	b	37	HIS
2	d	29	GLN
2	d	37	HIS
2	e	37	HIS
2	g	29	GLN
2	i	29	GLN
2	j	29	GLN
2	j	37	HIS
2	k	29	GLN
2	l	29	GLN
2	m	29	GLN
2	m	37	HIS
2	n	82	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.

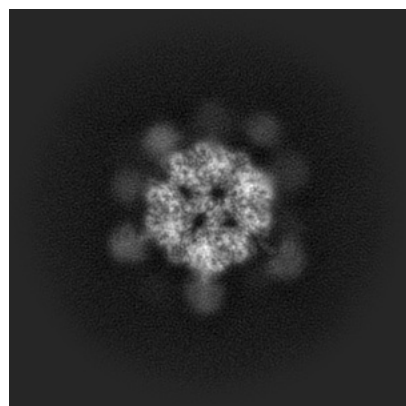
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70101. These allow visual inspection of the internal detail of the map and identification of artifacts.

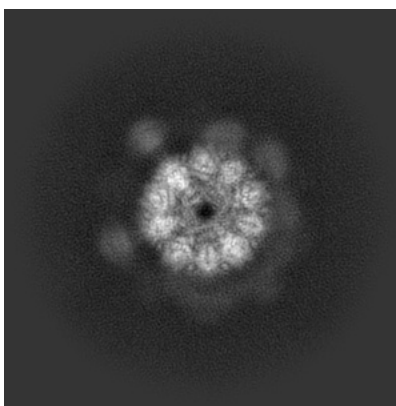
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

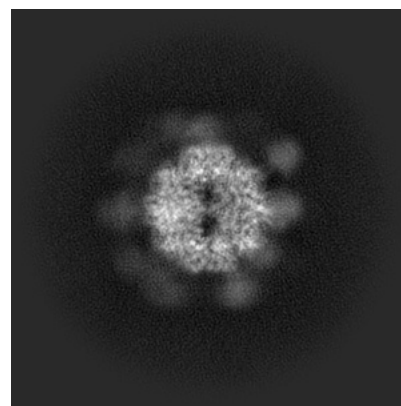
6.1.1 Primary map



X

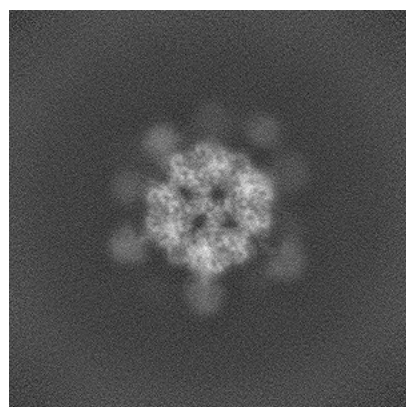


Y

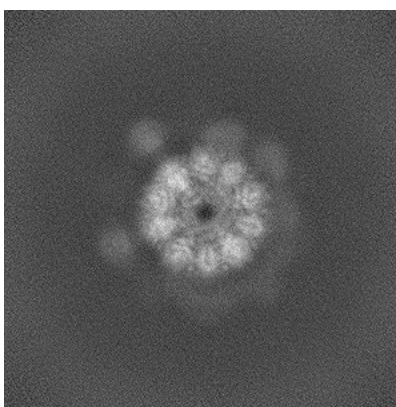


Z

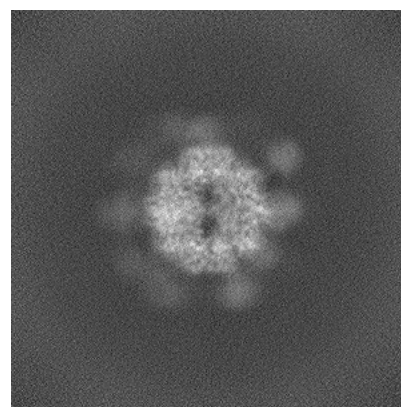
6.1.2 Raw map



X



Y

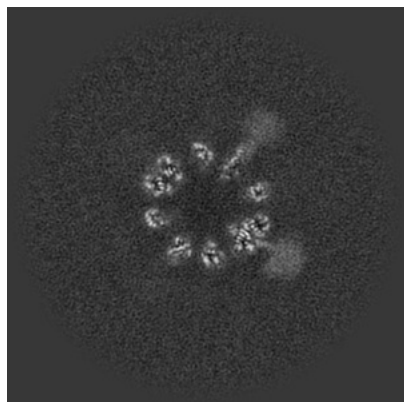


Z

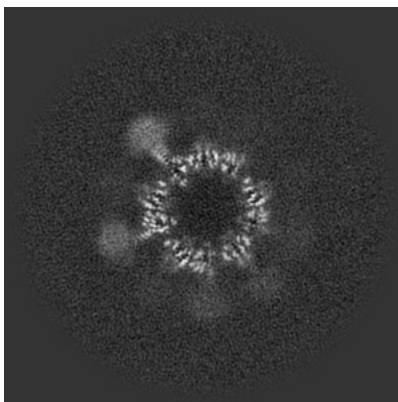
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

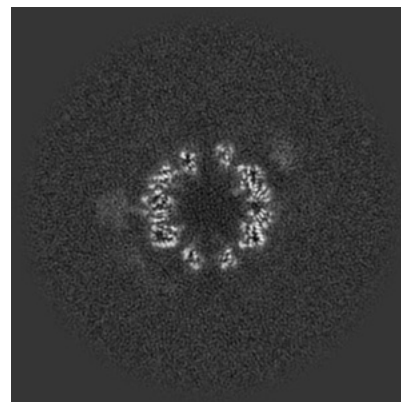
6.2.1 Primary map



X Index: 300

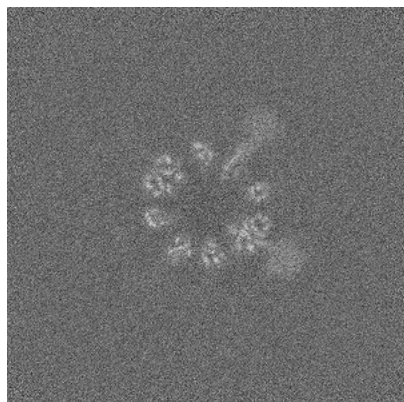


Y Index: 300

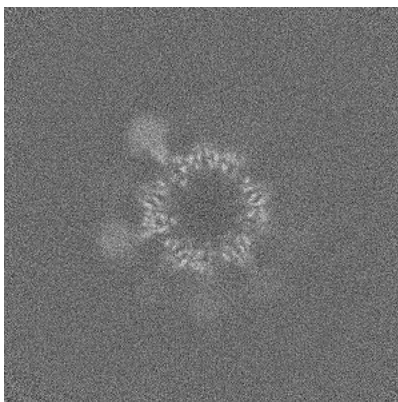


Z Index: 300

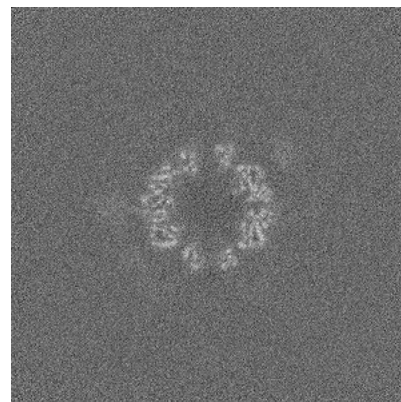
6.2.2 Raw map



X Index: 300



Y Index: 300

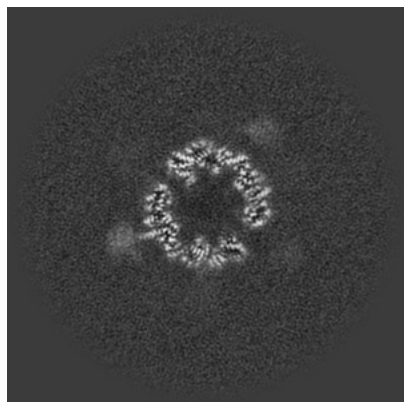


Z Index: 300

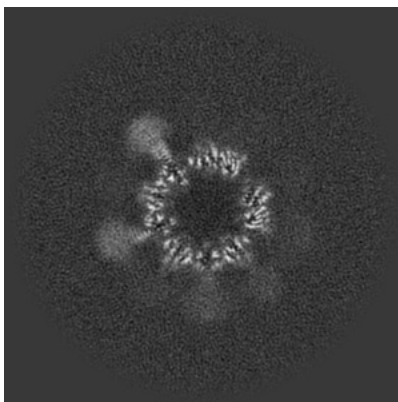
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

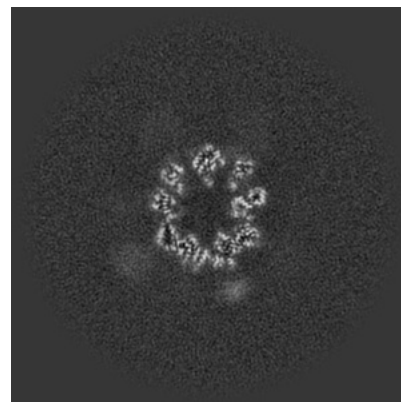
6.3.1 Primary map



X Index: 321

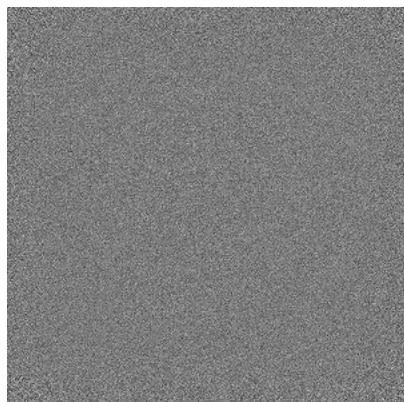


Y Index: 297

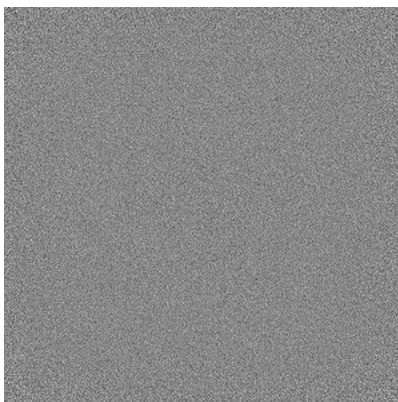


Z Index: 269

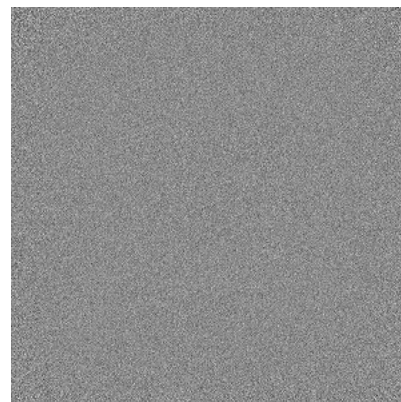
6.3.2 Raw map



X Index: 0



Y Index: 0

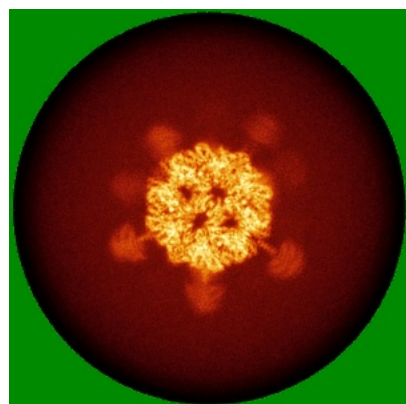


Z Index: 0

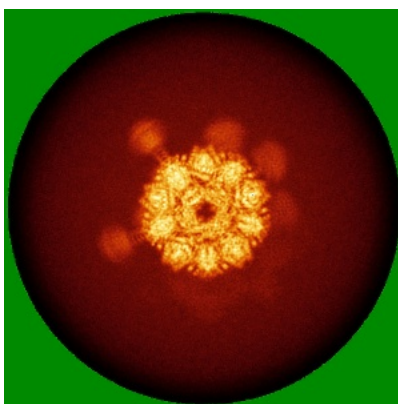
The images above show the largest variance slices of the map in three orthogonal directions.

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

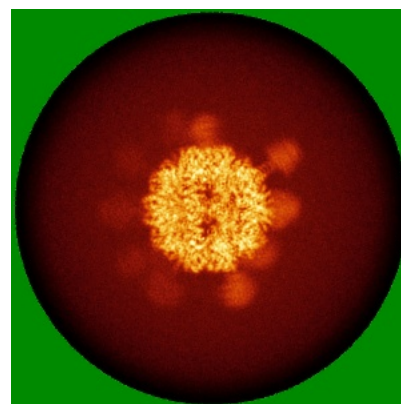
6.4.1 Primary map



X

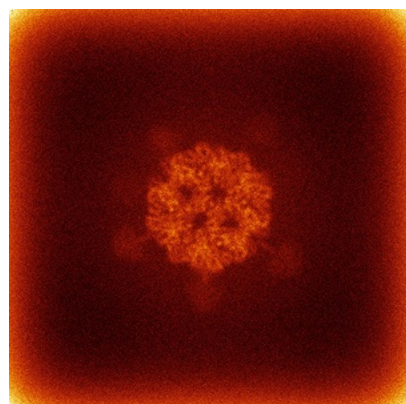


Y

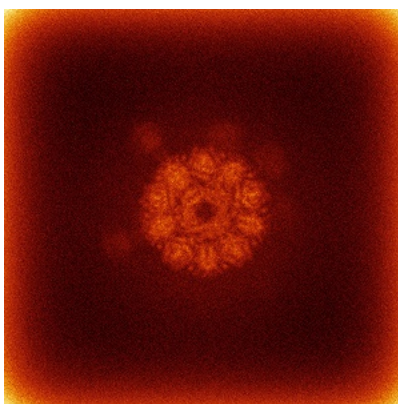


Z

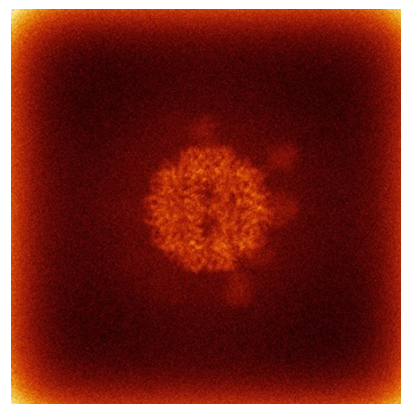
6.4.2 Raw map



X



Y

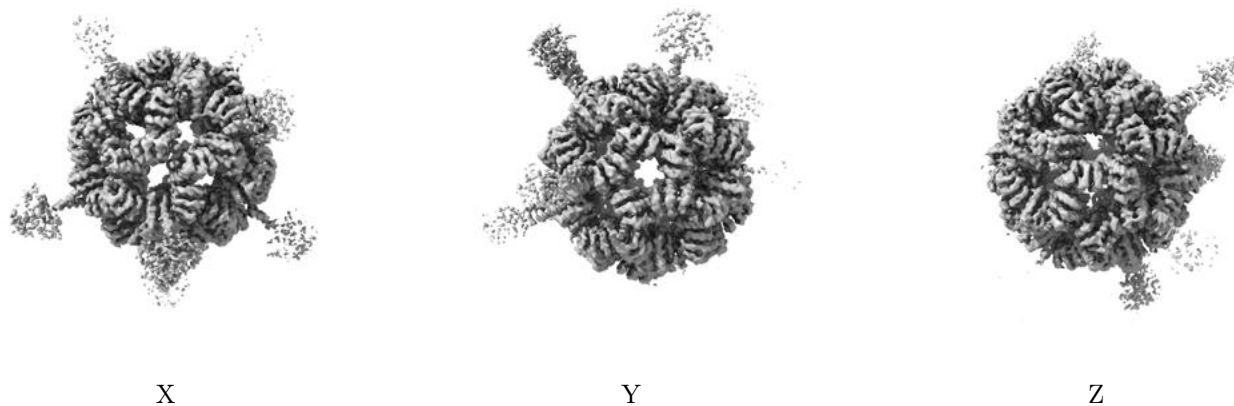


Z

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.

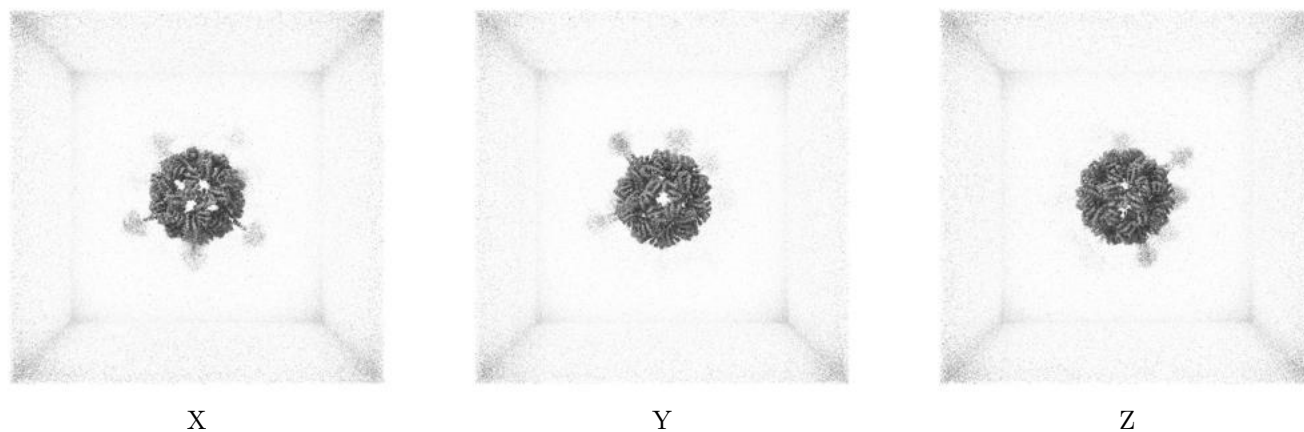
6.5 Orthogonal surface views [i](#)

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.

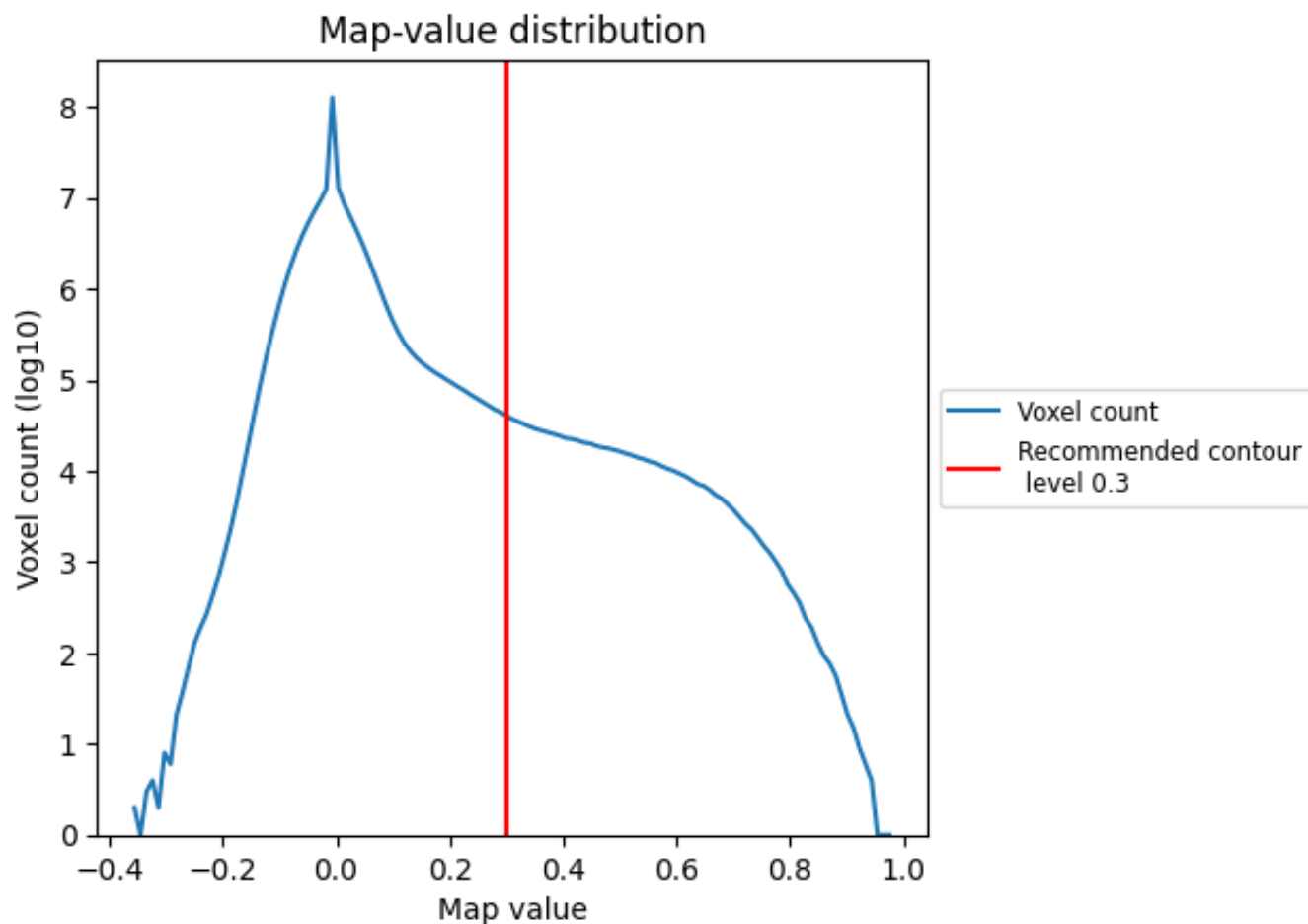
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

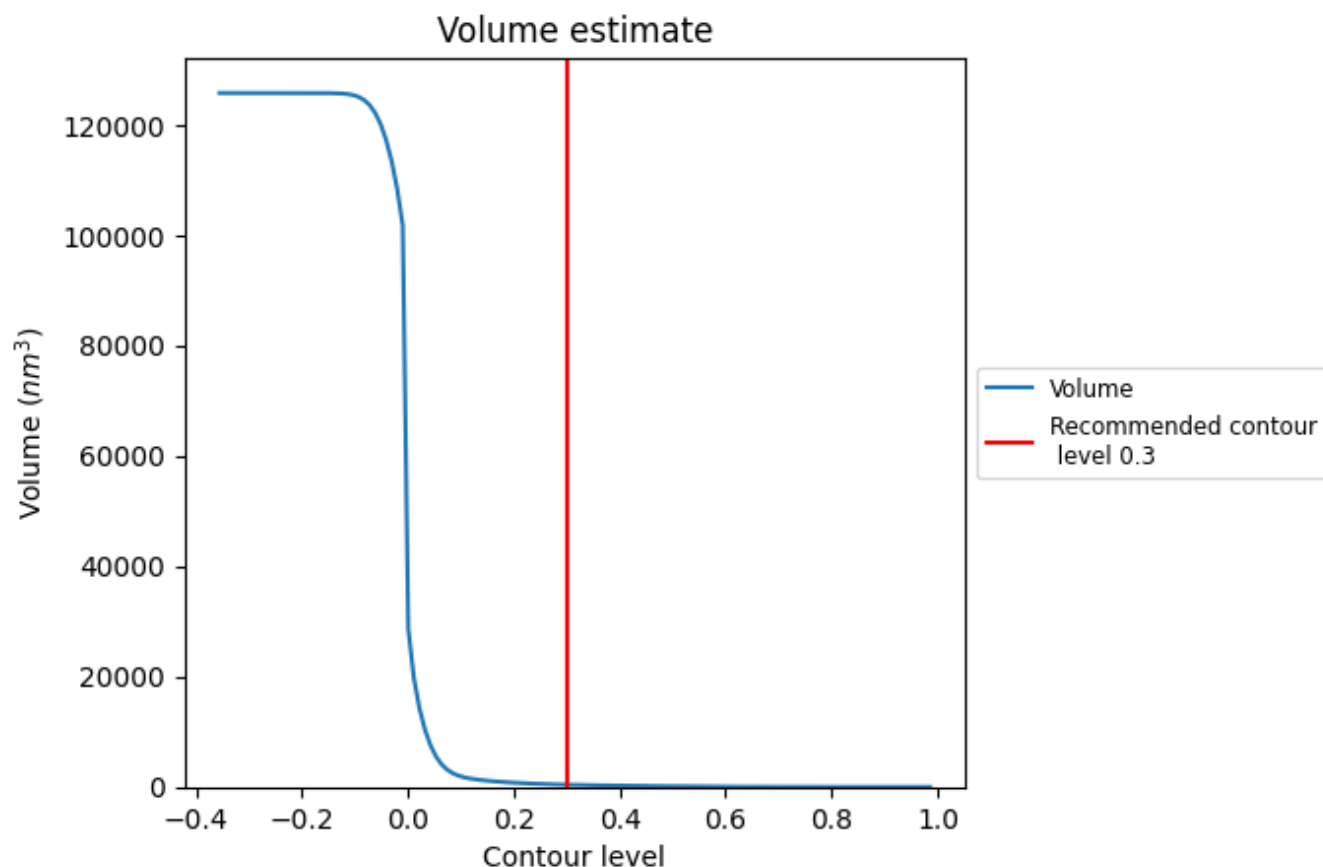
This section contains the results of statistical analysis of the map.

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.

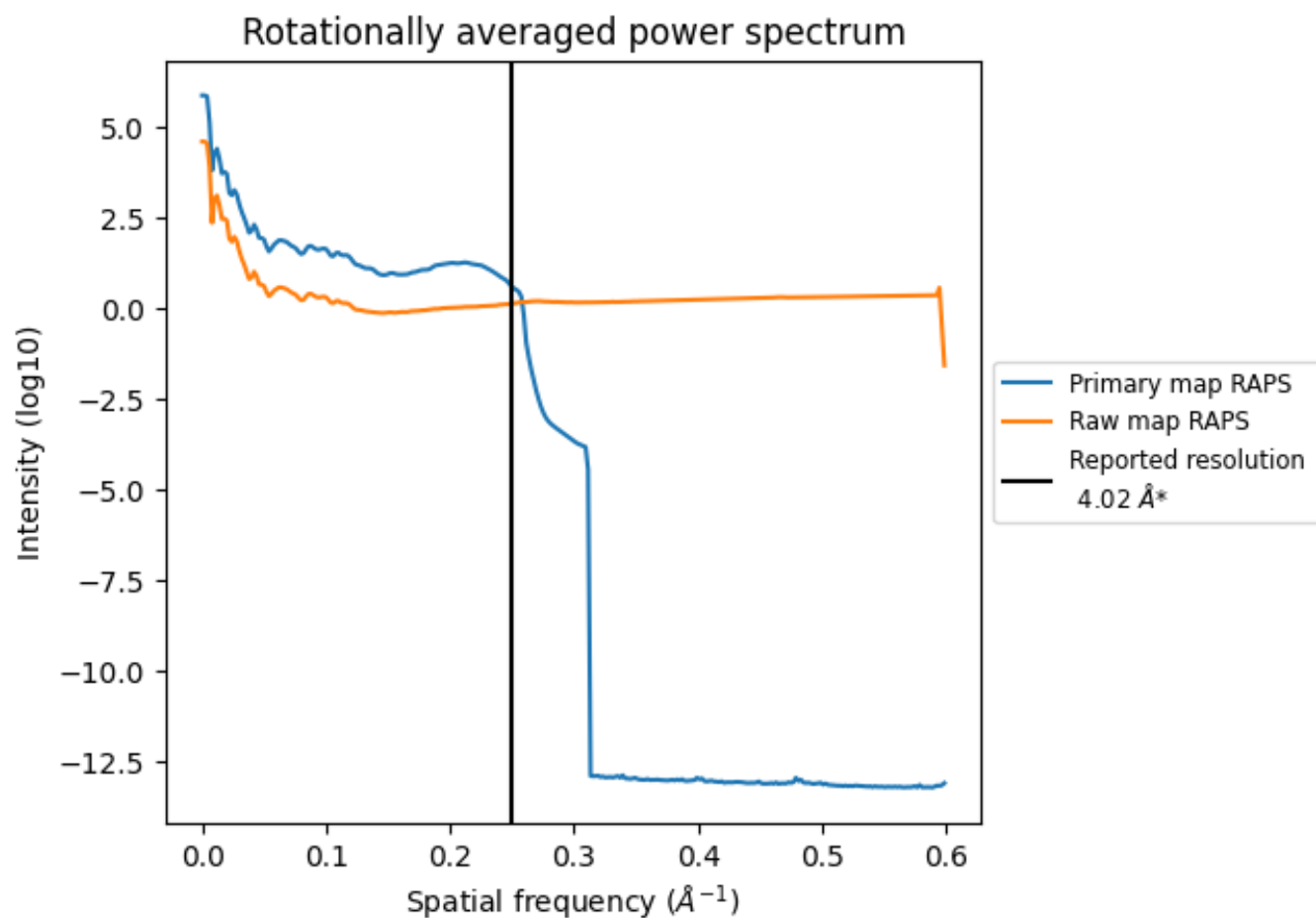
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 406 nm³; this corresponds to an approximate mass of 367 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 ⓘ

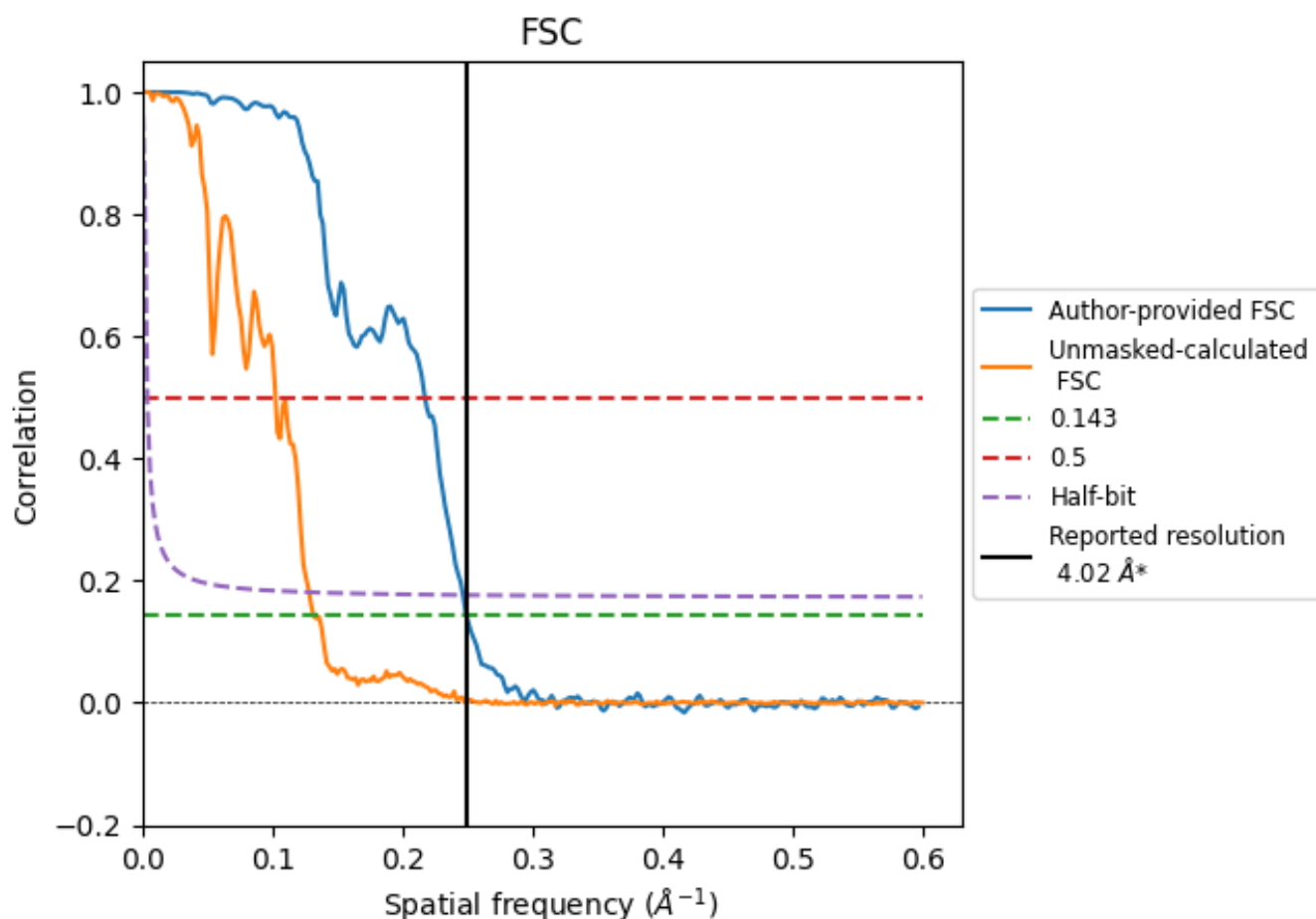


*Reported resolution corresponds to spatial frequency of 0.249 Å⁻¹

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 0.249 \AA^{-1}

8.2 Resolution estimates [i](#)

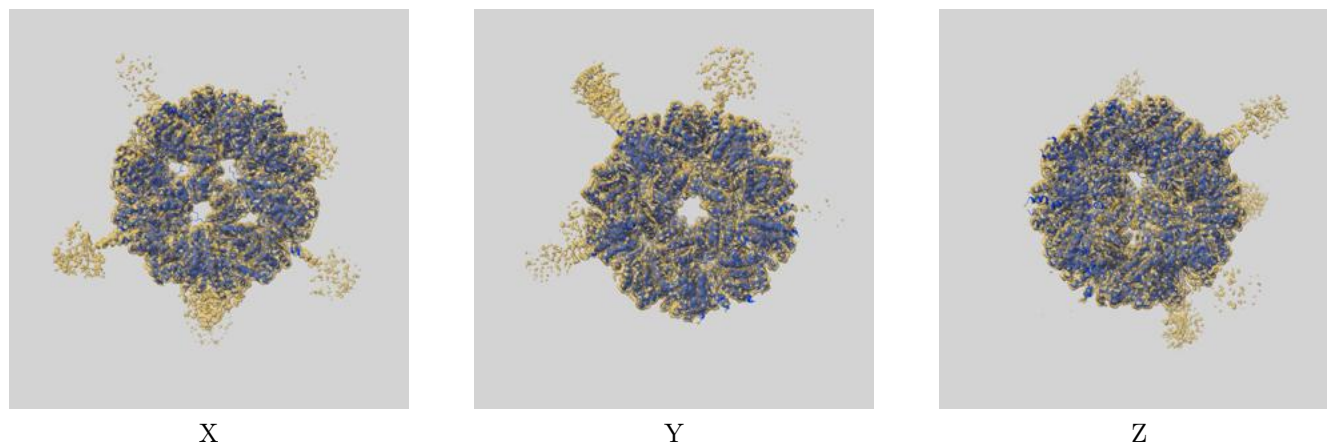
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.02	-	-
Author-provided FSC curve	4.02	4.61	4.06
Unmasked-calculated*	7.60	9.78	7.80

*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 7.60 differs from the reported value 4.02 by more than 10 %

9 Map-model fit [i](#)

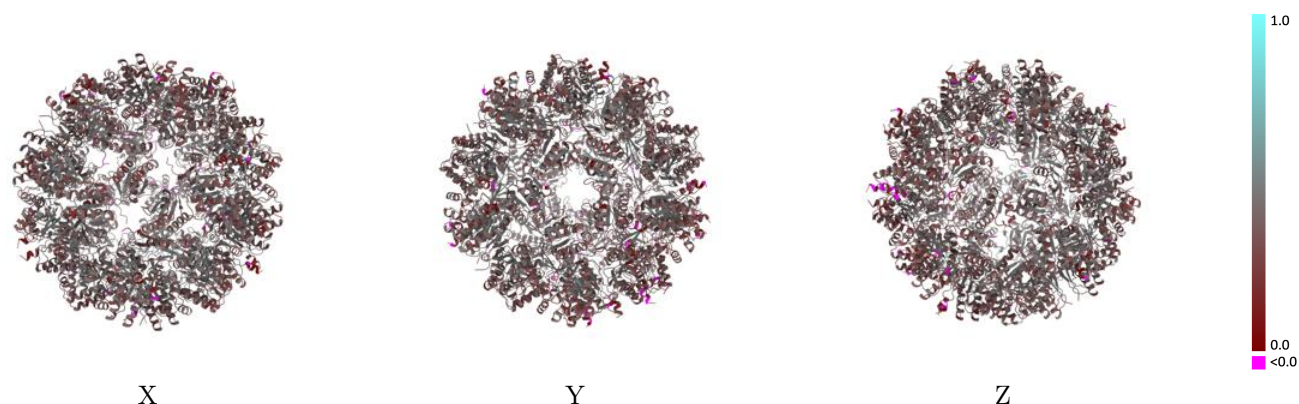
This section contains information regarding the fit between EMDB map EMD-70101 and PDB model 9O4H. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



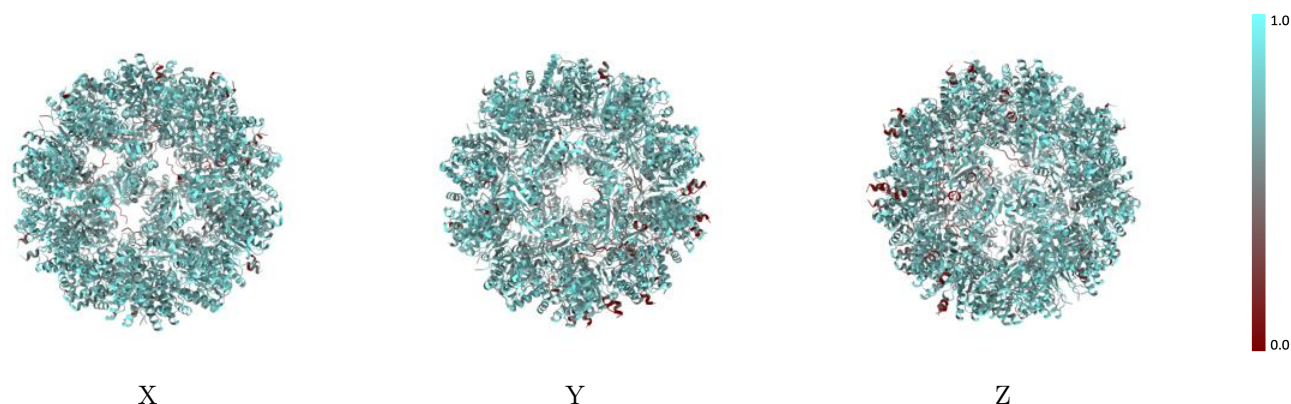
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



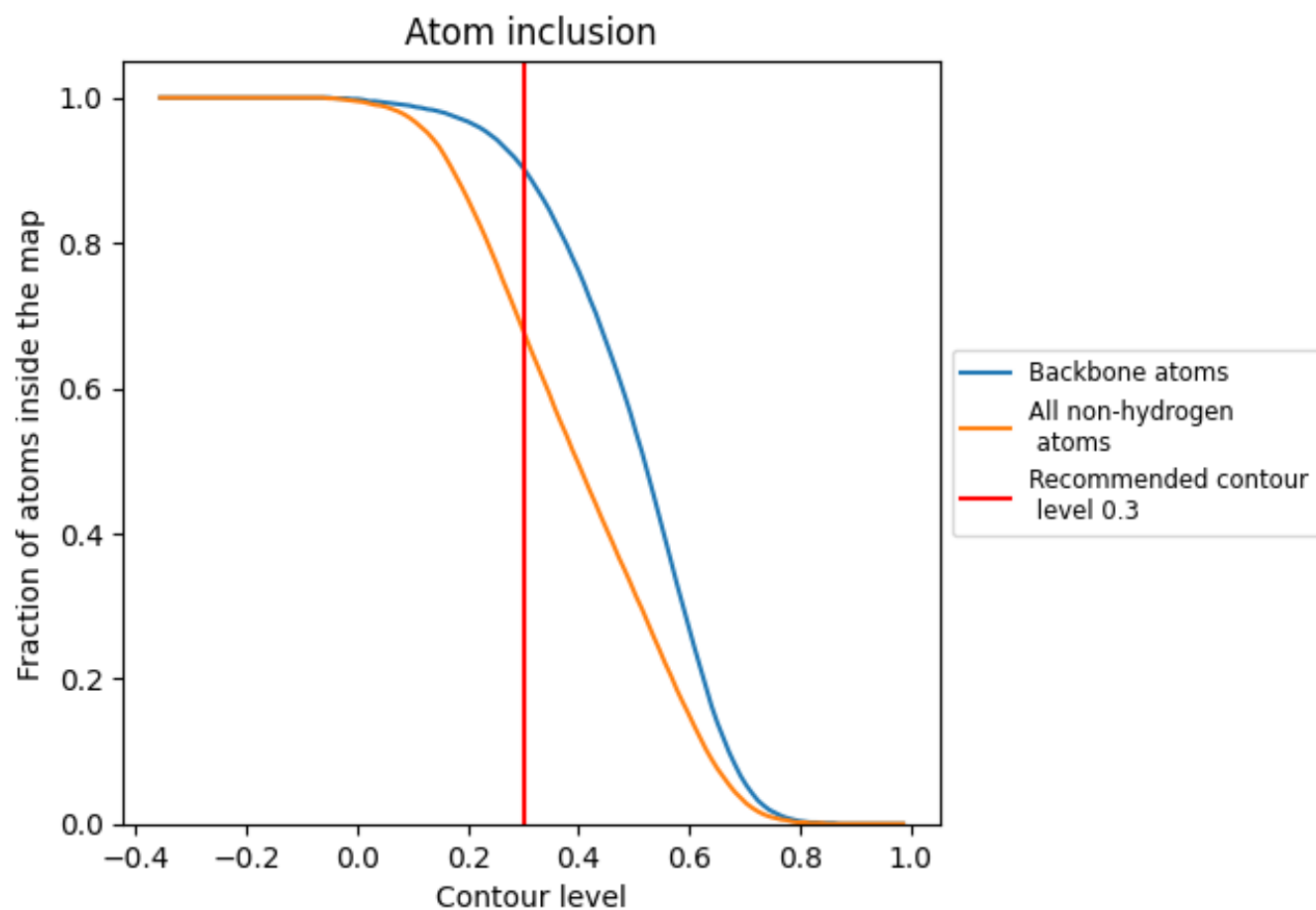
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 90% of all backbone atoms, 68% 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	 0.6800	 0.3700
A	 0.5900	 0.3240
AB	 0.6090	 0.3250
B	 0.6130	 0.3400
BB	 0.5920	 0.3310
C	 0.7020	 0.3720
CB	 0.7180	 0.3790
D	 0.7190	 0.3800
DB	 0.7180	 0.3730
E	 0.7300	 0.3790
EB	 0.7320	 0.3740
F	 0.7000	 0.3670
FB	 0.7020	 0.3700
G	 0.7000	 0.3780
GB	 0.6920	 0.3660
H	 0.7250	 0.3840
HB	 0.7220	 0.3830
I	 0.6530	 0.3650
IB	 0.6400	 0.3520
J	 0.6110	 0.3360
JB	 0.6110	 0.3390
K	 0.6120	 0.3430
KB	 0.6170	 0.3380
L	 0.6200	 0.3440
LB	 0.6180	 0.3420
M	 0.6350	 0.3570
MB	 0.6620	 0.3550
N	 0.6280	 0.3440
NB	 0.6270	 0.3520
O	 0.6170	 0.3360
OB	 0.6170	 0.3400
a	 0.7190	 0.3800
ab	 0.6960	 0.3850
b	 0.6880	 0.3880
bb	 0.6990	 0.3660



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Chain	Atom inclusion	Q-score
c	 0.7110	 0.3950
cb	 0.7240	 0.3980
d	 0.7130	 0.4040
db	 0.7030	 0.3920
e	 0.6840	 0.3780
eb	 0.6700	 0.3640
f	 0.6930	 0.3820
fb	 0.7160	 0.3950
g	 0.6940	 0.3850
gb	 0.7120	 0.3940
h	 0.6930	 0.3740
hb	 0.6960	 0.3780
i	 0.7130	 0.3930
ib	 0.7330	 0.3960
j	 0.7050	 0.3930
jb	 0.7010	 0.3810
k	 0.7070	 0.3770
kb	 0.6920	 0.3770
l	 0.7130	 0.3830
lb	 0.7250	 0.3970
m	 0.6890	 0.3720
mb	 0.6970	 0.3860
n	 0.7110	 0.4040
nb	 0.7220	 0.3970
o	 0.7000	 0.3800
ob	 0.7110	 0.3970