



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:38 AM UTC

PDB ID : 6QCM / pdb_00006qcm
EMDB ID : EMD-4508
Title : Cryo em structure of the Listeria stressosome
Authors : Williams, A.H.; Redzej, A.; Waksman, G.; Cossart, P.
Deposited on : 2018-12-28
Resolution : 4.21 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 : **NOT EXECUTED**
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

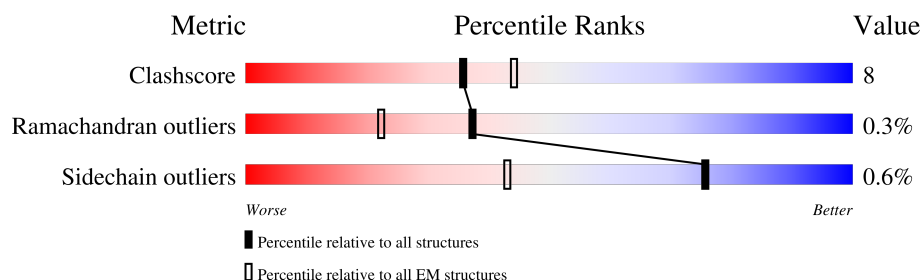
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.21 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	AB	128	90% 76% 13% • 10%
1	BC	128	90% 73% 17% 10%
1	DC	128	90% 70% 20% 10%
1	EB	128	90% 63% 26% • 10%
1	FA	128	90% 70% 20% 10%
1	FB	128	90% 71% 17% • 10%
1	FC	128	90% 73% 17% 10%
1	GC	128	90% 69% 21% 10%

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Mol	Chain	Length	Quality of chain
1	HC	128	
1	IC	128	
1	K	128	
1	KB	128	
1	L	128	
1	LB	128	
1	M	128	
1	OB	128	
1	P	128	
1	PB	128	
1	Q	128	
1	SB	128	
1	T	128	
1	TB	128	
1	U	128	
1	UB	128	
1	V	128	
1	VB	128	
1	W	128	
1	X	128	
1	Y	128	
1	Z	128	
2	CB	129	
2	DB	129	
2	E	129	

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Mol	Chain	Length	Quality of chain
2	F	129	
2	GB	129	
2	IB	129	
3	A	118	
3	B	118	
3	C	118	
3	D	118	
3	I	118	
3	J	118	
3	N	118	
3	O	118	
3	R	118	
3	S	118	
3	a	118	
3	b	118	
3	c	118	
3	d	118	
3	e	118	
3	f	118	
3	g	118	
3	h	118	
3	i	118	
3	j	118	
4	AD	123	
5	CD	136	

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Mol	Chain	Length	Quality of chain
5	FD	136	90% 72% 18% • 10%
5	HD	136	90% 65% 24% • 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 52697 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 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	BC	115	Total	C	N	O	S	0	0
			871	555	150	160	6		
1	DC	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	EB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	FA	115	Total	C	N	O	S	0	0
			871	555	150	160	6		
1	FB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	FC	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	GC	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	HC	115	Total	C	N	O	S	0	0
			871	555	150	160	6		
1	IC	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	K	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	KB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	L	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	LB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	M	115	Total	C	N	O	S	0	0
			871	555	150	160	6		
1	OB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	P	115	Total	C	N	O	S	0	0
			875	557	150	162	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	PB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	Q	115	Total	C	N	O	S	0	0
			871	554	149	162	6		
1	SB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	T	115	Total	C	N	O	S	0	0
			867	551	148	162	6		
1	TB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	U	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	UB	115	Total	C	N	O	S	0	0
			869	554	147	162	6		
1	V	115	Total	C	N	O	S	0	0
			871	554	149	162	6		
1	VB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	W	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	X	115	Total	C	N	O	S	0	0
			865	552	147	160	6		
1	Y	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	Z	115	Total	C	N	O	S	0	0
			875	557	150	162	6		

- Molecule 2 is a protein called RsbR protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CB	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	DB	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	E	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	F	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	GB	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	IB	116	Total	C	N	O	S	0	0
			884	563	152	163	6		

- Molecule 3 is a protein called RsbS protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	B	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	C	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	D	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	I	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	J	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	N	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	O	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	R	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	S	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	a	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	b	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	c	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	d	118	Total	C	N	O	S	0	0
			872	557	136	175	4		
3	e	118	Total	C	N	O	S	0	0
			868	555	135	173	5		
3	f	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	g	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	h	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	i	118	Total	C	N	O	S	0	0
			872	556	136	175	5		
3	j	118	Total	C	N	O	S	0	0
			871	556	135	175	5		

- Molecule 4 is a protein called RsbR protein,RsbR protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	123	Total	C	N	O	S	0	0
			935	594	160	175	6		

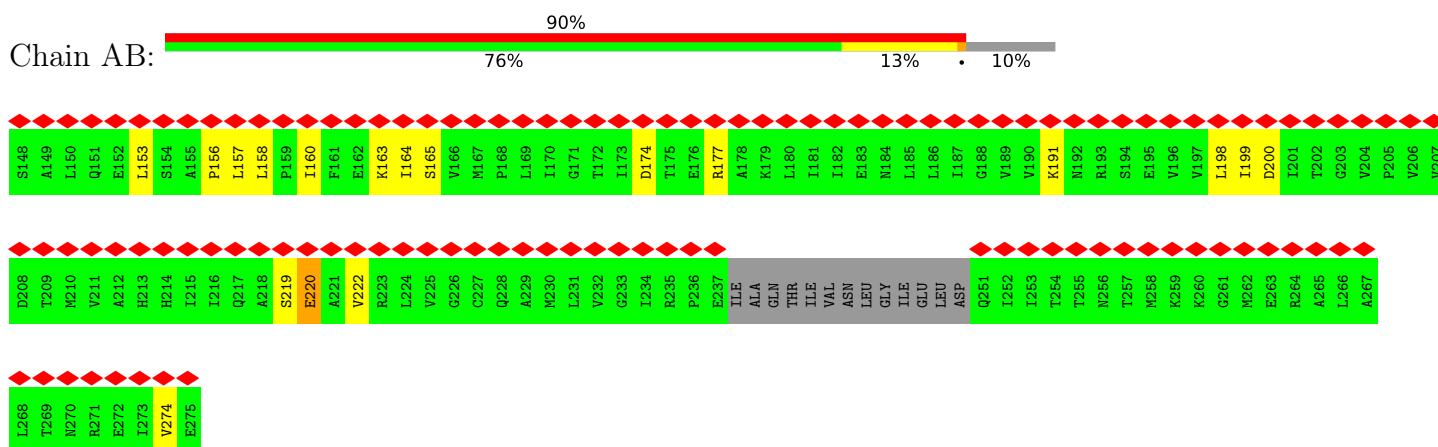
- Molecule 5 is a protein called RsbR protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CD	123	Total	C	N	O	S	0	0
			935	595	161	173	6		
5	FD	123	Total	C	N	O	S	0	0
			927	589	159	173	6		
5	HD	123	Total	C	N	O	S	0	0
			931	591	159	175	6		

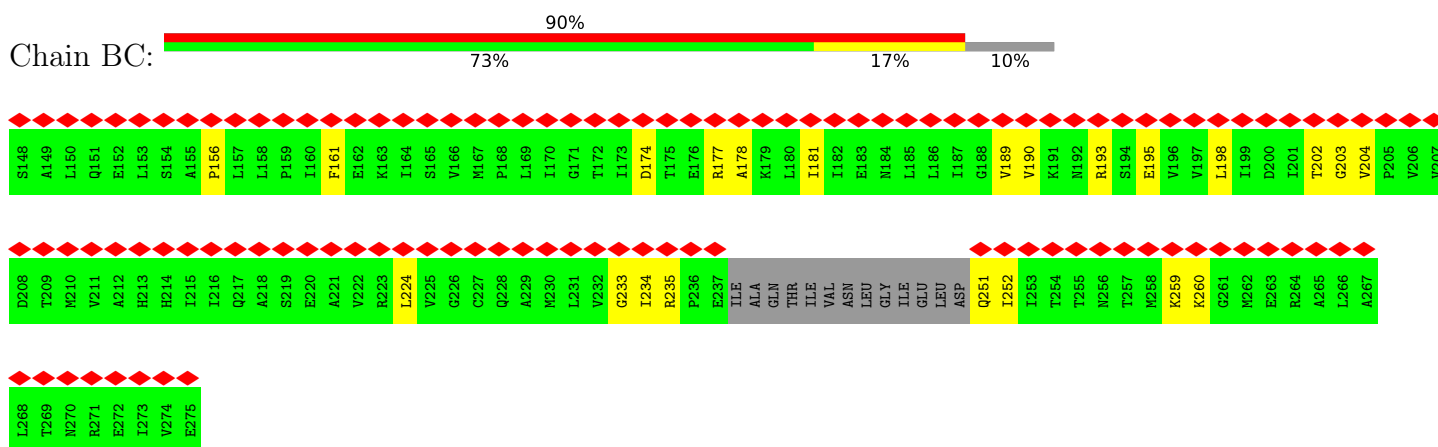
3 Residue-property plots

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

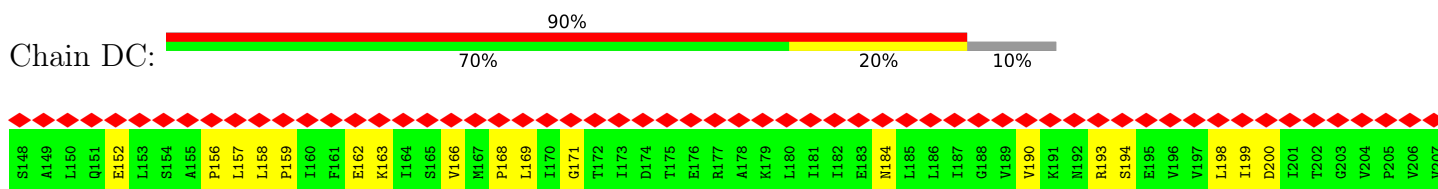
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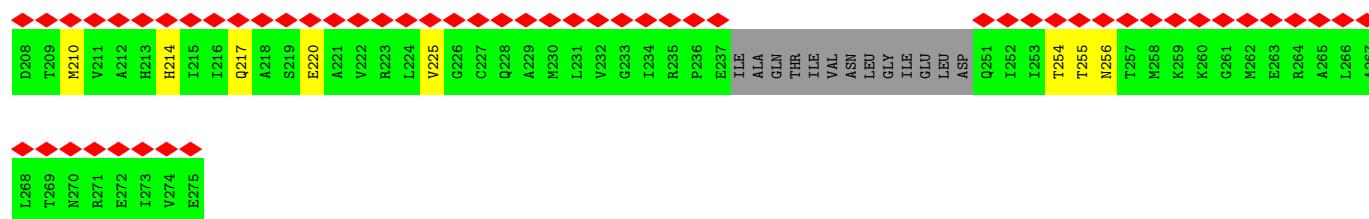


• Molecule 1: RsbR protein

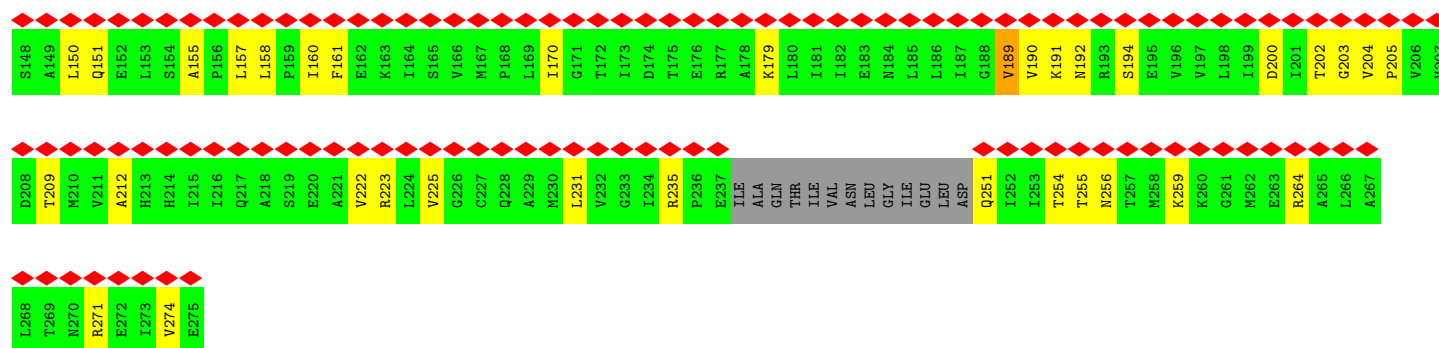


• Molecule 1: RsbR protein

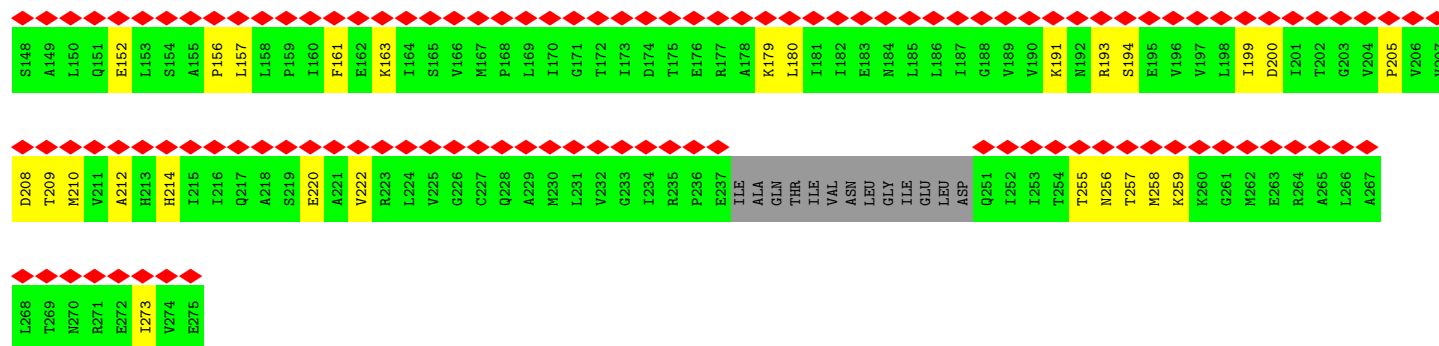
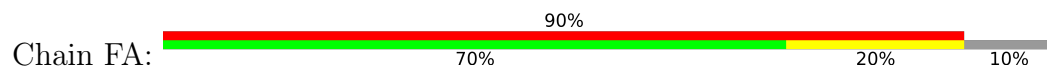




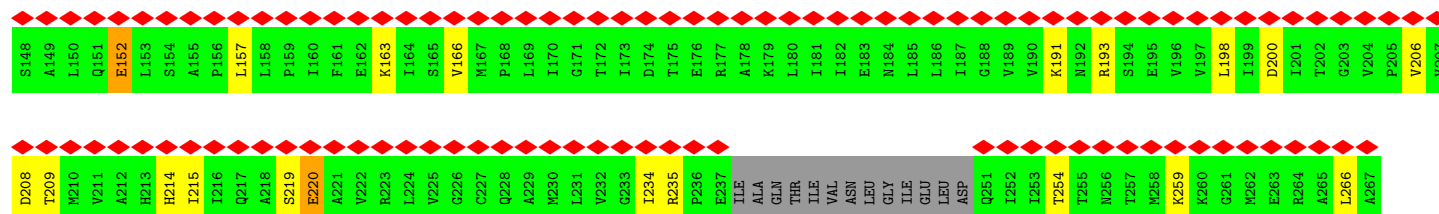
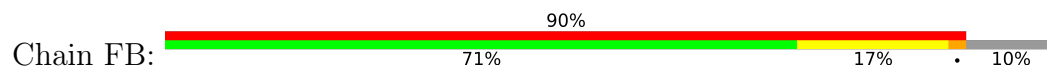
• Molecule 1: RsbR protein



• Molecule 1: RsbR protein

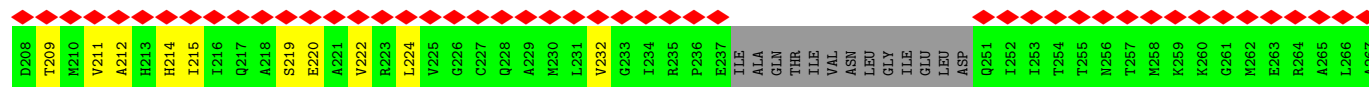
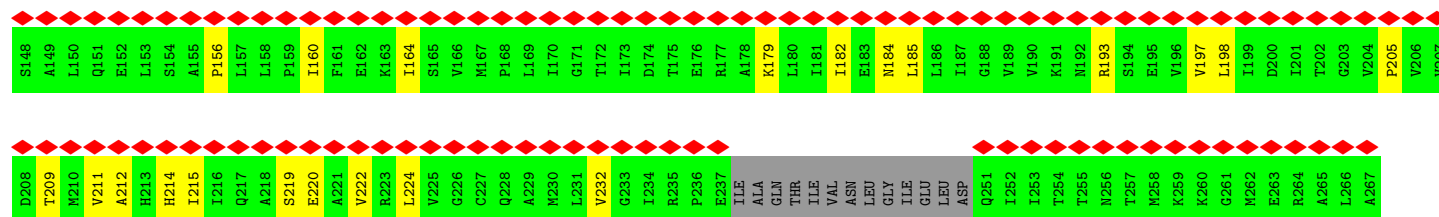
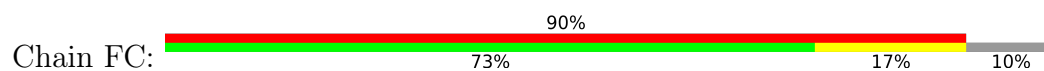


• Molecule 1: RsbR protein

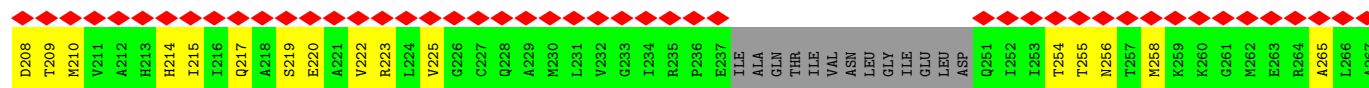
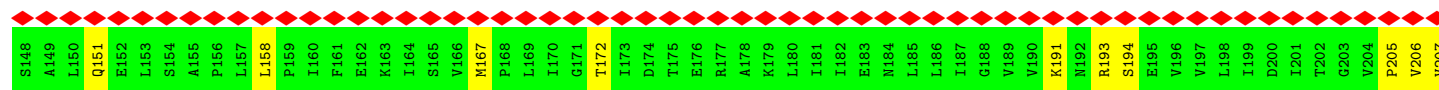
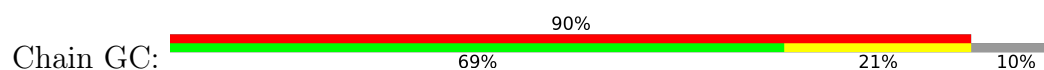




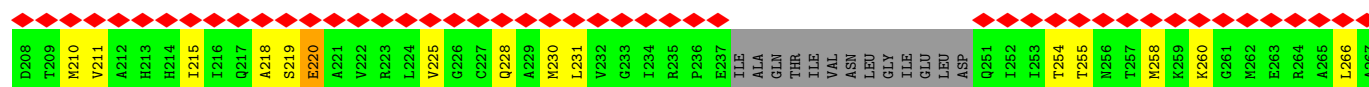
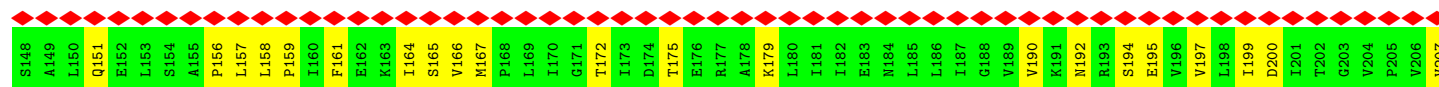
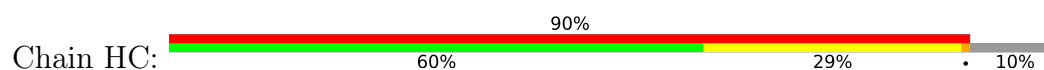
• Molecule 1: RsbR protein



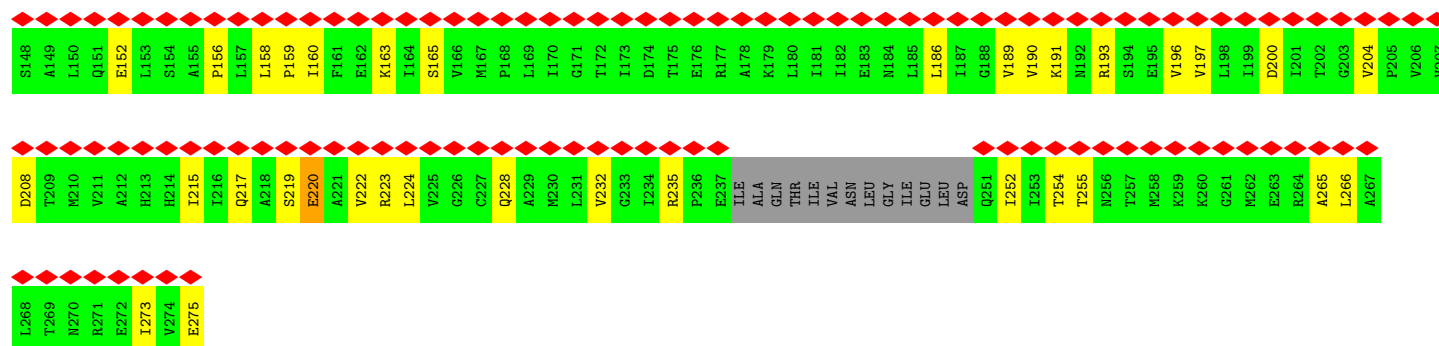
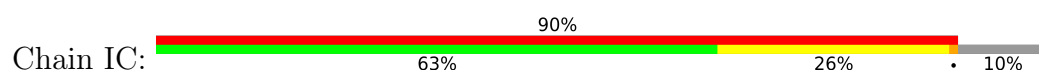
• Molecule 1: RsbR protein



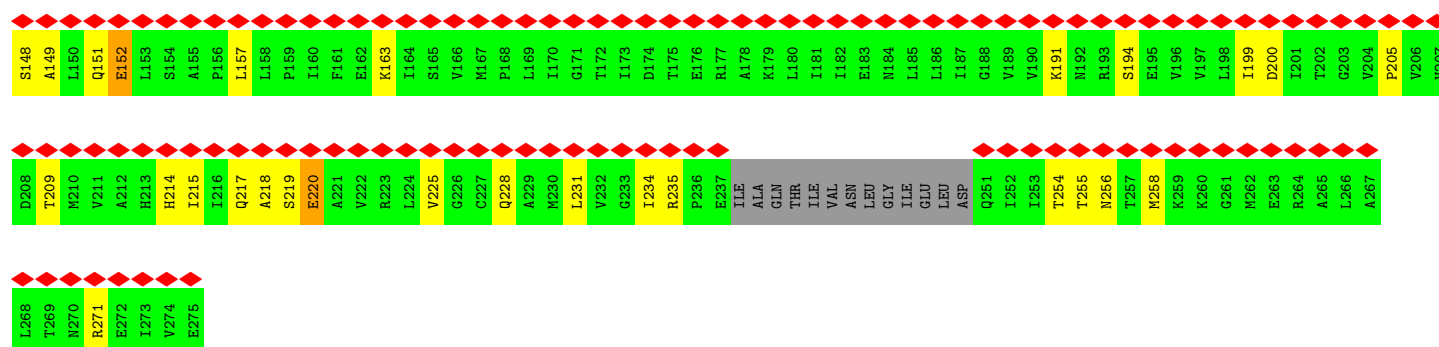
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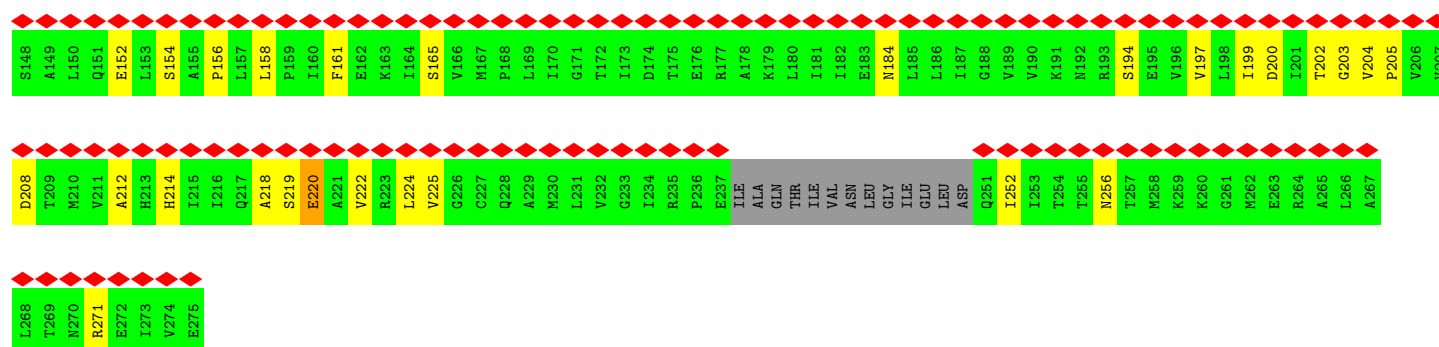
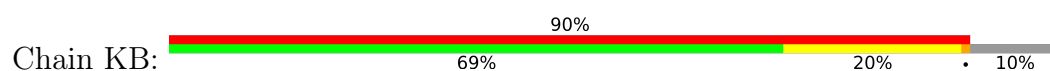
• Molecule 1: RsbR protein



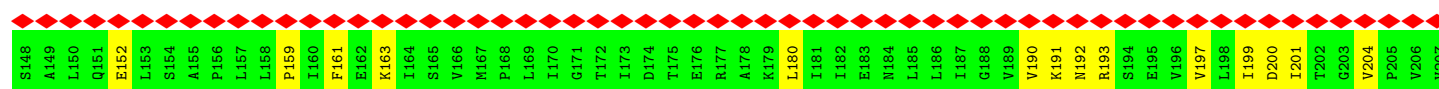
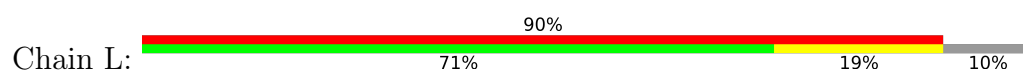
• Molecule 1: RsbR protein

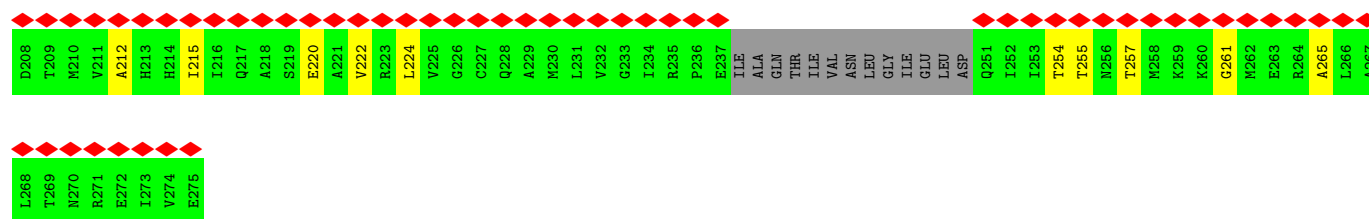


• Molecule 1: RsbR protein

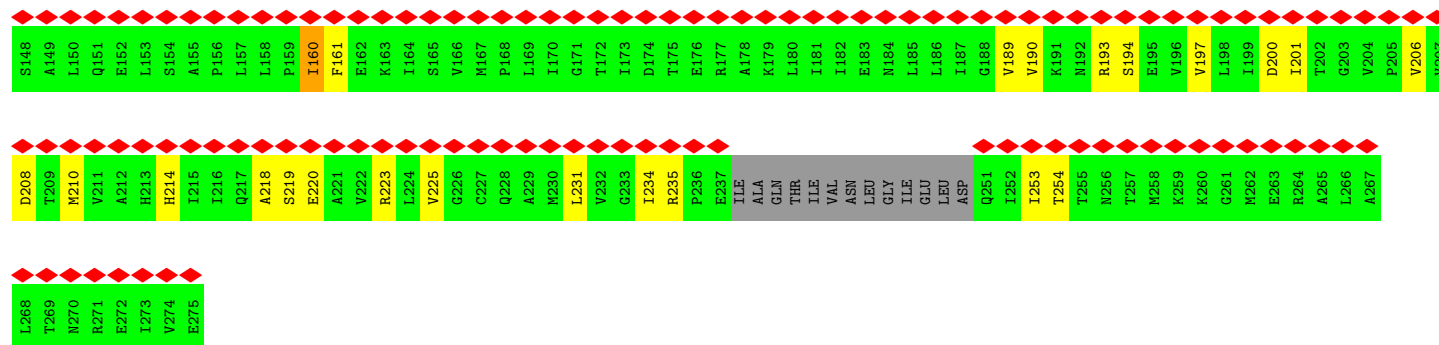
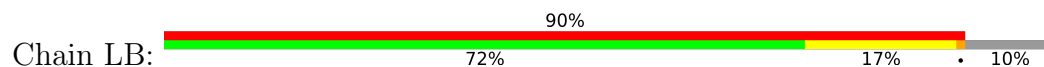


• Molecule 1: RsbR protein

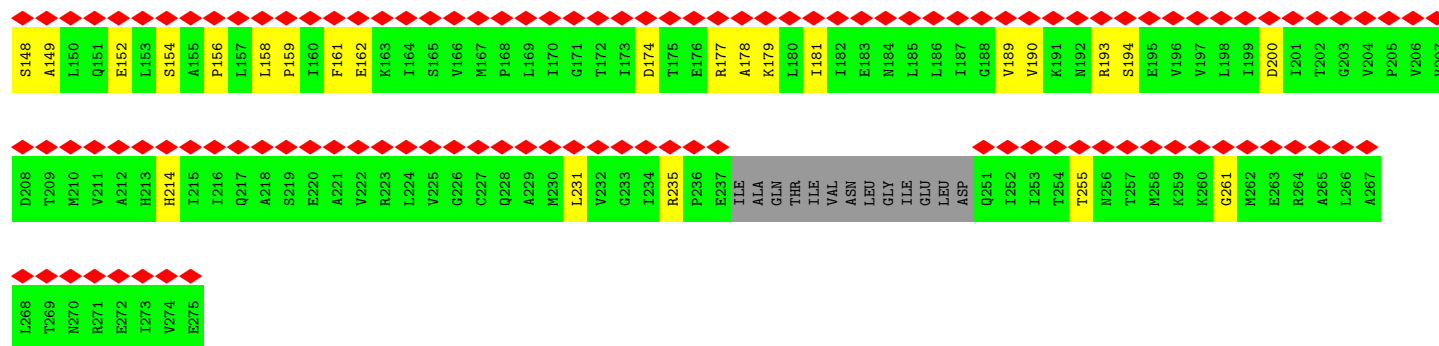




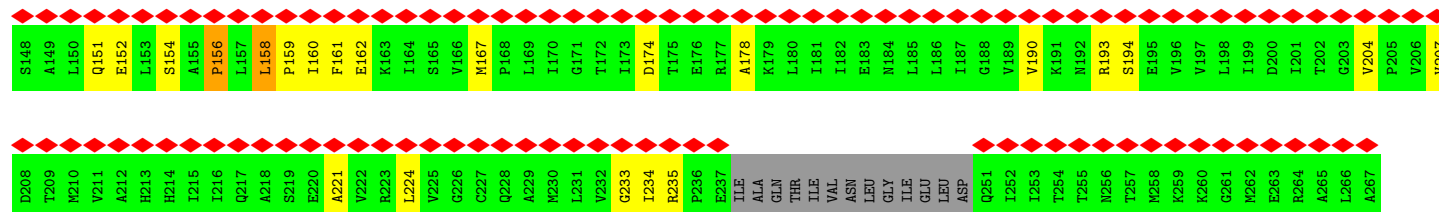
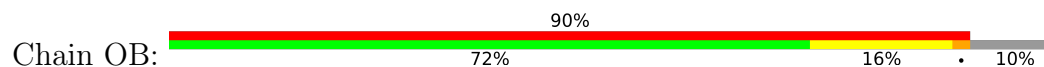
• Molecule 1: RsbR protein



• Molecule 1: RsbR protein

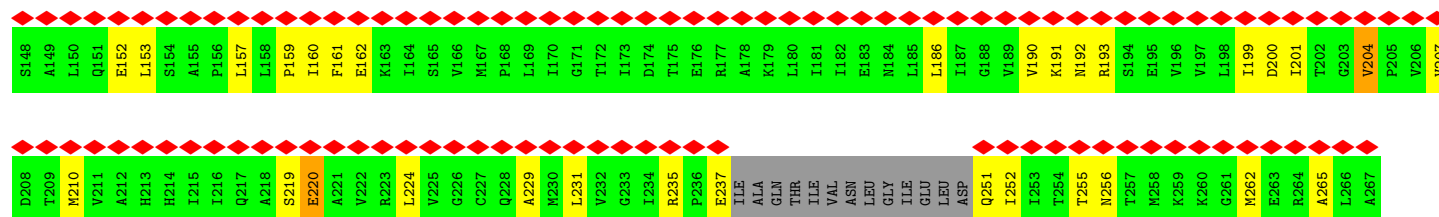


• Molecule 1: RsbR protein

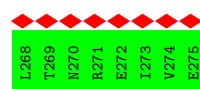
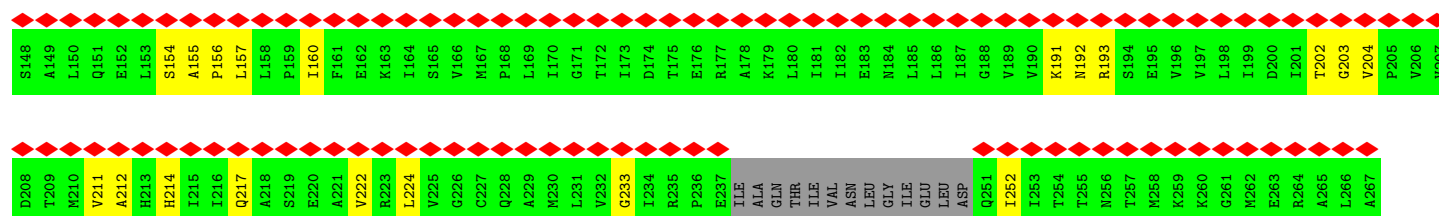
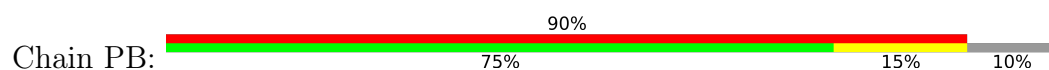




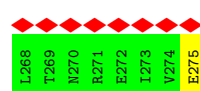
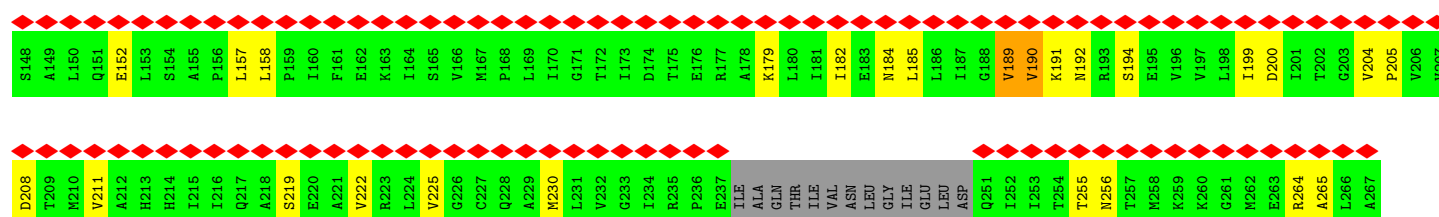
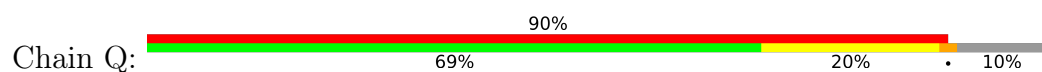
• Molecule 1: RsbR protein



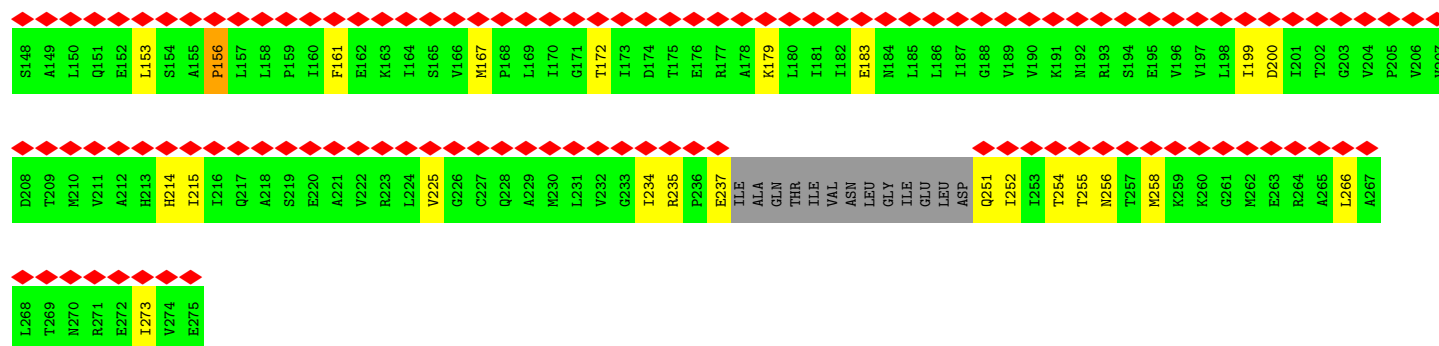
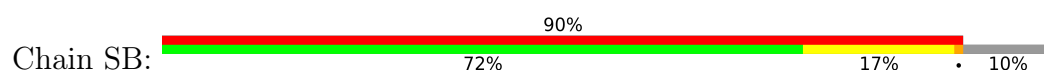
• Molecule 1: RsbR protein



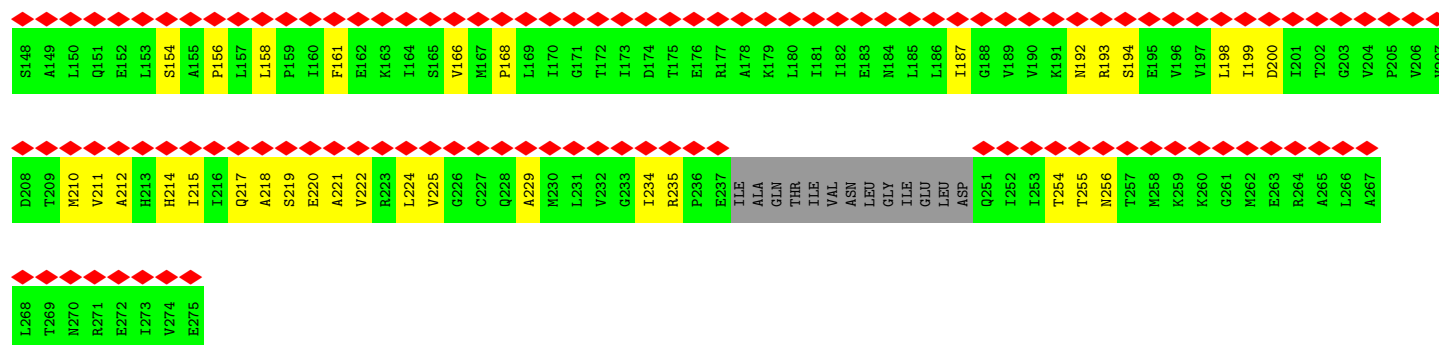
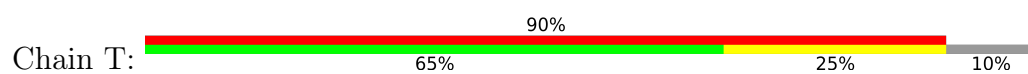
• Molecule 1: RsbR protein



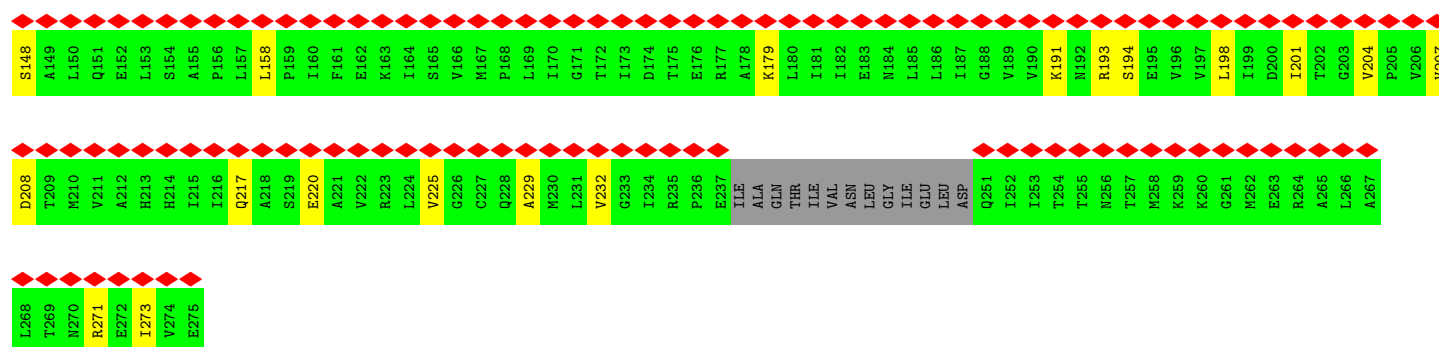
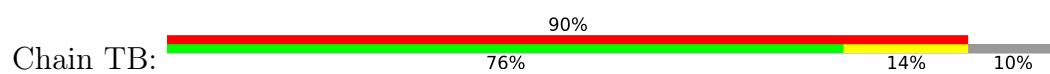
• Molecule 1: RsbR protein



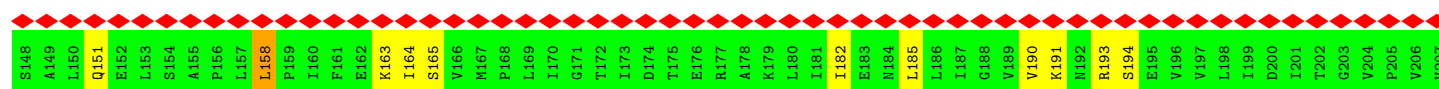
• Molecule 1: RsbR protein

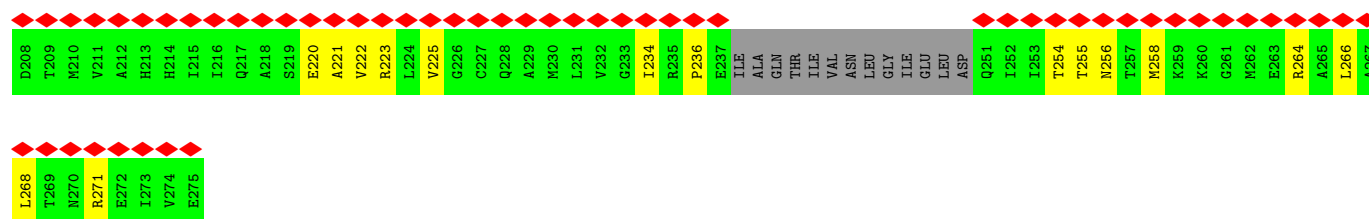


• Molecule 1: RsbR protein

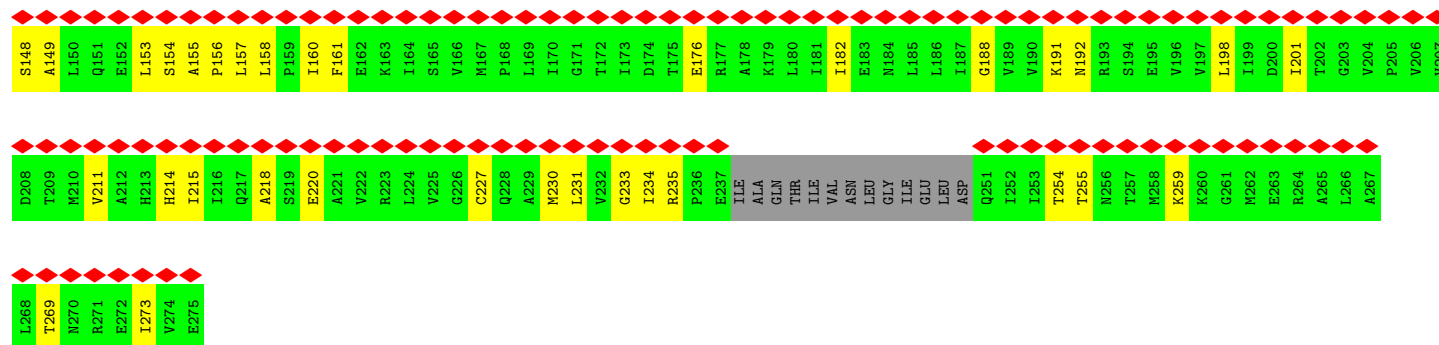


• Molecule 1: RsbR protein

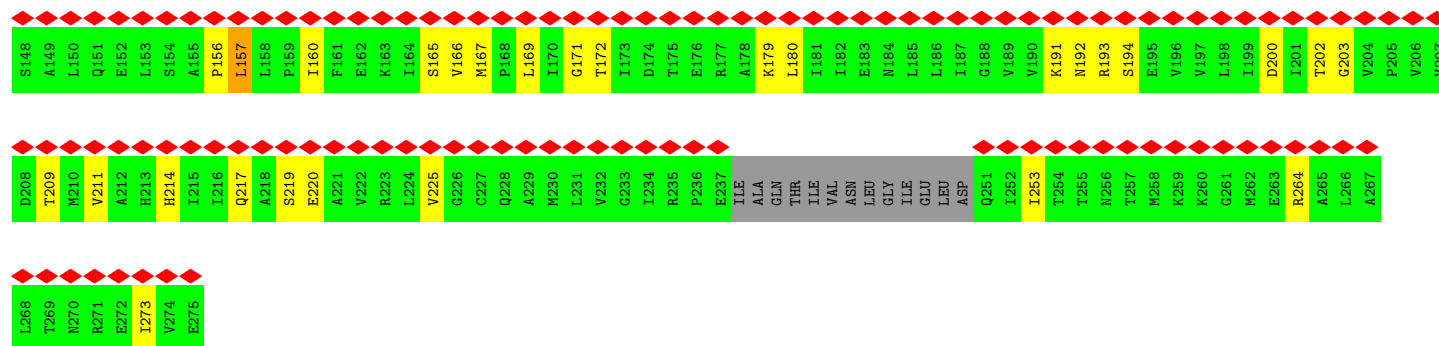




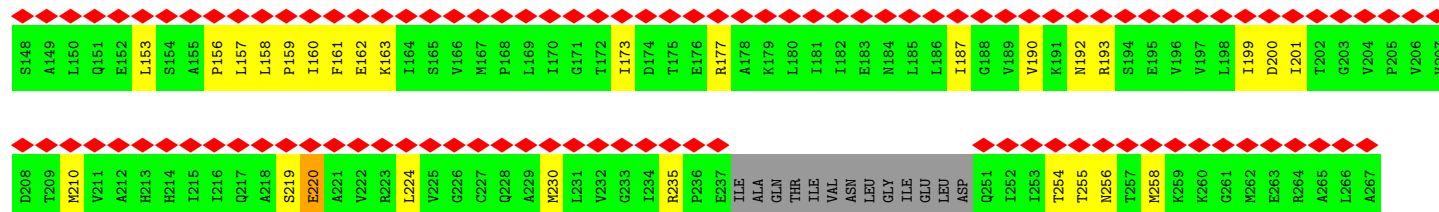
• Molecule 1: RsbR protein



• Molecule 1: RsbR protein

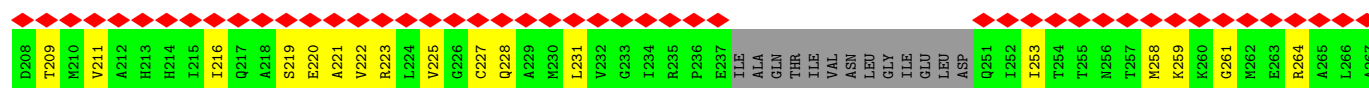
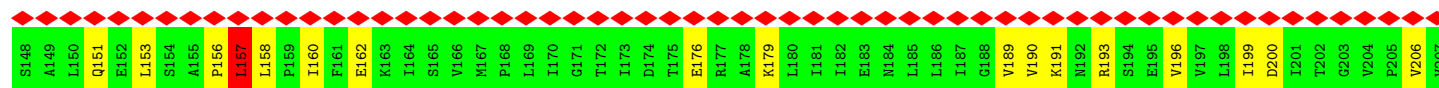


• Molecule 1: RsbR protein

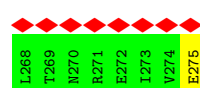
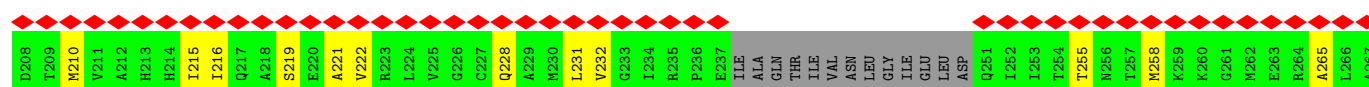
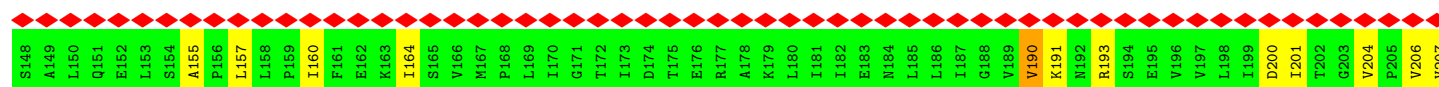
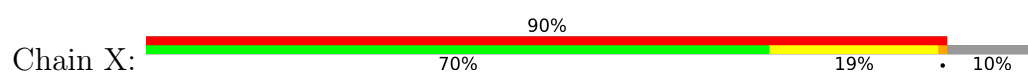




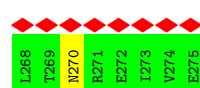
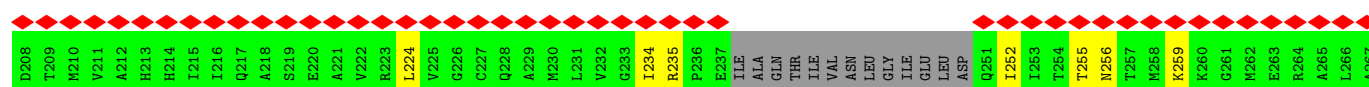
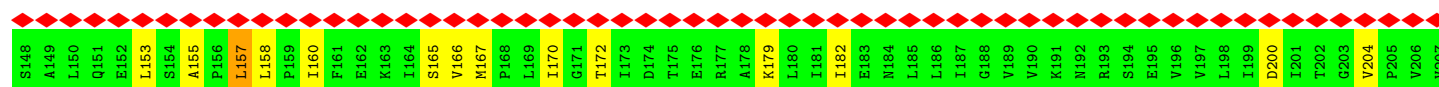
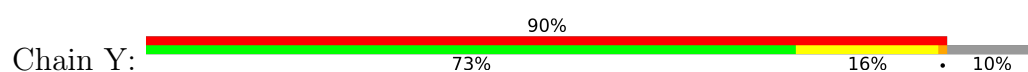
• Molecule 1: RsbR protein



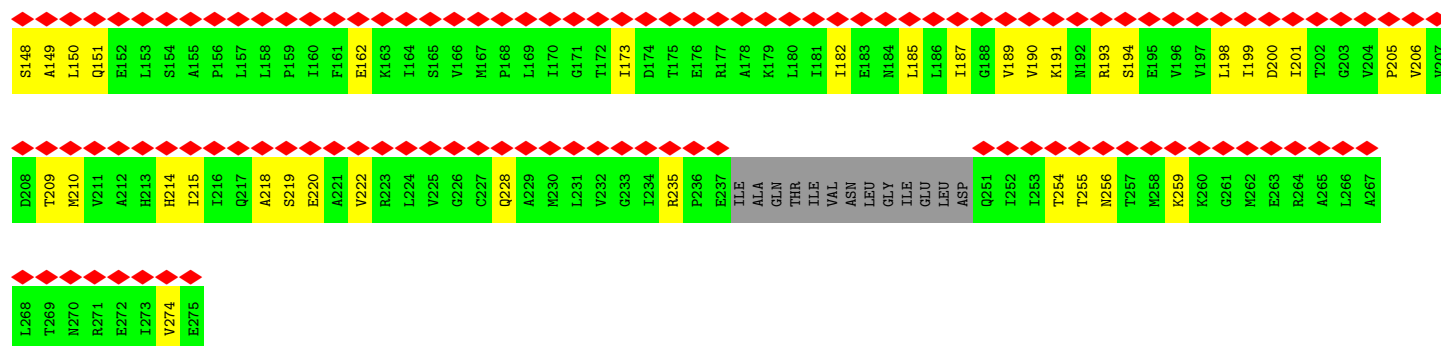
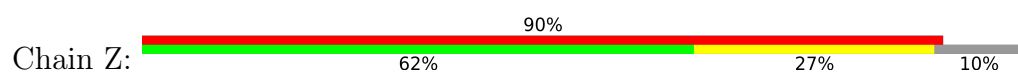
• Molecule 1: RsbR protein



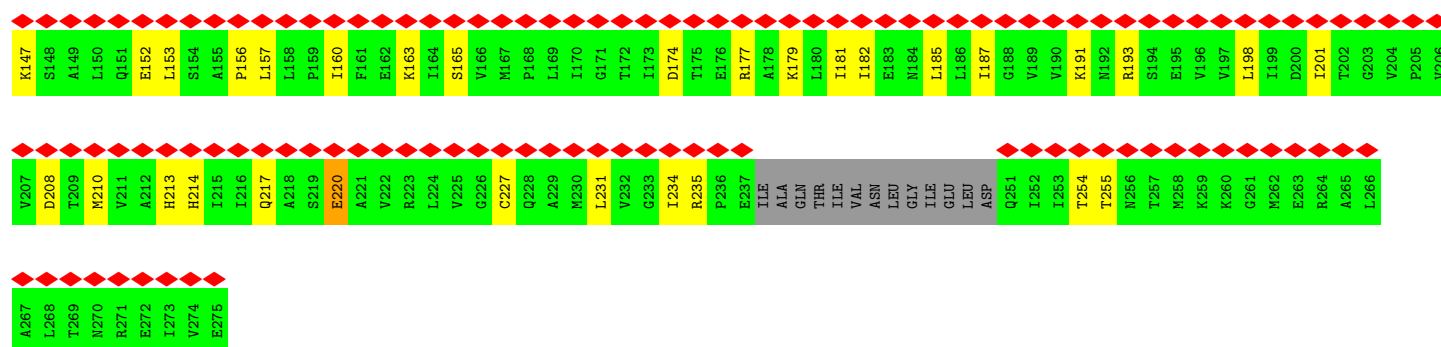
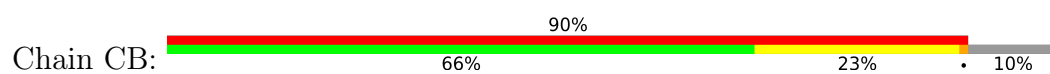
• Molecule 1: RsbR protein



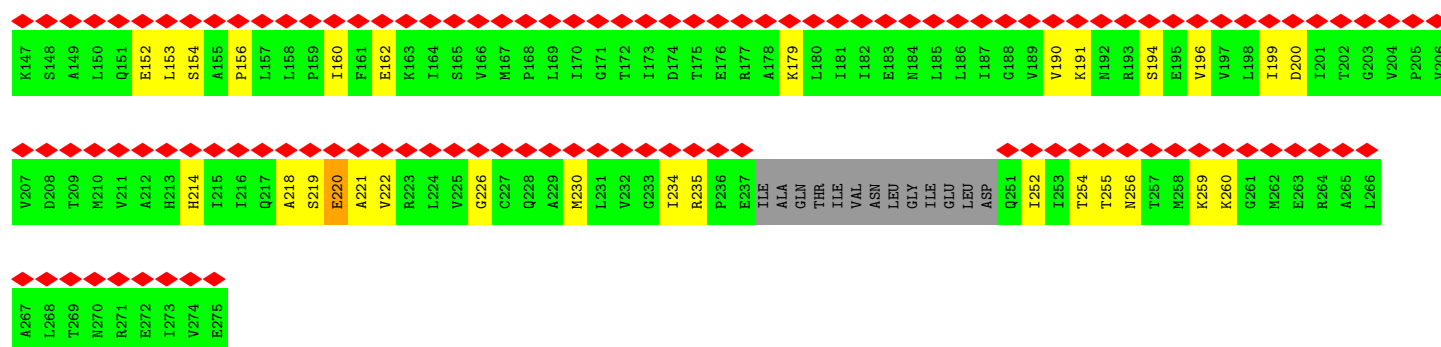
• Molecule 1: RsbR protein



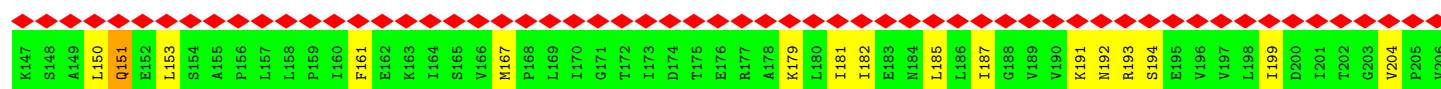
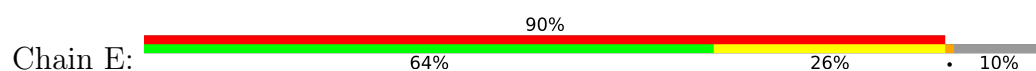
• Molecule 2: RsbR protein

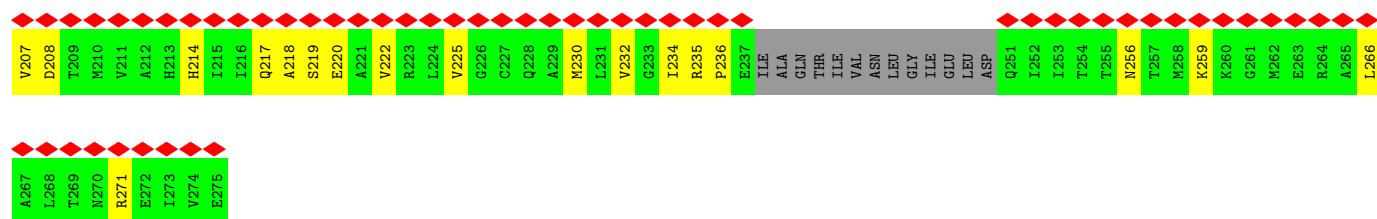


• Molecule 2: RsbR protein

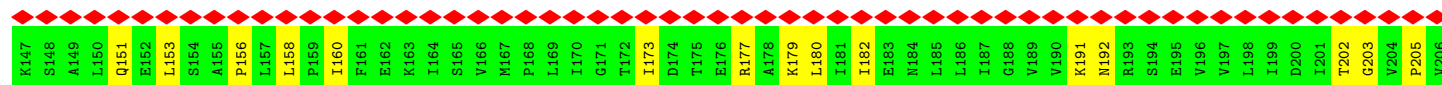
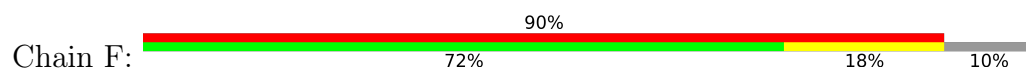


• Molecule 2: RsbR protein

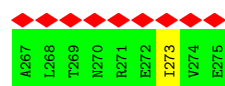




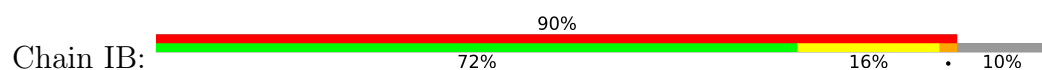
• Molecule 2: RsbR protein



• Molecule 2: RsbR protein

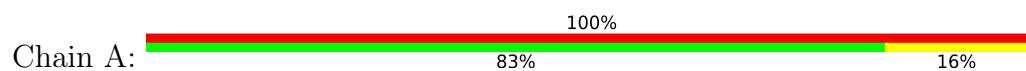


• Molecule 2: RsbR protein

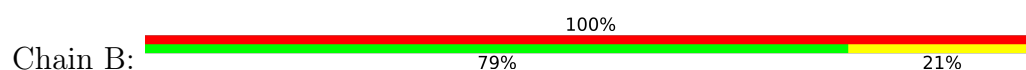




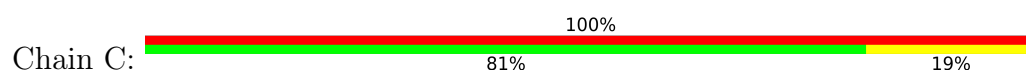
• Molecule 3: RsbS protein



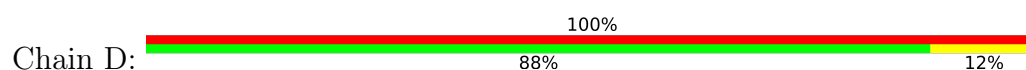
• Molecule 3: RsbS protein



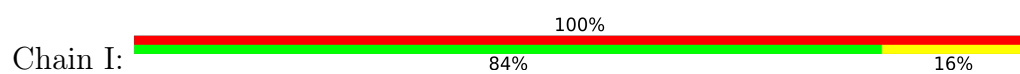
• Molecule 3: RsbS protein



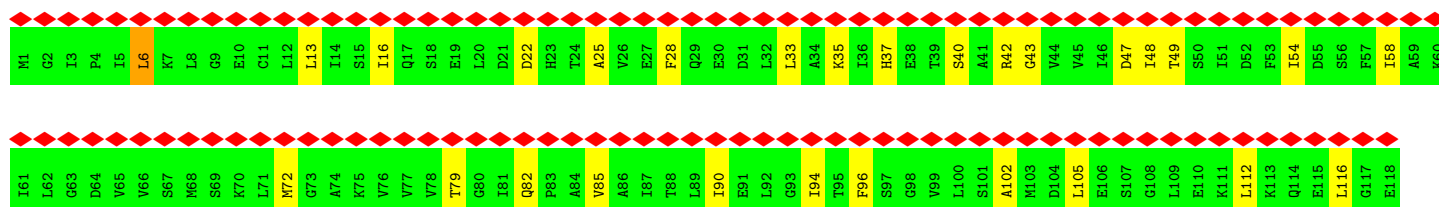
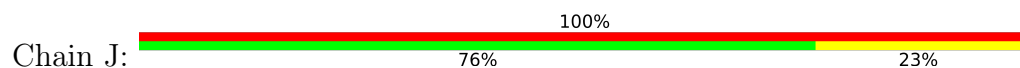
• Molecule 3: RsbS protein



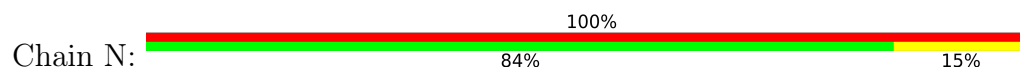
• Molecule 3: RsbS protein



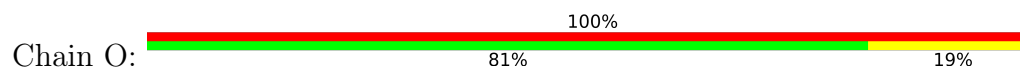
• Molecule 3: RsbS protein



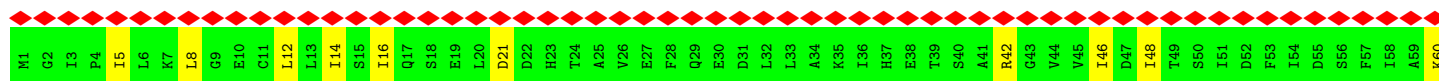
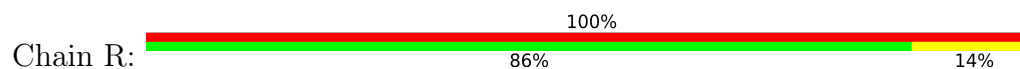
• Molecule 3: RsbS protein

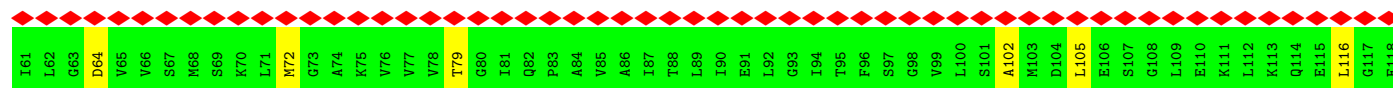


• Molecule 3: RsbS protein

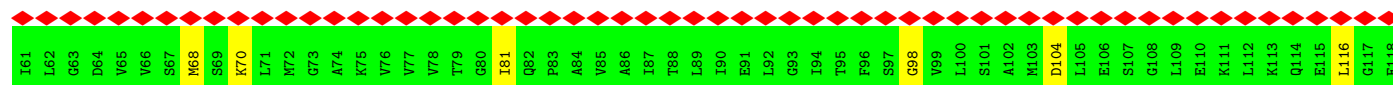
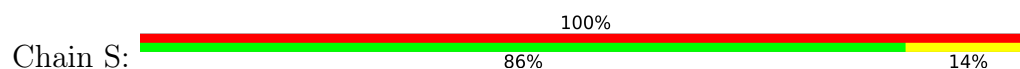


• Molecule 3: RsbS protein

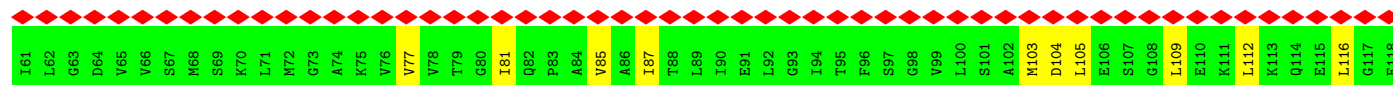
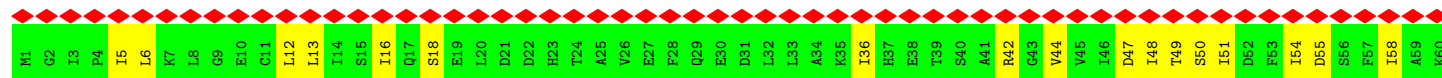
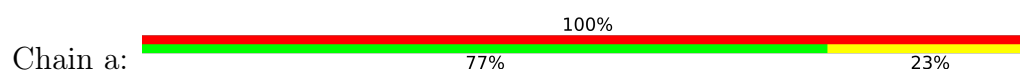




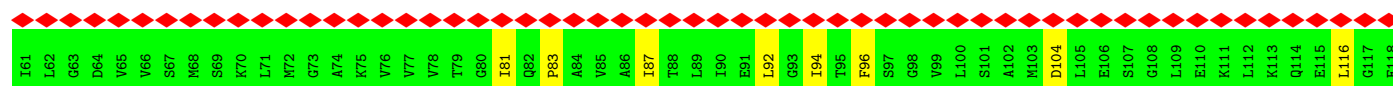
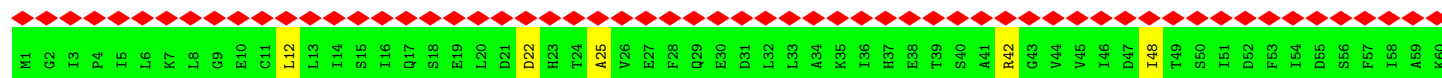
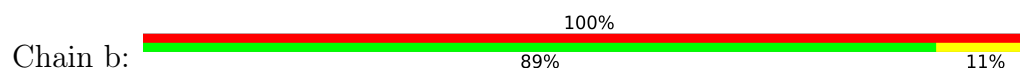
• Molecule 3: RsbS protein



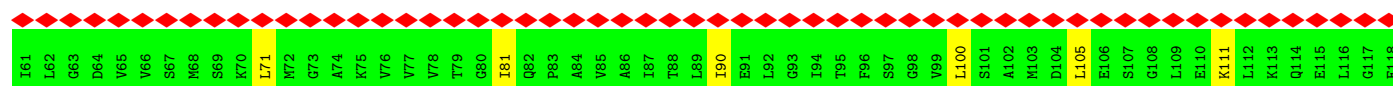
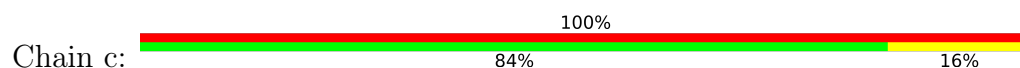
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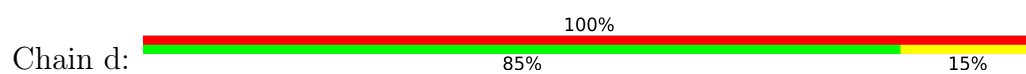
• Molecule 3: RsbS protein



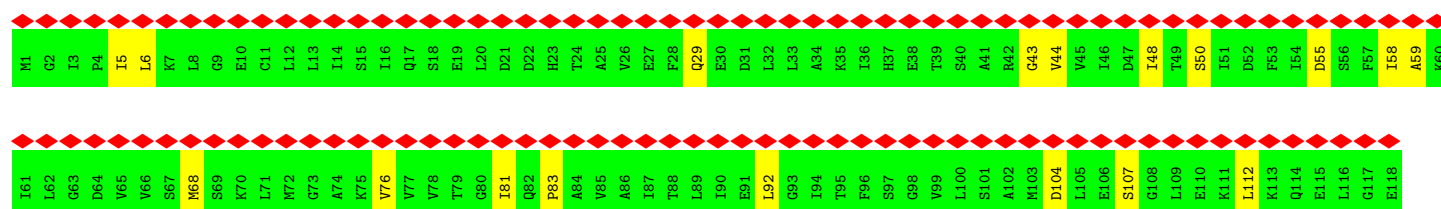
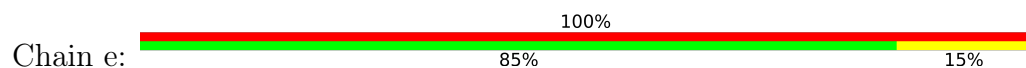
• Molecule 3: RsbS protein



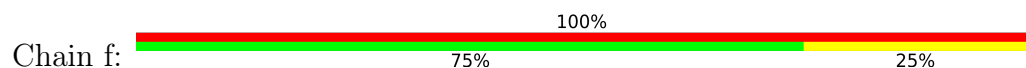
• Molecule 3: RsbS protein



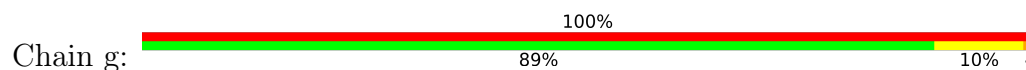
• Molecule 3: RsbS protein



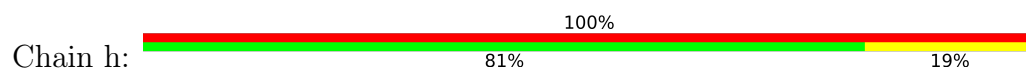
• Molecule 3: RsbS protein

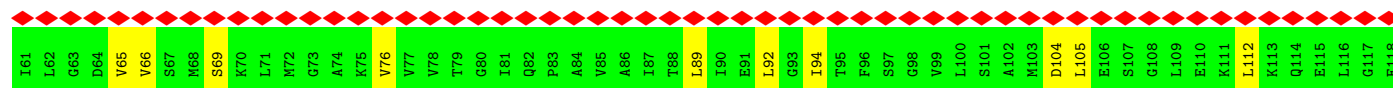


• Molecule 3: RsbS protein

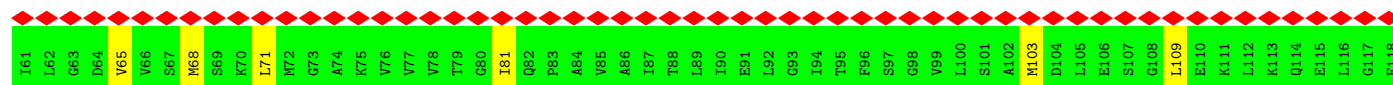
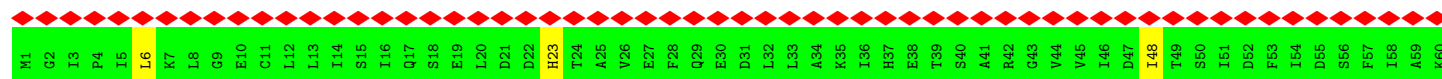
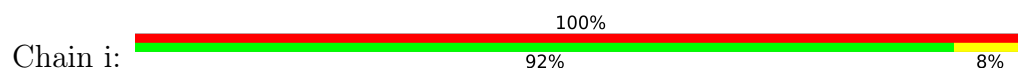


• Molecule 3: RsbS protein

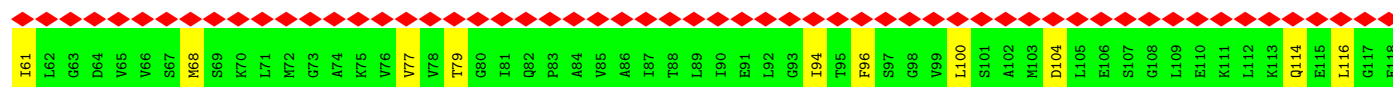
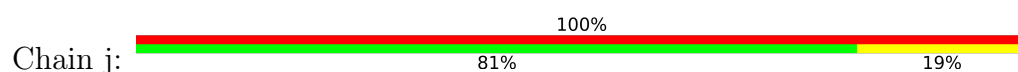




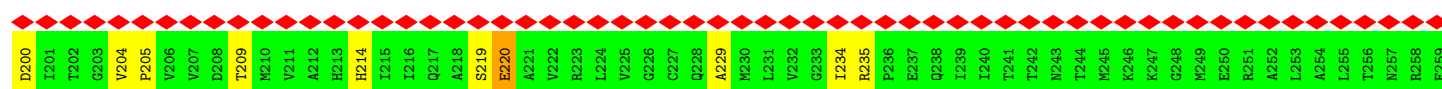
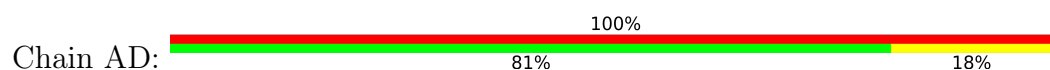
• Molecule 3: RsbS protein



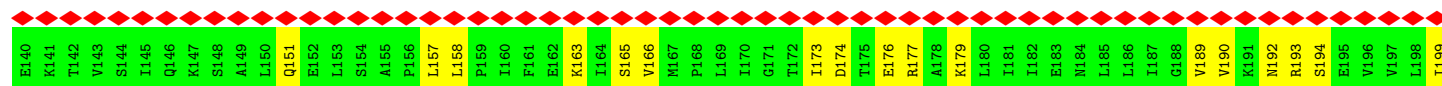
• Molecule 3: RsbS protein



• Molecule 4: RsbR protein, RsbR protein

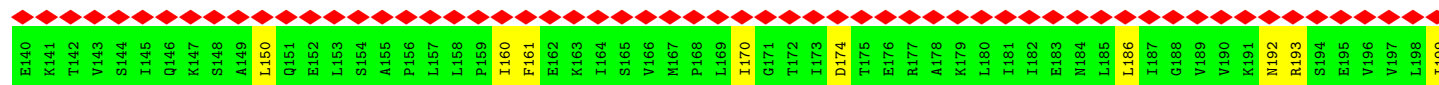
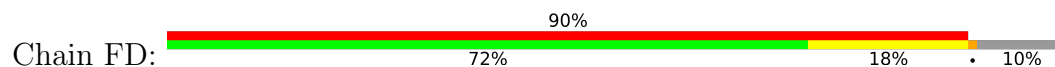


• Molecule 5: RsbR protein

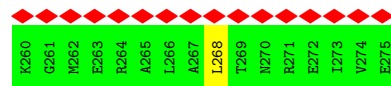
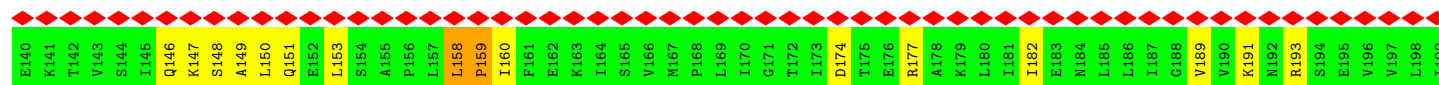




• Molecule 5: RsbR protein



• Molecule 5: RsbR protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	434.59998, 434.59998, 434.59998	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AB	0.26	0/881	0.68	0/1193
1	BC	0.23	0/877	0.63	0/1188
1	DC	0.23	0/881	0.69	2/1193 (0.2%)
1	EB	0.23	0/881	0.65	0/1193
1	FA	0.26	0/877	0.66	0/1188
1	FB	0.23	0/881	0.68	0/1193
1	FC	0.22	0/881	0.64	0/1193
1	GC	0.22	0/881	0.59	0/1193
1	HC	0.24	0/877	0.66	2/1188 (0.2%)
1	IC	0.24	0/881	0.67	2/1193 (0.2%)
1	K	0.25	0/881	0.68	0/1193
1	KB	0.24	0/881	0.62	0/1193
1	L	0.22	0/881	0.55	0/1193
1	LB	0.24	0/881	0.69	2/1193 (0.2%)
1	M	0.21	0/877	0.66	0/1188
1	OB	0.26	0/881	0.72	2/1193 (0.2%)
1	P	0.22	0/881	0.57	0/1193
1	PB	0.21	0/881	0.60	0/1193
1	Q	0.25	0/877	0.66	2/1189 (0.2%)
1	SB	0.23	0/881	0.58	0/1193
1	T	0.26	0/873	0.71	3/1185 (0.3%)
1	TB	0.24	0/881	0.66	0/1193
1	U	0.23	0/881	0.63	0/1193
1	UB	0.27	0/875	0.65	0/1186
1	V	0.24	0/877	0.62	0/1189
1	VB	0.26	0/881	0.70	2/1193 (0.2%)
1	W	0.24	0/881	0.71	0/1193
1	X	0.24	0/871	0.75	2/1181 (0.2%)
1	Y	0.23	0/881	0.62	0/1193
1	Z	0.24	0/881	0.69	1/1193 (0.1%)
2	CB	0.24	0/890	0.67	0/1204
2	DB	0.21	0/890	0.64	0/1204
2	E	0.22	0/890	0.61	0/1204
2	F	0.22	0/890	0.66	0/1204

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	GB	0.24	0/890	0.72	3/1204 (0.2%)
2	IB	0.21	0/890	0.59	0/1204
3	A	0.18	0/881	0.51	0/1188
3	B	0.16	0/881	0.40	0/1188
3	C	0.16	0/881	0.44	0/1188
3	D	0.19	0/881	0.53	0/1188
3	I	0.19	0/881	0.47	0/1188
3	J	0.18	0/881	0.47	0/1188
3	N	0.17	0/881	0.45	0/1188
3	O	0.17	0/881	0.40	0/1188
3	R	0.17	0/877	0.42	0/1184
3	S	0.17	0/877	0.45	0/1184
3	a	0.16	0/877	0.46	0/1184
3	b	0.15	0/877	0.39	0/1184
3	c	0.17	0/881	0.44	0/1188
3	d	0.16	0/878	0.45	0/1185
3	e	0.16	0/874	0.42	0/1180
3	f	0.20	0/881	0.47	0/1188
3	g	0.18	0/881	0.46	0/1188
3	h	0.17	0/877	0.45	0/1184
3	i	0.18	0/878	0.49	0/1184
3	j	0.17	0/877	0.43	0/1184
4	AD	0.24	0/941	0.66	0/1274
5	CD	0.23	0/941	0.62	0/1273
5	FD	0.24	0/933	0.67	0/1265
5	HD	0.22	0/935	0.70	0/1264
All	All	0.22	0/53055	0.60	23/71756 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	2
1	DC	0	1
1	FA	0	1
1	FB	0	2
1	FC	0	1
1	HC	0	2
1	IC	0	1
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	KB	0	2
1	L	0	1
1	P	0	2
1	PB	0	1
1	Q	0	1
1	TB	0	1
1	U	0	1
1	UB	0	1
1	VB	0	1
1	W	0	2
2	CB	0	1
2	DB	0	1
2	E	0	1
2	F	0	1
2	GB	0	3
2	IB	0	1
3	a	0	1
3	e	0	1
4	AD	0	1
5	CD	0	2
5	HD	0	1
All	All	0	39

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	219	SER	CA-C-N	8.03	136.16	121.70
1	X	219	SER	C-N-CA	8.03	136.16	121.70
1	Z	173	ILE	N-CA-C	-7.69	105.70	113.47
1	OB	156	PRO	CA-C-N	6.94	134.79	121.54
1	OB	156	PRO	C-N-CA	6.94	134.79	121.54
1	IC	156	PRO	CA-C-N	6.54	134.02	121.54
1	IC	156	PRO	C-N-CA	6.54	134.02	121.54
2	GB	156	PRO	CA-C-N	6.51	133.97	121.54
2	GB	156	PRO	C-N-CA	6.51	133.97	121.54
1	DC	156	PRO	CA-C-N	6.36	133.68	121.54
1	DC	156	PRO	C-N-CA	6.36	133.68	121.54
1	T	221	ALA	N-CA-C	6.35	118.95	111.02
1	HC	156	PRO	CA-C-N	6.35	133.66	121.54
1	HC	156	PRO	C-N-CA	6.35	133.66	121.54
1	T	156	PRO	CA-C-N	6.13	133.25	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	156	PRO	C-N-CA	6.13	133.25	121.54
1	VB	156	PRO	CA-C-N	6.12	133.22	121.54
1	VB	156	PRO	C-N-CA	6.12	133.22	121.54
1	Q	189	VAL	CA-C-N	5.31	131.53	121.97
1	Q	189	VAL	C-N-CA	5.31	131.53	121.97
1	LB	160	ILE	CA-C-N	5.11	131.29	121.54
1	LB	160	ILE	C-N-CA	5.11	131.29	121.54
2	GB	220	GLU	CA-CB-CG	5.10	124.30	114.10

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	158	LEU	Peptide
1	AB	220	GLU	Peptide
4	AD	220	GLU	Peptide
2	CB	220	GLU	Peptide
5	CD	151	GLN	Peptide
5	CD	157	LEU	Peptide
2	DB	220	GLU	Peptide
1	DC	220	GLU	Peptide
2	E	150	LEU	Peptide
2	F	151	GLN	Peptide
1	FA	220	GLU	Peptide
1	FB	152	GLU	Peptide
1	FB	220	GLU	Peptide
1	FC	215	ILE	Peptide
2	GB	157	LEU	Peptide
2	GB	166	VAL	Peptide
2	GB	220	GLU	Peptide
1	HC	157	LEU	Peptide
1	HC	220	GLU	Peptide
5	HD	158	LEU	Peptide
2	IB	220	GLU	Peptide
1	IC	220	GLU	Peptide
1	K	151	GLN	Peptide
1	K	220	GLU	Peptide
1	KB	204	VAL	Peptide
1	KB	220	GLU	Peptide
1	L	220	GLU	Peptide
1	P	204	VAL	Peptide
1	P	220	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	PB	157	LEU	Peptide
1	Q	204	VAL	Peptide
1	TB	220	GLU	Peptide
1	U	158	LEU	Peptide
1	UB	220	GLU	Peptide
1	VB	220	GLU	Peptide
1	W	151	GLN	Peptide
1	W	156	PRO	Peptide
3	a	5	ILE	Peptide
3	e	5	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	875	0	946	11	0
1	BC	871	0	942	12	0
1	DC	875	0	946	16	0
1	EB	875	0	946	23	0
1	FA	871	0	942	19	0
1	FB	875	0	946	17	0
1	FC	875	0	946	13	0
1	GC	875	0	946	18	0
1	HC	871	0	942	19	0
1	IC	875	0	946	21	0
1	K	875	0	946	18	0
1	KB	875	0	946	16	0
1	L	875	0	946	13	0
1	LB	875	0	946	12	0
1	M	871	0	942	14	0
1	OB	875	0	946	13	0
1	P	875	0	946	20	0
1	PB	875	0	946	12	0
1	Q	871	0	935	18	0
1	SB	875	0	946	16	0
1	T	867	0	924	19	0
1	TB	875	0	946	11	0
1	U	875	0	946	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UB	869	0	935	23	0
1	V	871	0	935	20	0
1	VB	875	0	946	23	0
1	W	875	0	946	20	0
1	X	865	0	931	15	0
1	Y	875	0	946	16	0
1	Z	875	0	946	24	0
2	CB	884	0	959	19	0
2	DB	884	0	959	17	0
2	E	884	0	959	23	0
2	F	884	0	959	15	0
2	GB	884	0	959	15	0
2	IB	884	0	959	15	0
3	A	875	0	921	14	0
3	B	875	0	921	16	0
3	C	875	0	921	16	0
3	D	875	0	921	9	0
3	I	875	0	921	14	0
3	J	875	0	921	16	0
3	N	875	0	921	10	0
3	O	875	0	921	15	0
3	R	871	0	910	10	0
3	S	871	0	910	10	0
3	a	871	0	910	15	0
3	b	871	0	910	11	0
3	c	875	0	921	11	0
3	d	872	0	914	11	0
3	e	868	0	908	11	0
3	f	875	0	921	18	0
3	g	875	0	921	9	0
3	h	871	0	910	14	0
3	i	872	0	912	5	0
3	j	871	0	910	15	0
4	AD	935	0	1007	15	0
5	CD	935	0	1014	20	0
5	FD	927	0	992	15	0
5	HD	931	0	994	25	0
All	All	52697	0	56380	847	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 8.

All (847) 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)
5:HD:219:SER:HG	5:HD:221:ALA:N	1.76	0.84
1:VB:162:GLU:HB3	1:VB:193:ARG:HH12	1.54	0.71
1:FA:163:LYS:HD2	1:K:152:GLU:HB2	1.73	0.70
1:U:190:VAL:HG21	1:U:223:ARG:HH21	1.60	0.67
1:FA:273:ILE:HD11	1:K:271:ARG:HB3	1.77	0.67
5:CD:223:ARG:HH12	5:CD:264:ARG:HG3	1.60	0.66
2:CB:152:GLU:HG3	2:CB:163:LYS:HB3	1.78	0.66
1:IC:152:GLU:HG3	1:IC:163:LYS:H	1.60	0.66
1:BC:259:LYS:HB2	1:DC:157:LEU:HB3	1.79	0.65
1:L:193:ARG:HG3	1:L:224:LEU:HD23	1.77	0.65
2:CB:198:LEU:HD21	2:CB:201:ILE:HG12	1.80	0.64
1:Z:198:LEU:HD21	1:Z:201:ILE:HG12	1.80	0.64
2:CB:179:LYS:HD2	2:CB:191:LYS:HE3	1.79	0.63
2:F:180:LEU:HB3	3:b:83:PRO:HB3	1.81	0.63
1:UB:198:LEU:HD21	1:UB:201:ILE:HD13	1.81	0.63
3:B:55:ASP:H	3:B:58:ILE:HD12	1.64	0.62
3:N:6:LEU:HD11	3:N:35:LYS:HG2	1.81	0.62
1:DC:169:LEU:HG	1:DC:171:GLY:H	1.65	0.62
1:BC:193:ARG:HG3	1:BC:224:LEU:HD23	1.82	0.62
1:UB:191:LYS:HD3	1:UB:215:ILE:HD13	1.81	0.62
1:FC:211:VAL:HA	1:FC:214:HIS:HB3	1.82	0.61
1:UB:259:LYS:HB2	1:VB:157:LEU:HB3	1.81	0.61
3:S:15:SER:HA	3:S:47:ASP:HB2	1.81	0.61
1:V:211:VAL:HA	1:V:214:HIS:HB2	1.83	0.61
5:HD:211:VAL:HA	5:HD:214:HIS:HB2	1.83	0.61
3:f:5:ILE:HG21	3:f:35:LYS:HG2	1.83	0.61
1:FC:164:ILE:HD11	1:FC:193:ARG:HH21	1.65	0.60
1:FB:152:GLU:HG2	1:FB:163:LYS:H	1.67	0.60
1:EB:157:LEU:HB2	1:FB:259:LYS:HD3	1.84	0.59
1:Y:157:LEU:HD12	1:Y:158:LEU:H	1.68	0.59
3:b:48:ILE:HD11	3:b:81:ILE:HG12	1.84	0.59
1:FA:152:GLU:HG2	1:FA:163:LYS:HG2	1.84	0.59
3:j:94:ILE:HD12	3:j:96:PHE:HB2	1.85	0.59
1:HC:207:VAL:HA	1:HC:210:MET:HB2	1.84	0.59
1:W:191:LYS:HG3	1:W:222:VAL:HG23	1.83	0.59
3:O:5:ILE:HG21	3:O:35:LYS:HG2	1.85	0.59
3:f:66:VAL:HG13	3:f:76:VAL:HG21	1.84	0.59
3:c:100:LEU:HB3	3:c:111:LYS:HE3	1.85	0.58
1:GC:217:GLN:HA	1:IC:254:THR:HG21	1.85	0.58
3:J:42:ARG:HG2	3:J:116:LEU:HD13	1.85	0.58
2:DB:191:LYS:HG3	2:DB:222:VAL:HG23	1.86	0.58
1:SB:225:VAL:HG11	1:SB:258:MET:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:199:ILE:HD12	1:W:200:ASP:HB3	1.85	0.58
1:X:191:LYS:HG3	1:X:222:VAL:HG23	1.83	0.58
5:CD:158:LEU:HB3	5:CD:271:ARG:HH22	1.69	0.58
1:BC:233:GLY:HA2	3:I:68:MET:HE1	1.84	0.58
1:GC:151:GLN:NE2	1:GC:167:MET:SD	2.76	0.58
1:K:254:THR:HG21	1:PB:217:GLN:HA	1.85	0.58
3:C:48:ILE:HD11	3:C:81:ILE:HG12	1.86	0.58
1:P:153:LEU:HD21	1:P:160:ILE:HD11	1.84	0.58
1:U:194:SER:HA	1:U:225:VAL:HB	1.85	0.58
3:b:42:ARG:HD2	3:b:116:LEU:HD11	1.84	0.58
3:C:65:VAL:HA	3:C:68:MET:HB2	1.86	0.58
4:AD:170:ILE:HD13	4:AD:204:VAL:HG21	1.84	0.58
2:E:151:GLN:NE2	2:E:167:MET:SD	2.76	0.58
1:KB:152:GLU:OE1	1:KB:154:SER:OG	2.22	0.58
1:OB:152:GLU:HG2	1:OB:162:GLU:HA	1.85	0.58
1:P:201:ILE:HG23	1:P:204:VAL:HB	1.86	0.58
1:PB:211:VAL:HA	1:PB:214:HIS:HB2	1.86	0.58
1:Q:190:VAL:HG11	1:Q:265:ALA:HB1	1.84	0.58
1:FA:193:ARG:NH2	1:FA:208:ASP:OD1	2.37	0.57
3:j:25:ALA:HA	3:j:28:PHE:HB3	1.86	0.57
2:E:193:ARG:NH2	2:E:208:ASP:OD1	2.37	0.57
1:UB:230:MET:SD	1:UB:230:MET:N	2.74	0.57
1:KB:156:PRO:HD3	1:KB:161:PHE:HD1	1.69	0.57
1:PB:191:LYS:HG3	1:PB:222:VAL:HG23	1.86	0.57
1:T:254:THR:HG21	1:V:217:GLN:HA	1.86	0.57
1:TB:204:VAL:HG23	1:TB:207:VAL:HB	1.86	0.57
1:V:156:PRO:HD2	1:V:160:ILE:HA	1.86	0.57
3:f:90:ILE:HG22	3:f:94:ILE:HD13	1.87	0.57
2:CB:157:LEU:HB2	2:DB:259:LYS:HD2	1.86	0.57
1:Q:191:LYS:HB3	1:Q:222:VAL:HG12	1.86	0.57
1:VB:153:LEU:HD11	1:VB:160:ILE:HD11	1.86	0.57
1:EB:231:LEU:O	1:EB:235:ARG:NH1	2.38	0.57
2:E:217:GLN:HA	1:VB:254:THR:HG21	1.87	0.56
2:DB:179:LYS:HD2	2:DB:191:LYS:HE3	1.87	0.56
5:FD:259:LYS:HD2	5:HD:158:LEU:HD23	1.88	0.56
1:Z:162:GLU:O	1:Z:194:SER:OG	2.23	0.56
5:CD:193:ARG:NH2	5:CD:208:ASP:OD1	2.38	0.56
1:P:161:PHE:HB3	1:P:192:ASN:HD22	1.70	0.56
1:Z:187:ILE:HG23	3:i:103:MET:HG2	1.88	0.56
2:CB:163:LYS:NZ	2:CB:165:SER:OG	2.38	0.56
2:CB:193:ARG:NH2	2:CB:208:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:237:GLU:O	1:P:251:GLN:NE2	2.39	0.56
1:FB:254:THR:HG21	2:IB:217:GLN:HA	1.86	0.55
1:K:163:LYS:NZ	1:K:258:MET:SD	2.79	0.55
1:VB:193:ARG:HG3	1:VB:224:LEU:HD23	1.89	0.55
1:W:216:ILE:HG12	1:W:221:ALA:HA	1.89	0.55
3:A:79:THR:HG22	3:A:102:ALA:HB3	1.87	0.55
1:IC:196:VAL:O	1:IC:228:GLN:NE2	2.40	0.55
1:PB:233:GLY:HA2	1:SB:214:HIS:HE1	1.71	0.55
3:A:42:ARG:HB3	3:A:116:LEU:HD22	1.88	0.55
3:O:55:ASP:H	3:O:58:ILE:HD12	1.72	0.55
1:FA:214:HIS:HE1	3:g:87:ILE:HA	1.70	0.55
1:EB:179:LYS:HD2	1:EB:191:LYS:HE3	1.88	0.55
1:M:214:HIS:HD2	3:d:90:ILE:HD12	1.72	0.55
3:B:66:VAL:HG12	3:B:70:LYS:HE2	1.88	0.55
1:P:152:GLU:HB3	1:Q:152:GLU:HG2	1.88	0.55
3:e:29:GLN:NE2	3:e:68:MET:SD	2.80	0.55
1:AB:164:ILE:HG22	1:AB:198:LEU:HD11	1.88	0.55
1:M:255:THR:HG21	1:M:261:GLY:HA2	1.89	0.55
1:OB:156:PRO:HG2	1:OB:159:PRO:HG2	1.89	0.55
3:D:22:ASP:N	3:D:22:ASP:OD1	2.40	0.55
1:PB:191:LYS:NZ	1:PB:192:ASN:O	2.40	0.55
2:F:191:LYS:HG3	2:F:222:VAL:HG23	1.87	0.54
1:FC:205:PRO:O	1:FC:209:THR:N	2.37	0.54
3:d:75:LYS:HE2	3:d:116:LEU:HD22	1.88	0.54
1:FB:193:ARG:NH2	1:FB:208:ASP:OD1	2.38	0.54
3:N:8:LEU:HB2	3:N:13:LEU:HD13	1.90	0.54
1:FB:214:HIS:HE2	3:J:90:ILE:HB	1.72	0.54
1:P:229:ALA:HB2	4:AD:184:ASN:HD21	1.72	0.54
1:W:223:ARG:NH1	1:W:261:GLY:O	2.40	0.54
3:j:36:ILE:HG13	3:j:41:ALA:HB3	1.90	0.54
1:X:157:LEU:HD12	1:Y:259:LYS:HD3	1.88	0.54
5:FD:201:ILE:HG22	5:FD:231:LEU:HD11	1.89	0.54
1:FA:191:LYS:HG3	1:FA:222:VAL:HG23	1.90	0.54
1:PB:193:ARG:HB2	1:PB:224:LEU:HA	1.90	0.54
1:V:191:LYS:NZ	1:V:192:ASN:O	2.41	0.54
3:c:22:ASP:HB3	3:c:58:ILE:HG12	1.89	0.54
3:d:44:VAL:HB	3:d:76:VAL:HG23	1.89	0.54
3:j:29:GLN:NE2	3:j:68:MET:SD	2.81	0.54
5:CD:192:ASN:HD21	5:CD:223:ARG:HH21	1.54	0.54
2:GB:179:LYS:HE3	2:GB:215:ILE:HD11	1.89	0.54
1:HC:199:ILE:HD11	1:HC:228:GLN:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:211:VAL:HA	2:F:214:HIS:HB2	1.89	0.53
1:TB:193:ARG:NH2	1:TB:208:ASP:OD1	2.41	0.53
3:j:15:SER:HA	3:j:47:ASP:HB3	1.90	0.53
1:W:223:ARG:HH12	1:W:264:ARG:HG3	1.72	0.53
3:O:65:VAL:HA	3:O:68:MET:HB2	1.90	0.53
3:d:104:ASP:OD1	3:d:104:ASP:N	2.41	0.53
1:BC:195:GLU:HB2	1:BC:198:LEU:HD22	1.91	0.53
1:VB:201:ILE:HD11	1:VB:235:ARG:HH22	1.73	0.53
1:X:200:ASP:OD1	1:X:200:ASP:N	2.39	0.53
2:DB:234:ILE:O	2:DB:235:ARG:NE	2.40	0.53
2:GB:153:LEU:HD22	2:GB:182:ILE:HG21	1.90	0.53
1:T:215:ILE:HA	1:T:218:ALA:HB3	1.91	0.53
1:UB:161:PHE:HB3	1:UB:192:ASN:HD22	1.73	0.53
3:B:5:ILE:HD11	3:B:12:LEU:HD21	1.91	0.53
5:HD:191:LYS:O	5:HD:223:ARG:N	2.41	0.53
1:L:159:PRO:HB3	1:L:190:VAL:HB	1.89	0.53
1:UB:188:GLY:H	3:a:103:MET:HE1	1.74	0.53
1:Z:206:VAL:O	1:Z:210:MET:N	2.41	0.53
3:R:79:THR:HG22	3:R:102:ALA:HB3	1.90	0.53
3:h:8:LEU:HD11	3:i:109:LEU:HD22	1.91	0.53
3:b:94:ILE:HG23	3:b:96:PHE:HD2	1.74	0.53
1:DC:217:GLN:HA	1:Z:254:THR:HG21	1.91	0.53
1:X:275:GLU:OE2	1:Y:270:ASN:ND2	2.42	0.53
3:B:15:SER:HB2	3:j:6:LEU:HD21	1.90	0.53
3:j:104:ASP:OD1	3:j:104:ASP:N	2.42	0.53
5:FD:234:ILE:O	5:FD:235:ARG:NE	2.42	0.53
3:a:42:ARG:HD2	3:a:116:LEU:HD12	1.91	0.53
3:d:8:LEU:HD22	3:d:13:LEU:HD11	1.91	0.53
4:AD:200:ASP:OD1	4:AD:200:ASP:N	2.42	0.53
5:FD:215:ILE:HG22	5:FD:219:SER:HB3	1.90	0.53
5:HD:159:PRO:HA	5:HD:189:VAL:HG23	1.91	0.53
5:HD:219:SER:O	5:HD:221:ALA:N	2.41	0.53
1:EB:150:LEU:O	1:EB:151:GLN:NE2	2.42	0.53
2:E:181:ILE:HD11	1:VB:230:MET:HE2	1.91	0.52
3:B:54:ILE:HG23	3:B:58:ILE:HB	1.92	0.52
3:N:12:LEU:HB2	3:N:44:VAL:HG22	1.89	0.52
3:O:79:THR:HG22	3:O:102:ALA:HB3	1.91	0.52
4:AD:234:ILE:O	4:AD:235:ARG:NE	2.42	0.52
1:L:161:PHE:HB2	1:L:192:ASN:HB2	1.91	0.52
3:i:48:ILE:HD11	3:i:81:ILE:HG12	1.91	0.52
1:BC:156:PRO:HD3	1:BC:161:PHE:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:65:VAL:HA	3:N:68:MET:HB2	1.91	0.52
1:DC:200:ASP:OD1	1:DC:200:ASP:N	2.43	0.52
2:E:199:ILE:HG21	2:E:230:MET:HE3	1.91	0.52
5:CD:215:ILE:HD13	5:CD:222:VAL:HG11	1.90	0.52
1:M:179:LYS:HE3	1:M:193:ARG:HH12	1.75	0.52
1:SB:235:ARG:NH1	1:SB:237:GLU:OE2	2.43	0.52
1:V:165:SER:OG	1:V:166:VAL:N	2.40	0.52
1:X:157:LEU:HB2	1:Y:259:LYS:HB2	1.92	0.52
1:UB:234:ILE:O	1:UB:235:ARG:NE	2.40	0.52
1:TB:179:LYS:HD2	1:TB:191:LYS:HD2	1.91	0.52
1:BC:260:LYS:HD3	3:I:42:ARG:HH21	1.74	0.52
1:FB:234:ILE:O	1:FB:235:ARG:NE	2.43	0.52
1:Z:191:LYS:HG3	1:Z:222:VAL:HG23	1.91	0.52
3:B:12:LEU:HB3	3:B:44:VAL:HG12	1.92	0.52
3:f:94:ILE:HD12	3:f:96:PHE:HB2	1.91	0.52
3:j:8:LEU:HD22	3:j:13:LEU:HD11	1.92	0.52
1:EB:200:ASP:OD1	1:EB:200:ASP:N	2.43	0.51
1:FB:166:VAL:HG22	1:FB:198:LEU:HA	1.92	0.51
1:GC:191:LYS:HG3	1:GC:222:VAL:HG23	1.90	0.51
1:M:200:ASP:OD1	1:M:200:ASP:N	2.43	0.51
3:f:7:LYS:HD2	3:f:39:THR:HG21	1.92	0.51
1:EB:191:LYS:NZ	1:EB:192:ASN:O	2.43	0.51
2:F:173:ILE:O	2:F:177:ARG:NH1	2.43	0.51
3:B:13:LEU:HD21	3:B:109:LEU:HD21	1.93	0.51
3:C:79:THR:HG22	3:C:102:ALA:HB3	1.91	0.51
2:CB:174:ASP:OD1	2:CB:174:ASP:N	2.43	0.51
2:DB:256:ASN:HB3	2:DB:260:LYS:HD2	1.91	0.51
1:K:194:SER:HA	1:K:225:VAL:HB	1.92	0.51
1:L:152:GLU:HG2	1:L:163:LYS:HB3	1.91	0.51
3:A:9:GLY:H	3:C:106:GLU:HG2	1.76	0.51
3:R:21:ASP:N	3:R:21:ASP:OD1	2.43	0.51
5:CD:223:ARG:HG3	5:CD:253:ILE:HB	1.92	0.51
1:KB:205:PRO:HA	1:KB:208:ASP:HB3	1.92	0.51
1:T:193:ARG:HG3	1:T:224:LEU:HD12	1.92	0.51
1:V:169:LEU:HG	1:V:171:GLY:H	1.75	0.51
1:DC:166:VAL:HG22	1:DC:198:LEU:HA	1.92	0.51
1:M:174:ASP:HA	1:M:177:ARG:HB3	1.91	0.51
1:OB:154:SER:HB2	1:OB:160:ILE:HG23	1.93	0.51
1:P:190:VAL:HG11	1:P:265:ALA:HB1	1.92	0.51
1:UB:254:THR:OG1	1:UB:255:THR:N	2.44	0.51
1:Z:219:SER:OG	1:Z:220:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:42:ARG:HH11	3:b:116:LEU:HD11	1.76	0.51
1:FB:191:LYS:HD3	1:FB:215:ILE:HG13	1.92	0.51
1:FB:206:VAL:HA	1:FB:209:THR:HG22	1.93	0.51
1:V:180:LEU:HD21	1:V:214:HIS:HB3	1.93	0.51
3:O:25:ALA:HB1	3:O:61:ILE:HG21	1.92	0.51
1:W:253:ILE:HD12	1:W:264:ARG:HH12	1.76	0.51
1:Y:165:SER:OG	1:Y:166:VAL:N	2.43	0.51
1:FC:156:PRO:HG2	1:FC:160:ILE:HA	1.93	0.51
1:VB:210:MET:HE3	1:Y:235:ARG:HB2	1.93	0.51
3:R:72:MET:O	5:CD:256:ASN:ND2	2.44	0.51
3:e:43:GLY:HA3	3:e:112:LEU:HD21	1.93	0.51
5:HD:234:ILE:O	5:HD:235:ARG:NE	2.41	0.51
1:P:162:GLU:OE1	1:P:193:ARG:NH1	2.44	0.51
3:g:54:ILE:HB	3:g:85:VAL:HG23	1.93	0.51
2:E:194:SER:HA	2:E:225:VAL:HB	1.93	0.51
3:J:16:ILE:HD12	3:J:48:ILE:HG22	1.93	0.51
3:f:68:MET:HE1	5:HD:233:GLY:HA2	1.92	0.51
3:S:6:LEU:HD23	3:S:13:LEU:HD12	1.93	0.50
1:HC:219:SER:OG	1:HC:220:GLU:N	2.44	0.50
1:IC:191:LYS:HZ2	1:IC:193:ARG:HD3	1.76	0.50
1:IC:217:GLN:HA	1:SB:254:THR:HG21	1.92	0.50
1:K:228:GLN:HB2	1:K:231:LEU:HB2	1.93	0.50
1:TB:194:SER:HA	1:TB:225:VAL:HB	1.94	0.50
3:C:66:VAL:HA	3:C:76:VAL:HG11	1.92	0.50
1:UB:148:SER:OG	1:UB:149:ALA:N	2.43	0.50
3:N:22:ASP:OD1	3:N:22:ASP:N	2.44	0.50
3:i:65:VAL:HA	3:i:68:MET:HB2	1.94	0.50
1:BC:189:VAL:HG12	1:BC:190:VAL:HG13	1.94	0.50
3:f:104:ASP:N	3:f:104:ASP:OD1	2.43	0.50
1:VB:219:SER:OG	1:VB:220:GLU:N	2.44	0.50
3:B:48:ILE:HD11	3:B:81:ILE:HG12	1.94	0.50
5:CD:174:ASP:HA	5:CD:177:ARG:HG3	1.92	0.50
1:OB:193:ARG:HB2	1:OB:224:LEU:HA	1.94	0.50
2:IB:193:ARG:HH12	2:IB:208:ASP:HA	1.77	0.50
1:FC:182:ILE:HG13	1:FC:185:LEU:HD22	1.94	0.50
1:GC:219:SER:OG	1:GC:220:GLU:N	2.40	0.50
1:IC:200:ASP:OD1	1:IC:200:ASP:N	2.44	0.50
3:f:29:GLN:NE2	3:f:64:ASP:OD2	2.44	0.50
1:EB:202:THR:OG1	1:EB:203:GLY:N	2.45	0.50
1:FA:210:MET:HB3	3:g:90:ILE:HD12	1.93	0.50
3:O:8:LEU:HD12	3:R:105:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:HD:219:SER:OG	5:HD:221:ALA:N	2.41	0.50
2:CB:213:HIS:HE2	1:EB:251:GLN:HG3	1.76	0.49
2:DB:190:VAL:HG12	2:DB:221:ALA:HB3	1.94	0.49
1:GC:223:ARG:HH21	1:GC:265:ALA:HA	1.77	0.49
1:K:219:SER:OG	1:K:220:GLU:N	2.44	0.49
2:E:266:LEU:HB3	2:E:271:ARG:HB2	1.94	0.49
1:X:228:GLN:HB2	1:X:231:LEU:HB2	1.93	0.49
3:A:96:PHE:HD1	3:A:99:VAL:HG21	1.77	0.49
3:S:3:ILE:HG12	3:S:28:PHE:HD1	1.77	0.49
3:g:104:ASP:OD1	3:g:104:ASP:N	2.45	0.49
1:X:164:ILE:HD11	1:X:193:ARG:HH21	1.76	0.49
1:LB:234:ILE:O	1:LB:235:ARG:NE	2.46	0.49
1:W:206:VAL:HA	1:W:209:THR:HG22	1.93	0.49
3:C:82:GLN:HB2	3:C:85:VAL:HG12	1.95	0.49
3:J:22:ASP:HB3	3:J:58:ILE:HG12	1.93	0.49
3:b:22:ASP:N	3:b:22:ASP:OD1	2.42	0.49
3:e:104:ASP:OD1	3:e:104:ASP:N	2.44	0.49
3:I:90:ILE:HA	3:I:94:ILE:HD11	1.93	0.49
1:GC:172:THR:HG23	1:GC:207:VAL:HG21	1.94	0.49
1:M:178:ALA:HA	1:M:181:ILE:HD12	1.93	0.49
4:AD:153:LEU:HD21	4:AD:182:ILE:HB	1.93	0.49
1:HC:228:GLN:H	1:HC:231:LEU:HD23	1.78	0.49
2:IB:214:HIS:O	2:IB:218:ALA:N	2.45	0.49
5:CD:176:GLU:HA	5:CD:179:LYS:HE3	1.94	0.49
3:C:64:ASP:O	3:C:68:MET:N	2.41	0.49
3:J:79:THR:HG22	3:J:102:ALA:HB3	1.93	0.49
5:HD:153:LEU:HG	5:HD:182:ILE:HG21	1.95	0.49
2:DB:219:SER:OG	2:DB:220:GLU:N	2.45	0.49
2:GB:234:ILE:O	2:GB:235:ARG:NE	2.46	0.49
1:SB:156:PRO:HD3	1:SB:161:PHE:HD2	1.77	0.49
1:VB:173:ILE:O	1:VB:177:ARG:NH1	2.46	0.49
3:f:48:ILE:HD11	3:f:81:ILE:HG12	1.94	0.49
1:DC:152:GLU:HG3	1:DC:163:LYS:HB3	1.94	0.48
1:FA:200:ASP:N	1:FA:200:ASP:OD1	2.46	0.48
2:IB:193:ARG:NH2	2:IB:208:ASP:OD1	2.44	0.48
3:d:48:ILE:HD11	3:d:81:ILE:HG12	1.94	0.48
2:F:191:LYS:NZ	2:F:192:ASN:O	2.45	0.48
1:M:152:GLU:OE2	1:M:154:SER:OG	2.27	0.48
1:W:227:CYS:HB3	1:W:231:LEU:HD23	1.94	0.48
3:O:48:ILE:HD11	3:O:81:ILE:HG12	1.95	0.48
2:F:156:PRO:HD2	2:F:160:ILE:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:266:LEU:HD22	1:FB:271:ARG:HH21	1.78	0.48
1:L:257:THR:O	1:L:261:GLY:N	2.45	0.48
1:P:160:ILE:HG23	1:P:191:LYS:HE2	1.95	0.48
1:Q:189:VAL:HG12	1:Q:219:SER:HB2	1.94	0.48
1:Q:264:ARG:NH2	5:HD:220:GLU:O	2.46	0.48
3:c:48:ILE:HD11	3:c:81:ILE:HG12	1.95	0.48
2:E:153:LEU:HD11	2:E:182:ILE:HG21	1.95	0.48
1:OB:194:SER:O	1:OB:194:SER:OG	2.31	0.48
1:UB:227:CYS:HB3	1:UB:231:LEU:HD22	1.95	0.48
3:e:50:SER:O	3:e:50:SER:OG	2.30	0.48
4:AD:152:GLU:HG3	5:CD:163:LYS:HG2	1.94	0.48
2:IB:200:ASP:OD1	2:IB:200:ASP:N	2.46	0.48
1:V:169:LEU:HD23	1:V:172:THR:HG23	1.95	0.48
1:Y:167:MET:HB3	1:Y:172:THR:HG21	1.95	0.48
3:S:10:GLU:OE1	3:S:42:ARG:NH1	2.47	0.48
3:e:55:ASP:H	3:e:58:ILE:HD12	1.78	0.48
1:L:200:ASP:OD1	1:L:200:ASP:N	2.46	0.48
1:V:219:SER:OG	1:V:220:GLU:N	2.46	0.48
3:a:109:LEU:HA	3:a:112:LEU:HB2	1.95	0.48
2:CB:227:CYS:HB3	2:CB:231:LEU:HD23	1.94	0.48
1:GC:193:ARG:NH2	1:GC:208:ASP:OD1	2.44	0.48
1:IC:165:SER:HA	1:IC:197:VAL:HG13	1.96	0.48
1:IC:223:ARG:HH22	1:IC:265:ALA:HA	1.79	0.48
1:K:234:ILE:O	1:K:235:ARG:NE	2.46	0.48
5:CD:165:SER:OG	5:CD:166:VAL:N	2.45	0.48
5:CD:200:ASP:OD1	5:CD:200:ASP:N	2.46	0.48
2:CB:234:ILE:O	2:CB:235:ARG:NE	2.44	0.48
1:X:204:VAL:HG23	1:X:207:VAL:HB	1.95	0.48
3:J:49:THR:O	3:J:82:GLN:NE2	2.47	0.48
3:R:60:LYS:NZ	3:R:64:ASP:OD2	2.41	0.48
1:AB:156:PRO:HD2	1:AB:160:ILE:HA	1.95	0.48
1:P:224:LEU:HD13	1:P:252:ILE:HD12	1.94	0.48
1:Y:155:ALA:HA	1:Y:160:ILE:HG13	1.95	0.48
2:IB:161:PHE:HB2	2:IB:192:ASN:HB2	1.96	0.48
3:C:104:ASP:OD1	3:C:104:ASP:N	2.45	0.48
3:e:48:ILE:HD11	3:e:81:ILE:HG12	1.96	0.48
1:LB:189:VAL:HG12	1:LB:190:VAL:HG23	1.96	0.47
1:X:232:VAL:HG11	3:d:71:LEU:HD22	1.95	0.47
1:GC:194:SER:HA	1:GC:225:VAL:HB	1.95	0.47
1:L:254:THR:OG1	1:L:255:THR:N	2.47	0.47
1:SB:153:LEU:HD11	1:SB:179:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:196:VAL:O	1:W:228:GLN:NE2	2.47	0.47
2:DB:156:PRO:HD2	2:DB:160:ILE:HG23	1.96	0.47
2:E:191:LYS:NZ	2:E:192:ASN:O	2.40	0.47
1:GC:191:LYS:HD3	1:GC:215:ILE:HD13	1.96	0.47
1:T:255:THR:OG1	1:T:256:ASN:N	2.45	0.47
1:VB:173:ILE:HG12	1:VB:177:ARG:HH12	1.79	0.47
3:B:43:GLY:HA2	3:B:75:LYS:H	1.78	0.47
2:DB:230:MET:SD	2:DB:230:MET:N	2.86	0.47
2:E:214:HIS:O	2:E:218:ALA:N	2.47	0.47
1:FC:193:ARG:HG3	1:FC:224:LEU:HD12	1.95	0.47
1:Q:194:SER:HA	1:Q:225:VAL:HB	1.95	0.47
3:c:25:ALA:HA	3:c:28:PHE:HB3	1.96	0.47
1:DC:217:GLN:HE22	1:Z:235:ARG:HD2	1.80	0.47
1:EB:254:THR:OG1	1:EB:255:THR:N	2.48	0.47
1:EB:259:LYS:HD2	1:FB:157:LEU:HG	1.96	0.47
1:FC:232:VAL:HG23	3:i:71:LEU:HD22	1.95	0.47
1:OB:233:GLY:HA2	3:e:68:MET:HE3	1.96	0.47
1:UB:153:LEU:HD23	1:UB:182:ILE:HD12	1.95	0.47
1:EB:161:PHE:HB2	1:EB:192:ASN:HB2	1.97	0.47
2:GB:214:HIS:O	2:GB:218:ALA:N	2.45	0.47
1:GC:206:VAL:HA	1:GC:210:MET:HB3	1.95	0.47
1:HC:151:GLN:HG2	1:HC:175:THR:HB	1.96	0.47
1:T:211:VAL:HA	1:T:214:HIS:HB2	1.97	0.47
1:T:234:ILE:O	1:T:235:ARG:NE	2.47	0.47
3:d:16:ILE:O	3:d:50:SER:OG	2.33	0.47
5:CD:194:SER:HA	5:CD:225:VAL:HB	1.96	0.47
2:E:179:LYS:HG3	2:E:191:LYS:HE3	1.97	0.47
1:K:205:PRO:O	1:K:209:THR:N	2.47	0.47
1:KB:158:LEU:HG	1:KB:271:ARG:HH12	1.79	0.47
1:KB:158:LEU:HB3	1:KB:271:ARG:HH22	1.80	0.47
1:KB:184:ASN:HD21	3:e:83:PRO:HD3	1.79	0.47
1:L:191:LYS:HD2	1:L:215:ILE:HG21	1.95	0.47
1:SB:273:ILE:HG23	1:TB:273:ILE:HB	1.95	0.47
3:J:6:LEU:HD11	3:J:35:LYS:HG2	1.97	0.47
3:a:104:ASP:N	3:a:104:ASP:OD1	2.44	0.47
3:g:72:MET:HE1	4:AD:229:ALA:HA	1.97	0.47
5:HD:200:ASP:OD1	5:HD:200:ASP:N	2.46	0.47
2:E:219:SER:OG	2:E:220:GLU:N	2.48	0.47
1:IC:160:ILE:HD11	1:IC:186:LEU:HD11	1.96	0.47
1:SB:167:MET:SD	1:SB:172:THR:OG1	2.72	0.47
1:Z:215:ILE:HA	1:Z:218:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:48:ILE:HD11	3:S:81:ILE:HG12	1.97	0.47
3:f:43:GLY:HA3	3:f:112:LEU:HD21	1.95	0.47
5:FD:199:ILE:HG13	5:FD:200:ASP:HB3	1.96	0.47
1:Q:199:ILE:HG12	1:Q:230:MET:HE3	1.95	0.47
1:T:219:SER:OG	1:T:220:GLU:N	2.47	0.47
1:Y:255:THR:OG1	1:Y:256:ASN:N	2.47	0.47
3:a:54:ILE:HD12	3:a:85:VAL:HG21	1.96	0.47
5:CD:201:ILE:HD11	5:CD:204:VAL:HG23	1.97	0.47
2:CB:217:GLN:HA	1:EB:254:THR:HG21	1.97	0.47
1:SB:234:ILE:O	1:SB:235:ARG:NE	2.48	0.47
1:Z:148:SER:OG	1:Z:149:ALA:N	2.43	0.47
3:J:25:ALA:HA	3:J:28:PHE:HB3	1.96	0.47
3:N:48:ILE:HD11	3:N:81:ILE:HG12	1.96	0.47
3:f:58:ILE:HA	3:f:61:ILE:HD12	1.96	0.47
3:j:14:ILE:HG23	3:j:46:ILE:HA	1.97	0.47
1:HC:165:SER:OG	1:HC:166:VAL:N	2.45	0.46
1:HC:179:LYS:HD3	1:HC:211:VAL:HG21	1.97	0.46
1:IC:232:VAL:HA	1:IC:235:ARG:HD2	1.96	0.46
1:KB:219:SER:OG	1:KB:220:GLU:N	2.48	0.46
1:OB:154:SER:OG	1:OB:161:PHE:O	2.27	0.46
1:P:271:ARG:NH1	1:Q:275:GLU:O	2.48	0.46
1:SB:266:LEU:HD13	1:SB:273:ILE:HG21	1.97	0.46
1:U:234:ILE:HG13	1:U:236:PRO:HD3	1.96	0.46
5:FD:160:ILE:HG12	5:FD:186:LEU:HD11	1.97	0.46
2:CB:156:PRO:HD2	2:CB:160:ILE:HA	1.97	0.46
1:HC:167:MET:HB2	1:HC:172:THR:HG21	1.96	0.46
1:OB:234:ILE:O	1:OB:235:ARG:NE	2.46	0.46
1:P:157:LEU:HG	1:P:159:PRO:HD2	1.97	0.46
1:W:153:LEU:HD11	1:W:160:ILE:HD11	1.97	0.46
3:a:55:ASP:H	3:a:58:ILE:HD12	1.80	0.46
4:AD:159:PRO:HA	4:AD:190:VAL:HG23	1.98	0.46
1:IC:266:LEU:HD13	1:IC:273:ILE:HA	1.98	0.46
1:Q:182:ILE:HD12	1:Q:185:LEU:HD12	1.96	0.46
3:C:86:ALA:HA	3:C:89:LEU:HB2	1.97	0.46
5:FD:193:ARG:NH1	5:FD:208:ASP:OD1	2.48	0.46
5:FD:205:PRO:HB2	5:FD:209:THR:HG22	1.97	0.46
1:AB:219:SER:OG	1:AB:220:GLU:N	2.48	0.46
1:BC:174:ASP:OD1	1:BC:177:ARG:NH1	2.48	0.46
1:DC:194:SER:HA	1:DC:225:VAL:HB	1.97	0.46
1:PB:154:SER:OG	1:PB:155:ALA:N	2.47	0.46
1:TB:217:GLN:HE22	3:h:89:LEU:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:191:LYS:HZ2	1:U:222:VAL:HG23	1.81	0.46
1:V:157:LEU:HD12	1:W:259:LYS:HE2	1.98	0.46
1:W:158:LEU:HB3	1:W:271:ARG:HH22	1.81	0.46
1:Z:205:PRO:O	1:Z:209:THR:OG1	2.31	0.46
5:CD:234:ILE:O	5:CD:235:ARG:NE	2.47	0.46
5:FD:260:LYS:HE3	5:FD:260:LYS:HB2	1.75	0.46
1:SB:199:ILE:HA	1:SB:200:ASP:HA	1.68	0.46
1:DC:159:PRO:HB3	1:DC:190:VAL:HB	1.96	0.46
1:DC:254:THR:OG1	1:DC:255:THR:N	2.48	0.46
1:T:161:PHE:HB2	1:T:192:ASN:HB2	1.98	0.46
3:A:55:ASP:H	3:A:58:ILE:HD12	1.80	0.46
4:AD:205:PRO:O	4:AD:209:THR:N	2.47	0.46
1:FA:205:PRO:O	1:FA:209:THR:N	2.42	0.46
1:KB:202:THR:OG1	1:KB:203:GLY:N	2.48	0.46
1:L:180:LEU:HB3	3:A:83:PRO:HB2	1.96	0.46
1:U:163:LYS:NZ	1:U:194:SER:O	2.49	0.46
1:U:225:VAL:HG11	1:U:258:MET:HG2	1.98	0.46
1:V:200:ASP:OD1	1:V:200:ASP:N	2.45	0.46
3:a:12:LEU:HD22	3:a:44:VAL:HG13	1.97	0.46
3:c:13:LEU:HD11	3:c:105:LEU:HD11	1.97	0.46
1:FA:156:PRO:HD2	1:FA:161:PHE:H	1.81	0.46
1:LB:200:ASP:OD1	1:LB:200:ASP:N	2.48	0.46
1:M:162:GLU:O	1:M:194:SER:OG	2.30	0.46
3:b:92:LEU:HD23	3:b:96:PHE:HZ	1.80	0.46
1:HC:194:SER:H	1:HC:225:VAL:HB	1.81	0.46
1:TB:198:LEU:HD21	1:TB:201:ILE:HG12	1.97	0.46
1:V:273:ILE:HD11	1:W:271:ARG:HB3	1.98	0.46
3:C:6:LEU:HD13	3:C:12:LEU:HD21	1.97	0.46
3:b:104:ASP:OD1	3:b:104:ASP:N	2.49	0.46
1:FA:179:LYS:HD2	1:FA:191:LYS:HZ1	1.81	0.46
1:GC:225:VAL:HG11	1:GC:258:MET:HG2	1.97	0.46
1:K:214:HIS:O	1:K:218:ALA:N	2.46	0.46
1:LB:219:SER:OG	1:LB:220:GLU:N	2.49	0.46
1:P:255:THR:OG1	1:P:256:ASN:N	2.49	0.46
1:FA:259:LYS:HD3	1:K:157:LEU:HD22	1.97	0.45
1:Y:153:LEU:HD21	1:Y:182:ILE:HD12	1.98	0.45
1:Y:179:LYS:HB3	1:Y:179:LYS:HE2	1.80	0.45
3:B:49:THR:O	3:B:82:GLN:NE2	2.41	0.45
5:CD:199:ILE:HD12	5:CD:200:ASP:HB3	1.98	0.45
2:CB:177:ARG:O	2:CB:181:ILE:N	2.48	0.45
2:F:173:ILE:HG23	2:F:177:ARG:HH22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:202:THR:OG1	2:F:203:GLY:N	2.49	0.45
1:FA:180:LEU:HD21	1:FA:214:HIS:HB3	1.98	0.45
1:M:156:PRO:HG2	1:M:159:PRO:HD2	1.97	0.45
1:OB:158:LEU:HB2	1:OB:271:ARG:HH22	1.81	0.45
3:B:92:LEU:HD22	3:B:94:ILE:HD13	1.98	0.45
1:FB:235:ARG:HD2	2:IB:217:GLN:HE22	1.81	0.45
1:L:212:ALA:HB1	1:L:222:VAL:HG11	1.98	0.45
1:U:254:THR:OG1	3:c:71:LEU:O	2.34	0.45
3:I:69:SER:OG	3:I:74:ALA:O	2.35	0.45
3:J:40:SER:O	3:J:40:SER:OG	2.34	0.45
5:HD:146:GLN:NE2	5:HD:149:ALA:O	2.49	0.45
1:TB:158:LEU:HD13	1:TB:271:ARG:HH12	1.82	0.45
1:U:191:LYS:HE2	1:U:191:LYS:HB2	1.87	0.45
3:S:68:MET:HE3	3:S:68:MET:HB3	1.76	0.45
2:E:191:LYS:HG3	2:E:222:VAL:HG23	1.98	0.45
2:GB:159:PRO:HB3	2:GB:190:VAL:HB	1.98	0.45
1:U:220:GLU:HG3	1:U:221:ALA:H	1.81	0.45
1:V:194:SER:HA	1:V:225:VAL:HB	1.98	0.45
3:O:64:ASP:O	3:O:68:MET:N	2.44	0.45
3:S:104:ASP:OD1	3:S:104:ASP:N	2.48	0.45
2:DB:152:GLU:HG2	2:DB:162:GLU:HG2	1.99	0.45
1:FB:200:ASP:OD1	1:FB:200:ASP:N	2.49	0.45
1:K:255:THR:OG1	1:K:256:ASN:N	2.50	0.45
1:P:235:ARG:H	4:AD:214:HIS:CE1	2.35	0.45
3:j:77:VAL:HG12	3:j:100:LEU:HB2	1.98	0.45
1:AB:174:ASP:OD1	1:AB:177:ARG:NH1	2.50	0.45
1:BC:202:THR:O	1:BC:204:VAL:N	2.50	0.45
1:EB:158:LEU:HB3	1:EB:271:ARG:HH12	1.82	0.45
1:EB:271:ARG:HB3	1:FB:273:ILE:HD11	1.98	0.45
1:FA:199:ILE:HA	1:FA:200:ASP:HA	1.69	0.45
1:FC:179:LYS:HE2	1:FC:179:LYS:HB3	1.69	0.45
1:L:201:ILE:HD12	1:L:204:VAL:HG13	1.98	0.45
1:P:219:SER:OG	1:P:220:GLU:N	2.50	0.45
1:UB:214:HIS:O	1:UB:218:ALA:N	2.47	0.45
3:O:25:ALA:HA	3:O:28:PHE:HB3	1.97	0.45
3:R:5:ILE:HD11	3:R:12:LEU:HB3	1.99	0.45
3:j:46:ILE:O	3:j:79:THR:OG1	2.32	0.45
1:DC:184:ASN:ND2	1:Z:228:GLN:OE1	2.49	0.45
1:FC:184:ASN:HA	3:C:103:MET:HE3	1.99	0.45
2:IB:219:SER:OG	2:IB:220:GLU:N	2.49	0.45
1:VB:159:PRO:HB3	1:VB:190:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:VB:199:ILE:HA	1:VB:200:ASP:HA	1.67	0.45
3:J:13:LEU:HD23	3:J:105:LEU:HD21	1.98	0.45
3:J:33:LEU:HB3	3:J:72:MET:HE1	1.98	0.45
3:a:18:SER:HA	3:a:51:ILE:HD13	1.99	0.45
5:CD:257:THR:OG1	5:CD:258:MET:N	2.50	0.45
2:CB:254:THR:OG1	2:CB:255:THR:N	2.49	0.45
2:E:161:PHE:HB2	2:E:192:ASN:HB2	1.98	0.45
1:EB:170:ILE:HD12	1:EB:204:VAL:HG11	1.98	0.45
3:N:55:ASP:H	3:N:58:ILE:HD12	1.81	0.45
3:S:42:ARG:HG3	3:S:116:LEU:HD13	1.99	0.45
4:AD:219:SER:OG	4:AD:220:GLU:N	2.50	0.45
5:FD:150:LEU:HD13	5:HD:150:LEU:HD22	1.99	0.45
1:HC:254:THR:OG1	1:HC:255:THR:N	2.49	0.45
1:Q:200:ASP:OD1	1:Q:200:ASP:N	2.47	0.45
1:T:166:VAL:HG22	1:T:198:LEU:HA	1.99	0.45
3:R:16:ILE:HD12	3:R:48:ILE:HG22	1.99	0.45
3:a:48:ILE:HD11	3:a:81:ILE:HG12	1.97	0.45
2:IB:194:SER:HA	2:IB:225:VAL:HB	1.98	0.44
1:Q:194:SER:O	1:Q:194:SER:OG	2.34	0.44
1:SB:255:THR:OG1	1:SB:256:ASN:N	2.47	0.44
1:U:158:LEU:HG	1:U:271:ARG:HH12	1.82	0.44
1:VB:255:THR:OG1	1:VB:256:ASN:N	2.50	0.44
3:e:104:ASP:OD1	3:e:107:SER:OG	2.34	0.44
2:E:187:ILE:HG23	1:VB:256:ASN:HD22	1.82	0.44
1:FA:194:SER:O	1:FA:194:SER:OG	2.36	0.44
1:K:148:SER:OG	1:K:149:ALA:N	2.50	0.44
1:PB:156:PRO:HD2	1:PB:160:ILE:HA	1.98	0.44
1:FA:193:ARG:HE	1:FA:193:ARG:HB3	1.63	0.44
2:GB:219:SER:OG	2:GB:220:GLU:N	2.48	0.44
1:HC:159:PRO:HB3	1:HC:190:VAL:HG13	1.99	0.44
1:UB:156:PRO:HD2	1:UB:160:ILE:HA	1.99	0.44
1:W:189:VAL:HG12	1:W:190:VAL:H	1.83	0.44
3:D:51:ILE:HD13	3:D:54:ILE:HD11	1.99	0.44
3:J:47:ASP:OD1	3:J:79:THR:OG1	2.36	0.44
3:O:109:LEU:HD22	3:R:8:LEU:HD11	2.00	0.44
2:CB:182:ILE:HA	2:CB:185:LEU:HB2	2.00	0.44
1:HC:266:LEU:HD22	1:HC:271:ARG:HD2	1.98	0.44
1:PB:202:THR:OG1	1:PB:203:GLY:N	2.50	0.44
1:SB:183:GLU:HG3	1:SB:215:ILE:HD13	1.99	0.44
1:VB:200:ASP:OD1	1:VB:200:ASP:N	2.44	0.44
3:I:22:ASP:OD1	3:I:22:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:104:ASP:OD1	3:I:104:ASP:N	2.50	0.44
3:e:59:ALA:HB1	3:e:92:LEU:HD12	2.00	0.44
3:g:43:GLY:HA3	3:g:112:LEU:HD21	1.99	0.44
1:K:200:ASP:N	1:K:200:ASP:OD1	2.50	0.44
1:KB:194:SER:HA	1:KB:225:VAL:HB	2.00	0.44
1:M:231:LEU:O	1:M:235:ARG:NH1	2.40	0.44
1:UB:154:SER:HA	1:VB:163:LYS:HE2	2.00	0.44
1:V:191:LYS:HE2	1:V:191:LYS:HB2	1.86	0.44
1:Z:214:HIS:O	1:Z:218:ALA:N	2.50	0.44
3:J:37:HIS:NE2	3:J:72:MET:SD	2.91	0.44
1:DC:162:GLU:OE1	1:DC:193:ARG:NH1	2.48	0.44
2:GB:205:PRO:O	2:GB:209:THR:OG1	2.33	0.44
1:OB:174:ASP:O	1:OB:178:ALA:N	2.39	0.44
3:f:32:LEU:HD11	3:f:44:VAL:HG21	1.99	0.44
3:j:25:ALA:HB1	3:j:61:ILE:HG21	2.00	0.44
5:HD:148:SER:O	5:HD:151:GLN:NE2	2.51	0.44
1:DC:166:VAL:HG12	1:DC:168:PRO:HD3	2.00	0.44
2:E:256:ASN:HD22	1:T:187:ILE:HG23	1.83	0.44
1:EB:212:ALA:HA	1:EB:222:VAL:HG11	2.00	0.44
1:PB:202:THR:HG23	1:PB:204:VAL:H	1.83	0.44
1:Q:157:LEU:HG	1:Q:158:LEU:H	1.83	0.44
1:TB:232:VAL:HG13	3:B:71:LEU:HD23	1.99	0.44
1:U:164:ILE:HD11	1:U:193:ARG:HH11	1.83	0.44
1:V:167:MET:SD	1:V:172:THR:OG1	2.68	0.44
1:Y:200:ASP:OD1	1:Y:200:ASP:N	2.49	0.44
1:Z:182:ILE:HA	1:Z:185:LEU:HB2	1.98	0.44
1:GC:214:HIS:O	1:GC:217:GLN:NE2	2.50	0.44
1:KB:224:LEU:HD13	1:KB:252:ILE:HD12	1.99	0.44
1:L:190:VAL:HG11	1:L:265:ALA:HB1	1.99	0.44
1:PB:191:LYS:HE2	1:PB:191:LYS:HB2	1.88	0.44
1:V:193:ARG:HE	1:V:193:ARG:HB3	1.57	0.44
3:C:70:LYS:NZ	3:C:98:GLY:O	2.49	0.44
3:d:39:THR:OG1	3:d:40:SER:N	2.51	0.44
3:j:42:ARG:HE	3:j:116:LEU:HD11	1.83	0.44
2:DB:199:ILE:HA	2:DB:200:ASP:HA	1.81	0.43
2:E:232:VAL:HB	1:T:217:GLN:HE22	1.83	0.43
1:P:199:ILE:HA	1:P:200:ASP:HA	1.69	0.43
1:VB:254:THR:OG1	1:VB:255:THR:N	2.51	0.43
1:Y:170:ILE:HD13	1:Y:204:VAL:HG11	1.99	0.43
3:O:104:ASP:OD1	3:O:104:ASP:N	2.50	0.43
1:AB:274:VAL:HB	1:Z:274:VAL:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:ILE:HA	2:E:185:LEU:HB2	2.00	0.43
2:F:217:GLN:H	2:F:217:GLN:HG2	1.65	0.43
1:IC:223:ARG:HH12	1:IC:265:ALA:HB2	1.82	0.43
1:K:215:ILE:HA	1:K:218:ALA:HB3	2.00	0.43
1:T:212:ALA:HA	1:T:222:VAL:HG21	1.99	0.43
5:FD:174:ASP:OD1	5:FD:174:ASP:N	2.44	0.43
5:FD:223:ARG:HH22	5:FD:265:ALA:HB2	1.83	0.43
1:KB:199:ILE:HA	1:KB:200:ASP:HA	1.76	0.43
3:D:5:ILE:HG12	3:D:12:LEU:HD11	2.00	0.43
3:D:13:LEU:HD13	3:D:45:VAL:HB	2.01	0.43
1:AB:199:ILE:HA	1:AB:200:ASP:HA	1.75	0.43
1:LB:194:SER:HA	1:LB:225:VAL:HB	2.01	0.43
1:M:148:SER:OG	1:M:149:ALA:N	2.51	0.43
1:P:207:VAL:HA	1:P:210:MET:HG2	1.98	0.43
1:T:199:ILE:HA	1:T:200:ASP:HA	1.74	0.43
1:TB:148:SER:O	1:TB:148:SER:OG	2.34	0.43
1:X:216:ILE:HG12	1:X:221:ALA:HA	2.00	0.43
3:A:3:ILE:HD12	3:A:28:PHE:HD1	1.83	0.43
3:h:12:LEU:HB2	3:h:44:VAL:HG23	2.01	0.43
2:E:191:LYS:HE2	2:E:191:LYS:HB2	1.82	0.43
1:HC:260:LYS:HD2	3:A:42:ARG:HH21	1.84	0.43
5:FD:161:PHE:HB2	5:FD:192:ASN:HB2	2.01	0.43
1:EB:223:ARG:HH12	1:EB:264:ARG:HG3	1.83	0.43
1:IC:193:ARG:HA	1:IC:193:ARG:HD2	1.88	0.43
1:LB:206:VAL:HA	1:LB:210:MET:HG2	2.00	0.43
1:Z:254:THR:OG1	1:Z:255:THR:N	2.48	0.43
3:I:5:ILE:HG21	3:I:35:LYS:HG2	2.01	0.43
3:e:44:VAL:HB	3:e:76:VAL:HG22	2.01	0.43
2:CB:210:MET:O	2:CB:214:HIS:ND1	2.50	0.43
2:E:235:ARG:HA	2:E:235:ARG:HD3	1.79	0.43
1:GC:205:PRO:O	1:GC:209:THR:N	2.43	0.43
1:SB:254:THR:OG1	1:SB:255:THR:N	2.49	0.43
1:T:229:ALA:HB1	1:V:180:LEU:HB3	2.00	0.43
1:TB:229:ALA:HA	3:B:72:MET:HE1	2.01	0.43
3:A:18:SER:O	3:A:18:SER:OG	2.34	0.43
5:HD:160:ILE:HD12	5:HD:160:ILE:HA	1.86	0.43
1:BC:234:ILE:O	1:BC:235:ARG:NE	2.52	0.43
2:DB:254:THR:OG1	2:DB:255:THR:N	2.52	0.43
2:E:234:ILE:HG13	2:E:236:PRO:HD3	2.01	0.43
1:FA:212:ALA:HA	1:FA:222:VAL:HG11	1.99	0.43
1:IC:193:ARG:NH2	1:IC:208:ASP:OD1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:223:ARG:HB3	1:LB:253:ILE:HG23	2.00	0.43
1:U:255:THR:OG1	1:U:256:ASN:N	2.52	0.43
3:D:21:ASP:N	3:D:24:THR:OG1	2.43	0.43
3:f:33:LEU:HD11	3:f:68:MET:HB3	1.99	0.43
3:g:6:LEU:HD11	3:g:35:LYS:HG2	2.00	0.43
2:DB:196:VAL:HG22	2:DB:226:GLY:HA3	2.00	0.43
2:F:179:LYS:HD2	2:F:191:LYS:HE3	2.01	0.43
2:IB:232:VAL:HG13	2:IB:235:ARG:HG3	2.01	0.43
1:KB:200:ASP:OD1	1:KB:200:ASP:N	2.51	0.43
3:f:71:LEU:HA	5:HD:254:THR:HG21	2.01	0.43
2:GB:199:ILE:HA	2:GB:200:ASP:HA	1.75	0.43
2:GB:273:ILE:HG12	2:IB:273:ILE:HG12	2.01	0.43
2:IB:254:THR:OG1	2:IB:255:THR:N	2.51	0.43
1:KB:212:ALA:HA	1:KB:222:VAL:HG11	2.01	0.43
1:LB:254:THR:HG21	5:CD:217:GLN:HA	2.00	0.43
1:Q:191:LYS:NZ	1:Q:192:ASN:O	2.50	0.43
1:U:264:ARG:H	1:U:264:ARG:HG2	1.70	0.43
1:Z:199:ILE:HA	1:Z:200:ASP:HA	1.73	0.43
3:O:89:LEU:HD13	3:O:94:ILE:HD11	1.99	0.43
5:HD:174:ASP:HA	5:HD:177:ARG:HG2	2.01	0.43
1:U:151:GLN:HE22	1:U:165:SER:HB2	1.84	0.42
1:UB:191:LYS:HE2	1:UB:191:LYS:HB2	1.82	0.42
1:X:155:ALA:HB2	1:X:160:ILE:HG12	2.01	0.42
3:C:54:ILE:HG23	3:C:58:ILE:HB	2.00	0.42
3:O:62:LEU:HD23	3:O:62:LEU:HA	1.92	0.42
3:d:14:ILE:HG23	3:d:46:ILE:HA	2.01	0.42
3:h:112:LEU:HD23	3:h:112:LEU:HA	1.92	0.42
4:AD:199:ILE:HA	4:AD:200:ASP:HA	1.77	0.42
5:HD:227:CYS:HB3	5:HD:231:LEU:HD23	2.00	0.42
1:V:202:THR:OG1	1:V:203:GLY:N	2.53	0.42
3:a:47:ASP:OD1	3:a:49:THR:OG1	2.34	0.42
1:FA:255:THR:OG1	1:FA:256:ASN:N	2.52	0.42
1:FC:219:SER:OG	1:FC:220:GLU:N	2.51	0.42
1:FC:273:ILE:HD12	1:IC:275:GLU:H	1.83	0.42
2:GB:193:ARG:HB2	2:GB:224:LEU:HA	2.01	0.42
1:HC:161:PHE:HB2	1:HC:192:ASN:H	1.85	0.42
3:O:13:LEU:HD21	3:O:109:LEU:HD13	2.00	0.42
1:DC:199:ILE:HA	1:DC:200:ASP:HA	1.80	0.42
2:E:259:LYS:HE2	2:E:259:LYS:HB2	1.95	0.42
1:Q:179:LYS:HZ3	1:Q:211:VAL:HG13	1.84	0.42
1:U:254:THR:HG21	3:c:71:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UB:273:ILE:HG23	1:VB:273:ILE:HD12	2.01	0.42
1:Z:193:ARG:HD3	1:Z:193:ARG:HA	1.81	0.42
3:f:11:CYS:SG	3:f:113:LYS:NZ	2.78	0.42
3:h:22:ASP:OD1	3:h:22:ASP:N	2.46	0.42
5:CD:189:VAL:HG12	5:CD:190:VAL:H	1.84	0.42
2:CB:187:ILE:HG23	1:EB:256:ASN:HD22	1.84	0.42
1:HC:164:ILE:HB	1:HC:195:GLU:HB3	2.00	0.42
1:P:231:LEU:O	1:P:235:ARG:NH1	2.53	0.42
1:GC:193:ARG:NH2	1:GC:208:ASP:O	2.50	0.42
1:U:223:ARG:HH22	1:U:268:LEU:HB2	1.85	0.42
1:UB:176:GLU:HA	1:UB:211:VAL:HG21	2.01	0.42
1:Z:189:VAL:HG12	1:Z:190:VAL:HG23	2.01	0.42
3:D:104:ASP:N	3:D:104:ASP:OD1	2.50	0.42
3:R:14:ILE:HG22	3:R:46:ILE:HA	2.00	0.42
3:g:47:ASP:OD1	3:g:49:THR:OG1	2.28	0.42
1:HC:215:ILE:HA	1:HC:218:ALA:HB3	2.02	0.42
1:KB:214:HIS:O	1:KB:218:ALA:N	2.52	0.42
1:M:156:PRO:HD3	1:M:161:PHE:CE1	2.55	0.42
1:T:166:VAL:HG12	1:T:168:PRO:HD3	2.02	0.42
3:N:54:ILE:HG23	3:N:58:ILE:HB	2.02	0.42
3:a:16:ILE:O	3:a:50:SER:OG	2.38	0.42
5:HD:193:ARG:NH2	5:HD:208:ASP:OD1	2.49	0.42
1:AB:157:LEU:HD12	1:Z:259:LYS:HD2	2.00	0.42
2:CB:153:LEU:HD13	2:CB:182:ILE:HG21	2.02	0.42
2:DB:153:LEU:HD23	2:DB:153:LEU:HA	1.86	0.42
2:DB:194:SER:O	2:DB:194:SER:OG	2.37	0.42
1:OB:190:VAL:HG12	1:OB:221:ALA:H	1.85	0.42
1:Q:255:THR:OG1	1:Q:256:ASN:N	2.46	0.42
1:VB:161:PHE:HB2	1:VB:192:ASN:HB2	2.01	0.42
3:D:48:ILE:HB	3:D:51:ILE:HD12	2.01	0.42
5:HD:160:ILE:HG22	5:HD:191:LYS:HA	2.01	0.42
1:AB:153:LEU:HD12	1:AB:153:LEU:HA	1.90	0.42
2:GB:187:ILE:HG23	1:KB:256:ASN:HD22	1.85	0.42
1:U:163:LYS:NZ	1:U:194:SER:OG	2.36	0.42
1:Z:255:THR:OG1	1:Z:256:ASN:N	2.51	0.42
3:A:64:ASP:O	3:A:67:SER:OG	2.33	0.42
3:A:75:LYS:HG3	3:A:116:LEU:HD11	2.01	0.42
3:J:43:GLY:HA3	3:J:112:LEU:HD21	2.01	0.42
3:h:54:ILE:HG23	3:h:58:ILE:HB	2.02	0.42
3:h:65:VAL:O	3:h:69:SER:OG	2.35	0.42
1:GC:158:LEU:HB3	1:GC:271:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IB:231:LEU:O	2:IB:235:ARG:NH1	2.49	0.42
1:M:158:LEU:HA	1:M:158:LEU:HD12	1.85	0.42
1:Q:184:ASN:HA	3:O:103:MET:HE1	2.00	0.42
1:VB:187:ILE:HG23	1:Y:256:ASN:HD22	1.84	0.42
3:D:9:GLY:H	3:I:106:GLU:HG2	1.85	0.42
3:I:24:THR:O	3:I:28:PHE:N	2.53	0.42
5:HD:202:THR:OG1	5:HD:203:GLY:N	2.53	0.42
5:HD:223:ARG:HG2	5:HD:253:ILE:HB	2.02	0.42
2:E:204:VAL:HB	2:E:207:VAL:HG22	2.02	0.41
1:FC:212:ALA:HA	1:FC:222:VAL:HG21	2.02	0.41
1:HC:199:ILE:HG21	1:HC:230:MET:HE3	2.02	0.41
1:IC:254:THR:OG1	1:IC:255:THR:N	2.52	0.41
1:K:199:ILE:HA	1:K:200:ASP:HA	1.79	0.41
1:OB:204:VAL:HG23	1:OB:207:VAL:HB	2.01	0.41
1:SB:251:GLN:HB3	1:SB:252:ILE:H	1.62	0.41
1:W:219:SER:OG	1:W:220:GLU:N	2.51	0.41
3:R:42:ARG:HB3	3:R:116:LEU:HD21	2.00	0.41
3:a:77:VAL:HG21	3:a:112:LEU:HD21	2.02	0.41
3:g:62:LEU:HD23	3:g:62:LEU:HA	1.91	0.41
3:h:26:VAL:HA	3:h:29:GLN:HE21	1.85	0.41
3:h:104:ASP:N	3:h:104:ASP:OD1	2.53	0.41
5:FD:170:ILE:HD13	5:FD:204:VAL:HG11	2.02	0.41
1:AB:199:ILE:HD12	1:AB:200:ASP:HB3	2.01	0.41
2:GB:179:LYS:HB3	2:GB:179:LYS:HE2	1.78	0.41
1:IC:219:SER:OG	1:IC:220:GLU:N	2.52	0.41
1:SB:199:ILE:HG13	1:SB:200:ASP:HB3	2.01	0.41
1:T:194:SER:HA	1:T:225:VAL:HB	2.02	0.41
1:W:176:GLU:HA	1:W:179:LYS:HE2	2.02	0.41
3:c:12:LEU:HD12	3:c:44:VAL:HG12	2.02	0.41
3:c:47:ASP:OD1	3:c:49:THR:OG1	2.37	0.41
1:AB:191:LYS:HB3	1:AB:222:VAL:HG23	2.02	0.41
1:DC:210:MET:O	1:DC:214:HIS:N	2.50	0.41
1:EB:155:ALA:HB2	1:EB:160:ILE:HG23	2.02	0.41
2:GB:255:THR:OG1	2:GB:256:ASN:N	2.53	0.41
1:HC:192:ASN:HD22	1:HC:258:MET:HE1	1.86	0.41
1:L:199:ILE:HA	1:L:200:ASP:HA	1.86	0.41
1:PB:212:ALA:HB1	1:PB:252:ILE:HG21	2.01	0.41
1:UB:215:ILE:HA	1:UB:218:ALA:HB3	2.01	0.41
1:Y:224:LEU:HD13	1:Y:252:ILE:HD12	2.01	0.41
3:N:49:THR:O	3:N:82:GLN:NE2	2.46	0.41
1:OB:151:GLN:NE2	1:OB:167:MET:SD	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:70:LYS:NZ	3:S:98:GLY:O	2.39	0.41
3:b:22:ASP:HA	3:b:25:ALA:HB3	2.01	0.41
3:h:13:LEU:HD23	3:h:105:LEU:HD11	2.03	0.41
3:h:51:ILE:HG21	3:h:54:ILE:HG13	2.02	0.41
3:h:92:LEU:HD22	3:h:94:ILE:HD13	2.02	0.41
5:FD:219:SER:OG	5:FD:220:GLU:N	2.52	0.41
1:UB:233:GLY:HA2	3:D:68:MET:HE1	2.01	0.41
1:X:206:VAL:O	1:X:210:MET:N	2.47	0.41
3:B:64:ASP:O	3:B:67:SER:OG	2.36	0.41
3:S:22:ASP:N	3:S:22:ASP:OD1	2.48	0.41
3:j:114:GLN:H	3:j:114:GLN:HG2	1.72	0.41
1:EB:194:SER:HA	1:EB:225:VAL:HB	2.03	0.41
1:FA:257:THR:OG1	1:FA:258:MET:N	2.54	0.41
1:FB:191:LYS:HE2	1:FB:191:LYS:HB2	1.90	0.41
1:HC:199:ILE:HA	1:HC:200:ASP:HA	1.69	0.41
1:K:191:LYS:HE2	1:K:191:LYS:HB2	1.90	0.41
1:T:154:SER:HB3	1:U:258:MET:HE2	2.02	0.41
1:U:266:LEU:O	1:U:271:ARG:N	2.50	0.41
1:UB:155:ALA:HB3	1:VB:258:MET:HB3	2.02	0.41
1:UB:158:LEU:HD11	1:UB:269:THR:HG21	2.03	0.41
1:UB:273:ILE:HD12	1:VB:273:ILE:HD12	2.02	0.41
3:A:35:LYS:HZ3	3:A:39:THR:HG1	1.67	0.41
3:C:90:ILE:HD12	3:C:90:ILE:HA	1.97	0.41
3:I:13:LEU:HD23	3:I:13:LEU:HA	1.91	0.41
3:j:42:ARG:HB3	3:j:116:LEU:HD21	2.03	0.41
1:AB:163:LYS:NZ	1:AB:165:SER:OG	2.43	0.41
1:BC:251:GLN:HB3	1:BC:252:ILE:H	1.66	0.41
2:DB:152:GLU:OE1	2:DB:154:SER:N	2.54	0.41
2:DB:214:HIS:O	2:DB:218:ALA:N	2.45	0.41
2:F:230:MET:SD	2:F:230:MET:N	2.91	0.41
1:GC:254:THR:HG21	1:K:217:GLN:HA	2.02	0.41
1:P:160:ILE:HD12	1:P:186:LEU:HD11	2.03	0.41
1:Q:199:ILE:HA	1:Q:200:ASP:HA	1.64	0.41
1:Q:205:PRO:HA	1:Q:208:ASP:HB3	2.03	0.41
1:T:215:ILE:H	1:T:215:ILE:HG13	1.70	0.41
1:V:253:ILE:HD11	1:V:264:ARG:HH21	1.86	0.41
3:B:116:LEU:HD12	3:B:116:LEU:HA	1.92	0.41
3:J:54:ILE:HD12	3:J:85:VAL:HG21	2.02	0.41
5:HD:147:LYS:HB3	5:HD:147:LYS:HE3	1.89	0.41
1:BC:178:ALA:HA	1:BC:181:ILE:HD12	2.03	0.41
1:EB:274:VAL:HG22	1:FB:274:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:205:PRO:HB2	2:F:209:THR:HG22	2.03	0.41
2:F:215:ILE:HD12	2:F:215:ILE:HA	1.87	0.41
2:IB:160:ILE:HD13	2:IB:188:GLY:HA2	2.01	0.41
1:W:157:LEU:HB2	1:W:158:LEU:H	1.80	0.41
1:W:162:GLU:HB3	1:W:193:ARG:HH12	1.85	0.41
1:X:258:MET:HE3	1:X:258:MET:HB3	1.84	0.41
1:Y:234:ILE:O	1:Y:235:ARG:NE	2.50	0.41
1:Z:150:LEU:O	1:Z:151:GLN:NE2	2.54	0.41
3:I:16:ILE:HD12	3:I:48:ILE:HG22	2.03	0.41
3:a:13:LEU:HD23	3:a:105:LEU:HD11	2.01	0.41
4:AD:158:LEU:HD13	4:AD:158:LEU:HA	1.96	0.41
2:F:158:LEU:HB2	2:F:271:ARG:HH22	1.86	0.41
1:GC:255:THR:OG1	1:GC:256:ASN:N	2.53	0.41
1:KB:165:SER:HA	1:KB:197:VAL:HG13	2.03	0.41
1:M:189:VAL:HG12	1:M:190:VAL:H	1.85	0.41
1:V:179:LYS:HZ3	1:V:191:LYS:HE3	1.86	0.41
1:W:176:GLU:HB2	1:W:211:VAL:HG21	2.03	0.41
1:Z:189:VAL:O	1:Z:219:SER:OG	2.35	0.41
3:I:5:ILE:HG12	3:I:14:ILE:HG12	2.03	0.41
3:I:21:ASP:N	3:I:21:ASP:OD1	2.54	0.41
3:J:94:ILE:HG22	3:J:96:PHE:H	1.85	0.41
3:a:36:ILE:HD12	3:a:36:ILE:HA	1.94	0.41
3:f:25:ALA:HB1	3:f:61:ILE:HG21	2.03	0.41
5:CD:173:ILE:HG23	5:CD:177:ARG:HG2	2.03	0.41
1:FB:219:SER:OG	1:FB:220:GLU:N	2.54	0.41
1:IC:189:VAL:HG12	1:IC:190:VAL:HG23	2.02	0.41
1:X:190:VAL:HG11	1:X:265:ALA:HB1	2.03	0.41
1:Z:199:ILE:HG13	1:Z:200:ASP:HB3	2.03	0.41
3:A:58:ILE:O	3:A:62:LEU:N	2.50	0.41
3:A:87:ILE:HD13	3:A:87:ILE:HA	1.95	0.41
3:h:16:ILE:O	3:h:50:SER:OG	2.36	0.41
3:h:66:VAL:HG12	3:h:76:VAL:HG11	2.02	0.41
4:AD:161:PHE:HB2	4:AD:192:ASN:HB2	2.02	0.41
1:DC:255:THR:OG1	1:DC:256:ASN:N	2.52	0.40
1:LB:193:ARG:NH2	1:LB:208:ASP:OD1	2.54	0.40
1:LB:214:HIS:O	1:LB:218:ALA:N	2.51	0.40
1:UB:214:HIS:CE1	3:a:87:ILE:HA	2.56	0.40
3:I:50:SER:O	3:I:50:SER:OG	2.31	0.40
1:EB:189:VAL:HG12	1:EB:190:VAL:H	1.86	0.40
2:F:153:LEU:HD21	2:F:182:ILE:HG21	2.02	0.40
1:FC:214:HIS:HB2	3:C:90:ILE:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GC:258:MET:HE3	1:GC:258:MET:HB3	1.86	0.40
2:IB:174:ASP:O	2:IB:178:ALA:N	2.49	0.40
1:T:210:MET:O	1:T:214:HIS:N	2.54	0.40
1:X:201:ILE:HG12	1:X:231:LEU:HD11	2.02	0.40
3:N:25:ALA:HA	3:N:28:PHE:HB3	2.04	0.40
3:b:12:LEU:HD23	3:b:12:LEU:HA	1.93	0.40
3:d:17:GLN:HE21	3:f:4:PRO:HA	1.86	0.40
4:AD:181:ILE:HG23	4:AD:182:ILE:HG13	2.03	0.40
1:EB:205:PRO:O	1:EB:209:THR:N	2.55	0.40
1:IC:159:PRO:HB3	1:IC:190:VAL:HB	2.04	0.40
1:IC:224:LEU:HD13	1:IC:252:ILE:HD12	2.03	0.40
1:LB:214:HIS:CD2	3:c:90:ILE:HG13	2.56	0.40
1:W:225:VAL:HG11	1:W:258:MET:HG2	2.03	0.40
3:B:62:LEU:HD23	3:B:62:LEU:HA	1.91	0.40
3:b:87:ILE:HD12	3:b:87:ILE:HA	1.93	0.40
3:c:4:PRO:HG3	3:c:15:SER:H	1.86	0.40
2:GB:212:ALA:HA	2:GB:222:VAL:HG11	2.03	0.40
1:IC:215:ILE:HD13	1:IC:222:VAL:HG21	2.02	0.40
1:U:182:ILE:HA	1:U:185:LEU:HB2	2.03	0.40
3:C:54:ILE:HD13	3:C:54:ILE:HA	1.95	0.40
5:HD:223:ARG:HH22	5:HD:268:LEU:HD23	1.86	0.40
2:CB:147:LYS:HD3	2:CB:147:LYS:HA	1.80	0.40
2:GB:194:SER:HA	2:GB:225:VAL:HB	2.03	0.40
1:LB:201:ILE:HB	1:LB:231:LEU:HD11	2.04	0.40
1:P:262:MET:HE2	1:P:262:MET:HB2	1.94	0.40
3:f:87:ILE:HG23	3:f:88:THR:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	AB	111/128 (87%)	95 (86%)	16 (14%)	0	100	100
1	BC	111/128 (87%)	91 (82%)	19 (17%)	1 (1%)	14	49
1	DC	111/128 (87%)	93 (84%)	17 (15%)	1 (1%)	14	49
1	EB	111/128 (87%)	90 (81%)	21 (19%)	0	100	100
1	FA	111/128 (87%)	83 (75%)	27 (24%)	1 (1%)	14	49
1	FB	111/128 (87%)	89 (80%)	22 (20%)	0	100	100
1	FC	111/128 (87%)	87 (78%)	23 (21%)	1 (1%)	14	49
1	GC	111/128 (87%)	98 (88%)	13 (12%)	0	100	100
1	HC	111/128 (87%)	90 (81%)	20 (18%)	1 (1%)	14	49
1	IC	111/128 (87%)	88 (79%)	22 (20%)	1 (1%)	14	49
1	K	111/128 (87%)	88 (79%)	23 (21%)	0	100	100
1	KB	111/128 (87%)	93 (84%)	18 (16%)	0	100	100
1	L	111/128 (87%)	90 (81%)	21 (19%)	0	100	100
1	LB	111/128 (87%)	91 (82%)	18 (16%)	2 (2%)	6	34
1	M	111/128 (87%)	88 (79%)	23 (21%)	0	100	100
1	OB	111/128 (87%)	94 (85%)	16 (14%)	1 (1%)	14	49
1	P	111/128 (87%)	96 (86%)	15 (14%)	0	100	100
1	PB	111/128 (87%)	93 (84%)	18 (16%)	0	100	100
1	Q	111/128 (87%)	89 (80%)	22 (20%)	0	100	100
1	SB	111/128 (87%)	94 (85%)	16 (14%)	1 (1%)	14	49
1	T	111/128 (87%)	93 (84%)	17 (15%)	1 (1%)	14	49
1	TB	111/128 (87%)	92 (83%)	19 (17%)	0	100	100
1	U	111/128 (87%)	94 (85%)	17 (15%)	0	100	100
1	UB	111/128 (87%)	92 (83%)	18 (16%)	1 (1%)	14	49
1	V	111/128 (87%)	91 (82%)	19 (17%)	1 (1%)	14	49
1	VB	111/128 (87%)	89 (80%)	21 (19%)	1 (1%)	14	49
1	W	111/128 (87%)	92 (83%)	18 (16%)	1 (1%)	14	49
1	X	111/128 (87%)	93 (84%)	18 (16%)	0	100	100
1	Y	111/128 (87%)	93 (84%)	18 (16%)	0	100	100
1	Z	111/128 (87%)	92 (83%)	19 (17%)	0	100	100
2	CB	112/129 (87%)	96 (86%)	16 (14%)	0	100	100
2	DB	112/129 (87%)	91 (81%)	21 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	112/129 (87%)	87 (78%)	24 (21%)	1 (1%)	14	49
2	F	112/129 (87%)	93 (83%)	19 (17%)	0	100	100
2	GB	112/129 (87%)	97 (87%)	14 (12%)	1 (1%)	14	49
2	IB	112/129 (87%)	93 (83%)	19 (17%)	0	100	100
3	A	116/118 (98%)	100 (86%)	16 (14%)	0	100	100
3	B	116/118 (98%)	103 (89%)	13 (11%)	0	100	100
3	C	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	D	116/118 (98%)	101 (87%)	15 (13%)	0	100	100
3	I	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
3	J	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
3	N	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
3	O	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
3	R	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
3	S	116/118 (98%)	100 (86%)	16 (14%)	0	100	100
3	a	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
3	b	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	c	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	d	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	e	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
3	f	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	g	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
3	h	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
3	i	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	j	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
4	AD	119/123 (97%)	99 (83%)	20 (17%)	0	100	100
5	CD	119/136 (88%)	104 (87%)	15 (13%)	0	100	100
5	FD	119/136 (88%)	98 (82%)	21 (18%)	0	100	100
5	HD	115/136 (85%)	93 (81%)	21 (18%)	1 (1%)	14	49
All	All	6794/7505 (90%)	5785 (85%)	991 (15%)	18 (0%)	37	71

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	HD	159	PRO
1	BC	203	GLY
1	FC	197	VAL
1	UB	157	LEU
1	W	157	LEU
1	FA	157	LEU
2	GB	158	LEU
1	LB	161	PHE
1	V	157	LEU
2	E	151	GLN
1	HC	158	LEU
1	LB	160	ILE
1	OB	158	LEU
1	SB	156	PRO
1	IC	158	LEU
1	DC	158	LEU
1	T	158	LEU
1	VB	158	LEU

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	AB	100/111 (90%)	100 (100%)	0	100	100
1	BC	99/111 (89%)	99 (100%)	0	100	100
1	DC	100/111 (90%)	100 (100%)	0	100	100
1	EB	100/111 (90%)	99 (99%)	1 (1%)	68	75
1	FA	99/111 (89%)	99 (100%)	0	100	100
1	FB	100/111 (90%)	99 (99%)	1 (1%)	68	75
1	FC	100/111 (90%)	99 (99%)	1 (1%)	68	75
1	GC	100/111 (90%)	100 (100%)	0	100	100
1	HC	99/111 (89%)	97 (98%)	2 (2%)	48	66
1	IC	100/111 (90%)	99 (99%)	1 (1%)	68	75
1	K	100/111 (90%)	99 (99%)	1 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	KB	100/111 (90%)	100 (100%)	0	100	100
1	L	100/111 (90%)	99 (99%)	1 (1%)	68	75
1	LB	100/111 (90%)	99 (99%)	1 (1%)	68	75
1	M	99/111 (89%)	99 (100%)	0	100	100
1	OB	100/111 (90%)	100 (100%)	0	100	100
1	P	100/111 (90%)	100 (100%)	0	100	100
1	PB	100/111 (90%)	100 (100%)	0	100	100
1	Q	99/111 (89%)	98 (99%)	1 (1%)	68	75
1	SB	100/111 (90%)	100 (100%)	0	100	100
1	T	98/111 (88%)	98 (100%)	0	100	100
1	TB	100/111 (90%)	100 (100%)	0	100	100
1	U	100/111 (90%)	100 (100%)	0	100	100
1	UB	99/111 (89%)	99 (100%)	0	100	100
1	V	99/111 (89%)	98 (99%)	1 (1%)	68	75
1	VB	100/111 (90%)	100 (100%)	0	100	100
1	W	100/111 (90%)	99 (99%)	1 (1%)	68	75
1	X	98/111 (88%)	95 (97%)	3 (3%)	35	56
1	Y	100/111 (90%)	99 (99%)	1 (1%)	68	75
1	Z	100/111 (90%)	100 (100%)	0	100	100
2	CB	101/112 (90%)	100 (99%)	1 (1%)	68	75
2	DB	101/112 (90%)	100 (99%)	1 (1%)	68	75
2	E	101/112 (90%)	101 (100%)	0	100	100
2	F	101/112 (90%)	101 (100%)	0	100	100
2	GB	101/112 (90%)	101 (100%)	0	100	100
2	IB	101/112 (90%)	98 (97%)	3 (3%)	36	57
3	A	99/100 (99%)	98 (99%)	1 (1%)	68	75
3	B	99/100 (99%)	99 (100%)	0	100	100
3	C	99/100 (99%)	98 (99%)	1 (1%)	68	75
3	D	99/100 (99%)	98 (99%)	1 (1%)	68	75
3	I	99/100 (99%)	99 (100%)	0	100	100
3	J	99/100 (99%)	98 (99%)	1 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	99/100 (99%)	97 (98%)	2 (2%)	48	66
3	O	99/100 (99%)	99 (100%)	0	100	100
3	R	98/100 (98%)	98 (100%)	0	100	100
3	S	98/100 (98%)	98 (100%)	0	100	100
3	a	98/100 (98%)	97 (99%)	1 (1%)	68	75
3	b	98/100 (98%)	98 (100%)	0	100	100
3	c	99/100 (99%)	98 (99%)	1 (1%)	68	75
3	d	98/100 (98%)	98 (100%)	0	100	100
3	e	97/100 (97%)	96 (99%)	1 (1%)	68	75
3	f	99/100 (99%)	99 (100%)	0	100	100
3	g	99/100 (99%)	98 (99%)	1 (1%)	68	75
3	h	98/100 (98%)	97 (99%)	1 (1%)	68	75
3	i	98/100 (98%)	96 (98%)	2 (2%)	48	66
3	j	98/100 (98%)	98 (100%)	0	100	100
4	AD	107/108 (99%)	106 (99%)	1 (1%)	70	76
5	CD	107/119 (90%)	107 (100%)	0	100	100
5	FD	105/119 (88%)	104 (99%)	1 (1%)	68	75
5	HD	106/119 (89%)	106 (100%)	0	100	100
All	All	5990/6467 (93%)	5954 (99%)	36 (1%)	76	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CB	220	GLU
2	DB	252	ILE
1	EB	189	VAL
1	FB	269	THR
1	FC	198	LEU
1	HC	197	VAL
1	HC	273	ILE
2	IB	174	ASP
2	IB	197	VAL
2	IB	232	VAL
1	IC	204	VAL
1	K	152	GLU
1	L	197	VAL

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Mol	Chain	Res	Type
1	LB	197	VAL
1	Q	190	VAL
1	V	209	THR
1	W	157	LEU
1	X	190	VAL
1	X	215	ILE
1	X	255	THR
1	Y	157	LEU
3	A	99	VAL
3	C	6	LEU
3	D	99	VAL
3	J	6	LEU
3	N	6	LEU
3	N	94	ILE
3	a	6	LEU
3	c	6	LEU
3	e	6	LEU
3	g	6	LEU
3	h	6	LEU
3	i	6	LEU
3	i	23	HIS
4	AD	157	LEU
5	FD	215	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	217	GLN
1	BC	228	GLN
1	BC	270	ASN
2	CB	151	GLN
1	DC	228	GLN
1	EB	256	ASN
2	F	151	GLN
2	F	192	ASN
2	F	228	GLN
1	FA	151	GLN
1	FA	213	HIS
1	FA	214	HIS
1	FB	151	GLN
1	FB	228	GLN
1	FC	192	ASN

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Mol	Chain	Res	Type
2	GB	228	GLN
2	GB	270	ASN
1	HC	151	GLN
1	HC	192	ASN
1	K	192	ASN
1	K	256	ASN
1	KB	228	GLN
1	KB	256	ASN
1	M	214	HIS
1	M	228	GLN
1	OB	228	GLN
1	P	192	ASN
1	P	213	HIS
1	P	228	GLN
1	PB	151	GLN
1	PB	270	ASN
1	Q	228	GLN
1	SB	214	HIS
1	SB	256	ASN
1	T	228	GLN
1	T	256	ASN
1	T	270	ASN
1	TB	151	GLN
1	TB	184	ASN
1	TB	217	GLN
1	TB	228	GLN
1	U	151	GLN
1	U	228	GLN
1	UB	192	ASN
1	UB	228	GLN
1	VB	192	ASN
1	VB	228	GLN
1	X	214	HIS
1	X	228	GLN
1	X	270	ASN
1	Y	228	GLN
1	Y	256	ASN
1	Z	151	GLN
3	A	17	GLN
3	A	29	GLN
3	I	29	GLN
3	a	29	GLN

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Mol	Chain	Res	Type
3	a	82	GLN
3	c	37	HIS
3	d	37	HIS
3	e	23	HIS
3	e	29	GLN
3	h	29	GLN
3	i	29	GLN
3	j	37	HIS
4	AD	146	GLN
4	AD	184	ASN
5	CD	146	GLN
5	CD	151	GLN
5	CD	192	ASN
5	CD	213	HIS
5	CD	228	GLN
5	CD	256	ASN
5	FD	192	ASN
5	HD	146	GLN
5	HD	151	GLN
5	HD	228	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	HD	2
4	AD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AD	237:GLU	C	238:GLN	N	11.07
1	HD	220:GLU	C	221:ALA	N	5.35
1	HD	222:VAL	C	223:ARG	N	3.25

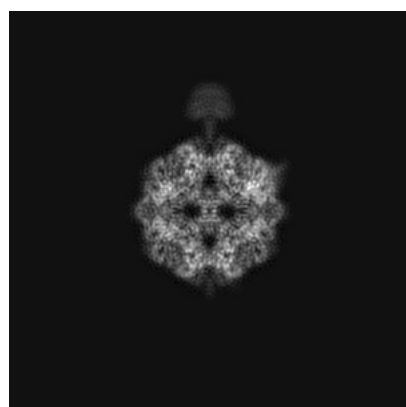
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4508. These allow visual inspection of the internal detail of the map and identification of artifacts.

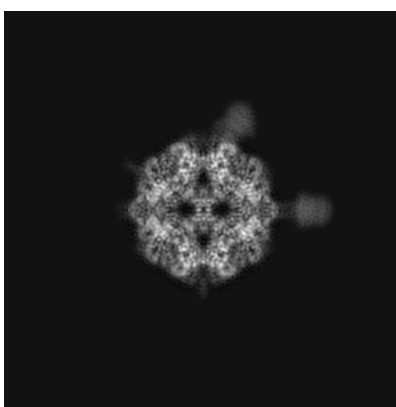
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

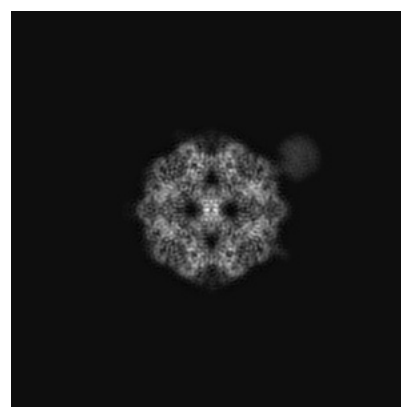
6.1.1 Primary map



X



Y

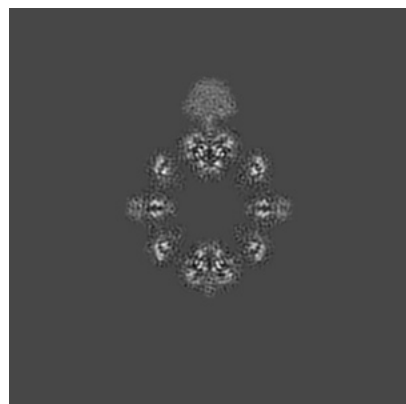


Z

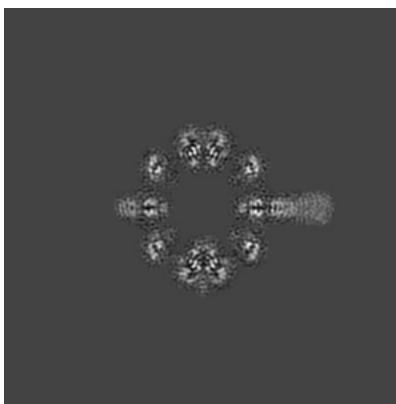
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

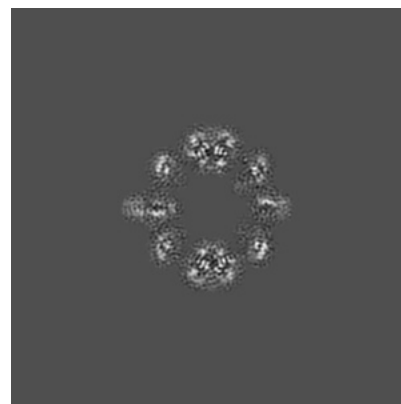
6.2.1 Primary map



X Index: 205



Y Index: 205

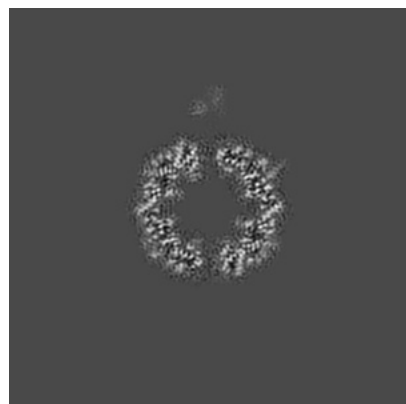


Z Index: 205

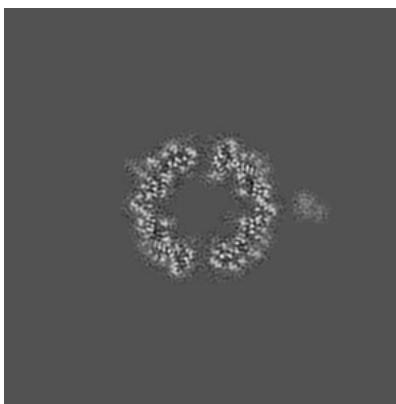
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

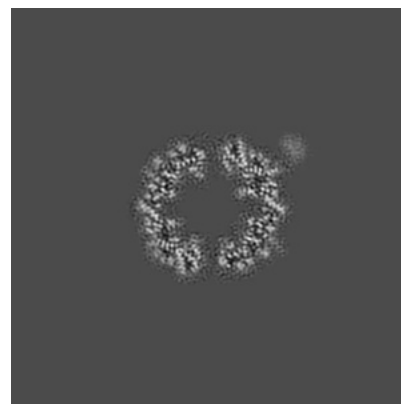
6.3.1 Primary map



X Index: 187



Y Index: 224

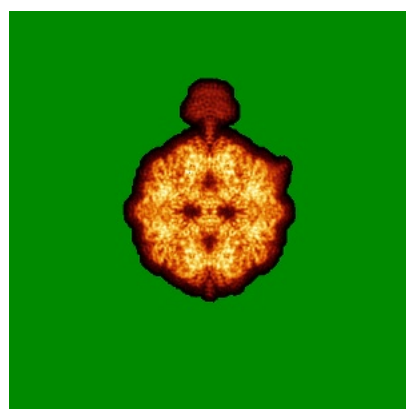


Z Index: 222

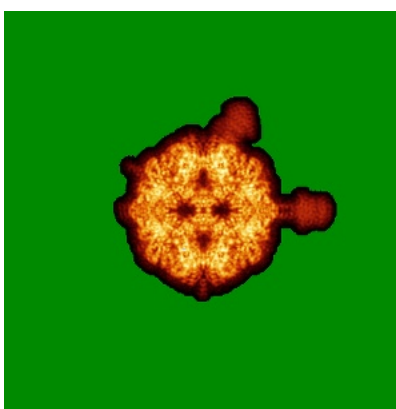
The images above show the largest variance slices of the map in three orthogonal directions.

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

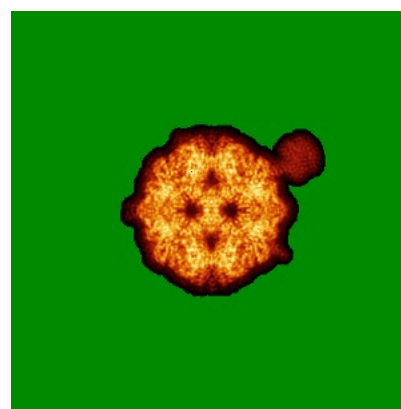
6.4.1 Primary map



X



Y

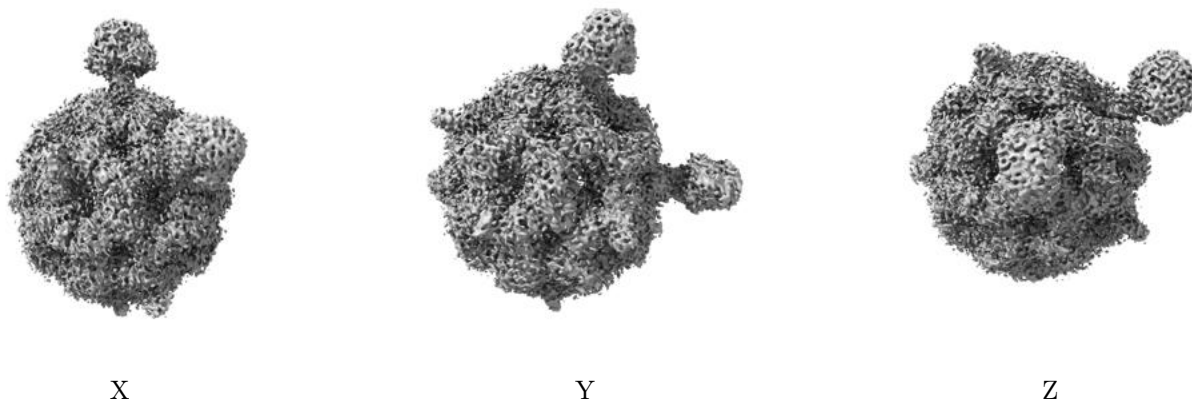


Z

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 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

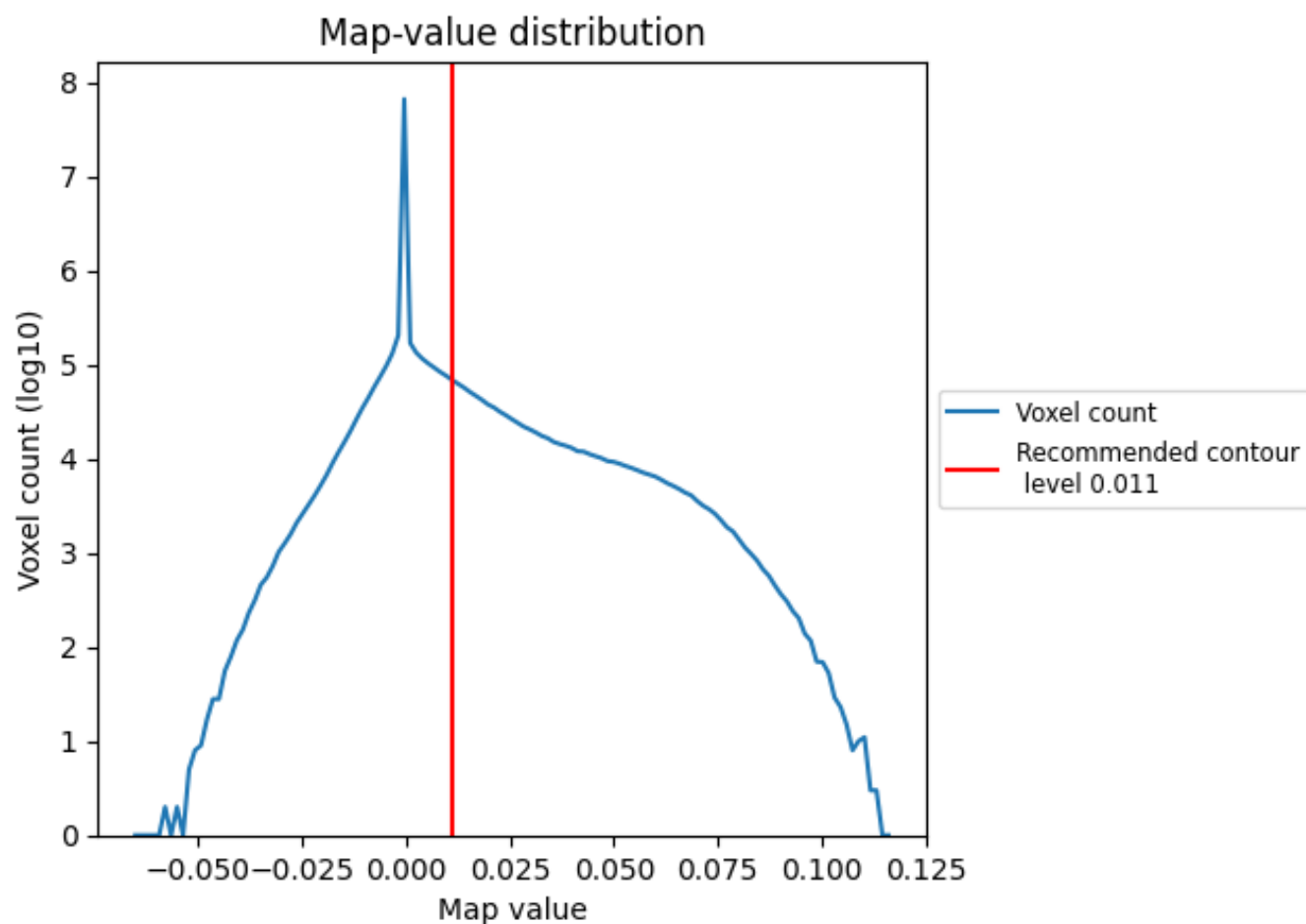
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

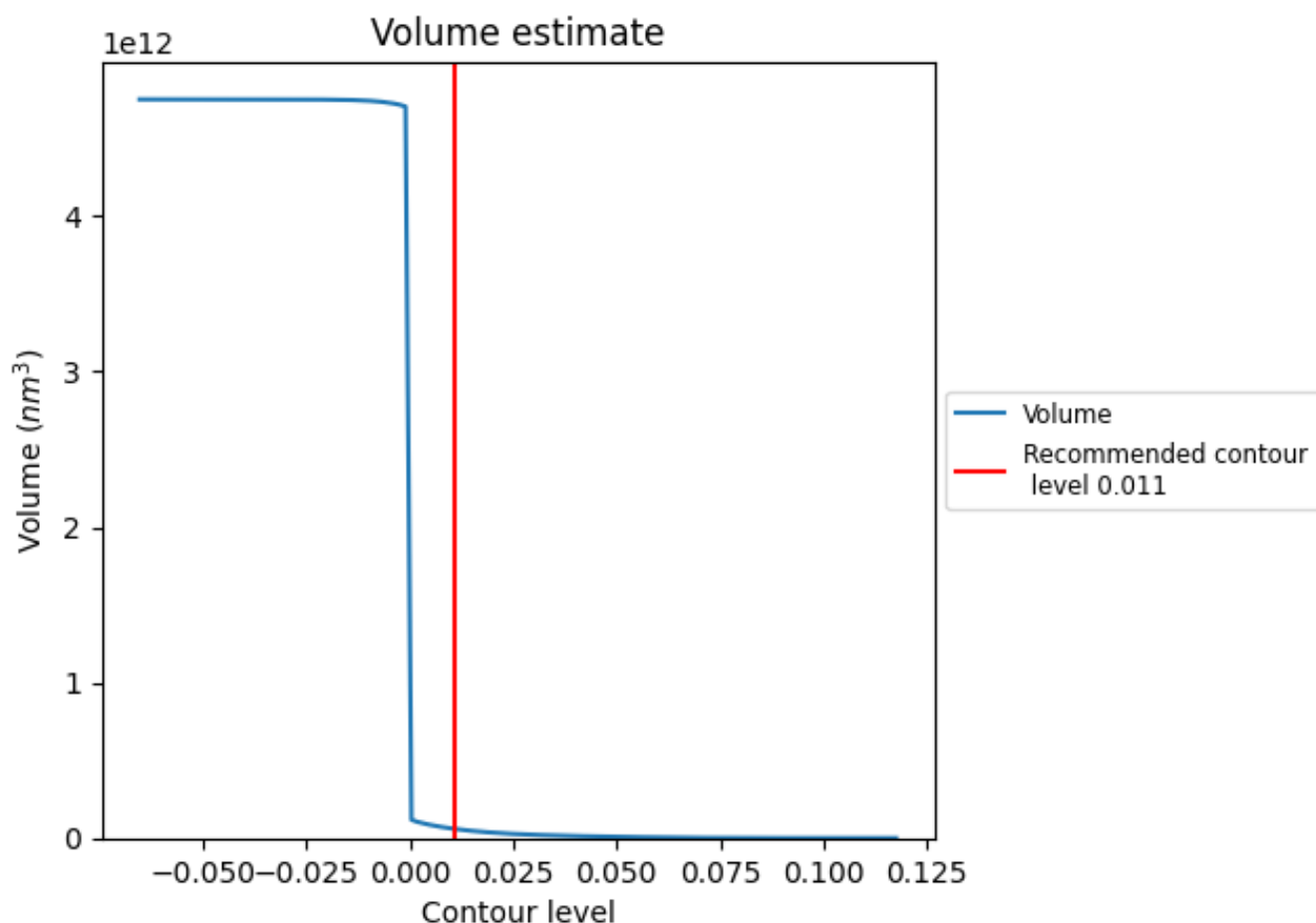
This section contains the results of statistical analysis of the map.

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.

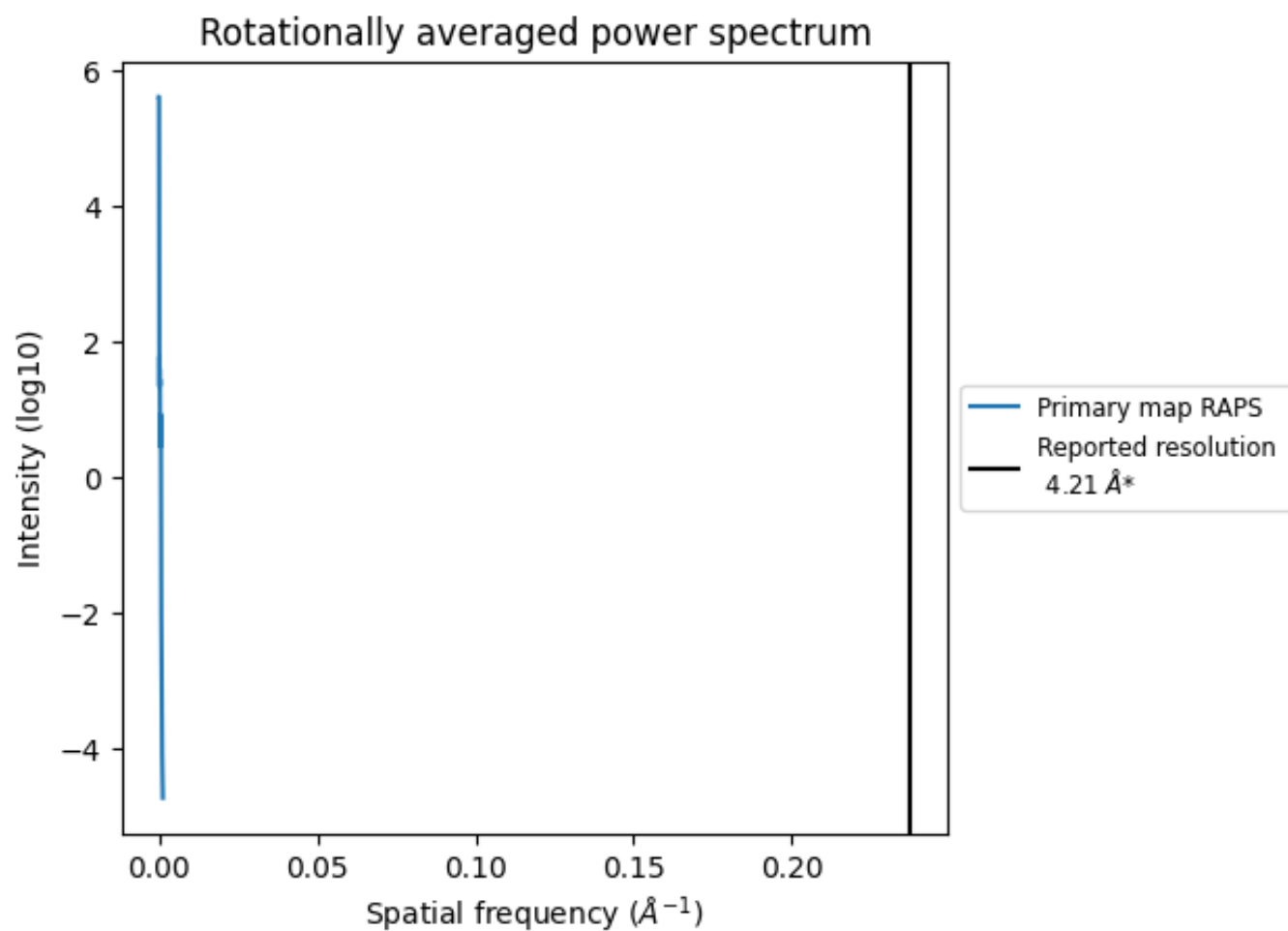
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58726214163 nm^3 ; this corresponds to an approximate mass of 53048918866 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 ⓘ

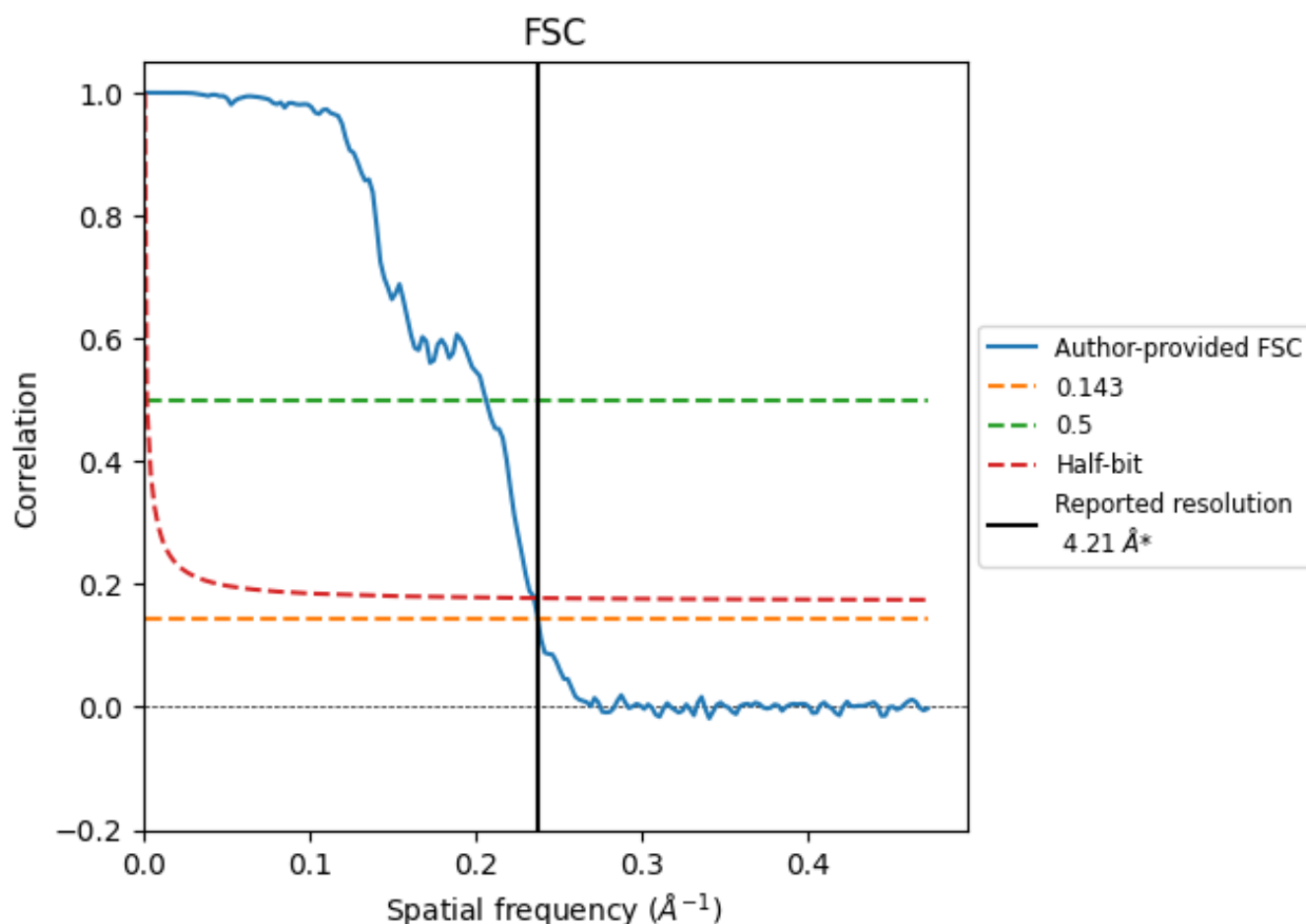


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

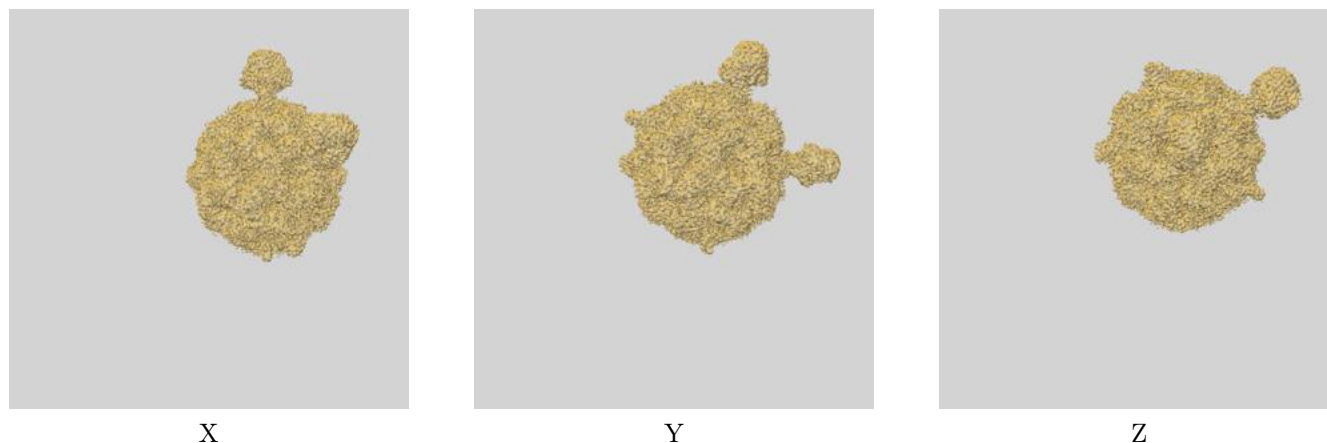
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.21	-	-
Author-provided FSC curve	4.21	4.85	4.26
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

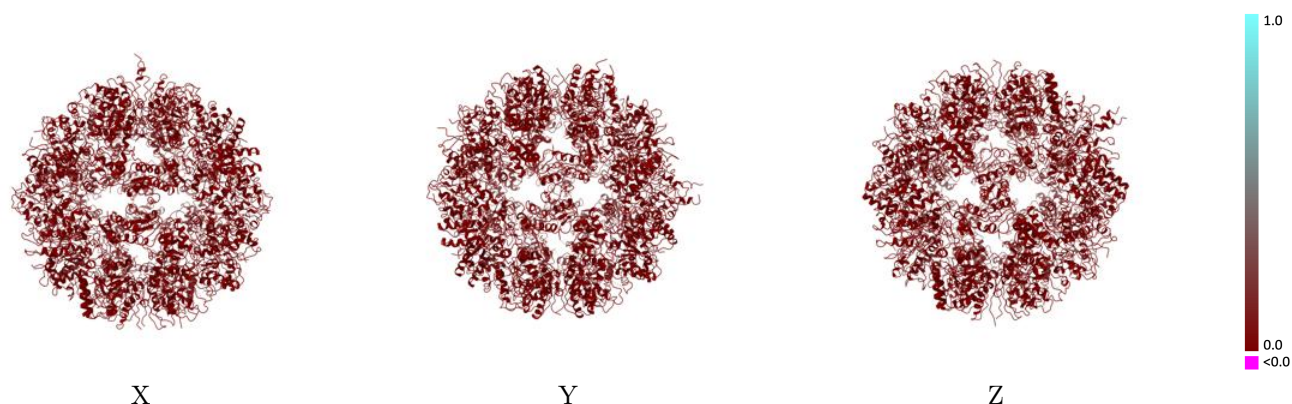
This section contains information regarding the fit between EMDB map EMD-4508 and PDB model 6QCM. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



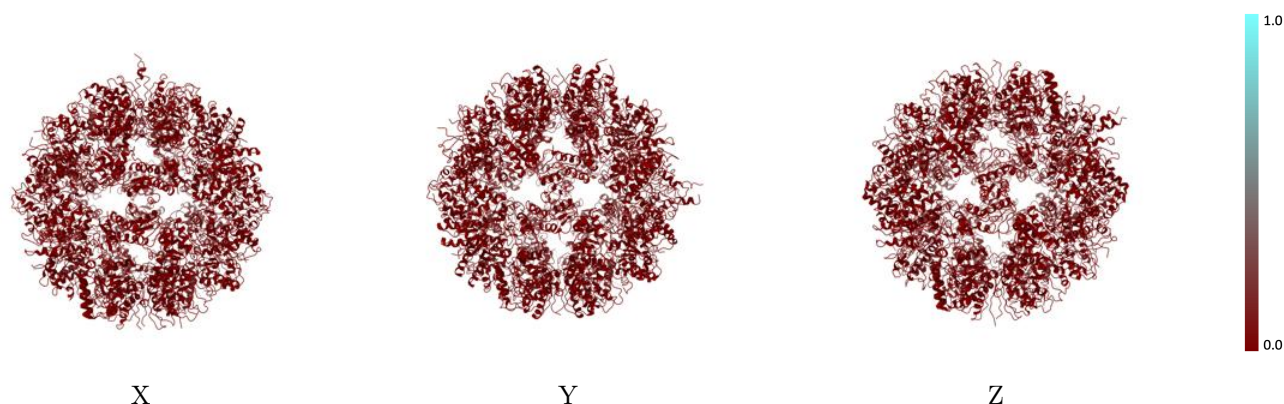
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



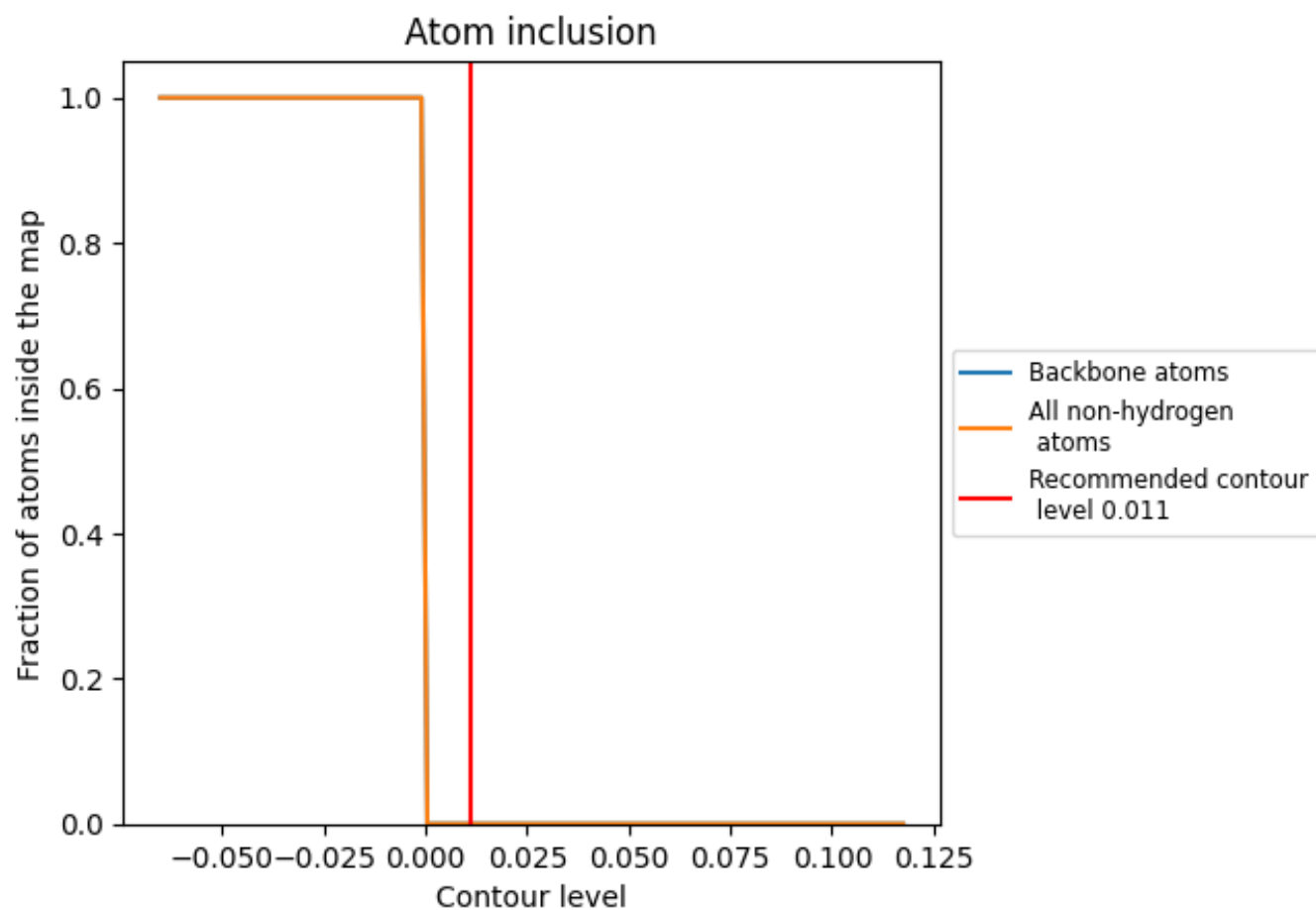
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A	0.0000	0.0000
AB	0.0000	0.0000
AD	0.0000	0.0000
B	0.0000	0.0000
BC	0.0000	0.0000
C	0.0000	0.0000
CB	0.0000	0.0000
CD	0.0000	0.0000
D	0.0000	0.0000
DB	0.0000	0.0000
DC	0.0000	0.0000
E	0.0000	0.0000
EB	0.0000	0.0000
F	0.0000	0.0000
FA	0.0000	0.0000
FB	0.0000	0.0000
FC	0.0000	0.0000
FD	0.0000	0.0000
GB	0.0000	0.0000
GC	0.0000	0.0000
HC	0.0000	0.0000
HD	0.0000	0.0000
I	0.0000	0.0000
IB	0.0000	0.0000
IC	0.0000	0.0000
J	0.0000	0.0000
K	0.0000	0.0000
KB	0.0000	0.0000
L	0.0000	0.0000
LB	0.0000	0.0000
M	0.0000	0.0000
N	0.0000	0.0000
O	0.0000	0.0000
OB	0.0000	0.0000



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Chain	Atom inclusion	Q-score
P	 0.0000	 0.0000
PB	 0.0000	 0.0000
Q	 0.0000	 0.0000
R	 0.0000	 0.0000
S	 0.0000	 0.0000
SB	 0.0000	 0.0000
T	 0.0000	 0.0000
TB	 0.0000	 0.0000
U	 0.0000	 0.0000
UB	 0.0000	 0.0000
V	 0.0000	 0.0000
VB	 0.0000	 0.0000
W	 0.0000	 0.0000
X	 0.0000	 0.0000
Y	 0.0000	 0.0000
Z	 0.0000	 0.0000
a	 0.0000	 0.0000
b	 0.0000	 0.0000
c	 0.0000	 0.0000
d	 0.0000	 0.0000
e	 0.0000	 0.0000
f	 0.0000	 0.0000
g	 0.0000	 0.0000
h	 0.0000	 0.0000
i	 0.0000	 0.0000
j	 0.0000	 0.0000