



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:37 AM UTC

PDB ID : 7B0U / pdb_00007b0u
EMDB ID : EMD-11971
Title : Stressosome complex from *Listeria innocua*
Authors : Miksys, A.; Fu, L.; Madej, M.G.; Ziegler, C.
Deposited on : 2020-11-22
Resolution : 3.86 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:

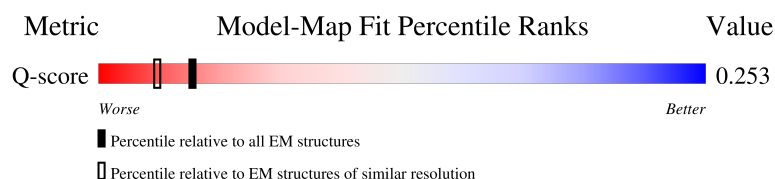
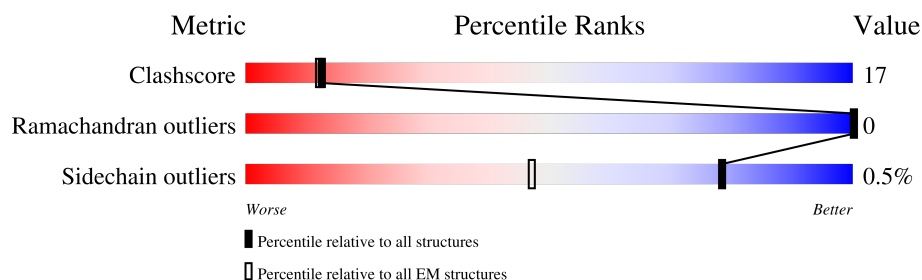
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8889 (3.36 - 4.35)

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	7	278	55% 80% 18% .
1	A	278	51% 82% 17% .
1	C	278	53% 86% 13% .
1	G	278	53% 86% 13% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	278	51% 81% 17%
1	Q	278	55% 81% 17%
1	R	278	53% 87% 12%
1	V	278	53% 86% 13%
1	d	278	55% 82% 16%
1	e	278	51% 82% 17%
1	g	278	53% 86% 12%
1	k	278	53% 85% 14%
1	s	278	55% 81% 17%
1	t	278	51% 82% 17%
1	v	278	53% 86% 13%
1	z	278	53% 85% 14%
2	0	278	53% 86% 13%
2	2	278	52% 80% 19%
2	B	278	51% 79% 19%
2	D	278	53% 79% 19%
2	H	278	53% 86% 13%
2	J	278	52% 81% 17%
2	L	278	51% 79% 19%
2	S	278	53% 78% 20%
2	W	278	53% 86% 13%
2	Y	278	52% 81% 18%
2	f	278	51% 79% 19%
2	h	278	53% 77% 21%
2	l	278	53% 86% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	n	278	
2	u	278	
2	w	278	
3	1	118	
3	4	118	
3	5	118	
3	E	118	
3	F	118	
3	I	118	
3	N	118	
3	O	118	
3	T	118	
3	U	118	
3	X	118	
3	a	118	
3	b	118	
3	i	118	
3	j	118	
3	m	118	
3	p	118	
3	q	118	
3	x	118	
3	y	118	
4	3	278	
4	M	278	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Z	278	55% 77% 21% ..
4	o	278	55% 76% 22% ..
5	6	278	56% 84% 14% .
5	P	278	56% 84% 14% .
5	c	278	56% 84% 14% .
5	r	278	56% 84% 14% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 105492 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	A	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	C	274	Total	C	N	O	S	1	0
			2201	1410	360	419	12		
1	G	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	Q	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	K	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	R	274	Total	C	N	O	S	1	0
			2201	1410	360	419	12		
1	V	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	d	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	e	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	g	274	Total	C	N	O	S	1	0
			2201	1410	360	419	12		
1	k	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	s	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	t	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	v	274	Total	C	N	O	S	1	0
			2201	1410	360	419	12		
1	z	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		
1	7	274	Total	C	N	O	S	0	0
			2192	1405	359	416	12		

- Molecule 2 is a protein called RsbR protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	D	274	Total	C	N	O	P	S	1	0
			2207	1409	360	424	2	12		
2	H	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	J	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	L	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	S	274	Total	C	N	O	P	S	1	0
			2207	1409	360	424	2	12		
2	W	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	Y	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	f	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	h	274	Total	C	N	O	P	S	1	0
			2207	1409	360	424	2	12		
2	l	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	n	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	u	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	w	274	Total	C	N	O	P	S	1	0
			2207	1409	360	424	2	12		
2	0	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
2	2	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		

- Molecule 3 is a protein called RsbS protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
3	F	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
3	I	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
3	N	118	Total	C	N	O	S	0	0
			881	565	136	175	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	T	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	U	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	X	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	a	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	b	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	i	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	j	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	m	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	p	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	q	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	x	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	y	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	1	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	4	118	Total 881	C 565	N 136	O 175	S 5	0	0
3	5	118	Total 881	C 565	N 136	O 175	S 5	0	0

- Molecule 4 is a protein called RsbR protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	M	274	Total 2200	C 1405	N 359	O 422	P 2	S 12	0	0
4	Z	274	Total 2200	C 1405	N 359	O 422	P 2	S 12	0	0
4	o	274	Total 2200	C 1405	N 359	O 422	P 2	S 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	274	Total	C	N	O	P	S	0	0
			2200	1405	359	422	2	12		

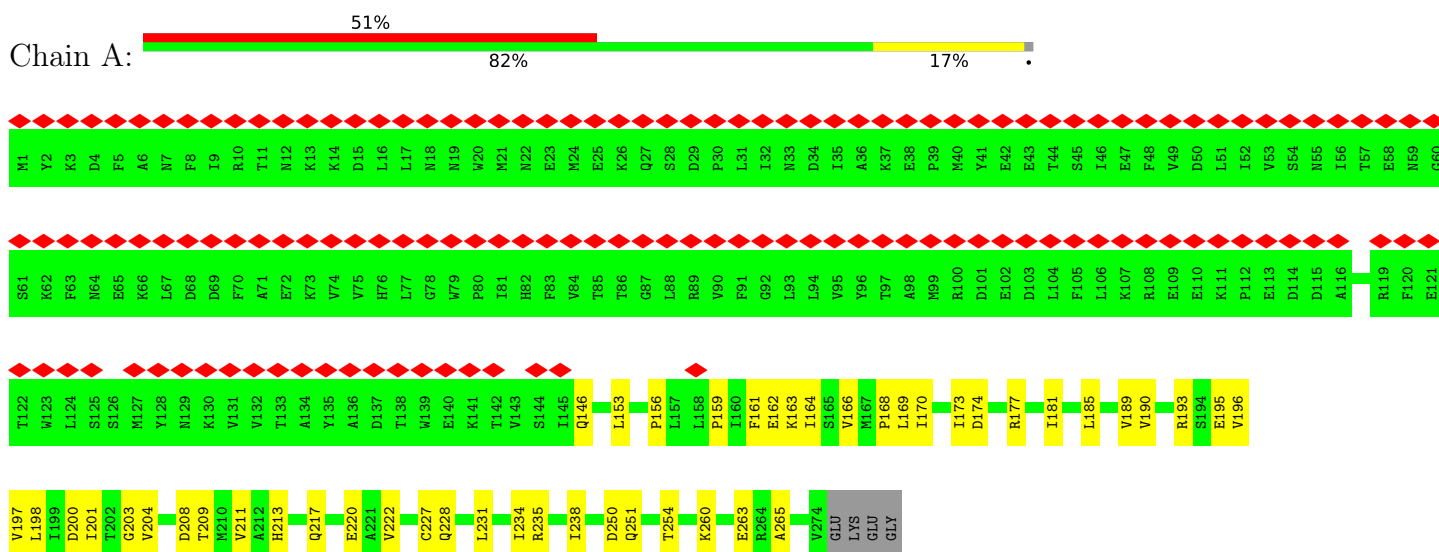
- Molecule 5 is a protein called RsbR protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	P	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
5	c	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
5	r	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		
5	6	274	Total	C	N	O	P	S	0	0
			2196	1405	359	419	1	12		

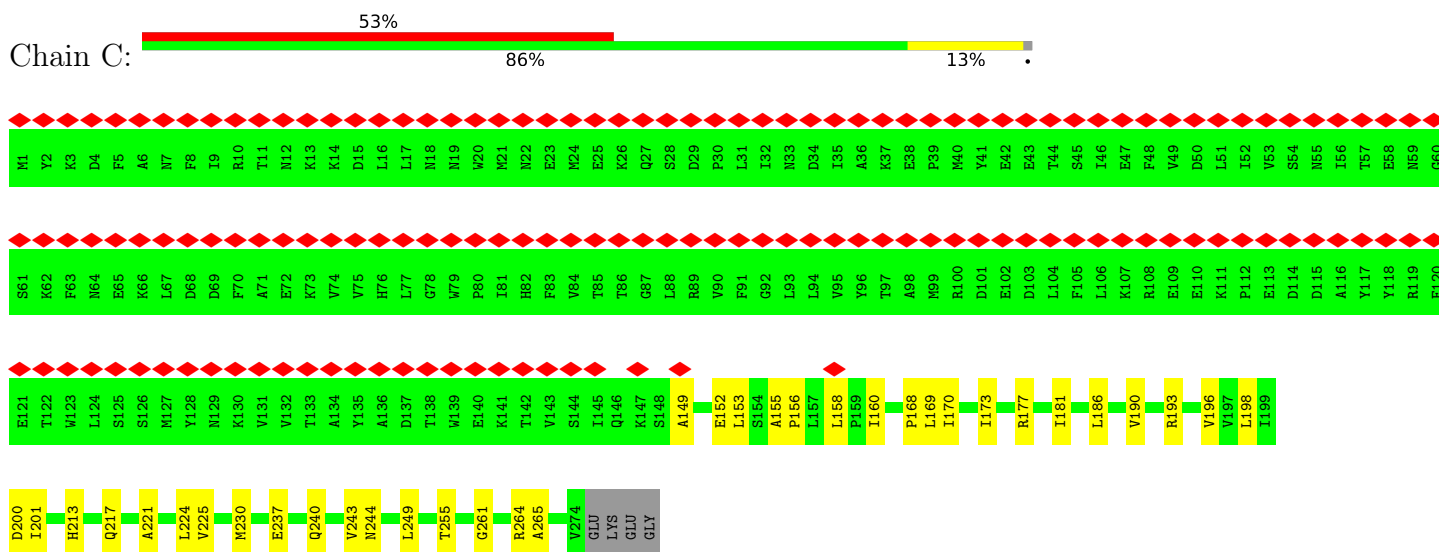
3 Residue-property plots

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

• Molecule 1: RsbR protein

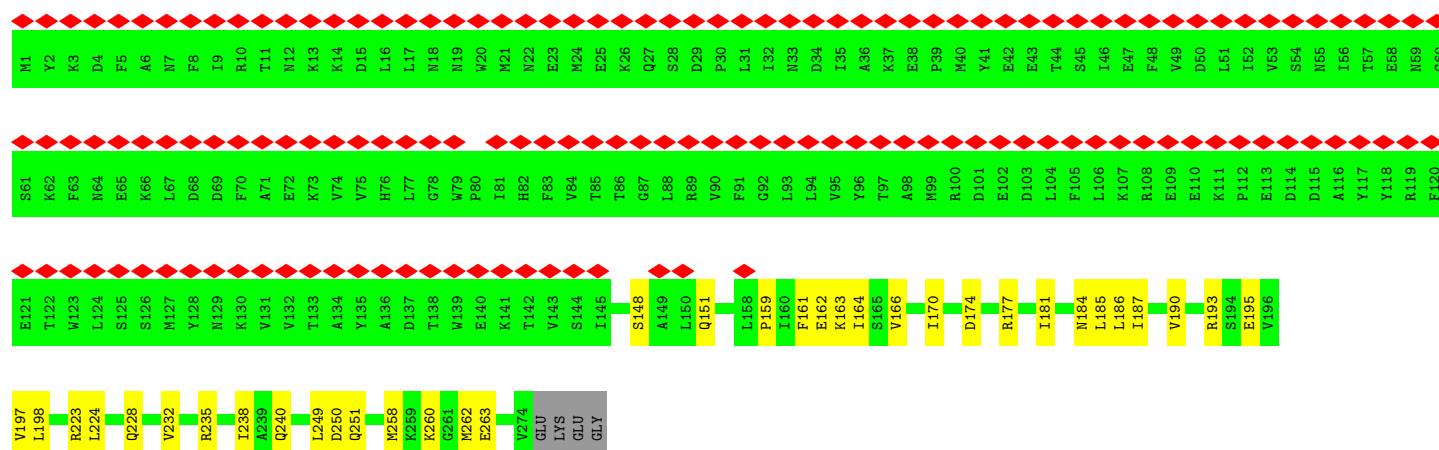


• Molecule 1: RsbR protein



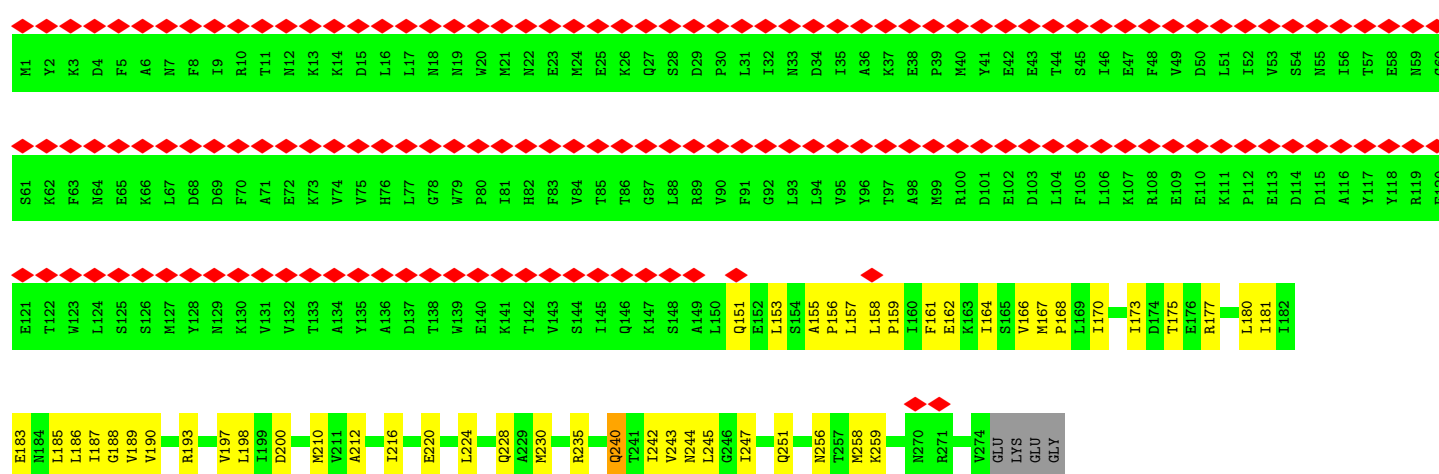
• Molecule 1: RsbR protein

Chain G: 



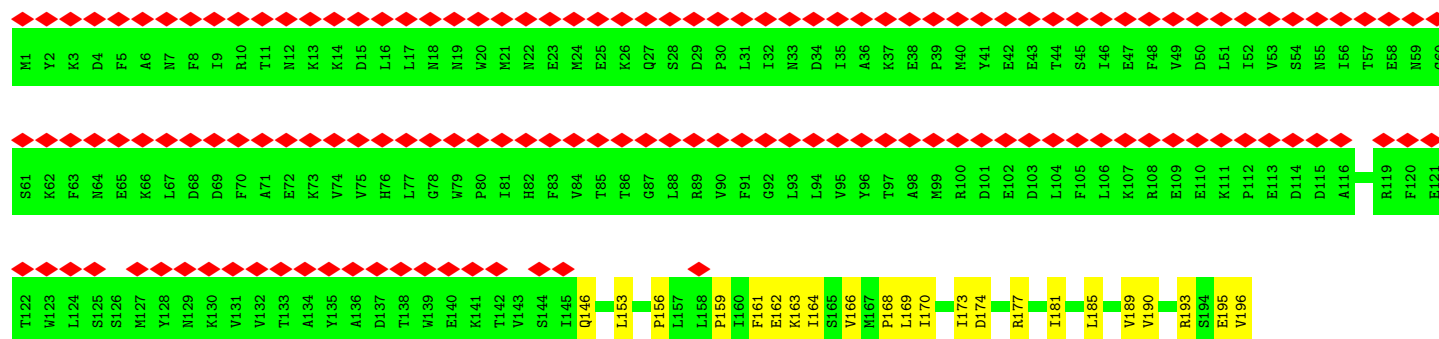
• Molecule 1: RsbR protein

Chain Q: 



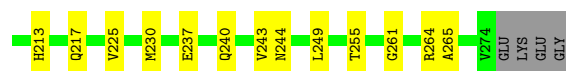
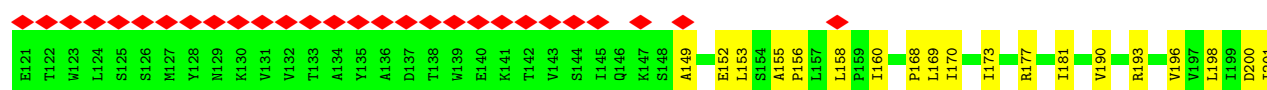
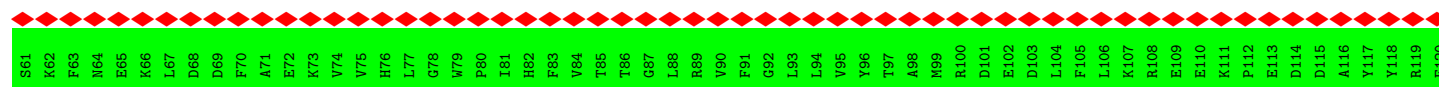
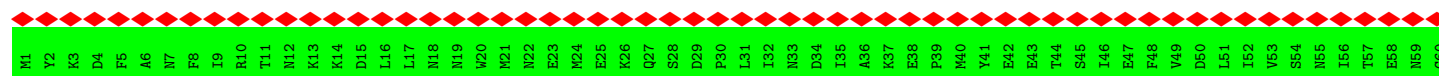
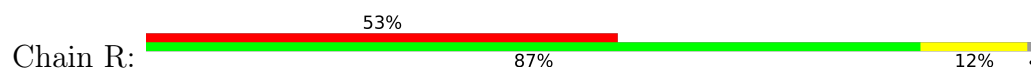
• Molecule 1: RsbR protein

Chain K: 

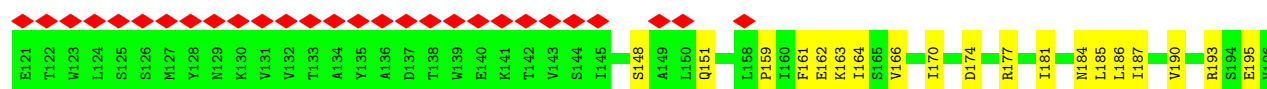
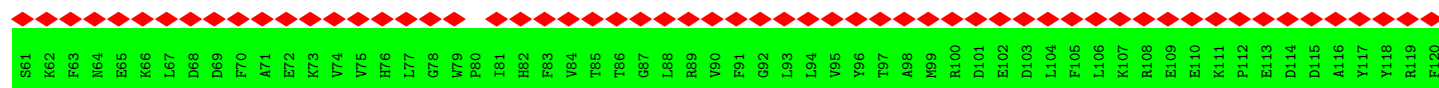
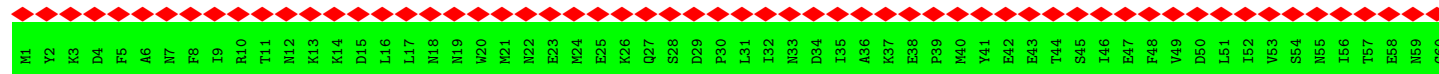
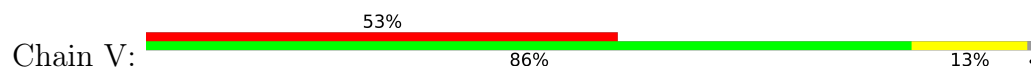




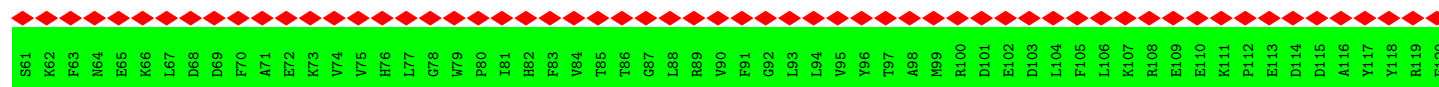
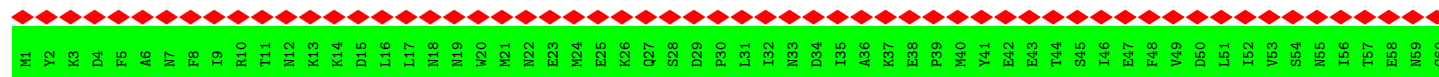
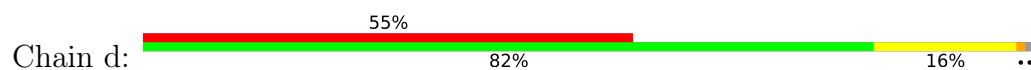
• Molecule 1: RsbR protein

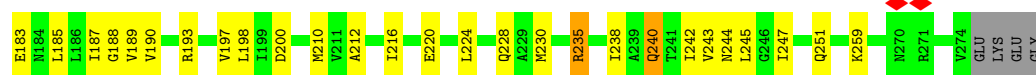
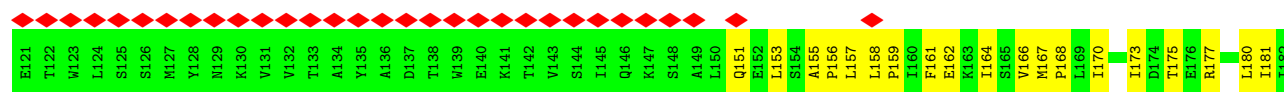


• Molecule 1: RsbR protein

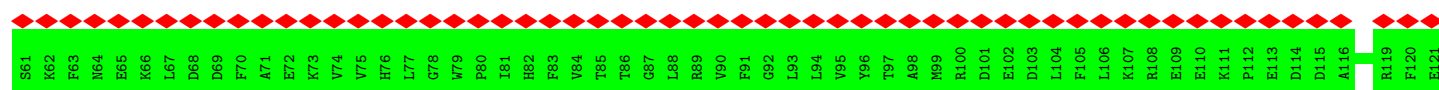
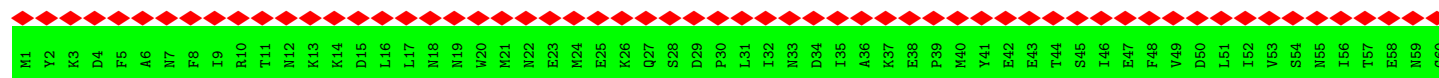
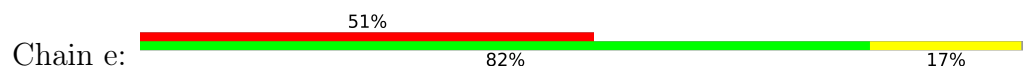


• Molecule 1: RsbR protein

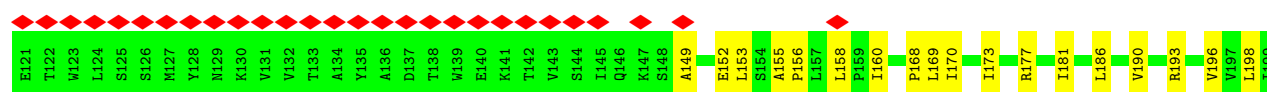
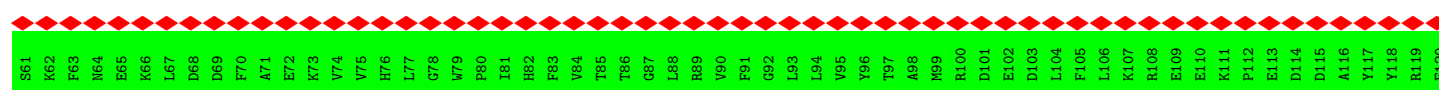
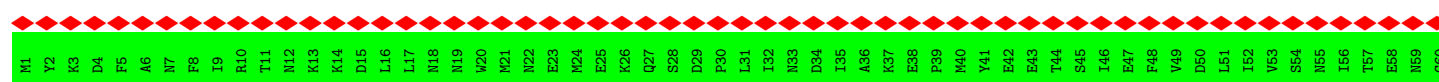
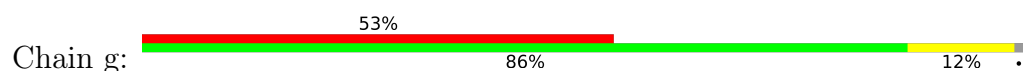




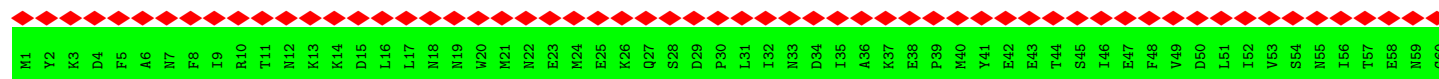
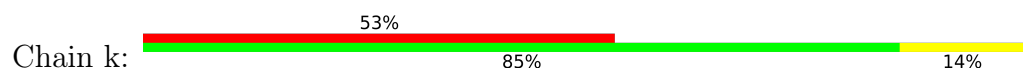
• Molecule 1: RsbR protein



• Molecule 1: RsbR protein

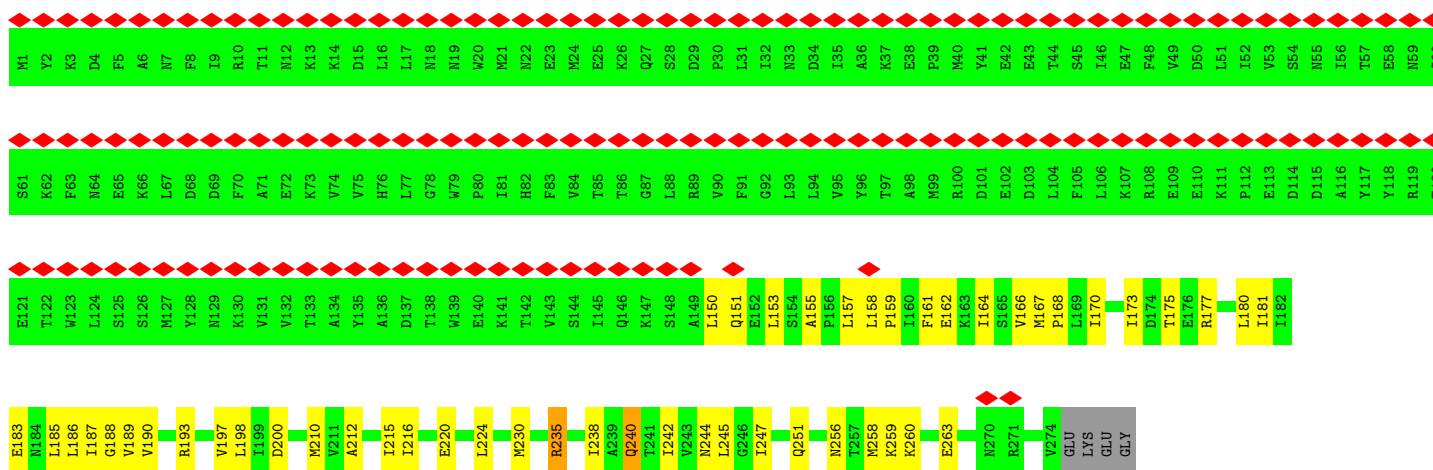
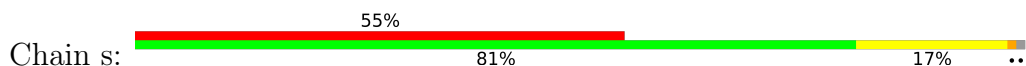


• Molecule 1: RsbR protein

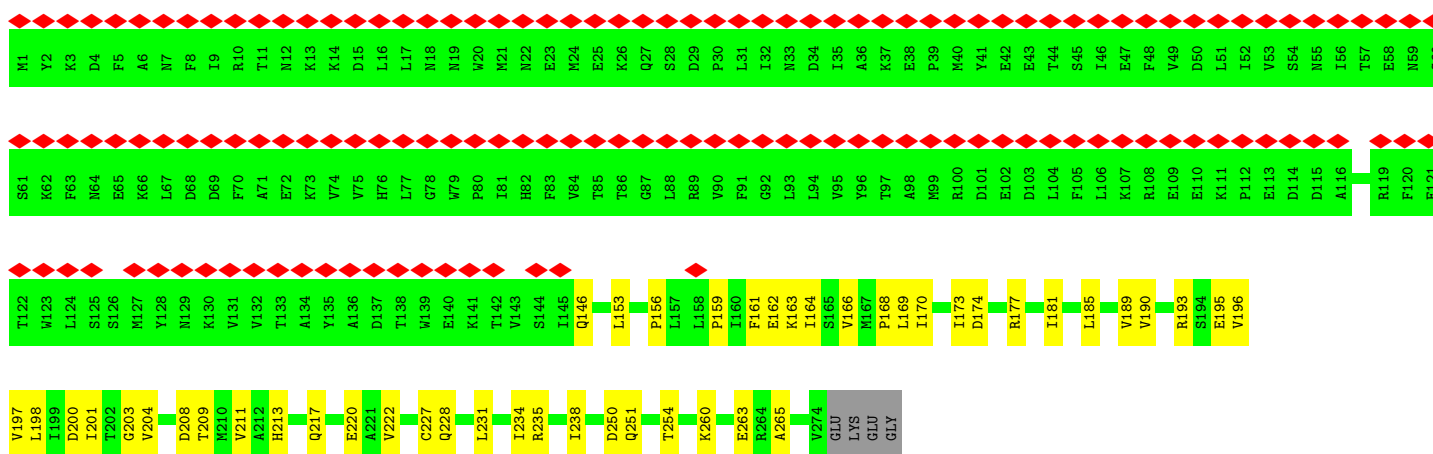
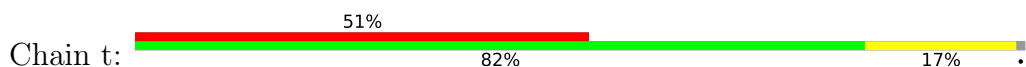




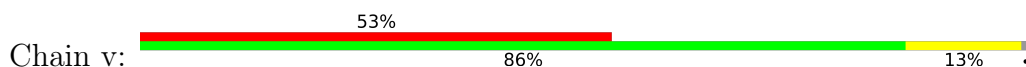
• Molecule 1: RsbR protein

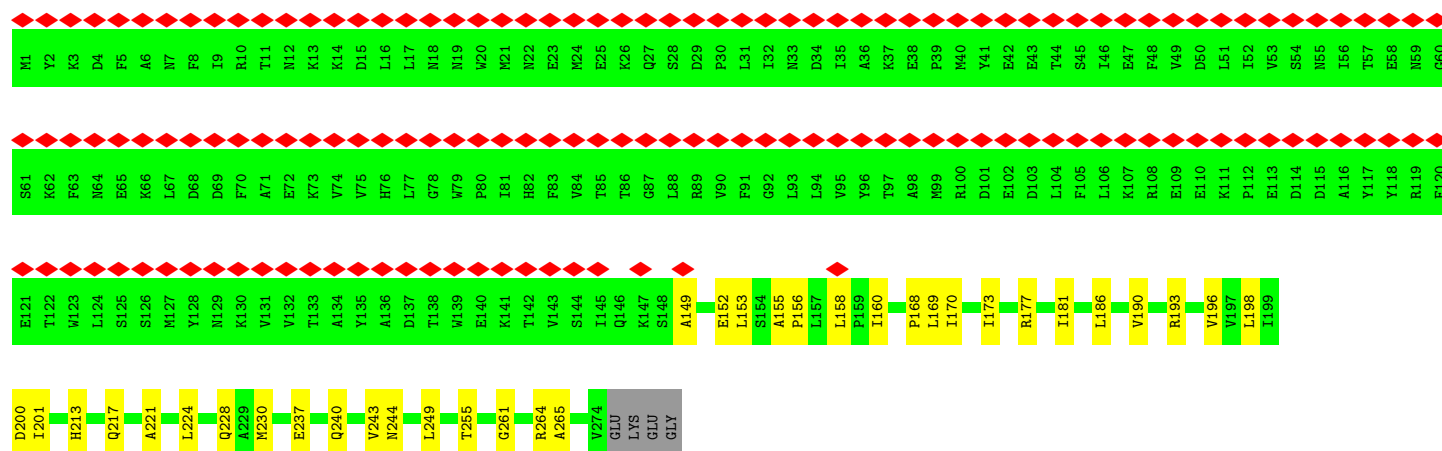


• Molecule 1: RsbR protein

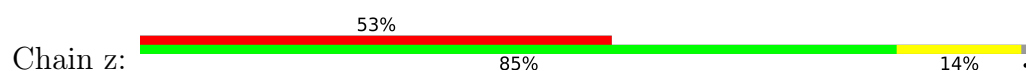


• Molecule 1: RsbR protein

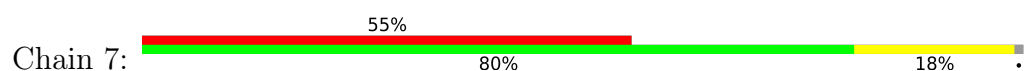




• Molecule 1: RsbR protein

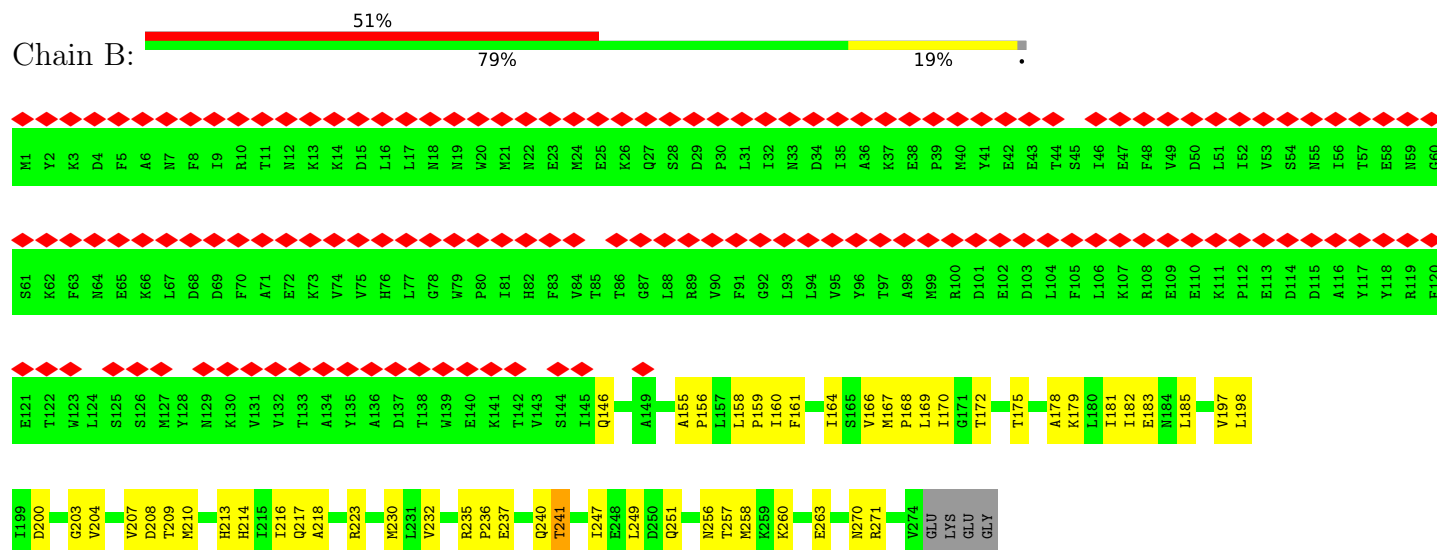


• Molecule 1: RsbR protein



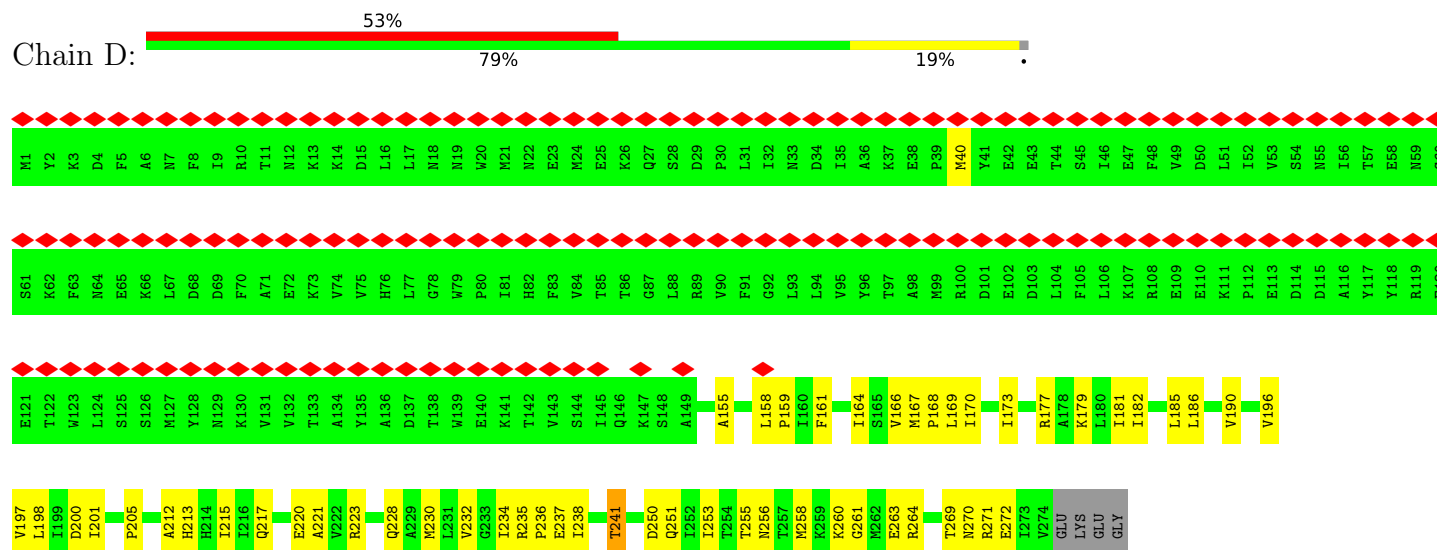
- Molecule 2: RsbR protein

Chain B:



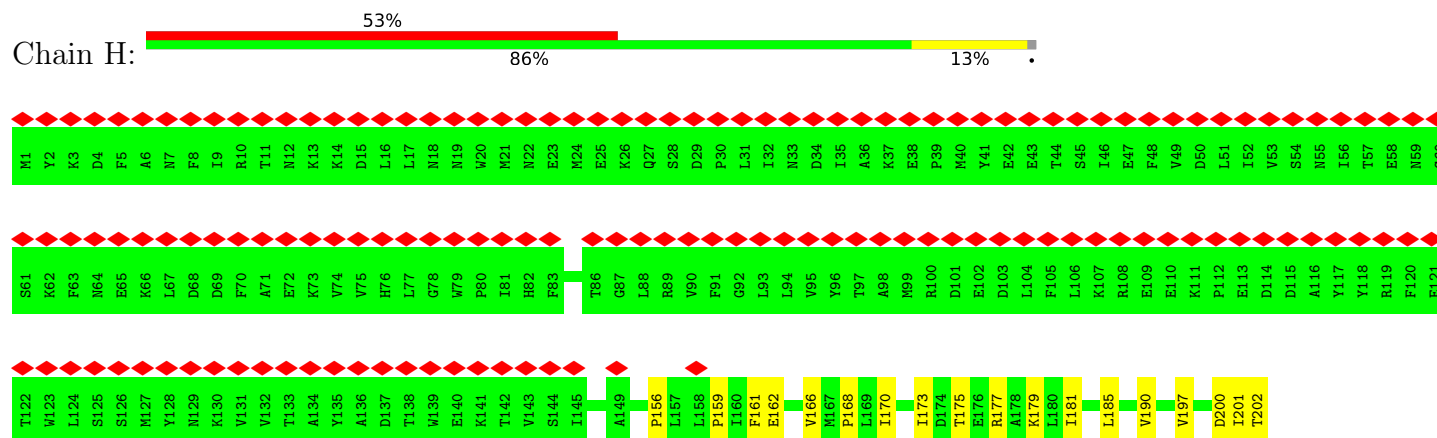
- Molecule 2: RsbR protein

Chain D:



- Molecule 2: RsbR protein

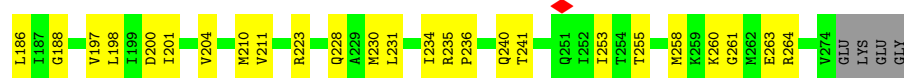
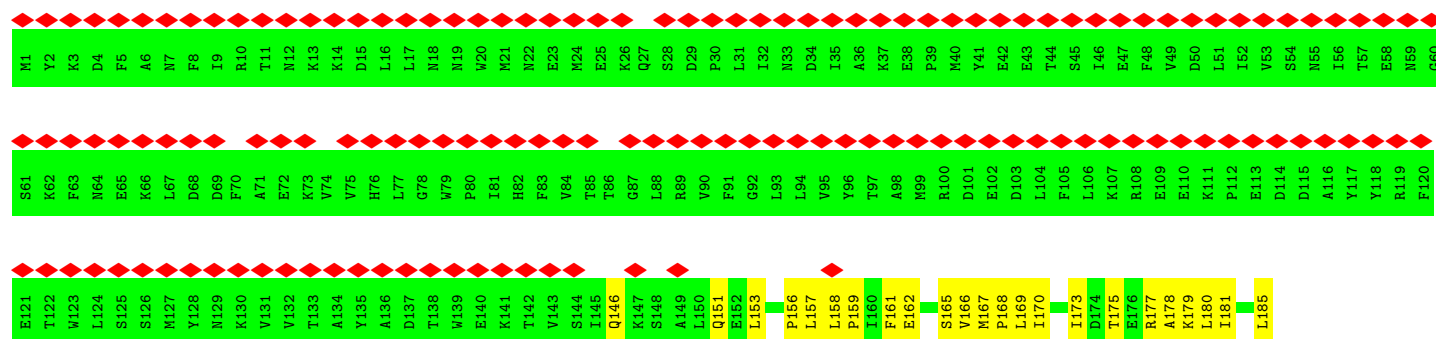
Chain H:





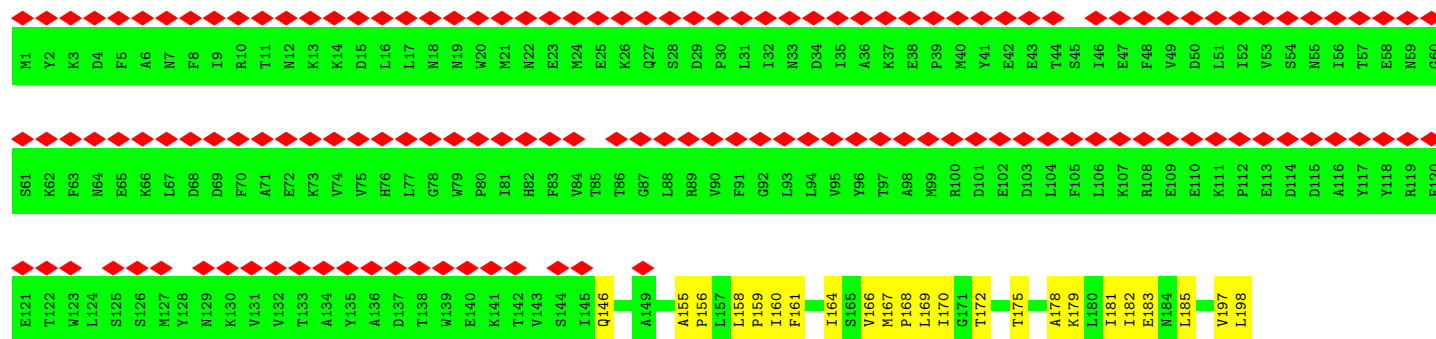
• Molecule 2: RsbR protein

Chain J: 52% 81% 17%



• Molecule 2: RsbR protein

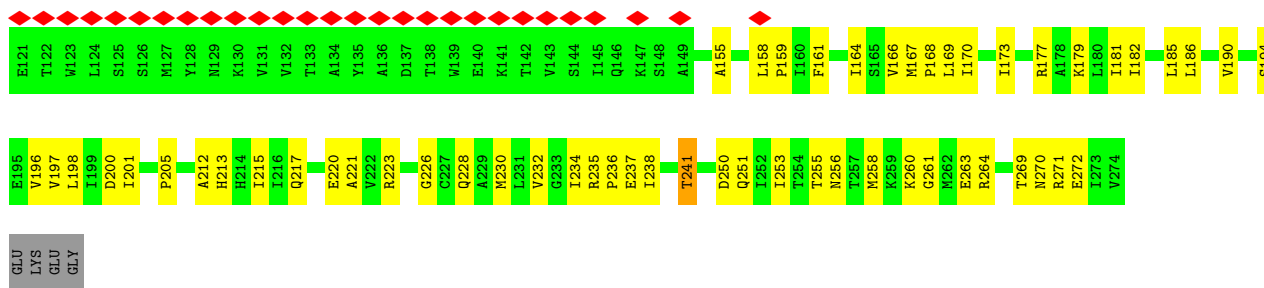
Chain L: 51% 79% 19%



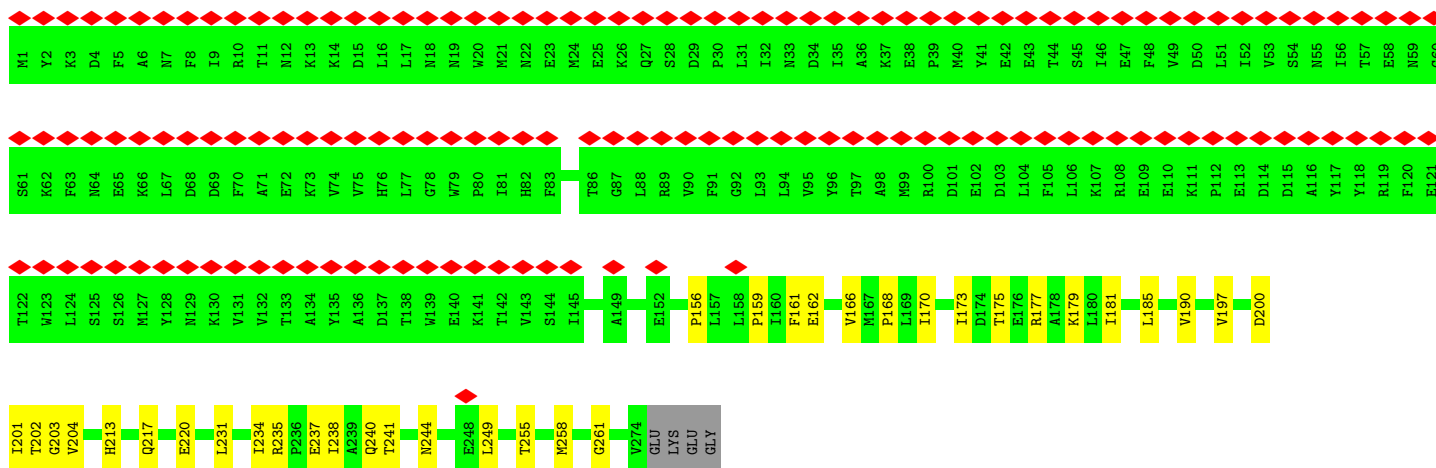
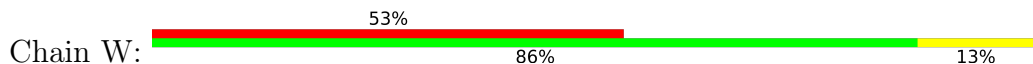
• Molecule 2: RsbR protein

Chain S: 53% 78% 20%

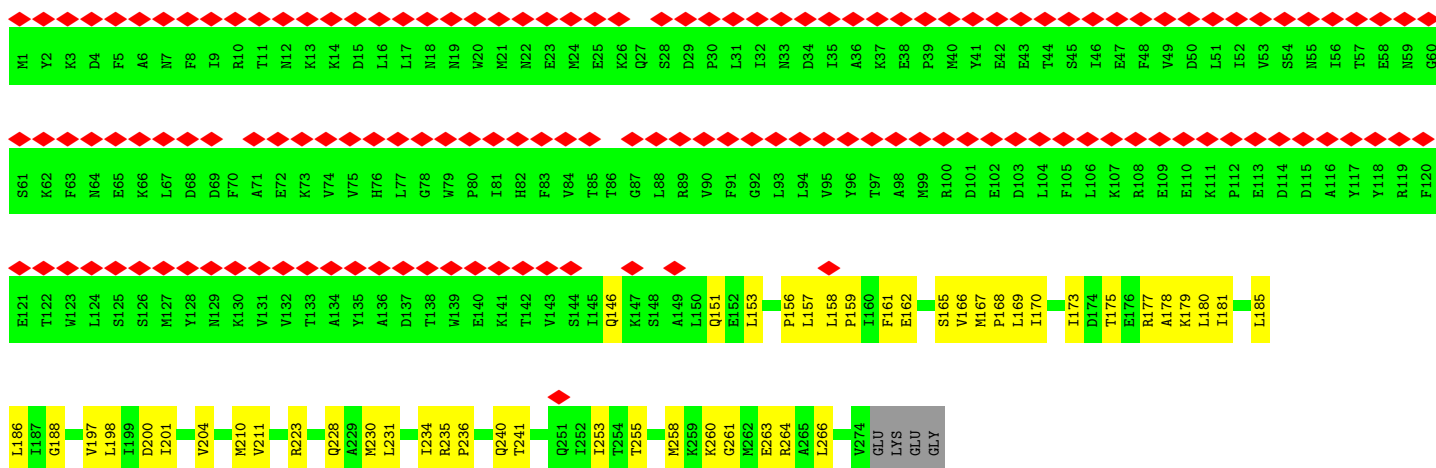
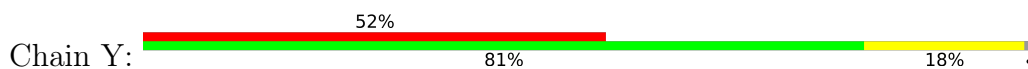




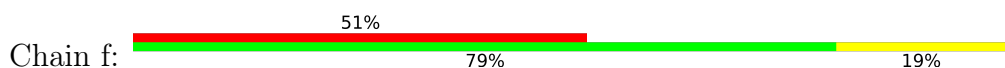
• Molecule 2: RsbR protein

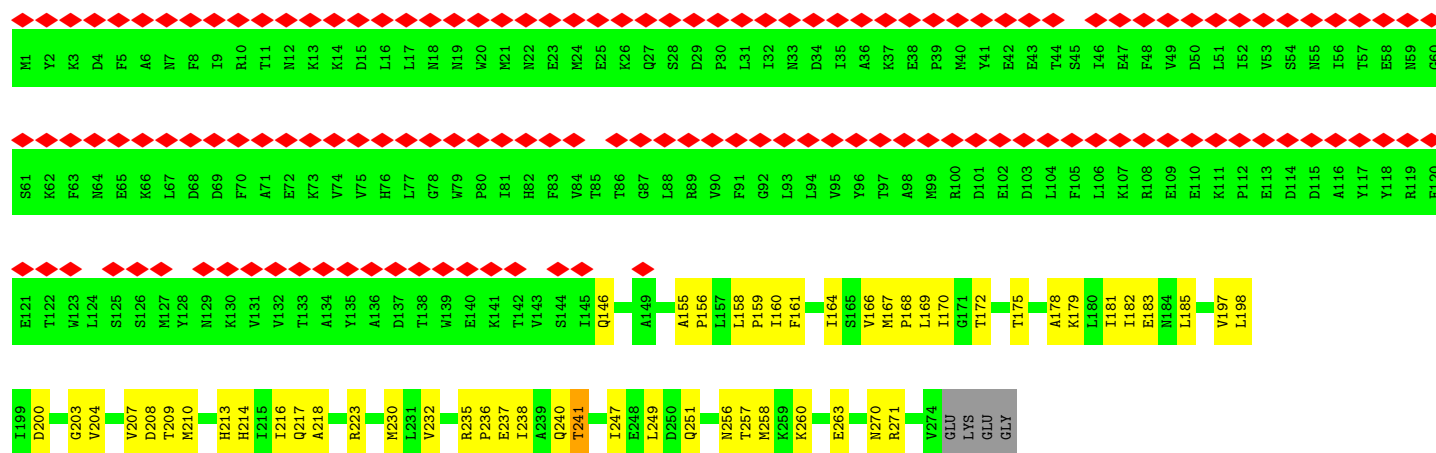


• Molecule 2: RsbR protein

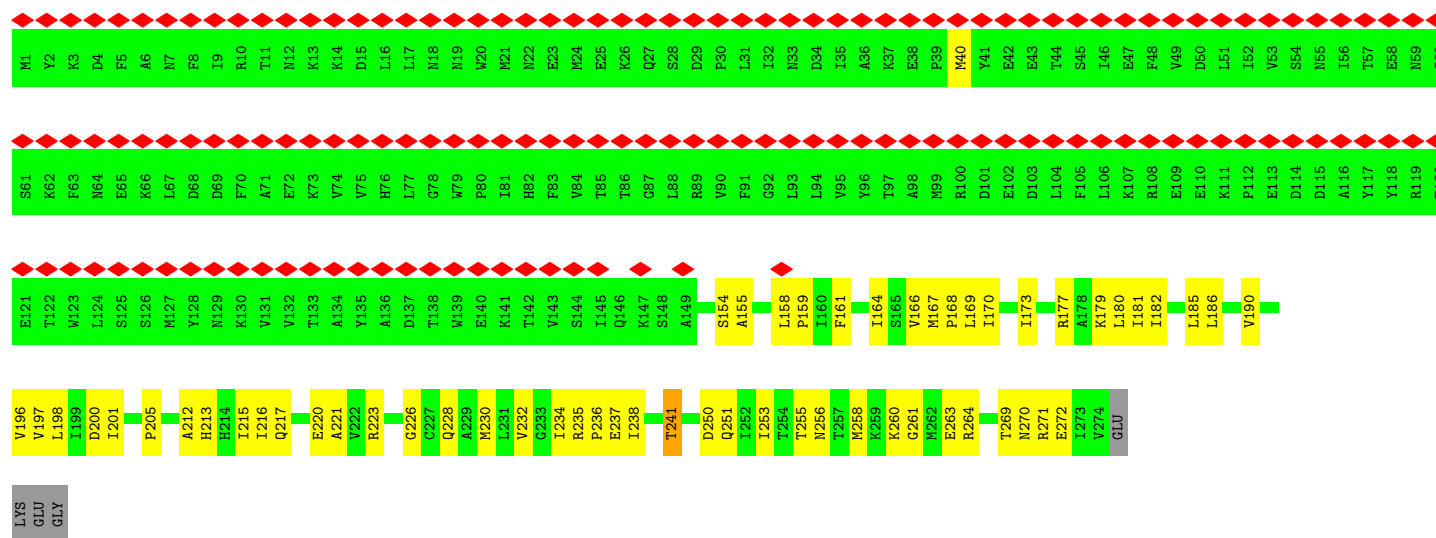
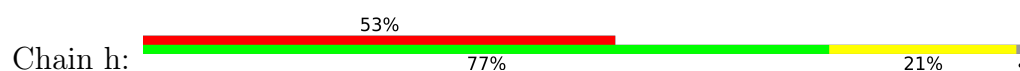


• Molecule 2: RsbR protein

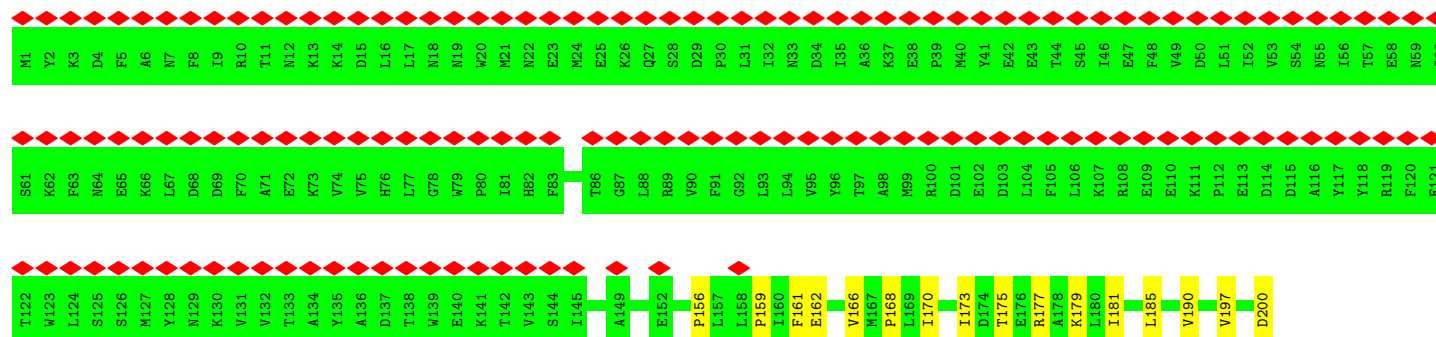
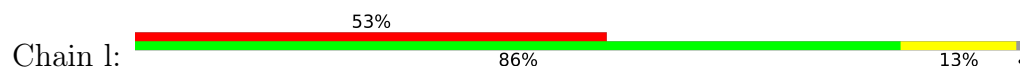




• Molecule 2: RsbR protein

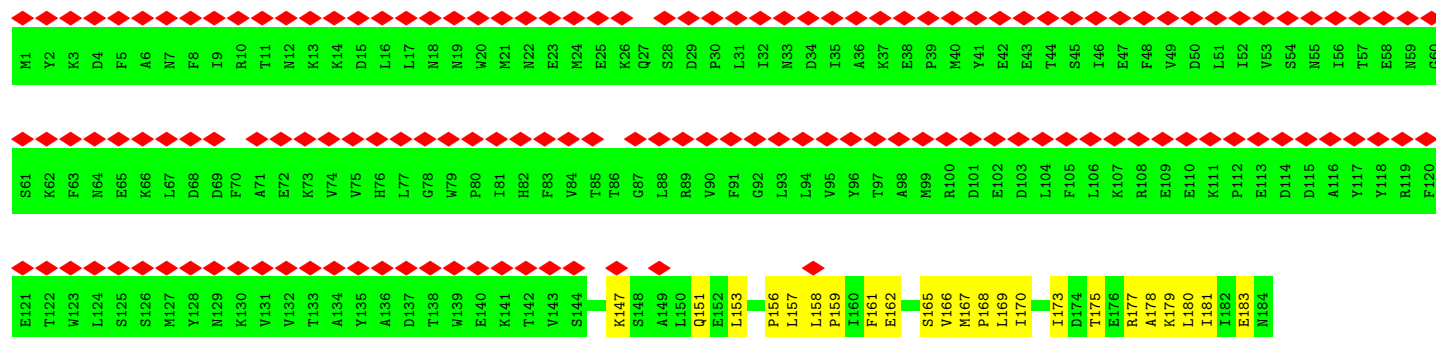
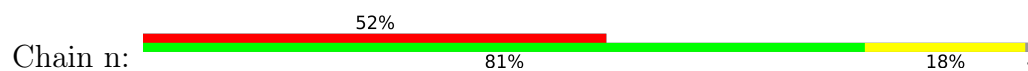


• Molecule 2: RsbR protein

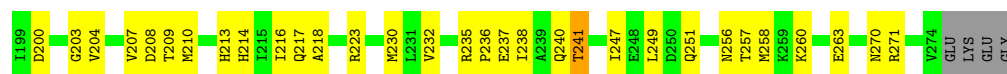
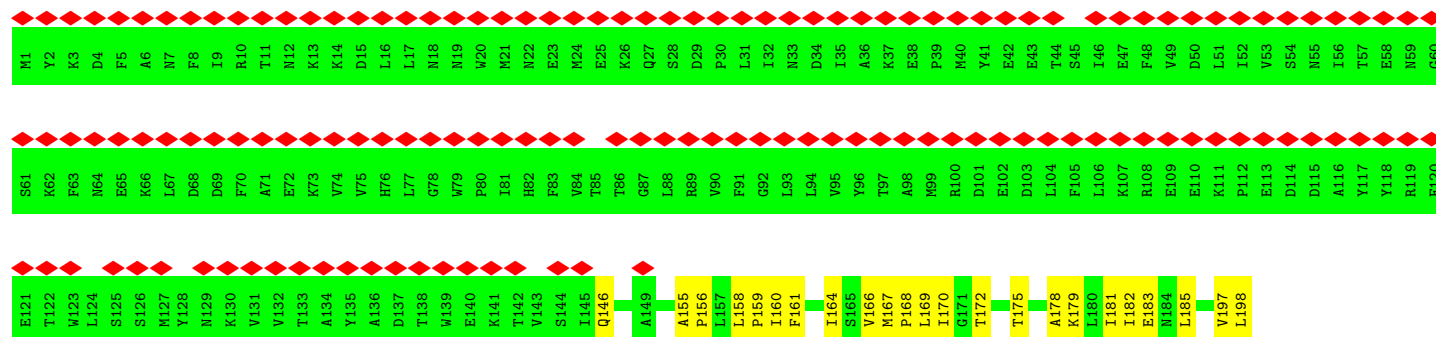
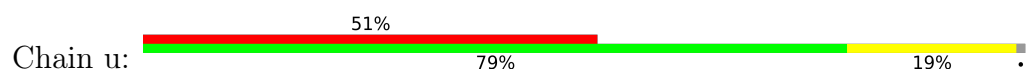




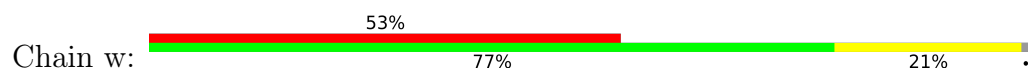
• Molecule 2: RsbR protein

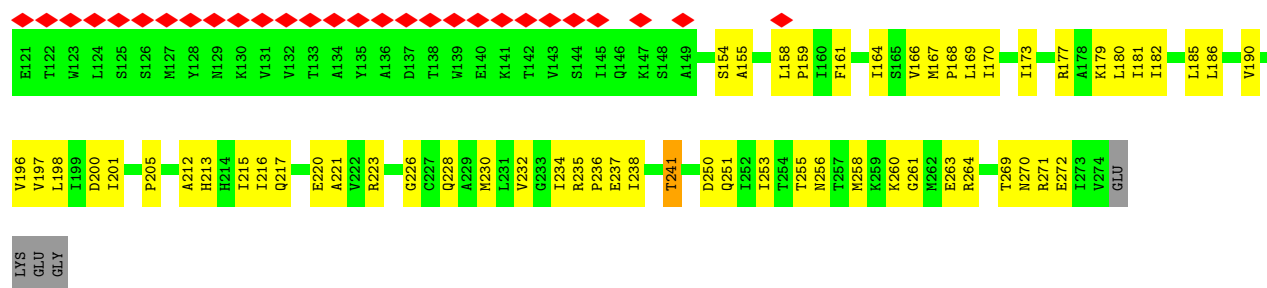


• Molecule 2: RsbR protein

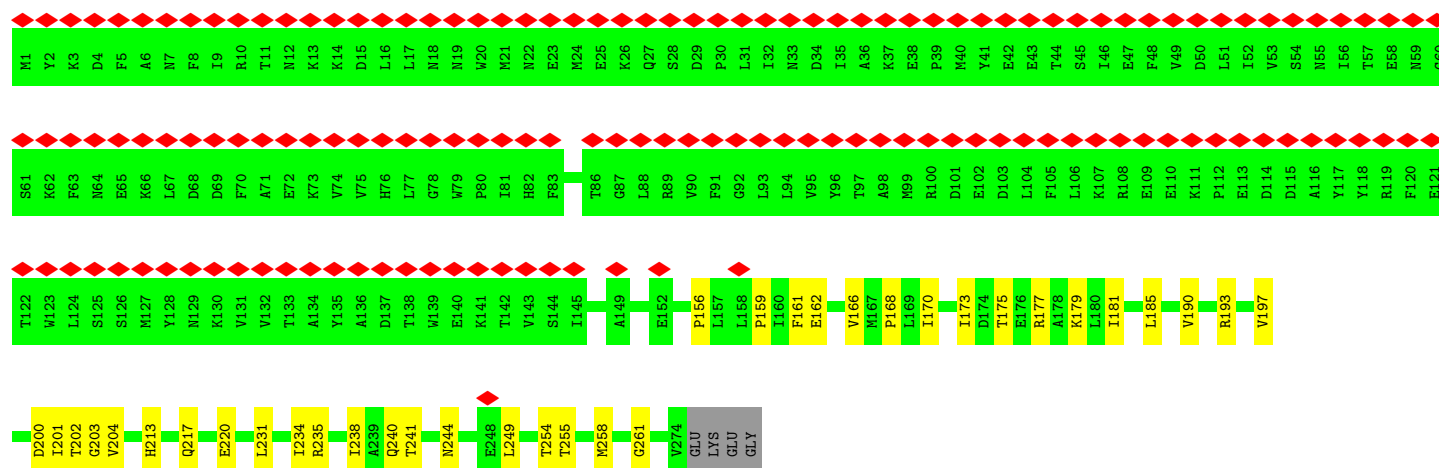
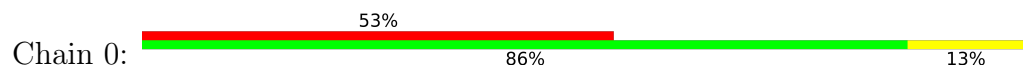


• Molecule 2: RsbR protein

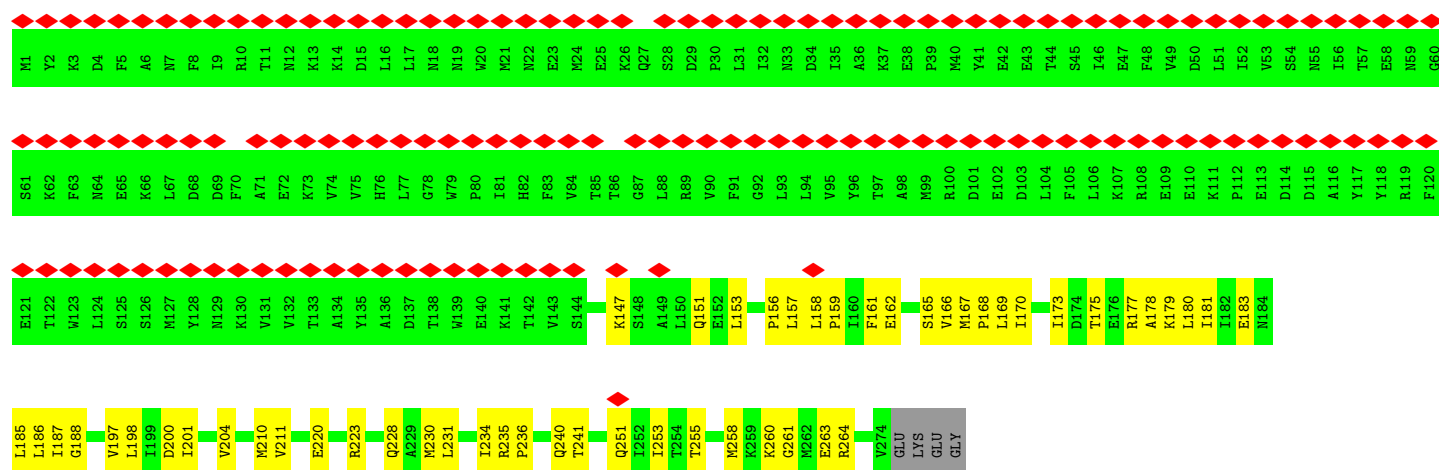
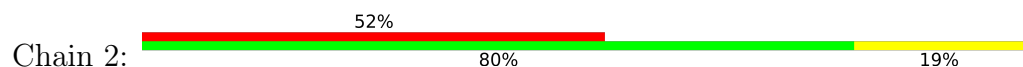




• Molecule 2: RsbR protein



• Molecule 2: RsbR protein

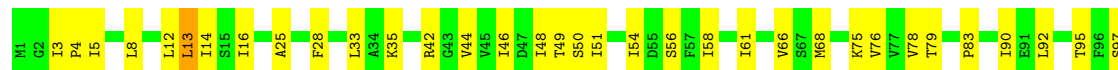


• Molecule 3: RsbS protein

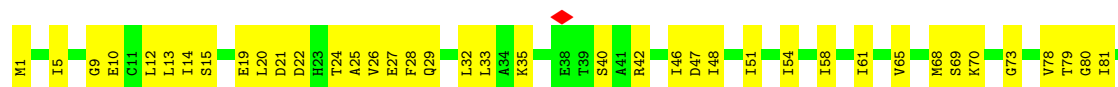




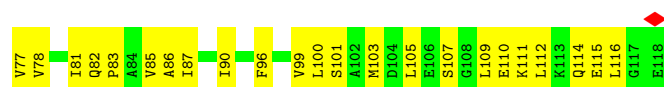
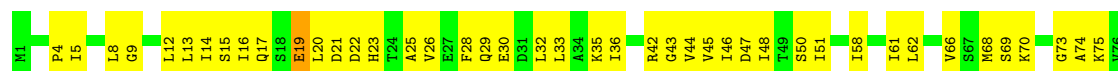
• Molecule 3: RsbS protein



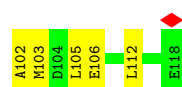
• Molecule 3: RsbS protein



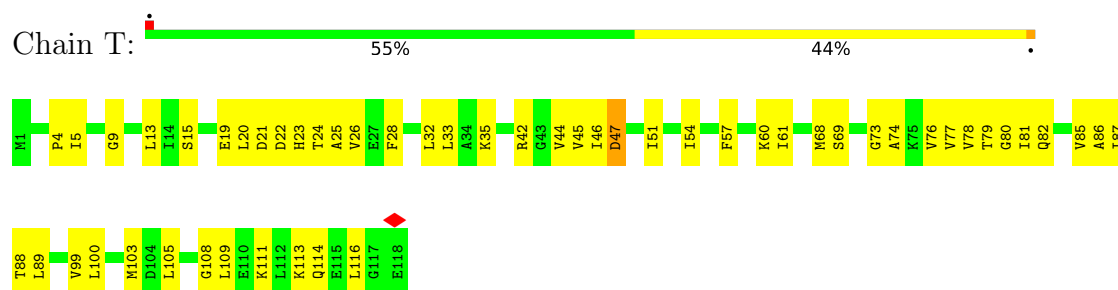
• Molecule 3: RsbS protein



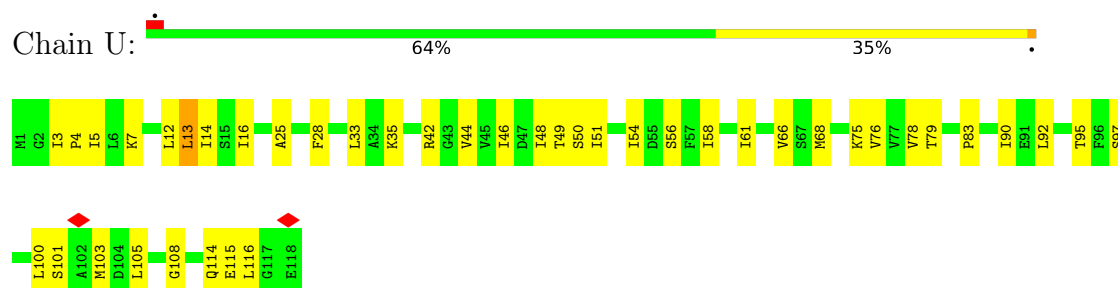
• Molecule 3: RsbS protein



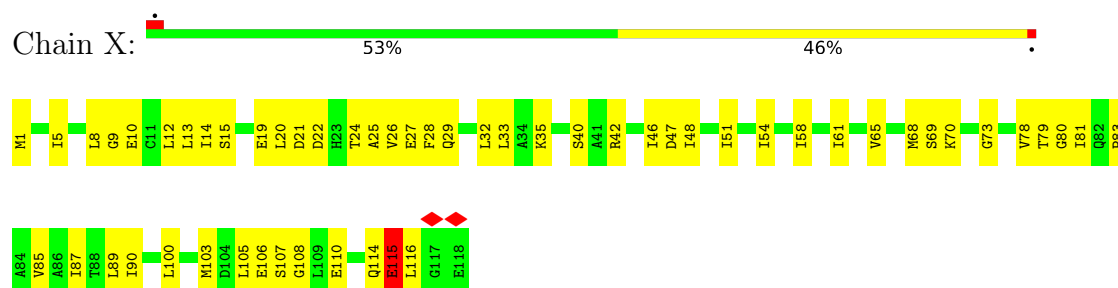
- Molecule 3: RsbS protein



- Molecule 3: RsbS protein



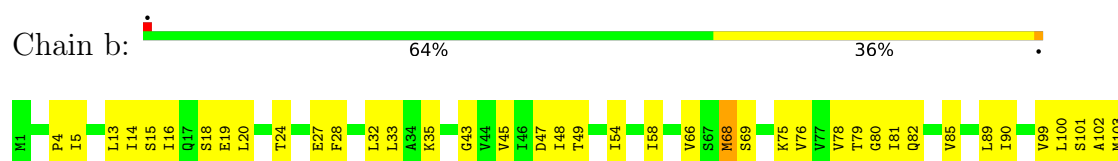
- Molecule 3: RsbS protein



- Molecule 3: RsbS protein



- Molecule 3: RsbS protein

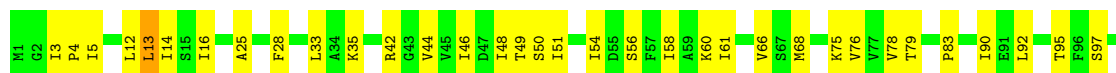




• Molecule 3: RsbS protein



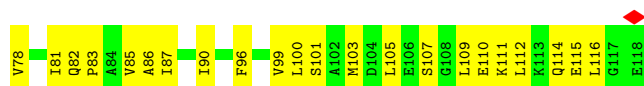
• Molecule 3: RsbS protein



• Molecule 3: RsbS protein



• Molecule 3: RsbS protein



• Molecule 3: RsbS protein

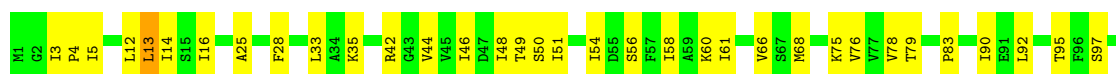




• Molecule 3: RsbS protein



• Molecule 3: RsbS protein



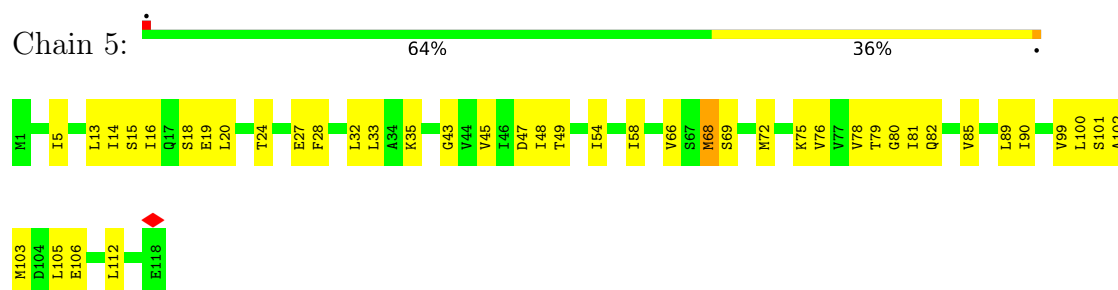
• Molecule 3: RsbS protein



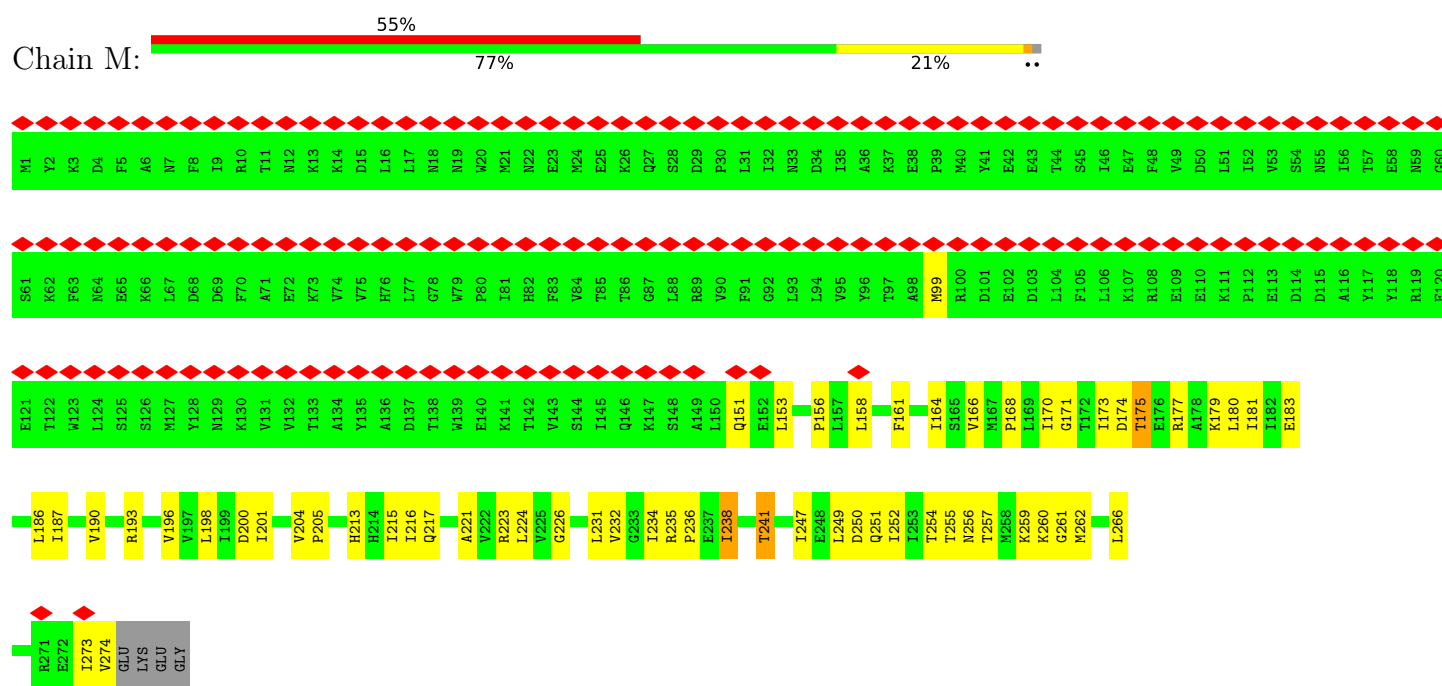
• Molecule 3: RsbS protein



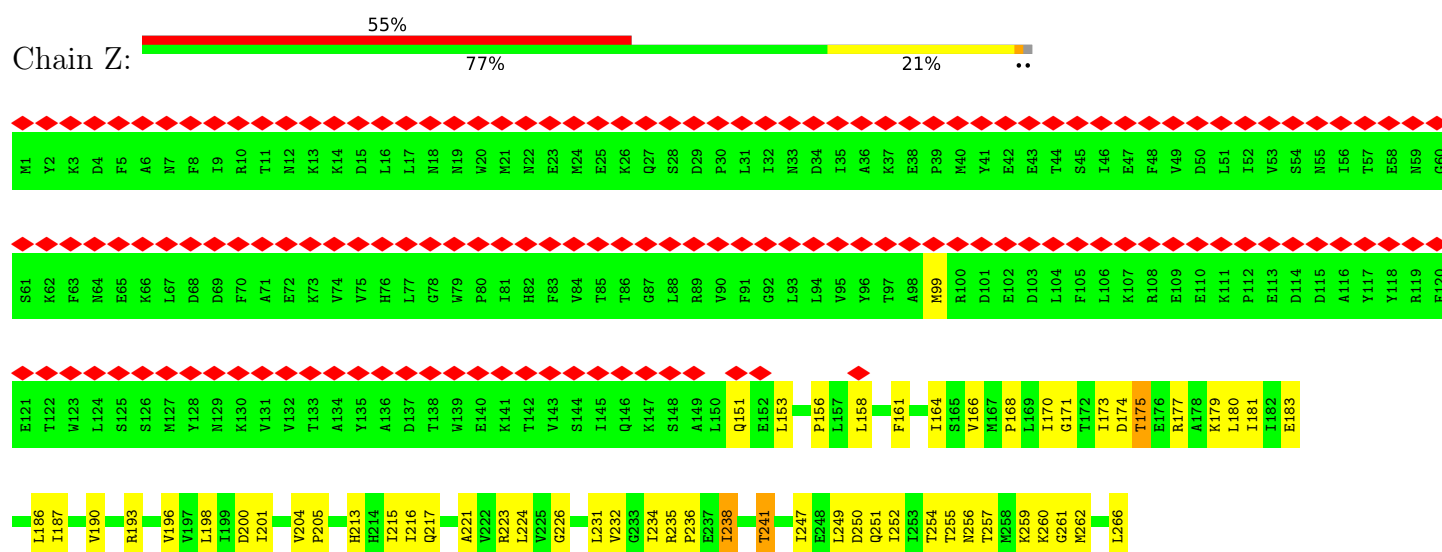
- Molecule 3: RsbS protein

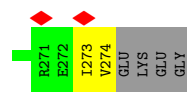


- Molecule 4: RsbR protein

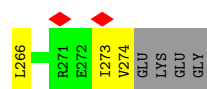
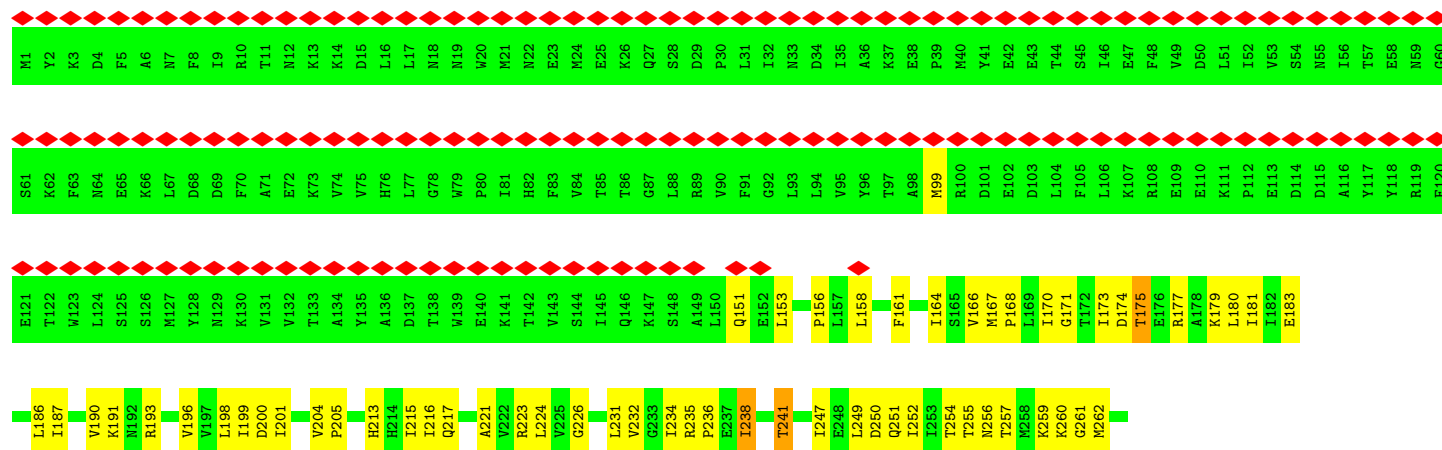
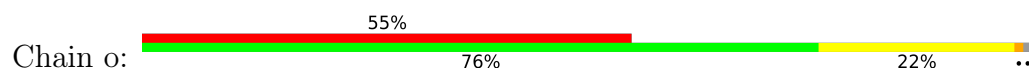


- Molecule 4: RsbR protein

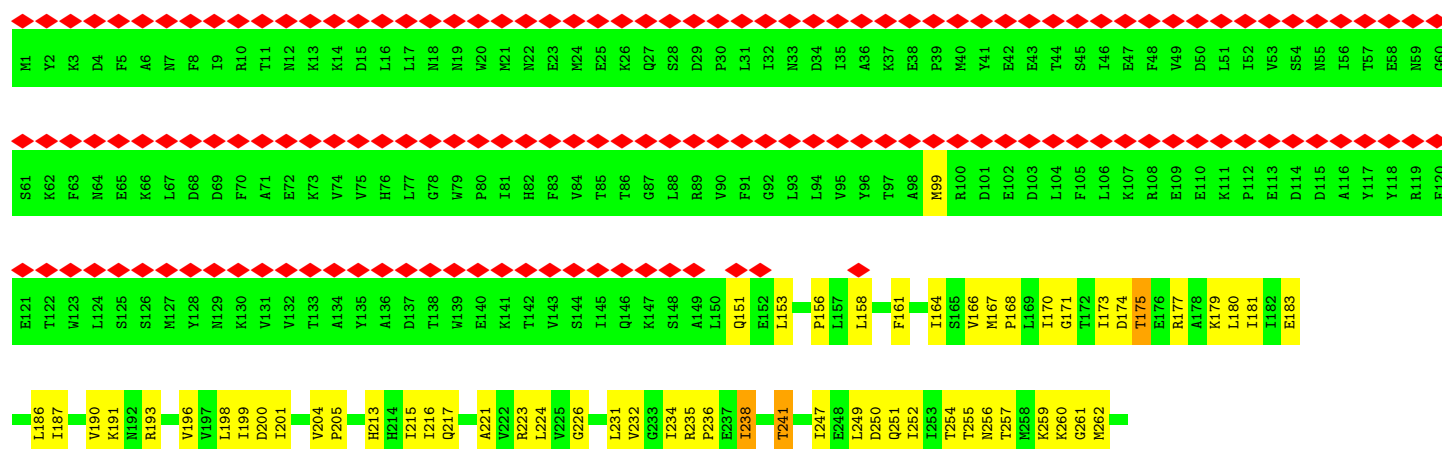
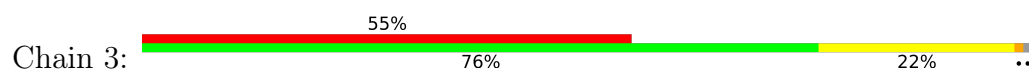




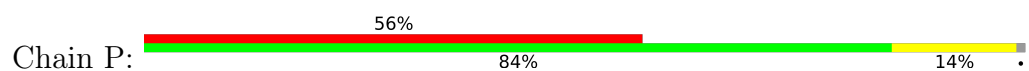
• Molecule 4: RsbR protein

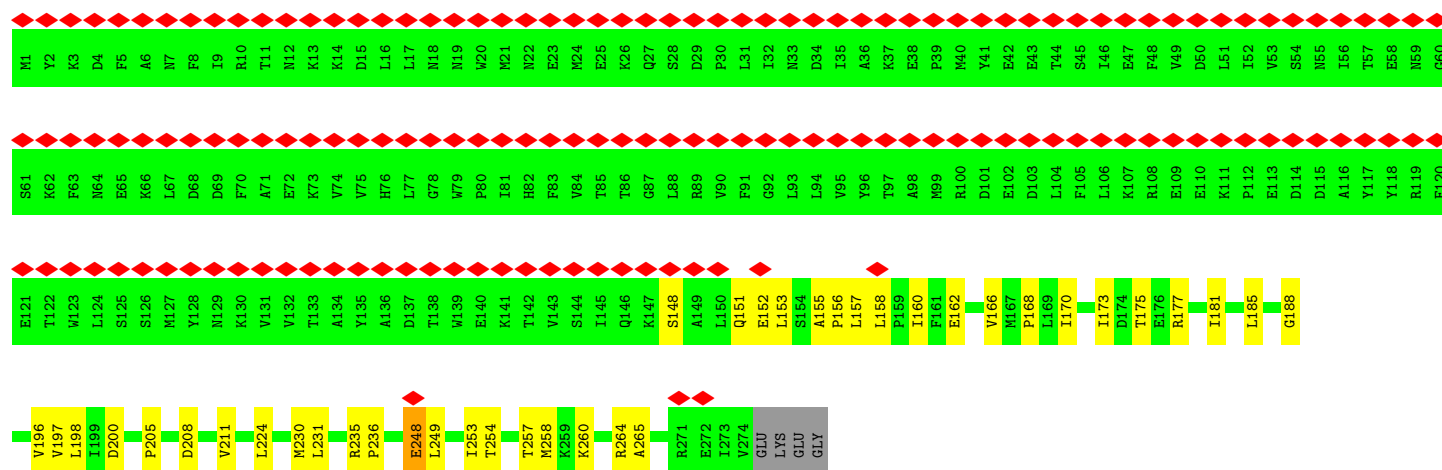


• Molecule 4: RsbR protein

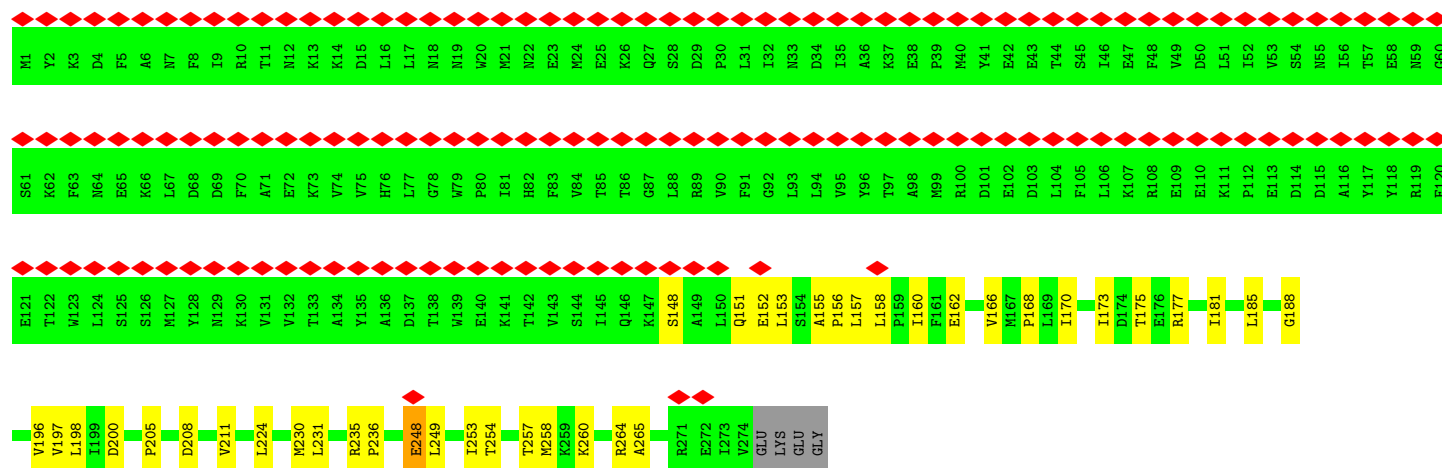
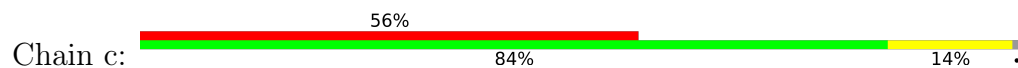


• Molecule 5: RsbR protein

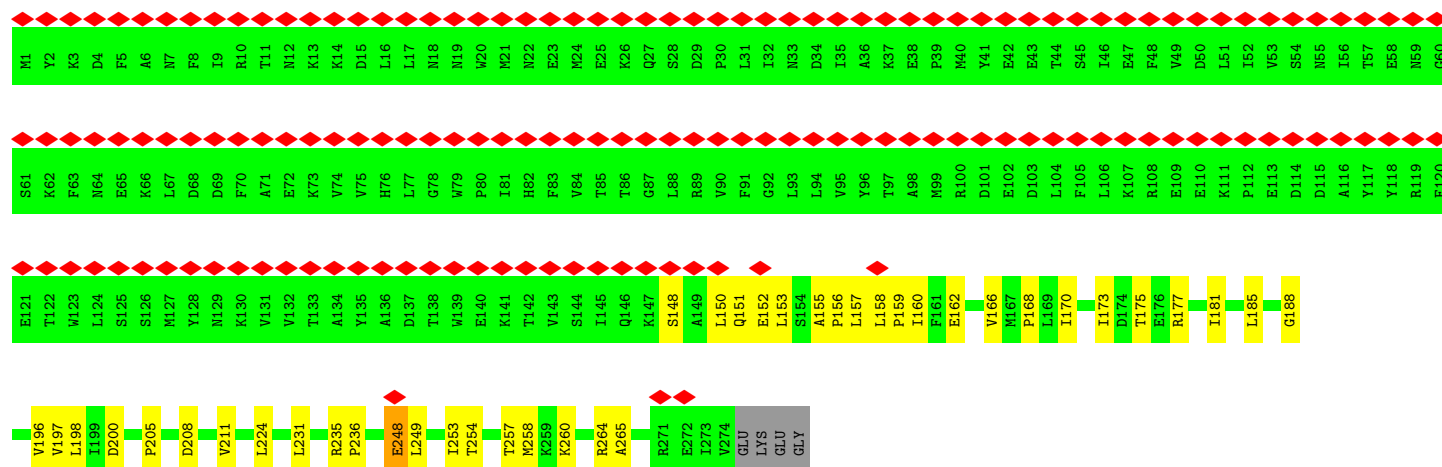
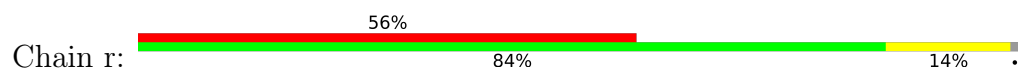




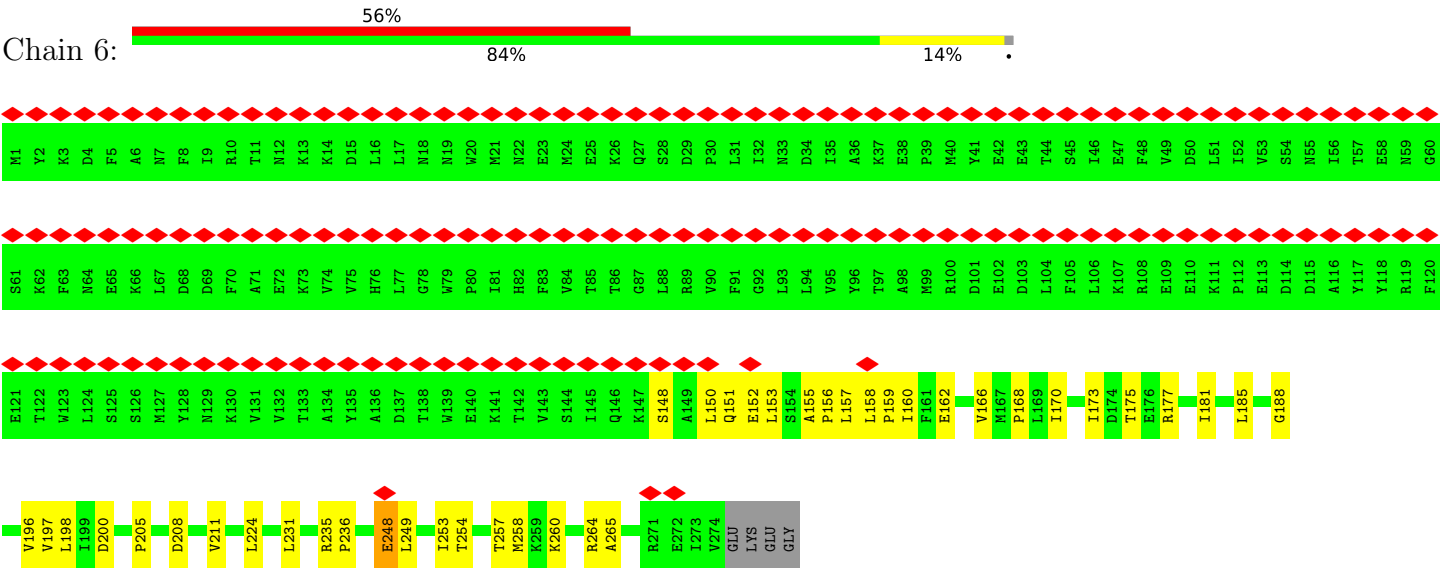
• Molecule 5: RsbR protein



• Molecule 5: RsbR protein



● Molecule 5: RsbR protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	32031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.517	Depositor
Minimum map value	-3.399	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.240	Depositor
Recommended contour level	0.735	Depositor
Map size (Å)	408.38403, 408.38403, 408.38403	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO

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	7	0.15	0/2229	0.35	0/3021
1	A	0.12	0/2229	0.30	0/3021
1	C	0.12	0/2238	0.32	0/3033
1	G	0.13	0/2229	0.33	0/3021
1	K	0.12	0/2229	0.30	0/3021
1	Q	0.15	0/2229	0.35	0/3021
1	R	0.12	0/2238	0.32	0/3033
1	V	0.13	0/2229	0.33	0/3021
1	d	0.15	0/2229	0.35	0/3021
1	e	0.13	0/2229	0.30	0/3021
1	g	0.12	0/2238	0.32	0/3033
1	k	0.13	0/2229	0.33	0/3021
1	s	0.15	0/2229	0.35	0/3021
1	t	0.12	0/2229	0.30	0/3021
1	v	0.12	0/2238	0.32	0/3033
1	z	0.13	0/2229	0.33	0/3021
2	0	0.13	0/2221	0.31	0/3008
2	2	0.14	0/2221	0.33	0/3008
2	B	0.14	0/2221	0.33	0/3008
2	D	0.14	0/2221	0.33	0/3008
2	H	0.13	0/2221	0.31	0/3008
2	J	0.14	0/2221	0.33	0/3008
2	L	0.14	0/2221	0.33	0/3008
2	S	0.14	0/2221	0.33	0/3008
2	W	0.13	0/2221	0.31	0/3008
2	Y	0.14	0/2221	0.33	0/3008
2	f	0.14	0/2221	0.33	0/3008
2	h	0.14	0/2221	0.33	0/3008
2	l	0.13	0/2221	0.31	0/3008
2	n	0.14	0/2221	0.33	0/3008
2	u	0.14	0/2221	0.33	0/3008
2	w	0.14	0/2221	0.33	0/3008

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	1	0.20	0/888	0.46	1/1197 (0.1%)
3	4	0.19	0/888	0.54	2/1197 (0.2%)
3	5	0.21	0/888	0.50	2/1197 (0.2%)
3	E	0.17	0/888	0.36	0/1197
3	F	0.19	0/888	0.42	0/1197
3	I	0.20	0/888	0.46	1/1197 (0.1%)
3	N	0.19	0/888	0.54	2/1197 (0.2%)
3	O	0.21	0/888	0.50	2/1197 (0.2%)
3	T	0.17	0/888	0.35	0/1197
3	U	0.19	0/888	0.42	0/1197
3	X	0.20	0/888	0.46	1/1197 (0.1%)
3	a	0.19	0/888	0.54	2/1197 (0.2%)
3	b	0.21	0/888	0.50	2/1197 (0.2%)
3	i	0.16	0/888	0.36	0/1197
3	j	0.19	0/888	0.42	0/1197
3	m	0.20	0/888	0.46	1/1197 (0.1%)
3	p	0.19	0/888	0.54	2/1197 (0.2%)
3	q	0.21	0/888	0.50	2/1197 (0.2%)
3	x	0.17	0/888	0.36	0/1197
3	y	0.19	0/888	0.42	0/1197
4	3	0.15	0/2213	0.34	0/2995
4	M	0.15	0/2213	0.34	0/2995
4	Z	0.14	0/2213	0.34	0/2995
4	o	0.15	0/2213	0.34	0/2995
5	6	0.14	0/2221	0.37	0/3008
5	P	0.14	0/2221	0.37	0/3008
5	c	0.14	0/2221	0.37	0/3008
5	r	0.14	0/2221	0.37	0/3008
All	All	0.15	0/106732	0.36	20/144464 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	19	GLU	N-CA-C	7.46	121.45	111.30
3	N	19	GLU	N-CA-C	7.33	121.27	111.30
3	4	19	GLU	N-CA-C	7.32	121.25	111.30
3	p	19	GLU	N-CA-C	7.29	121.22	111.30
3	4	19	GLU	CA-CB-CG	6.78	127.67	114.10
3	p	19	GLU	CA-CB-CG	6.78	127.66	114.10
3	N	19	GLU	CA-CB-CG	6.77	127.64	114.10
3	a	19	GLU	CA-CB-CG	6.75	127.61	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	19	GLU	CA-CB-CG	6.74	127.58	114.10
3	5	19	GLU	CA-CB-CG	6.73	127.57	114.10
3	q	19	GLU	CA-CB-CG	6.72	127.53	114.10
3	b	19	GLU	CA-CB-CG	6.71	127.52	114.10
3	m	115	GLU	CA-CB-CG	5.67	125.43	114.10
3	I	115	GLU	CA-CB-CG	5.66	125.42	114.10
3	X	115	GLU	CA-CB-CG	5.66	125.42	114.10
3	1	115	GLU	CA-CB-CG	5.65	125.41	114.10
3	5	19	GLU	CB-CG-CD	5.51	121.96	112.60
3	O	19	GLU	CB-CG-CD	5.50	121.95	112.60
3	q	19	GLU	CB-CG-CD	5.49	121.93	112.60
3	b	19	GLU	CB-CG-CD	5.49	121.93	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7	2192	0	2237	41	0
1	A	2192	0	2237	33	0
1	C	2201	0	2242	29	0
1	G	2192	0	2237	30	0
1	K	2192	0	2237	34	0
1	Q	2192	0	2237	38	0
1	R	2201	0	2242	25	0
1	V	2192	0	2237	28	0
1	d	2192	0	2237	37	0
1	e	2192	0	2237	33	0
1	g	2201	0	2242	27	0
1	k	2192	0	2237	31	0
1	s	2192	0	2237	43	0
1	t	2192	0	2237	33	0
1	v	2201	0	2242	28	0
1	z	2192	0	2237	31	0
2	0	2196	0	2236	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	2196	0	2236	37	0
2	B	2196	0	2236	40	0
2	D	2207	0	2241	38	0
2	H	2196	0	2236	21	0
2	J	2196	0	2236	36	0
2	L	2196	0	2236	39	0
2	S	2207	0	2241	40	0
2	W	2196	0	2236	21	0
2	Y	2196	0	2236	37	0
2	f	2196	0	2236	40	0
2	h	2207	0	2241	41	0
2	l	2196	0	2236	21	0
2	n	2196	0	2236	36	0
2	u	2196	0	2236	40	0
2	w	2207	0	2241	41	0
3	1	881	0	928	47	0
3	4	881	0	928	56	0
3	5	881	0	928	41	0
3	E	881	0	928	41	0
3	F	881	0	928	29	0
3	I	881	0	928	47	0
3	N	881	0	928	57	0
3	O	881	0	928	44	0
3	T	881	0	928	41	0
3	U	881	0	928	31	0
3	X	881	0	928	48	0
3	a	881	0	928	58	0
3	b	881	0	928	44	0
3	i	881	0	928	39	0
3	j	881	0	928	30	0
3	m	881	0	928	47	0
3	p	881	0	928	58	0
3	q	881	0	928	41	0
3	x	881	0	928	38	0
3	y	881	0	928	30	0
4	3	2200	0	2235	57	0
4	M	2200	0	2235	56	0
4	Z	2200	0	2235	58	0
4	o	2200	0	2235	56	0
5	6	2196	0	2236	30	0
5	P	2196	0	2236	28	0
5	c	2196	0	2236	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	r	2196	0	2236	30	0
All	All	105492	0	108052	1995	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 17.

All (1995) 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)
4:M:170:ILE:HD13	4:o:156:PRO:HB3	1.55	0.88
4:Z:170:ILE:HD13	4:3:156:PRO:HB3	1.55	0.88
3:I:103:MET:HE1	1:R:190:VAL:HA	1.56	0.87
4:Z:156:PRO:HB3	4:3:170:ILE:HD13	1.54	0.87
1:C:190:VAL:HA	3:X:103:MET:HE1	1.57	0.86
1:A:146:GLN:HG2	2:B:146:GLN:HE22	1.41	0.85
1:K:146:GLN:HG2	2:L:146:GLN:HE22	1.41	0.85
4:M:156:PRO:HB3	4:o:170:ILE:HD13	1.56	0.85
1:t:146:GLN:HG2	2:u:146:GLN:HE22	1.41	0.84
1:e:146:GLN:HG2	2:f:146:GLN:HE22	1.41	0.84
3:p:15:SER:HA	3:p:47:ASP:HB3	1.63	0.81
3:4:15:SER:HA	3:4:47:ASP:HB3	1.63	0.81
3:m:103:MET:HE1	1:v:190:VAL:HA	1.61	0.80
4:o:161:PHE:HB3	4:o:164:ILE:HB	1.64	0.80
4:3:161:PHE:HB3	4:3:164:ILE:HB	1.64	0.80
3:a:15:SER:HA	3:a:47:ASP:HB3	1.63	0.80
3:N:15:SER:HA	3:N:47:ASP:HB3	1.63	0.79
3:m:79:THR:HA	3:m:103:MET:HA	1.64	0.79
3:1:79:THR:HA	3:1:103:MET:HA	1.64	0.79
3:X:79:THR:HA	3:X:103:MET:HA	1.64	0.78
3:I:79:THR:HA	3:I:103:MET:HA	1.64	0.77
4:Z:161:PHE:HB3	4:Z:164:ILE:HB	1.64	0.77
4:M:161:PHE:HB3	4:M:164:ILE:HB	1.64	0.77
3:5:66:VAL:HA	3:5:75:LYS:HZ2	1.47	0.77
3:q:66:VAL:HA	3:q:75:LYS:HZ2	1.48	0.77
2:u:235:ARG:HG2	2:u:236:PRO:HD2	1.67	0.77
2:f:235:ARG:HG2	2:f:236:PRO:HD2	1.67	0.77
2:D:236:PRO:HG3	2:H:190:VAL:HG21	1.67	0.76
2:S:236:PRO:HG3	2:W:190:VAL:HG21	1.67	0.76
3:U:5:ILE:HG21	3:U:35:LYS:HG2	1.68	0.76
2:h:236:PRO:HG3	2:l:190:VAL:HG21	1.67	0.76
2:w:161:PHE:HB3	2:w:164:ILE:HB	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:w:236:PRO:HG3	2:0:190:VAL:HG21	1.67	0.76
3:F:5:ILE:HG21	3:F:35:LYS:HG2	1.68	0.76
2:B:235:ARG:HG2	2:B:236:PRO:HD2	1.67	0.76
2:h:161:PHE:HB3	2:h:164:ILE:HB	1.67	0.76
1:g:190:VAL:HA	3:1:103:MET:HE1	1.66	0.76
3:F:54:ILE:HG23	3:F:58:ILE:HB	1.68	0.76
3:j:5:ILE:HG21	3:j:35:LYS:HG2	1.67	0.76
3:y:5:ILE:HG21	3:y:35:LYS:HG2	1.68	0.76
2:L:235:ARG:HG2	2:L:236:PRO:HD2	1.67	0.76
3:U:54:ILE:HG23	3:U:58:ILE:HB	1.68	0.76
3:j:54:ILE:HG23	3:j:58:ILE:HB	1.68	0.76
3:y:54:ILE:HG23	3:y:58:ILE:HB	1.68	0.76
2:S:161:PHE:HB3	2:S:164:ILE:HB	1.67	0.75
2:D:161:PHE:HB3	2:D:164:ILE:HB	1.67	0.75
4:o:204:VAL:O	4:o:235:ARG:NH1	2.20	0.75
4:3:204:VAL:O	4:3:235:ARG:NH1	2.20	0.75
3:a:12:LEU:HD22	3:a:44:VAL:HG23	1.69	0.75
3:b:66:VAL:HA	3:b:75:LYS:HZ2	1.50	0.75
3:N:12:LEU:HD22	3:N:44:VAL:HG23	1.69	0.75
3:O:66:VAL:HA	3:O:75:LYS:HZ2	1.50	0.74
4:M:204:VAL:O	4:M:235:ARG:NH1	2.20	0.74
4:Z:204:VAL:O	4:Z:235:ARG:NH1	2.20	0.74
3:x:103:MET:HE1	1:7:190:VAL:HG13	1.70	0.74
3:T:103:MET:HE1	1:d:190:VAL:HG13	1.70	0.74
1:C:255:THR:HG21	1:C:261:GLY:HA2	1.70	0.73
3:E:103:MET:HE1	1:Q:190:VAL:HG13	1.70	0.73
4:M:193:ARG:NH1	3:O:102:ALA:O	2.21	0.73
1:R:255:THR:HG21	1:R:261:GLY:HA2	1.70	0.73
3:p:12:LEU:HD22	3:p:44:VAL:HG23	1.69	0.73
4:Z:193:ARG:NH1	3:b:102:ALA:O	2.22	0.73
3:i:15:SER:HA	3:i:47:ASP:HB2	1.70	0.73
3:x:15:SER:HA	3:x:47:ASP:HB2	1.70	0.73
3:4:12:LEU:HD22	3:4:44:VAL:HG23	1.69	0.73
1:d:173:ILE:HD13	1:d:177:ARG:HE	1.54	0.72
2:l:240:GLN:NE2	2:l:244:ASN:OD1	2.22	0.72
2:0:240:GLN:NE2	2:0:244:ASN:OD1	2.22	0.72
1:Q:173:ILE:HD13	1:Q:177:ARG:HE	1.54	0.72
3:X:21:ASP:HA	3:X:58:ILE:HD11	1.70	0.72
3:I:21:ASP:HA	3:I:58:ILE:HD11	1.70	0.72
3:T:15:SER:HA	3:T:47:ASP:HB2	1.70	0.72
3:T:78:VAL:HG23	3:T:108:GLY:HA3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:68:MET:HE2	2:u:240:GLN:HA	1.70	0.72
3:E:15:SER:HA	3:E:47:ASP:HB2	1.70	0.72
3:E:78:VAL:HG23	3:E:108:GLY:HA3	1.72	0.72
3:m:78:VAL:HG13	3:m:79:THR:HG23	1.72	0.72
2:H:240:GLN:NE2	2:H:244:ASN:OD1	2.22	0.72
3:O:78:VAL:HG21	3:O:105:LEU:HA	1.72	0.72
3:X:78:VAL:HG13	3:X:79:THR:HG23	1.72	0.72
3:b:78:VAL:HG21	3:b:105:LEU:HA	1.72	0.72
3:1:78:VAL:HG13	3:1:79:THR:HG23	1.72	0.72
3:I:78:VAL:HG13	3:I:79:THR:HG23	1.72	0.72
2:W:240:GLN:NE2	2:W:244:ASN:OD1	2.22	0.72
3:m:21:ASP:HA	3:m:58:ILE:HD11	1.70	0.71
3:5:78:VAL:HG21	3:5:105:LEU:HA	1.72	0.71
1:7:173:ILE:HD13	1:7:177:ARG:HE	1.54	0.71
3:q:78:VAL:HG21	3:q:105:LEU:HA	1.72	0.71
1:s:173:ILE:HD13	1:s:177:ARG:HE	1.54	0.71
3:1:21:ASP:HA	3:1:58:ILE:HD11	1.70	0.71
3:N:68:MET:HE2	2:f:240:GLN:HA	1.70	0.71
3:i:78:VAL:HG23	3:i:108:GLY:HA3	1.71	0.71
3:x:78:VAL:HG23	3:x:108:GLY:HA3	1.71	0.71
1:g:255:THR:HG21	1:g:261:GLY:HA2	1.70	0.71
1:v:255:THR:HG21	1:v:261:GLY:HA2	1.70	0.71
2:L:240:GLN:HA	3:4:68:MET:HE2	1.70	0.71
5:P:231:LEU:HB3	5:P:254:THR:HG22	1.73	0.70
3:I:106:GLU:HG3	3:X:9:GLY:H	1.56	0.70
5:c:231:LEU:HB3	5:c:254:THR:HG22	1.73	0.70
3:y:68:MET:HE1	2:2:240:GLN:HA	1.73	0.70
3:N:14:ILE:HG21	3:N:28:PHE:HE1	1.55	0.70
3:a:14:ILE:HG21	3:a:28:PHE:HE1	1.55	0.70
3:j:68:MET:HE1	2:n:240:GLN:HA	1.73	0.70
3:T:4:PRO:HG3	3:U:4:PRO:HG3	1.74	0.70
1:z:249:LEU:O	3:1:70:LYS:NZ	2.24	0.70
2:B:240:GLN:HA	3:p:68:MET:HE2	1.71	0.70
3:p:5:ILE:HG21	3:p:35:LYS:HG2	1.74	0.69
3:4:5:ILE:HG21	3:4:35:LYS:HG2	1.74	0.69
3:U:42:ARG:HE	3:U:116:LEU:HD22	1.57	0.69
3:m:69:SER:O	3:m:73:GLY:N	2.24	0.69
3:F:42:ARG:HE	3:F:116:LEU:HD22	1.58	0.69
3:p:14:ILE:HG21	3:p:28:PHE:HE1	1.55	0.69
3:1:69:SER:O	3:1:73:GLY:N	2.24	0.69
3:4:14:ILE:HG21	3:4:28:PHE:HE1	1.55	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:231:LEU:HB3	5:6:254:THR:HG22	1.73	0.69
3:j:42:ARG:HE	3:j:116:LEU:HD22	1.58	0.69
5:r:231:LEU:HB3	5:r:254:THR:HG22	1.73	0.69
2:J:170:ILE:HD13	2:2:156:PRO:HB3	1.73	0.69
3:y:42:ARG:HE	3:y:116:LEU:HD22	1.58	0.69
2:J:156:PRO:HB3	2:2:170:ILE:HD13	1.75	0.69
2:h:169:LEU:HD11	2:h:201:ILE:HD12	1.75	0.69
2:w:169:LEU:HD11	2:w:201:ILE:HD12	1.75	0.69
4:o:193:ARG:NH1	3:q:102:ALA:O	2.26	0.68
3:a:5:ILE:HG21	3:a:35:LYS:HG2	1.74	0.68
3:N:5:ILE:HG21	3:N:35:LYS:HG2	1.74	0.68
1:V:249:LEU:O	3:X:70:LYS:NZ	2.26	0.68
4:3:193:ARG:NH1	3:5:102:ALA:O	2.26	0.68
5:6:162:GLU:OE1	1:7:259:LYS:NZ	2.27	0.68
3:O:54:ILE:HG23	3:O:58:ILE:HB	1.75	0.68
3:b:54:ILE:HG23	3:b:58:ILE:HB	1.75	0.68
5:c:155:ALA:HB2	5:c:181:ILE:HD13	1.76	0.67
5:P:155:ALA:HB2	5:P:181:ILE:HD13	1.76	0.67
3:5:15:SER:HA	3:5:47:ASP:HB2	1.76	0.67
2:S:169:LEU:HD11	2:S:201:ILE:HD12	1.75	0.67
2:Y:156:PRO:HB3	2:n:170:ILE:HD13	1.77	0.67
3:q:15:SER:HA	3:q:47:ASP:HB2	1.76	0.67
2:u:155:ALA:HB2	2:u:181:ILE:HD13	1.76	0.67
3:x:4:PRO:HG3	3:y:4:PRO:HG3	1.76	0.67
3:4:78:VAL:HG21	3:4:105:LEU:HA	1.77	0.67
2:D:169:LEU:HD11	2:D:201:ILE:HD12	1.75	0.67
2:H:249:LEU:HD13	5:6:224:LEU:HD11	1.76	0.67
2:f:155:ALA:HB2	2:f:181:ILE:HD13	1.76	0.67
3:1:25:ALA:HB1	3:1:61:ILE:HG13	1.77	0.67
3:5:13:LEU:HD13	3:5:45:VAL:HB	1.77	0.67
2:L:155:ALA:HB2	2:L:181:ILE:HD13	1.76	0.66
3:m:15:SER:HA	3:m:47:ASP:HB3	1.77	0.66
3:m:25:ALA:HB1	3:m:61:ILE:HG13	1.77	0.66
3:p:78:VAL:HG21	3:p:105:LEU:HA	1.77	0.66
3:q:13:LEU:HD13	3:q:45:VAL:HB	1.77	0.66
3:q:54:ILE:HG23	3:q:58:ILE:HB	1.75	0.66
3:1:15:SER:HA	3:1:47:ASP:HB3	1.77	0.66
3:E:4:PRO:HG3	3:F:4:PRO:HG3	1.77	0.66
2:Y:170:ILE:HD13	2:n:156:PRO:HB3	1.76	0.66
3:5:54:ILE:HG23	3:5:58:ILE:HB	1.75	0.66
2:B:155:ALA:HB2	2:B:181:ILE:HD13	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:69:SER:O	3:X:73:GLY:N	2.24	0.66
3:i:4:PRO:HG3	3:j:4:PRO:HG3	1.76	0.66
3:I:69:SER:O	3:I:73:GLY:N	2.24	0.66
3:U:68:MET:HE1	2:Y:240:GLN:HA	1.77	0.66
2:2:178:ALA:HB2	2:2:211:VAL:HG13	1.77	0.66
3:O:15:SER:HA	3:O:47:ASP:HB2	1.76	0.66
2:n:178:ALA:HB2	2:n:211:VAL:HG13	1.78	0.66
1:C:173:ILE:HG22	1:C:177:ARG:HD3	1.77	0.66
1:Q:240:GLN:O	1:Q:244:ASN:ND2	2.26	0.66
1:R:173:ILE:HG22	1:R:177:ARG:HD3	1.77	0.66
3:b:15:SER:HA	3:b:47:ASP:HB2	1.76	0.66
3:p:12:LEU:HD11	3:p:35:LYS:HG3	1.78	0.66
5:P:162:GLU:OE1	1:Q:259:LYS:NZ	2.27	0.66
1:d:240:GLN:O	1:d:244:ASN:ND2	2.26	0.66
3:4:12:LEU:HD11	3:4:35:LYS:HG3	1.78	0.66
1:G:161:PHE:HB3	1:G:164:ILE:HB	1.78	0.65
3:N:33:LEU:HB3	2:f:236:PRO:HB3	1.77	0.65
1:V:161:PHE:HB3	1:V:164:ILE:HB	1.78	0.65
3:b:13:LEU:HD13	3:b:45:VAL:HB	1.77	0.65
5:c:162:GLU:OE1	1:d:259:LYS:NZ	2.27	0.65
3:O:13:LEU:HD13	3:O:45:VAL:HB	1.77	0.65
5:P:224:LEU:HD11	2:0:249:LEU:HD13	1.78	0.65
2:Y:178:ALA:HB2	2:Y:211:VAL:HG13	1.78	0.65
1:7:240:GLN:O	1:7:244:ASN:ND2	2.26	0.65
3:E:24:THR:O	3:E:28:PHE:HB2	1.97	0.65
2:J:178:ALA:HB2	2:J:211:VAL:HG13	1.78	0.65
3:T:24:THR:O	3:T:28:PHE:HB2	1.97	0.65
3:I:25:ALA:HB1	3:I:61:ILE:HG13	1.77	0.65
5:6:155:ALA:HB2	5:6:181:ILE:HD13	1.76	0.65
3:N:78:VAL:HG21	3:N:105:LEU:HA	1.77	0.65
3:a:33:LEU:HB3	2:u:236:PRO:HB3	1.77	0.65
3:a:78:VAL:HG21	3:a:105:LEU:HA	1.77	0.65
1:g:173:ILE:HG22	1:g:177:ARG:HD3	1.76	0.65
3:i:24:THR:O	3:i:28:PHE:HB2	1.97	0.65
5:r:155:ALA:HB2	5:r:181:ILE:HD13	1.76	0.65
3:E:82:GLN:O	3:E:86:ALA:N	2.28	0.65
1:G:249:LEU:O	3:I:70:LYS:NZ	2.29	0.65
3:X:15:SER:HA	3:X:47:ASP:HB3	1.77	0.65
3:x:24:THR:O	3:x:28:PHE:HB2	1.97	0.65
1:Q:198:LEU:HD23	1:Q:230:MET:HB2	1.78	0.65
5:c:224:LEU:HD11	2:l:249:LEU:HD13	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:240:GLN:O	1:s:244:ASN:ND2	2.26	0.65
3:X:25:ALA:HB1	3:X:61:ILE:HG13	1.77	0.65
1:d:198:LEU:HD23	1:d:230:MET:HB2	1.78	0.65
3:I:15:SER:HA	3:I:47:ASP:HB3	1.77	0.64
3:T:57:PHE:HD1	3:T:60:LYS:HZ3	1.45	0.64
3:a:78:VAL:HG23	3:a:101:SER:HB2	1.79	0.64
1:v:173:ILE:HG22	1:v:177:ARG:HD3	1.77	0.64
3:F:78:VAL:HG23	3:F:108:GLY:HA3	1.79	0.64
3:N:12:LEU:HD11	3:N:35:LYS:HG3	1.78	0.64
3:N:78:VAL:HG23	3:N:101:SER:HB2	1.80	0.64
3:U:78:VAL:HG23	3:U:108:GLY:HA3	1.79	0.64
2:W:249:LEU:HD13	5:r:224:LEU:HD11	1.77	0.64
3:a:12:LEU:HD11	3:a:35:LYS:HG3	1.78	0.64
1:k:161:PHE:HB3	1:k:164:ILE:HB	1.78	0.64
1:z:161:PHE:HB3	1:z:164:ILE:HB	1.78	0.64
3:E:57:PHE:HD1	3:E:60:LYS:HZ3	1.46	0.64
2:L:223:ARG:NH2	1:R:249:LEU:O	2.30	0.64
2:f:223:ARG:NH2	1:g:249:LEU:O	2.30	0.64
2:B:223:ARG:NH2	1:C:249:LEU:O	2.31	0.64
3:F:68:MET:HE1	2:J:240:GLN:HA	1.79	0.64
4:M:170:ILE:HG22	4:o:158:LEU:HD22	1.80	0.64
2:u:223:ARG:NH2	1:v:249:LEU:O	2.30	0.64
2:B:185:LEU:HD11	2:B:197:VAL:HG11	1.80	0.64
3:T:82:GLN:O	3:T:86:ALA:N	2.29	0.64
4:Z:205:PRO:O	4:Z:235:ARG:NH2	2.29	0.64
2:D:168:PRO:HA	2:D:200:ASP:HB3	1.80	0.64
4:M:205:PRO:O	4:M:235:ARG:NH2	2.29	0.64
2:L:236:PRO:HB3	3:4:33:LEU:HB3	1.79	0.64
2:S:168:PRO:HA	2:S:200:ASP:HB3	1.80	0.64
2:L:185:LEU:HD11	2:L:197:VAL:HG11	1.80	0.64
2:h:167:MET:HE1	2:h:169:LEU:HD23	1.80	0.64
1:s:198:LEU:HD23	1:s:230:MET:HB2	1.78	0.64
2:w:167:MET:HE1	2:w:169:LEU:HD23	1.80	0.64
2:D:167:MET:HE1	2:D:169:LEU:HD23	1.80	0.64
3:j:78:VAL:HG23	3:j:108:GLY:HA3	1.79	0.64
3:j:95:THR:HG22	3:j:97:SER:H	1.63	0.64
2:S:167:MET:HE1	2:S:169:LEU:HD23	1.80	0.63
3:y:95:THR:HG22	3:y:97:SER:H	1.63	0.63
2:S:173:ILE:HA	2:S:177:ARG:HD3	1.80	0.63
3:y:78:VAL:HG23	3:y:108:GLY:HA3	1.79	0.63
2:D:173:ILE:HA	2:D:177:ARG:HD3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:158:LEU:HD22	4:o:170:ILE:HG22	1.81	0.63
4:o:205:PRO:O	4:o:235:ARG:NH2	2.29	0.63
1:7:198:LEU:HD23	1:7:230:MET:HB2	1.78	0.63
1:C:224:LEU:HD21	3:X:89:LEU:HD22	1.81	0.63
3:U:51:ILE:HG21	3:U:54:ILE:HD11	1.80	0.63
2:B:236:PRO:HB3	3:p:33:LEU:HB3	1.80	0.63
2:D:270:ASN:OD1	2:D:271:ARG:N	2.32	0.63
3:I:12:LEU:HD21	3:I:35:LYS:HG3	1.80	0.63
3:i:103:MET:HE1	1:s:190:VAL:HG13	1.79	0.63
3:F:51:ILE:HG21	3:F:54:ILE:HD11	1.81	0.63
2:S:270:ASN:OD1	2:S:271:ARG:N	2.32	0.63
4:3:205:PRO:O	4:3:235:ARG:NH2	2.29	0.63
5:6:196:VAL:HG21	5:6:265:ALA:HB1	1.80	0.63
3:X:12:LEU:HD21	3:X:35:LYS:HG3	1.80	0.63
5:r:196:VAL:HG21	5:r:265:ALA:HB1	1.80	0.63
3:X:78:VAL:HG23	3:X:108:GLY:HA3	1.80	0.63
3:I:78:VAL:HG23	3:I:108:GLY:HA3	1.80	0.62
3:U:95:THR:HG22	3:U:97:SER:H	1.63	0.62
4:Z:158:LEU:HD22	4:3:170:ILE:HG22	1.81	0.62
3:j:51:ILE:HG21	3:j:54:ILE:HD11	1.81	0.62
2:w:270:ASN:OD1	2:w:271:ARG:N	2.32	0.62
3:y:51:ILE:HG21	3:y:54:ILE:HD11	1.80	0.62
2:h:168:PRO:HA	2:h:200:ASP:HB3	1.80	0.62
2:h:270:ASN:OD1	2:h:271:ARG:N	2.32	0.62
3:p:78:VAL:HG23	3:p:101:SER:HB2	1.80	0.62
2:w:168:PRO:HA	2:w:200:ASP:HB3	1.80	0.62
3:4:78:VAL:HG23	3:4:101:SER:HB2	1.80	0.62
3:F:95:THR:HG22	3:F:97:SER:H	1.63	0.62
4:Z:170:ILE:HG22	4:3:158:LEU:HD22	1.81	0.62
3:m:12:LEU:HD21	3:m:35:LYS:HG3	1.80	0.62
3:i:82:GLN:O	3:i:86:ALA:N	2.29	0.62
2:u:185:LEU:HD11	2:u:197:VAL:HG11	1.80	0.62
1:z:240:GLN:HA	3:1:68:MET:HE2	1.82	0.62
3:1:12:LEU:HD21	3:1:35:LYS:HG3	1.80	0.62
5:c:196:VAL:HG21	5:c:265:ALA:HB1	1.80	0.62
3:O:48:ILE:N	3:O:79:THR:OG1	2.28	0.62
5:P:196:VAL:HG21	5:P:265:ALA:HB1	1.80	0.62
2:f:185:LEU:HD11	2:f:197:VAL:HG11	1.80	0.62
1:g:156:PRO:HB3	2:h:170:ILE:HD13	1.82	0.62
1:v:156:PRO:HB3	2:w:170:ILE:HD13	1.82	0.62
3:m:21:ASP:OD1	3:m:22:ASP:N	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:x:82:GLN:O	3:x:86:ALA:N	2.29	0.62
3:1:78:VAL:HG23	3:1:108:GLY:HA3	1.80	0.62
3:I:21:ASP:OD1	3:I:22:ASP:N	2.33	0.62
3:b:48:ILE:N	3:b:79:THR:OG1	2.28	0.62
3:m:78:VAL:HG23	3:m:108:GLY:HA3	1.80	0.62
3:1:21:ASP:OD1	3:1:22:ASP:N	2.33	0.62
3:N:87:ILE:HA	3:N:90:ILE:HG22	1.81	0.62
3:a:87:ILE:HA	3:a:90:ILE:HG22	1.81	0.62
2:h:155:ALA:HB2	2:h:181:ILE:HD13	1.82	0.62
2:h:173:ILE:HA	2:h:177:ARG:HD3	1.80	0.62
2:w:155:ALA:HB2	2:w:181:ILE:HD13	1.82	0.62
2:w:173:ILE:HA	2:w:177:ARG:HD3	1.80	0.62
1:K:161:PHE:HB3	1:K:164:ILE:HB	1.81	0.61
3:X:21:ASP:OD1	3:X:22:ASP:N	2.33	0.61
1:A:161:PHE:HB3	1:A:164:ILE:HB	1.81	0.61
1:e:161:PHE:HB3	1:e:164:ILE:HB	1.81	0.61
1:G:186:LEU:HB3	3:4:83:PRO:HB3	1.83	0.61
1:R:156:PRO:HB3	2:S:170:ILE:HD13	1.82	0.61
3:p:87:ILE:HA	3:p:90:ILE:HG22	1.81	0.61
3:4:87:ILE:HA	3:4:90:ILE:HG22	1.81	0.61
2:J:198:LEU:HD23	2:J:230:MET:HB2	1.83	0.61
2:n:198:LEU:HD23	2:n:230:MET:HB2	1.83	0.61
2:2:198:LEU:HD23	2:2:230:MET:HB2	1.83	0.61
1:C:156:PRO:HB3	2:D:170:ILE:HD13	1.82	0.61
2:Y:198:LEU:HD23	2:Y:230:MET:HB2	1.83	0.61
1:t:161:PHE:HB3	1:t:164:ILE:HB	1.81	0.61
3:b:54:ILE:HD12	3:b:58:ILE:HG21	1.83	0.61
2:B:178:ALA:O	2:B:182:ILE:HG12	2.01	0.61
3:O:54:ILE:HD12	3:O:58:ILE:HG21	1.83	0.61
2:L:178:ALA:O	2:L:182:ILE:HG12	2.01	0.61
2:S:155:ALA:HB2	2:S:181:ILE:HD13	1.82	0.61
2:n:173:ILE:HG22	2:n:177:ARG:HH11	1.66	0.61
2:D:155:ALA:HB2	2:D:181:ILE:HD13	1.82	0.61
2:2:173:ILE:HG22	2:2:177:ARG:HH11	1.66	0.61
1:d:159:PRO:HB2	1:d:166:VAL:HG23	1.83	0.60
3:q:54:ILE:HD12	3:q:58:ILE:HG21	1.83	0.60
2:h:205:PRO:O	2:h:235:ARG:NH1	2.34	0.60
1:Q:159:PRO:HB2	1:Q:166:VAL:HG23	1.83	0.60
2:w:205:PRO:O	2:w:235:ARG:NH1	2.34	0.60
3:5:54:ILE:HD12	3:5:58:ILE:HG21	1.83	0.60
1:7:159:PRO:HB2	1:7:166:VAL:HG23	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:9:GLY:H	3:X:106:GLU:HG3	1.66	0.60
2:J:173:ILE:HG22	2:J:177:ARG:HH11	1.66	0.60
2:Y:173:ILE:HG22	2:Y:177:ARG:HH11	1.66	0.60
1:k:249:LEU:O	3:m:70:LYS:NZ	2.34	0.60
1:s:159:PRO:HB2	1:s:166:VAL:HG23	1.83	0.60
2:u:178:ALA:O	2:u:182:ILE:HG12	2.01	0.60
3:x:25:ALA:HB1	3:x:61:ILE:HG13	1.84	0.60
3:4:14:ILE:HD11	3:4:32:LEU:HD13	1.84	0.60
3:T:25:ALA:HB1	3:T:61:ILE:HG13	1.84	0.60
2:f:178:ALA:O	2:f:182:ILE:HG12	2.01	0.60
3:i:25:ALA:HB1	3:i:61:ILE:HG13	1.84	0.60
3:p:14:ILE:HD11	3:p:32:LEU:HD13	1.84	0.60
3:i:13:LEU:HD23	3:i:45:VAL:HB	1.84	0.60
3:x:13:LEU:HD23	3:x:45:VAL:HB	1.84	0.60
3:E:25:ALA:HB1	3:E:61:ILE:HG13	1.84	0.60
3:1:14:ILE:HG21	3:1:28:PHE:HE1	1.66	0.59
3:T:78:VAL:HG13	3:T:79:THR:HG23	1.84	0.59
3:m:14:ILE:HG21	3:m:28:PHE:HE1	1.66	0.59
3:N:13:LEU:HD23	3:N:45:VAL:HB	1.83	0.59
3:a:13:LEU:HD23	3:a:45:VAL:HB	1.83	0.59
2:u:207:VAL:O	2:u:241:TPO:O1P	2.20	0.59
3:X:14:ILE:HG21	3:X:28:PHE:HE1	1.67	0.59
2:f:207:VAL:O	2:f:241:TPO:O2P	2.20	0.59
3:i:78:VAL:HG13	3:i:79:THR:HG23	1.84	0.59
3:E:78:VAL:HG13	3:E:79:THR:HG23	1.84	0.59
3:p:13:LEU:HD23	3:p:45:VAL:HB	1.83	0.59
3:x:78:VAL:HG13	3:x:79:THR:HG23	1.84	0.59
3:I:14:ILE:HG21	3:I:28:PHE:HE1	1.66	0.59
1:v:169:LEU:HD11	1:v:201:ILE:HD12	1.84	0.59
1:C:169:LEU:HD11	1:C:201:ILE:HD12	1.84	0.59
1:g:169:LEU:HD11	1:g:201:ILE:HD12	1.84	0.59
3:N:21:ASP:OD1	3:N:22:ASP:N	2.35	0.59
1:R:169:LEU:HD11	1:R:201:ILE:HD12	1.84	0.59
3:a:21:ASP:OD1	3:a:22:ASP:N	2.36	0.59
3:4:13:LEU:HD23	3:4:45:VAL:HB	1.83	0.59
3:4:21:ASP:OD1	3:4:22:ASP:N	2.36	0.59
1:A:222:VAL:HG22	1:A:227:CYS:HB2	1.85	0.59
1:K:222:VAL:HG22	1:K:227:CYS:HB2	1.85	0.59
2:L:207:VAL:O	2:L:241:TPO:O2P	2.20	0.59
3:a:14:ILE:HD11	3:a:32:LEU:HD13	1.84	0.59
3:E:13:LEU:HD23	3:E:45:VAL:HB	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:GLN:HA	3:I:68:MET:HE2	1.83	0.59
2:H:185:LEU:HD11	2:H:197:VAL:HG11	1.85	0.59
3:N:14:ILE:HD11	3:N:32:LEU:HD13	1.84	0.59
3:O:14:ILE:HD11	3:O:32:LEU:HD13	1.83	0.59
3:T:13:LEU:HD23	3:T:45:VAL:HB	1.84	0.59
2:W:185:LEU:HD11	2:W:197:VAL:HG11	1.85	0.59
1:s:166:VAL:HG12	1:s:198:LEU:HD12	1.85	0.59
3:5:68:MET:HE1	1:7:240:GLN:HA	1.85	0.59
2:B:207:VAL:O	2:B:241:TPO:O1P	2.20	0.58
3:b:14:ILE:HD11	3:b:32:LEU:HD13	1.83	0.58
1:g:224:LEU:HD21	3:1:89:LEU:HD22	1.86	0.58
1:7:166:VAL:HG12	1:7:198:LEU:HD12	1.85	0.58
1:G:224:LEU:O	3:4:100:LEU:HD22	2.03	0.58
3:p:29:GLN:O	3:p:33:LEU:HG	2.04	0.58
3:4:29:GLN:O	3:4:33:LEU:HG	2.04	0.58
3:5:14:ILE:HD11	3:5:32:LEU:HD13	1.83	0.58
1:e:222:VAL:HG22	1:e:227:CYS:HB2	1.85	0.58
1:C:240:GLN:OE1	1:C:244:ASN:ND2	2.37	0.58
4:Z:262:MET:HE1	4:3:161:PHE:CD1	2.39	0.58
3:q:14:ILE:HD11	3:q:32:LEU:HD13	1.83	0.58
2:0:185:LEU:HD11	2:0:197:VAL:HG11	1.85	0.58
3:F:12:LEU:HB3	3:F:44:VAL:HG23	1.85	0.58
1:R:240:GLN:OE1	1:R:244:ASN:ND2	2.37	0.58
3:U:12:LEU:HB3	3:U:44:VAL:HG23	1.85	0.58
3:j:12:LEU:HB3	3:j:44:VAL:HG23	1.85	0.58
2:l:185:LEU:HD11	2:l:197:VAL:HG11	1.85	0.58
1:t:222:VAL:HG22	1:t:227:CYS:HB2	1.85	0.58
3:y:12:LEU:HB3	3:y:44:VAL:HG23	1.85	0.58
3:x:9:GLY:O	3:x:113:LYS:NZ	2.37	0.58
3:O:69:SER:HB3	3:O:75:LYS:HZ3	1.69	0.58
3:b:69:SER:HB3	3:b:75:LYS:HZ3	1.69	0.58
2:h:169:LEU:HD13	2:h:173:ILE:HD11	1.86	0.58
3:i:9:GLY:O	3:i:113:LYS:NZ	2.37	0.58
2:S:205:PRO:O	2:S:235:ARG:NH1	2.34	0.58
3:a:69:SER:O	3:a:73:GLY:N	2.26	0.58
3:m:9:GLY:H	3:1:106:GLU:HG3	1.68	0.58
2:w:169:LEU:HD13	2:w:173:ILE:HD11	1.86	0.58
3:N:83:PRO:HB3	1:z:186:LEU:HB3	1.85	0.58
3:N:100:LEU:HD22	1:z:224:LEU:O	2.04	0.58
3:a:100:LEU:HD22	1:k:224:LEU:O	2.04	0.58
2:D:205:PRO:O	2:D:235:ARG:NH1	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:9:GLY:O	3:T:113:LYS:NZ	2.37	0.57
4:Z:161:PHE:CD1	4:3:262:MET:HE1	2.39	0.57
1:d:166:VAL:HG12	1:d:198:LEU:HD12	1.85	0.57
4:3:190:VAL:HG22	3:5:103:MET:HE1	1.86	0.57
3:E:9:GLY:O	3:E:113:LYS:NZ	2.37	0.57
3:N:29:GLN:O	3:N:33:LEU:HG	2.04	0.57
3:a:29:GLN:O	3:a:33:LEU:HG	2.04	0.57
1:g:240:GLN:OE1	1:g:244:ASN:ND2	2.37	0.57
3:p:21:ASP:OD1	3:p:22:ASP:N	2.36	0.57
1:Q:166:VAL:HG12	1:Q:198:LEU:HD12	1.85	0.57
2:L:203:GLY:H	2:L:235:ARG:HH22	1.52	0.57
1:v:240:GLN:OE1	1:v:244:ASN:ND2	2.37	0.57
2:B:203:GLY:H	2:B:235:ARG:HH22	1.52	0.57
3:E:20:LEU:HG	3:E:21:ASP:H	1.70	0.57
2:J:169:LEU:HD11	2:J:181:ILE:HD13	1.86	0.57
4:M:262:MET:HE1	4:o:161:PHE:CD1	2.39	0.57
3:T:20:LEU:HG	3:T:21:ASP:H	1.70	0.57
3:a:46:ILE:HB	3:a:77:VAL:HG23	1.86	0.57
3:N:46:ILE:HB	3:N:77:VAL:HG23	1.86	0.57
2:Y:169:LEU:HD11	2:Y:181:ILE:HD13	1.87	0.57
5:c:249:LEU:O	2:n:223:ARG:NH1	2.37	0.57
4:o:190:VAL:HG22	3:q:103:MET:HE1	1.86	0.57
4:M:161:PHE:CD1	4:o:262:MET:HE1	2.39	0.57
1:d:235:ARG:HG2	1:d:238:ILE:HG12	1.85	0.57
1:R:177:ARG:O	1:R:181:ILE:HG12	2.05	0.57
4:o:256:ASN:OD1	4:o:257:THR:N	2.38	0.57
1:v:177:ARG:O	1:v:181:ILE:HG12	2.05	0.57
1:v:213:HIS:O	1:v:217:GLN:HG2	2.05	0.57
4:3:256:ASN:OD1	4:3:257:THR:N	2.38	0.57
1:A:173:ILE:HG22	1:A:177:ARG:HE	1.70	0.57
1:C:221:ALA:HB2	3:X:90:ILE:HD13	1.87	0.57
1:g:177:ARG:O	1:g:181:ILE:HG12	2.05	0.57
1:g:213:HIS:O	1:g:217:GLN:HG2	2.05	0.57
2:u:213:HIS:O	2:u:217:GLN:HG3	2.05	0.57
4:M:256:ASN:OD1	4:M:257:THR:N	2.38	0.57
3:O:68:MET:HE1	1:Q:240:GLN:HA	1.86	0.57
2:f:213:HIS:O	2:f:217:GLN:HG3	2.05	0.57
3:i:20:LEU:HG	3:i:21:ASP:H	1.70	0.57
3:p:26:VAL:O	3:p:30:GLU:HG3	2.05	0.57
3:x:20:LEU:HG	3:x:21:ASP:H	1.70	0.57
2:B:213:HIS:O	2:B:217:GLN:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:O	1:C:181:ILE:HG12	2.05	0.57
1:K:173:ILE:HA	1:K:177:ARG:HD3	1.86	0.57
2:u:203:GLY:H	2:u:235:ARG:HH22	1.52	0.57
3:4:26:VAL:O	3:4:30:GLU:HG3	2.05	0.57
1:A:173:ILE:HA	1:A:177:ARG:HD3	1.86	0.56
3:E:22:ASP:HA	3:E:57:PHE:HE2	1.70	0.56
5:P:249:LEU:O	2:2:223:ARG:NH1	2.38	0.56
1:K:173:ILE:HG22	1:K:177:ARG:HE	1.70	0.56
3:T:22:ASP:HA	3:T:57:PHE:HE2	1.70	0.56
4:Z:256:ASN:OD1	4:Z:257:THR:N	2.38	0.56
3:p:46:ILE:HB	3:p:77:VAL:HG23	1.86	0.56
1:C:213:HIS:O	1:C:217:GLN:HG2	2.05	0.56
2:L:213:HIS:O	2:L:217:GLN:HG3	2.05	0.56
1:R:213:HIS:O	1:R:217:GLN:HG2	2.05	0.56
1:e:173:ILE:HG22	1:e:177:ARG:HE	1.70	0.56
1:e:173:ILE:HA	1:e:177:ARG:HD3	1.86	0.56
2:f:203:GLY:H	2:f:235:ARG:HH22	1.52	0.56
1:t:173:ILE:HG22	1:t:177:ARG:HE	1.70	0.56
3:a:83:PRO:HB3	1:k:186:LEU:HB3	1.87	0.56
3:m:14:ILE:HD11	3:m:32:LEU:HD13	1.88	0.56
1:s:161:PHE:HB3	1:s:164:ILE:HB	1.87	0.56
1:t:173:ILE:HA	1:t:177:ARG:HD3	1.86	0.56
3:1:14:ILE:HD11	3:1:32:LEU:HD13	1.88	0.56
3:4:46:ILE:HB	3:4:77:VAL:HG23	1.86	0.56
2:B:168:PRO:HA	2:B:200:ASP:HB3	1.87	0.56
3:I:81:ILE:HD12	3:I:85:VAL:HG12	1.88	0.56
3:N:26:VAL:O	3:N:30:GLU:HG3	2.05	0.56
3:a:26:VAL:O	3:a:30:GLU:HG3	2.05	0.56
3:x:57:PHE:HD1	3:x:60:LYS:HZ3	1.53	0.56
1:7:161:PHE:HB3	1:7:164:ILE:HB	1.87	0.56
2:B:172:THR:HA	2:B:204:VAL:HG23	1.87	0.56
3:E:89:LEU:HD22	1:Q:224:LEU:HD21	1.87	0.56
3:X:81:ILE:HD12	3:X:85:VAL:HG12	1.88	0.56
2:n:169:LEU:HD11	2:n:181:ILE:HD13	1.87	0.56
2:2:169:LEU:HD11	2:2:181:ILE:HD13	1.87	0.56
3:4:69:SER:O	3:4:73:GLY:N	2.26	0.56
2:D:169:LEU:HD13	2:D:173:ILE:HD11	1.86	0.56
2:L:168:PRO:HA	2:L:200:ASP:HB3	1.87	0.56
1:d:161:PHE:HB3	1:d:164:ILE:HB	1.87	0.56
1:e:170:ILE:HD13	2:f:156:PRO:HB3	1.88	0.56
2:f:168:PRO:HA	2:f:200:ASP:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:r:258:MET:HE3	1:s:159:PRO:HA	1.88	0.56
1:t:170:ILE:HD13	2:u:156:PRO:HB3	1.88	0.56
3:F:3:ILE:HD13	3:F:28:PHE:HD1	1.71	0.56
3:I:51:ILE:HG21	3:I:54:ILE:HD11	1.88	0.56
2:S:169:LEU:HD13	2:S:173:ILE:HD11	1.86	0.56
3:U:3:ILE:HD13	3:U:28:PHE:HD1	1.71	0.56
2:h:220:GLU:OE2	2:h:223:ARG:NH2	2.33	0.56
2:u:168:PRO:HA	2:u:200:ASP:HB3	1.87	0.56
1:G:166:VAL:HG21	1:G:258:MET:HE1	1.88	0.56
1:Q:161:PHE:HB3	1:Q:164:ILE:HB	1.87	0.56
2:S:198:LEU:HD23	2:S:230:MET:HB2	1.87	0.56
1:V:166:VAL:HG21	1:V:258:MET:HE1	1.88	0.56
3:a:82:GLN:O	3:a:86:ALA:N	2.35	0.56
5:c:258:MET:HE3	1:d:159:PRO:HA	1.88	0.56
5:P:258:MET:HE3	1:Q:159:PRO:HA	1.88	0.56
2:L:172:THR:HA	2:L:204:VAL:HG23	1.87	0.56
1:V:174:ASP:H	1:V:177:ARG:HB2	1.70	0.56
3:X:51:ILE:HG21	3:X:54:ILE:HD11	1.88	0.56
5:c:166:VAL:HG23	5:c:198:LEU:HB2	1.88	0.56
1:g:221:ALA:HB2	3:1:90:ILE:HD13	1.87	0.56
1:z:174:ASP:H	1:z:177:ARG:HB2	1.70	0.56
3:1:19:GLU:HG3	3:1:51:ILE:HD13	1.88	0.56
3:4:82:GLN:O	3:4:86:ALA:N	2.35	0.56
2:B:179:LYS:O	2:B:183:GLU:HG2	2.06	0.56
2:D:198:LEU:HD23	2:D:230:MET:HB2	1.88	0.56
3:N:82:GLN:O	3:N:86:ALA:N	2.35	0.56
2:f:179:LYS:O	2:f:183:GLU:HG2	2.06	0.56
1:k:174:ASP:H	1:k:177:ARG:HB2	1.70	0.56
3:m:19:GLU:HG3	3:m:51:ILE:HD13	1.88	0.56
3:m:81:ILE:HD12	3:m:85:VAL:HG12	1.88	0.56
3:p:82:GLN:O	3:p:86:ALA:N	2.35	0.56
2:u:179:LYS:O	2:u:183:GLU:HG2	2.06	0.56
3:1:81:ILE:HD12	3:1:85:VAL:HG12	1.88	0.56
2:D:235:ARG:HB2	2:D:238:ILE:HD13	1.88	0.55
1:G:174:ASP:H	1:G:177:ARG:HB2	1.70	0.55
3:I:19:GLU:HG3	3:I:51:ILE:HD13	1.88	0.55
4:M:221:ALA:HA	3:O:90:ILE:HD11	1.88	0.55
3:N:9:GLY:H	3:O:106:GLU:HB3	1.70	0.55
5:P:166:VAL:HG23	5:P:198:LEU:HB2	1.88	0.55
2:L:179:LYS:O	2:L:183:GLU:HG2	2.06	0.55
1:V:170:ILE:HD13	2:W:156:PRO:HB3	1.86	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:19:GLU:HG3	3:X:51:ILE:HD13	1.88	0.55
3:p:69:SER:O	3:p:73:GLY:N	2.26	0.55
2:w:220:GLU:OE2	2:w:223:ARG:NH2	2.33	0.55
3:4:48:ILE:HG23	3:4:51:ILE:HD12	1.88	0.55
1:A:250:ASP:OD1	1:A:251:GLN:N	2.39	0.55
1:K:250:ASP:OD1	1:K:251:GLN:N	2.39	0.55
2:L:270:ASN:OD1	2:L:271:ARG:N	2.39	0.55
3:i:57:PHE:HD1	3:i:60:LYS:HZ3	1.54	0.55
3:p:48:ILE:HG23	3:p:51:ILE:HD12	1.88	0.55
4:3:164:ILE:HG23	4:3:196:VAL:HB	1.88	0.55
5:6:258:MET:HE3	1:7:159:PRO:HA	1.88	0.55
1:G:170:ILE:HD13	2:H:156:PRO:HB3	1.86	0.55
3:N:8:LEU:HB3	3:O:105:LEU:HD22	1.88	0.55
3:q:81:ILE:HG22	3:q:85:VAL:HG13	1.88	0.55
2:w:235:ARG:HB2	2:w:238:ILE:HD13	1.88	0.55
2:B:270:ASN:OD1	2:B:271:ARG:N	2.40	0.55
2:S:235:ARG:HB2	2:S:238:ILE:HD13	1.88	0.55
2:Y:223:ARG:NH1	5:r:249:LEU:O	2.38	0.55
4:Z:190:VAL:HG22	3:b:103:MET:HE1	1.89	0.55
1:e:250:ASP:OD1	1:e:251:GLN:N	2.39	0.55
3:j:66:VAL:HG22	3:j:75:LYS:HD3	1.88	0.55
4:o:164:ILE:HG23	4:o:196:VAL:HB	1.88	0.55
3:y:66:VAL:HG22	3:y:75:LYS:HD3	1.88	0.55
1:z:170:ILE:HD13	2:0:156:PRO:HB3	1.86	0.55
3:4:66:VAL:HG13	3:4:75:LYS:HD3	1.88	0.55
1:A:170:ILE:HD13	2:B:156:PRO:HB3	1.88	0.55
2:f:172:THR:HA	2:f:204:VAL:HG23	1.87	0.55
2:f:198:LEU:HG	2:f:230:MET:HB2	1.88	0.55
2:h:235:ARG:HB2	2:h:238:ILE:HD13	1.88	0.55
3:j:3:ILE:HD13	3:j:28:PHE:HD1	1.71	0.55
1:k:170:ILE:HD13	2:l:156:PRO:HB3	1.86	0.55
3:p:66:VAL:HG13	3:p:75:LYS:HD3	1.88	0.55
1:t:250:ASP:OD1	1:t:251:GLN:N	2.39	0.55
3:y:3:ILE:HD13	3:y:28:PHE:HD1	1.71	0.55
3:5:81:ILE:HG22	3:5:85:VAL:HG13	1.88	0.55
3:I:14:ILE:HD11	3:I:32:LEU:HD13	1.87	0.55
3:O:43:GLY:HA3	3:O:112:LEU:HD21	1.88	0.55
2:Y:151:GLN:NE2	2:Y:180:LEU:HD21	2.21	0.55
1:g:186:LEU:HB3	3:1:83:PRO:HB3	1.89	0.55
1:k:166:VAL:HG21	1:k:258:MET:HE1	1.88	0.55
2:u:172:THR:HA	2:u:204:VAL:HG23	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:u:198:LEU:HG	2:u:230:MET:HB2	1.88	0.55
1:K:170:ILE:HD13	2:L:156:PRO:HB3	1.88	0.55
3:b:43:GLY:HA3	3:b:112:LEU:HD21	1.88	0.55
2:w:198:LEU:HD23	2:w:230:MET:HB2	1.87	0.55
1:z:166:VAL:HG21	1:z:258:MET:HE1	1.88	0.55
2:J:151:GLN:NE2	2:J:180:LEU:HD21	2.21	0.55
2:h:198:LEU:HD23	2:h:230:MET:HB2	1.88	0.55
3:i:22:ASP:HA	3:i:57:PHE:HE2	1.70	0.55
3:X:14:ILE:HD11	3:X:32:LEU:HD13	1.87	0.55
3:i:46:ILE:O	3:i:78:VAL:HG12	2.07	0.55
3:x:46:ILE:O	3:x:78:VAL:HG12	2.07	0.55
3:X:48:ILE:N	3:X:79:THR:OG1	2.29	0.55
3:b:81:ILE:HG22	3:b:85:VAL:HG13	1.88	0.55
3:q:43:GLY:HA3	3:q:112:LEU:HD21	1.88	0.55
2:2:151:GLN:NE2	2:2:180:LEU:HD21	2.21	0.55
4:M:164:ILE:HG23	4:M:196:VAL:HB	1.88	0.54
3:O:81:ILE:HG22	3:O:85:VAL:HG13	1.88	0.54
3:U:66:VAL:HG22	3:U:75:LYS:HD3	1.88	0.54
3:q:48:ILE:N	3:q:79:THR:OG1	2.28	0.54
3:x:22:ASP:HA	3:x:57:PHE:HE2	1.70	0.54
2:B:198:LEU:HG	2:B:230:MET:HB2	1.88	0.54
3:F:66:VAL:HG22	3:F:75:LYS:HD3	1.88	0.54
2:S:220:GLU:OE2	2:S:223:ARG:NH2	2.33	0.54
2:n:151:GLN:NE2	2:n:180:LEU:HD21	2.22	0.54
3:5:43:GLY:HA3	3:5:112:LEU:HD21	1.88	0.54
2:L:198:LEU:HG	2:L:230:MET:HB2	1.88	0.54
3:T:46:ILE:O	3:T:78:VAL:HG12	2.07	0.54
1:V:186:LEU:HB3	3:p:83:PRO:HB3	1.90	0.54
5:r:166:VAL:HG23	5:r:198:LEU:HB2	1.88	0.54
3:y:49:THR:OG1	3:y:79:THR:HB	2.07	0.54
2:D:220:GLU:OE2	2:D:223:ARG:NH2	2.33	0.54
4:Z:164:ILE:HG23	4:Z:196:VAL:HB	1.88	0.54
3:a:48:ILE:HG23	3:a:51:ILE:HD12	1.88	0.54
3:a:66:VAL:HG13	3:a:75:LYS:HD3	1.88	0.54
2:f:270:ASN:OD1	2:f:271:ARG:N	2.40	0.54
1:g:168:PRO:HA	1:g:200:ASP:HB3	1.89	0.54
3:j:49:THR:OG1	3:j:79:THR:HB	2.07	0.54
1:v:168:PRO:HA	1:v:200:ASP:HB3	1.89	0.54
2:w:177:ARG:O	2:w:181:ILE:HG12	2.08	0.54
3:1:42:ARG:HH11	3:1:116:LEU:HD22	1.73	0.54
4:3:226:GLY:HA3	3:5:102:ALA:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:48:ILE:N	3:I:79:THR:OG1	2.29	0.54
3:N:48:ILE:HG23	3:N:51:ILE:HD12	1.88	0.54
3:X:10:GLU:HG2	3:X:42:ARG:NH2	2.23	0.54
2:h:177:ARG:O	2:h:181:ILE:HG12	2.08	0.54
3:m:42:ARG:HH11	3:m:116:LEU:HD22	1.73	0.54
2:u:270:ASN:OD1	2:u:271:ARG:N	2.39	0.54
3:5:48:ILE:N	3:5:79:THR:OG1	2.28	0.54
3:E:46:ILE:O	3:E:78:VAL:HG12	2.07	0.54
3:I:10:GLU:HG2	3:I:42:ARG:NH2	2.23	0.54
2:J:223:ARG:NH1	5:6:249:LEU:O	2.39	0.54
3:N:66:VAL:HG13	3:N:75:LYS:HD3	1.88	0.54
1:V:224:LEU:O	3:p:100:LEU:HD22	2.07	0.54
3:i:19:GLU:HG3	3:i:51:ILE:HD13	1.90	0.54
4:o:226:GLY:HA3	3:q:102:ALA:HB2	1.89	0.54
3:q:68:MET:HE1	1:s:240:GLN:HA	1.89	0.54
3:x:19:GLU:HG3	3:x:51:ILE:HD13	1.90	0.54
3:1:51:ILE:HG21	3:1:54:ILE:HD11	1.88	0.54
5:6:166:VAL:HG23	5:6:198:LEU:HB2	1.88	0.54
1:C:186:LEU:HB3	3:X:83:PRO:HB3	1.90	0.54
2:D:177:ARG:O	2:D:181:ILE:HG12	2.08	0.54
3:E:19:GLU:HG3	3:E:51:ILE:HD13	1.90	0.54
3:T:19:GLU:HG3	3:T:51:ILE:HD13	1.90	0.54
2:n:228:GLN:OE1	2:n:228:GLN:N	2.41	0.54
2:2:228:GLN:OE1	2:2:228:GLN:N	2.41	0.54
2:S:177:ARG:O	2:S:181:ILE:HG12	2.08	0.54
3:m:51:ILE:HG21	3:m:54:ILE:HD11	1.88	0.54
3:U:49:THR:OG1	3:U:79:THR:HB	2.07	0.54
4:Z:224:LEU:HD21	3:b:89:LEU:HD22	1.90	0.54
3:b:68:MET:HE1	1:d:240:GLN:HA	1.89	0.54
1:k:185:LEU:HD11	1:k:197:VAL:HG11	1.90	0.54
1:z:185:LEU:HD11	1:z:197:VAL:HG11	1.90	0.54
3:F:49:THR:OG1	3:F:79:THR:HB	2.07	0.54
3:j:25:ALA:HB1	3:j:61:ILE:HG21	1.90	0.53
3:q:72:MET:HB3	1:s:256:ASN:ND2	2.24	0.53
1:s:155:ALA:HB2	1:s:181:ILE:HD13	1.90	0.53
2:u:158:LEU:O	2:u:160:ILE:HG13	2.08	0.53
2:f:158:LEU:O	2:f:160:ILE:HG13	2.08	0.53
3:1:10:GLU:HG2	3:1:42:ARG:NH2	2.23	0.53
1:7:155:ALA:HB2	1:7:181:ILE:HD13	1.90	0.53
3:m:10:GLU:HG2	3:m:42:ARG:NH2	2.23	0.53
3:y:25:ALA:HB1	3:y:61:ILE:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:16:ILE:O	3:U:50:SER:OG	2.22	0.53
1:C:168:PRO:HA	1:C:200:ASP:HB3	1.89	0.53
1:G:185:LEU:HD11	1:G:197:VAL:HG11	1.90	0.53
3:U:25:ALA:HB1	3:U:61:ILE:HG21	1.90	0.53
1:V:185:LEU:HD11	1:V:197:VAL:HG11	1.90	0.53
3:q:72:MET:O	1:s:256:ASN:ND2	2.41	0.53
3:F:25:ALA:HB1	3:F:61:ILE:HG21	1.90	0.53
5:P:253:ILE:HG21	5:P:264:ARG:HH22	1.74	0.53
1:R:168:PRO:HA	1:R:200:ASP:HB3	1.89	0.53
5:c:253:ILE:HG21	5:c:264:ARG:HH22	1.74	0.53
5:r:162:GLU:OE1	1:s:259:LYS:NZ	2.38	0.53
3:5:69:SER:HB3	3:5:75:LYS:HZ3	1.74	0.53
2:D:185:LEU:HD11	2:D:197:VAL:HG11	1.90	0.53
3:F:16:ILE:O	3:F:50:SER:OG	2.22	0.53
1:K:190:VAL:HG21	4:Z:236:PRO:HG3	1.90	0.53
2:S:185:LEU:HD11	2:S:197:VAL:HG11	1.90	0.53
3:T:89:LEU:HD22	1:d:224:LEU:HD21	1.91	0.53
3:a:69:SER:HB3	3:a:75:LYS:HD2	1.91	0.53
1:d:155:ALA:HB2	1:d:181:ILE:HD13	1.90	0.53
3:p:20:LEU:HD23	3:p:21:ASP:H	1.74	0.53
3:q:69:SER:HB3	3:q:75:LYS:HZ3	1.74	0.53
2:B:158:LEU:O	2:B:160:ILE:HG13	2.08	0.53
1:Q:155:ALA:HB2	1:Q:181:ILE:HD13	1.90	0.53
1:V:240:GLN:HA	3:X:68:MET:HE2	1.90	0.53
3:q:78:VAL:HA	3:q:101:SER:HB3	1.91	0.53
3:4:20:LEU:HD23	3:4:21:ASP:H	1.74	0.53
5:6:156:PRO:HB3	1:7:170:ILE:HD13	1.91	0.53
2:D:166:VAL:HG23	2:D:198:LEU:HB2	1.90	0.53
3:I:42:ARG:HH11	3:I:116:LEU:HD22	1.73	0.53
2:J:228:GLN:OE1	2:J:228:GLN:N	2.41	0.53
3:N:69:SER:HB3	3:N:75:LYS:HD2	1.91	0.53
2:S:166:VAL:HG23	2:S:198:LEU:HB2	1.91	0.53
2:Y:228:GLN:N	2:Y:228:GLN:OE1	2.41	0.53
4:Z:221:ALA:HA	3:b:90:ILE:HD11	1.91	0.53
3:5:78:VAL:HA	3:5:101:SER:HB3	1.91	0.53
5:P:153:LEU:HA	1:Q:170:ILE:HD11	1.92	0.52
2:L:158:LEU:O	2:L:160:ILE:HG13	2.08	0.52
3:X:42:ARG:HH11	3:X:116:LEU:HD22	1.73	0.52
3:a:43:GLY:HA3	3:a:112:LEU:HD11	1.91	0.52
5:c:153:LEU:HA	1:d:170:ILE:HD11	1.92	0.52
2:J:153:LEU:HA	2:2:170:ILE:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:20:LEU:HD23	3:a:21:ASP:H	1.74	0.52
3:N:43:GLY:HA3	3:N:112:LEU:HD11	1.91	0.52
1:g:255:THR:HG22	1:g:264:ARG:NH2	2.25	0.52
3:p:20:LEU:HD23	3:p:21:ASP:N	2.24	0.52
5:r:253:ILE:HG21	5:r:264:ARG:HH22	1.74	0.52
1:v:255:THR:HG22	1:v:264:ARG:NH2	2.25	0.52
1:z:262:MET:HE2	1:z:262:MET:HA	1.91	0.52
1:C:255:THR:HG22	1:C:264:ARG:NH2	2.25	0.52
3:N:20:LEU:HD23	3:N:21:ASP:H	1.74	0.52
1:R:255:THR:HG22	1:R:264:ARG:NH2	2.25	0.52
4:Z:223:ARG:NH2	4:Z:251:GLN:O	2.43	0.52
1:k:262:MET:HE2	1:k:262:MET:HA	1.91	0.52
1:z:163:LYS:HG2	1:z:195:GLU:HG3	1.91	0.52
4:M:223:ARG:NH2	4:M:251:GLN:O	2.43	0.52
1:k:163:LYS:HG2	1:k:195:GLU:HG3	1.91	0.52
2:w:185:LEU:HD11	2:w:197:VAL:HG11	1.90	0.52
3:4:20:LEU:HD23	3:4:21:ASP:N	2.24	0.52
5:6:253:ILE:HG21	5:6:264:ARG:HH22	1.74	0.52
3:N:16:ILE:HD11	3:N:28:PHE:CE1	2.45	0.52
1:V:262:MET:HA	1:V:262:MET:HE2	1.91	0.52
4:o:223:ARG:NH2	4:o:251:GLN:O	2.43	0.52
3:p:69:SER:HB3	3:p:75:LYS:HD2	1.91	0.52
3:4:43:GLY:HA3	3:4:112:LEU:HD11	1.91	0.52
1:G:190:VAL:HA	3:4:103:MET:HE1	1.92	0.52
1:G:262:MET:HE2	1:G:262:MET:HA	1.91	0.52
3:O:78:VAL:HA	3:O:101:SER:HB3	1.91	0.52
3:a:16:ILE:HD11	3:a:28:PHE:CE1	2.45	0.52
5:c:156:PRO:HB3	1:d:170:ILE:HD13	1.91	0.52
2:h:185:LEU:HD11	2:h:197:VAL:HG11	1.90	0.52
3:p:43:GLY:HA3	3:p:112:LEU:HD11	1.91	0.52
4:3:223:ARG:NH2	4:3:251:GLN:O	2.43	0.52
5:P:156:PRO:HB3	1:Q:170:ILE:HD13	1.91	0.52
3:b:78:VAL:HA	3:b:101:SER:HB3	1.91	0.52
5:c:177:ARG:HH22	1:d:153:LEU:HD21	1.74	0.52
2:h:166:VAL:HG23	2:h:198:LEU:HB2	1.91	0.52
3:4:69:SER:HB3	3:4:75:LYS:HD2	1.91	0.52
5:P:177:ARG:HH22	1:Q:153:LEU:HD21	1.74	0.52
3:X:42:ARG:NH1	3:X:116:LEU:HD13	2.25	0.52
1:e:190:VAL:HG21	4:o:236:PRO:HG3	1.92	0.52
2:w:166:VAL:HG23	2:w:198:LEU:HB2	1.91	0.52
3:x:69:SER:O	3:x:73:GLY:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:42:ARG:NH1	3:1:116:LEU:HD13	2.25	0.52
3:1:42:ARG:NH1	3:1:116:LEU:HD13	2.25	0.52
3:m:42:ARG:NH1	3:m:116:LEU:HD13	2.25	0.52
5:r:177:ARG:HH22	1:s:153:LEU:HD21	1.74	0.52
1:t:190:VAL:HG21	4:3:236:PRO:HG3	1.92	0.52
3:i:69:SER:O	3:i:73:GLY:N	2.42	0.51
3:4:16:ILE:HD11	3:4:28:PHE:CE1	2.45	0.51
2:L:249:LEU:O	3:4:70:LYS:NZ	2.43	0.51
3:a:20:LEU:HD23	3:a:21:ASP:N	2.24	0.51
3:p:16:ILE:HD11	3:p:28:PHE:CE1	2.45	0.51
1:A:190:VAL:HG21	4:M:236:PRO:HG3	1.92	0.51
3:E:46:ILE:HG22	3:E:77:VAL:HA	1.92	0.51
4:Z:190:VAL:HG13	3:b:103:MET:HE1	1.93	0.51
1:e:208:ASP:HB3	1:e:211:VAL:HG23	1.92	0.51
4:M:164:ILE:HD12	4:M:196:VAL:HB	1.91	0.51
4:M:224:LEU:HD21	3:O:89:LEU:HD22	1.91	0.51
3:N:20:LEU:HD23	3:N:21:ASP:N	2.24	0.51
3:N:70:LYS:NZ	2:f:249:LEU:O	2.43	0.51
1:K:159:PRO:HB2	1:K:166:VAL:HG13	1.93	0.51
3:T:13:LEU:HD21	3:T:109:LEU:HD21	1.92	0.51
4:o:164:ILE:HD12	4:o:196:VAL:HB	1.91	0.51
1:t:208:ASP:HB3	1:t:211:VAL:HG23	1.92	0.51
3:5:68:MET:HE2	1:7:243:VAL:HG11	1.93	0.51
1:A:159:PRO:HB2	1:A:166:VAL:HG13	1.93	0.51
3:E:13:LEU:HD21	3:E:109:LEU:HD21	1.92	0.51
2:H:175:THR:HG22	2:H:179:LYS:HE2	1.93	0.51
4:M:226:GLY:HA3	3:O:102:ALA:HB2	1.92	0.51
2:W:175:THR:HG22	2:W:179:LYS:HE2	1.93	0.51
3:p:22:ASP:OD1	3:p:23:HIS:N	2.41	0.51
1:t:173:ILE:HG13	1:t:211:VAL:HG11	1.91	0.51
5:6:153:LEU:HA	1:7:170:ILE:HD11	1.92	0.51
5:6:177:ARG:HH22	1:7:153:LEU:HD21	1.74	0.51
1:V:163:LYS:HG2	1:V:195:GLU:HG3	1.91	0.51
4:Z:164:ILE:HD12	4:Z:196:VAL:HB	1.91	0.51
4:3:164:ILE:HD12	4:3:196:VAL:HB	1.91	0.51
3:T:46:ILE:HG22	3:T:77:VAL:HA	1.92	0.51
1:e:173:ILE:HG13	1:e:211:VAL:HG11	1.91	0.51
2:h:232:VAL:HG11	2:h:258:MET:HA	1.92	0.51
4:o:168:PRO:O	4:o:200:ASP:HB2	2.11	0.51
1:s:235:ARG:HG2	1:s:238:ILE:HG12	1.93	0.51
1:G:163:LYS:HG2	1:G:195:GLU:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:13:LEU:HD11	3:U:105:LEU:HD21	1.93	0.51
3:y:13:LEU:HD11	3:y:105:LEU:HD21	1.93	0.51
4:3:168:PRO:O	4:3:200:ASP:HB2	2.11	0.51
3:4:22:ASP:OD1	3:4:23:HIS:N	2.41	0.51
1:C:170:ILE:HG12	2:D:158:LEU:HD13	1.92	0.51
3:F:13:LEU:HD11	3:F:105:LEU:HD21	1.93	0.51
3:N:69:SER:O	3:N:73:GLY:N	2.26	0.51
5:P:168:PRO:HA	5:P:200:ASP:HB3	1.93	0.51
5:c:168:PRO:HA	5:c:200:ASP:HB3	1.93	0.51
1:d:193:ARG:HA	1:d:193:ARG:CZ	2.41	0.51
3:j:13:LEU:HD11	3:j:105:LEU:HD21	1.93	0.51
1:t:156:PRO:HB3	2:u:170:ILE:HD13	1.93	0.51
1:7:193:ARG:CZ	1:7:193:ARG:HA	2.41	0.51
3:I:24:THR:O	3:I:28:PHE:HB3	2.10	0.51
1:Q:193:ARG:HA	1:Q:193:ARG:CZ	2.41	0.51
1:R:170:ILE:HG12	2:S:158:LEU:HD13	1.92	0.51
3:X:24:THR:O	3:X:28:PHE:HB3	2.10	0.51
3:X:29:GLN:O	3:X:33:LEU:HG	2.11	0.51
2:Y:185:LEU:HD11	2:Y:197:VAL:HG11	1.92	0.51
1:e:156:PRO:HB3	2:f:170:ILE:HD13	1.93	0.51
1:e:159:PRO:HB2	1:e:166:VAL:HG13	1.93	0.51
3:i:46:ILE:HG22	3:i:77:VAL:HA	1.92	0.51
2:n:185:LEU:HD11	2:n:197:VAL:HG11	1.92	0.51
1:s:193:ARG:CZ	1:s:193:ARG:HA	2.41	0.51
2:w:232:VAL:HG11	2:w:258:MET:HA	1.92	0.51
3:1:24:THR:O	3:1:28:PHE:HB3	2.10	0.51
1:A:208:ASP:HB3	1:A:211:VAL:HG23	1.92	0.50
3:I:29:GLN:O	3:I:33:LEU:HG	2.11	0.50
2:J:185:LEU:HD11	2:J:197:VAL:HG11	1.93	0.50
4:M:168:PRO:O	4:M:200:ASP:HB2	2.11	0.50
1:Q:168:PRO:HA	1:Q:200:ASP:HB3	1.93	0.50
4:Z:168:PRO:O	4:Z:200:ASP:HB2	2.11	0.50
3:x:89:LEU:HD22	1:7:224:LEU:HD21	1.92	0.50
2:2:185:LEU:HD11	2:2:197:VAL:HG11	1.92	0.50
4:3:255:THR:HG21	4:3:261:GLY:N	2.27	0.50
1:7:168:PRO:HA	1:7:200:ASP:HB3	1.93	0.50
4:M:255:THR:HG21	4:M:261:GLY:N	2.26	0.50
1:K:173:ILE:HG13	1:K:211:VAL:HG11	1.91	0.50
1:K:208:ASP:HB3	1:K:211:VAL:HG23	1.92	0.50
1:d:168:PRO:HA	1:d:200:ASP:HB3	1.93	0.50
3:m:24:THR:O	3:m:28:PHE:HB3	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:o:255:THR:HG21	4:o:261:GLY:N	2.27	0.50
1:s:168:PRO:HA	1:s:200:ASP:HB3	1.93	0.50
3:x:46:ILE:HG22	3:x:77:VAL:HA	1.92	0.50
1:t:159:PRO:HB2	1:t:166:VAL:HG13	1.93	0.50
1:A:173:ILE:HG13	1:A:211:VAL:HG11	1.91	0.50
2:J:170:ILE:HD11	2:2:153:LEU:HA	1.93	0.50
1:g:170:ILE:HG12	2:h:158:LEU:HD13	1.92	0.50
3:i:13:LEU:HD21	3:i:109:LEU:HD21	1.92	0.50
2:l:175:THR:HG22	2:l:179:LYS:HE2	1.93	0.50
1:V:177:ARG:O	1:V:181:ILE:HG12	2.11	0.50
4:Z:255:THR:HG21	4:Z:261:GLY:N	2.27	0.50
5:r:168:PRO:HA	5:r:200:ASP:HB3	1.93	0.50
3:x:13:LEU:HD21	3:x:109:LEU:HD21	1.92	0.50
2:0:175:THR:HG22	2:0:179:LYS:HE2	1.93	0.50
3:1:48:ILE:N	3:1:79:THR:OG1	2.29	0.50
1:G:177:ARG:O	1:G:181:ILE:HG12	2.11	0.50
1:k:235:ARG:HB2	1:k:238:ILE:HD13	1.94	0.50
1:v:170:ILE:HG12	2:w:158:LEU:HD13	1.92	0.50
5:6:168:PRO:HA	5:6:200:ASP:HB3	1.93	0.50
3:E:5:ILE:HG21	3:E:35:LYS:HD2	1.94	0.50
3:a:70:LYS:NZ	2:u:249:LEU:O	2.45	0.50
1:Q:216:ILE:HG21	1:Q:247:ILE:HD12	1.94	0.50
4:Z:170:ILE:HD11	4:3:153:LEU:HA	1.94	0.50
1:d:216:ILE:HG21	1:d:247:ILE:HD12	1.94	0.50
1:e:203:GLY:H	1:e:235:ARG:HH21	1.60	0.50
2:l:159:PRO:HB2	2:l:166:VAL:HG13	1.93	0.50
3:m:48:ILE:N	3:m:79:THR:OG1	2.29	0.50
1:A:203:GLY:H	1:A:235:ARG:HH21	1.60	0.50
3:T:5:ILE:HG21	3:T:35:LYS:HD2	1.94	0.50
1:t:203:GLY:H	1:t:235:ARG:HH21	1.60	0.50
1:z:235:ARG:HB2	1:z:238:ILE:HD13	1.94	0.50
1:A:156:PRO:HB3	2:B:170:ILE:HD13	1.93	0.49
4:M:153:LEU:HA	4:o:170:ILE:HD11	1.93	0.49
1:Q:212:ALA:HB1	1:Q:242:ILE:HG12	1.93	0.49
1:K:203:GLY:H	1:K:235:ARG:HH21	1.60	0.49
2:Y:153:LEU:HA	2:n:170:ILE:HD11	1.93	0.49
1:k:148:SER:HA	1:k:151:GLN:HG3	1.94	0.49
2:n:235:ARG:HG2	2:n:236:PRO:HD2	1.95	0.49
5:r:153:LEU:HA	1:s:170:ILE:HD11	1.94	0.49
2:0:159:PRO:HB2	2:0:166:VAL:HG13	1.93	0.49
2:2:235:ARG:HG2	2:2:236:PRO:HD2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:19:GLU:HB3	3:N:51:ILE:HG12	1.94	0.49
3:N:25:ALA:HB1	3:N:61:ILE:HG13	1.94	0.49
3:N:111:LYS:O	3:N:114:GLN:HG3	2.11	0.49
1:K:156:PRO:HB3	2:L:170:ILE:HD13	1.93	0.49
3:a:25:ALA:HB1	3:a:61:ILE:HG13	1.94	0.49
1:d:212:ALA:HB1	1:d:242:ILE:HG12	1.93	0.49
3:i:5:ILE:HG21	3:i:35:LYS:HD2	1.94	0.49
3:x:5:ILE:HG21	3:x:35:LYS:HD2	1.94	0.49
2:J:157:LEU:HD23	2:J:188:GLY:HA3	1.94	0.49
1:V:148:SER:HA	1:V:151:GLN:HG3	1.94	0.49
3:a:19:GLU:HB3	3:a:51:ILE:HG12	1.94	0.49
3:a:111:LYS:O	3:a:114:GLN:HG3	2.12	0.49
3:m:29:GLN:O	3:m:33:LEU:HG	2.11	0.49
3:q:99:VAL:C	3:q:100:LEU:HD12	2.37	0.49
1:z:148:SER:HA	1:z:151:GLN:HG3	1.94	0.49
1:z:177:ARG:O	1:z:181:ILE:HG12	2.11	0.49
3:1:29:GLN:O	3:1:33:LEU:HG	2.11	0.49
3:4:77:VAL:O	3:4:100:LEU:HG	2.12	0.49
3:5:99:VAL:C	3:5:100:LEU:HD12	2.37	0.49
1:7:212:ALA:HB1	1:7:242:ILE:HG12	1.93	0.49
2:D:232:VAL:HG11	2:D:258:MET:HA	1.92	0.49
2:H:159:PRO:HB2	2:H:166:VAL:HG13	1.93	0.49
2:S:232:VAL:HG11	2:S:258:MET:HA	1.92	0.49
2:W:159:PRO:HB2	2:W:166:VAL:HG13	1.93	0.49
3:m:89:LEU:HD22	1:v:224:LEU:HD21	1.94	0.49
3:1:48:ILE:H	3:1:79:THR:HG1	1.57	0.49
3:4:19:GLU:HB3	3:4:51:ILE:HG12	1.94	0.49
1:G:148:SER:HA	1:G:151:GLN:HG3	1.94	0.49
2:S:196:VAL:HG22	2:S:228:GLN:HB3	1.95	0.49
2:Y:157:LEU:HD23	2:Y:188:GLY:HA3	1.94	0.49
1:e:196:VAL:HG21	1:e:265:ALA:HB1	1.94	0.49
1:k:159:PRO:HA	2:l:258:MET:HE3	1.94	0.49
1:k:177:ARG:O	1:k:181:ILE:HG12	2.11	0.49
3:m:48:ILE:H	3:m:79:THR:HG1	1.57	0.49
3:p:19:GLU:HB3	3:p:51:ILE:HG12	1.94	0.49
3:p:77:VAL:O	3:p:100:LEU:HG	2.12	0.49
1:t:196:VAL:HG21	1:t:265:ALA:HB1	1.94	0.49
2:D:196:VAL:HG22	2:D:228:GLN:HB3	1.95	0.49
2:J:235:ARG:HG2	2:J:236:PRO:HD2	1.95	0.49
1:V:159:PRO:HA	2:W:258:MET:HE3	1.94	0.49
2:Y:235:ARG:HG2	2:Y:236:PRO:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:77:VAL:O	3:a:100:LEU:HG	2.12	0.49
3:b:99:VAL:C	3:b:100:LEU:HD12	2.37	0.49
2:h:255:THR:HG21	2:h:261:GLY:N	2.27	0.49
3:q:78:VAL:HG23	3:q:101:SER:HB3	1.95	0.49
1:s:212:ALA:HB1	1:s:242:ILE:HG12	1.93	0.49
2:w:255:THR:HG21	2:w:261:GLY:N	2.28	0.49
1:z:159:PRO:HA	2:0:258:MET:HE3	1.94	0.49
3:4:111:LYS:O	3:4:114:GLN:HG3	2.12	0.49
3:5:78:VAL:HG23	3:5:101:SER:HB3	1.95	0.49
1:G:159:PRO:HA	2:H:258:MET:HE3	1.94	0.49
3:N:77:VAL:O	3:N:100:LEU:HG	2.12	0.49
3:T:20:LEU:HG	3:T:21:ASP:N	2.27	0.49
3:m:83:PRO:HB3	1:v:186:LEU:HB3	1.95	0.49
3:p:111:LYS:O	3:p:114:GLN:HG3	2.12	0.49
4:3:161:PHE:CE2	4:3:266:LEU:HD21	2.47	0.49
1:C:196:VAL:HG21	1:C:265:ALA:HB1	1.94	0.49
3:E:20:LEU:HG	3:E:21:ASP:N	2.27	0.49
4:M:190:VAL:HG22	3:O:103:MET:HE1	1.95	0.49
3:O:99:VAL:C	3:O:100:LEU:HD12	2.37	0.49
1:R:196:VAL:HG21	1:R:265:ALA:HB1	1.95	0.49
2:S:255:THR:HG21	2:S:261:GLY:N	2.27	0.49
4:o:161:PHE:CE2	4:o:266:LEU:HD21	2.47	0.49
5:r:177:ARG:O	5:r:181:ILE:HG12	2.13	0.49
5:6:177:ARG:O	5:6:181:ILE:HG12	2.13	0.49
5:P:177:ARG:O	5:P:181:ILE:HG12	2.13	0.49
4:Z:156:PRO:HG2	4:Z:168:PRO:HG2	1.95	0.49
4:Z:161:PHE:CE2	4:Z:266:LEU:HD21	2.48	0.49
2:f:203:GLY:H	2:f:235:ARG:NH2	2.10	0.49
3:p:99:VAL:C	3:p:100:LEU:HD12	2.38	0.49
2:w:250:ASP:OD1	2:w:251:GLN:N	2.46	0.49
2:B:203:GLY:H	2:B:235:ARG:NH2	2.10	0.49
2:D:255:THR:HG21	2:D:261:GLY:N	2.27	0.49
1:G:235:ARG:HB2	1:G:238:ILE:HD13	1.94	0.49
3:I:115:GLU:C	3:I:115:GLU:OE1	2.56	0.49
4:M:156:PRO:HG2	4:M:168:PRO:HG2	1.95	0.49
4:M:161:PHE:CE2	4:M:266:LEU:HD21	2.48	0.49
4:M:193:ARG:HH12	3:O:102:ALA:CB	2.26	0.49
3:N:99:VAL:C	3:N:100:LEU:HD12	2.38	0.49
3:N:103:MET:HE1	1:z:190:VAL:HA	1.95	0.49
3:O:78:VAL:HG23	3:O:101:SER:HB3	1.95	0.49
3:T:21:ASP:OD1	3:T:22:ASP:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:235:ARG:HB2	1:V:238:ILE:HD13	1.94	0.49
3:X:115:GLU:C	3:X:115:GLU:OE1	2.56	0.49
2:h:250:ASP:OD1	2:h:251:GLN:N	2.46	0.49
2:u:203:GLY:H	2:u:235:ARG:NH2	2.10	0.49
3:E:21:ASP:OD1	3:E:22:ASP:N	2.46	0.48
3:E:69:SER:O	3:E:73:GLY:N	2.42	0.48
3:E:81:ILE:HD12	3:E:81:ILE:H	1.78	0.48
2:J:210:MET:HA	2:J:210:MET:HE2	1.94	0.48
3:T:69:SER:O	3:T:73:GLY:N	2.42	0.48
2:Y:210:MET:HE2	2:Y:210:MET:HA	1.94	0.48
3:a:99:VAL:C	3:a:100:LEU:HD12	2.38	0.48
3:b:78:VAL:HG23	3:b:101:SER:HB3	1.95	0.48
5:c:177:ARG:O	5:c:181:ILE:HG12	2.13	0.48
2:f:167:MET:HE1	2:f:169:LEU:HD23	1.95	0.48
3:i:42:ARG:O	3:i:74:ALA:N	2.46	0.48
3:i:81:ILE:H	3:i:81:ILE:HD12	1.78	0.48
3:m:115:GLU:C	3:m:115:GLU:OE1	2.56	0.48
3:x:42:ARG:O	3:x:74:ALA:N	2.46	0.48
3:1:115:GLU:OE1	3:1:115:GLU:C	2.56	0.48
3:4:8:LEU:HD21	3:4:13:LEU:HD12	1.95	0.48
3:4:99:VAL:C	3:4:100:LEU:HD12	2.38	0.48
3:I:102:ALA:HA	1:R:225:VAL:O	2.12	0.48
4:M:170:ILE:HD11	4:o:153:LEU:HA	1.95	0.48
2:L:203:GLY:H	2:L:235:ARG:NH2	2.10	0.48
2:Y:170:ILE:HD11	2:n:153:LEU:HA	1.94	0.48
3:p:8:LEU:HD21	3:p:13:LEU:HD12	1.95	0.48
1:s:185:LEU:HD11	1:s:197:VAL:HG11	1.95	0.48
1:s:216:ILE:HG21	1:s:247:ILE:HD12	1.94	0.48
2:u:167:MET:HE1	2:u:169:LEU:HD23	1.96	0.48
3:x:81:ILE:HD12	3:x:81:ILE:H	1.78	0.48
3:i:5:ILE:HG13	3:i:35:LYS:HG3	1.95	0.48
3:p:25:ALA:HB1	3:p:61:ILE:HG13	1.94	0.48
3:x:21:ASP:OD1	3:x:22:ASP:N	2.46	0.48
3:4:25:ALA:HB1	3:4:61:ILE:HG13	1.94	0.48
2:D:221:ALA:HA	3:F:90:ILE:HD11	1.96	0.48
3:E:5:ILE:HG13	3:E:35:LYS:HG3	1.95	0.48
1:G:240:GLN:CA	3:I:68:MET:HE2	2.43	0.48
2:L:210:MET:HG3	2:L:214:HIS:CE1	2.49	0.48
3:T:5:ILE:HG13	3:T:35:LYS:HG3	1.95	0.48
3:T:81:ILE:H	3:T:81:ILE:HD12	1.78	0.48
3:a:22:ASP:OD1	3:a:23:HIS:N	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:21:ASP:OD1	3:i:22:ASP:N	2.46	0.48
3:x:5:ILE:HG13	3:x:35:LYS:HG3	1.95	0.48
1:7:216:ILE:HG21	1:7:247:ILE:HD12	1.94	0.48
2:B:210:MET:HG3	2:B:214:HIS:CE1	2.49	0.48
3:N:8:LEU:HD21	3:N:13:LEU:HD12	1.95	0.48
3:T:42:ARG:O	3:T:74:ALA:N	2.46	0.48
4:Z:153:LEU:HA	4:3:170:ILE:HD11	1.94	0.48
4:3:156:PRO:HG2	4:3:168:PRO:HG2	1.95	0.48
2:D:250:ASP:OD1	2:D:251:GLN:N	2.46	0.48
3:I:87:ILE:HA	3:I:90:ILE:HG12	1.96	0.48
3:N:107:SER:O	3:N:110:GLU:HG3	2.14	0.48
1:K:196:VAL:HG21	1:K:265:ALA:HB1	1.94	0.48
2:n:210:MET:HE2	2:n:210:MET:HA	1.94	0.48
4:o:156:PRO:HG2	4:o:168:PRO:HG2	1.95	0.48
3:x:20:LEU:HG	3:x:21:ASP:N	2.27	0.48
2:2:157:LEU:HD23	2:2:188:GLY:HA3	1.94	0.48
2:2:210:MET:HE2	2:2:210:MET:HA	1.94	0.48
4:3:166:VAL:HG12	4:3:198:LEU:HD12	1.96	0.48
1:A:196:VAL:HG21	1:A:265:ALA:HB1	1.94	0.48
3:E:42:ARG:O	3:E:74:ALA:N	2.46	0.48
2:S:250:ASP:OD1	2:S:251:GLN:N	2.46	0.48
3:X:87:ILE:HA	3:X:90:ILE:HG12	1.96	0.48
4:Z:193:ARG:HH12	3:b:102:ALA:CB	2.27	0.48
3:a:8:LEU:HD21	3:a:13:LEU:HD12	1.95	0.48
1:e:174:ASP:H	1:e:177:ARG:HB3	1.79	0.48
2:n:157:LEU:HD23	2:n:188:GLY:HA3	1.94	0.48
4:o:166:VAL:HG12	4:o:198:LEU:HD12	1.96	0.48
3:p:21:ASP:HA	3:p:58:ILE:HD11	1.96	0.48
3:p:81:ILE:HG22	3:p:85:VAL:HG23	1.96	0.48
3:p:107:SER:O	3:p:110:GLU:HG3	2.14	0.48
1:t:174:ASP:H	1:t:177:ARG:HB3	1.79	0.48
1:v:196:VAL:HG21	1:v:265:ALA:HB1	1.94	0.48
1:7:185:LEU:HD11	1:7:197:VAL:HG11	1.95	0.48
3:N:22:ASP:OD1	3:N:23:HIS:N	2.41	0.48
3:a:107:SER:O	3:a:110:GLU:HG3	2.14	0.48
1:g:193:ARG:HG2	1:g:193:ARG:HH11	1.79	0.48
1:g:196:VAL:HG21	1:g:265:ALA:HB1	1.95	0.48
2:h:196:VAL:HG22	2:h:228:GLN:HB3	1.95	0.48
1:v:193:ARG:HG2	1:v:193:ARG:HH11	1.79	0.48
2:w:196:VAL:HG22	2:w:228:GLN:HB3	1.95	0.48
3:4:21:ASP:HA	3:4:58:ILE:HD11	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:107:SER:O	3:4:110:GLU:HG3	2.14	0.48
3:X:115:GLU:OE1	3:X:116:LEU:HD23	2.14	0.48
3:b:24:THR:HA	3:b:27:GLU:HG2	1.96	0.48
2:f:210:MET:HG3	2:f:214:HIS:CE1	2.49	0.48
3:i:20:LEU:HG	3:i:21:ASP:N	2.27	0.48
3:j:46:ILE:O	3:j:78:VAL:HG12	2.14	0.48
5:r:170:ILE:HG22	1:s:158:LEU:HD22	1.94	0.48
2:u:210:MET:HG3	2:u:214:HIS:CE1	2.49	0.48
3:y:46:ILE:O	3:y:78:VAL:HG12	2.14	0.48
3:4:81:ILE:HG22	3:4:85:VAL:HG23	1.96	0.48
3:5:24:THR:HA	3:5:27:GLU:HG2	1.96	0.48
4:Z:226:GLY:HA3	3:b:102:ALA:HB2	1.95	0.48
1:d:190:VAL:O	1:d:193:ARG:NH1	2.47	0.48
4:o:175:TPO:HG22	4:o:179:LYS:HE3	1.96	0.48
3:q:24:THR:HA	3:q:27:GLU:HG2	1.96	0.48
5:r:148:SER:O	5:r:151:GLN:HG3	2.14	0.48
5:6:148:SER:O	5:6:151:GLN:HG3	2.14	0.48
3:F:56:SER:HB3	3:F:92:LEU:HD13	1.96	0.47
4:M:273:ILE:HG23	4:M:274:VAL:HG13	1.96	0.47
3:O:24:THR:HA	3:O:27:GLU:HG2	1.96	0.47
3:O:80:GLY:HA3	3:O:103:MET:HG3	1.96	0.47
1:Q:190:VAL:O	1:Q:193:ARG:NH1	2.47	0.47
1:R:193:ARG:HG2	1:R:193:ARG:HH11	1.79	0.47
3:U:56:SER:HB3	3:U:92:LEU:HD13	1.96	0.47
2:Y:170:ILE:HG22	2:n:158:LEU:HD22	1.95	0.47
4:Z:273:ILE:HG23	4:Z:274:VAL:HG13	1.96	0.47
3:a:9:GLY:H	3:b:106:GLU:HB3	1.79	0.47
4:3:175:TPO:HG22	4:3:179:LYS:HE3	1.96	0.47
3:I:115:GLU:OE1	3:I:116:LEU:HD23	2.14	0.47
3:a:8:LEU:HB3	3:b:105:LEU:HD22	1.96	0.47
3:b:80:GLY:HA3	3:b:103:MET:HG3	1.96	0.47
4:o:151:GLN:O	4:o:180:LEU:HD21	2.15	0.47
4:o:161:PHE:HE2	4:o:266:LEU:HD21	1.79	0.47
3:1:20:LEU:HD23	3:1:21:ASP:N	2.29	0.47
4:3:151:GLN:O	4:3:180:LEU:HD21	2.15	0.47
4:3:161:PHE:HE2	4:3:266:LEU:HD21	1.79	0.47
2:J:159:PRO:HB2	2:J:166:VAL:HG13	1.97	0.47
1:V:190:VAL:HA	3:p:103:MET:HE1	1.96	0.47
2:Y:159:PRO:HB2	2:Y:166:VAL:HG13	1.97	0.47
1:k:240:GLN:HA	3:m:68:MET:HE2	1.96	0.47
3:m:20:LEU:HD23	3:m:21:ASP:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:106:GLU:HG3	3:1:9:GLY:H	1.79	0.47
3:q:54:ILE:HB	3:q:85:VAL:HG23	1.96	0.47
3:5:54:ILE:HB	3:5:85:VAL:HG23	1.96	0.47
1:C:193:ARG:HG2	1:C:193:ARG:HH11	1.79	0.47
3:U:46:ILE:O	3:U:78:VAL:HG12	2.14	0.47
3:m:115:GLU:OE1	3:m:116:LEU:HD23	2.14	0.47
3:1:115:GLU:OE1	3:1:116:LEU:HD23	2.14	0.47
4:3:221:ALA:HA	3:5:90:ILE:HD11	1.96	0.47
4:3:273:ILE:HG23	4:3:274:VAL:HG13	1.96	0.47
1:7:183:GLU:O	1:7:187:ILE:HG12	2.15	0.47
1:A:163:LYS:HG2	1:A:195:GLU:HG3	1.97	0.47
1:A:185:LEU:HD11	1:A:197:VAL:HG11	1.97	0.47
1:A:260:LYS:O	1:A:263:GLU:HG3	2.14	0.47
3:F:46:ILE:O	3:F:78:VAL:HG12	2.14	0.47
1:K:163:LYS:HG2	1:K:195:GLU:HG3	1.97	0.47
1:K:174:ASP:H	1:K:177:ARG:HB3	1.79	0.47
1:t:260:LYS:O	1:t:263:GLU:HG3	2.14	0.47
2:w:186:LEU:HB3	3:y:83:PRO:HB3	1.97	0.47
1:7:190:VAL:O	1:7:193:ARG:NH1	2.47	0.47
1:A:174:ASP:H	1:A:177:ARG:HB3	1.79	0.47
4:M:166:VAL:HG12	4:M:198:LEU:HD12	1.96	0.47
1:K:185:LEU:HD11	1:K:197:VAL:HG11	1.97	0.47
1:K:260:LYS:O	1:K:263:GLU:HG3	2.14	0.47
3:b:54:ILE:HB	3:b:85:VAL:HG23	1.96	0.47
4:o:273:ILE:HG23	4:o:274:VAL:HG13	1.96	0.47
1:s:183:GLU:O	1:s:187:ILE:HG12	2.15	0.47
1:s:190:VAL:O	1:s:193:ARG:NH1	2.47	0.47
4:3:255:THR:HG23	4:3:260:LYS:HD2	1.96	0.47
2:B:249:LEU:O	3:p:70:LYS:NZ	2.47	0.47
3:I:20:LEU:HD23	3:I:21:ASP:N	2.29	0.47
4:M:161:PHE:HE2	4:M:266:LEU:HD21	1.79	0.47
3:N:21:ASP:HA	3:N:58:ILE:HD11	1.96	0.47
3:O:54:ILE:HB	3:O:85:VAL:HG23	1.96	0.47
5:P:205:PRO:O	5:P:235:ARG:NH1	2.47	0.47
2:L:167:MET:HE1	2:L:169:LEU:HD23	1.95	0.47
4:Z:166:VAL:HG12	4:Z:198:LEU:HD12	1.96	0.47
3:a:4:PRO:HG3	3:b:4:PRO:HG3	1.96	0.47
5:c:205:PRO:O	5:c:235:ARG:NH1	2.47	0.47
1:e:163:LYS:HG2	1:e:195:GLU:HG3	1.97	0.47
1:e:260:LYS:O	1:e:263:GLU:HG3	2.14	0.47
4:o:221:ALA:HA	3:q:90:ILE:HD11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:o:255:THR:HG23	4:o:260:LYS:HD2	1.96	0.47
5:r:205:PRO:O	5:r:235:ARG:NH1	2.47	0.47
1:t:163:LYS:HG2	1:t:195:GLU:HG3	1.97	0.47
3:y:76:VAL:HG23	3:y:100:LEU:HA	1.97	0.47
5:6:205:PRO:O	5:6:235:ARG:NH1	2.47	0.47
3:F:76:VAL:HG23	3:F:100:LEU:HA	1.97	0.47
1:G:187:ILE:HA	1:G:190:VAL:HG12	1.97	0.47
2:J:167:MET:HE1	2:J:181:ILE:HG23	1.97	0.47
3:U:76:VAL:HG23	3:U:100:LEU:HA	1.97	0.47
1:V:187:ILE:HA	1:V:190:VAL:HG12	1.97	0.47
4:Z:161:PHE:HE2	4:Z:266:LEU:HD21	1.79	0.47
3:a:21:ASP:HA	3:a:58:ILE:HD11	1.96	0.47
3:a:103:MET:HE1	1:k:190:VAL:HA	1.97	0.47
3:j:33:LEU:HD11	3:j:68:MET:HG2	1.96	0.47
3:j:56:SER:HB3	3:j:92:LEU:HD13	1.96	0.47
3:j:76:VAL:HG23	3:j:100:LEU:HA	1.97	0.47
3:q:20:LEU:HB3	3:q:24:THR:OG1	2.14	0.47
5:r:248:GLU:OE1	5:r:248:GLU:HA	2.15	0.47
3:5:20:LEU:HB3	3:5:24:THR:OG1	2.14	0.47
2:B:167:MET:HE1	2:B:169:LEU:HD23	1.96	0.47
3:X:20:LEU:HD23	3:X:21:ASP:N	2.29	0.47
2:Y:167:MET:HE1	2:Y:181:ILE:HG23	1.97	0.47
3:5:80:GLY:HA3	3:5:103:MET:HG3	1.96	0.47
5:6:248:GLU:OE1	5:6:248:GLU:HA	2.15	0.47
3:F:33:LEU:HD11	3:F:68:MET:HG2	1.96	0.47
4:M:175:TPO:HG22	4:M:179:LYS:HE3	1.96	0.47
3:T:33:LEU:HD11	3:T:68:MET:HB3	1.96	0.47
2:Y:158:LEU:HD22	2:n:170:ILE:HG22	1.96	0.47
1:k:187:ILE:HA	1:k:190:VAL:HG12	1.97	0.47
2:n:159:PRO:HB2	2:n:166:VAL:HG13	1.97	0.47
3:y:33:LEU:HD11	3:y:68:MET:HG2	1.96	0.47
3:y:56:SER:HB3	3:y:92:LEU:HD13	1.96	0.47
2:D:190:VAL:HG21	3:F:83:PRO:HD3	1.97	0.46
3:E:33:LEU:HD11	3:E:68:MET:HB3	1.96	0.46
3:U:33:LEU:HD11	3:U:68:MET:HG2	1.96	0.46
4:Z:175:TPO:HG22	4:Z:179:LYS:HE3	1.96	0.46
4:Z:255:THR:HG23	4:Z:260:LYS:HD2	1.96	0.46
3:m:90:ILE:HD13	1:v:221:ALA:HB2	1.97	0.46
1:z:187:ILE:HA	1:z:190:VAL:HG12	1.97	0.46
2:2:159:PRO:HB2	2:2:166:VAL:HG13	1.97	0.46
2:H:213:HIS:O	2:H:217:GLN:HG2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:81:ILE:HG22	3:N:85:VAL:HG23	1.96	0.46
5:P:170:ILE:HD13	1:Q:156:PRO:HB3	1.97	0.46
1:Q:185:LEU:HD11	1:Q:197:VAL:HG11	1.95	0.46
2:W:213:HIS:O	2:W:217:GLN:HG2	2.16	0.46
5:c:170:ILE:HD13	1:d:156:PRO:HB3	1.97	0.46
2:f:161:PHE:HB3	2:f:164:ILE:HB	1.98	0.46
1:k:228:GLN:OE1	1:k:228:GLN:N	2.47	0.46
3:m:46:ILE:O	3:m:78:VAL:HG12	2.15	0.46
3:q:80:GLY:HA3	3:q:103:MET:HG3	1.96	0.46
2:u:182:ILE:HD12	2:u:218:ALA:HB2	1.97	0.46
3:1:46:ILE:O	3:1:78:VAL:HG12	2.15	0.46
3:5:72:MET:O	1:7:256:ASN:ND2	2.47	0.46
3:E:106:GLU:HB3	3:F:8:LEU:HA	1.96	0.46
4:M:201:ILE:O	4:M:204:VAL:HG12	2.16	0.46
4:M:255:THR:HG23	4:M:260:LYS:HD2	1.96	0.46
4:Z:201:ILE:O	4:Z:204:VAL:HG12	2.16	0.46
3:a:81:ILE:HG22	3:a:85:VAL:HG23	1.96	0.46
3:a:96:PHE:HA	1:k:223:ARG:HH22	1.80	0.46
5:c:148:SER:O	5:c:151:GLN:HG3	2.14	0.46
1:e:185:LEU:HD11	1:e:197:VAL:HG11	1.97	0.46
2:f:182:ILE:HD12	2:f:218:ALA:HB2	1.97	0.46
1:s:151:GLN:O	1:s:180:LEU:HD21	2.15	0.46
2:u:161:PHE:HB3	2:u:164:ILE:HB	1.98	0.46
1:z:228:GLN:OE1	1:z:228:GLN:N	2.47	0.46
1:7:151:GLN:O	1:7:180:LEU:HD21	2.15	0.46
3:F:14:ILE:HB	3:F:46:ILE:HA	1.98	0.46
1:G:228:GLN:OE1	1:G:228:GLN:N	2.47	0.46
2:J:170:ILE:HG22	2:2:158:LEU:HD22	1.96	0.46
4:M:151:GLN:O	4:M:180:LEU:HD21	2.15	0.46
1:Q:175:THR:HG23	1:Q:210:MET:HE1	1.97	0.46
4:Z:151:GLN:O	4:Z:180:LEU:HD21	2.15	0.46
1:d:185:LEU:HD11	1:d:197:VAL:HG11	1.95	0.46
2:h:256:ASN:OD1	2:h:260:LYS:NZ	2.48	0.46
4:o:256:ASN:OD1	4:o:257:THR:HG22	2.15	0.46
3:q:69:SER:HB3	3:q:75:LYS:NZ	2.31	0.46
1:t:185:LEU:HD11	1:t:197:VAL:HG11	1.97	0.46
3:x:33:LEU:HD11	3:x:68:MET:HB3	1.96	0.46
3:5:69:SER:HB3	3:5:75:LYS:NZ	2.31	0.46
3:E:113:LYS:HD3	3:E:113:LYS:HA	1.77	0.46
3:I:46:ILE:O	3:I:78:VAL:HG12	2.15	0.46
5:P:148:SER:O	5:P:151:GLN:HG3	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:228:GLN:N	1:V:228:GLN:OE1	2.47	0.46
3:X:46:ILE:O	3:X:78:VAL:HG12	2.15	0.46
1:d:175:THR:HG23	1:d:210:MET:HE1	1.97	0.46
2:h:186:LEU:HB3	3:j:83:PRO:HB3	1.98	0.46
3:i:33:LEU:HD11	3:i:68:MET:HB3	1.96	0.46
3:p:9:GLY:H	3:q:106:GLU:HB3	1.79	0.46
2:w:256:ASN:OD1	2:w:260:LYS:NZ	2.48	0.46
4:3:256:ASN:OD1	4:3:257:THR:HG22	2.15	0.46
1:7:177:ARG:O	1:7:181:ILE:HG12	2.15	0.46
3:I:106:GLU:HB2	3:X:8:LEU:HA	1.96	0.46
1:Q:183:GLU:O	1:Q:187:ILE:HG12	2.15	0.46
3:U:14:ILE:HB	3:U:46:ILE:HA	1.98	0.46
1:d:151:GLN:O	1:d:180:LEU:HD21	2.15	0.46
2:f:216:ILE:HG21	2:f:247:ILE:HD13	1.98	0.46
2:f:256:ASN:OD1	2:f:257:THR:N	2.49	0.46
3:j:14:ILE:HB	3:j:46:ILE:HA	1.98	0.46
3:m:87:ILE:HA	3:m:90:ILE:HG12	1.96	0.46
2:u:216:ILE:HG21	2:u:247:ILE:HD13	1.98	0.46
2:0:213:HIS:O	2:0:217:GLN:HG2	2.16	0.46
2:2:167:MET:HE1	2:2:181:ILE:HG23	1.97	0.46
3:I:13:LEU:HD23	3:I:105:LEU:HD21	1.98	0.46
2:L:161:PHE:HB3	2:L:164:ILE:HB	1.97	0.46
3:T:45:VAL:HG13	3:T:78:VAL:HB	1.98	0.46
2:l:213:HIS:O	2:l:217:GLN:HG2	2.16	0.46
1:s:177:ARG:O	1:s:181:ILE:HG12	2.15	0.46
3:y:14:ILE:HB	3:y:46:ILE:HA	1.98	0.46
3:1:87:ILE:HA	3:1:90:ILE:HG12	1.96	0.46
5:6:257:THR:HG23	5:6:260:LYS:H	1.81	0.46
3:E:45:VAL:HG13	3:E:78:VAL:HB	1.98	0.46
1:Q:151:GLN:O	1:Q:180:LEU:HD21	2.15	0.46
2:S:256:ASN:OD1	2:S:260:LYS:NZ	2.48	0.46
3:X:13:LEU:HD23	3:X:105:LEU:HD21	1.98	0.46
3:i:45:VAL:HG13	3:i:78:VAL:HB	1.98	0.46
3:m:14:ILE:HG21	3:m:28:PHE:CE1	2.50	0.46
2:n:167:MET:HE1	2:n:181:ILE:HG23	1.97	0.46
4:o:201:ILE:O	4:o:204:VAL:HG12	2.16	0.46
2:u:256:ASN:OD1	2:u:257:THR:N	2.49	0.46
3:1:14:ILE:HG21	3:1:28:PHE:CE1	2.50	0.46
4:3:201:ILE:O	4:3:204:VAL:HG12	2.16	0.46
5:6:170:ILE:HD13	1:7:156:PRO:HB3	1.97	0.46
2:B:216:ILE:HG21	2:B:247:ILE:HD13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:ASN:OD1	2:D:260:LYS:NZ	2.48	0.46
4:M:256:ASN:OD1	4:M:257:THR:HG22	2.15	0.46
5:P:236:PRO:HB3	2:2:186:LEU:HB3	1.98	0.46
1:d:183:GLU:O	1:d:187:ILE:HG12	2.15	0.46
1:7:245:LEU:HG	1:7:247:ILE:HG23	1.98	0.46
2:B:161:PHE:HB3	2:B:164:ILE:HB	1.98	0.46
4:M:170:ILE:HG13	4:M:171:GLY:N	2.31	0.46
1:Q:177:ARG:O	1:Q:181:ILE:HG12	2.15	0.46
2:L:216:ILE:HG21	2:L:247:ILE:HD13	1.98	0.46
3:b:20:LEU:HB3	3:b:24:THR:OG1	2.15	0.46
5:c:236:PRO:HB3	2:n:186:LEU:HB3	1.98	0.46
5:c:257:THR:HG23	5:c:260:LYS:H	1.81	0.46
1:k:210:MET:HE3	1:k:210:MET:HB3	1.81	0.46
1:s:175:THR:HG23	1:s:210:MET:HE1	1.97	0.46
2:w:237:GLU:O	2:w:241[A]:TPO:O2P	2.34	0.46
3:x:45:VAL:HG13	3:x:78:VAL:HB	1.98	0.46
1:z:210:MET:HE3	1:z:210:MET:HB3	1.82	0.46
2:B:256:ASN:OD1	2:B:257:THR:N	2.49	0.45
3:O:20:LEU:HB3	3:O:24:THR:OG1	2.14	0.45
4:Z:256:ASN:OD1	4:Z:257:THR:HG22	2.15	0.45
2:h:269:THR:OG1	2:h:272:GLU:OE1	2.26	0.45
5:r:257:THR:HG23	5:r:260:LYS:H	1.81	0.45
5:P:257:THR:HG23	5:P:260:LYS:H	1.81	0.45
2:L:256:ASN:OD1	2:L:257:THR:N	2.49	0.45
4:Z:193:ARG:HH12	3:b:102:ALA:HB3	1.82	0.45
1:d:177:ARG:O	1:d:181:ILE:HG12	2.15	0.45
2:h:237:GLU:O	2:h:241[A]:TPO:O1P	2.34	0.45
4:o:173:ILE:HG22	4:o:177:ARG:CZ	2.46	0.45
1:s:245:LEU:HG	1:s:247:ILE:HG23	1.98	0.45
3:y:60:LYS:HE3	3:y:60:LYS:HB3	1.83	0.45
3:1:22:ASP:O	3:1:26:VAL:HG22	2.16	0.45
4:3:173:ILE:HG22	4:3:177:ARG:CZ	2.46	0.45
1:7:175:THR:HG23	1:7:210:MET:HE1	1.97	0.45
2:B:182:ILE:HD12	2:B:218:ALA:HB2	1.97	0.45
3:O:18:SER:HB2	3:O:24:THR:HG21	1.98	0.45
1:Q:245:LEU:HG	1:Q:247:ILE:HG23	1.98	0.45
2:L:182:ILE:HD12	2:L:218:ALA:HB2	1.97	0.45
4:Z:170:ILE:HG13	4:Z:171:GLY:N	2.31	0.45
3:b:18:SER:HB2	3:b:24:THR:HG21	1.98	0.45
5:c:248:GLU:OE1	5:c:248:GLU:HA	2.15	0.45
1:d:245:LEU:HG	1:d:247:ILE:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:213:HIS:O	1:e:217:GLN:HG2	2.17	0.45
1:g:149:ALA:HA	1:g:152:GLU:HG2	1.99	0.45
1:t:213:HIS:O	1:t:217:GLN:HG2	2.17	0.45
1:v:149:ALA:HA	1:v:152:GLU:HG2	1.99	0.45
2:0:170:ILE:HG22	2:0:203:GLY:HA3	1.98	0.45
4:3:173:ILE:HG22	4:3:177:ARG:NE	2.31	0.45
2:B:237:GLU:O	2:B:241:TPO:O3P	2.35	0.45
1:C:149:ALA:HA	1:C:152:GLU:HG2	1.99	0.45
5:P:248:GLU:OE1	5:P:248:GLU:HA	2.15	0.45
1:R:149:ALA:HA	1:R:152:GLU:HG2	1.99	0.45
3:m:22:ASP:O	3:m:26:VAL:HG22	2.16	0.45
4:o:216:ILE:HG21	4:o:247:ILE:HG12	1.99	0.45
5:r:159:PRO:HG3	1:s:168:PRO:HG3	1.98	0.45
5:r:185:LEU:HD11	5:r:197:VAL:HG11	1.99	0.45
2:w:269:THR:OG1	2:w:272:GLU:OE1	2.26	0.45
2:2:204:VAL:C	2:2:235:ARG:HH21	2.25	0.45
5:6:185:LEU:HD11	5:6:197:VAL:HG11	1.99	0.45
3:I:14:ILE:HG21	3:I:28:PHE:CE1	2.50	0.45
2:J:186:LEU:HB3	5:6:236:PRO:HB3	1.97	0.45
4:M:173:ILE:HG22	4:M:177:ARG:NE	2.31	0.45
3:N:4:PRO:HG3	3:O:4:PRO:HG3	1.98	0.45
2:f:260:LYS:O	2:f:263:GLU:HG3	2.17	0.45
2:l:170:ILE:HG22	2:l:203:GLY:HA3	1.98	0.45
2:n:204:VAL:C	2:n:235:ARG:HH21	2.25	0.45
4:o:173:ILE:HG22	4:o:177:ARG:NE	2.31	0.45
4:3:170:ILE:HG13	4:3:171:GLY:N	2.31	0.45
1:A:193:ARG:HE	4:M:256:ASN:HD22	1.65	0.45
2:L:237:GLU:O	2:L:241:TPO:O3P	2.35	0.45
2:S:237:GLU:O	2:S:241[A]:TPO:O1P	2.34	0.45
4:Z:173:ILE:HG22	4:Z:177:ARG:NE	2.31	0.45
3:p:77:VAL:O	3:p:77:VAL:HG13	2.17	0.45
2:u:260:LYS:O	2:u:263:GLU:HG3	2.17	0.45
4:3:216:ILE:HG21	4:3:247:ILE:HG12	1.99	0.45
2:D:237:GLU:O	2:D:241[A]:TPO:O2P	2.34	0.45
3:I:22:ASP:O	3:I:26:VAL:HG22	2.16	0.45
3:X:14:ILE:HG21	3:X:28:PHE:CE1	2.50	0.45
2:h:190:VAL:HG21	3:j:83:PRO:HD3	1.98	0.45
3:i:100:LEU:HG	1:s:224:LEU:O	2.16	0.45
3:j:60:LYS:HE3	3:j:60:LYS:HB3	1.83	0.45
4:o:170:ILE:HG13	4:o:171:GLY:N	2.31	0.45
2:2:168:PRO:HA	2:2:200:ASP:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:77:VAL:O	3:4:77:VAL:HG13	2.17	0.45
1:e:228:GLN:OE1	1:e:228:GLN:N	2.49	0.45
2:u:237:GLU:O	2:u:241:TPO:O3P	2.35	0.45
3:x:111:LYS:O	3:x:114:GLN:HG3	2.17	0.45
1:A:231:LEU:O	1:A:254:THR:HA	2.17	0.45
4:M:151:GLN:HE21	4:M:180:LEU:HD13	1.82	0.45
3:N:13:LEU:HD21	3:N:109:LEU:HD21	1.99	0.45
3:O:72:MET:O	1:Q:256:ASN:ND2	2.50	0.45
5:P:185:LEU:HD11	5:P:197:VAL:HG11	1.99	0.45
3:U:54:ILE:HD12	3:U:58:ILE:HG21	1.99	0.45
3:X:22:ASP:O	3:X:26:VAL:HG22	2.16	0.45
4:Z:151:GLN:HE21	4:Z:180:LEU:HD13	1.82	0.45
1:e:193:ARG:HE	4:o:256:ASN:HD22	1.64	0.45
2:f:237:GLU:O	2:f:241:TPO:O3P	2.35	0.45
1:g:173:ILE:HG22	1:g:177:ARG:HH11	1.82	0.45
3:i:111:LYS:O	3:i:114:GLN:HG3	2.17	0.45
2:n:168:PRO:HA	2:n:200:ASP:HB3	1.98	0.45
1:v:173:ILE:HG22	1:v:177:ARG:HH11	1.82	0.45
1:A:213:HIS:O	1:A:217:GLN:HG2	2.17	0.45
3:O:69:SER:HB3	3:O:75:LYS:NZ	2.31	0.45
1:K:231:LEU:O	1:K:254:THR:HA	2.17	0.45
4:Z:216:ILE:HG21	4:Z:247:ILE:HG12	1.99	0.45
3:b:69:SER:HB3	3:b:75:LYS:NZ	2.31	0.45
5:c:185:LEU:HD11	5:c:197:VAL:HG11	1.99	0.45
1:t:193:ARG:HE	4:3:256:ASN:HD22	1.64	0.45
1:C:237[A]:GLU:O	1:C:240:GLN:HG3	2.17	0.44
3:F:54:ILE:HD12	3:F:58:ILE:HG21	1.99	0.44
2:J:156:PRO:O	2:J:168:PRO:HD2	2.17	0.44
2:J:158:LEU:HD22	2:2:170:ILE:HG22	1.98	0.44
4:M:216:ILE:HG21	4:M:247:ILE:HG12	1.99	0.44
5:P:208:ASP:HB3	5:P:211:VAL:HG23	1.99	0.44
1:R:237[A]:GLU:O	1:R:240:GLN:HG3	2.17	0.44
3:X:46:ILE:HG22	3:X:48:ILE:HD11	1.99	0.44
3:a:13:LEU:HD21	3:a:109:LEU:HD21	1.99	0.44
1:e:231:LEU:O	1:e:254:THR:HA	2.17	0.44
3:m:13:LEU:HD23	3:m:105:LEU:HD21	1.98	0.44
2:n:156:PRO:O	2:n:168:PRO:HD2	2.17	0.44
3:4:81:ILE:H	3:4:81:ILE:HD12	1.82	0.44
2:B:260:LYS:O	2:B:263:GLU:HG3	2.17	0.44
3:I:106:GLU:HG3	3:X:9:GLY:N	2.29	0.44
2:L:260:LYS:O	2:L:263:GLU:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:186:LEU:HB3	5:r:236:PRO:HB3	1.98	0.44
5:c:208:ASP:HB3	5:c:211:VAL:HG23	1.99	0.44
1:e:169:LEU:HD22	1:e:181:ILE:HD13	1.99	0.44
4:o:151:GLN:HE21	4:o:180:LEU:HD13	1.82	0.44
3:q:18:SER:HB2	3:q:24:THR:HG21	1.98	0.44
1:t:169:LEU:HD22	1:t:181:ILE:HD13	1.99	0.44
3:1:13:LEU:HD23	3:1:105:LEU:HD21	1.98	0.44
2:2:156:PRO:O	2:2:168:PRO:HD2	2.17	0.44
4:3:151:GLN:HE21	4:3:180:LEU:HD13	1.82	0.44
2:D:186:LEU:HB3	3:F:83:PRO:HB3	1.98	0.44
3:E:78:VAL:CG2	3:E:105:LEU:HA	2.48	0.44
3:I:46:ILE:HG22	3:I:48:ILE:HD11	1.99	0.44
3:O:68:MET:HE2	1:Q:243:VAL:HG11	1.99	0.44
2:Y:156:PRO:O	2:Y:168:PRO:HD2	2.17	0.44
1:e:234:ILE:HD11	1:e:238:ILE:HG22	1.99	0.44
2:h:159:PRO:HB2	2:h:166:VAL:HG13	1.99	0.44
3:p:13:LEU:HD21	3:p:109:LEU:HD21	1.99	0.44
3:q:45:VAL:HG13	3:q:76:VAL:HG23	1.99	0.44
1:t:231:LEU:O	1:t:254:THR:HA	2.17	0.44
2:w:190:VAL:HG21	3:y:83:PRO:HD3	1.99	0.44
3:4:9:GLY:H	3:5:106:GLU:HB3	1.81	0.44
3:4:29:GLN:HG3	3:4:30:GLU:N	2.32	0.44
3:5:18:SER:HB2	3:5:24:THR:HG21	1.98	0.44
2:D:159:PRO:HB2	2:D:166:VAL:HG13	2.00	0.44
3:N:77:VAL:O	3:N:77:VAL:HG13	2.17	0.44
1:K:213:HIS:O	1:K:217:GLN:HG2	2.17	0.44
1:R:198:LEU:HD13	1:R:230:MET:HB3	2.00	0.44
2:S:159:PRO:HB2	2:S:166:VAL:HG13	2.00	0.44
3:T:78:VAL:CG2	3:T:105:LEU:HA	2.48	0.44
3:j:16:ILE:O	3:j:50:SER:OG	2.22	0.44
2:n:260:LYS:O	2:n:263:GLU:HG3	2.18	0.44
3:p:81:ILE:HD12	3:p:81:ILE:H	1.82	0.44
2:w:159:PRO:HB2	2:w:166:VAL:HG13	1.99	0.44
3:y:33:LEU:HD23	3:y:33:LEU:HA	1.81	0.44
3:4:13:LEU:HD21	3:4:109:LEU:HD21	1.99	0.44
3:5:45:VAL:HG13	3:5:76:VAL:HG23	1.99	0.44
1:C:198:LEU:HD13	1:C:230:MET:HB3	2.00	0.44
4:M:241:TPO:O1P	4:M:241:TPO:HA	2.17	0.44
3:N:96:PHE:HA	1:z:223:ARG:HH22	1.83	0.44
1:K:193:ARG:HE	4:Z:256:ASN:HD22	1.66	0.44
3:X:61:ILE:O	3:X:65:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:29:GLN:HG3	3:a:30:GLU:N	2.32	0.44
3:a:77:VAL:O	3:a:77:VAL:HG13	2.17	0.44
2:l:168:PRO:HA	2:l:200:ASP:HB3	2.00	0.44
3:m:46:ILE:HG22	3:m:48:ILE:HD11	1.99	0.44
3:m:61:ILE:O	3:m:65:VAL:HG23	2.17	0.44
2:n:253:ILE:HG21	2:n:264:ARG:HH12	1.83	0.44
3:p:29:GLN:HG3	3:p:30:GLU:N	2.32	0.44
1:t:234:ILE:HD11	1:t:238:ILE:HG22	1.99	0.44
2:u:258:MET:HE3	2:u:258:MET:HB3	1.78	0.44
2:0:168:PRO:HA	2:0:200:ASP:HB3	2.00	0.44
3:1:61:ILE:O	3:1:65:VAL:HG23	2.17	0.44
2:2:260:LYS:O	2:2:263:GLU:HG3	2.18	0.44
2:H:170:ILE:HG22	2:H:203:GLY:HA3	1.98	0.44
3:I:61:ILE:O	3:I:65:VAL:HG23	2.18	0.44
2:J:204:VAL:C	2:J:235:ARG:HH21	2.25	0.44
3:N:29:GLN:HG3	3:N:30:GLU:N	2.32	0.44
1:K:169:LEU:HD22	1:K:181:ILE:HD13	1.99	0.44
2:L:159:PRO:HB2	2:L:166:VAL:HG13	2.00	0.44
2:W:170:ILE:HG22	2:W:203:GLY:HA3	1.98	0.44
4:Z:241:TPO:O2P	4:Z:241:TPO:HA	2.17	0.44
3:p:16:ILE:O	3:p:50:SER:OG	2.25	0.44
1:s:189:VAL:O	1:s:193:ARG:NH2	2.50	0.44
2:2:253:ILE:HG21	2:2:264:ARG:HH12	1.83	0.44
4:3:166:VAL:HG12	4:3:198:LEU:HB2	1.99	0.44
1:A:169:LEU:HD22	1:A:181:ILE:HD13	1.99	0.44
2:B:159:PRO:HB2	2:B:166:VAL:HG13	2.00	0.44
3:E:51:ILE:HG21	3:E:54:ILE:HD11	1.99	0.44
4:M:173:ILE:HG22	4:M:177:ARG:CZ	2.46	0.44
4:M:177:ARG:O	4:M:181:ILE:HG13	2.18	0.44
3:O:45:VAL:HG13	3:O:76:VAL:HG23	1.99	0.44
2:Y:204:VAL:C	2:Y:235:ARG:HH21	2.25	0.44
3:p:8:LEU:HB3	3:q:105:LEU:HD22	2.00	0.44
3:x:78:VAL:CG2	3:x:105:LEU:HA	2.47	0.44
3:y:16:ILE:O	3:y:50:SER:OG	2.22	0.44
3:1:46:ILE:HG22	3:1:48:ILE:HD11	1.99	0.44
1:7:189:VAL:O	1:7:193:ARG:NH2	2.50	0.44
3:F:66:VAL:HA	3:F:75:LYS:HD3	2.00	0.44
2:J:201:ILE:HG21	2:J:234:ILE:HG13	1.99	0.44
2:J:260:LYS:O	2:J:263:GLU:HG3	2.18	0.44
2:S:226:GLY:HA3	3:U:101:SER:O	2.18	0.44
2:Y:168:PRO:HA	2:Y:200:ASP:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:173:ILE:HG22	4:Z:177:ARG:CZ	2.46	0.44
4:Z:177:ARG:O	4:Z:181:ILE:HG13	2.18	0.44
3:b:45:VAL:HG13	3:b:76:VAL:HG23	1.99	0.44
3:b:68:MET:HE2	1:d:243:VAL:HG11	2.00	0.44
2:f:258:MET:HE3	2:f:258:MET:HB3	1.78	0.44
3:i:78:VAL:CG2	3:i:105:LEU:HA	2.48	0.44
3:j:33:LEU:HD23	3:j:33:LEU:HA	1.81	0.44
4:3:250:ASP:OD1	4:3:251:GLN:N	2.50	0.44
1:A:168:PRO:HA	1:A:200:ASP:HB3	2.00	0.44
2:J:157:LEU:HD11	2:J:165:SER:HB3	2.00	0.44
2:J:168:PRO:HA	2:J:200:ASP:HB3	1.98	0.44
2:J:175:THR:O	2:J:179:LYS:HG2	2.18	0.44
4:M:250:ASP:OD1	4:M:251:GLN:N	2.50	0.44
3:T:51:ILE:HG21	3:T:54:ILE:HD11	2.00	0.44
3:U:66:VAL:HA	3:U:75:LYS:HD3	2.00	0.44
2:Y:175:THR:O	2:Y:179:LYS:HG2	2.18	0.44
2:Y:201:ILE:HG21	2:Y:234:ILE:HG13	1.99	0.44
2:Y:260:LYS:O	2:Y:263:GLU:HG3	2.18	0.44
3:i:22:ASP:O	3:i:26:VAL:HG22	2.18	0.44
4:o:166:VAL:HG12	4:o:198:LEU:HB2	1.99	0.44
4:o:250:ASP:OD1	4:o:251:GLN:N	2.50	0.44
1:t:189:VAL:O	1:t:193:ARG:HD2	2.18	0.44
1:v:237[A]:GLU:O	1:v:240:GLN:HG3	2.17	0.44
2:D:269:THR:OG1	2:D:272:GLU:OE1	2.26	0.43
3:E:22:ASP:O	3:E:26:VAL:HG22	2.18	0.43
2:H:168:PRO:HA	2:H:200:ASP:HB3	2.00	0.43
3:N:17:GLN:HA	3:N:50:SER:OG	2.18	0.43
3:N:33:LEU:HD11	3:N:68:MET:SD	2.58	0.43
1:K:168:PRO:HA	1:K:200:ASP:HB3	2.00	0.43
3:T:22:ASP:O	3:T:26:VAL:HG22	2.18	0.43
2:Y:253:ILE:CG2	2:Y:264:ARG:HH12	2.30	0.43
4:Z:250:ASP:OD1	4:Z:251:GLN:N	2.50	0.43
3:a:33:LEU:HD11	3:a:68:MET:SD	2.58	0.43
1:e:189:VAL:O	1:e:193:ARG:HD2	2.18	0.43
1:g:237[A]:GLU:O	1:g:240:GLN:HG3	2.17	0.43
3:x:22:ASP:O	3:x:26:VAL:HG22	2.18	0.43
2:0:235:ARG:HB2	2:0:238:ILE:HD12	2.00	0.43
2:H:235:ARG:HB2	2:H:238:ILE:HD12	2.00	0.43
4:M:190:VAL:HG13	3:O:103:MET:HE1	2.01	0.43
1:R:173:ILE:HG22	1:R:177:ARG:HH11	1.82	0.43
2:W:168:PRO:HA	2:W:200:ASP:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:235:ARG:HB2	2:W:238:ILE:HD12	2.00	0.43
2:Y:157:LEU:HD11	2:Y:165:SER:HB3	2.00	0.43
3:b:78:VAL:HG13	3:b:79:THR:HG23	2.00	0.43
1:e:161:PHE:CG	1:e:162:GLU:N	2.87	0.43
2:l:235:ARG:HB2	2:l:238:ILE:HD12	2.00	0.43
2:n:175:THR:O	2:n:179:LYS:HG2	2.18	0.43
3:5:33:LEU:HB3	1:7:236:PRO:HB3	2.00	0.43
3:E:111:LYS:O	3:E:114:GLN:HG3	2.17	0.43
2:J:253:ILE:CG2	2:J:264:ARG:HH12	2.30	0.43
3:N:81:ILE:H	3:N:81:ILE:HD12	1.82	0.43
1:K:201:ILE:O	1:K:204:VAL:HG22	2.19	0.43
2:S:269:THR:OG1	2:S:272:GLU:OE1	2.26	0.43
3:a:17:GLN:HA	3:a:50:SER:OG	2.18	0.43
2:l:161:PHE:CG	2:l:162:GLU:N	2.86	0.43
4:o:241:TPO:O2P	4:o:241:TPO:HA	2.17	0.43
3:q:78:VAL:HG13	3:q:79:THR:HG23	2.00	0.43
1:t:161:PHE:CG	1:t:162:GLU:N	2.87	0.43
2:0:161:PHE:CG	2:0:162:GLU:N	2.86	0.43
2:2:253:ILE:CG2	2:2:264:ARG:HH12	2.30	0.43
4:3:241:TPO:O1P	4:3:241:TPO:HA	2.17	0.43
3:5:14:ILE:HG21	3:5:28:PHE:CE1	2.53	0.43
1:A:201:ILE:O	1:A:204:VAL:HG22	2.19	0.43
2:H:161:PHE:CG	2:H:162:GLU:N	2.86	0.43
2:J:253:ILE:HG21	2:J:264:ARG:HH12	1.83	0.43
4:M:166:VAL:HG12	4:M:198:LEU:HB2	1.99	0.43
3:O:78:VAL:HG13	3:O:79:THR:HG23	2.00	0.43
5:P:157:LEU:HD23	5:P:188:GLY:HA3	2.00	0.43
1:K:189:VAL:O	1:K:193:ARG:HD2	2.18	0.43
5:c:157:LEU:HD23	5:c:188:GLY:HA3	2.00	0.43
2:n:201:ILE:HG21	2:n:234:ILE:HG13	1.99	0.43
4:o:177:ARG:O	4:o:181:ILE:HG13	2.18	0.43
3:q:14:ILE:HG21	3:q:28:PHE:CE1	2.54	0.43
3:y:54:ILE:HD12	3:y:58:ILE:HG21	1.99	0.43
2:2:175:THR:O	2:2:179:LYS:HG2	2.18	0.43
2:2:201:ILE:HG21	2:2:234:ILE:HG13	1.99	0.43
3:5:78:VAL:HG13	3:5:79:THR:HG23	2.00	0.43
1:A:189:VAL:O	1:A:193:ARG:HD2	2.18	0.43
1:C:173:ILE:HG22	1:C:177:ARG:HH11	1.82	0.43
3:T:111:LYS:O	3:T:114:GLN:HG3	2.17	0.43
3:T:113:LYS:HA	3:T:113:LYS:HD3	1.77	0.43
2:Y:253:ILE:HG21	2:Y:264:ARG:HH12	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:166:VAL:HG12	4:Z:198:LEU:HB2	1.99	0.43
1:d:189:VAL:O	1:d:193:ARG:NH2	2.50	0.43
1:g:240:GLN:HA	1:g:243:VAL:HG12	2.01	0.43
3:j:54:ILE:HD12	3:j:58:ILE:HG21	1.99	0.43
2:n:253:ILE:CG2	2:n:264:ARG:HH12	2.30	0.43
5:r:208:ASP:HB3	5:r:211:VAL:HG23	1.99	0.43
2:u:159:PRO:HB2	2:u:166:VAL:HG13	2.00	0.43
1:z:260:LYS:O	1:z:263:GLU:HG3	2.18	0.43
3:1:35:LYS:O	3:1:39:THR:OG1	2.26	0.43
4:3:177:ARG:O	4:3:181:ILE:HG13	2.18	0.43
5:6:157:LEU:HD23	5:6:188:GLY:HA3	2.00	0.43
5:6:208:ASP:HB3	5:6:211:VAL:HG23	1.99	0.43
3:F:48:ILE:N	3:F:79:THR:OG1	2.46	0.43
1:G:260:LYS:O	1:G:263:GLU:HG3	2.18	0.43
5:P:158:LEU:O	5:P:160:ILE:HG13	2.19	0.43
1:Q:189:VAL:O	1:Q:193:ARG:NH2	2.50	0.43
1:K:234:ILE:HD11	1:K:238:ILE:HG22	1.99	0.43
1:V:223:ARG:HH22	3:p:96:PHE:HA	1.84	0.43
2:W:161:PHE:CG	2:W:162:GLU:N	2.86	0.43
3:a:81:ILE:H	3:a:81:ILE:HD12	1.82	0.43
2:f:159:PRO:HB2	2:f:166:VAL:HG13	2.00	0.43
1:g:198:LEU:HD13	1:g:230:MET:HB3	2.00	0.43
3:j:48:ILE:N	3:j:79:THR:OG1	2.46	0.43
1:k:260:LYS:O	1:k:263:GLU:HG3	2.18	0.43
3:m:35:LYS:O	3:m:39:THR:OG1	2.26	0.43
5:r:157:LEU:HD23	5:r:188:GLY:HA3	2.00	0.43
2:u:160:ILE:HG22	2:u:161:PHE:O	2.19	0.43
1:v:198:LEU:HD13	1:v:230:MET:HB3	2.00	0.43
1:v:240:GLN:HA	1:v:243:VAL:HG12	2.01	0.43
3:y:48:ILE:N	3:y:79:THR:OG1	2.46	0.43
3:4:33:LEU:HD11	3:4:68:MET:SD	2.58	0.43
2:D:234:ILE:HD11	2:D:238:ILE:HG22	2.01	0.43
3:I:9:GLY:N	3:X:106:GLU:HG3	2.32	0.43
1:V:260:LYS:O	1:V:263:GLU:HG3	2.18	0.43
2:W:177:ARG:O	2:W:181:ILE:HG13	2.19	0.43
5:c:158:LEU:O	5:c:160:ILE:HG13	2.19	0.43
2:h:237:GLU:HG2	2:h:238:ILE:HD12	2.00	0.43
3:m:8:LEU:HA	3:1:106:GLU:HB2	1.99	0.43
2:n:255:THR:HG21	2:n:261:GLY:N	2.34	0.43
1:t:208:ASP:OD1	1:t:209:THR:N	2.51	0.43
2:2:255:THR:HG21	2:2:261:GLY:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HD11	1:A:238:ILE:HG22	2.00	0.43
2:H:177:ARG:O	2:H:181:ILE:HG13	2.19	0.43
4:M:249:LEU:HD22	4:M:252:ILE:HD11	2.01	0.43
2:L:160:ILE:HG22	2:L:161:PHE:O	2.19	0.43
4:Z:249:LEU:HD22	4:Z:252:ILE:HD11	2.01	0.43
1:e:208:ASP:OD1	1:e:209:THR:N	2.51	0.43
2:f:160:ILE:HG22	2:f:161:PHE:O	2.19	0.43
1:g:160:ILE:O	2:h:258:MET:HE2	2.18	0.43
3:p:33:LEU:HD11	3:p:68:MET:SD	2.58	0.43
2:0:177:ARG:O	2:0:181:ILE:HG13	2.19	0.43
2:B:160:ILE:HG22	2:B:161:PHE:O	2.19	0.43
1:C:155:ALA:HB2	1:C:181:ILE:HD12	2.01	0.43
1:C:240:GLN:HA	1:C:243:VAL:HG12	2.01	0.43
2:D:260:LYS:O	2:D:263:GLU:HG3	2.19	0.43
1:K:161:PHE:CG	1:K:162:GLU:N	2.87	0.43
1:K:166:VAL:HG23	1:K:198:LEU:HB2	2.01	0.43
2:S:234:ILE:HD11	2:S:238:ILE:HG22	2.01	0.43
3:b:14:ILE:HG21	3:b:28:PHE:CE1	2.53	0.43
1:e:166:VAL:HG23	1:e:198:LEU:HB2	2.01	0.43
2:l:177:ARG:O	2:l:181:ILE:HG13	2.19	0.43
3:m:5:ILE:HG21	3:m:35:LYS:HG2	2.01	0.43
1:t:166:VAL:HG23	1:t:198:LEU:HB2	2.01	0.43
1:v:160:ILE:O	2:w:258:MET:HE2	2.18	0.43
2:w:237:GLU:HG2	2:w:238:ILE:HD12	2.00	0.43
1:7:258:MET:HE2	1:7:258:MET:HB3	1.91	0.43
1:A:161:PHE:CG	1:A:162:GLU:N	2.87	0.43
1:A:166:VAL:HG23	1:A:198:LEU:HB2	2.01	0.43
1:C:160:ILE:O	2:D:258:MET:HE2	2.18	0.43
2:D:253:ILE:HG21	2:D:264:ARG:HH22	1.84	0.43
2:J:255:THR:HG21	2:J:261:GLY:N	2.34	0.43
3:O:14:ILE:HG21	3:O:28:PHE:CE1	2.54	0.43
1:K:231:LEU:HD21	1:K:234:ILE:HB	2.01	0.43
1:R:160:ILE:O	2:S:258:MET:HE2	2.18	0.43
1:R:237[B]:GLU:O	1:R:240:GLN:HG3	2.18	0.43
1:R:240:GLN:HA	1:R:243:VAL:HG12	2.01	0.43
2:S:260:LYS:O	2:S:263:GLU:HG3	2.19	0.43
2:Y:255:THR:HG21	2:Y:261:GLY:N	2.34	0.43
3:q:82:GLN:HB2	3:q:85:VAL:HG12	2.01	0.43
3:1:5:ILE:HG21	3:1:35:LYS:HG2	2.01	0.43
1:A:231:LEU:HD21	1:A:234:ILE:HB	2.01	0.42
3:E:87:ILE:HG13	3:E:88:THR:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:155:ALA:HB2	1:R:181:ILE:HD12	2.01	0.42
2:S:253:ILE:HG21	2:S:264:ARG:HH22	1.84	0.42
3:T:87:ILE:HG13	3:T:88:THR:N	2.34	0.42
1:e:168:PRO:HA	1:e:200:ASP:HB3	2.00	0.42
2:l:255:THR:HG21	2:l:261:GLY:N	2.34	0.42
3:m:26:VAL:HG23	3:m:27:GLU:OE1	2.19	0.42
3:x:100:LEU:HG	1:7:224:LEU:O	2.19	0.42
3:5:82:GLN:HB2	3:5:85:VAL:HG12	2.01	0.42
1:C:237[B]:GLU:O	1:C:240:GLN:HG3	2.18	0.42
2:H:255:THR:HG21	2:H:261:GLY:N	2.34	0.42
3:O:81:ILE:H	3:O:81:ILE:HD12	1.84	0.42
3:U:48:ILE:N	3:U:79:THR:OG1	2.46	0.42
2:Y:166:VAL:HG21	2:Y:258:MET:HE1	2.02	0.42
3:b:81:ILE:H	3:b:81:ILE:HD12	1.84	0.42
1:g:237[B]:GLU:O	1:g:240:GLN:HG3	2.18	0.42
2:h:213:HIS:O	2:h:217:GLN:HG2	2.19	0.42
3:p:42:ARG:HG2	3:p:116:LEU:HD13	2.01	0.42
5:r:158:LEU:O	5:r:160:ILE:HG13	2.19	0.42
1:s:258:MET:HE2	1:s:258:MET:HB3	1.91	0.42
1:v:237[B]:GLU:O	1:v:240:GLN:HG3	2.18	0.42
2:0:255:THR:HG21	2:0:261:GLY:N	2.34	0.42
3:1:26:VAL:HG23	3:1:27:GLU:OE1	2.19	0.42
3:4:42:ARG:HG2	3:4:116:LEU:HD13	2.01	0.42
5:6:158:LEU:O	5:6:160:ILE:HG13	2.19	0.42
3:E:80:GLY:H	3:E:103:MET:HA	1.84	0.42
3:I:48:ILE:H	3:I:79:THR:HG1	1.57	0.42
2:J:166:VAL:HG21	2:J:258:MET:HE1	2.02	0.42
2:S:237:GLU:HG2	2:S:238:ILE:HD12	2.00	0.42
3:T:80:GLY:H	3:T:103:MET:HA	1.85	0.42
2:W:255:THR:HG21	2:W:261:GLY:N	2.34	0.42
4:Z:213:HIS:O	4:Z:217:GLN:HG2	2.20	0.42
3:a:16:ILE:O	3:a:50:SER:OG	2.25	0.42
3:i:51:ILE:HG21	3:i:54:ILE:HD11	2.00	0.42
1:t:220:GLU:OE2	1:t:251:GLN:NE2	2.52	0.42
1:v:153:LEU:HA	2:w:170:ILE:HD11	2.02	0.42
2:w:213:HIS:O	2:w:217:GLN:HG2	2.19	0.42
2:B:240:GLN:OE1	3:p:68:MET:HE1	2.19	0.42
2:D:213:HIS:O	2:D:217:GLN:HG2	2.19	0.42
2:D:237:GLU:HG2	2:D:238:ILE:HD12	2.00	0.42
4:M:213:HIS:O	4:M:217:GLN:HG2	2.20	0.42
2:S:213:HIS:O	2:S:217:GLN:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:220:GLU:OE2	1:e:251:GLN:NE2	2.53	0.42
1:g:153:LEU:HA	2:h:170:ILE:HD11	2.02	0.42
1:k:223:ARG:HD2	1:k:223:ARG:O	2.19	0.42
2:n:157:LEU:HD11	2:n:165:SER:HB3	2.00	0.42
4:o:249:LEU:HD22	4:o:252:ILE:HD11	2.01	0.42
1:s:215:ILE:HD13	1:s:215:ILE:HA	1.92	0.42
1:t:168:PRO:HA	1:t:200:ASP:HB3	2.00	0.42
1:t:201:ILE:O	1:t:204:VAL:HG22	2.19	0.42
2:w:216:ILE:HD13	2:w:216:ILE:HA	1.91	0.42
3:x:51:ILE:HG21	3:x:54:ILE:HD11	1.99	0.42
3:y:66:VAL:HA	3:y:75:LYS:HD3	2.00	0.42
2:2:157:LEU:HD11	2:2:165:SER:HB3	2.00	0.42
4:3:249:LEU:HD22	4:3:252:ILE:HD11	2.01	0.42
2:S:194:SER:H	3:U:103:MET:HE1	1.84	0.42
3:X:26:VAL:HG23	3:X:27:GLU:OE1	2.20	0.42
3:a:42:ARG:HG2	3:a:116:LEU:HD13	2.01	0.42
2:h:216:ILE:HD13	2:h:216:ILE:HA	1.91	0.42
3:j:66:VAL:HA	3:j:75:LYS:HD3	2.00	0.42
2:l:200:ASP:OD1	2:l:202:THR:N	2.53	0.42
4:o:213:HIS:O	4:o:217:GLN:HG2	2.20	0.42
3:p:81:ILE:CG2	3:p:85:VAL:HG23	2.49	0.42
1:z:223:ARG:O	1:z:223:ARG:HD2	2.20	0.42
3:1:80:GLY:N	3:1:103:MET:HB3	2.35	0.42
4:3:193:ARG:HH12	3:5:102:ALA:CB	2.32	0.42
1:C:225:VAL:C	3:X:100:LEU:HD11	2.45	0.42
3:E:20:LEU:HD23	3:E:23:HIS:CD2	2.55	0.42
4:M:186:LEU:O	4:M:190:VAL:HG23	2.20	0.42
3:N:35:LYS:HD2	3:N:35:LYS:O	2.20	0.42
3:N:42:ARG:HG2	3:N:116:LEU:HD13	2.01	0.42
1:Q:157:LEU:HD12	1:Q:167:MET:HB2	2.02	0.42
2:S:186:LEU:HB3	3:U:83:PRO:HB3	2.01	0.42
4:Z:186:LEU:O	4:Z:190:VAL:HG23	2.20	0.42
1:e:201:ILE:O	1:e:204:VAL:HG22	2.19	0.42
3:m:80:GLY:N	3:m:103:MET:HB3	2.35	0.42
4:o:183:GLU:O	4:o:187:ILE:HG12	2.20	0.42
1:t:228:GLN:OE1	1:t:228:GLN:N	2.49	0.42
2:w:234:ILE:HD11	2:w:238:ILE:HG22	2.01	0.42
3:x:20:LEU:HD23	3:x:23:HIS:CD2	2.55	0.42
1:z:198:LEU:HD23	1:z:232:VAL:HG21	2.01	0.42
2:0:200:ASP:OD1	2:0:202:THR:N	2.53	0.42
4:3:213:HIS:O	4:3:217:GLN:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:32:LEU:HD11	3:E:44:VAL:HG21	2.01	0.42
3:I:26:VAL:HG23	3:I:27:GLU:OE1	2.20	0.42
3:O:5:ILE:HG21	3:O:35:LYS:HG3	2.02	0.42
2:S:221:ALA:HA	3:U:90:ILE:HD11	2.02	0.42
3:T:20:LEU:HD23	3:T:23:HIS:CD2	2.55	0.42
3:T:32:LEU:HD11	3:T:44:VAL:HG21	2.01	0.42
2:W:173:ILE:HG22	2:W:177:ARG:CZ	2.50	0.42
3:b:5:ILE:HG21	3:b:35:LYS:HG3	2.02	0.42
1:d:157:LEU:HD12	1:d:167:MET:HB2	2.02	0.42
2:h:221:ALA:HA	3:j:90:ILE:HD11	2.00	0.42
2:h:234:ILE:HD11	2:h:238:ILE:HG22	2.01	0.42
3:i:20:LEU:HD23	3:i:23:HIS:CD2	2.55	0.42
1:k:198:LEU:HD23	1:k:232:VAL:HG21	2.01	0.42
4:o:232:VAL:HG23	4:o:255:THR:HB	2.02	0.42
4:3:183:GLU:O	4:3:187:ILE:HG12	2.20	0.42
4:3:232:VAL:HG23	4:3:255:THR:HB	2.02	0.42
3:5:16:ILE:HD11	3:5:28:PHE:CE1	2.55	0.42
1:A:220:GLU:OE2	1:A:251:GLN:NE2	2.52	0.42
1:G:223:ARG:HD2	1:G:223:ARG:C	2.45	0.42
2:H:173:ILE:HG22	2:H:177:ARG:CZ	2.50	0.42
2:J:258:MET:HE3	2:J:258:MET:HB3	1.89	0.42
4:M:183:GLU:O	4:M:187:ILE:HG12	2.20	0.42
4:Z:183:GLU:O	4:Z:187:ILE:HG12	2.20	0.42
3:a:35:LYS:HD2	3:a:35:LYS:O	2.20	0.42
4:o:193:ARG:HH12	3:q:102:ALA:CB	2.32	0.42
3:q:16:ILE:HD11	3:q:28:PHE:CE1	2.55	0.42
3:q:81:ILE:H	3:q:81:ILE:HD12	1.84	0.42
2:w:260:LYS:O	2:w:263:GLU:HG3	2.19	0.42
3:4:81:ILE:CG2	3:4:85:VAL:HG23	2.50	0.42
3:5:81:ILE:HD12	3:5:81:ILE:H	1.84	0.42
2:H:220:GLU:HA	2:H:220:GLU:OE1	2.20	0.42
1:K:220:GLU:OE2	1:K:251:GLN:NE2	2.52	0.42
2:W:220:GLU:OE1	2:W:220:GLU:HA	2.20	0.42
2:f:198:LEU:HD23	2:f:232:VAL:HG21	2.02	0.42
1:k:223:ARG:HD2	1:k:223:ARG:C	2.44	0.42
2:2:177:ARG:O	2:2:181:ILE:HG13	2.20	0.42
1:G:198:LEU:HD23	1:G:232:VAL:HG21	2.01	0.42
1:G:235:ARG:HB2	1:G:238:ILE:CD1	2.50	0.42
2:H:200:ASP:OD1	2:H:202:THR:N	2.53	0.42
3:N:81:ILE:CG2	3:N:85:VAL:HG23	2.50	0.42
2:S:190:VAL:HG21	3:U:83:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:223:ARG:HD2	1:V:223:ARG:C	2.45	0.42
1:V:235:ARG:HB2	1:V:238:ILE:CD1	2.50	0.42
3:a:81:ILE:CG2	3:a:85:VAL:HG23	2.50	0.42
2:h:260:LYS:O	2:h:263:GLU:HG3	2.19	0.42
2:l:231:LEU:HD23	2:l:234:ILE:HD11	2.01	0.42
2:n:177:ARG:O	2:n:181:ILE:HG13	2.20	0.42
3:p:14:ILE:HG22	3:p:15:SER:N	2.35	0.42
2:u:198:LEU:HD23	2:u:232:VAL:HG21	2.02	0.42
1:A:228:GLN:OE1	1:A:228:GLN:N	2.49	0.41
1:G:193:ARG:NE	1:G:193:ARG:HA	2.35	0.41
5:P:152:GLU:HG3	5:P:153:LEU:HD12	2.03	0.41
1:K:208:ASP:OD1	1:K:209:THR:N	2.51	0.41
3:T:42:ARG:HD2	3:T:116:LEU:HD22	2.01	0.41
1:V:193:ARG:HA	1:V:193:ARG:NE	2.35	0.41
2:Y:258:MET:HE3	2:Y:258:MET:HB3	1.89	0.41
5:r:156:PRO:HB3	1:s:170:ILE:HD13	2.02	0.41
1:t:231:LEU:HD21	1:t:234:ILE:HB	2.01	0.41
2:0:231:LEU:HD23	2:0:234:ILE:HD11	2.01	0.41
2:2:220:GLU:OE1	2:2:251:GLN:NE2	2.36	0.41
3:4:14:ILE:HG22	3:4:15:SER:N	2.35	0.41
1:A:208:ASP:OD1	1:A:209:THR:N	2.51	0.41
3:E:42:ARG:HD2	3:E:116:LEU:HD22	2.01	0.41
3:E:81:ILE:CG2	3:E:85:VAL:HG23	2.51	0.41
3:O:82:GLN:HB2	3:O:85:VAL:HG12	2.00	0.41
1:V:198:LEU:HD23	1:V:232:VAL:HG21	2.01	0.41
2:W:200:ASP:OD1	2:W:202:THR:N	2.53	0.41
3:X:80:GLY:N	3:X:103:MET:HB3	2.35	0.41
3:b:82:GLN:HB2	3:b:85:VAL:HG12	2.01	0.41
5:c:152:GLU:HG3	5:c:153:LEU:HD12	2.03	0.41
2:f:208:ASP:OD1	2:f:209:THR:N	2.53	0.41
3:i:42:ARG:HD2	3:i:116:LEU:HD22	2.01	0.41
3:q:33:LEU:HD21	3:q:68:MET:HG3	2.02	0.41
5:r:150:LEU:HB2	1:s:150:LEU:HD21	2.02	0.41
3:x:87:ILE:HG13	3:x:88:THR:N	2.34	0.41
1:z:223:ARG:HD2	1:z:223:ARG:C	2.45	0.41
2:2:161:PHE:CG	2:2:162:GLU:N	2.88	0.41
3:5:33:LEU:HD21	3:5:68:MET:HG3	2.02	0.41
1:7:157:LEU:HD22	1:7:188:GLY:HA3	2.01	0.41
1:7:215:ILE:HD13	1:7:215:ILE:HA	1.92	0.41
1:G:223:ARG:HD2	1:G:223:ARG:O	2.20	0.41
3:I:80:GLY:N	3:I:103:MET:HB3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:80:GLY:H	3:I:103:MET:HB3	1.86	0.41
4:M:193:ARG:HH12	3:O:102:ALA:HB3	1.85	0.41
4:M:234:ILE:HD13	4:M:238:ILE:HD11	2.02	0.41
1:Q:157:LEU:HD22	1:Q:188:GLY:HA3	2.01	0.41
1:R:153:LEU:HA	2:S:170:ILE:HD11	2.02	0.41
3:T:81:ILE:CG2	3:T:85:VAL:HG23	2.51	0.41
4:Z:170:ILE:HG13	4:3:153:LEU:HD23	2.02	0.41
4:Z:234:ILE:HD13	4:Z:238:ILE:HD11	2.02	0.41
1:d:157:LEU:HD22	1:d:188:GLY:HA3	2.01	0.41
1:e:231:LEU:HD21	1:e:234:ILE:HB	2.01	0.41
3:i:87:ILE:HG13	3:i:88:THR:N	2.34	0.41
3:i:89:LEU:HD22	1:s:224:LEU:HD21	2.01	0.41
2:l:201:ILE:O	2:l:204:VAL:HG12	2.21	0.41
2:n:161:PHE:CG	2:n:162:GLU:N	2.88	0.41
5:r:152:GLU:HG3	5:r:153:LEU:HD12	2.03	0.41
1:s:157:LEU:HD22	1:s:188:GLY:HA3	2.01	0.41
2:u:208:ASP:OD1	2:u:209:THR:N	2.53	0.41
3:y:114:GLN:NE2	3:y:115:GLU:HB2	2.35	0.41
2:0:201:ILE:O	2:0:204:VAL:HG12	2.21	0.41
2:0:220:GLU:HA	2:0:220:GLU:OE1	2.20	0.41
5:6:152:GLU:HG3	5:6:153:LEU:HD12	2.03	0.41
1:7:157:LEU:HD12	1:7:167:MET:HB2	2.02	0.41
1:C:153:LEU:HA	2:D:170:ILE:HD11	2.02	0.41
1:G:223:ARG:HH22	3:4:96:PHE:HA	1.86	0.41
3:I:107:SER:O	3:I:110:GLU:HG3	2.20	0.41
2:J:146:GLN:NE2	2:2:147:LYS:HE2	2.36	0.41
5:P:230:MET:HE2	5:P:230:MET:HB3	1.90	0.41
1:K:228:GLN:OE1	1:K:228:GLN:N	2.49	0.41
2:L:258:MET:HB3	2:L:258:MET:HE3	1.78	0.41
1:V:223:ARG:HD2	1:V:223:ARG:O	2.19	0.41
3:X:80:GLY:H	3:X:103:MET:HB3	1.85	0.41
3:i:80:GLY:H	3:i:103:MET:HA	1.84	0.41
3:j:114:GLN:NE2	3:j:115:GLU:HB2	2.35	0.41
4:o:224:LEU:HD21	3:q:89:LEU:HD22	2.01	0.41
3:p:35:LYS:HD2	3:p:35:LYS:O	2.20	0.41
3:x:42:ARG:HD2	3:x:116:LEU:HD22	2.01	0.41
3:x:80:GLY:H	3:x:103:MET:HA	1.85	0.41
1:z:193:ARG:NE	1:z:193:ARG:HA	2.35	0.41
5:6:170:ILE:HG22	1:7:158:LEU:HD22	2.02	0.41
5:6:253:ILE:HG21	5:6:264:ARG:NH2	2.35	0.41
3:O:16:ILE:HD11	3:O:28:PHE:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:179:LYS:HA	2:S:182:ILE:HG22	2.02	0.41
3:X:107:SER:O	3:X:110:GLU:HG3	2.20	0.41
2:Y:177:ARG:O	2:Y:181:ILE:HG13	2.20	0.41
4:Z:174:ASP:H	4:Z:177:ARG:HB2	1.85	0.41
4:Z:231:LEU:O	4:Z:254:THR:HA	2.20	0.41
4:Z:232:VAL:HG23	4:Z:255:THR:HB	2.02	0.41
1:d:220:GLU:OE1	1:d:251:GLN:HG3	2.21	0.41
1:g:155:ALA:HB2	1:g:181:ILE:HD12	2.01	0.41
2:h:179:LYS:HA	2:h:182:ILE:HG22	2.02	0.41
1:k:193:ARG:NE	1:k:193:ARG:HA	2.35	0.41
2:l:220:GLU:OE1	2:l:220:GLU:HA	2.20	0.41
5:r:173:ILE:HG22	5:r:177:ARG:NE	2.35	0.41
1:s:157:LEU:HD12	1:s:167:MET:HB2	2.02	0.41
1:v:155:ALA:HB2	1:v:181:ILE:HD12	2.01	0.41
3:4:17:GLN:HA	3:4:50:SER:OG	2.19	0.41
1:7:220:GLU:OE1	1:7:251:GLN:HG3	2.21	0.41
2:B:251:GLN:OE1	2:B:251:GLN:N	2.53	0.41
2:J:177:ARG:O	2:J:181:ILE:HG13	2.20	0.41
4:M:215:ILE:HD13	4:M:215:ILE:HA	1.92	0.41
4:M:232:VAL:HG23	4:M:255:THR:HB	2.02	0.41
3:N:62:LEU:O	3:N:66:VAL:HG23	2.20	0.41
3:N:112:LEU:O	3:N:115:GLU:HG3	2.21	0.41
1:Q:220:GLU:OE1	1:Q:251:GLN:HG3	2.21	0.41
2:L:251:GLN:OE1	2:L:251:GLN:N	2.53	0.41
3:a:43:GLY:HA2	3:a:74:ALA:O	2.20	0.41
3:a:112:LEU:O	3:a:115:GLU:HG3	2.21	0.41
3:b:16:ILE:HD11	3:b:28:PHE:CE1	2.55	0.41
5:c:230:MET:HE2	5:c:230:MET:HB3	1.90	0.41
2:h:253:ILE:HG21	2:h:264:ARG:HH22	1.84	0.41
1:k:161:PHE:CG	1:k:162:GLU:N	2.89	0.41
2:n:166:VAL:HG21	2:n:258:MET:HE1	2.02	0.41
3:p:4:PRO:HG3	3:q:4:PRO:HG3	2.02	0.41
3:p:17:GLN:HA	3:p:50:SER:OG	2.18	0.41
3:p:43:GLY:HA2	3:p:74:ALA:O	2.20	0.41
2:w:179:LYS:HA	2:w:182:ILE:HG22	2.03	0.41
2:w:221:ALA:HA	3:y:90:ILE:HD11	2.01	0.41
2:w:253:ILE:HG21	2:w:264:ARG:HH22	1.84	0.41
2:2:166:VAL:HG21	2:2:258:MET:HE1	2.02	0.41
4:3:224:LEU:HD21	3:5:89:LEU:HD22	2.01	0.41
3:4:8:LEU:HB3	3:5:105:LEU:HD22	2.03	0.41
3:4:35:LYS:O	3:4:35:LYS:HD2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:43:GLY:HA2	3:4:74:ALA:O	2.20	0.41
5:6:173:ILE:HG22	5:6:177:ARG:NE	2.35	0.41
2:H:201:ILE:O	2:H:204:VAL:HG12	2.21	0.41
4:M:174:ASP:H	4:M:177:ARG:HB2	1.85	0.41
4:M:231:LEU:O	4:M:254:THR:HA	2.20	0.41
3:N:43:GLY:HA2	3:N:74:ALA:O	2.20	0.41
5:P:173:ILE:HG22	5:P:177:ARG:NE	2.35	0.41
2:L:210:MET:HG3	2:L:214:HIS:HE1	1.86	0.41
1:R:158:LEU:O	1:R:160:ILE:HG13	2.20	0.41
2:Y:161:PHE:CG	2:Y:162:GLU:N	2.88	0.41
4:Z:215:ILE:HD13	4:Z:215:ILE:HA	1.92	0.41
4:o:231:LEU:O	4:o:254:THR:HA	2.20	0.41
3:p:112:LEU:O	3:p:115:GLU:HG3	2.21	0.41
1:s:220:GLU:OE1	1:s:251:GLN:HG3	2.21	0.41
2:0:173:ILE:HG22	2:0:177:ARG:CZ	2.50	0.41
3:4:112:LEU:O	3:4:115:GLU:HG3	2.21	0.41
2:B:210:MET:HG3	2:B:214:HIS:HE1	1.86	0.41
2:B:237:GLU:O	2:B:240:GLN:HB3	2.21	0.41
2:D:179:LYS:HA	2:D:182:ILE:HG22	2.03	0.41
2:J:161:PHE:CG	2:J:162:GLU:N	2.88	0.41
4:M:153:LEU:HD23	4:o:170:ILE:HG13	2.02	0.41
2:L:237:GLU:O	2:L:240:GLN:HB3	2.21	0.41
3:U:114:GLN:NE2	3:U:115:GLU:HB2	2.35	0.41
2:W:201:ILE:O	2:W:204:VAL:HG12	2.21	0.41
3:X:5:ILE:HG21	3:X:35:LYS:HG2	2.01	0.41
3:a:62:LEU:O	3:a:66:VAL:HG23	2.21	0.41
3:b:33:LEU:HD21	3:b:68:MET:HG3	2.02	0.41
2:l:173:ILE:HG22	2:l:177:ARG:CZ	2.50	0.41
4:o:234:ILE:HD13	4:o:238:ILE:HD11	2.02	0.41
3:q:49:THR:HG23	3:q:79:THR:HB	2.03	0.41
1:z:161:PHE:CG	1:z:162:GLU:N	2.89	0.41
4:3:231:LEU:O	4:3:254:THR:HA	2.20	0.41
1:A:153:LEU:HD23	2:B:170:ILE:HG13	2.03	0.41
2:B:166:VAL:HG21	2:B:258:MET:HE1	2.02	0.41
2:B:208:ASP:OD1	2:B:209:THR:N	2.53	0.41
2:B:258:MET:HB3	2:B:258:MET:HE3	1.78	0.41
1:C:158:LEU:O	1:C:160:ILE:HG13	2.20	0.41
1:C:190:VAL:CA	3:X:103:MET:HE1	2.39	0.41
3:F:114:GLN:NE2	3:F:115:GLU:HB2	2.35	0.41
1:G:190:VAL:HG23	3:4:103:MET:SD	2.60	0.41
3:I:5:ILE:HG21	3:I:35:LYS:HG2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:33:LEU:HD21	3:O:68:MET:HG3	2.02	0.41
5:P:170:ILE:HG22	1:Q:158:LEU:HD22	2.02	0.41
1:K:153:LEU:HD23	2:L:170:ILE:HG13	2.03	0.41
3:U:75:LYS:HE3	3:U:75:LYS:HB2	1.85	0.41
1:V:184:ASN:HA	1:V:187:ILE:HG22	2.03	0.41
2:Y:146:GLN:NE2	2:n:147:LYS:HE2	2.36	0.41
4:Z:153:LEU:HD23	4:3:170:ILE:HG13	2.02	0.41
5:c:173:ILE:HG22	5:c:177:ARG:NE	2.35	0.41
2:f:204:VAL:C	2:f:235:ARG:HH21	2.27	0.41
1:g:158:LEU:O	1:g:160:ILE:HG13	2.20	0.41
1:k:184:ASN:HA	1:k:187:ILE:HG22	2.03	0.41
1:k:208:ASP:OD1	1:k:209:THR:N	2.54	0.41
4:o:186:LEU:O	4:o:190:VAL:HG23	2.20	0.41
4:o:215:ILE:HD13	4:o:215:ILE:HA	1.92	0.41
3:p:3:ILE:O	3:p:5:ILE:HD12	2.21	0.41
3:q:5:ILE:HG21	3:q:35:LYS:HG3	2.02	0.41
5:r:168:PRO:CG	1:s:159:PRO:HG3	2.51	0.41
2:u:251:GLN:OE1	2:u:251:GLN:N	2.53	0.41
1:v:158:LEU:O	1:v:160:ILE:HG13	2.20	0.41
3:x:32:LEU:HD11	3:x:44:VAL:HG21	2.01	0.41
3:x:81:ILE:CG2	3:x:85:VAL:HG23	2.51	0.41
1:z:184:ASN:HA	1:z:187:ILE:HG22	2.03	0.41
1:z:208:ASP:OD1	1:z:209:THR:N	2.54	0.41
4:3:186:LEU:O	4:3:190:VAL:HG23	2.20	0.41
4:3:234:ILE:HD13	4:3:238:ILE:HD11	2.02	0.41
3:4:3:ILE:O	3:4:5:ILE:HD12	2.21	0.41
3:5:5:ILE:HG21	3:5:35:LYS:HG3	2.02	0.41
3:5:49:THR:HG23	3:5:79:THR:HB	2.03	0.41
3:E:83:PRO:HB3	1:Q:186:LEU:HB3	2.03	0.41
1:G:184:ASN:HA	1:G:187:ILE:HG22	2.03	0.41
4:Z:224:LEU:O	3:b:100:LEU:HD23	2.21	0.41
2:f:251:GLN:OE1	2:f:251:GLN:N	2.53	0.41
3:i:32:LEU:HD11	3:i:44:VAL:HG21	2.01	0.41
3:i:81:ILE:CG2	3:i:85:VAL:HG23	2.51	0.41
1:k:235:ARG:HB2	1:k:238:ILE:CD1	2.50	0.41
2:n:183:GLU:O	2:n:187:ILE:HG12	2.21	0.41
4:o:167:MET:HE3	4:o:199:ILE:HG23	2.03	0.41
2:u:204:VAL:C	2:u:235:ARG:HH21	2.27	0.41
1:z:235:ARG:HB2	1:z:238:ILE:CD1	2.50	0.41
2:2:183:GLU:O	2:2:187:ILE:HG12	2.21	0.41
2:B:198:LEU:HD23	2:B:232:VAL:HG21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:ALA:O	2:D:215:ILE:HG22	2.21	0.40
2:L:166:VAL:HG21	2:L:258:MET:HE1	2.02	0.40
2:L:208:ASP:OD1	2:L:209:THR:N	2.53	0.40
1:V:161:PHE:CG	1:V:162:GLU:N	2.89	0.40
3:a:14:ILE:HG22	3:a:15:SER:N	2.35	0.40
5:c:170:ILE:HG22	1:d:158:LEU:HD22	2.02	0.40
1:d:161:PHE:CG	1:d:162:GLU:N	2.89	0.40
2:f:237:GLU:O	2:f:240:GLN:HB3	2.21	0.40
2:h:212:ALA:O	2:h:215:ILE:HG22	2.21	0.40
3:m:80:GLY:H	3:m:103:MET:HB3	1.86	0.40
4:o:174:ASP:H	4:o:177:ARG:HB2	1.85	0.40
2:u:207:VAL:HB	2:u:238:ILE:HG23	2.04	0.40
2:w:212:ALA:O	2:w:215:ILE:HG22	2.21	0.40
1:z:247:ILE:O	1:z:249:LEU:HG	2.21	0.40
4:3:167:MET:HE3	4:3:199:ILE:HG23	2.03	0.40
4:3:174:ASP:H	4:3:177:ARG:HB2	1.85	0.40
5:6:150:LEU:HB2	1:7:150:LEU:HD21	2.03	0.40
3:F:75:LYS:HE3	3:F:75:LYS:HB2	1.85	0.40
3:N:14:ILE:HG22	3:N:15:SER:N	2.35	0.40
1:Q:258:MET:HE2	1:Q:258:MET:HB3	1.91	0.40
1:K:258:MET:HE2	1:K:258:MET:HB2	1.99	0.40
2:L:198:LEU:HD23	2:L:232:VAL:HG21	2.02	0.40
3:T:105:LEU:HD22	3:U:7:LYS:O	2.21	0.40
2:W:231:LEU:HD23	2:W:234:ILE:HD11	2.01	0.40
3:b:49:THR:HG23	3:b:79:THR:HB	2.03	0.40
1:k:247:ILE:O	1:k:249:LEU:HG	2.22	0.40
1:k:250:ASP:OD1	1:k:251:GLN:N	2.54	0.40
5:r:159:PRO:HB2	5:r:166:VAL:HG13	2.03	0.40
1:s:161:PHE:CG	1:s:162:GLU:N	2.89	0.40
1:t:153:LEU:HD23	2:u:170:ILE:HG13	2.03	0.40
1:z:250:ASP:OD1	1:z:251:GLN:N	2.54	0.40
2:0:231:LEU:O	2:0:254:THR:HA	2.22	0.40
3:1:80:GLY:H	3:1:103:MET:HB3	1.86	0.40
4:3:215:ILE:HD13	4:3:215:ILE:HA	1.92	0.40
5:6:159:PRO:HB2	5:6:166:VAL:HG13	2.03	0.40
3:E:76:VAL:HG23	3:E:99:VAL:HG23	2.04	0.40
1:G:161:PHE:CG	1:G:162:GLU:N	2.89	0.40
2:H:231:LEU:HD23	2:H:234:ILE:HD11	2.01	0.40
3:O:54:ILE:HD12	3:O:58:ILE:CG2	2.50	0.40
1:Q:161:PHE:CG	1:Q:162:GLU:N	2.89	0.40
2:S:212:ALA:O	2:S:215:ILE:HG22	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:76:VAL:HG23	3:T:99:VAL:HG23	2.04	0.40
2:Y:266:LEU:HD23	2:Y:266:LEU:HA	1.93	0.40
1:e:153:LEU:HD23	2:f:170:ILE:HG13	2.03	0.40
2:f:166:VAL:HG21	2:f:258:MET:HE1	2.02	0.40
2:f:207:VAL:HB	2:f:238:ILE:HG23	2.04	0.40
2:h:226:GLY:HA3	3:j:101:SER:O	2.21	0.40
3:i:83:PRO:HB3	1:s:186:LEU:HD13	2.02	0.40
2:l:231:LEU:O	2:l:254:THR:HA	2.22	0.40
3:m:107:SER:O	3:m:110:GLU:HG3	2.20	0.40
2:u:166:VAL:HG21	2:u:258:MET:HE1	2.02	0.40
2:u:237:GLU:O	2:u:240:GLN:HB3	2.21	0.40
2:w:226:GLY:HA3	3:y:101:SER:O	2.21	0.40
3:1:92:LEU:HD12	3:1:93:GLY:N	2.37	0.40
3:I:92:LEU:HD12	3:I:93:GLY:N	2.36	0.40
3:O:49:THR:HG23	3:O:79:THR:HB	2.03	0.40
3:b:54:ILE:HD12	3:b:58:ILE:CG2	2.50	0.40
1:d:228:GLN:OE1	1:d:228:GLN:N	2.51	0.40
3:m:92:LEU:HD12	3:m:93:GLY:N	2.37	0.40
4:o:187:ILE:O	4:o:191:LYS:HG2	2.22	0.40
1:s:260:LYS:O	1:s:263:GLU:HG3	2.22	0.40
1:v:228:GLN:OE1	1:v:228:GLN:N	2.49	0.40
3:1:107:SER:O	3:1:110:GLU:HG3	2.20	0.40
4:3:187:ILE:O	4:3:191:LYS:HG2	2.22	0.40
1:7:161:PHE:CG	1:7:162:GLU:N	2.89	0.40
1:7:260:LYS:O	1:7:263:GLU:HG3	2.22	0.40
1:G:250:ASP:OD1	1:G:251:GLN:N	2.54	0.40
2:H:237:GLU:H	2:H:237:GLU:CD	2.30	0.40
3:N:32:LEU:O	3:N:36:ILE:HG22	2.22	0.40
1:Q:228:GLN:OE1	1:Q:228:GLN:N	2.51	0.40
3:T:100:LEU:HG	1:d:224:LEU:O	2.21	0.40
1:V:250:ASP:OD1	1:V:251:GLN:N	2.54	0.40
2:W:237:GLU:H	2:W:237:GLU:CD	2.30	0.40
3:a:3:ILE:O	3:a:5:ILE:HD12	2.21	0.40
2:h:154:SER:HB3	2:h:180:LEU:HD22	2.04	0.40
2:w:154:SER:HB3	2:w:180:LEU:HD22	2.04	0.40
2:0:190:VAL:O	2:0:193:ARG:NH2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7	272/278 (98%)	259 (95%)	13 (5%)	0	100	100
1	A	272/278 (98%)	256 (94%)	16 (6%)	0	100	100
1	C	273/278 (98%)	261 (96%)	12 (4%)	0	100	100
1	G	272/278 (98%)	255 (94%)	17 (6%)	0	100	100
1	K	272/278 (98%)	256 (94%)	16 (6%)	0	100	100
1	Q	272/278 (98%)	259 (95%)	13 (5%)	0	100	100
1	R	273/278 (98%)	261 (96%)	12 (4%)	0	100	100
1	V	272/278 (98%)	254 (93%)	18 (7%)	0	100	100
1	d	272/278 (98%)	259 (95%)	13 (5%)	0	100	100
1	e	272/278 (98%)	256 (94%)	16 (6%)	0	100	100
1	g	273/278 (98%)	261 (96%)	12 (4%)	0	100	100
1	k	272/278 (98%)	255 (94%)	17 (6%)	0	100	100
1	s	272/278 (98%)	259 (95%)	13 (5%)	0	100	100
1	t	272/278 (98%)	256 (94%)	16 (6%)	0	100	100
1	v	273/278 (98%)	261 (96%)	12 (4%)	0	100	100
1	z	272/278 (98%)	255 (94%)	17 (6%)	0	100	100
2	0	271/278 (98%)	259 (96%)	12 (4%)	0	100	100
2	2	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	B	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	D	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	H	271/278 (98%)	259 (96%)	12 (4%)	0	100	100
2	J	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	L	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	S	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	W	271/278 (98%)	259 (96%)	12 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	f	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	h	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	l	271/278 (98%)	259 (96%)	12 (4%)	0	100	100
2	n	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	u	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
2	w	271/278 (98%)	256 (94%)	15 (6%)	0	100	100
3	1	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	4	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	5	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	E	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
3	F	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
3	I	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	N	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	O	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	T	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
3	U	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
3	X	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	a	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	b	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	i	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
3	j	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
3	m	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	p	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	q	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	x	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
3	y	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
4	3	270/278 (97%)	249 (92%)	21 (8%)	0	100	100
4	M	270/278 (97%)	249 (92%)	21 (8%)	0	100	100
4	Z	270/278 (97%)	248 (92%)	22 (8%)	0	100	100
4	o	270/278 (97%)	249 (92%)	21 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	6	271/278 (98%)	255 (94%)	16 (6%)	0	100	100
5	P	271/278 (98%)	255 (94%)	16 (6%)	0	100	100
5	c	271/278 (98%)	255 (94%)	16 (6%)	0	100	100
5	r	271/278 (98%)	255 (94%)	16 (6%)	0	100	100
All	All	13176/13480 (98%)	12406 (94%)	770 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	246/249 (99%)	244 (99%)	2 (1%)	73	77
1	A	246/249 (99%)	246 (100%)	0	100	100
1	C	247/249 (99%)	247 (100%)	0	100	100
1	G	246/249 (99%)	246 (100%)	0	100	100
1	K	246/249 (99%)	246 (100%)	0	100	100
1	Q	246/249 (99%)	244 (99%)	2 (1%)	73	77
1	R	247/249 (99%)	247 (100%)	0	100	100
1	V	246/249 (99%)	246 (100%)	0	100	100
1	d	246/249 (99%)	244 (99%)	2 (1%)	73	77
1	e	246/249 (99%)	246 (100%)	0	100	100
1	g	247/249 (99%)	247 (100%)	0	100	100
1	k	246/249 (99%)	246 (100%)	0	100	100
1	s	246/249 (99%)	244 (99%)	2 (1%)	73	77
1	t	246/249 (99%)	246 (100%)	0	100	100
1	v	247/249 (99%)	247 (100%)	0	100	100
1	z	246/249 (99%)	246 (100%)	0	100	100
2	0	245/248 (99%)	245 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	B	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	D	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	H	245/248 (99%)	245 (100%)	0	100	100
2	J	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	L	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	S	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	W	245/248 (99%)	245 (100%)	0	100	100
2	Y	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	f	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	h	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	l	245/248 (99%)	245 (100%)	0	100	100
2	n	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	u	245/248 (99%)	244 (100%)	1 (0%)	84	83
2	w	245/248 (99%)	244 (100%)	1 (0%)	84	83
3	1	100/100 (100%)	96 (96%)	4 (4%)	28	52
3	4	100/100 (100%)	100 (100%)	0	100	100
3	5	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	E	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	F	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	I	100/100 (100%)	96 (96%)	4 (4%)	28	52
3	N	100/100 (100%)	100 (100%)	0	100	100
3	O	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	T	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	U	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	X	100/100 (100%)	96 (96%)	4 (4%)	28	52
3	a	100/100 (100%)	100 (100%)	0	100	100
3	b	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	i	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	j	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	m	100/100 (100%)	96 (96%)	4 (4%)	28	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	p	100/100 (100%)	100 (100%)	0	100	100
3	q	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	x	100/100 (100%)	99 (99%)	1 (1%)	68	75
3	y	100/100 (100%)	99 (99%)	1 (1%)	68	75
4	3	244/247 (99%)	241 (99%)	3 (1%)	63	72
4	M	244/247 (99%)	241 (99%)	3 (1%)	63	72
4	Z	244/247 (99%)	241 (99%)	3 (1%)	63	72
4	o	244/247 (99%)	241 (99%)	3 (1%)	63	72
5	6	245/248 (99%)	244 (100%)	1 (0%)	84	83
5	P	245/248 (99%)	244 (100%)	1 (0%)	84	83
5	c	245/248 (99%)	244 (100%)	1 (0%)	84	83
5	r	245/248 (99%)	244 (100%)	1 (0%)	84	83
All	All	11816/11932 (99%)	11752 (100%)	64 (0%)	78	82

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	175	THR
2	D	40	MET
3	E	47	ASP
3	F	13	LEU
3	I	1	MET
3	I	40	SER
3	I	114	GLN
3	I	115	GLU
2	J	231	LEU
4	M	99	MET
4	M	238	ILE
4	M	259	LYS
3	O	68	MET
5	P	248	GLU
1	Q	235	ARG
1	Q	240	GLN
2	L	175	THR
2	S	40	MET
3	T	47	ASP
3	U	13	LEU
3	X	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	X	40	SER
3	X	114	GLN
3	X	115	GLU
2	Y	231	LEU
4	Z	99	MET
4	Z	238	ILE
4	Z	259	LYS
3	b	68	MET
5	c	248	GLU
1	d	235	ARG
1	d	240	GLN
2	f	175	THR
2	h	40	MET
3	i	47	ASP
3	j	13	LEU
3	m	1	MET
3	m	40	SER
3	m	114	GLN
3	m	115	GLU
2	n	231	LEU
4	o	99	MET
4	o	238	ILE
4	o	259	LYS
3	q	68	MET
5	r	248	GLU
1	s	235	ARG
1	s	240	GLN
2	u	175	THR
2	w	40	MET
3	x	47	ASP
3	y	13	LEU
3	1	1	MET
3	1	40	SER
3	1	114	GLN
3	1	115	GLU
2	2	231	LEU
4	3	99	MET
4	3	238	ILE
4	3	259	LYS
3	5	68	MET
5	6	248	GLU
1	7	235	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7	240	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	244	ASN
1	C	146	GLN
1	C	244	ASN
2	D	240	GLN
3	F	114	GLN
1	G	146	GLN
1	G	240	GLN
2	H	240	GLN
3	I	114	GLN
2	J	151	GLN
2	J	184	ASN
4	M	151	GLN
4	M	192	ASN
5	P	244	ASN
1	Q	256	ASN
1	K	213	HIS
1	K	244	ASN
1	R	146	GLN
1	R	244	ASN
2	S	240	GLN
3	U	114	GLN
1	V	146	GLN
1	V	240	GLN
2	W	240	GLN
3	X	114	GLN
2	Y	151	GLN
2	Y	184	ASN
4	Z	151	GLN
4	Z	192	ASN
5	c	244	ASN
1	d	256	ASN
1	e	213	HIS
1	g	146	GLN
1	g	244	ASN
2	h	240	GLN
3	j	114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	k	146	GLN
1	k	240	GLN
2	l	240	GLN
3	m	114	GLN
2	n	151	GLN
2	n	184	ASN
4	o	151	GLN
4	o	192	ASN
3	q	29	GLN
5	r	244	ASN
1	s	256	ASN
1	t	213	HIS
1	t	244	ASN
1	v	146	GLN
1	v	244	ASN
2	w	240	GLN
3	y	114	GLN
1	z	146	GLN
1	z	240	GLN
2	0	240	GLN
3	1	114	GLN
2	2	151	GLN
2	2	184	ASN
4	3	151	GLN
4	3	192	ASN
3	5	29	GLN
5	6	244	ASN
1	7	256	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

32 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TPO	l	241	2	8,10,11	1.08	0	10,14,16	2.04	1 (10%)
2	TPO	J	241	2	8,10,11	1.71	1 (12%)	10,14,16	1.32	1 (10%)
2	TPO	Y	241	2	8,10,11	1.72	1 (12%)	10,14,16	1.28	1 (10%)
5	TPO	c	175	5	8,10,11	1.62	1 (12%)	10,14,16	2.03	1 (10%)
2	TPO	W	241	2	8,10,11	1.08	0	10,14,16	2.03	1 (10%)
2	TPO	S	241[A]	2	8,10,11	1.64	1 (12%)	10,14,16	2.05	1 (10%)
4	TPO	M	241	4	8,10,11	1.25	0	10,14,16	1.31	1 (10%)
2	TPO	S	241[B]	2	8,10,11	1.65	1 (12%)	10,14,16	1.97	1 (10%)
2	TPO	u	241	2	8,10,11	1.63	1 (12%)	10,14,16	2.01	1 (10%)
4	TPO	Z	241	4	8,10,11	1.74	1 (12%)	10,14,16	1.40	1 (10%)
2	TPO	w	241[A]	2	8,10,11	1.64	1 (12%)	10,14,16	2.05	1 (10%)
2	TPO	w	241[B]	2	8,10,11	1.65	1 (12%)	10,14,16	1.97	1 (10%)
4	TPO	3	175	4	8,10,11	1.73	1 (12%)	10,14,16	1.44	2 (20%)
4	TPO	M	175	4	8,10,11	1.73	1 (12%)	10,14,16	1.44	2 (20%)
5	TPO	P	175	5	8,10,11	1.62	1 (12%)	10,14,16	2.03	1 (10%)
4	TPO	o	241	4	8,10,11	1.73	1 (12%)	10,14,16	1.39	1 (10%)
2	TPO	0	241	2	8,10,11	1.63	1 (12%)	10,14,16	2.04	1 (10%)
2	TPO	f	241	2	8,10,11	1.09	0	10,14,16	2.00	1 (10%)
2	TPO	H	241	2	8,10,11	1.63	1 (12%)	10,14,16	2.03	1 (10%)
2	TPO	B	241	2	8,10,11	1.63	1 (12%)	10,14,16	2.01	1 (10%)
4	TPO	Z	175	4	8,10,11	1.75	1 (12%)	10,14,16	1.32	1 (10%)
5	TPO	r	175	5	8,10,11	1.62	1 (12%)	10,14,16	2.04	1 (10%)
2	TPO	n	241	2	8,10,11	1.71	1 (12%)	10,14,16	1.29	1 (10%)
4	TPO	3	241	4	8,10,11	1.25	0	10,14,16	1.31	1 (10%)
2	TPO	h	241[A]	2	8,10,11	1.64	1 (12%)	10,14,16	2.05	1 (10%)
2	TPO	h	241[B]	2	8,10,11	1.64	1 (12%)	10,14,16	1.97	1 (10%)
2	TPO	L	241	2	8,10,11	1.08	0	10,14,16	2.01	1 (10%)
2	TPO	2	241	2	8,10,11	1.72	1 (12%)	10,14,16	1.33	1 (10%)
2	TPO	D	241[B]	2	8,10,11	1.64	1 (12%)	10,14,16	1.97	1 (10%)
2	TPO	D	241[A]	2	8,10,11	1.64	1 (12%)	10,14,16	2.05	1 (10%)
5	TPO	6	175	5	8,10,11	1.63	1 (12%)	10,14,16	2.04	1 (10%)
4	TPO	o	175	4	8,10,11	1.74	1 (12%)	10,14,16	1.32	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	l	241	2	-	4/9/11/13	-
2	TPO	J	241	2	-	3/9/11/13	-
2	TPO	Y	241	2	-	2/9/11/13	-
5	TPO	c	175	5	-	2/9/11/13	-
2	TPO	W	241	2	-	4/9/11/13	-
2	TPO	S	241[A]	2	-	5/9/11/13	-
4	TPO	M	241	4	-	6/9/11/13	-
2	TPO	S	241[B]	2	-	1/9/11/13	-
2	TPO	u	241	2	-	5/9/11/13	-
4	TPO	Z	241	4	-	6/9/11/13	-
2	TPO	w	241[A]	2	-	5/9/11/13	-
2	TPO	w	241[B]	2	-	1/9/11/13	-
4	TPO	3	175	4	-	6/9/11/13	-
4	TPO	M	175	4	-	6/9/11/13	-
5	TPO	P	175	5	-	2/9/11/13	-
4	TPO	o	241	4	-	6/9/11/13	-
2	TPO	0	241	2	-	5/9/11/13	-
2	TPO	f	241	2	-	5/9/11/13	-
2	TPO	H	241	2	-	5/9/11/13	-
2	TPO	B	241	2	-	5/9/11/13	-
4	TPO	Z	175	4	-	5/9/11/13	-
5	TPO	r	175	5	-	2/9/11/13	-
2	TPO	n	241	2	-	2/9/11/13	-
4	TPO	3	241	4	-	6/9/11/13	-
2	TPO	h	241[A]	2	-	5/9/11/13	-
2	TPO	h	241[B]	2	-	1/9/11/13	-
2	TPO	L	241	2	-	5/9/11/13	-
2	TPO	2	241	2	-	3/9/11/13	-
2	TPO	D	241[B]	2	-	1/9/11/13	-
2	TPO	D	241[A]	2	-	5/9/11/13	-
5	TPO	6	175	5	-	2/9/11/13	-
4	TPO	o	175	4	-	5/9/11/13	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	241	TPO	P-O1P	3.61	1.61	1.50
2	n	241	TPO	P-O1P	3.58	1.61	1.50
4	o	175	TPO	P-O1P	3.58	1.61	1.50
4	Z	175	TPO	P-O1P	3.57	1.61	1.50
2	2	241	TPO	P-O1P	3.56	1.61	1.50
2	S	241[B]	TPO	P-O1P	3.56	1.61	1.50
2	h	241[B]	TPO	P-O1P	3.56	1.61	1.50
2	w	241[B]	TPO	P-O1P	3.55	1.61	1.50
2	J	241	TPO	P-O1P	3.54	1.61	1.50
4	Z	241	TPO	P-O1P	3.54	1.61	1.50
2	D	241[B]	TPO	P-O1P	3.53	1.61	1.50
2	D	241[A]	TPO	P-O1P	3.53	1.61	1.50
2	H	241	TPO	P-O1P	3.52	1.61	1.50
2	0	241	TPO	P-O1P	3.52	1.61	1.50
2	B	241	TPO	P-O1P	3.52	1.61	1.50
2	u	241	TPO	P-O1P	3.52	1.61	1.50
2	h	241[A]	TPO	P-O1P	3.52	1.61	1.50
5	6	175	TPO	P-O1P	3.52	1.61	1.50
2	w	241[A]	TPO	P-O1P	3.52	1.61	1.50
2	S	241[A]	TPO	P-O1P	3.51	1.61	1.50
4	o	241	TPO	P-O1P	3.50	1.61	1.50
5	r	175	TPO	P-O1P	3.50	1.61	1.50
5	P	175	TPO	P-O1P	3.49	1.61	1.50
5	c	175	TPO	P-O1P	3.48	1.61	1.50
4	M	175	TPO	P-O1P	3.46	1.61	1.50
4	3	175	TPO	P-O1P	3.46	1.61	1.50

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	241[A]	TPO	P-OG1-CB	-6.06	106.87	123.33
2	w	241[A]	TPO	P-OG1-CB	-6.06	106.87	123.33
2	h	241[A]	TPO	P-OG1-CB	-6.05	106.88	123.33
2	D	241[A]	TPO	P-OG1-CB	-6.05	106.88	123.33
2	l	241	TPO	P-OG1-CB	-6.05	106.90	123.33
2	0	241	TPO	P-OG1-CB	-6.05	106.90	123.33
2	W	241	TPO	P-OG1-CB	-6.04	106.92	123.33
2	H	241	TPO	P-OG1-CB	-6.03	106.94	123.33
5	r	175	TPO	P-OG1-CB	-5.98	107.09	123.33
5	6	175	TPO	P-OG1-CB	-5.97	107.10	123.33
5	P	175	TPO	P-OG1-CB	-5.96	107.12	123.33
5	c	175	TPO	P-OG1-CB	-5.96	107.12	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	241	TPO	P-OG1-CB	-5.93	107.21	123.33
2	u	241	TPO	P-OG1-CB	-5.93	107.22	123.33
2	f	241	TPO	P-OG1-CB	-5.93	107.22	123.33
2	B	241	TPO	P-OG1-CB	-5.92	107.23	123.33
2	w	241[B]	TPO	P-OG1-CB	-5.59	108.13	123.33
2	D	241[B]	TPO	P-OG1-CB	-5.59	108.15	123.33
2	h	241[B]	TPO	P-OG1-CB	-5.58	108.15	123.33
2	S	241[B]	TPO	P-OG1-CB	-5.58	108.16	123.33
4	Z	175	TPO	P-OG1-CB	-3.05	115.03	123.33
4	M	175	TPO	P-OG1-CB	-3.05	115.03	123.33
4	o	175	TPO	P-OG1-CB	-3.04	115.07	123.33
4	3	175	TPO	P-OG1-CB	-3.04	115.07	123.33
4	Z	241	TPO	P-OG1-CB	-2.99	115.20	123.33
4	M	241	TPO	P-OG1-CB	-2.98	115.22	123.33
4	3	241	TPO	P-OG1-CB	-2.98	115.24	123.33
2	2	241	TPO	P-OG1-CB	-2.97	115.25	123.33
2	J	241	TPO	P-OG1-CB	-2.97	115.25	123.33
2	n	241	TPO	P-OG1-CB	-2.97	115.26	123.33
4	o	241	TPO	P-OG1-CB	-2.96	115.29	123.33
2	Y	241	TPO	P-OG1-CB	-2.95	115.31	123.33
4	3	175	TPO	O3P-P-OG1	2.21	114.45	105.85
4	M	175	TPO	O3P-P-OG1	2.21	114.45	105.85

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	241	TPO	N-CA-CB-OG1
2	B	241	TPO	C-CA-CB-CG2
2	B	241	TPO	O-C-CA-CB
2	D	241[A]	TPO	N-CA-CB-OG1
2	D	241[A]	TPO	C-CA-CB-CG2
2	D	241[A]	TPO	O-C-CA-CB
2	D	241[B]	TPO	N-CA-CB-OG1
2	H	241	TPO	N-CA-CB-CG2
2	H	241	TPO	N-CA-CB-OG1
2	H	241	TPO	C-CA-CB-CG2
2	H	241	TPO	O-C-CA-CB
4	M	175	TPO	N-CA-CB-CG2
4	M	175	TPO	N-CA-CB-OG1
4	M	175	TPO	C-CA-CB-CG2
4	M	175	TPO	CA-CB-OG1-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	M	241	TPO	N-CA-CB-CG2
4	M	241	TPO	N-CA-CB-OG1
4	M	241	TPO	C-CA-CB-CG2
4	M	241	TPO	O-C-CA-CB
4	M	241	TPO	CA-CB-OG1-P
5	P	175	TPO	N-CA-CB-OG1
5	P	175	TPO	O-C-CA-CB
2	L	241	TPO	N-CA-CB-OG1
2	L	241	TPO	C-CA-CB-CG2
2	L	241	TPO	O-C-CA-CB
2	S	241[A]	TPO	N-CA-CB-OG1
2	S	241[A]	TPO	C-CA-CB-CG2
2	S	241[A]	TPO	O-C-CA-CB
2	S	241[B]	TPO	N-CA-CB-OG1
2	W	241	TPO	N-CA-CB-CG2
2	W	241	TPO	N-CA-CB-OG1
2	W	241	TPO	C-CA-CB-CG2
2	W	241	TPO	O-C-CA-CB
4	Z	175	TPO	N-CA-CB-CG2
4	Z	175	TPO	N-CA-CB-OG1
4	Z	175	TPO	C-CA-CB-CG2
4	Z	175	TPO	CA-CB-OG1-P
4	Z	241	TPO	N-CA-CB-CG2
4	Z	241	TPO	N-CA-CB-OG1
4	Z	241	TPO	C-CA-CB-CG2
4	Z	241	TPO	O-C-CA-CB
4	Z	241	TPO	CA-CB-OG1-P
5	c	175	TPO	N-CA-CB-OG1
5	c	175	TPO	O-C-CA-CB
2	f	241	TPO	N-CA-CB-OG1
2	f	241	TPO	C-CA-CB-CG2
2	f	241	TPO	O-C-CA-CB
2	h	241[A]	TPO	N-CA-CB-OG1
2	h	241[A]	TPO	C-CA-CB-CG2
2	h	241[A]	TPO	O-C-CA-CB
2	h	241[B]	TPO	N-CA-CB-OG1
2	l	241	TPO	N-CA-CB-CG2
2	l	241	TPO	N-CA-CB-OG1
2	l	241	TPO	C-CA-CB-CG2
2	l	241	TPO	O-C-CA-CB
4	o	175	TPO	N-CA-CB-CG2
4	o	175	TPO	N-CA-CB-OG1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	o	175	TPO	C-CA-CB-CG2
4	o	175	TPO	CA-CB-OG1-P
4	o	241	TPO	N-CA-CB-CG2
4	o	241	TPO	N-CA-CB-OG1
4	o	241	TPO	C-CA-CB-CG2
4	o	241	TPO	O-C-CA-CB
4	o	241	TPO	CA-CB-OG1-P
5	r	175	TPO	N-CA-CB-OG1
5	r	175	TPO	O-C-CA-CB
2	u	241	TPO	N-CA-CB-OG1
2	u	241	TPO	C-CA-CB-CG2
2	u	241	TPO	O-C-CA-CB
2	w	241[A]	TPO	N-CA-CB-OG1
2	w	241[A]	TPO	C-CA-CB-CG2
2	w	241[A]	TPO	O-C-CA-CB
2	w	241[B]	TPO	N-CA-CB-OG1
2	0	241	TPO	N-CA-CB-CG2
2	0	241	TPO	N-CA-CB-OG1
2	0	241	TPO	C-CA-CB-CG2
2	0	241	TPO	O-C-CA-CB
4	3	175	TPO	N-CA-CB-CG2
4	3	175	TPO	N-CA-CB-OG1
4	3	175	TPO	C-CA-CB-CG2
4	3	175	TPO	CA-CB-OG1-P
4	3	241	TPO	N-CA-CB-CG2
4	3	241	TPO	N-CA-CB-OG1
4	3	241	TPO	C-CA-CB-CG2
4	3	241	TPO	O-C-CA-CB
4	3	241	TPO	CA-CB-OG1-P
5	6	175	TPO	N-CA-CB-OG1
5	6	175	TPO	O-C-CA-CB
2	J	241	TPO	CG2-CB-OG1-P
2	Y	241	TPO	CG2-CB-OG1-P
2	n	241	TPO	CG2-CB-OG1-P
2	2	241	TPO	CG2-CB-OG1-P
2	B	241	TPO	N-CA-CB-CG2
2	D	241[A]	TPO	N-CA-CB-CG2
2	L	241	TPO	N-CA-CB-CG2
2	S	241[A]	TPO	N-CA-CB-CG2
2	f	241	TPO	N-CA-CB-CG2
2	h	241[A]	TPO	N-CA-CB-CG2
2	u	241	TPO	N-CA-CB-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	w	241[A]	TPO	N-CA-CB-CG2
2	L	241	TPO	CB-OG1-P-O1P
2	f	241	TPO	CB-OG1-P-O1P
2	D	241[A]	TPO	CB-OG1-P-O1P
2	H	241	TPO	CB-OG1-P-O1P
2	J	241	TPO	CB-OG1-P-O1P
4	M	175	TPO	CB-OG1-P-O1P
4	M	241	TPO	CB-OG1-P-O1P
2	S	241[A]	TPO	CB-OG1-P-O1P
2	h	241[A]	TPO	CB-OG1-P-O1P
2	w	241[A]	TPO	CB-OG1-P-O1P
2	0	241	TPO	CB-OG1-P-O1P
2	2	241	TPO	CB-OG1-P-O1P
4	3	175	TPO	CB-OG1-P-O1P
4	3	241	TPO	CB-OG1-P-O1P
2	J	241	TPO	O-C-CA-CB
4	M	175	TPO	O-C-CA-CB
2	Y	241	TPO	O-C-CA-CB
4	Z	175	TPO	O-C-CA-CB
2	n	241	TPO	O-C-CA-CB
4	o	175	TPO	O-C-CA-CB
2	2	241	TPO	O-C-CA-CB
4	3	175	TPO	O-C-CA-CB
2	B	241	TPO	CB-OG1-P-O1P
4	Z	241	TPO	CB-OG1-P-O1P
4	o	241	TPO	CB-OG1-P-O1P
2	u	241	TPO	CB-OG1-P-O1P

There are no ring outliers.

16 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	241[A]	TPO	1	0
4	M	241	TPO	1	0
2	u	241	TPO	2	0
4	Z	241	TPO	1	0
2	w	241[A]	TPO	1	0
4	3	175	TPO	1	0
4	M	175	TPO	1	0
4	o	241	TPO	1	0
2	f	241	TPO	2	0
2	B	241	TPO	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	175	TPO	1	0
4	3	241	TPO	1	0
2	h	241[A]	TPO	1	0
2	L	241	TPO	2	0
2	D	241[A]	TPO	1	0
4	o	175	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

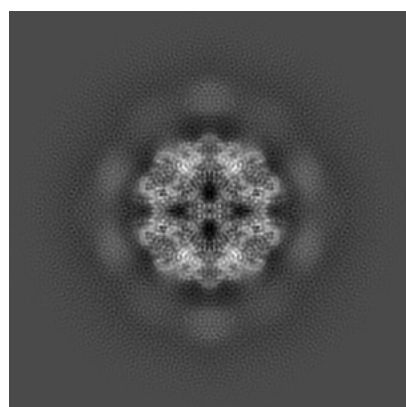
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11971. These allow visual inspection of the internal detail of the map and identification of artifacts.

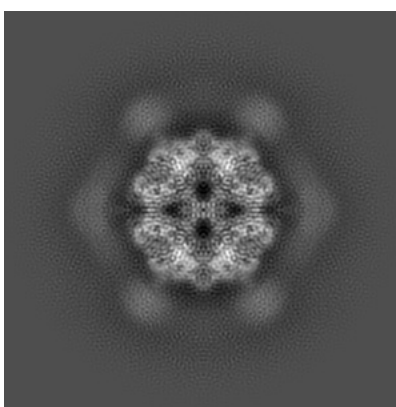
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

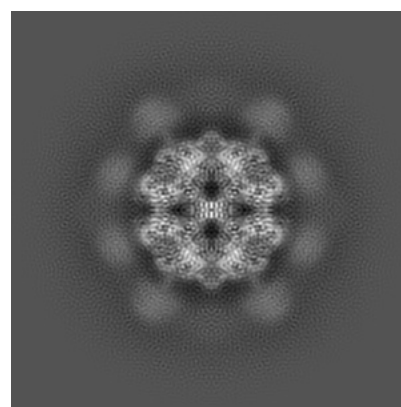
6.1.1 Primary map



X



Y

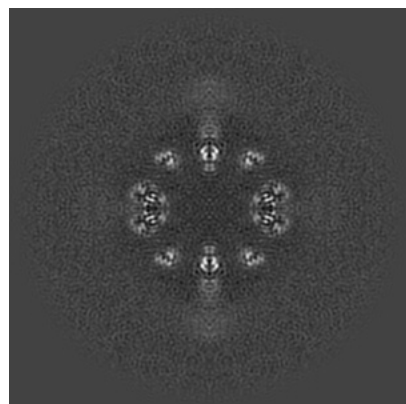


Z

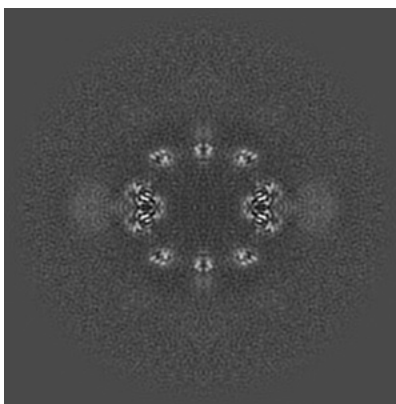
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

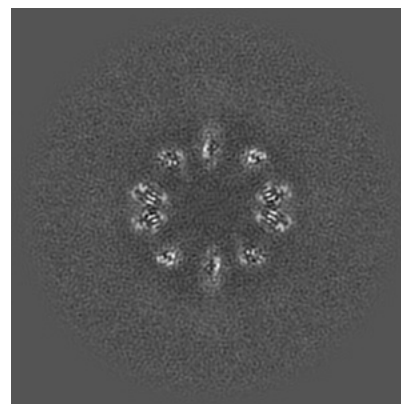
6.2.1 Primary map



X Index: 192



Y Index: 192

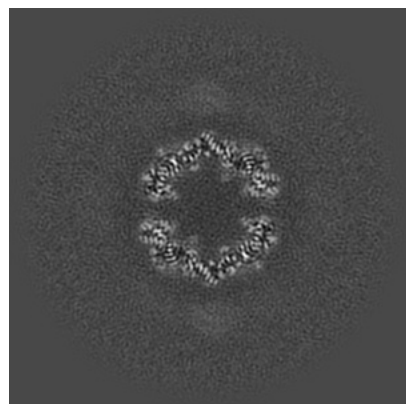


Z Index: 192

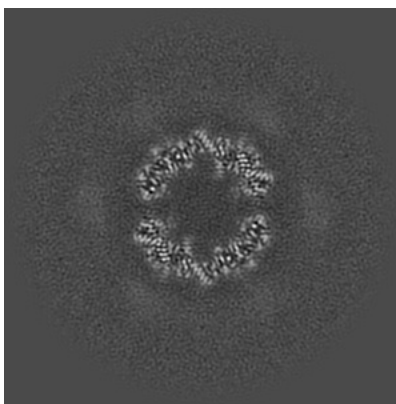
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

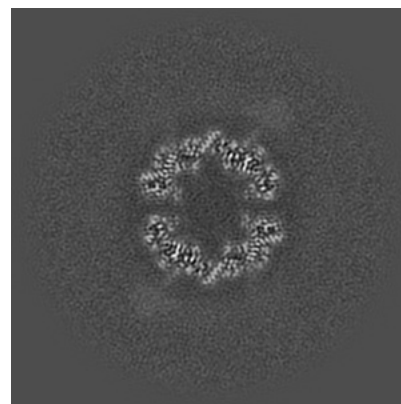
6.3.1 Primary map



X Index: 175



Y Index: 174

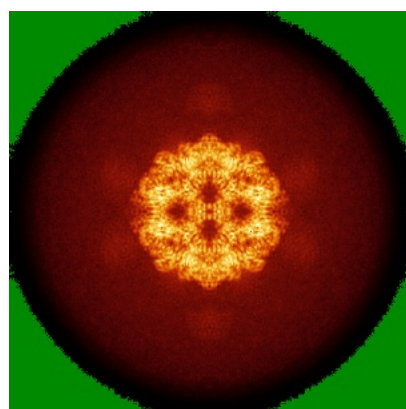


Z Index: 209

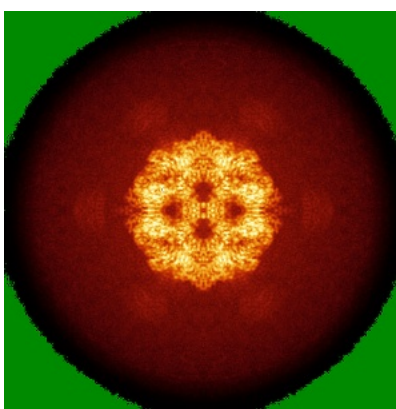
The images above show the largest variance slices of the map in three orthogonal directions.

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

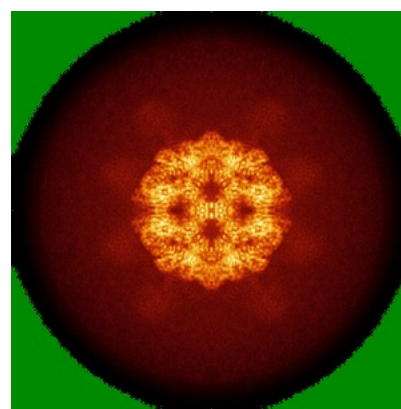
6.4.1 Primary map



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

This section was not generated.

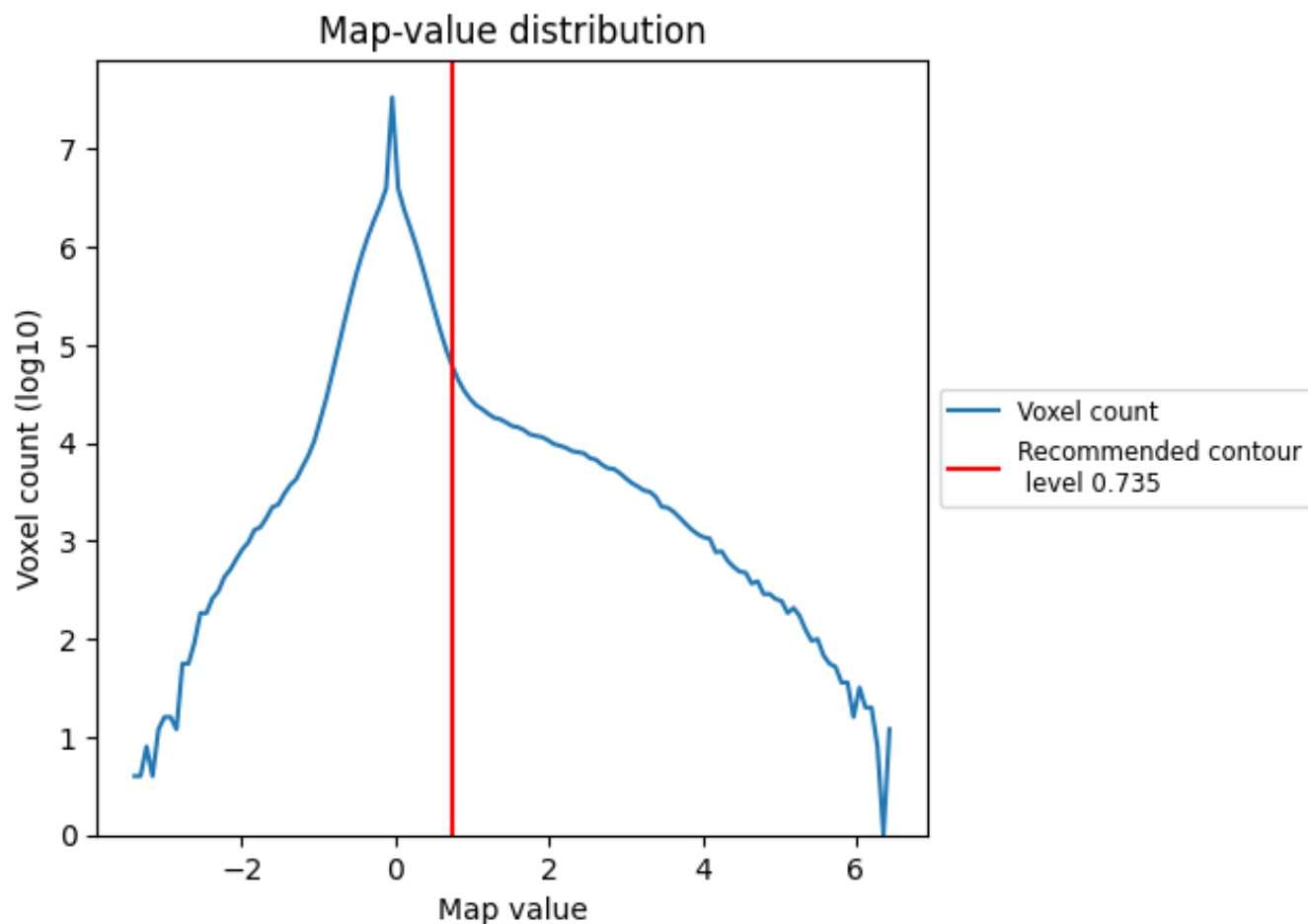
6.6 Mask visualisation

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

7 Map analysis [i](#)

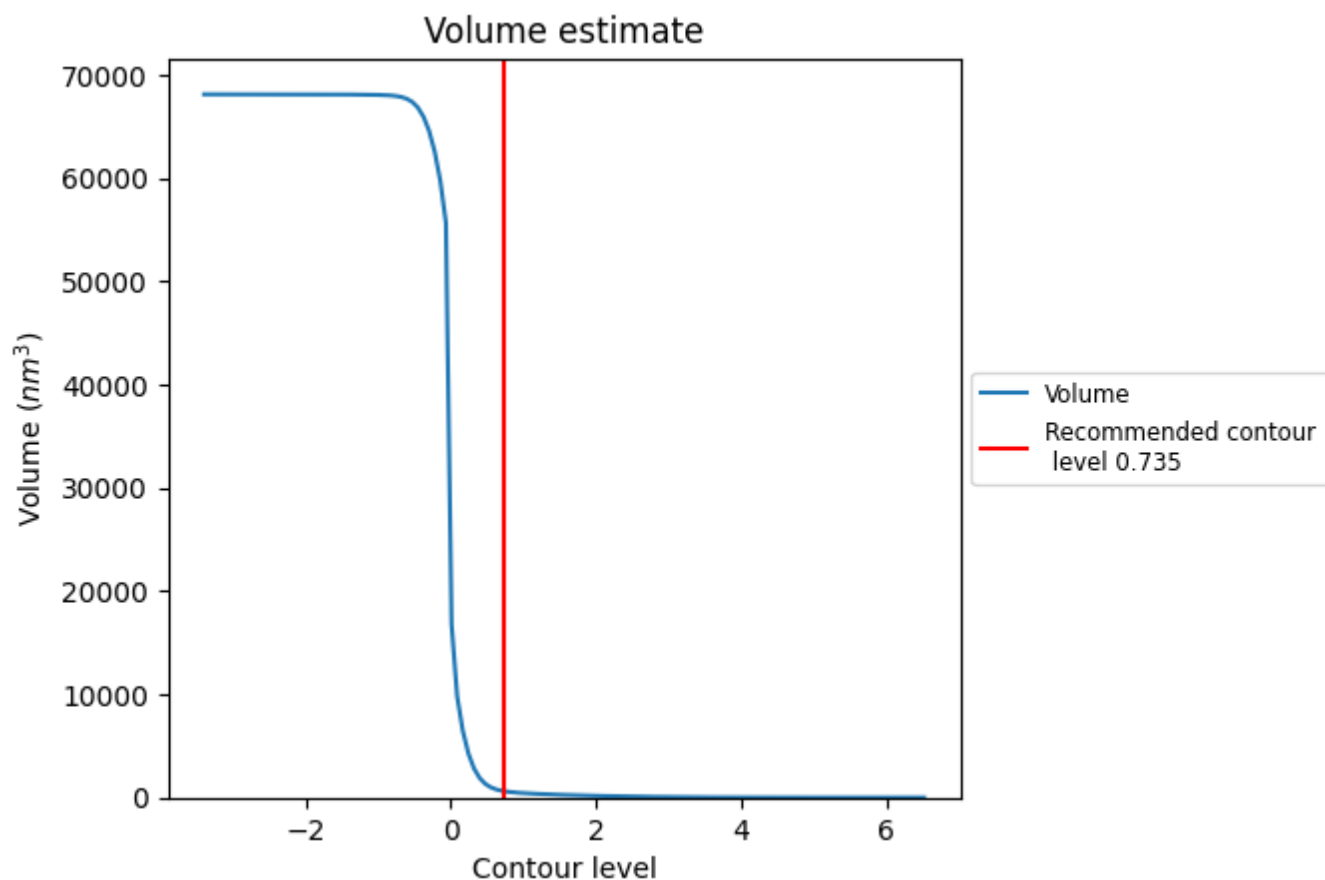
This section contains the results of statistical analysis of the map.

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.

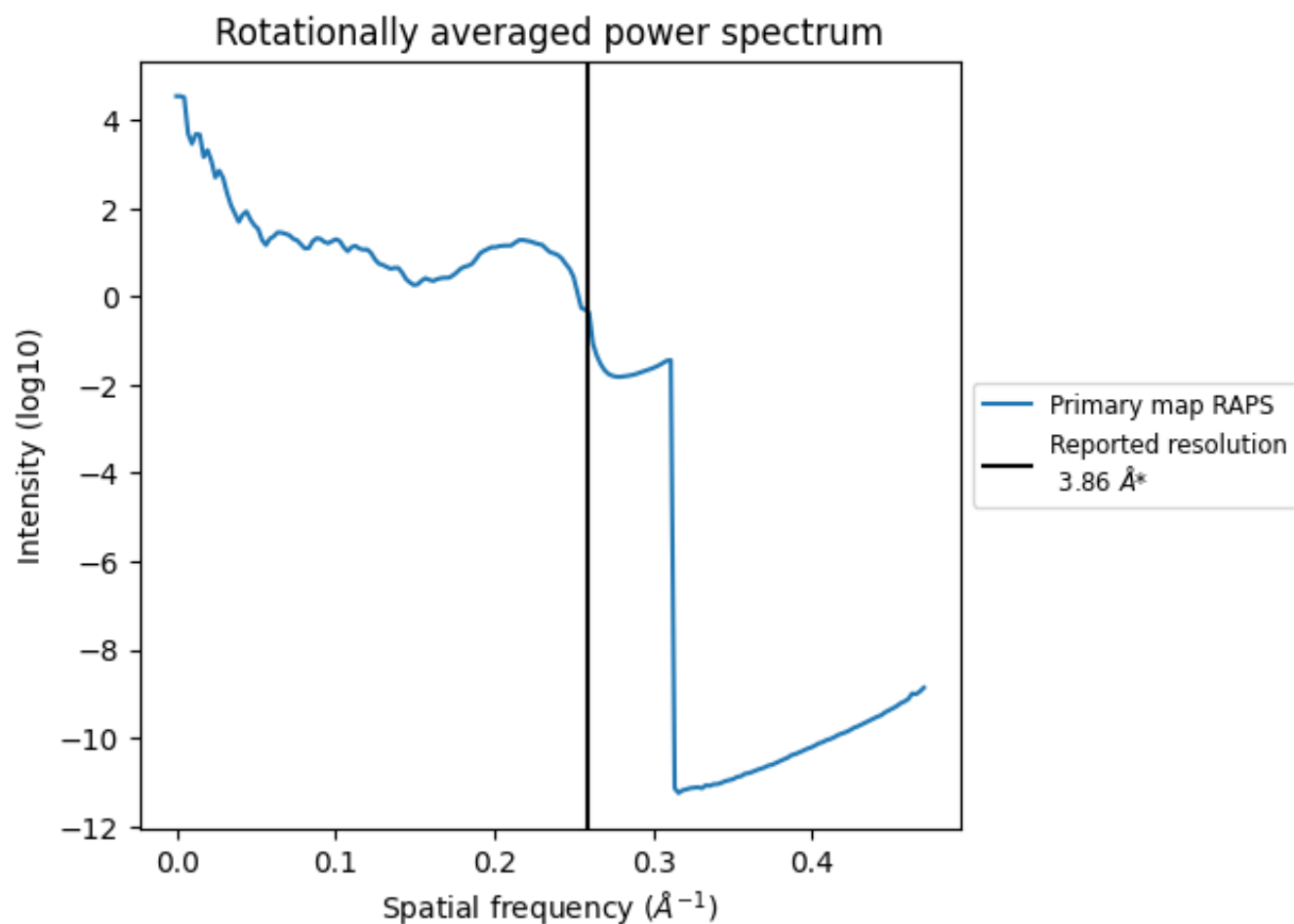
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm³; this corresponds to an approximate mass of 557 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 0.259 Å⁻¹

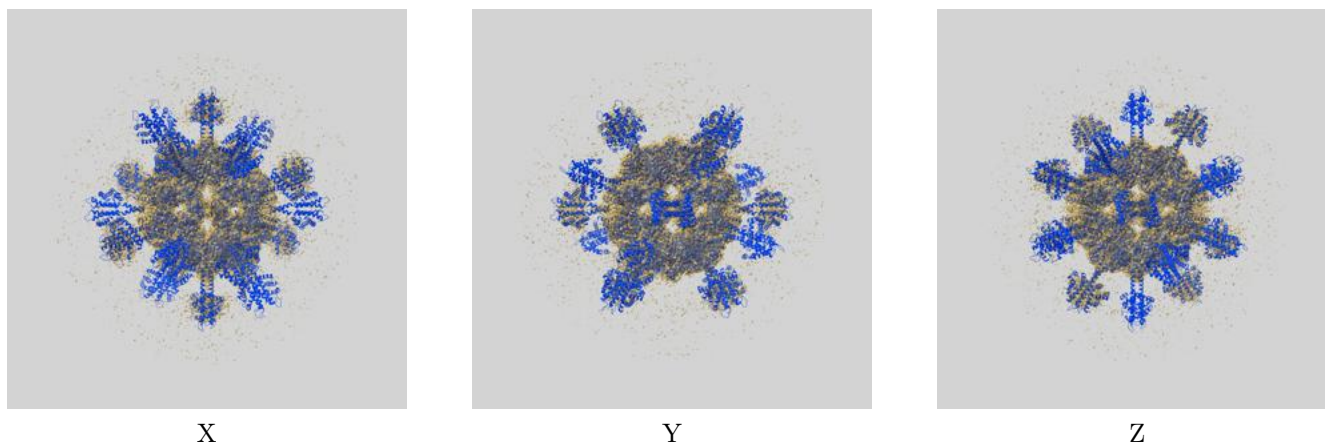
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

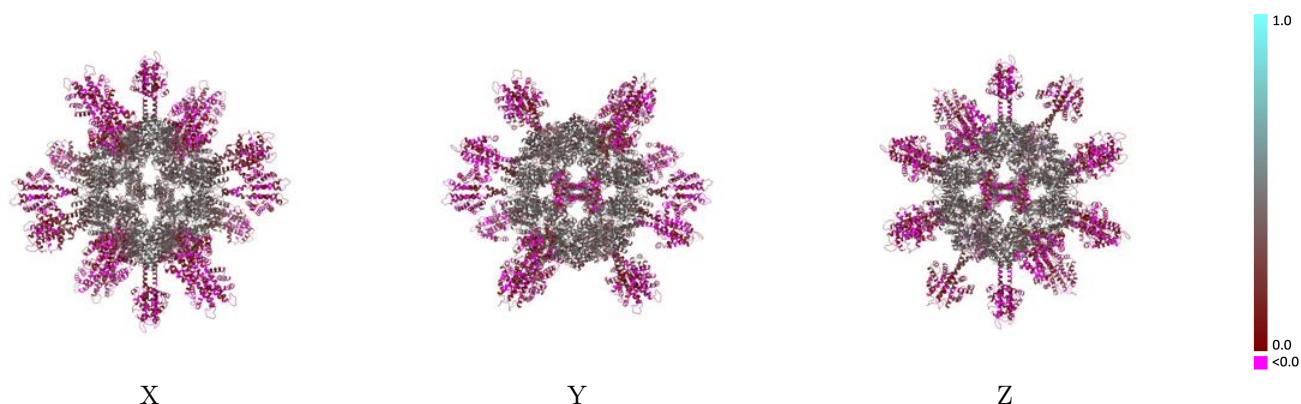
This section contains information regarding the fit between EMDB map EMD-11971 and PDB model 7B0U. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



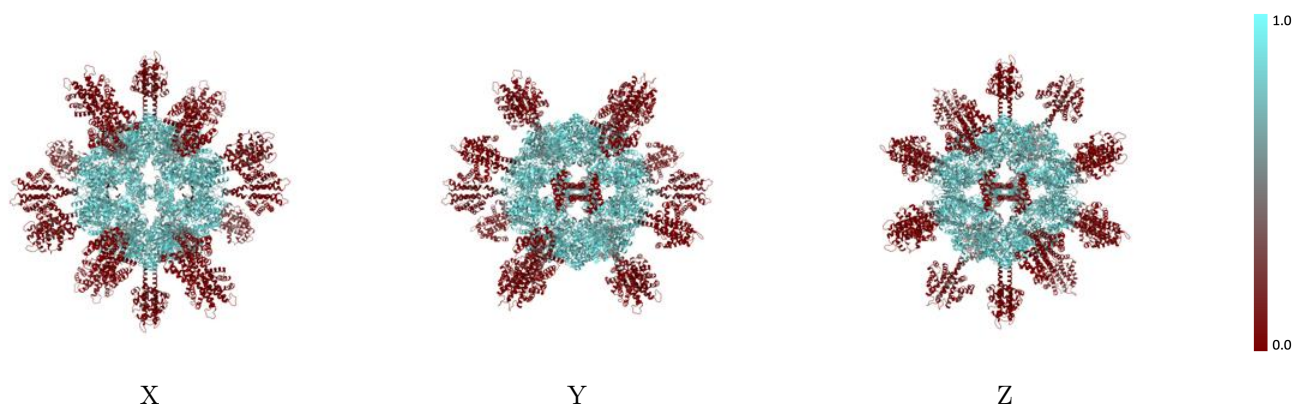
The images above show the 3D surface view of the map at the recommended contour level 0.735 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



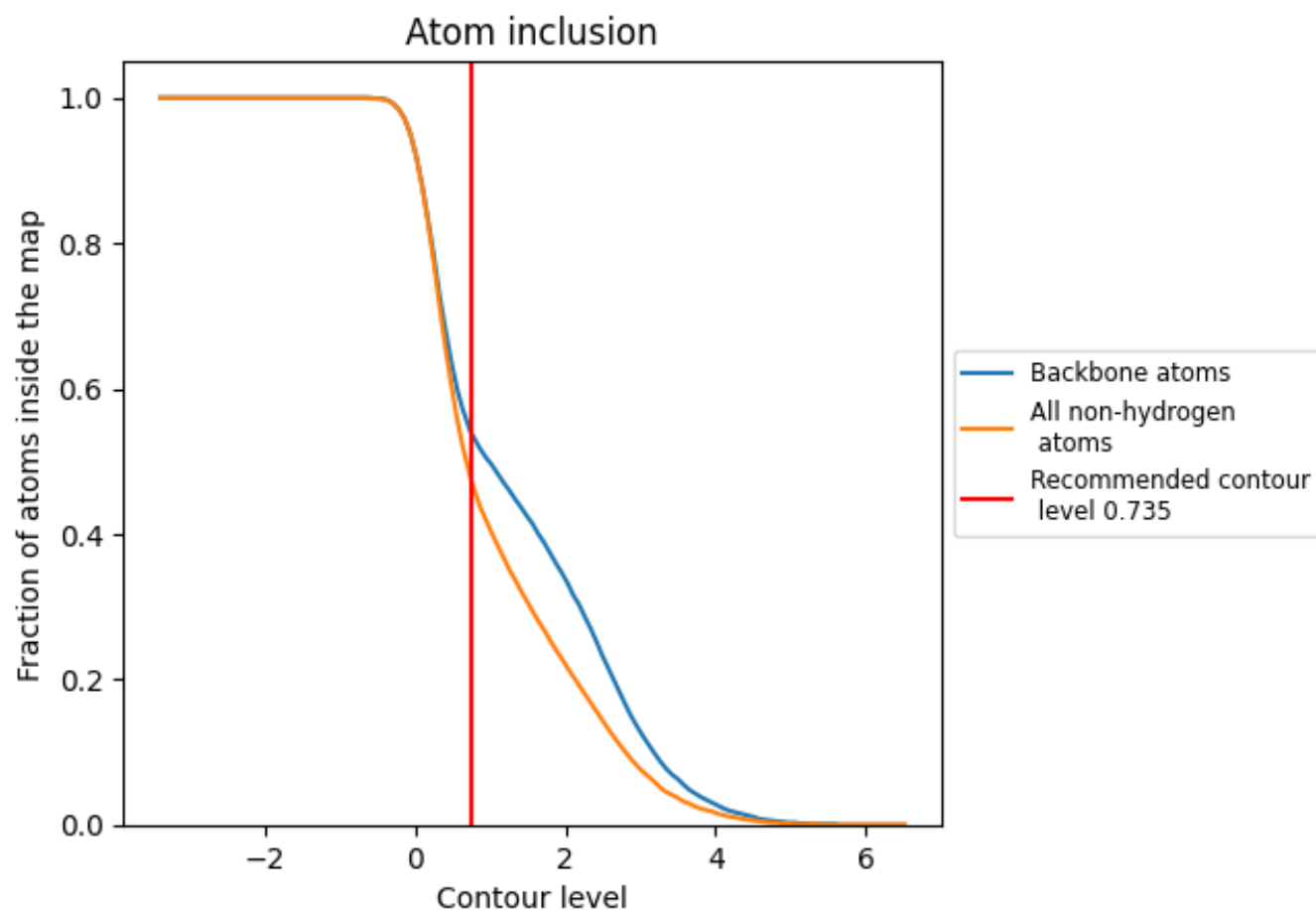
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.735).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 48% 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 (0.735) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4760	 0.2530
0	 0.4050	 0.2160
1	 0.8430	 0.3680
2	 0.4100	 0.2130
3	 0.3670	 0.2040
4	 0.8600	 0.3920
5	 0.8560	 0.3720
6	 0.3620	 0.2050
7	 0.3720	 0.2030
A	 0.4420	 0.2700
B	 0.4420	 0.2620
C	 0.3880	 0.2350
D	 0.3850	 0.2420
E	 0.8590	 0.3900
F	 0.8600	 0.4000
G	 0.4140	 0.2210
H	 0.4060	 0.2170
I	 0.8390	 0.3590
J	 0.4100	 0.2120
K	 0.4420	 0.2680
L	 0.4420	 0.2610
M	 0.3670	 0.2020
N	 0.8620	 0.3950
O	 0.8580	 0.3790
P	 0.3610	 0.2050
Q	 0.3720	 0.2000
R	 0.3880	 0.2380
S	 0.3840	 0.2420
T	 0.8600	 0.3920
U	 0.8610	 0.4000
V	 0.4150	 0.2220
W	 0.4060	 0.2150
X	 0.8350	 0.3620
Y	 0.4100	 0.2120
Z	 0.3670	 0.2030



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.8600	 0.3960
b	 0.8600	 0.3790
c	 0.3620	 0.2040
d	 0.3720	 0.2030
e	 0.4440	 0.2710
f	 0.4410	 0.2630
g	 0.3890	 0.2360
h	 0.3850	 0.2410
i	 0.8610	 0.3900
j	 0.8620	 0.4020
k	 0.4150	 0.2210
l	 0.4040	 0.2170
m	 0.8310	 0.3670
n	 0.4100	 0.2130
o	 0.3670	 0.2020
p	 0.8640	 0.3950
q	 0.8540	 0.3720
r	 0.3620	 0.2040
s	 0.3700	 0.2040
t	 0.4430	 0.2700
u	 0.4420	 0.2610
v	 0.3880	 0.2370
w	 0.3850	 0.2420
x	 0.8610	 0.3900
y	 0.8610	 0.4010
z	 0.4140	 0.2200