



Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 11:56 pm BST

PDB ID : 9RCB / pdb_00009rcb
EMDB ID : EMD-53912
Title : Unsheathed flagellar filament in *Vibrio alginolyticus*
Authors : Qin, K.; Eikenkel, R.; Zhao, W.; Erhardt, M.; Bergeron, J.R.C.
Deposited on : 2025-05-27
Resolution : 3.10 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

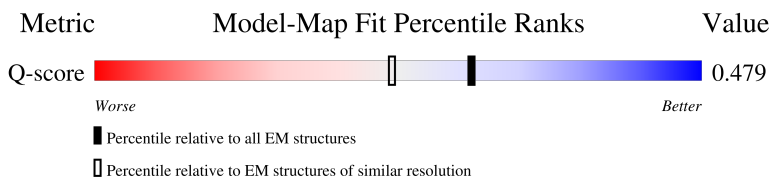
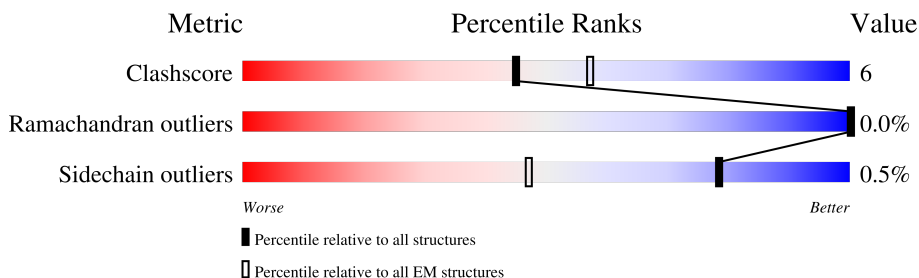
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	377	 6% 91% 9%
1	B	377	 7% 89% 11%
1	C	377	 8% 91% 8%
1	D	377	 7% 92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	377	
1	F	377	
1	G	377	
1	H	377	
1	I	377	
1	J	377	
1	K	377	
1	L	377	
1	M	377	
1	N	377	
1	O	377	
1	P	377	
1	Q	377	
1	R	377	
1	S	377	
1	T	377	
1	U	377	
1	V	377	
1	X	377	
1	Z	377	
1	b	377	
1	c	377	
1	d	377	
1	e	377	
1	f	377	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	g	377	<div> <div>45%</div> <div>82%</div> <div>17%</div> </div>
1	h	377	<div> <div>13%</div> <div>86%</div> <div>14%</div> </div>
1	i	377	<div> <div>24%</div> <div>86%</div> <div>13%</div> </div>
1	j	377	<div> <div>11%</div> <div>86%</div> <div>14%</div> </div>
1	k	377	<div> <div>21%</div> <div>84%</div> <div>15%</div> </div>
1	l	377	<div> <div>11%</div> <div>87%</div> <div>12%</div> </div>
1	m	377	<div> <div>20%</div> <div>87%</div> <div>13%</div> </div>
1	n	377	<div> <div>31%</div> <div>83%</div> <div>16%</div> </div>
1	o	377	<div> <div>15%</div> <div>91%</div> <div>8%</div> </div>
1	p	377	<div> <div>26%</div> <div>87%</div> <div>13%</div> </div>
1	q	377	<div> <div>13%</div> <div>87%</div> <div>12%</div> </div>
1	r	377	<div> <div>25%</div> <div>88%</div> <div>12%</div> </div>
1	s	377	<div> <div>42%</div> <div>82%</div> <div>17%</div> </div>
1	u	377	<div> <div>40%</div> <div>86%</div> <div>13%</div> </div>
1	w	377	<div> <div>34%</div> <div>82%</div> <div>18%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 243936 atoms, of which 120824 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 Flagellin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	B	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	C	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	D	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	E	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	F	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	G	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	H	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	I	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	J	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	K	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	L	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	M	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	N	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	O	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	P	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	Q	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	S	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	T	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	U	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	V	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	X	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	Z	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	b	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	c	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	d	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	e	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	f	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	g	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	h	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	i	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	j	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	k	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	l	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	m	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	n	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0
1	o	376	Total 5544	C 1692	H 2746	N 503	O 594	S 9	0	0

Continued on next page...

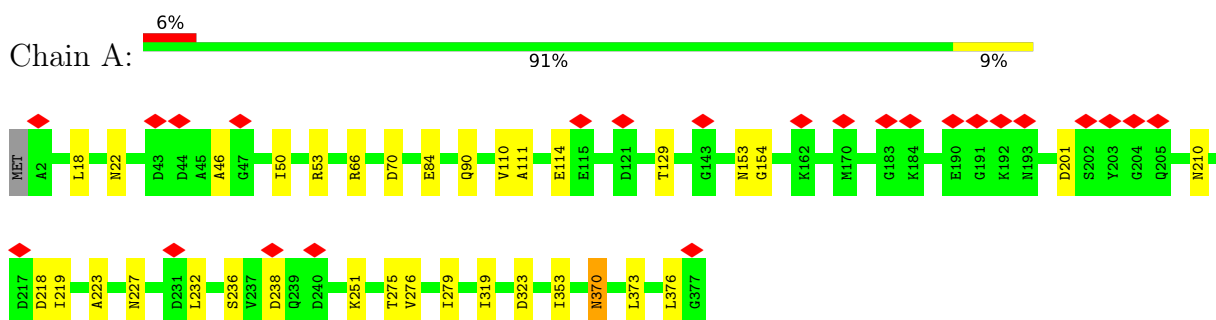
Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
1	p	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	q	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	r	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	s	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	u	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		
1	w	376	Total	C	H	N	O	S	0	0
			5544	1692	2746	503	594	9		

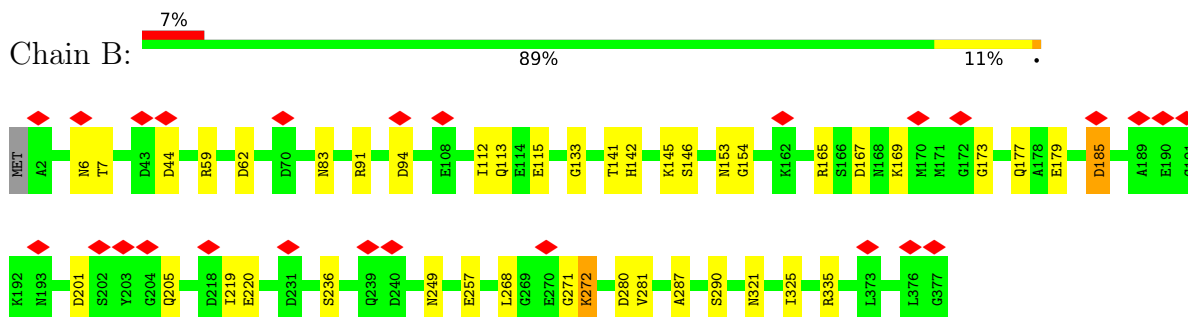
3 Residue-property plots [i](#)

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.

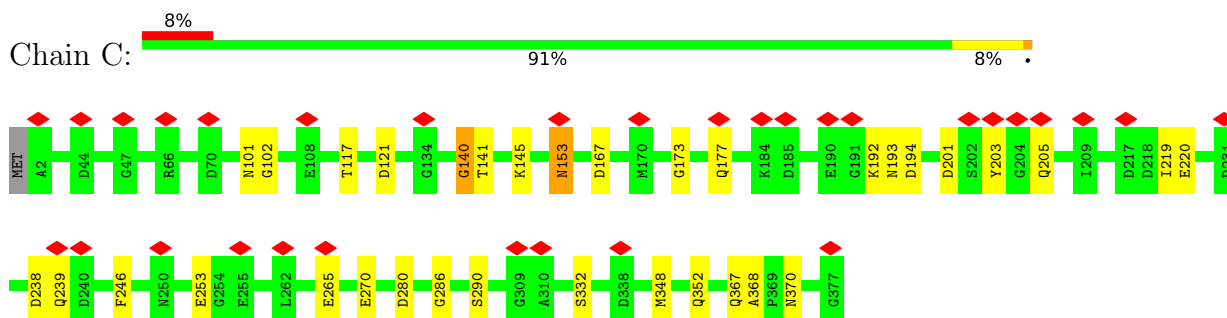
- Molecule 1: Flagellin



- Molecule 1: Flagellin

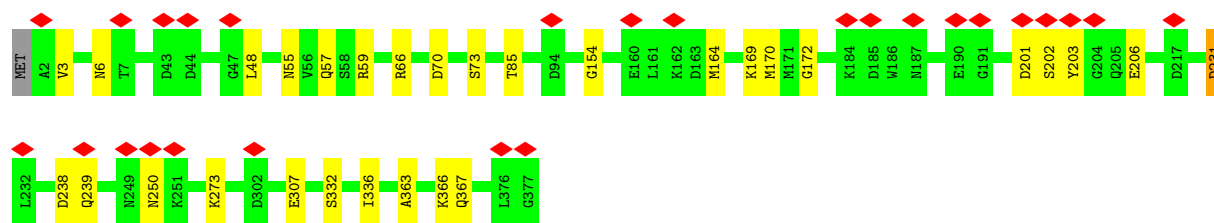


- Molecule 1: Flagellin

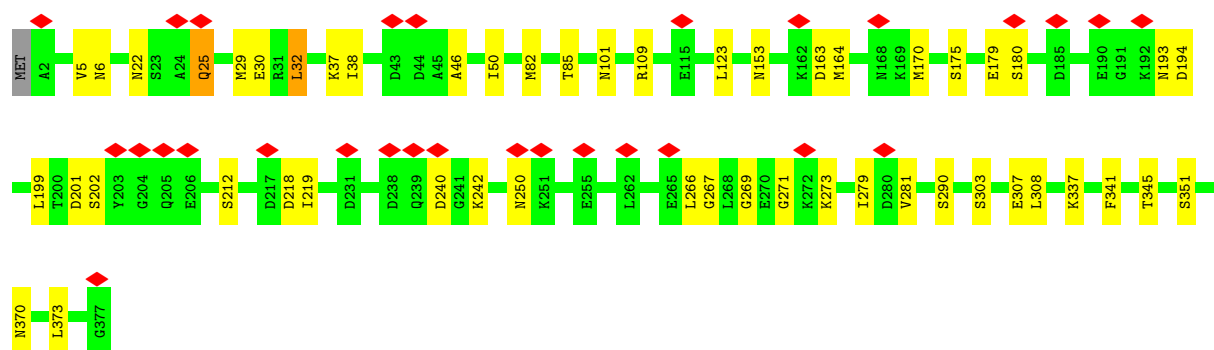
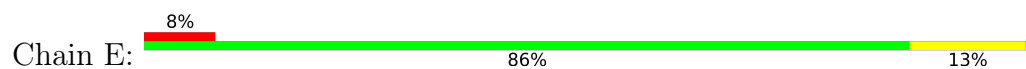


- Molecule 1: Flagellin

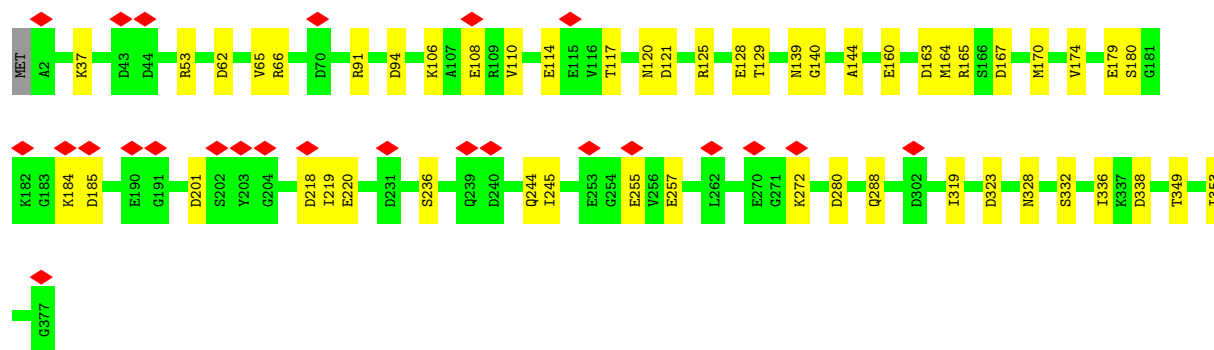
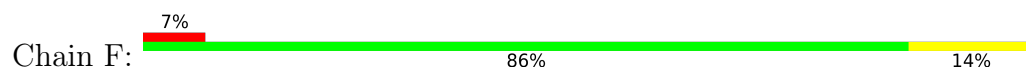




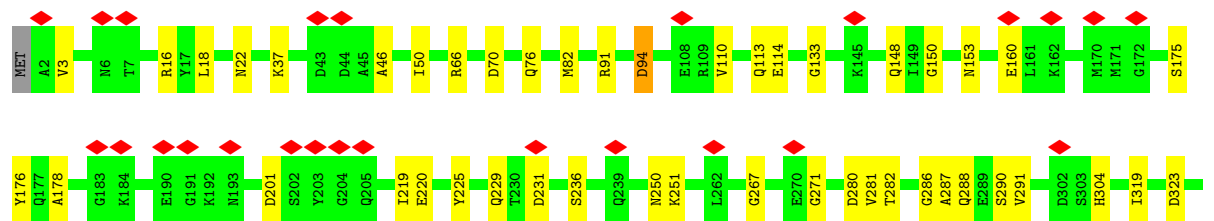
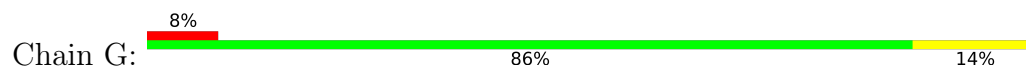
• Molecule 1: Flagellin

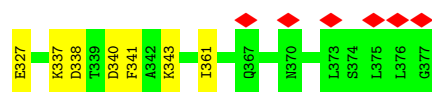


• Molecule 1: Flagellin

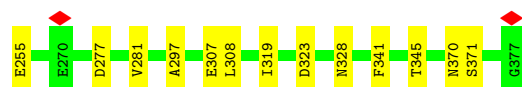
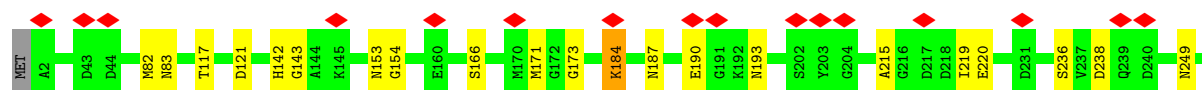


• Molecule 1: Flagellin

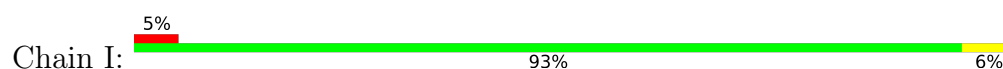




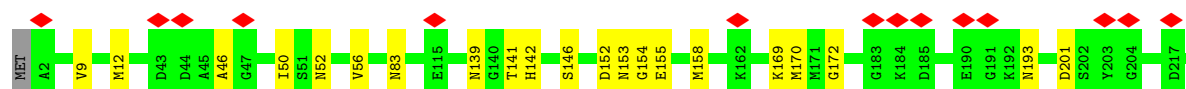
- Molecule 1: Flagellin



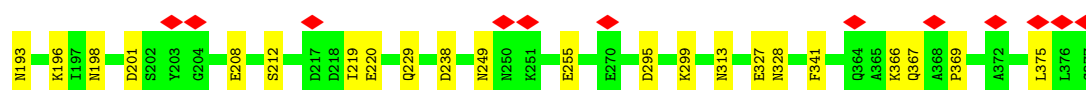
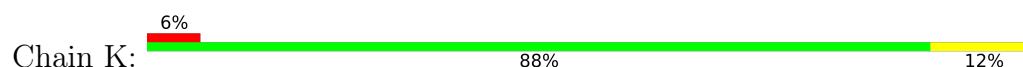
- Molecule 1: Flagellin



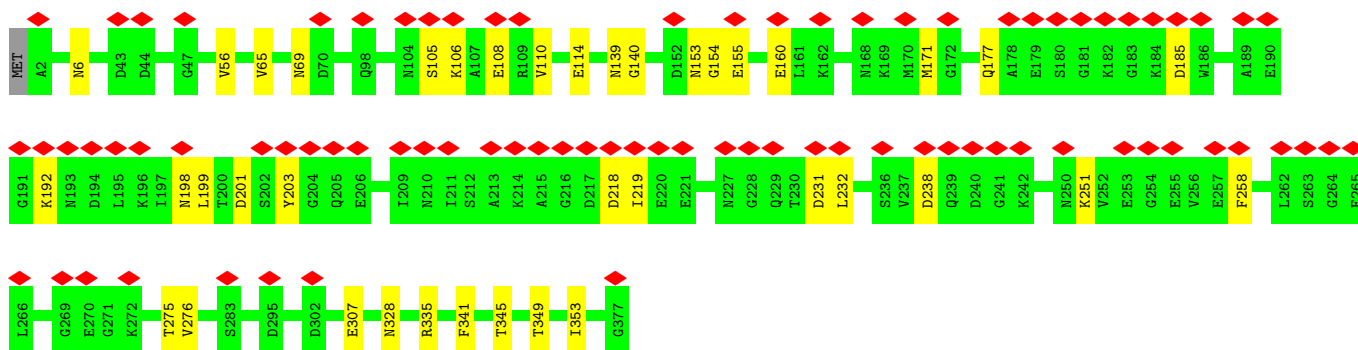
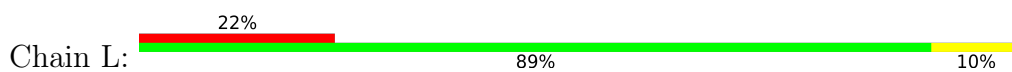
- Molecule 1: Flagellin



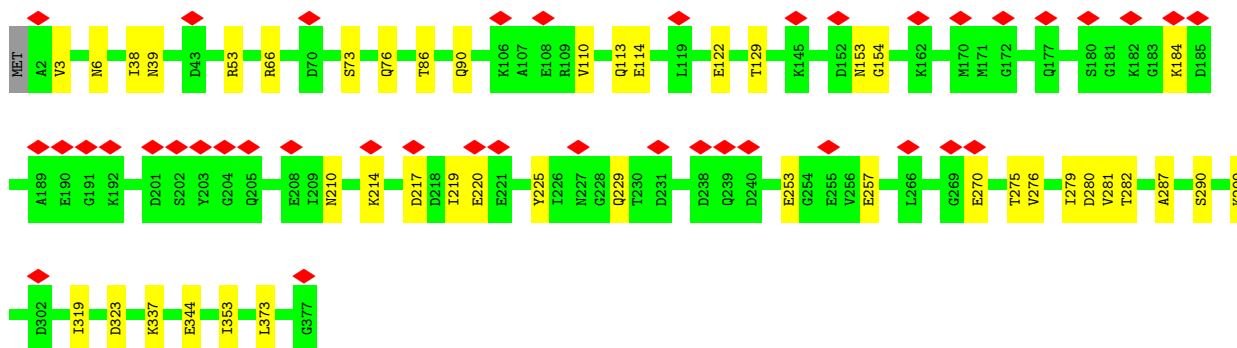
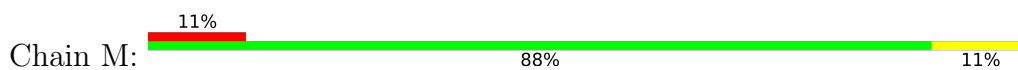
- Molecule 1: Flagellin



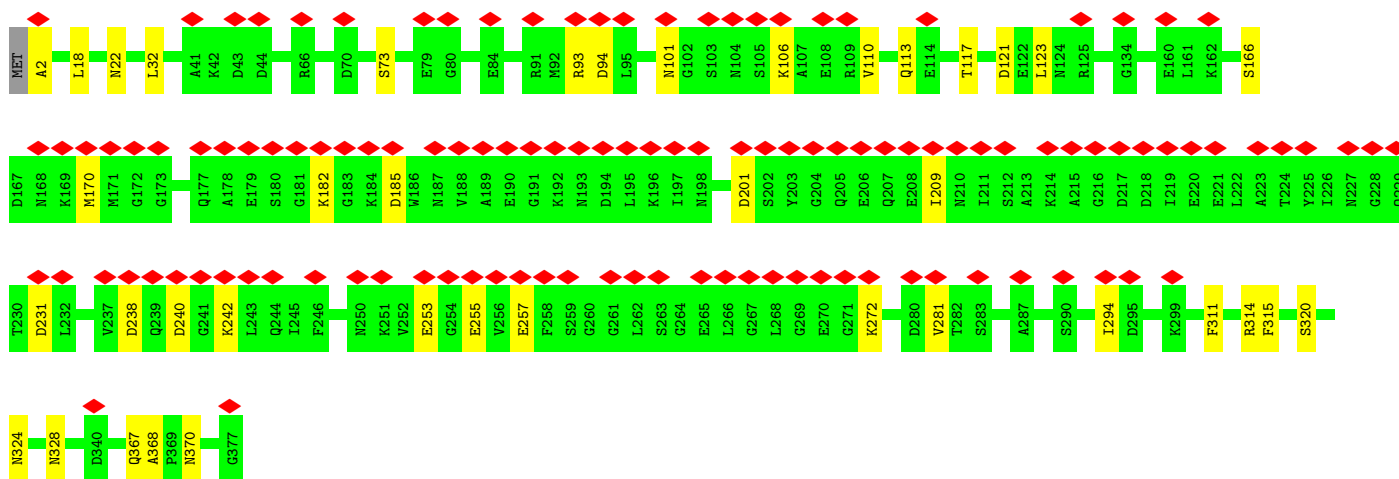
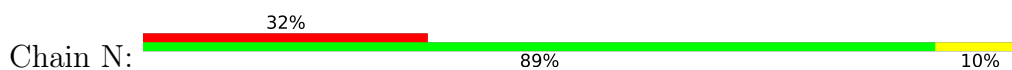
- Molecule 1: Flagellin



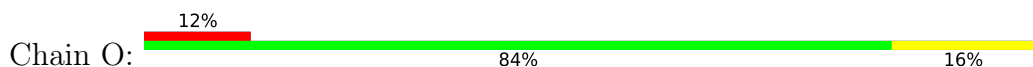
• Molecule 1: Flagellin

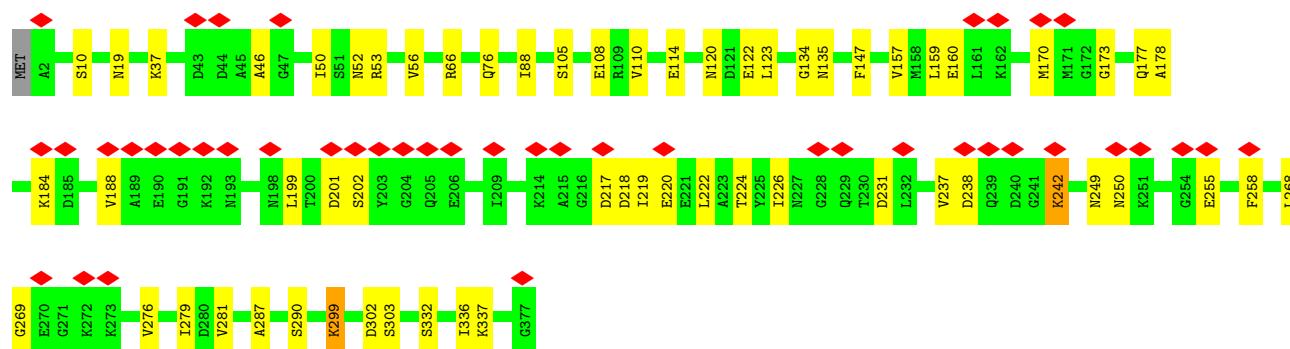


• Molecule 1: Flagellin

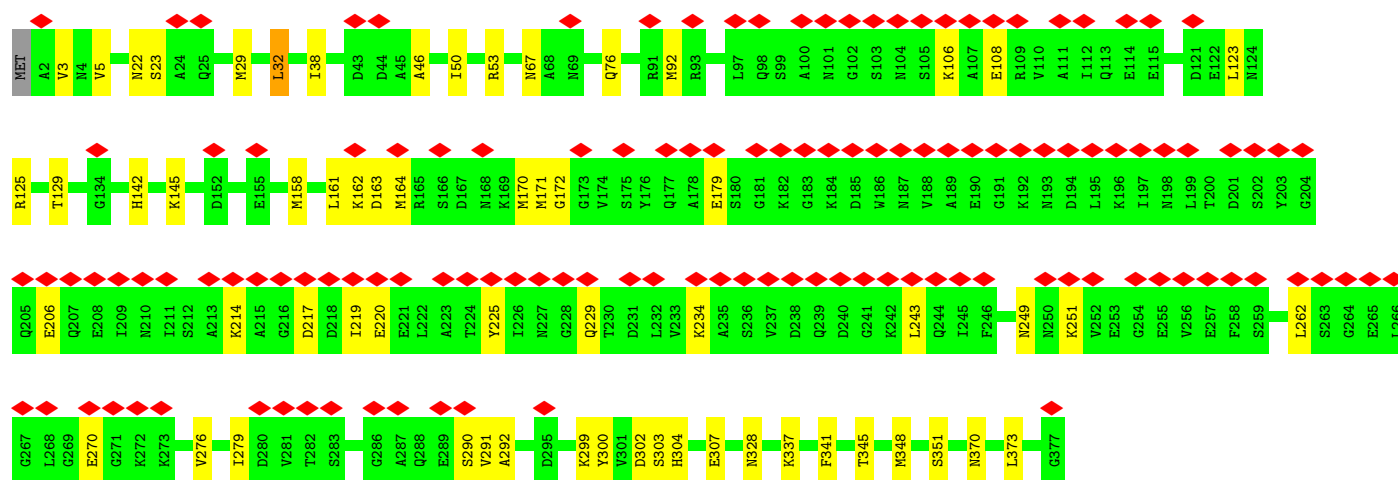
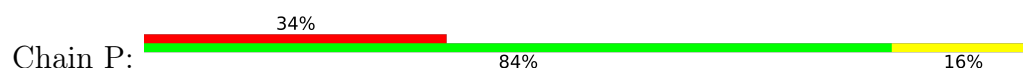


• Molecule 1: Flagellin

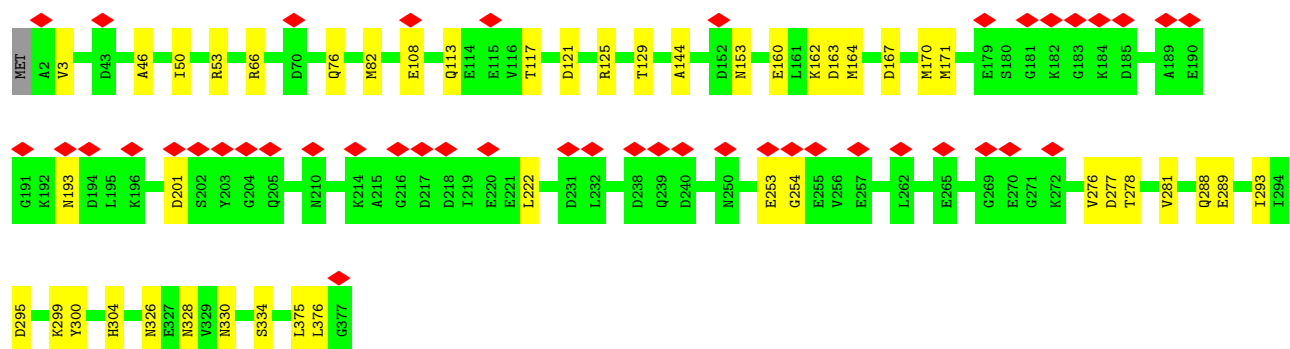
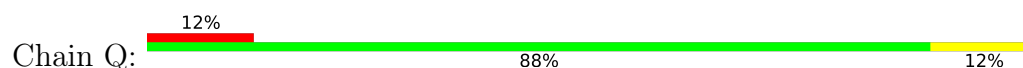




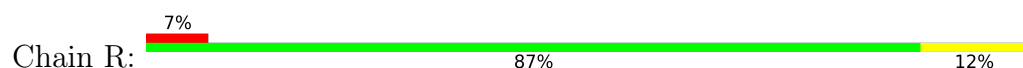
• Molecule 1: Flagellin

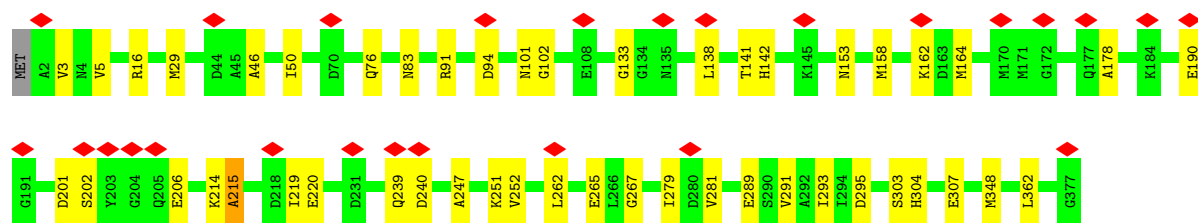


• Molecule 1: Flagellin

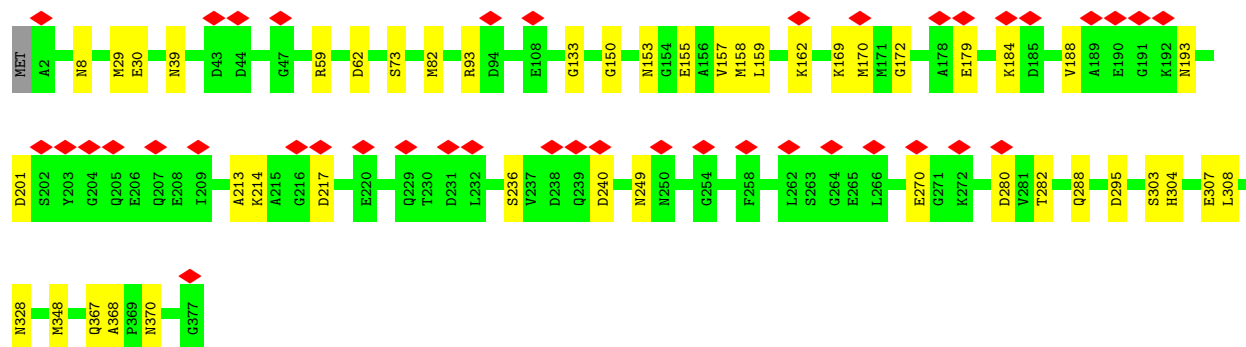
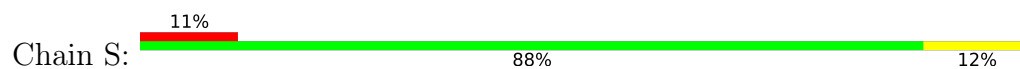


• Molecule 1: Flagellin

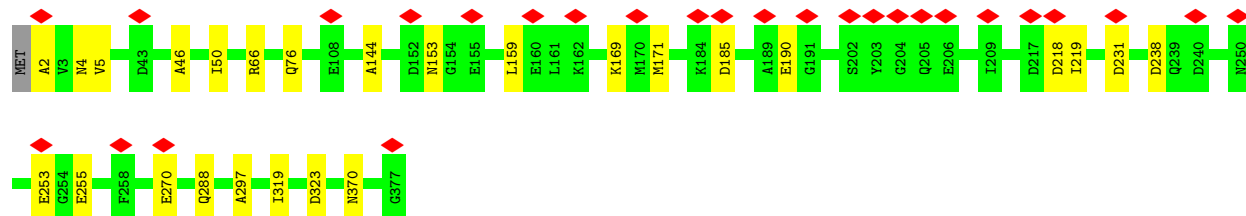
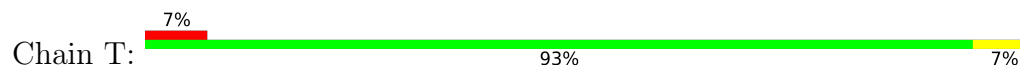




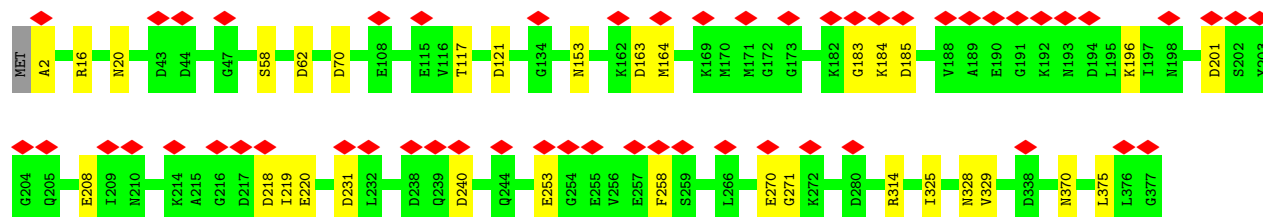
• Molecule 1: Flagellin



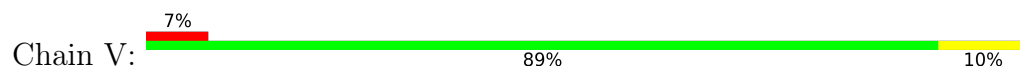
• Molecule 1: Flagellin

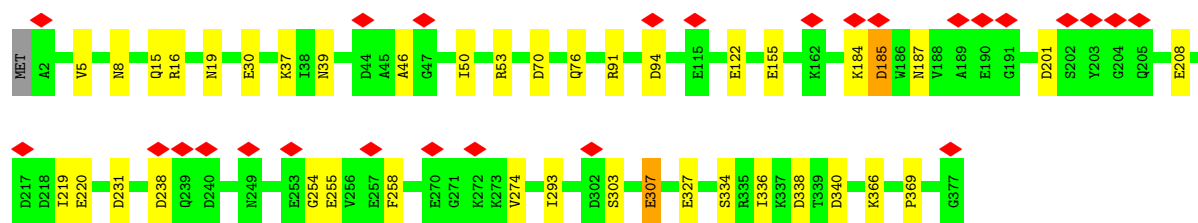


• Molecule 1: Flagellin

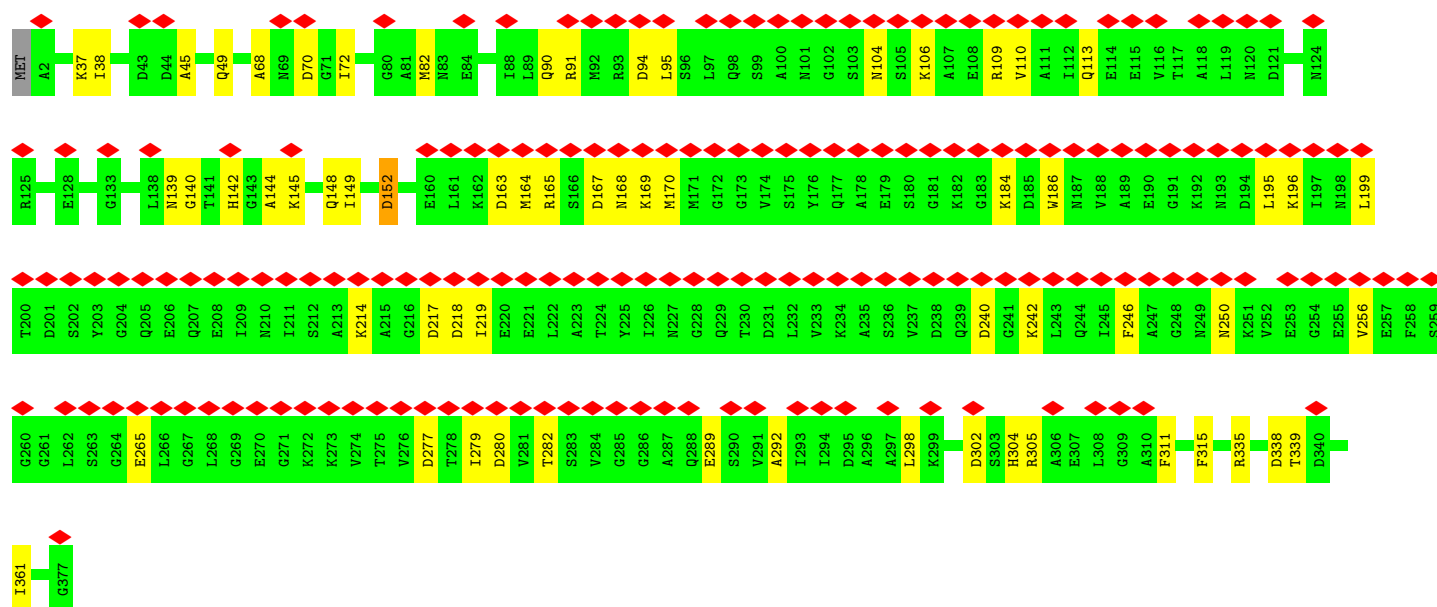
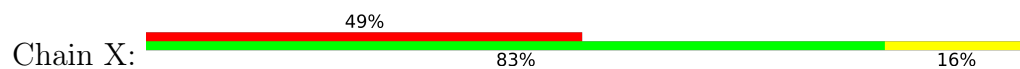


• Molecule 1: Flagellin

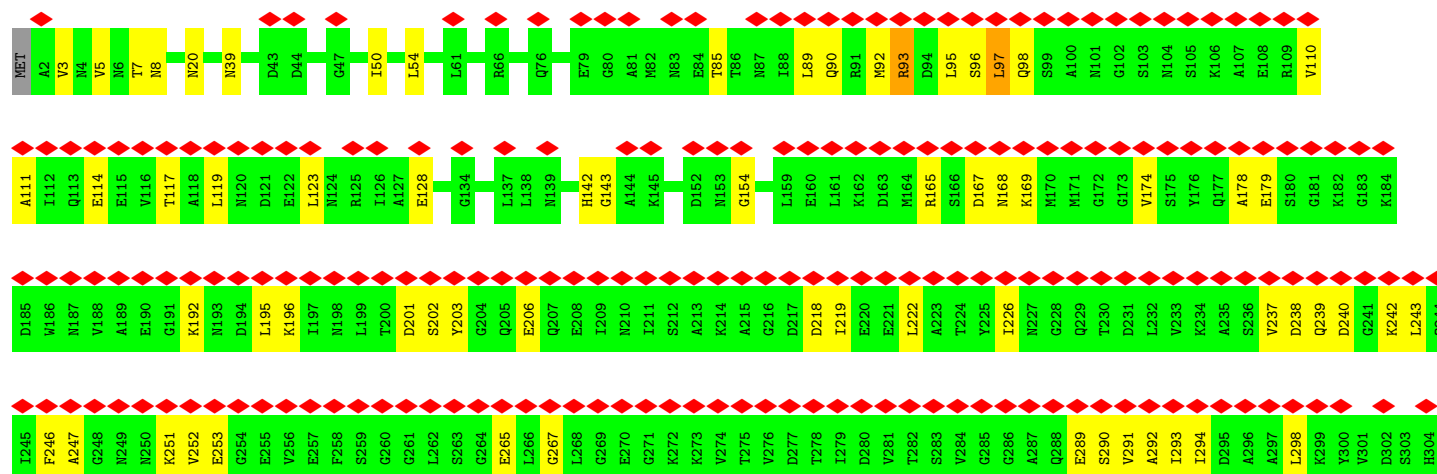
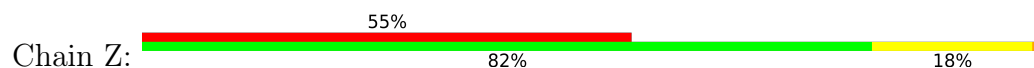


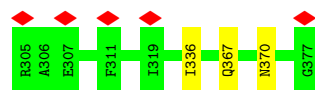


• Molecule 1: Flagellin

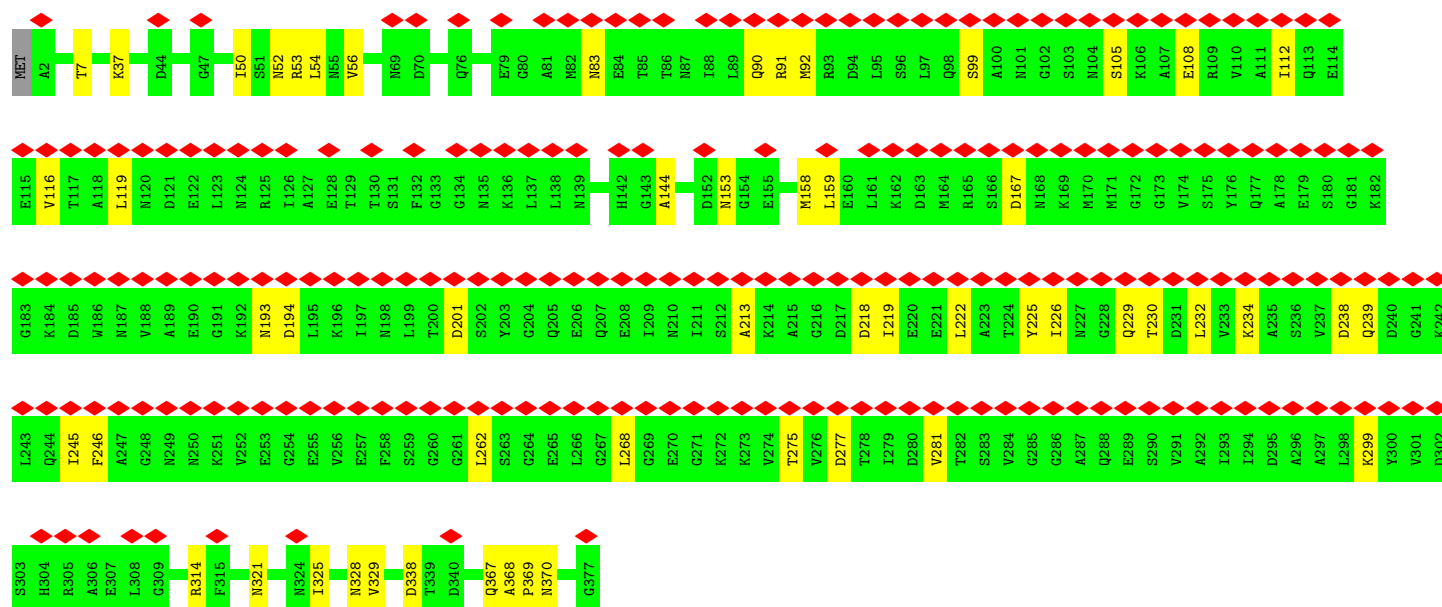
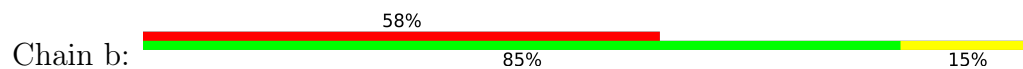


• Molecule 1: Flagellin

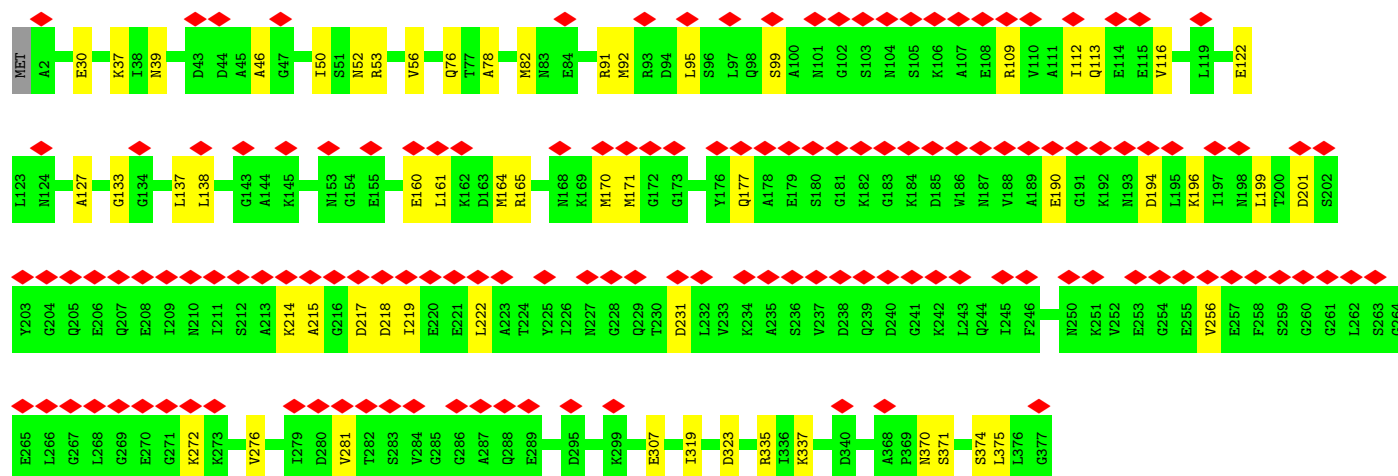
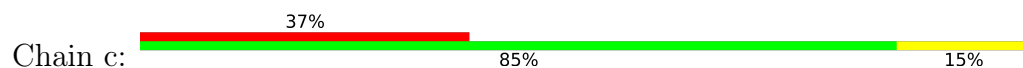




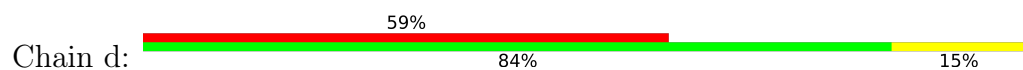
• Molecule 1: Flagellin



• Molecule 1: Flagellin

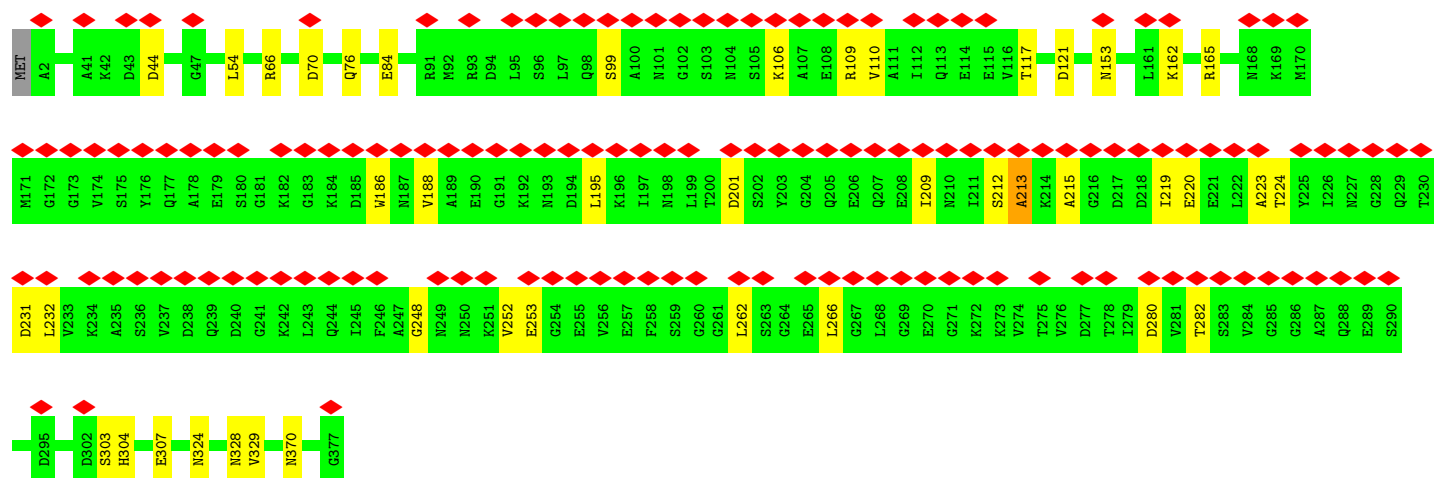
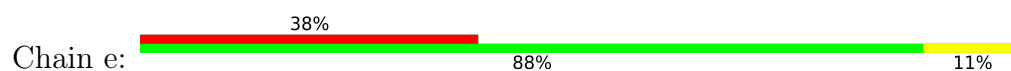


• Molecule 1: Flagellin

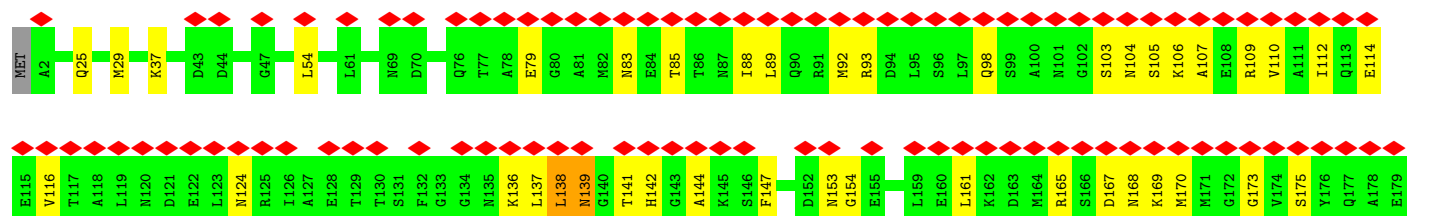
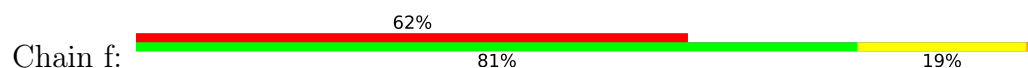


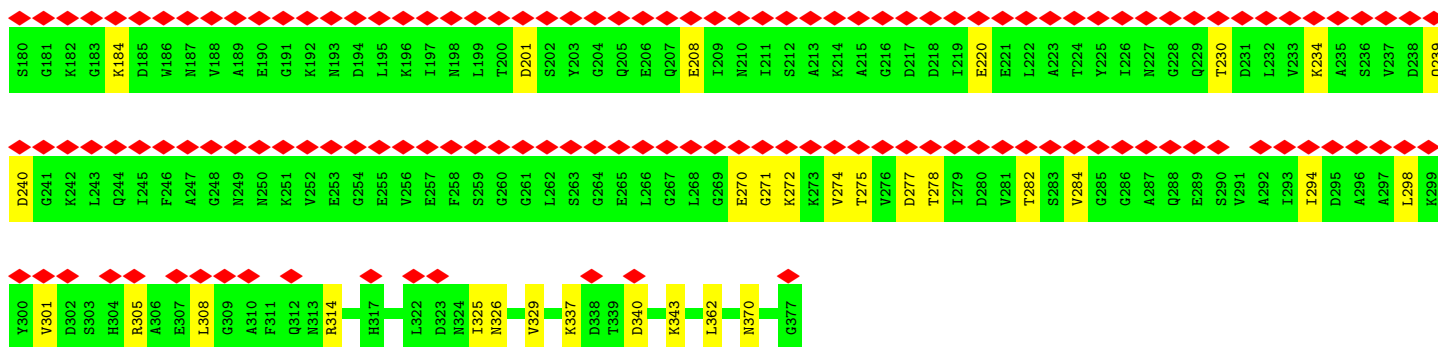


• Molecule 1: Flagellin

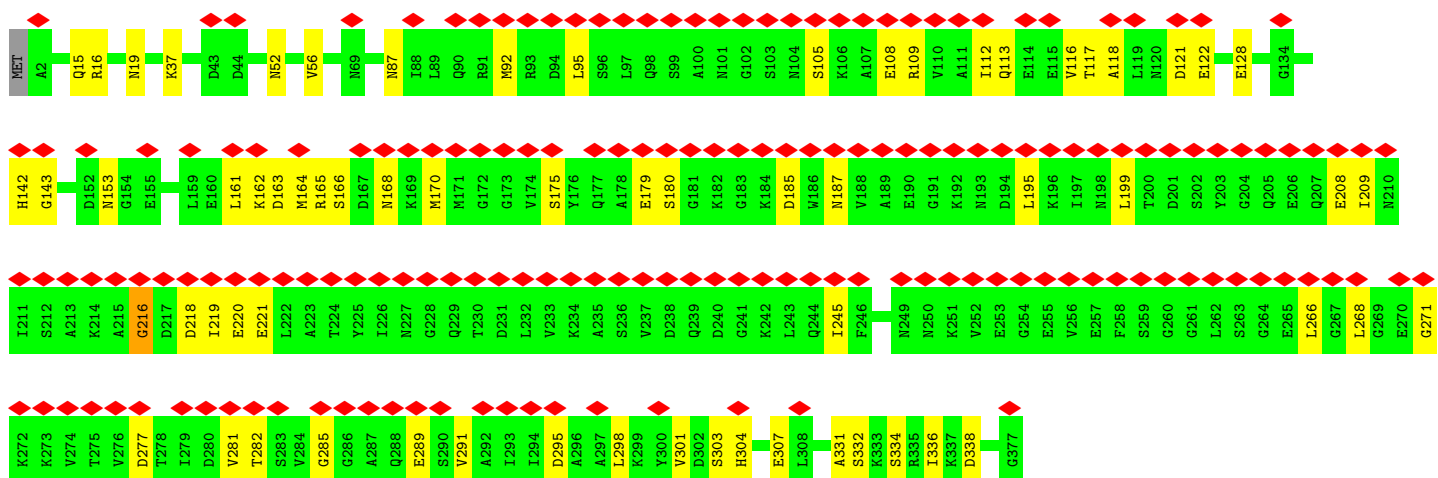
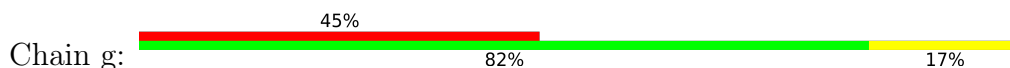


• Molecule 1: Flagellin

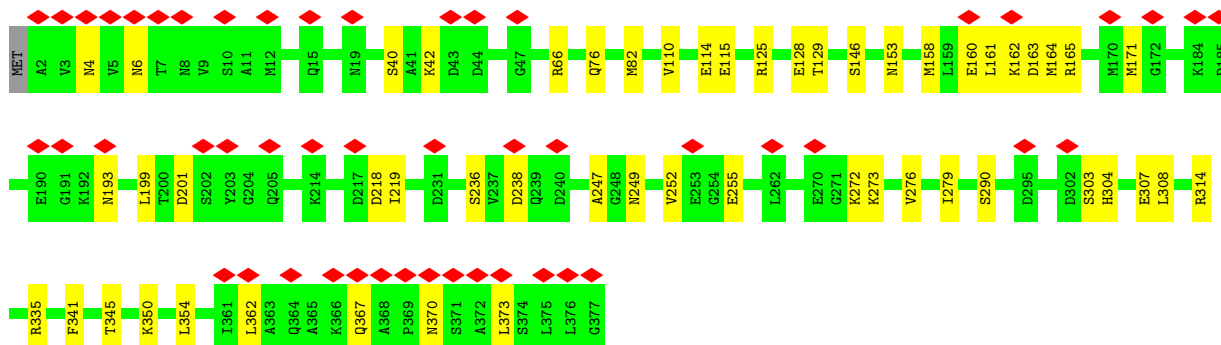
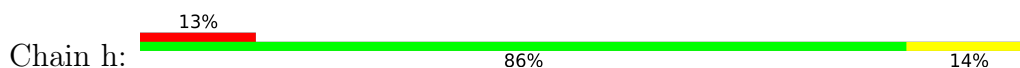




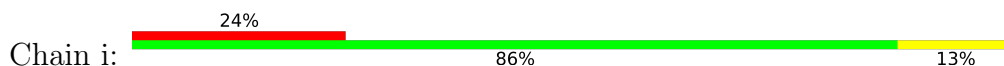
• Molecule 1: Flagellin

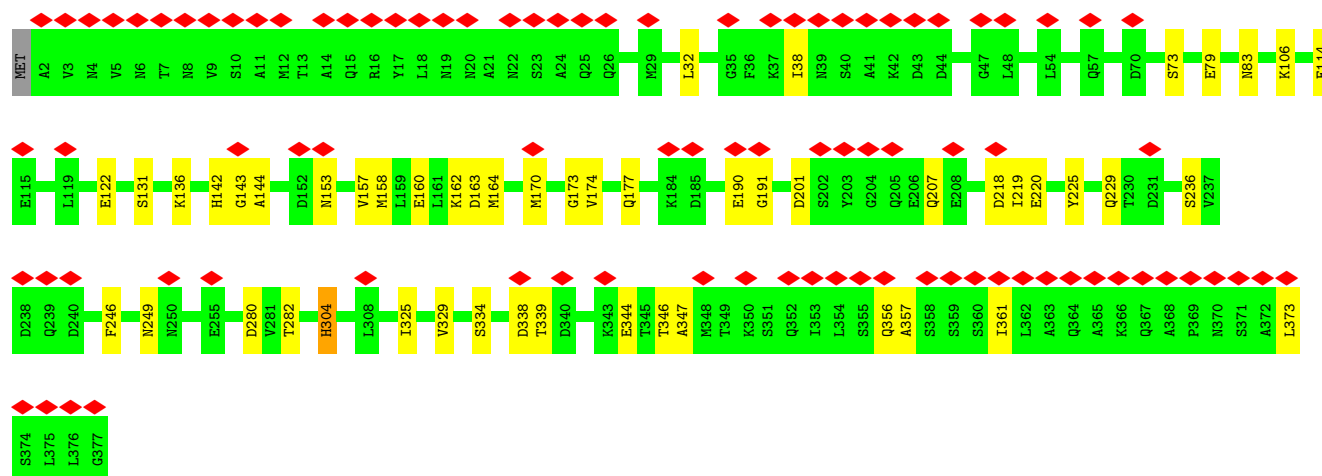


• Molecule 1: Flagellin

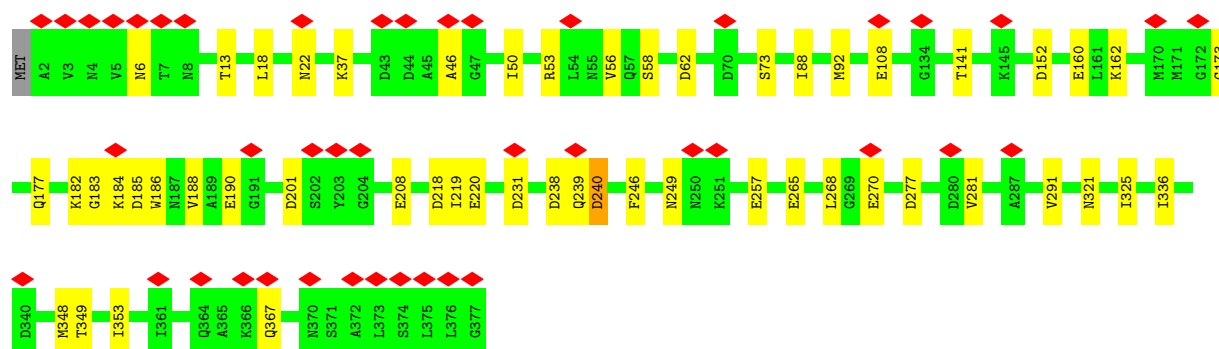
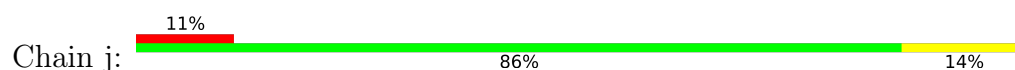


• Molecule 1: Flagellin

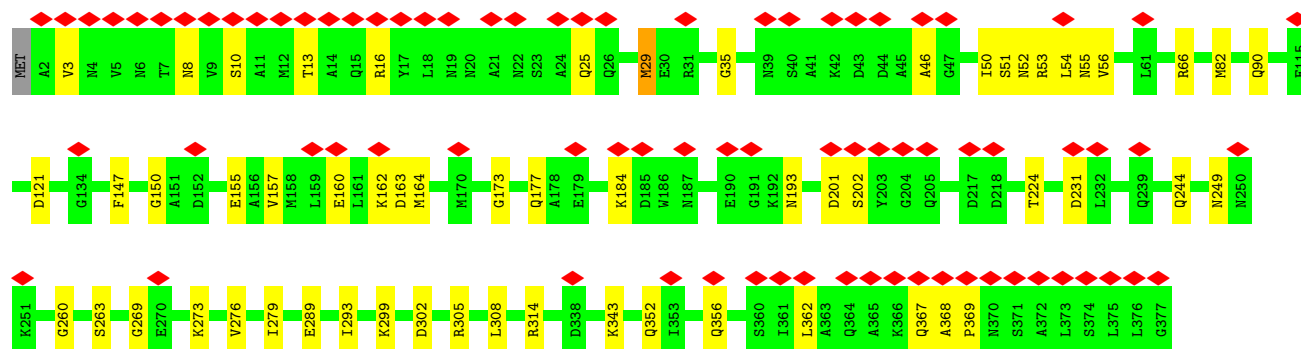
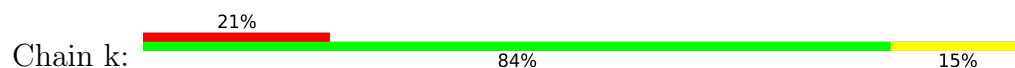




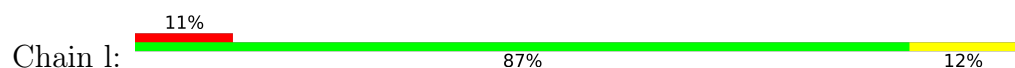
• Molecule 1: Flagellin

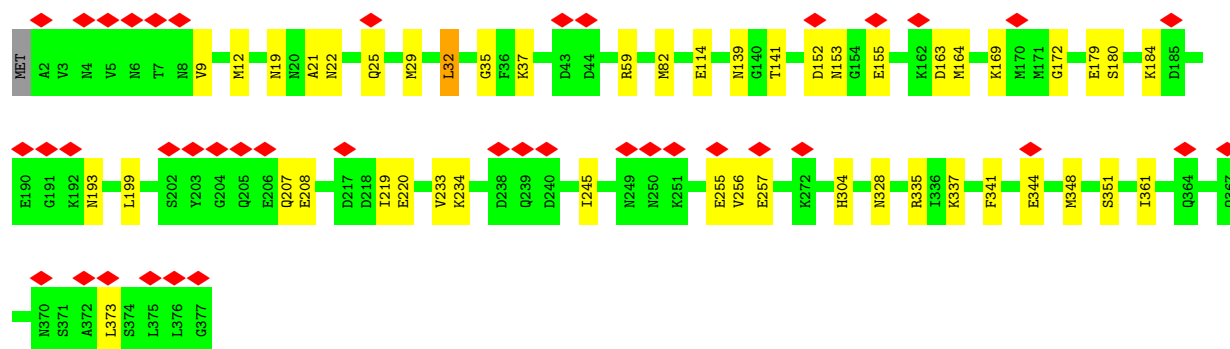


• Molecule 1: Flagellin

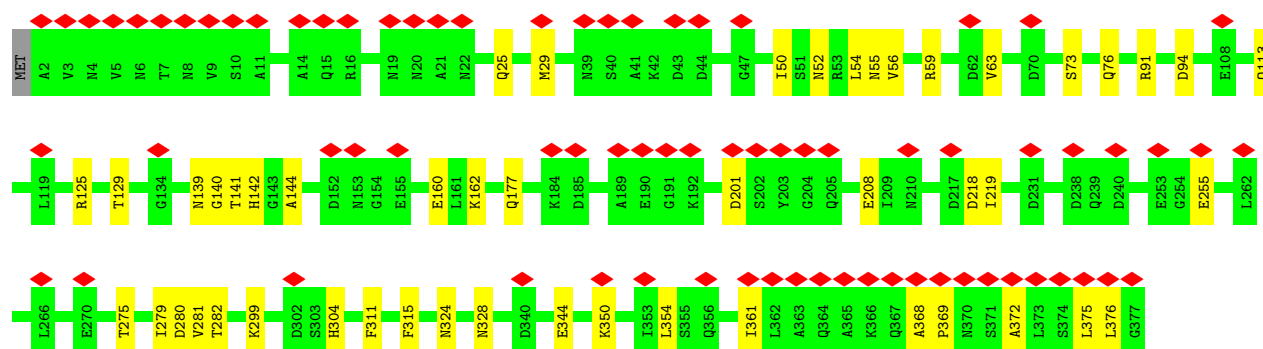
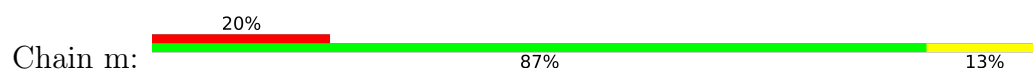


• Molecule 1: Flagellin

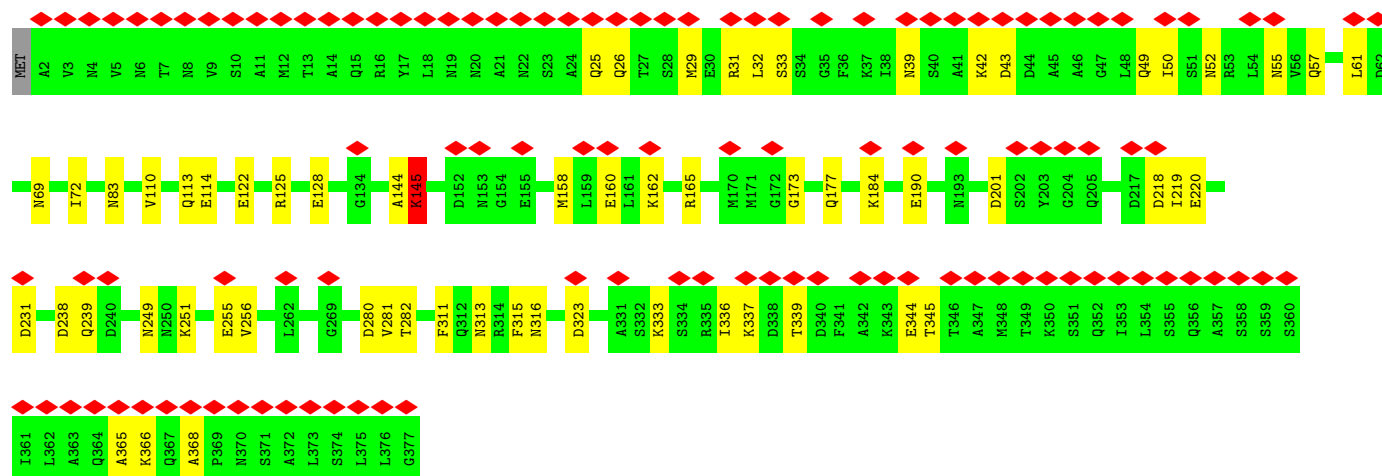
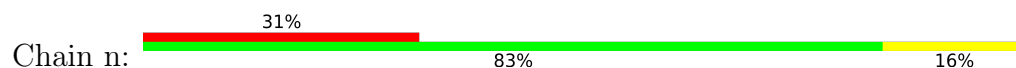




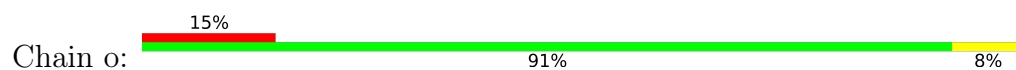
• Molecule 1: Flagellin

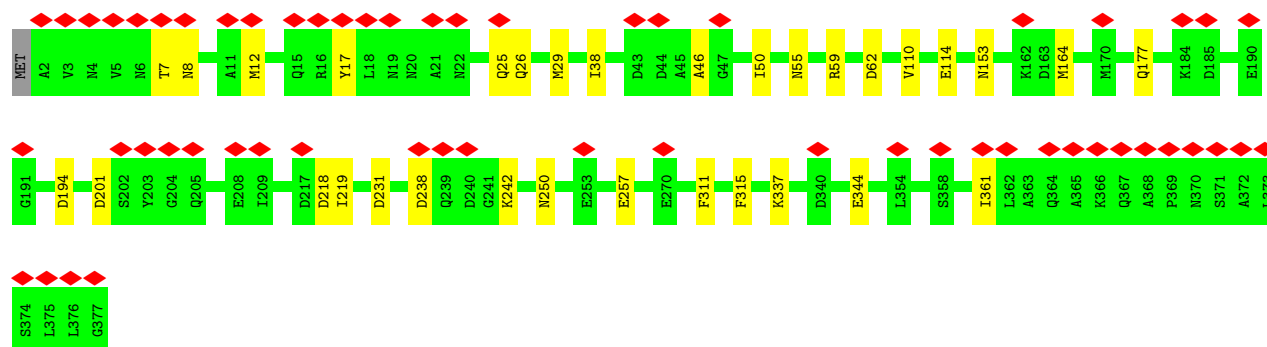


• Molecule 1: Flagellin

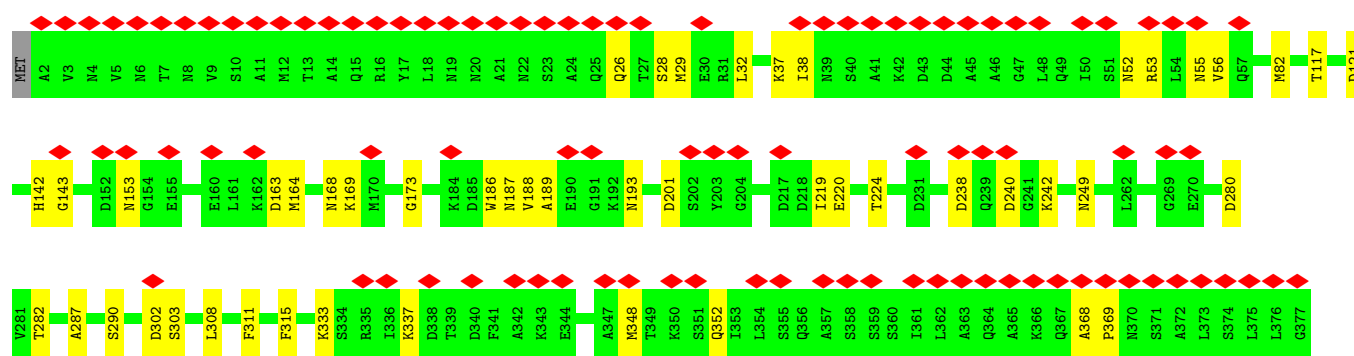
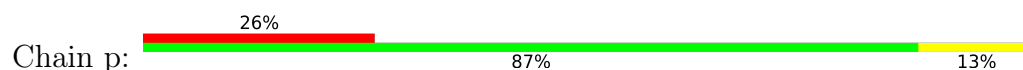


• Molecule 1: Flagellin

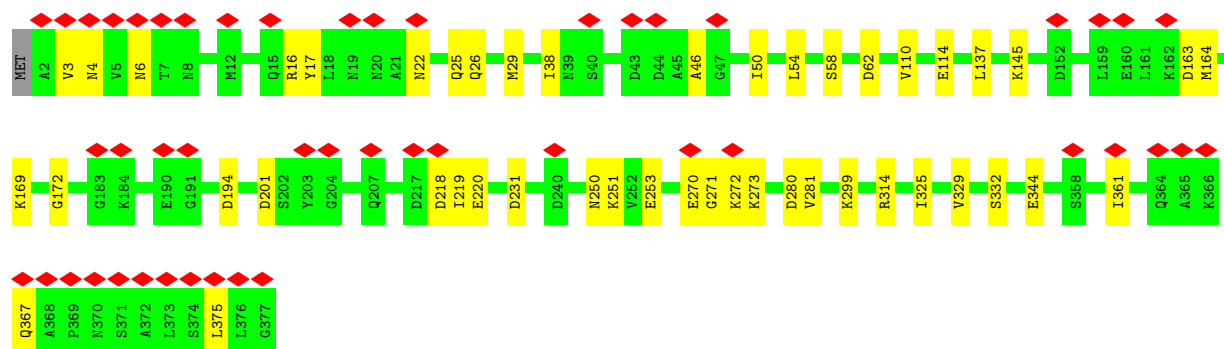
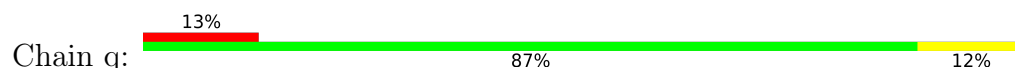




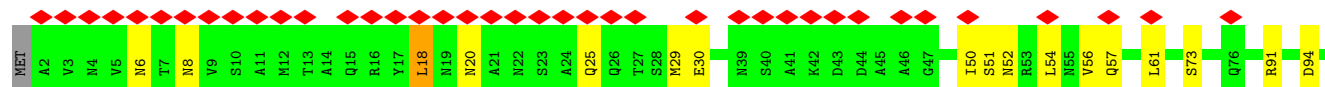
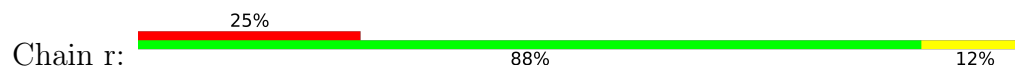
• Molecule 1: Flagellin

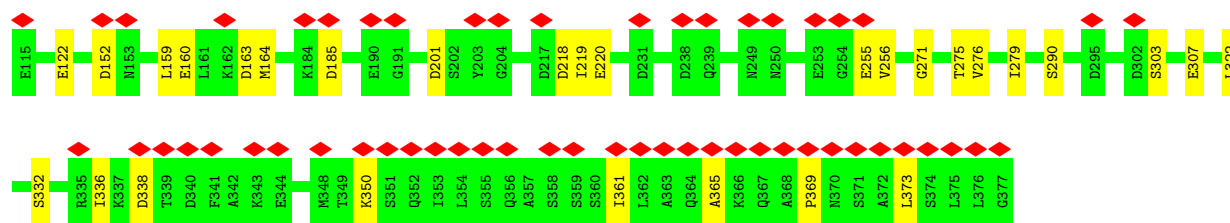


• Molecule 1: Flagellin

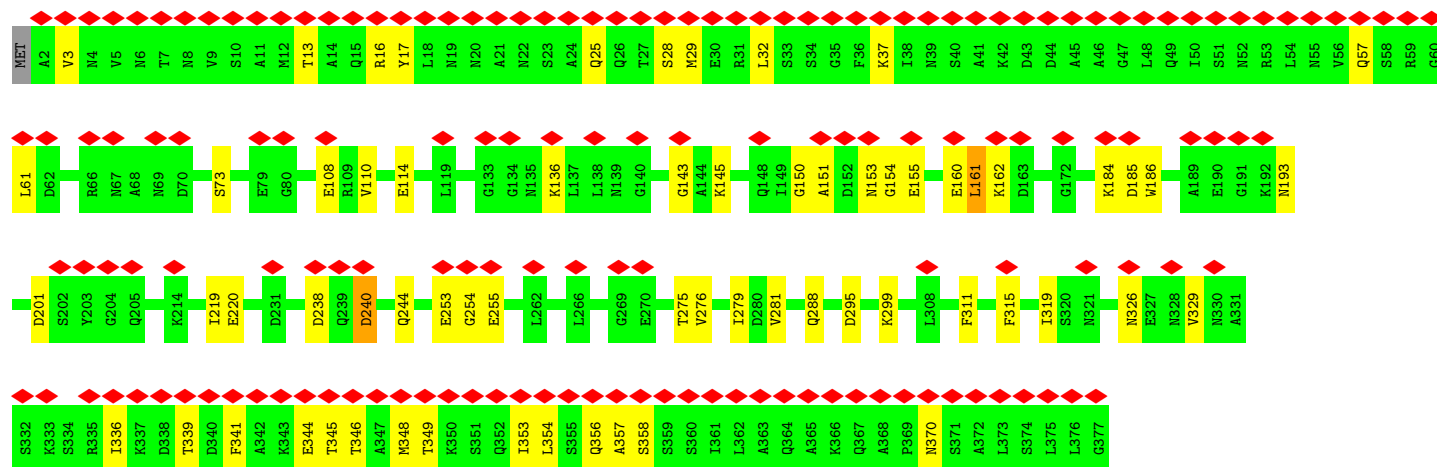
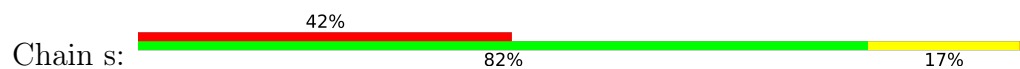


• Molecule 1: Flagellin

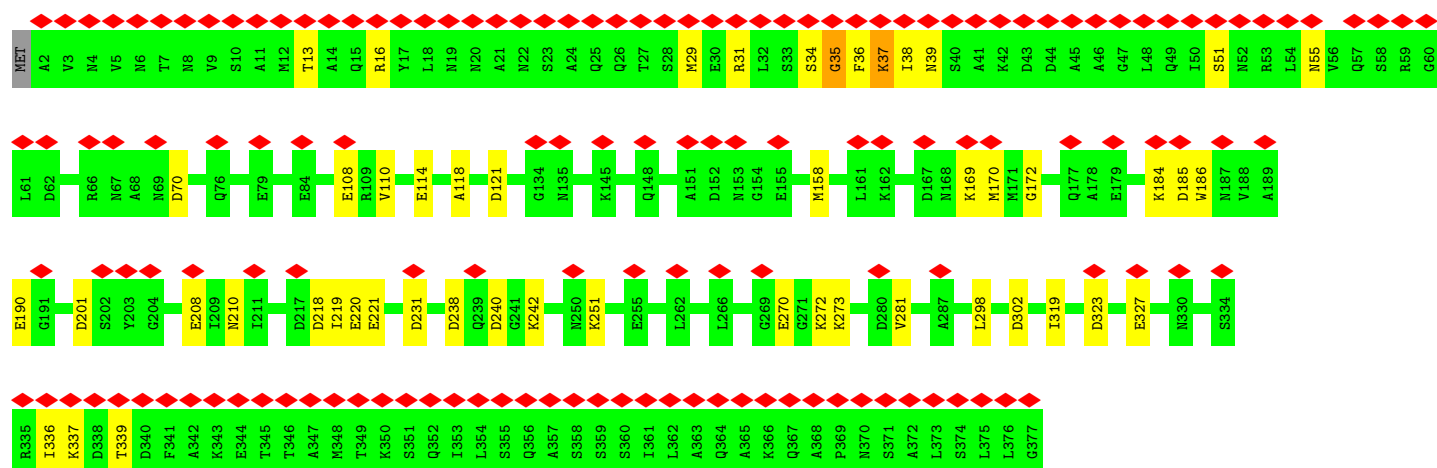
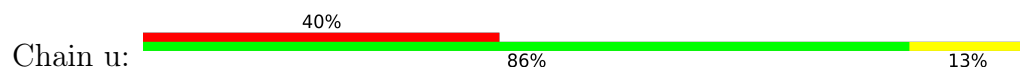




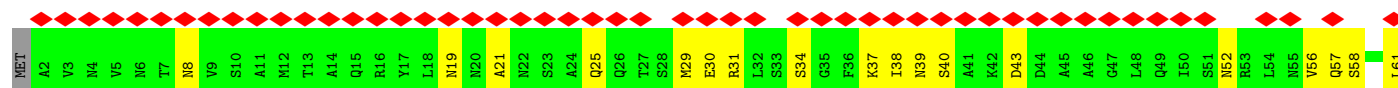
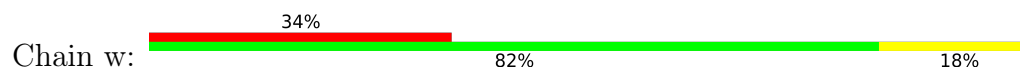
• Molecule 1: Flagellin

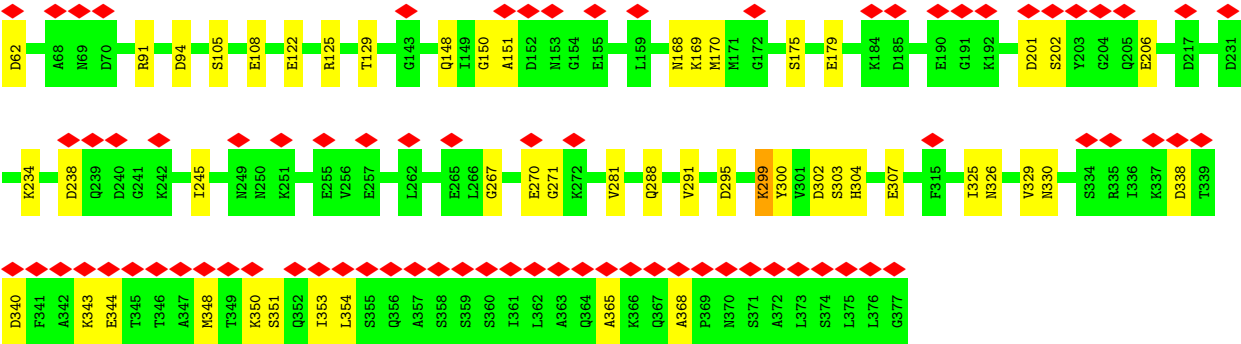


• Molecule 1: Flagellin



• Molecule 1: Flagellin





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	439378	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.080	Depositor
Minimum map value	-0.712	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	550.0, 550.0, 550.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/2816	0.48	0/3790
1	B	0.32	0/2816	0.53	1/3790 (0.0%)
1	C	0.29	0/2816	0.52	1/3790 (0.0%)
1	D	0.25	0/2816	0.49	0/3790
1	E	0.30	0/2816	0.50	0/3790
1	F	0.31	0/2816	0.52	0/3790
1	G	0.31	0/2816	0.51	1/3790 (0.0%)
1	H	0.25	0/2816	0.49	0/3790
1	I	0.25	0/2816	0.49	0/3790
1	J	0.28	0/2816	0.49	0/3790
1	K	0.26	0/2816	0.51	0/3790
1	L	0.29	0/2816	0.51	0/3790
1	M	0.24	0/2816	0.48	0/3790
1	N	0.27	0/2816	0.51	0/3790
1	O	0.31	0/2816	0.53	0/3790
1	P	0.27	0/2816	0.52	0/3790
1	Q	0.34	0/2816	0.51	0/3790
1	R	0.29	0/2816	0.54	0/3790
1	S	0.25	0/2816	0.49	0/3790
1	T	0.30	0/2816	0.52	0/3790
1	U	0.28	0/2816	0.51	1/3790 (0.0%)
1	V	0.26	0/2816	0.51	1/3790 (0.0%)
1	X	0.30	0/2816	0.56	1/3790 (0.0%)
1	Z	0.28	0/2816	0.52	0/3790
1	b	0.26	0/2816	0.51	0/3790
1	c	0.25	0/2816	0.50	0/3790
1	d	0.22	0/2816	0.47	0/3790
1	e	0.32	1/2816 (0.0%)	0.58	0/3790
1	f	0.24	0/2816	0.50	1/3790 (0.0%)
1	g	0.27	0/2816	0.54	2/3790 (0.1%)
1	h	0.27	1/2816 (0.0%)	0.49	0/3790
1	i	0.24	0/2816	0.51	0/3790
1	j	0.32	0/2816	0.54	0/3790
1	k	0.28	0/2816	0.50	0/3790

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	l	0.27	0/2816	0.51	0/3790
1	m	0.31	0/2816	0.51	0/3790
1	n	0.27	0/2816	0.53	0/3790
1	o	0.25	0/2816	0.50	0/3790
1	p	0.28	0/2816	0.51	1/3790 (0.0%)
1	q	0.30	0/2816	0.52	1/3790 (0.0%)
1	r	0.24	0/2816	0.50	2/3790 (0.1%)
1	s	0.23	0/2816	0.49	0/3790
1	u	0.26	0/2816	0.50	2/3790 (0.1%)
1	w	0.30	0/2816	0.53	0/3790
All	All	0.28	2/123904 (0.0%)	0.51	15/166760 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	h	247	ALA	C-N	-5.89	1.29	1.33
1	e	248	GLY	CA-C	-5.52	1.48	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	GLY	N-CA-C	-7.56	100.51	112.61
1	u	35	GLY	N-CA-C	-6.30	107.22	115.47
1	u	37	LYS	N-CA-C	-6.17	105.01	112.54
1	r	185	ASP	N-CA-C	-5.99	106.95	114.56
1	U	185	ASP	N-CA-C	-5.99	106.61	114.04
1	f	139	ASN	N-CA-C	-5.88	106.34	112.93
1	B	146	SER	N-CA-C	5.87	119.04	109.24
1	q	137	LEU	N-CA-C	5.79	120.85	113.55
1	g	185	ASP	N-CA-C	-5.75	107.25	114.56
1	X	152	ASP	N-CA-C	5.61	116.67	108.14
1	r	271	GLY	N-CA-C	5.59	117.90	111.36
1	g	216	GLY	N-CA-C	-5.54	105.39	113.48
1	V	185	ASP	N-CA-C	-5.31	106.69	114.39
1	p	186	TRP	N-CA-C	-5.29	100.69	108.79
1	G	251	LYS	N-CA-C	-5.00	108.21	114.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2798	2746	2745	24	0
1	B	2798	2746	2745	31	0
1	C	2798	2746	2745	23	0
1	D	2798	2746	2745	24	0
1	E	2798	2746	2745	43	0
1	F	2798	2746	2745	34	0
1	G	2798	2746	2745	39	0
1	H	2798	2746	2745	28	0
1	I	2798	2746	2745	21	0
1	J	2798	2746	2745	20	0
1	K	2798	2746	2745	36	0
1	L	2798	2746	2745	32	0
1	M	2798	2746	2745	33	0
1	N	2798	2746	2745	33	0
1	O	2798	2746	2745	52	0
1	P	2798	2746	2745	46	0
1	Q	2798	2746	2745	33	0
1	R	2798	2746	2745	37	0
1	S	2798	2746	2745	37	0
1	T	2798	2746	2745	25	0
1	U	2798	2746	2745	23	0
1	V	2798	2746	2745	31	0
1	X	2798	2746	2745	48	0
1	Z	2798	2746	2745	47	0
1	b	2798	2746	2745	46	0
1	c	2798	2746	2745	40	0
1	d	2798	2746	2745	50	0
1	e	2798	2746	2745	31	0
1	f	2798	2746	2745	51	0
1	g	2798	2746	2745	48	0
1	h	2798	2746	2745	43	0
1	i	2798	2746	2745	47	0
1	j	2798	2746	2745	47	0
1	k	2798	2746	2745	42	0
1	l	2798	2746	2745	41	0
1	m	2798	2746	2745	37	0
1	n	2798	2746	2745	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	o	2798	2746	2745	27	0
1	p	2798	2746	2745	31	0
1	q	2798	2746	2745	30	0
1	r	2798	2746	2745	36	0
1	s	2798	2746	2745	60	0
1	u	2798	2746	2745	42	0
1	w	2798	2746	2745	54	0
All	All	123112	120824	120780	1528	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 6.

All (1528) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:15:GLN:O	1:V:19:ASN:ND2	2.08	0.87
1:w:40:SER:OG	1:w:43:ASP:OD1	1.91	0.86
1:X:338:ASP:OD1	1:X:339:THR:N	2.08	0.86
1:h:218:ASP:OD1	1:h:219:ILE:N	2.10	0.85
1:C:205:GLN:OE1	1:C:205:GLN:N	2.10	0.85
1:C:253:GLU:OE1	1:C:253:GLU:N	2.11	0.84
1:U:196:LYS:NZ	1:U:208:GLU:OE2	2.09	0.84
1:j:108:GLU:N	1:j:108:GLU:OE1	2.10	0.84
1:q:253:GLU:OE1	1:q:253:GLU:N	2.10	0.84
1:w:326:ASN:OD1	1:w:330:ASN:ND2	2.12	0.83
1:o:257:GLU:N	1:o:257:GLU:OE2	2.13	0.82
1:f:314:ARG:NE	1:g:122:GLU:OE1	2.13	0.82
1:i:177:GLN:N	1:i:177:GLN:OE1	2.13	0.81
1:c:92:MET:HE3	1:c:116:VAL:HG13	1.63	0.81
1:m:218:ASP:OD1	1:m:219:ILE:N	2.14	0.81
1:A:218:ASP:OD1	1:A:219:ILE:N	2.13	0.81
1:o:218:ASP:OD1	1:o:219:ILE:N	2.14	0.81
1:P:179:GLU:OE1	1:P:179:GLU:N	2.14	0.80
1:K:295:ASP:OD1	1:K:299:LYS:NZ	2.15	0.80
1:h:255:GLU:N	1:h:255:GLU:OE2	2.15	0.80
1:b:90:GLN:OE1	1:b:91:ARG:N	2.15	0.80
1:V:307:GLU:OE2	1:V:307:GLU:N	2.15	0.79
1:w:179:GLU:OE1	1:w:179:GLU:N	2.16	0.79
1:L:177:GLN:N	1:L:177:GLN:OE1	2.16	0.78
1:w:201:ASP:OD1	1:w:202:SER:N	2.17	0.78
1:R:247:ALA:HB1	1:R:252:VAL:HG21	1.62	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:352:GLN:O	1:k:356:GLN:NE2	2.17	0.78
1:B:236:SER:OG	1:M:153:ASN:OD1	2.02	0.78
1:R:206:GLU:OE2	1:R:206:GLU:N	2.16	0.78
1:h:367:GLN:O	1:h:370:ASN:ND2	2.17	0.77
1:f:168:ASN:OD1	1:f:169:LYS:N	2.18	0.77
1:w:295:ASP:OD1	1:w:299:LYS:NZ	2.18	0.77
1:n:339:THR:OG1	1:n:344:GLU:OE1	2.01	0.77
1:s:255:GLU:OE2	1:s:255:GLU:N	2.18	0.77
1:O:160:GLU:N	1:O:160:GLU:OE1	2.17	0.76
1:D:154:GLY:O	1:k:224:THR:OG1	2.03	0.76
1:l:184:LYS:HE3	1:l:184:LYS:HA	1.68	0.76
1:m:55:ASN:OD1	1:m:56:VAL:N	2.19	0.76
1:N:253:GLU:N	1:N:253:GLU:OE1	2.19	0.76
1:B:153:ASN:OD1	1:i:236:SER:OG	2.03	0.76
1:f:208:GLU:OE1	1:f:208:GLU:N	2.19	0.75
1:Q:144:ALA:HB2	1:Q:160:GLU:OE1	1.87	0.75
1:R:190:GLU:N	1:R:190:GLU:OE1	2.19	0.75
1:c:127:ALA:HB2	1:c:164:MET:CE	2.16	0.75
1:f:340:ASP:OD1	1:f:343:LYS:NZ	2.19	0.75
1:J:170:MET:HE3	1:J:170:MET:HA	1.69	0.75
1:P:307:GLU:OE1	1:P:307:GLU:N	2.19	0.74
1:Z:97:LEU:HD23	1:Z:98:GLN:N	2.03	0.74
1:P:328:ASN:OD1	1:Q:76:GLN:NE2	2.21	0.74
1:L:218:ASP:OD1	1:L:219:ILE:N	2.22	0.73
1:e:307:GLU:N	1:e:307:GLU:OE1	2.20	0.73
1:U:253:GLU:N	1:U:253:GLU:OE1	2.21	0.73
1:b:325:ILE:O	1:b:329:VAL:HG23	1.89	0.73
1:d:168:ASN:OD1	1:d:169:LYS:N	2.22	0.73
1:C:101:ASN:OD1	1:C:102:GLY:N	2.21	0.72
1:b:238:ASP:OD1	1:b:239:GLN:NE2	2.22	0.72
1:d:328:ASN:OD1	1:e:76:GLN:NE2	2.22	0.72
1:w:25:GLN:N	1:w:25:GLN:OE1	2.23	0.72
1:j:190:GLU:N	1:j:190:GLU:OE2	2.22	0.72
1:Q:326:ASN:O	1:Q:330:ASN:ND2	2.22	0.72
1:X:218:ASP:OD1	1:X:219:ILE:N	2.22	0.72
1:p:168:ASN:OD1	1:p:169:LYS:N	2.23	0.72
1:q:250:ASN:OD1	1:q:299:LYS:NZ	2.23	0.72
1:h:307:GLU:N	1:h:307:GLU:OE2	2.21	0.72
1:B:153:ASN:OD1	1:B:154:GLY:N	2.23	0.71
1:b:275:THR:OG1	1:b:277:ASP:OD1	2.07	0.71
1:F:170:MET:HE2	1:F:170:MET:HA	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ASN:ND2	1:l:35:GLY:O	2.24	0.71
1:n:239:GLN:OE1	1:n:239:GLN:N	2.23	0.71
1:Z:253:GLU:OE2	1:Z:253:GLU:N	2.24	0.70
1:c:370:ASN:ND2	1:c:370:ASN:O	2.25	0.70
1:u:270:GLU:OE1	1:u:270:GLU:N	2.23	0.70
1:I:206:GLU:N	1:I:206:GLU:OE2	2.25	0.70
1:G:327:GLU:OE1	1:R:16:ARG:NH2	2.25	0.69
1:g:105:SER:OG	1:g:108:GLU:OE1	2.06	0.69
1:j:257:GLU:OE1	1:j:257:GLU:N	2.26	0.69
1:N:272:LYS:HE2	1:N:272:LYS:HA	1.72	0.69
1:R:307:GLU:OE2	1:R:307:GLU:N	2.23	0.68
1:P:303:SER:O	1:P:307:GLU:OE1	2.12	0.68
1:S:158:MET:SD	1:S:159:LEU:N	2.67	0.68
1:E:101:ASN:O	1:E:109:ARG:NH2	2.27	0.68
1:C:286:GLY:O	1:C:290:SER:OG	2.12	0.68
1:s:114:GLU:N	1:s:114:GLU:OE2	2.26	0.67
1:P:108:GLU:OE1	1:P:108:GLU:N	2.24	0.66
1:e:303:SER:O	1:e:307:GLU:OE1	2.11	0.66
1:H:82:MET:HE1	1:H:308:LEU:CD1	2.26	0.66
1:P:299:LYS:HA	1:P:299:LYS:HE3	1.77	0.66
1:K:53:ARG:NH2	1:s:108:GLU:OE2	2.28	0.66
1:Z:97:LEU:HD23	1:Z:97:LEU:C	2.21	0.66
1:w:288:GLN:O	1:w:291:VAL:HG12	1.95	0.66
1:I:218:ASP:OD1	1:I:219:ILE:N	2.29	0.66
1:L:153:ASN:OD1	1:L:154:GLY:N	2.28	0.66
1:m:50:ILE:O	1:m:54:LEU:HD22	1.95	0.66
1:r:50:ILE:O	1:r:54:LEU:HD13	1.96	0.66
1:T:270:GLU:N	1:T:270:GLU:OE2	2.28	0.65
1:X:82:MET:HE1	1:X:304:HIS:HB3	1.77	0.65
1:u:190:GLU:OE2	1:u:190:GLU:N	2.29	0.65
1:d:30:GLU:OE1	1:d:39:ASN:ND2	2.29	0.65
1:o:177:GLN:N	1:o:177:GLN:OE1	2.30	0.65
1:T:218:ASP:OD1	1:T:219:ILE:N	2.30	0.65
1:U:328:ASN:OD1	1:V:76:GLN:NE2	2.30	0.65
1:f:239:GLN:NE2	1:f:240:ASP:OD2	2.29	0.65
1:k:244:GLN:NE2	1:k:289:GLU:OE1	2.29	0.65
1:E:180:SER:OG	1:E:266:LEU:O	2.13	0.65
1:b:144:ALA:HB1	1:b:158:MET:SD	2.36	0.65
1:p:52:ASN:O	1:p:55:ASN:OD1	2.14	0.65
1:s:28:SER:O	1:s:32:LEU:HD13	1.97	0.65
1:V:255:GLU:OE1	1:V:255:GLU:N	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:49:GLN:OE1	1:X:49:GLN:N	2.29	0.64
1:Z:367:GLN:O	1:Z:370:ASN:ND2	2.30	0.64
1:D:170:MET:HE2	1:D:170:MET:HA	1.80	0.64
1:N:170:MET:HE2	1:N:170:MET:HA	1.80	0.64
1:u:38:ILE:HD13	1:u:337:LYS:HA	1.79	0.64
1:X:163:ASP:OD1	1:X:164:MET:N	2.30	0.64
1:X:91:ARG:O	1:X:94:ASP:OD2	2.15	0.64
1:X:149:ILE:HD11	1:X:315:PHE:CE2	2.32	0.64
1:k:164:MET:HE3	1:k:164:MET:O	1.97	0.64
1:O:105:SER:OG	1:O:108:GLU:OE1	2.14	0.64
1:G:110:VAL:O	1:G:114:GLU:OE1	2.15	0.63
1:A:53:ARG:NH1	1:B:133:GLY:O	2.32	0.63
1:E:218:ASP:OD1	1:E:219:ILE:N	2.31	0.63
1:F:218:ASP:OD1	1:F:219:ILE:N	2.30	0.63
1:w:37:LYS:NZ	1:w:338:ASP:O	2.27	0.63
1:E:201:ASP:OD1	1:E:202:SER:N	2.32	0.63
1:c:30:GLU:OE1	1:c:39:ASN:ND2	2.32	0.63
1:Q:82:MET:HE1	1:Q:304:HIS:CD2	2.34	0.63
1:b:50:ILE:O	1:b:54:LEU:HD23	1.98	0.63
1:s:295:ASP:OD1	1:s:299:LYS:NZ	2.31	0.63
1:M:53:ARG:NH2	1:j:108:GLU:OE2	2.31	0.62
1:Z:218:ASP:OD2	1:Z:219:ILE:N	2.31	0.62
1:Z:168:ASN:OD1	1:Z:169:LYS:N	2.32	0.62
1:g:168:ASN:OD1	1:g:170:MET:N	2.32	0.62
1:s:110:VAL:O	1:s:114:GLU:OE2	2.18	0.62
1:g:92:MET:HE1	1:g:116:VAL:HG22	1.81	0.62
1:O:281:VAL:O	1:O:281:VAL:HG12	1.99	0.62
1:i:325:ILE:O	1:i:329:VAL:HG23	2.00	0.62
1:g:92:MET:HE3	1:g:92:MET:HA	1.82	0.62
1:k:53:ARG:O	1:k:56:VAL:HG22	2.00	0.62
1:F:328:ASN:OD1	1:G:76:GLN:NE2	2.33	0.61
1:X:196:LYS:HB3	1:X:196:LYS:HZ3	1.64	0.61
1:M:253:GLU:OE1	1:M:253:GLU:O	2.16	0.61
1:l:139:ASN:OD1	1:l:141:THR:OG1	2.12	0.61
1:m:299:LYS:O	1:m:299:LYS:HD3	2.00	0.61
1:E:37:LYS:O	1:E:37:LYS:HD3	2.00	0.61
1:V:8:ASN:OD1	1:V:8:ASN:O	2.18	0.61
1:L:105:SER:OG	1:L:108:GLU:OE1	2.16	0.61
1:T:253:GLU:OE1	1:T:253:GLU:O	2.19	0.61
1:k:314:ARG:NE	1:w:122:GLU:OE1	2.28	0.61
1:q:325:ILE:O	1:q:329:VAL:HG23	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:O	1:B:62:ASP:OD1	2.19	0.61
1:M:257:GLU:N	1:M:257:GLU:OE2	2.34	0.61
1:S:29:MET:HG3	1:S:348:MET:HE3	1.83	0.60
1:V:46:ALA:O	1:V:50:ILE:HG13	2.01	0.60
1:b:238:ASP:OD1	1:b:239:GLN:N	2.34	0.60
1:S:59:ARG:O	1:S:62:ASP:OD2	2.19	0.60
1:K:367:GLN:N	1:K:367:GLN:OE1	2.33	0.60
1:O:46:ALA:O	1:O:50:ILE:HG13	2.01	0.60
1:A:353:ILE:HG23	1:M:373:LEU:HD13	1.84	0.60
1:Q:46:ALA:O	1:Q:50:ILE:HG13	2.00	0.60
1:R:101:ASN:OD1	1:R:102:GLY:N	2.34	0.60
1:h:163:ASP:OD1	1:h:164:MET:N	2.34	0.60
1:Z:92:MET:HE1	1:Z:119:LEU:CB	2.32	0.60
1:k:201:ASP:OD1	1:k:202:SER:N	2.34	0.59
1:e:212:SER:O	1:e:213:ALA:HB2	2.01	0.59
1:o:59:ARG:O	1:o:62:ASP:OD1	2.20	0.59
1:f:370:ASN:O	1:f:370:ASN:ND2	2.35	0.59
1:A:129:THR:HG23	1:V:155:GLU:OE2	2.02	0.59
1:M:270:GLU:OE2	1:M:270:GLU:N	2.31	0.59
1:Z:92:MET:HE1	1:Z:119:LEU:HB2	1.85	0.59
1:w:31:ARG:NH2	1:w:37:LYS:O	2.36	0.59
1:d:90:GLN:NE2	1:d:94:ASP:OD2	2.35	0.59
1:m:350:LYS:O	1:m:354:LEU:HD12	2.02	0.59
1:X:37:LYS:NZ	1:X:338:ASP:O	2.34	0.59
1:e:370:ASN:C	1:e:370:ASN:HD22	2.11	0.59
1:q:361:ILE:HG12	1:r:29:MET:HE2	1.83	0.59
1:A:319:ILE:O	1:A:323:ASP:OD2	2.21	0.59
1:X:104:ASN:O	1:X:109:ARG:NH1	2.36	0.59
1:d:282:THR:HG22	1:d:282:THR:O	2.02	0.59
1:j:141:THR:HG22	1:j:141:THR:O	2.03	0.59
1:w:148:GLN:NE2	1:w:150:GLY:O	2.34	0.59
1:k:160:GLU:OE2	1:k:162:LYS:NZ	2.31	0.59
1:q:375:LEU:O	1:q:375:LEU:HD23	2.03	0.59
1:F:91:ARG:O	1:F:94:ASP:OD1	2.21	0.58
1:X:169:LYS:HD2	1:X:169:LYS:N	2.17	0.58
1:N:238:ASP:OD2	1:N:242:LYS:NZ	2.37	0.58
1:N:281:VAL:O	1:N:281:VAL:HG22	2.03	0.58
1:b:92:MET:HE2	1:b:92:MET:N	2.18	0.58
1:Q:53:ARG:NH1	1:R:133:GLY:O	2.36	0.58
1:D:201:ASP:OD1	1:D:202:SER:N	2.37	0.58
1:k:8:ASN:OD1	1:k:8:ASN:O	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:142:HIS:CE1	1:P:161:LEU:HD12	2.39	0.58
1:H:281:VAL:HG12	1:H:281:VAL:O	2.04	0.58
1:J:328:ASN:OD1	1:K:76:GLN:NE2	2.36	0.58
1:e:186:TRP:CG	1:e:186:TRP:O	2.57	0.58
1:h:303:SER:O	1:h:307:GLU:OE2	2.21	0.58
1:s:143:GLY:HA3	1:s:145:LYS:HE3	1.86	0.58
1:d:83:ASN:OD1	1:d:87:ASN:ND2	2.36	0.58
1:j:281:VAL:HG12	1:j:281:VAL:O	2.04	0.58
1:w:31:ARG:O	1:w:34:SER:OG	2.19	0.58
1:E:307:GLU:N	1:E:307:GLU:OE1	2.37	0.58
1:U:58:SER:O	1:U:62:ASP:OD2	2.22	0.58
1:b:54:LEU:HD12	1:b:329:VAL:HG13	1.84	0.58
1:w:58:SER:O	1:w:62:ASP:OD1	2.22	0.57
1:R:91:ARG:O	1:R:94:ASP:OD1	2.21	0.57
1:X:149:ILE:HD11	1:X:315:PHE:CZ	2.39	0.57
1:s:160:GLU:OE1	1:s:162:LYS:NZ	2.36	0.57
1:r:350:LYS:HB3	1:r:350:LYS:HZ2	1.68	0.57
1:T:288:GLN:O	1:e:153:ASN:ND2	2.38	0.57
1:s:238:ASP:OD1	1:s:244:GLN:NE2	2.35	0.57
1:w:21:ALA:O	1:w:25:GLN:OE1	2.22	0.57
1:T:255:GLU:OE2	1:T:255:GLU:N	2.29	0.57
1:Z:3:VAL:HG13	1:Z:3:VAL:O	2.04	0.57
1:n:313:ASN:O	1:n:316:ASN:OD1	2.21	0.57
1:E:179:GLU:OE2	1:E:267:GLY:O	2.23	0.57
1:X:167:ASP:OD1	1:X:167:ASP:O	2.22	0.57
1:q:231:ASP:OD2	1:q:251:LYS:NZ	2.38	0.57
1:r:332:SER:O	1:r:336:ILE:HD12	2.04	0.57
1:s:341:PHE:O	1:s:345:THR:HG23	2.05	0.57
1:X:277:ASP:N	1:X:277:ASP:OD1	2.36	0.57
1:C:238:ASP:OD1	1:C:239:GLN:NE2	2.37	0.56
1:f:161:LEU:HD11	1:f:308:LEU:HD21	1.87	0.56
1:l:32:LEU:HD23	1:l:32:LEU:O	2.05	0.56
1:L:110:VAL:O	1:L:114:GLU:OE1	2.23	0.56
1:s:354:LEU:O	1:s:354:LEU:HD23	2.04	0.56
1:d:184:LYS:HA	1:d:184:LYS:HE2	1.88	0.56
1:K:91:ARG:O	1:K:94:ASP:OD1	2.23	0.56
1:Z:128:GLU:OE2	1:Z:165:ARG:NH1	2.39	0.56
1:u:281:VAL:HG12	1:u:281:VAL:O	2.05	0.56
1:G:18:LEU:O	1:G:22:ASN:OD1	2.24	0.56
1:Z:93:ARG:HB2	1:Z:294:ILE:HG21	1.87	0.56
1:i:190:GLU:OE1	1:i:191:GLY:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:31:ARG:HA	1:u:39:ASN:HD21	1.71	0.56
1:d:85:THR:O	1:d:88:ILE:HG22	2.04	0.56
1:r:52:ASN:O	1:r:56:VAL:HG23	2.05	0.56
1:N:231:ASP:C	1:N:231:ASP:OD1	2.49	0.56
1:T:185:ASP:OD1	1:T:185:ASP:N	2.38	0.56
1:j:240:ASP:OD2	1:j:240:ASP:N	2.37	0.56
1:m:55:ASN:OD1	1:m:55:ASN:C	2.49	0.56
1:q:110:VAL:O	1:q:114:GLU:OE2	2.23	0.56
1:s:356:GLN:OE1	1:s:357:ALA:N	2.38	0.56
1:T:231:ASP:OD1	1:T:231:ASP:C	2.49	0.56
1:Z:110:VAL:O	1:Z:114:GLU:OE1	2.24	0.56
1:s:339:THR:HG23	1:s:344:GLU:OE1	2.06	0.56
1:u:208:GLU:OE1	1:u:210:ASN:OD1	2.24	0.56
1:B:91:ARG:O	1:B:94:ASP:OD1	2.24	0.56
1:k:66:ARG:HB3	1:k:66:ARG:NH1	2.20	0.56
1:s:61:LEU:HD23	1:s:151:ALA:HB2	1.87	0.56
1:Z:206:GLU:OE1	1:Z:206:GLU:N	2.38	0.56
1:E:46:ALA:O	1:E:50:ILE:HG13	2.05	0.55
1:N:2:ALA:N	1:O:19:ASN:OD1	2.39	0.55
1:u:110:VAL:O	1:u:114:GLU:OE1	2.24	0.55
1:m:113:GLN:OE1	1:m:281:VAL:HG22	2.06	0.55
1:A:46:ALA:O	1:A:50:ILE:HG13	2.05	0.55
1:B:44:ASP:OD1	1:B:44:ASP:O	2.24	0.55
1:Z:201:ASP:OD1	1:Z:202:SER:N	2.40	0.55
1:s:184:LYS:N	1:s:184:LYS:HD3	2.22	0.55
1:L:198:ASN:OD1	1:L:199:LEU:N	2.39	0.55
1:h:110:VAL:O	1:h:114:GLU:OE2	2.25	0.55
1:m:91:ARG:O	1:m:94:ASP:OD1	2.23	0.55
1:C:270:GLU:OE2	1:C:270:GLU:N	2.30	0.55
1:m:255:GLU:N	1:m:255:GLU:OE2	2.40	0.55
1:n:69:ASN:O	1:n:72:ILE:HG22	2.07	0.55
1:n:162:LYS:HB3	1:n:162:LYS:HZ2	1.72	0.55
1:u:238:ASP:C	1:u:238:ASP:OD1	2.50	0.55
1:I:91:ARG:O	1:I:94:ASP:OD2	2.25	0.55
1:N:117:THR:O	1:N:121:ASP:OD2	2.25	0.55
1:S:193:ASN:ND2	1:S:213:ALA:O	2.40	0.55
1:U:231:ASP:OD1	1:U:231:ASP:C	2.49	0.55
1:g:208:GLU:C	1:g:209:ILE:HD12	2.32	0.55
1:H:370:ASN:OD1	1:H:370:ASN:C	2.49	0.55
1:I:288:GLN:O	1:T:153:ASN:ND2	2.40	0.55
1:e:162:LYS:HD2	1:e:304:HIS:CG	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:192:LYS:HE3	1:L:192:LYS:HA	1.87	0.54
1:V:91:ARG:O	1:V:94:ASP:OD1	2.25	0.54
1:p:53:ARG:O	1:p:56:VAL:HG12	2.06	0.54
1:O:170:MET:HE3	1:O:170:MET:HA	1.90	0.54
1:T:238:ASP:OD1	1:T:238:ASP:C	2.51	0.54
1:n:184:LYS:O	1:n:184:LYS:CD	2.55	0.54
1:B:287:ALA:O	1:B:290:SER:OG	2.21	0.54
1:J:169:LYS:O	1:J:172:GLY:N	2.38	0.54
1:O:201:ASP:OD2	1:O:202:SER:N	2.41	0.54
1:O:299:LYS:HE2	1:O:299:LYS:HA	1.89	0.54
1:Z:111:ALA:HA	1:Z:114:GLU:OE1	2.08	0.54
1:h:314:ARG:NE	1:i:122:GLU:OE1	2.35	0.54
1:u:38:ILE:N	1:u:38:ILE:HD12	2.23	0.54
1:f:170:MET:HE3	1:f:170:MET:HA	1.90	0.54
1:f:184:LYS:NZ	1:f:220:GLU:OE1	2.40	0.54
1:p:302:ASP:OD1	1:p:303:SER:N	2.40	0.54
1:u:37:LYS:HG3	1:u:38:ILE:HD12	1.90	0.54
1:w:303:SER:O	1:w:307:GLU:OE1	2.26	0.54
1:G:82:MET:HE1	1:G:304:HIS:CD2	2.43	0.54
1:S:133:GLY:O	1:c:53:ARG:NH1	2.40	0.54
1:d:270:GLU:OE1	1:d:271:GLY:N	2.41	0.54
1:p:38:ILE:HD13	1:p:337:LYS:HA	1.90	0.54
1:r:91:ARG:O	1:r:94:ASP:OD1	2.25	0.54
1:r:152:ASP:OD2	1:s:136:LYS:NZ	2.39	0.54
1:K:169:LYS:HE2	1:K:169:LYS:HA	1.89	0.54
1:O:258:PHE:CD1	1:O:268:LEU:HD13	2.43	0.54
1:P:225:TYR:O	1:P:229:GLN:OE1	2.26	0.54
1:g:121:ASP:N	1:g:121:ASP:OD2	2.37	0.54
1:q:46:ALA:O	1:q:50:ILE:HG13	2.07	0.54
1:B:257:GLU:OE2	1:B:257:GLU:N	2.40	0.54
1:O:299:LYS:NZ	1:O:302:ASP:OD1	2.35	0.54
1:d:88:ILE:HD11	1:d:119:LEU:O	2.07	0.54
1:M:153:ASN:OD1	1:M:154:GLY:N	2.41	0.54
1:S:303:SER:O	1:S:307:GLU:OE1	2.24	0.54
1:f:89:LEU:HA	1:f:92:MET:SD	2.48	0.54
1:s:57:GLN:OE1	1:s:329:VAL:HG21	2.07	0.54
1:A:153:ASN:OD1	1:h:236:SER:HB3	2.08	0.54
1:n:231:ASP:O	1:n:231:ASP:OD1	2.26	0.54
1:H:153:ASN:OD1	1:H:154:GLY:N	2.41	0.54
1:X:45:ALA:O	1:X:49:GLN:OE1	2.26	0.54
1:q:367:GLN:OE1	1:q:367:GLN:O	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:125:ARG:O	1:w:129:THR:HG23	2.08	0.54
1:E:25:GLN:HG2	1:E:351:SER:OG	2.08	0.53
1:J:52:ASN:O	1:J:56:VAL:HG23	2.08	0.53
1:r:164:MET:HE3	1:r:164:MET:HA	1.90	0.53
1:J:193:ASN:OD1	1:J:193:ASN:O	2.27	0.53
1:c:112:ILE:O	1:c:116:VAL:HG23	2.07	0.53
1:j:257:GLU:N	1:j:257:GLU:CD	2.66	0.53
1:S:8:ASN:OD1	1:S:8:ASN:O	2.25	0.53
1:g:298:LEU:O	1:g:301:VAL:HG12	2.08	0.53
1:o:194:ASP:OD2	1:o:194:ASP:N	2.41	0.53
1:P:279:ILE:HD12	1:P:290:SER:HB2	1.90	0.53
1:j:58:SER:O	1:j:62:ASP:OD2	2.26	0.53
1:f:93:ARG:HG3	1:f:294:ILE:HG21	1.89	0.53
1:k:52:ASN:O	1:k:55:ASN:ND2	2.42	0.53
1:u:240:ASP:OD1	1:u:240:ASP:N	2.41	0.53
1:G:94:ASP:OD1	1:G:94:ASP:N	2.41	0.53
1:b:53:ARG:NH1	1:c:133:GLY:O	2.42	0.53
1:c:231:ASP:OD1	1:c:231:ASP:C	2.52	0.53
1:d:169:LYS:O	1:d:172:GLY:N	2.31	0.53
1:p:153:ASN:OD1	1:p:153:ASN:C	2.52	0.53
1:s:281:VAL:HG12	1:s:281:VAL:O	2.09	0.53
1:u:240:ASP:OD1	1:u:242:LYS:NZ	2.40	0.53
1:G:231:ASP:C	1:G:231:ASP:OD1	2.51	0.53
1:Z:179:GLU:OE1	1:Z:267:GLY:O	2.27	0.53
1:f:107:ALA:O	1:f:110:VAL:HG12	2.09	0.53
1:E:25:GLN:O	1:E:29:MET:SD	2.67	0.53
1:J:153:ASN:OD1	1:J:154:GLY:N	2.41	0.53
1:T:319:ILE:O	1:T:323:ASP:OD1	2.26	0.53
1:Z:98:GLN:OE1	1:Z:98:GLN:HA	2.09	0.53
1:Z:142:HIS:CG	1:Z:143:GLY:H	2.27	0.53
1:k:82:MET:HE1	1:k:308:LEU:CD1	2.39	0.53
1:l:25:GLN:O	1:l:29:MET:HE2	2.09	0.53
1:A:153:ASN:OD1	1:A:153:ASN:C	2.51	0.53
1:G:220:GLU:OE1	1:R:158:MET:HE3	2.08	0.53
1:X:170:MET:HE2	1:X:170:MET:HA	1.90	0.53
1:g:118:ALA:O	1:g:121:ASP:OD2	2.27	0.53
1:i:153:ASN:OD1	1:i:153:ASN:C	2.51	0.53
1:k:25:GLN:O	1:k:29:MET:HG3	2.08	0.53
1:c:281:VAL:HG22	1:c:281:VAL:O	2.09	0.52
1:f:109:ARG:O	1:f:112:ILE:HG22	2.09	0.52
1:u:272:LYS:NZ	1:u:273:LYS:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:328:ASN:OD1	1:O:76:GLN:NE2	2.42	0.52
1:P:348:MET:O	1:P:351:SER:OG	2.27	0.52
1:H:238:ASP:OD1	1:H:238:ASP:C	2.53	0.52
1:l:179:GLU:OE2	1:l:180:SER:OG	2.20	0.52
1:m:368:ALA:HB3	1:m:369:PRO:HD3	1.92	0.52
1:n:255:GLU:C	1:n:255:GLU:OE1	2.51	0.52
1:X:250:ASN:C	1:X:250:ASN:OD1	2.51	0.52
1:i:218:ASP:OD2	1:i:219:ILE:N	2.42	0.52
1:j:367:GLN:C	1:j:367:GLN:OE1	2.53	0.52
1:p:37:LYS:HG2	1:p:38:ILE:HD12	1.92	0.52
1:c:170:MET:HE3	1:c:170:MET:HA	1.91	0.52
1:i:225:TYR:CE1	1:i:229:GLN:NE2	2.75	0.52
1:m:361:ILE:HD11	1:n:29:MET:HB3	1.90	0.52
1:u:184:LYS:O	1:u:184:LYS:HG3	2.09	0.52
1:C:117:THR:O	1:C:121:ASP:OD2	2.27	0.52
1:I:187:ASN:OD1	1:I:187:ASN:C	2.53	0.52
1:K:58:SER:O	1:K:62:ASP:OD1	2.28	0.52
1:r:218:ASP:OD1	1:r:219:ILE:N	2.36	0.52
1:r:361:ILE:HG23	1:s:29:MET:SD	2.50	0.52
1:A:153:ASN:OD1	1:A:154:GLY:N	2.43	0.52
1:j:160:GLU:OE2	1:j:160:GLU:C	2.52	0.52
1:o:46:ALA:O	1:o:50:ILE:HG13	2.10	0.52
1:u:118:ALA:O	1:u:121:ASP:OD1	2.28	0.52
1:B:205:GLN:HA	1:B:205:GLN:OE1	2.09	0.52
1:c:164:MET:O	1:c:164:MET:SD	2.67	0.52
1:f:109:ARG:NH2	1:f:284:VAL:HG23	2.25	0.52
1:D:206:GLU:OE1	1:D:206:GLU:N	2.42	0.52
1:I:94:ASP:OD2	1:I:94:ASP:N	2.39	0.52
1:g:187:ASN:HB3	1:g:216:GLY:HA2	1.92	0.52
1:j:160:GLU:OE1	1:j:162:LYS:NZ	2.38	0.52
1:l:348:MET:O	1:l:351:SER:HB2	2.10	0.52
1:s:153:ASN:OD1	1:s:154:GLY:N	2.43	0.52
1:B:6:ASN:HB2	1:i:338:ASP:OD2	2.10	0.52
1:D:6:ASN:ND2	1:k:35:GLY:O	2.43	0.52
1:O:159:LEU:C	1:O:160:GLU:OE1	2.53	0.52
1:l:207:GLN:NE2	1:l:208:GLU:O	2.43	0.52
1:w:281:VAL:HG12	1:w:281:VAL:O	2.09	0.52
1:e:188:VAL:HG13	1:e:215:ALA:HA	1.91	0.51
1:G:91:ARG:O	1:G:94:ASP:OD1	2.29	0.51
1:I:153:ASN:OD1	1:I:153:ASN:N	2.42	0.51
1:h:199:LEU:HD13	1:h:252:VAL:HG22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:25:GLN:CG	1:l:351:SER:OG	2.58	0.51
1:V:303:SER:O	1:V:307:GLU:OE2	2.28	0.51
1:d:125:ARG:HG3	1:d:126:ILE:N	2.26	0.51
1:f:79:GLU:OE2	1:f:305:ARG:NH1	2.42	0.51
1:s:185:ASP:OD2	1:s:185:ASP:C	2.53	0.51
1:F:62:ASP:O	1:F:65:VAL:HG22	2.10	0.51
1:j:53:ARG:O	1:j:56:VAL:HG22	2.10	0.51
1:T:4:ASN:C	1:T:4:ASN:OD1	2.53	0.51
1:c:190:GLU:CD	1:c:190:GLU:H	2.18	0.51
1:d:298:LEU:O	1:d:302:ASP:OD1	2.28	0.51
1:h:160:GLU:OE1	1:h:161:LEU:N	2.44	0.51
1:l:32:LEU:HD23	1:l:32:LEU:C	2.36	0.51
1:H:190:GLU:OE2	1:H:215:ALA:HB2	2.11	0.51
1:M:113:GLN:OE1	1:M:281:VAL:HG12	2.10	0.51
1:h:238:ASP:OD1	1:h:238:ASP:C	2.53	0.51
1:j:349:THR:O	1:j:353:ILE:HG12	2.10	0.51
1:k:362:LEU:C	1:k:362:LEU:HD23	2.35	0.51
1:n:158:MET:C	1:n:158:MET:SD	2.93	0.51
1:K:159:LEU:HD12	1:K:160:GLU:H	1.76	0.51
1:Z:5:VAL:HG22	1:Z:5:VAL:O	2.10	0.51
1:f:230:THR:O	1:f:234:LYS:NZ	2.43	0.51
1:f:325:ILE:O	1:f:329:VAL:HG12	2.11	0.51
1:s:253:GLU:OE2	1:s:253:GLU:C	2.54	0.51
1:B:153:ASN:OD1	1:B:153:ASN:C	2.53	0.51
1:u:51:SER:O	1:u:55:ASN:OD1	2.28	0.51
1:L:160:GLU:HA	1:L:160:GLU:OE1	2.11	0.51
1:Q:162:LYS:HD3	1:Q:162:LYS:N	2.25	0.51
1:X:186:TRP:NE1	1:X:265:GLU:OE2	2.44	0.51
1:k:51:SER:HA	1:k:54:LEU:HD12	1.92	0.51
1:m:141:THR:O	1:m:142:HIS:C	2.54	0.51
1:o:8:ASN:CG	1:o:8:ASN:O	2.54	0.51
1:w:25:GLN:HG2	1:w:351:SER:HB3	1.93	0.51
1:E:193:ASN:O	1:E:212:SER:HA	2.10	0.51
1:E:218:ASP:OD2	1:P:158:MET:HE3	2.11	0.51
1:S:153:ASN:OD1	1:S:153:ASN:C	2.53	0.51
1:f:25:GLN:O	1:f:29:MET:HG3	2.11	0.51
1:p:368:ALA:HB3	1:p:369:PRO:HD3	1.92	0.51
1:H:153:ASN:OD1	1:H:153:ASN:C	2.54	0.50
1:I:340:ASP:OD2	1:T:2:ALA:N	2.44	0.50
1:X:106:LYS:O	1:X:110:VAL:HG23	2.11	0.50
1:i:357:ALA:O	1:i:361:ILE:HG12	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:66:ARG:HB3	1:k:66:ARG:CZ	2.41	0.50
1:k:289:GLU:O	1:k:293:ILE:HG22	2.11	0.50
1:m:177:GLN:OE1	1:m:177:GLN:N	2.44	0.50
1:s:3:VAL:O	1:s:3:VAL:HG13	2.11	0.50
1:N:22:ASN:OD1	1:N:22:ASN:C	2.55	0.50
1:O:222:LEU:O	1:O:226:ILE:HD12	2.11	0.50
1:R:29:MET:HG3	1:R:348:MET:HE3	1.93	0.50
1:Z:222:LEU:HG	1:Z:226:ILE:HD11	1.93	0.50
1:j:182:LYS:HE3	1:j:265:GLU:HG3	1.94	0.50
1:l:19:ASN:OD1	1:l:19:ASN:C	2.55	0.50
1:P:142:HIS:NE2	1:P:145:LYS:HG3	2.26	0.50
1:R:214:LYS:O	1:R:215:ALA:HB3	2.12	0.50
1:S:270:GLU:OE2	1:S:270:GLU:HA	2.10	0.50
1:d:218:ASP:OD1	1:d:219:ILE:N	2.44	0.50
1:f:103:SER:O	1:f:104:ASN:ND2	2.39	0.50
1:s:315:PHE:O	1:s:319:ILE:HD12	2.12	0.50
1:F:244:GLN:O	1:F:245:ILE:HD13	2.10	0.50
1:H:370:ASN:OD1	1:H:371:SER:N	2.44	0.50
1:m:125:ARG:O	1:m:129:THR:OG1	2.21	0.50
1:q:3:VAL:HG23	1:r:18:LEU:HD21	1.93	0.50
1:s:57:GLN:O	1:s:61:LEU:HG	2.11	0.50
1:I:3:VAL:HG13	1:I:3:VAL:O	2.12	0.50
1:P:270:GLU:HA	1:P:270:GLU:OE1	2.11	0.50
1:e:219:ILE:HG23	1:e:220:GLU:N	2.27	0.50
1:f:83:ASN:C	1:f:83:ASN:OD1	2.55	0.50
1:l:361:ILE:HG23	1:m:29:MET:HG2	1.92	0.50
1:n:42:LYS:HD2	1:n:42:LYS:N	2.27	0.50
1:K:341:PHE:CE1	1:V:5:VAL:HG23	2.47	0.50
1:P:29:MET:O	1:P:32:LEU:HB3	2.11	0.50
1:P:370:ASN:C	1:P:370:ASN:HD22	2.18	0.50
1:B:219:ILE:HG23	1:B:220:GLU:N	2.27	0.50
1:D:66:ARG:O	1:D:70:ASP:OD2	2.30	0.50
1:O:302:ASP:OD1	1:O:303:SER:N	2.45	0.50
1:V:30:GLU:OE2	1:V:39:ASN:ND2	2.45	0.50
1:b:37:LYS:NZ	1:b:338:ASP:O	2.38	0.50
1:c:99:SER:O	1:c:109:ARG:NH1	2.45	0.50
1:i:32:LEU:HD21	1:i:344:GLU:CB	2.42	0.50
1:i:361:ILE:CG2	1:u:29:MET:HE2	2.42	0.50
1:o:25:GLN:HG2	1:o:29:MET:HE2	1.94	0.50
1:p:55:ASN:HB3	1:p:333:LYS:HD2	1.94	0.50
1:w:365:ALA:O	1:w:368:ALA:HB3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:GLN:O	1:C:370:ASN:OD1	2.30	0.50
1:O:37:LYS:NZ	1:O:336:ILE:O	2.43	0.50
1:R:3:VAL:HG13	1:R:3:VAL:O	2.11	0.50
1:d:83:ASN:OD1	1:d:83:ASN:C	2.54	0.50
1:l:169:LYS:O	1:l:169:LYS:HD3	2.12	0.50
1:u:158:MET:SD	1:u:158:MET:C	2.95	0.50
1:u:270:GLU:H	1:u:270:GLU:CD	2.17	0.50
1:Q:334:SER:HB2	1:b:7:THR:HG21	1.94	0.50
1:X:338:ASP:OD1	1:X:338:ASP:C	2.55	0.50
1:Z:174:VAL:N	1:Z:247:ALA:O	2.40	0.50
1:c:177:GLN:OE1	1:c:272:LYS:NZ	2.45	0.50
1:j:37:LYS:NZ	1:j:336:ILE:O	2.45	0.50
1:l:59:ARG:HD2	1:w:94:ASP:OD2	2.12	0.50
1:n:122:GLU:O	1:n:122:GLU:OE2	2.30	0.50
1:p:117:THR:O	1:p:121:ASP:OD1	2.30	0.50
1:M:225:TYR:CE1	1:M:229:GLN:NE2	2.68	0.49
1:O:188:VAL:HG23	1:O:217:ASP:O	2.11	0.49
1:R:281:VAL:HG12	1:R:281:VAL:O	2.10	0.49
1:c:214:LYS:O	1:c:215:ALA:HB3	2.12	0.49
1:w:61:LEU:HD12	1:w:326:ASN:HB2	1.94	0.49
1:B:321:ASN:O	1:B:325:ILE:HG13	2.12	0.49
1:F:319:ILE:O	1:F:323:ASP:OD1	2.28	0.49
1:G:3:VAL:HG13	1:G:3:VAL:O	2.12	0.49
1:H:82:MET:HE1	1:H:308:LEU:HD12	1.93	0.49
1:L:153:ASN:OD1	1:L:153:ASN:C	2.54	0.49
1:X:184:LYS:O	1:X:184:LYS:HG3	2.10	0.49
1:h:66:ARG:HB3	1:h:66:ARG:NH1	2.27	0.49
1:s:61:LEU:HD12	1:s:326:ASN:HB2	1.94	0.49
1:A:66:ARG:O	1:A:70:ASP:OD2	2.30	0.49
1:J:153:ASN:OD1	1:J:153:ASN:C	2.56	0.49
1:K:53:ARG:CZ	1:s:108:GLU:OE2	2.61	0.49
1:K:155:GLU:OE1	1:h:129:THR:HG22	2.12	0.49
1:U:375:LEU:O	1:U:375:LEU:HD12	2.12	0.49
1:b:116:VAL:HG21	1:b:281:VAL:HG21	1.93	0.49
1:n:184:LYS:O	1:n:184:LYS:HD3	2.12	0.49
1:q:22:ASN:O	1:q:26:GLN:HG3	2.12	0.49
1:w:340:ASP:HB3	1:w:343:LYS:HE2	1.93	0.49
1:E:341:PHE:O	1:E:345:THR:HG23	2.12	0.49
1:M:86:THR:O	1:M:90:GLN:OE1	2.30	0.49
1:O:110:VAL:O	1:O:114:GLU:OE2	2.30	0.49
1:R:281:VAL:O	1:R:281:VAL:CG1	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:54:LEU:HD22	1:f:329:VAL:HG23	1.94	0.49
1:j:270:GLU:OE1	1:j:270:GLU:N	2.42	0.49
1:m:280:ASP:OD1	1:m:282:THR:HG23	2.12	0.49
1:o:26:GLN:C	1:o:26:GLN:OE1	2.55	0.49
1:D:238:ASP:C	1:D:238:ASP:OD1	2.55	0.49
1:E:240:ASP:O	1:E:240:ASP:OD2	2.31	0.49
1:V:258:PHE:CD1	1:V:258:PHE:N	2.80	0.49
1:o:238:ASP:OD1	1:o:238:ASP:C	2.55	0.49
1:H:117:THR:O	1:H:121:ASP:OD2	2.30	0.49
1:H:341:PHE:O	1:H:345:THR:HG23	2.12	0.49
1:I:238:ASP:C	1:I:238:ASP:OD1	2.55	0.49
1:S:188:VAL:HG23	1:S:217:ASP:O	2.13	0.49
1:b:230:THR:HG22	1:b:232:LEU:HD12	1.95	0.49
1:n:144:ALA:O	1:n:145:LYS:CB	2.59	0.49
1:r:20:ASN:OD1	1:r:20:ASN:C	2.56	0.49
1:r:201:ASP:OD1	1:r:201:ASP:C	2.56	0.49
1:s:61:LEU:HD23	1:s:151:ALA:CB	2.43	0.49
1:w:325:ILE:O	1:w:329:VAL:HG13	2.12	0.49
1:F:125:ARG:NH1	1:F:129:THR:HG21	2.27	0.49
1:Q:108:GLU:OE1	1:Q:108:GLU:N	2.36	0.49
1:c:319:ILE:O	1:c:323:ASP:OD1	2.30	0.49
1:h:373:LEU:C	1:h:373:LEU:HD13	2.37	0.49
1:j:6:ASN:ND2	1:u:36:PHE:CZ	2.81	0.49
1:n:311:PHE:CZ	1:n:315:PHE:CE1	3.01	0.49
1:L:155:GLU:OE1	1:M:129:THR:HG23	2.13	0.49
1:R:262:LEU:HA	1:R:265:GLU:HB3	1.95	0.49
1:m:144:ALA:HB2	1:m:160:GLU:HG2	1.94	0.49
1:o:201:ASP:C	1:o:201:ASP:OD1	2.56	0.49
1:p:201:ASP:OD1	1:p:201:ASP:C	2.56	0.49
1:u:319:ILE:O	1:u:323:ASP:OD1	2.30	0.49
1:F:144:ALA:HB2	1:F:160:GLU:HG2	1.93	0.49
1:F:280:ASP:C	1:F:280:ASP:OD1	2.56	0.49
1:O:224:THR:OG1	1:Z:154:GLY:O	2.27	0.49
1:S:82:MET:HE1	1:S:308:LEU:HD11	1.94	0.49
1:U:117:THR:O	1:U:121:ASP:OD2	2.31	0.49
1:Z:167:ASP:OD2	1:Z:167:ASP:C	2.56	0.49
1:j:231:ASP:OD1	1:j:231:ASP:O	2.31	0.49
1:I:154:GLY:O	1:p:224:THR:OG1	2.28	0.48
1:M:3:VAL:HG13	1:M:3:VAL:O	2.12	0.48
1:M:319:ILE:O	1:M:323:ASP:OD1	2.31	0.48
1:O:177:GLN:NE2	1:O:178:ALA:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:222:LEU:C	1:Q:222:LEU:HD23	2.38	0.48
1:b:167:ASP:OD2	1:b:167:ASP:C	2.56	0.48
1:n:255:GLU:OE1	1:n:256:VAL:N	2.46	0.48
1:s:185:ASP:OD2	1:s:186:TRP:N	2.46	0.48
1:K:366:LYS:O	1:K:369:PRO:HD2	2.13	0.48
1:L:307:GLU:C	1:L:307:GLU:OE1	2.55	0.48
1:N:73:SER:OG	1:X:335:ARG:NH1	2.46	0.48
1:h:276:VAL:O	1:h:279:ILE:HG13	2.13	0.48
1:l:234:LYS:O	1:l:245:ILE:HD12	2.13	0.48
1:o:231:ASP:OD2	1:o:231:ASP:C	2.56	0.48
1:F:125:ARG:HH11	1:F:129:THR:HG21	1.78	0.48
1:O:238:ASP:OD2	1:O:242:LYS:NZ	2.43	0.48
1:b:218:ASP:OD1	1:b:219:ILE:N	2.46	0.48
1:g:142:HIS:CG	1:g:143:GLY:H	2.30	0.48
1:C:140:GLY:O	1:C:141:THR:CB	2.60	0.48
1:D:367:GLN:OE1	1:D:367:GLN:HA	2.13	0.48
1:E:271:GLY:O	1:E:273:LYS:NZ	2.40	0.48
1:F:120:ASN:OD1	1:F:120:ASN:C	2.56	0.48
1:Z:239:GLN:NE2	1:Z:240:ASP:OD1	2.35	0.48
1:h:201:ASP:OD1	1:h:201:ASP:C	2.56	0.48
1:w:326:ASN:OD1	1:w:326:ASN:C	2.56	0.48
1:B:179:GLU:N	1:B:179:GLU:OE1	2.46	0.48
1:H:319:ILE:O	1:H:323:ASP:OD1	2.30	0.48
1:O:231:ASP:OD1	1:O:231:ASP:C	2.57	0.48
1:S:179:GLU:OE2	1:S:179:GLU:O	2.30	0.48
1:V:238:ASP:OD1	1:V:238:ASP:C	2.56	0.48
1:X:142:HIS:NE2	1:X:145:LYS:HG3	2.28	0.48
1:h:218:ASP:OD1	1:h:219:ILE:HG22	2.14	0.48
1:i:190:GLU:OE1	1:i:190:GLU:C	2.56	0.48
1:j:321:ASN:O	1:j:325:ILE:HG12	2.14	0.48
1:n:162:LYS:HB3	1:n:162:LYS:NZ	2.29	0.48
1:o:238:ASP:OD2	1:o:242:LYS:NZ	2.46	0.48
1:Z:192:LYS:HZ2	1:Z:265:GLU:HB2	1.78	0.48
1:b:83:ASN:C	1:b:83:ASN:OD1	2.56	0.48
1:G:176:TYR:CE2	1:G:271:GLY:HA3	2.48	0.48
1:e:195:LEU:HB2	1:e:262:LEU:HD12	1.95	0.48
1:r:61:LEU:HD12	1:r:322:LEU:HD22	1.94	0.48
1:s:339:THR:HG22	1:s:341:PHE:HD1	1.78	0.48
1:G:114:GLU:OE1	1:G:114:GLU:N	2.46	0.48
1:J:146:SER:HB3	1:J:158:MET:HE3	1.95	0.48
1:K:176:TYR:OH	1:K:255:GLU:OE1	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:185:ASP:OD1	1:N:185:ASP:N	2.47	0.48
1:U:163:ASP:OD1	1:U:164:MET:N	2.47	0.48
1:f:175:SER:O	1:f:272:LYS:N	2.46	0.48
1:B:141:THR:HG23	1:B:142:HIS:N	2.29	0.48
1:I:184:LYS:NZ	1:I:218:ASP:OD2	2.43	0.48
1:Z:246:PHE:CD1	1:Z:292:ALA:HB1	2.48	0.48
1:b:218:ASP:OD1	1:b:219:ILE:HG22	2.14	0.48
1:g:117:THR:O	1:g:121:ASP:OD2	2.31	0.48
1:g:209:ILE:HD12	1:g:209:ILE:N	2.28	0.48
1:j:184:LYS:O	1:j:185:ASP:CB	2.62	0.48
1:j:231:ASP:OD1	1:j:231:ASP:C	2.57	0.48
1:m:361:ILE:HD13	1:n:33:SER:HB3	1.95	0.48
1:E:179:GLU:OE1	1:E:269:GLY:N	2.47	0.48
1:G:319:ILE:O	1:G:323:ASP:OD1	2.32	0.48
1:P:3:VAL:HG13	1:P:3:VAL:O	2.14	0.48
1:P:219:ILE:HG23	1:P:220:GLU:N	2.29	0.48
1:R:291:VAL:O	1:R:295:ASP:OD2	2.32	0.48
1:U:153:ASN:OD1	1:U:153:ASN:C	2.57	0.48
1:Z:246:PHE:CE1	1:Z:292:ALA:HB1	2.49	0.48
1:d:176:TYR:HA	1:d:271:GLY:HA3	1.96	0.48
1:l:32:LEU:HD12	1:l:344:GLU:HB3	1.96	0.48
1:l:257:GLU:N	1:l:257:GLU:OE1	2.47	0.48
1:G:236:SER:OG	1:R:153:ASN:OD1	2.32	0.47
1:J:141:THR:HG23	1:J:142:HIS:N	2.29	0.47
1:P:162:LYS:HD3	1:P:304:HIS:ND1	2.29	0.47
1:e:84:GLU:HA	1:e:84:GLU:OE2	2.13	0.47
1:h:162:LYS:HD2	1:h:304:HIS:ND1	2.28	0.47
1:h:362:LEU:HD23	1:h:362:LEU:C	2.38	0.47
1:w:179:GLU:OE1	1:w:267:GLY:O	2.32	0.47
1:w:344:GLU:OE1	1:w:344:GLU:HA	2.13	0.47
1:D:48:LEU:HD21	1:k:305:ARG:HH21	1.78	0.47
1:Q:193:ASN:OD1	1:Q:193:ASN:C	2.56	0.47
1:g:142:HIS:CE1	1:g:161:LEU:HD12	2.49	0.47
1:n:32:LEU:HD21	1:n:345:THR:HG22	1.95	0.47
1:D:250:ASN:OD1	1:D:250:ASN:C	2.57	0.47
1:K:46:ALA:O	1:K:50:ILE:HG13	2.15	0.47
1:N:367:GLN:O	1:N:370:ASN:OD1	2.31	0.47
1:g:164:MET:HE1	1:g:301:VAL:HG23	1.96	0.47
1:l:233:VAL:HB	1:l:245:ILE:HD11	1.96	0.47
1:F:201:ASP:OD1	1:F:201:ASP:C	2.57	0.47
1:R:303:SER:O	1:R:307:GLU:OE2	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:85:THR:HG23	1:Z:123:LEU:HD22	1.97	0.47
1:Z:195:LEU:C	1:Z:196:LYS:HD3	2.39	0.47
1:d:199:LEU:C	1:d:199:LEU:HD12	2.40	0.47
1:g:219:ILE:HG23	1:g:220:GLU:N	2.28	0.47
1:L:203:TYR:O	1:L:203:TYR:CD2	2.67	0.47
1:N:240:ASP:CG	1:N:242:LYS:HZ1	2.22	0.47
1:Q:201:ASP:OD1	1:Q:201:ASP:C	2.57	0.47
1:S:30:GLU:OE2	1:S:39:ASN:ND2	2.47	0.47
1:e:201:ASP:C	1:e:201:ASP:OD1	2.57	0.47
1:j:367:GLN:OE1	1:j:367:GLN:O	2.32	0.47
1:u:298:LEU:O	1:u:302:ASP:OD2	2.33	0.47
1:G:70:ASP:N	1:G:70:ASP:OD1	2.47	0.47
1:e:117:THR:O	1:e:121:ASP:OD1	2.31	0.47
1:f:112:ILE:O	1:f:116:VAL:HG13	2.14	0.47
1:E:170:MET:SD	1:E:250:ASN:ND2	2.83	0.47
1:E:175:SER:O	1:E:271:GLY:HA2	2.15	0.47
1:G:66:ARG:HG3	1:G:66:ARG:HH11	1.79	0.47
1:L:232:LEU:HA	1:L:251:LYS:HE3	1.96	0.47
1:M:110:VAL:O	1:M:114:GLU:OE2	2.32	0.47
1:M:214:LYS:N	1:M:217:ASP:OD2	2.47	0.47
1:P:262:LEU:HD23	1:P:262:LEU:O	2.15	0.47
1:Q:163:ASP:OD1	1:Q:164:MET:N	2.47	0.47
1:c:214:LYS:HB2	1:c:217:ASP:OD2	2.15	0.47
1:f:136:LYS:C	1:f:137:LEU:HD23	2.39	0.47
1:h:4:ASN:OD1	1:h:6:ASN:N	2.44	0.47
1:k:367:GLN:C	1:k:367:GLN:OE1	2.58	0.47
1:n:49:GLN:OE1	1:n:49:GLN:C	2.58	0.47
1:o:361:ILE:HD11	1:p:29:MET:HG2	1.97	0.47
1:p:121:ASP:OD1	1:p:121:ASP:N	2.48	0.47
1:q:16:ARG:NH2	1:q:17:TYR:OH	2.48	0.47
1:r:303:SER:O	1:r:307:GLU:OE2	2.33	0.47
1:U:184:LYS:NZ	1:U:240:ASP:O	2.47	0.47
1:k:276:VAL:O	1:k:279:ILE:HG23	2.15	0.47
1:n:83:ASN:C	1:n:83:ASN:OD1	2.58	0.47
1:p:163:ASP:OD1	1:p:164:MET:N	2.47	0.47
1:p:219:ILE:HG23	1:p:220:GLU:N	2.29	0.47
1:E:38:ILE:HD12	1:E:337:LYS:HA	1.97	0.47
1:J:46:ALA:O	1:J:50:ILE:HG13	2.15	0.47
1:L:198:ASN:OD1	1:L:198:ASN:C	2.57	0.47
1:P:46:ALA:O	1:P:50:ILE:HG22	2.15	0.47
1:U:183:GLY:C	1:U:184:LYS:HD2	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:54:LEU:HD12	1:b:329:VAL:CG1	2.44	0.47
1:b:92:MET:HE1	1:b:119:LEU:HD13	1.97	0.47
1:b:222:LEU:HD11	1:b:226:ILE:HD11	1.96	0.47
1:h:350:LYS:O	1:h:354:LEU:HD23	2.15	0.47
1:o:344:GLU:OE2	1:o:344:GLU:HA	2.14	0.47
1:s:17:TYR:HB3	1:s:358:SER:OG	2.15	0.47
1:s:219:ILE:HG23	1:s:220:GLU:N	2.30	0.47
1:s:240:ASP:OD1	1:s:240:ASP:N	2.39	0.47
1:E:163:ASP:OD1	1:E:164:MET:N	2.48	0.47
1:G:46:ALA:O	1:G:50:ILE:HG13	2.14	0.47
1:G:286:GLY:O	1:G:290:SER:OG	2.22	0.47
1:L:335:ARG:NH2	1:M:73:SER:OG	2.48	0.47
1:b:368:ALA:HB3	1:b:369:PRO:HD3	1.97	0.47
1:d:111:ALA:O	1:d:115:GLU:OE2	2.33	0.47
1:d:144:ALA:HB2	1:d:160:GLU:OE1	2.14	0.47
1:h:249:ASN:HA	1:h:252:VAL:O	2.15	0.47
1:n:31:ARG:HD3	1:n:344:GLU:OE2	2.15	0.47
1:q:54:LEU:HD22	1:q:329:VAL:HG13	1.97	0.47
1:B:169:LYS:HD3	1:B:169:LYS:C	2.40	0.46
1:H:187:ASN:C	1:H:187:ASN:OD1	2.57	0.46
1:V:201:ASP:C	1:V:201:ASP:OD1	2.58	0.46
1:X:196:LYS:HZ3	1:X:196:LYS:CB	2.28	0.46
1:X:214:LYS:O	1:X:217:ASP:HB2	2.15	0.46
1:b:314:ARG:O	1:c:122:GLU:OE2	2.32	0.46
1:h:193:ASN:C	1:h:193:ASN:OD1	2.58	0.46
1:m:344:GLU:OE2	1:m:344:GLU:HA	2.14	0.46
1:n:177:GLN:N	1:n:177:GLN:OE1	2.48	0.46
1:s:346:THR:O	1:s:349:THR:HG22	2.16	0.46
1:A:111:ALA:HA	1:A:114:GLU:OE1	2.15	0.46
1:B:83:ASN:C	1:B:83:ASN:OD1	2.58	0.46
1:E:179:GLU:N	1:E:179:GLU:CD	2.73	0.46
1:F:139:ASN:OD1	1:F:140:GLY:N	2.49	0.46
1:F:332:SER:O	1:F:336:ILE:HG12	2.15	0.46
1:N:32:LEU:HB3	1:X:361:ILE:HD11	1.98	0.46
1:P:234:LYS:HD2	1:P:234:LYS:N	2.29	0.46
1:g:291:VAL:O	1:g:295:ASP:OD2	2.33	0.46
1:l:155:GLU:OE2	1:m:129:THR:HG23	2.15	0.46
1:n:280:ASP:OD1	1:n:282:THR:HG23	2.15	0.46
1:q:314:ARG:NE	1:r:122:GLU:OE1	2.43	0.46
1:u:170:MET:HE2	1:u:170:MET:HA	1.96	0.46
1:P:234:LYS:HE2	1:P:234:LYS:HA	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:299:LYS:O	1:P:302:ASP:OD2	2.33	0.46
1:b:193:ASN:ND2	1:b:213:ALA:O	2.37	0.46
1:g:199:LEU:C	1:g:199:LEU:HD12	2.41	0.46
1:i:114:GLU:OE1	1:i:114:GLU:HA	2.15	0.46
1:p:28:SER:O	1:p:32:LEU:HD23	2.15	0.46
1:J:201:ASP:C	1:J:201:ASP:OD1	2.57	0.46
1:U:70:ASP:N	1:U:70:ASP:OD1	2.49	0.46
1:U:314:ARG:NE	1:V:122:GLU:OE1	2.32	0.46
1:X:148:GLN:CG	1:X:148:GLN:O	2.61	0.46
1:f:139:ASN:CG	1:f:141:THR:HG23	2.41	0.46
1:f:314:ARG:CZ	1:g:122:GLU:OE1	2.63	0.46
1:s:29:MET:HE2	1:s:348:MET:HE1	1.97	0.46
1:N:281:VAL:O	1:N:281:VAL:CG2	2.63	0.46
1:O:276:VAL:O	1:O:279:ILE:HG12	2.15	0.46
1:Q:113:GLN:OE1	1:Q:281:VAL:HG12	2.16	0.46
1:V:37:LYS:NZ	1:V:336:ILE:O	2.47	0.46
1:V:231:ASP:OD1	1:V:231:ASP:N	2.47	0.46
1:X:148:GLN:O	1:X:148:GLN:HG3	2.16	0.46
1:d:175:SER:N	1:d:272:LYS:O	2.47	0.46
1:j:277:ASP:OD2	1:j:277:ASP:C	2.59	0.46
1:o:250:ASN:OD1	1:o:250:ASN:C	2.59	0.46
1:B:271:GLY:O	1:B:272:LYS:C	2.57	0.46
1:K:375:LEU:HD21	1:h:362:LEU:HD22	1.98	0.46
1:S:370:ASN:C	1:S:370:ASN:OD1	2.58	0.46
1:g:113:GLN:OE1	1:g:281:VAL:HG22	2.16	0.46
1:k:164:MET:HE3	1:k:164:MET:CA	2.46	0.46
1:n:26:GLN:HA	1:n:29:MET:SD	2.56	0.46
1:q:201:ASP:C	1:q:201:ASP:OD1	2.59	0.46
1:r:8:ASN:O	1:r:8:ASN:OD1	2.33	0.46
1:s:25:GLN:C	1:s:25:GLN:OE1	2.59	0.46
1:s:253:GLU:OE2	1:s:254:GLY:N	2.49	0.46
1:E:22:ASN:C	1:E:22:ASN:OD1	2.58	0.46
1:P:172:GLY:C	1:P:249:ASN:OD1	2.59	0.46
1:V:94:ASP:OD1	1:V:94:ASP:N	2.44	0.46
1:j:219:ILE:HG23	1:j:220:GLU:HG2	1.97	0.46
1:E:101:ASN:HD21	1:P:67:ASN:ND2	2.13	0.46
1:F:128:GLU:OE2	1:F:165:ARG:NH1	2.47	0.46
1:c:199:LEU:HB3	1:c:256:VAL:HG22	1.97	0.46
1:l:373:LEU:C	1:l:373:LEU:HD23	2.41	0.46
1:n:42:LYS:HD2	1:n:42:LYS:H	1.81	0.46
1:q:169:LYS:O	1:q:172:GLY:N	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:255:GLU:OE1	1:r:256:VAL:N	2.49	0.46
1:u:13:THR:OG1	1:u:16:ARG:NH2	2.43	0.46
1:D:70:ASP:OD2	1:D:70:ASP:N	2.49	0.46
1:E:82:MET:SD	1:E:164:MET:HE3	2.56	0.46
1:I:219:ILE:HG23	1:I:220:GLU:N	2.31	0.46
1:O:184:LYS:N	1:O:184:LYS:HD2	2.31	0.46
1:e:280:ASP:OD1	1:e:282:THR:HG23	2.15	0.46
1:i:373:LEU:CD1	1:s:353:ILE:HG23	2.46	0.46
1:p:37:LYS:CG	1:p:38:ILE:HD12	2.46	0.46
1:p:348:MET:SD	1:p:348:MET:C	2.98	0.46
1:q:58:SER:O	1:q:62:ASP:OD2	2.34	0.46
1:q:194:ASP:OD1	1:q:194:ASP:N	2.48	0.46
1:C:194:ASP:OD1	1:C:194:ASP:C	2.59	0.46
1:S:201:ASP:OD1	1:S:201:ASP:C	2.59	0.46
1:V:340:ASP:O	1:V:340:ASP:OD2	2.33	0.46
1:Z:251:LYS:O	1:Z:252:VAL:HG23	2.16	0.46
1:A:18:LEU:O	1:A:22:ASN:OD1	2.35	0.45
1:G:280:ASP:OD1	1:G:282:THR:HG23	2.16	0.45
1:R:141:THR:HG22	1:R:141:THR:O	2.15	0.45
1:d:238:ASP:OD1	1:d:238:ASP:C	2.59	0.45
1:e:219:ILE:HG23	1:e:220:GLU:H	1.82	0.45
1:l:335:ARG:NH2	1:m:73:SER:OG	2.48	0.45
1:n:238:ASP:C	1:n:238:ASP:OD1	2.60	0.45
1:q:38:ILE:O	1:q:38:ILE:HG22	2.15	0.45
1:B:185:ASP:C	1:B:185:ASP:OD1	2.60	0.45
1:E:281:VAL:HG12	1:E:281:VAL:O	2.15	0.45
1:F:53:ARG:NH1	1:G:133:GLY:O	2.49	0.45
1:M:184:LYS:HZ3	1:X:144:ALA:HB1	1.81	0.45
1:M:279:ILE:HG13	1:M:279:ILE:O	2.15	0.45
1:O:66:ARG:HG2	1:O:66:ARG:HH11	1.81	0.45
1:P:300:TYR:CE1	1:P:304:HIS:CE1	3.04	0.45
1:R:202:SER:HB3	1:R:251:LYS:HA	1.98	0.45
1:U:370:ASN:O	1:U:370:ASN:OD1	2.35	0.45
1:X:289:GLU:C	1:X:289:GLU:OE1	2.59	0.45
1:h:279:ILE:HG21	1:h:290:SER:HB2	1.99	0.45
1:k:163:ASP:OD1	1:k:164:MET:N	2.50	0.45
1:n:219:ILE:HG23	1:n:220:GLU:N	2.31	0.45
1:n:231:ASP:OD1	1:n:251:LYS:NZ	2.39	0.45
1:w:57:GLN:O	1:w:61:LEU:HG	2.16	0.45
1:G:16:ARG:HD3	1:n:323:ASP:OD2	2.17	0.45
1:K:5:VAL:HG21	1:r:338:ASP:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:299:LYS:HA	1:P:299:LYS:CE	2.43	0.45
1:U:218:ASP:CG	1:U:219:ILE:N	2.74	0.45
1:d:193:ASN:OD1	1:d:193:ASN:N	2.49	0.45
1:e:99:SER:O	1:e:109:ARG:NH1	2.49	0.45
1:f:153:ASN:OD1	1:f:154:GLY:N	2.50	0.45
1:j:18:LEU:HD23	1:j:18:LEU:O	2.15	0.45
1:j:88:ILE:O	1:j:92:MET:HG3	2.16	0.45
1:n:49:GLN:OE1	1:n:50:ILE:HD13	2.15	0.45
1:p:240:ASP:OD2	1:p:242:LYS:NZ	2.48	0.45
1:s:193:ASN:N	1:s:193:ASN:OD1	2.48	0.45
1:B:142:HIS:CD2	1:B:145:LYS:HE2	2.52	0.45
1:N:113:GLN:HA	1:N:113:GLN:OE1	2.17	0.45
1:Z:237:VAL:HG22	1:Z:243:LEU:HG	1.98	0.45
1:i:32:LEU:HD21	1:i:344:GLU:HB3	1.98	0.45
1:i:361:ILE:N	1:i:361:ILE:HD13	2.31	0.45
1:w:234:LYS:O	1:w:245:ILE:HD12	2.17	0.45
1:F:163:ASP:OD1	1:F:164:MET:N	2.48	0.45
1:G:288:GLN:NE2	1:R:153:ASN:OD1	2.50	0.45
1:K:238:ASP:C	1:K:238:ASP:OD1	2.59	0.45
1:P:214:LYS:HB2	1:P:217:ASP:OD1	2.15	0.45
1:d:175:SER:HB3	1:d:272:LYS:O	2.17	0.45
1:k:231:ASP:OD1	1:k:231:ASP:C	2.60	0.45
1:k:299:LYS:O	1:k:302:ASP:OD1	2.35	0.45
1:l:328:ASN:OD1	1:m:76:GLN:NE2	2.50	0.45
1:m:52:ASN:O	1:m:56:VAL:HG23	2.16	0.45
1:m:162:LYS:HG2	1:m:304:HIS:CE1	2.51	0.45
1:u:31:ARG:HG2	1:u:39:ASN:ND2	2.32	0.45
1:E:30:GLU:OE1	1:O:10:SER:OG	2.31	0.45
1:G:113:GLN:OE1	1:G:281:VAL:HG22	2.17	0.45
1:G:201:ASP:OD1	1:G:201:ASP:C	2.60	0.45
1:L:231:ASP:OD2	1:L:251:LYS:NZ	2.33	0.45
1:O:120:ASN:C	1:O:120:ASN:OD1	2.59	0.45
1:R:219:ILE:HG23	1:R:220:GLU:N	2.32	0.45
1:T:171:MET:SD	1:T:297:ALA:HB1	2.56	0.45
1:T:218:ASP:OD1	1:T:219:ILE:HG22	2.17	0.45
1:b:105:SER:OG	1:b:108:GLU:OE1	2.21	0.45
1:b:367:GLN:O	1:b:370:ASN:OD1	2.35	0.45
1:h:335:ARG:NH2	1:i:73:SER:OG	2.50	0.45
1:i:201:ASP:OD1	1:i:201:ASP:C	2.60	0.45
1:n:110:VAL:O	1:n:114:GLU:OE1	2.35	0.45
1:n:201:ASP:OD1	1:n:201:ASP:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:7:THR:O	1:o:8:ASN:ND2	2.50	0.45
1:o:218:ASP:OD1	1:o:219:ILE:HG22	2.17	0.45
1:p:193:ASN:OD1	1:p:193:ASN:C	2.60	0.45
1:r:57:GLN:O	1:r:61:LEU:HD23	2.17	0.45
1:u:169:LYS:O	1:u:172:GLY:N	2.36	0.45
1:A:236:SER:HB3	1:L:153:ASN:OD1	2.17	0.45
1:C:192:LYS:NZ	1:C:265:GLU:OE1	2.32	0.45
1:C:280:ASP:OD1	1:C:280:ASP:C	2.60	0.45
1:E:194:ASP:OD1	1:E:194:ASP:N	2.50	0.45
1:K:153:ASN:OD1	1:K:153:ASN:C	2.60	0.45
1:L:341:PHE:O	1:L:345:THR:HG23	2.17	0.45
1:M:323:ASP:OD1	1:M:323:ASP:N	2.50	0.45
1:P:38:ILE:HD12	1:P:337:LYS:HA	1.97	0.45
1:f:173:GLY:O	1:f:274:VAL:HG22	2.17	0.45
1:g:92:MET:HE3	1:g:92:MET:CA	2.44	0.45
1:k:155:GLU:OE1	1:w:129:THR:CG2	2.65	0.45
1:m:139:ASN:OD1	1:m:140:GLY:N	2.50	0.45
1:q:25:GLN:HG2	1:q:29:MET:HE3	1.99	0.45
1:w:52:ASN:O	1:w:56:VAL:HG12	2.16	0.45
1:C:348:MET:O	1:C:352:GLN:HG3	2.16	0.45
1:N:123:LEU:HD23	1:N:166:SER:HB3	1.99	0.45
1:O:52:ASN:O	1:O:56:VAL:HG13	2.17	0.45
1:R:239:GLN:N	1:R:239:GLN:OE1	2.50	0.45
1:Z:50:ILE:HG22	1:Z:54:LEU:HD12	1.99	0.45
1:c:194:ASP:OD2	1:c:196:LYS:NZ	2.39	0.45
1:g:142:HIS:HE1	1:g:161:LEU:HD12	1.82	0.45
1:h:110:VAL:HG12	1:h:114:GLU:OE2	2.17	0.45
1:n:190:GLU:OE1	1:n:190:GLU:HA	2.16	0.45
1:r:279:ILE:HD12	1:r:290:SER:OG	2.17	0.45
1:u:31:ARG:HA	1:u:34:SER:HB3	1.97	0.45
1:w:105:SER:N	1:w:108:GLU:OE1	2.49	0.45
1:w:300:TYR:CE1	1:w:304:HIS:NE2	2.85	0.45
1:F:117:THR:O	1:F:121:ASP:OD2	2.34	0.45
1:H:83:ASN:OD1	1:H:83:ASN:C	2.59	0.45
1:H:171:MET:SD	1:H:297:ALA:HB1	2.57	0.45
1:L:139:ASN:OD1	1:L:140:GLY:N	2.50	0.45
1:M:353:ILE:HD11	1:N:370:ASN:HD22	1.82	0.45
1:S:93:ARG:NE	1:S:295:ASP:OD1	2.48	0.45
1:X:246:PHE:CD2	1:X:292:ALA:HB1	2.52	0.45
1:c:222:LEU:HD23	1:c:222:LEU:C	2.42	0.45
1:e:231:ASP:OD1	1:e:232:LEU:HD23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:ASP:OD1	1:I:121:ASP:N	2.49	0.45
1:O:336:ILE:N	1:O:336:ILE:HD12	2.32	0.45
1:e:70:ASP:OD1	1:e:70:ASP:N	2.50	0.45
1:g:95:LEU:HD12	1:g:112:ILE:HG23	1.99	0.45
1:g:266:LEU:CD2	1:g:268:LEU:HD21	2.47	0.45
1:h:82:MET:HE1	1:h:308:LEU:HD11	1.99	0.45
1:h:146:SER:HA	1:h:158:MET:HA	1.98	0.45
1:m:208:GLU:OE2	1:m:208:GLU:N	2.45	0.45
1:n:128:GLU:OE2	1:n:165:ARG:NH1	2.47	0.45
1:o:17:TYR:CD1	1:o:17:TYR:N	2.85	0.45
1:E:279:ILE:HD12	1:E:290:SER:OG	2.17	0.44
1:E:341:PHE:CE2	1:P:5:VAL:HG23	2.52	0.44
1:H:187:ASN:OD1	1:H:187:ASN:O	2.35	0.44
1:J:139:ASN:OD1	1:J:141:THR:HG22	2.17	0.44
1:Q:144:ALA:CB	1:Q:160:GLU:OE1	2.60	0.44
1:b:54:LEU:CD1	1:b:329:VAL:HG13	2.47	0.44
1:b:230:THR:CG2	1:b:232:LEU:HD12	2.47	0.44
1:d:91:ARG:NE	1:d:91:ARG:HA	2.32	0.44
1:d:170:MET:HE2	1:d:170:MET:HA	1.99	0.44
1:k:173:GLY:HA2	1:k:249:ASN:OD1	2.17	0.44
1:u:31:ARG:HG2	1:u:39:ASN:CG	2.42	0.44
1:I:117:THR:O	1:I:121:ASP:OD1	2.35	0.44
1:V:53:ARG:HG2	1:V:53:ARG:HH11	1.82	0.44
1:X:311:PHE:CZ	1:X:315:PHE:CE1	3.06	0.44
1:f:37:LYS:HG2	1:f:337:LYS:O	2.17	0.44
1:i:170:MET:HA	1:i:170:MET:HE3	1.99	0.44
1:i:173:GLY:HA3	1:i:246:PHE:CZ	2.52	0.44
1:j:201:ASP:OD1	1:j:201:ASP:C	2.61	0.44
1:p:287:ALA:HA	1:p:290:SER:OG	2.18	0.44
1:A:238:ASP:OD1	1:A:238:ASP:C	2.61	0.44
1:E:370:ASN:OD1	1:E:370:ASN:O	2.35	0.44
1:K:201:ASP:OD1	1:K:201:ASP:C	2.59	0.44
1:L:201:ASP:OD1	1:L:201:ASP:C	2.60	0.44
1:P:22:ASN:OD1	1:P:22:ASN:C	2.60	0.44
1:V:274:VAL:HG21	1:V:293:ILE:HD11	1.99	0.44
1:b:314:ARG:HG3	1:c:122:GLU:OE2	2.18	0.44
1:g:331:ALA:O	1:g:334:SER:OG	2.30	0.44
1:l:25:GLN:HG2	1:l:351:SER:OG	2.16	0.44
1:q:219:ILE:HG23	1:q:220:GLU:N	2.32	0.44
1:r:6:ASN:O	1:r:6:ASN:CG	2.61	0.44
1:C:203:TYR:C	1:C:205:GLN:OE1	2.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:307:GLU:CD	1:H:307:GLU:H	2.26	0.44
1:M:287:ALA:HA	1:M:290:SER:OG	2.17	0.44
1:S:367:GLN:OE1	1:S:367:GLN:HA	2.18	0.44
1:k:3:VAL:HB	1:w:19:ASN:OD1	2.18	0.44
1:l:163:ASP:OD1	1:l:164:MET:N	2.49	0.44
1:D:206:GLU:N	1:D:206:GLU:CD	2.75	0.44
1:G:287:ALA:O	1:G:291:VAL:HG23	2.17	0.44
1:P:163:ASP:OD1	1:P:164:MET:N	2.50	0.44
1:P:373:LEU:HD23	1:P:373:LEU:O	2.17	0.44
1:V:70:ASP:OD1	1:V:70:ASP:N	2.49	0.44
1:X:82:MET:HE2	1:X:305:ARG:HG2	2.00	0.44
1:c:46:ALA:O	1:c:50:ILE:HG13	2.17	0.44
1:c:52:ASN:O	1:c:56:VAL:HG23	2.17	0.44
1:d:169:LYS:HD3	1:d:169:LYS:C	2.43	0.44
1:f:138:LEU:N	1:f:138:LEU:HD13	2.32	0.44
1:g:179:GLU:OE1	1:g:179:GLU:N	2.46	0.44
1:g:332:SER:O	1:g:336:ILE:HD12	2.17	0.44
1:C:193:ASN:O	1:C:193:ASN:OD1	2.35	0.44
1:D:332:SER:O	1:D:336:ILE:HD12	2.18	0.44
1:H:166:SER:OG	1:H:277:ASP:OD1	2.24	0.44
1:K:160:GLU:OE2	1:K:162:LYS:HE3	2.17	0.44
1:K:198:ASN:OD1	1:K:198:ASN:C	2.59	0.44
1:O:53:ARG:O	1:O:56:VAL:HG22	2.18	0.44
1:O:281:VAL:O	1:O:281:VAL:CG1	2.66	0.44
1:Q:3:VAL:O	1:Q:3:VAL:HG23	2.17	0.44
1:Q:167:ASP:OD1	1:Q:167:ASP:N	2.50	0.44
1:d:250:ASN:CG	1:d:250:ASN:O	2.60	0.44
1:d:299:LYS:HA	1:d:302:ASP:OD1	2.18	0.44
1:e:109:ARG:HB3	1:e:282:THR:HA	2.00	0.44
1:g:37:LYS:HE3	1:g:338:ASP:O	2.17	0.44
1:h:128:GLU:OE2	1:h:165:ARG:NH1	2.50	0.44
1:n:160:GLU:OE1	1:n:162:LYS:HG3	2.18	0.44
1:w:350:LYS:O	1:w:354:LEU:HD13	2.18	0.44
1:F:165:ARG:HB3	1:F:167:ASP:OD1	2.18	0.44
1:K:193:ASN:O	1:K:212:SER:HA	2.18	0.44
1:X:90:GLN:C	1:X:90:GLN:CD	2.86	0.44
1:X:195:LEU:HD12	1:X:196:LYS:N	2.33	0.44
1:X:279:ILE:HG22	1:X:280:ASP:N	2.33	0.44
1:c:137:LEU:HB2	1:c:138:LEU:HD22	1.99	0.44
1:d:169:LYS:O	1:d:169:LYS:HD3	2.18	0.44
1:f:277:ASP:N	1:f:277:ASP:OD2	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:128:GLU:OE2	1:g:165:ARG:NH1	2.51	0.44
1:i:207:GLN:N	1:i:207:GLN:OE1	2.51	0.44
1:o:12:MET:SD	1:o:12:MET:C	3.01	0.44
1:A:275:THR:HG22	1:A:276:VAL:N	2.33	0.44
1:D:169:LYS:O	1:D:172:GLY:N	2.42	0.44
1:F:184:LYS:NZ	1:F:220:GLU:OE1	2.51	0.44
1:G:66:ARG:O	1:G:70:ASP:OD1	2.36	0.44
1:O:173:GLY:HA2	1:O:249:ASN:OD1	2.18	0.44
1:d:144:ALA:HB1	1:d:159:LEU:O	2.17	0.44
1:i:162:LYS:HG2	1:i:304:HIS:CE1	2.52	0.44
1:j:238:ASP:OD1	1:j:238:ASP:C	2.61	0.44
1:l:255:GLU:OE1	1:l:255:GLU:N	2.51	0.44
1:m:299:LYS:HD3	1:m:299:LYS:C	2.42	0.44
1:p:82:MET:HE1	1:p:308:LEU:HD11	2.00	0.44
1:u:218:ASP:OD1	1:u:221:GLU:HB2	2.18	0.44
1:w:168:ASN:OD1	1:w:169:LYS:N	2.51	0.44
1:B:280:ASP:OD1	1:B:280:ASP:C	2.60	0.44
1:L:275:THR:HG22	1:L:276:VAL:N	2.33	0.44
1:R:239:GLN:HG2	1:R:240:ASP:OD2	2.18	0.44
1:X:70:ASP:N	1:X:70:ASP:OD1	2.51	0.44
1:d:164:MET:SD	1:d:164:MET:N	2.91	0.44
1:h:279:ILE:HG21	1:h:290:SER:CB	2.48	0.44
1:i:142:HIS:CG	1:i:143:GLY:H	2.36	0.44
1:j:13:THR:HG22	1:u:327:GLU:OE1	2.18	0.44
1:j:177:GLN:O	1:j:268:LEU:HA	2.17	0.44
1:m:311:PHE:CZ	1:m:315:PHE:CE1	3.05	0.44
1:r:365:ALA:O	1:r:369:PRO:HD2	2.18	0.44
1:r:373:LEU:HD13	1:r:373:LEU:C	2.43	0.44
1:s:184:LYS:HD3	1:s:184:LYS:H	1.83	0.44
1:w:302:ASP:OD2	1:w:303:SER:N	2.51	0.44
1:B:141:THR:CG2	1:B:142:HIS:N	2.80	0.43
1:L:106:LYS:HD3	1:L:110:VAL:HG23	1.98	0.43
1:N:201:ASP:OD1	1:N:201:ASP:C	2.61	0.43
1:R:3:VAL:O	1:R:3:VAL:CG1	2.66	0.43
1:X:68:ALA:O	1:X:72:ILE:HG12	2.18	0.43
1:f:98:GLN:OE1	1:f:98:GLN:O	2.36	0.43
1:f:161:LEU:HD11	1:f:308:LEU:CD2	2.48	0.43
1:f:167:ASP:OD1	1:f:167:ASP:N	2.49	0.43
1:i:144:ALA:HB2	1:i:160:GLU:OE1	2.18	0.43
1:s:311:PHE:CZ	1:s:315:PHE:CE2	3.06	0.43
1:u:219:ILE:HG23	1:u:220:GLU:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:LYS:HE2	1:F:338:ASP:O	2.18	0.43
1:O:147:PHE:N	1:O:157:VAL:O	2.45	0.43
1:Q:170:MET:HE3	1:Q:170:MET:HA	2.00	0.43
1:S:307:GLU:OE1	1:S:307:GLU:N	2.48	0.43
1:U:201:ASP:OD1	1:U:201:ASP:C	2.59	0.43
1:Z:97:LEU:C	1:Z:97:LEU:CD2	2.89	0.43
1:b:92:MET:HE2	1:b:92:MET:CA	2.47	0.43
1:c:201:ASP:OD1	1:c:201:ASP:C	2.62	0.43
1:g:37:LYS:NZ	1:g:336:ILE:O	2.44	0.43
1:k:13:THR:O	1:k:16:ARG:HB3	2.18	0.43
1:o:8:ASN:O	1:o:8:ASN:OD1	2.35	0.43
1:E:153:ASN:OD1	1:E:153:ASN:O	2.36	0.43
1:F:288:GLN:O	1:Q:153:ASN:ND2	2.51	0.43
1:J:231:ASP:OD2	1:J:231:ASP:C	2.61	0.43
1:K:327:GLU:OE2	1:V:16:ARG:HD3	2.18	0.43
1:L:65:VAL:O	1:L:69:ASN:OD1	2.36	0.43
1:L:106:LYS:HA	1:L:106:LYS:HE2	2.00	0.43
1:O:287:ALA:O	1:O:290:SER:OG	2.29	0.43
1:O:332:SER:O	1:O:336:ILE:CD1	2.67	0.43
1:Q:289:GLU:OE1	1:Q:293:ILE:HD11	2.18	0.43
1:S:328:ASN:OD1	1:T:76:GLN:NE2	2.45	0.43
1:T:190:GLU:OE2	1:T:190:GLU:N	2.30	0.43
1:V:366:LYS:O	1:V:369:PRO:HD2	2.18	0.43
1:X:199:LEU:HB3	1:X:256:VAL:HG23	2.00	0.43
1:f:109:ARG:HD3	1:f:282:THR:O	2.18	0.43
1:A:110:VAL:O	1:A:114:GLU:OE1	2.37	0.43
1:B:7:THR:HG21	1:i:334:SER:OG	2.18	0.43
1:F:255:GLU:N	1:F:255:GLU:CD	2.76	0.43
1:O:299:LYS:O	1:O:302:ASP:OD1	2.37	0.43
1:X:139:ASN:OD1	1:X:140:GLY:N	2.51	0.43
1:d:298:LEU:O	1:d:301:VAL:HG22	2.18	0.43
1:g:109:ARG:HB3	1:g:282:THR:HA	2.01	0.43
1:j:182:LYS:O	1:j:183:GLY:C	2.60	0.43
1:k:46:ALA:O	1:k:50:ILE:HG13	2.18	0.43
1:o:110:VAL:O	1:o:114:GLU:OE1	2.36	0.43
1:p:173:GLY:HA2	1:p:249:ASN:OD1	2.18	0.43
1:s:61:LEU:HD12	1:s:326:ASN:HA	1.99	0.43
1:w:29:MET:SD	1:w:348:MET:HB2	2.58	0.43
1:E:85:THR:HG23	1:E:123:LEU:HD22	2.00	0.43
1:F:174:VAL:HG13	1:F:272:LYS:O	2.19	0.43
1:F:236:SER:OG	1:Q:153:ASN:ND2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:38:ILE:O	1:M:337:LYS:NZ	2.51	0.43
1:U:16:ARG:O	1:U:20:ASN:OD1	2.36	0.43
1:Z:92:MET:HE1	1:Z:119:LEU:HB3	1.99	0.43
1:c:371:SER:O	1:c:374:SER:OG	2.31	0.43
1:f:298:LEU:O	1:f:301:VAL:HG12	2.17	0.43
1:f:314:ARG:NH2	1:g:122:GLU:OE1	2.52	0.43
1:g:303:SER:O	1:g:307:GLU:OE1	2.35	0.43
1:h:82:MET:HG3	1:h:164:MET:HE3	2.01	0.43
1:j:219:ILE:HG23	1:j:220:GLU:N	2.33	0.43
1:k:82:MET:HE1	1:k:308:LEU:HD12	2.00	0.43
1:m:375:LEU:O	1:n:366:LYS:NZ	2.49	0.43
1:n:218:ASP:CG	1:n:219:ILE:N	2.77	0.43
1:B:201:ASP:OD1	1:B:201:ASP:C	2.61	0.43
1:D:59:ARG:NH2	1:k:90:GLN:HB3	2.32	0.43
1:D:307:GLU:OE2	1:l:114:GLU:OE1	2.37	0.43
1:G:37:LYS:NZ	1:G:338:ASP:O	2.39	0.43
1:P:291:VAL:HG13	1:P:292:ALA:N	2.34	0.43
1:S:184:LYS:HE3	1:d:144:ALA:HB3	2.00	0.43
1:X:113:GLN:HG3	1:X:282:THR:HG23	2.00	0.43
1:c:218:ASP:OD1	1:c:219:ILE:N	2.52	0.43
1:f:147:PHE:N	1:f:147:PHE:CD1	2.86	0.43
1:g:179:GLU:CD	1:g:180:SER:N	2.77	0.43
1:j:141:THR:O	1:j:141:THR:CG2	2.67	0.43
1:w:206:GLU:OE2	1:w:206:GLU:C	2.62	0.43
1:C:167:ASP:OD1	1:C:167:ASP:N	2.45	0.43
1:F:257:GLU:HA	1:F:257:GLU:OE2	2.18	0.43
1:H:184:LYS:NZ	1:H:220:GLU:OE2	2.49	0.43
1:L:349:THR:O	1:L:353:ILE:HD12	2.18	0.43
1:M:219:ILE:HG23	1:M:220:GLU:N	2.33	0.43
1:S:236:SER:HB3	1:d:153:ASN:OD1	2.19	0.43
1:U:184:LYS:HE2	1:f:144:ALA:HB1	2.00	0.43
1:Z:96:SER:HB3	1:Z:291:VAL:HG22	2.01	0.43
1:Z:290:SER:HA	1:Z:293:ILE:HG22	1.99	0.43
1:b:225:TYR:O	1:b:229:GLN:HG2	2.19	0.43
1:e:66:ARG:NH1	1:e:66:ARG:HB3	2.34	0.43
1:e:223:ALA:O	1:e:224:THR:C	2.59	0.43
1:i:356:GLN:OE1	1:i:357:ALA:N	2.51	0.43
1:i:361:ILE:HG13	1:u:29:MET:HE2	2.01	0.43
1:j:218:ASP:CG	1:j:219:ILE:N	2.77	0.43
1:k:150:GLY:HA3	1:k:155:GLU:HB3	2.00	0.43
1:u:35:GLY:C	1:u:339:THR:HG22	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:ALA:O	1:D:366:LYS:HG2	2.18	0.43
1:N:311:PHE:CZ	1:N:315:PHE:CE1	3.07	0.43
1:R:83:ASN:OD1	1:R:83:ASN:C	2.62	0.43
1:R:138:LEU:HD22	1:R:164:MET:CE	2.48	0.43
1:T:144:ALA:HA	1:T:159:LEU:O	2.18	0.43
1:X:37:LYS:HG3	1:X:38:ILE:HG13	1.99	0.43
1:c:307:GLU:C	1:c:307:GLU:OE1	2.62	0.43
1:f:85:THR:O	1:f:88:ILE:HG22	2.18	0.43
1:s:37:LYS:HZ3	1:s:336:ILE:C	2.24	0.43
1:A:223:ALA:O	1:A:227:ASN:ND2	2.46	0.43
1:B:335:ARG:NH1	1:j:73:SER:OG	2.52	0.43
1:C:173:GLY:HA3	1:C:246:PHE:CZ	2.54	0.43
1:G:160:GLU:C	1:G:160:GLU:CD	2.87	0.43
1:G:225:TYR:CZ	1:G:229:GLN:NE2	2.84	0.43
1:K:313:ASN:ND2	1:h:115:GLU:OE2	2.51	0.43
1:O:219:ILE:HD12	1:O:237:VAL:HG21	2.00	0.43
1:P:92:MET:HE1	1:P:123:LEU:HD11	1.99	0.43
1:S:169:LYS:HE2	1:S:249:ASN:HB3	2.00	0.43
1:S:214:LYS:HE3	1:e:165:ARG:NH2	2.34	0.43
1:T:270:GLU:N	1:T:270:GLU:CD	2.77	0.43
1:V:8:ASN:OD1	1:V:8:ASN:C	2.62	0.43
1:b:232:LEU:HD12	1:b:232:LEU:H	1.83	0.43
1:c:113:GLN:OE1	1:c:113:GLN:O	2.37	0.43
1:f:153:ASN:OD1	1:f:153:ASN:C	2.62	0.43
1:k:193:ASN:OD1	1:k:193:ASN:C	2.62	0.43
1:m:201:ASP:OD1	1:m:201:ASP:C	2.61	0.43
1:q:272:LYS:HD2	1:q:273:LYS:N	2.33	0.43
1:r:6:ASN:O	1:r:6:ASN:OD1	2.37	0.43
1:r:275:THR:HG22	1:r:276:VAL:H	1.84	0.43
1:w:304:HIS:HA	1:w:307:GLU:OE1	2.19	0.43
1:F:114:GLU:OE1	1:F:114:GLU:HA	2.19	0.43
1:Q:66:ARG:NH1	1:Q:66:ARG:HB3	2.34	0.43
1:S:158:MET:SD	1:S:158:MET:C	3.02	0.43
1:S:162:LYS:HG2	1:S:304:HIS:CE1	2.54	0.43
1:Z:39:ASN:OD1	1:Z:39:ASN:N	2.51	0.43
1:Z:89:LEU:O	1:Z:90:GLN:C	2.61	0.43
1:Z:336:ILE:HD12	1:Z:336:ILE:H	1.84	0.43
1:g:15:GLN:O	1:g:19:ASN:ND2	2.52	0.43
1:g:166:SER:OG	1:g:277:ASP:OD1	2.34	0.43
1:g:175:SER:O	1:g:271:GLY:HA2	2.19	0.43
1:i:219:ILE:HG23	1:i:220:GLU:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:57:GLN:O	1:n:61:LEU:HD22	2.18	0.43
1:w:108:GLU:CD	1:w:108:GLU:H	2.26	0.43
1:w:175:SER:O	1:w:271:GLY:HA2	2.19	0.43
1:B:112:ILE:HA	1:B:115:GLU:OE1	2.18	0.42
1:D:201:ASP:OD1	1:D:201:ASP:C	2.62	0.42
1:E:303:SER:O	1:E:307:GLU:OE1	2.36	0.42
1:G:250:ASN:OD1	1:G:250:ASN:C	2.62	0.42
1:H:142:HIS:CG	1:H:143:GLY:H	2.37	0.42
1:K:18:LEU:C	1:K:18:LEU:HD23	2.44	0.42
1:K:229:GLN:HE21	1:K:229:GLN:HA	1.84	0.42
1:N:106:LYS:HD2	1:N:106:LYS:HA	1.91	0.42
1:R:279:ILE:O	1:R:279:ILE:HG13	2.18	0.42
1:S:280:ASP:OD1	1:S:282:THR:HG23	2.19	0.42
1:d:121:ASP:O	1:d:121:ASP:OD2	2.36	0.42
1:d:163:ASP:C	1:d:164:MET:SD	3.02	0.42
1:k:50:ILE:HG22	1:k:54:LEU:HD11	2.00	0.42
1:q:231:ASP:OD2	1:q:231:ASP:C	2.62	0.42
1:r:365:ALA:O	1:r:369:PRO:CD	2.67	0.42
1:J:240:ASP:OD1	1:J:240:ASP:N	2.52	0.42
1:M:275:THR:HG22	1:M:276:VAL:N	2.33	0.42
1:O:219:ILE:HG13	1:O:220:GLU:N	2.34	0.42
1:O:255:GLU:OE1	1:O:255:GLU:HA	2.19	0.42
1:Q:328:ASN:OD1	1:R:76:GLN:NE2	2.52	0.42
1:R:162:LYS:HG2	1:R:304:HIS:CE1	2.54	0.42
1:R:252:VAL:O	1:R:252:VAL:HG23	2.19	0.42
1:X:298:LEU:O	1:X:302:ASP:OD2	2.37	0.42
1:b:99:SER:HB2	1:b:112:ILE:HG21	2.01	0.42
1:d:122:GLU:HA	1:d:125:ARG:HG2	2.01	0.42
1:d:167:ASP:OD1	1:d:167:ASP:N	2.49	0.42
1:f:114:GLU:CD	1:f:114:GLU:C	2.87	0.42
1:g:245:ILE:HD12	1:g:245:ILE:N	2.34	0.42
1:i:174:VAL:HG23	1:i:249:ASN:OD1	2.19	0.42
1:k:177:GLN:O	1:k:269:GLY:N	2.41	0.42
1:l:82:MET:HE1	1:l:304:HIS:ND1	2.34	0.42
1:m:324:ASN:OD1	1:m:328:ASN:ND2	2.52	0.42
1:s:143:GLY:CA	1:s:145:LYS:HE3	2.49	0.42
1:u:38:ILE:N	1:u:38:ILE:CD1	2.82	0.42
1:w:91:ARG:HG3	1:w:91:ARG:HH11	1.83	0.42
1:E:199:LEU:C	1:E:199:LEU:HD12	2.44	0.42
1:O:122:GLU:HA	1:O:122:GLU:OE1	2.18	0.42
1:O:336:ILE:HD12	1:O:336:ILE:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:219:ILE:HD11	1:P:243:LEU:HD13	2.00	0.42
1:P:341:PHE:O	1:P:345:THR:HG23	2.18	0.42
1:Q:288:GLN:O	1:b:153:ASN:ND2	2.52	0.42
1:S:240:ASP:OD1	1:S:240:ASP:N	2.52	0.42
1:U:325:ILE:O	1:U:329:VAL:HG13	2.20	0.42
1:V:254:GLY:C	1:V:255:GLU:OE1	2.62	0.42
1:b:52:ASN:O	1:b:56:VAL:HG23	2.19	0.42
1:b:328:ASN:OD1	1:c:76:GLN:NE2	2.52	0.42
1:d:37:LYS:HG2	1:d:337:LYS:O	2.20	0.42
1:i:373:LEU:HD12	1:s:353:ILE:HG23	2.02	0.42
1:k:10:SER:CB	1:w:30:GLU:OE1	2.67	0.42
1:k:121:ASP:OD1	1:k:121:ASP:C	2.61	0.42
1:m:25:GLN:HG2	1:m:29:MET:CE	2.48	0.42
1:r:163:ASP:OD1	1:r:164:MET:N	2.52	0.42
1:C:201:ASP:C	1:C:201:ASP:OD1	2.63	0.42
1:J:9:VAL:HA	1:J:12:MET:HG3	2.00	0.42
1:N:314:ARG:NE	1:O:122:GLU:OE1	2.47	0.42
1:P:170:MET:HE2	1:P:170:MET:HA	2.00	0.42
1:X:109:ARG:HB3	1:X:282:THR:HA	2.01	0.42
1:d:168:ASN:OD1	1:d:168:ASN:C	2.63	0.42
1:g:218:ASP:HB3	1:g:221:GLU:HG3	2.01	0.42
1:h:272:LYS:HD3	1:h:273:LYS:N	2.35	0.42
1:h:341:PHE:O	1:h:345:THR:HG23	2.19	0.42
1:l:25:GLN:HB3	1:l:351:SER:OG	2.19	0.42
1:p:142:HIS:CG	1:p:143:GLY:H	2.38	0.42
1:q:163:ASP:OD1	1:q:164:MET:N	2.52	0.42
1:r:25:GLN:C	1:r:25:GLN:CD	2.86	0.42
1:u:201:ASP:OD1	1:u:201:ASP:C	2.62	0.42
1:G:219:ILE:HG23	1:G:220:GLU:N	2.34	0.42
1:I:201:ASP:OD1	1:I:201:ASP:C	2.62	0.42
1:L:258:PHE:CD1	1:L:258:PHE:N	2.87	0.42
1:Z:178:ALA:HA	1:Z:267:GLY:O	2.18	0.42
1:b:158:MET:SD	1:b:159:LEU:N	2.92	0.42
1:b:234:LYS:O	1:b:246:PHE:N	2.48	0.42
1:b:245:ILE:HD13	1:b:268:LEU:HD11	2.00	0.42
1:f:326:ASN:HA	1:f:329:VAL:HG12	2.02	0.42
1:i:83:ASN:OD1	1:i:83:ASN:C	2.61	0.42
1:i:339:THR:OG1	1:i:344:GLU:OE1	2.38	0.42
1:l:153:ASN:OD1	1:l:153:ASN:C	2.63	0.42
1:l:199:LEU:HD12	1:l:199:LEU:C	2.45	0.42
1:m:279:ILE:O	1:m:279:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:238:ASP:C	1:w:238:ASP:OD1	2.62	0.42
1:G:178:ALA:HA	1:G:267:GLY:O	2.19	0.42
1:H:219:ILE:HG23	1:H:220:GLU:N	2.34	0.42
1:I:173:GLY:HA2	1:I:249:ASN:OD1	2.20	0.42
1:J:152:ASP:N	1:J:155:GLU:OE2	2.51	0.42
1:J:368:ALA:HB3	1:J:369:PRO:HD3	2.02	0.42
1:K:183:GLY:C	1:K:185:ASP:H	2.27	0.42
1:O:88:ILE:HB	1:O:123:LEU:HD21	2.02	0.42
1:X:165:ARG:O	1:X:168:ASN:HB2	2.20	0.42
1:X:169:LYS:N	1:X:169:LYS:CD	2.81	0.42
1:Z:92:MET:HG2	1:Z:294:ILE:HD11	2.00	0.42
1:b:201:ASP:OD1	1:b:201:ASP:C	2.62	0.42
1:g:162:LYS:HG3	1:g:304:HIS:CG	2.54	0.42
1:l:29:MET:O	1:l:32:LEU:CB	2.68	0.42
1:l:152:ASP:OD2	1:l:155:GLU:OE1	2.37	0.42
1:l:193:ASN:OD1	1:l:193:ASN:C	2.62	0.42
1:p:187:ASN:O	1:p:189:ALA:N	2.53	0.42
1:s:201:ASP:OD1	1:s:201:ASP:C	2.61	0.42
1:I:367:GLN:OE1	1:I:367:GLN:HA	2.20	0.42
1:N:255:GLU:OE2	1:N:255:GLU:HA	2.18	0.42
1:R:178:ALA:HA	1:R:267:GLY:O	2.19	0.42
1:S:288:GLN:O	1:d:153:ASN:ND2	2.52	0.42
1:c:171:MET:HB3	1:c:276:VAL:HG23	2.02	0.42
1:d:219:ILE:HG13	1:d:237:VAL:HG21	2.01	0.42
1:e:186:TRP:CH2	1:e:266:LEU:HD21	2.55	0.42
1:h:125:ARG:HH11	1:h:129:THR:HG21	1.85	0.42
1:n:231:ASP:OD1	1:n:231:ASP:C	2.62	0.42
1:o:311:PHE:CZ	1:o:315:PHE:CE1	3.07	0.42
1:s:13:THR:HG23	1:s:16:ARG:HH21	1.85	0.42
1:s:356:GLN:OE1	1:s:356:GLN:C	2.63	0.42
1:u:185:ASP:OD1	1:u:186:TRP:N	2.53	0.42
1:w:39:ASN:ND2	1:w:39:ASN:O	2.53	0.42
1:A:276:VAL:HA	1:A:279:ILE:HD11	2.01	0.42
1:E:179:GLU:HA	1:E:242:LYS:NZ	2.35	0.42
1:N:93:ARG:HB2	1:N:294:ILE:HG21	2.02	0.42
1:Q:125:ARG:NH1	1:Q:129:THR:HG21	2.35	0.42
1:Z:7:THR:HG22	1:Z:8:ASN:N	2.35	0.42
1:b:299:LYS:HD2	1:b:299:LYS:O	2.19	0.42
1:c:78:ALA:O	1:c:82:MET:HG3	2.20	0.42
1:h:272:LYS:NZ	1:h:273:LYS:O	2.31	0.42
1:j:46:ALA:O	1:j:50:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:239:GLN:CD	1:j:239:GLN:H	2.27	0.42
1:k:260:GLY:O	1:k:263:SER:HB3	2.20	0.42
1:k:368:ALA:HB3	1:k:369:PRO:HD3	2.01	0.42
1:p:311:PHE:CZ	1:p:315:PHE:CE1	3.07	0.42
1:r:30:GLU:OE1	1:r:30:GLU:HA	2.20	0.42
1:r:50:ILE:CG2	1:r:51:SER:N	2.83	0.42
1:E:201:ASP:OD1	1:E:201:ASP:C	2.63	0.42
1:E:373:LEU:HD12	1:E:373:LEU:O	2.20	0.42
1:P:125:ARG:NH1	1:P:129:THR:HG21	2.34	0.42
1:Q:253:GLU:CD	1:Q:254:GLY:N	2.78	0.42
1:R:46:ALA:O	1:R:50:ILE:HG13	2.20	0.42
1:T:4:ASN:OD1	1:T:4:ASN:O	2.38	0.42
1:Z:114:GLU:HA	1:Z:117:THR:OG1	2.20	0.42
1:i:106:LYS:NZ	1:i:282:THR:O	2.53	0.42
1:i:157:VAL:HG12	1:i:158:MET:N	2.35	0.42
1:k:10:SER:HB2	1:w:30:GLU:OE1	2.19	0.42
1:n:365:ALA:O	1:n:368:ALA:HB3	2.20	0.42
1:w:61:LEU:HD23	1:w:151:ALA:HB2	2.02	0.42
1:D:231:ASP:OD2	1:D:231:ASP:N	2.51	0.42
1:E:5:VAL:HG23	1:l:341:PHE:CE1	2.55	0.42
1:E:82:MET:HE1	1:E:308:LEU:HD11	2.02	0.42
1:L:328:ASN:OD1	1:M:76:GLN:NE2	2.52	0.42
1:M:66:ARG:NH1	1:M:66:ARG:HB3	2.35	0.42
1:X:240:ASP:OD2	1:X:242:LYS:HD2	2.20	0.42
1:Z:238:ASP:OD1	1:Z:242:LYS:HB2	2.19	0.42
1:A:201:ASP:OD1	1:A:201:ASP:C	2.63	0.41
1:C:140:GLY:O	1:C:141:THR:HB	2.20	0.41
1:M:344:GLU:OE2	1:M:344:GLU:HA	2.18	0.41
1:O:218:ASP:CG	1:O:219:ILE:N	2.78	0.41
1:P:125:ARG:HH11	1:P:129:THR:HG21	1.84	0.41
1:S:370:ASN:OD1	1:S:370:ASN:O	2.38	0.41
1:U:258:PHE:N	1:U:258:PHE:CD1	2.88	0.41
1:c:160:GLU:HG3	1:c:161:LEU:N	2.35	0.41
1:f:270:GLU:CD	1:f:271:GLY:H	2.28	0.41
1:h:153:ASN:ND2	1:s:288:GLN:O	2.53	0.41
1:i:218:ASP:CG	1:i:219:ILE:N	2.78	0.41
1:l:21:ALA:O	1:l:22:ASN:C	2.63	0.41
1:q:270:GLU:CD	1:q:271:GLY:N	2.78	0.41
1:w:168:ASN:OD1	1:w:170:MET:N	2.45	0.41
1:E:273:LYS:N	1:E:273:LYS:CD	2.82	0.41
1:G:340:ASP:OD1	1:G:343:LYS:HD3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:ASP:N	1:L:185:ASP:OD1	2.52	0.41
1:L:238:ASP:OD1	1:L:238:ASP:C	2.63	0.41
1:O:199:LEU:HD12	1:O:199:LEU:C	2.45	0.41
1:P:142:HIS:HE2	1:P:145:LYS:HG3	1.85	0.41
1:e:54:LEU:HD22	1:e:329:VAL:HG13	2.00	0.41
1:g:153:ASN:OD1	1:g:153:ASN:N	2.52	0.41
1:g:195:LEU:C	1:g:195:LEU:HD23	2.45	0.41
1:j:208:GLU:C	1:j:208:GLU:CD	2.88	0.41
1:k:147:PHE:N	1:k:157:VAL:O	2.52	0.41
1:m:59:ARG:O	1:m:63:VAL:HG23	2.20	0.41
1:u:31:ARG:NH2	1:u:37:LYS:HB2	2.34	0.41
1:u:208:GLU:CD	1:u:208:GLU:C	2.88	0.41
1:u:336:ILE:HG23	1:u:337:LYS:N	2.35	0.41
1:C:332:SER:OG	1:D:73:SER:HB2	2.20	0.41
1:F:185:ASP:OD1	1:F:185:ASP:N	2.53	0.41
1:J:340:ASP:OD2	1:U:2:ALA:HB1	2.20	0.41
1:K:328:ASN:ND2	1:h:76:GLN:OE1	2.51	0.41
1:M:39:ASN:OD1	1:M:39:ASN:N	2.53	0.41
1:N:257:GLU:C	1:N:257:GLU:CD	2.88	0.41
1:Q:375:LEU:HD11	1:R:362:LEU:HD23	2.02	0.41
1:S:172:GLY:C	1:S:249:ASN:OD1	2.63	0.41
1:Z:142:HIS:CG	1:Z:143:GLY:N	2.89	0.41
1:b:108:GLU:O	1:b:112:ILE:HG12	2.20	0.41
1:d:170:MET:HG3	1:d:300:TYR:CD1	2.55	0.41
1:e:188:VAL:O	1:e:215:ALA:CB	2.68	0.41
1:i:131:SER:HB3	1:i:136:LYS:HD3	2.02	0.41
1:j:173:GLY:HA3	1:j:246:PHE:CZ	2.55	0.41
1:l:22:ASN:C	1:l:22:ASN:OD1	2.63	0.41
1:l:37:LYS:HG2	1:l:337:LYS:O	2.20	0.41
1:l:169:LYS:O	1:l:172:GLY:N	2.34	0.41
1:n:25:GLN:HG2	1:n:29:MET:SD	2.59	0.41
1:n:55:ASN:OD1	1:n:333:LYS:HD2	2.21	0.41
1:s:184:LYS:N	1:s:184:LYS:CD	2.83	0.41
1:A:84:GLU:OE2	1:A:84:GLU:HA	2.20	0.41
1:A:232:LEU:HA	1:A:251:LYS:HD3	2.02	0.41
1:E:370:ASN:OD1	1:E:370:ASN:C	2.64	0.41
1:H:193:ASN:O	1:H:193:ASN:CG	2.63	0.41
1:K:169:LYS:O	1:K:172:GLY:N	2.41	0.41
1:N:106:LYS:O	1:N:110:VAL:HG23	2.20	0.41
1:S:170:MET:HA	1:S:170:MET:HE3	2.02	0.41
1:i:373:LEU:HD11	1:s:356:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:218:ASP:CG	1:j:219:ILE:H	2.28	0.41
1:m:372:ALA:HB3	1:w:353:ILE:HG21	2.02	0.41
1:n:49:GLN:C	1:n:49:GLN:CD	2.88	0.41
1:n:57:GLN:O	1:n:61:LEU:CD2	2.69	0.41
1:A:90:GLN:OE1	1:L:56:VAL:HG22	2.20	0.41
1:B:113:GLN:OE1	1:B:281:VAL:HG22	2.19	0.41
1:C:367:GLN:O	1:C:368:ALA:C	2.63	0.41
1:M:153:ASN:OD1	1:M:153:ASN:C	2.63	0.41
1:P:171:MET:HB3	1:P:276:VAL:HG23	2.01	0.41
1:T:66:ARG:HH11	1:T:66:ARG:HG3	1.86	0.41
1:T:169:LYS:HE3	1:T:169:LYS:HB2	1.92	0.41
1:V:334:SER:HA	1:V:338:ASP:OD2	2.21	0.41
1:f:175:SER:O	1:f:271:GLY:HA2	2.20	0.41
1:i:160:GLU:OE1	1:i:160:GLU:HA	2.20	0.41
1:m:218:ASP:OD1	1:m:218:ASP:C	2.62	0.41
1:u:281:VAL:O	1:u:281:VAL:CG1	2.68	0.41
1:w:25:GLN:HG2	1:w:351:SER:CB	2.51	0.41
1:B:177:GLN:C	1:B:268:LEU:HD23	2.45	0.41
1:C:219:ILE:HG23	1:C:220:GLU:N	2.34	0.41
1:H:82:MET:HE3	1:H:82:MET:HB2	1.96	0.41
1:I:341:PHE:CE1	1:T:5:VAL:HG23	2.56	0.41
1:J:83:ASN:OD1	1:J:83:ASN:C	2.64	0.41
1:K:173:GLY:HA2	1:K:249:ASN:HD22	1.86	0.41
1:K:219:ILE:HG23	1:K:220:GLU:N	2.35	0.41
1:Q:299:LYS:O	1:Q:300:TYR:C	2.63	0.41
1:R:201:ASP:C	1:R:201:ASP:OD1	2.64	0.41
1:S:150:GLY:HA3	1:S:155:GLU:HB2	2.02	0.41
1:U:219:ILE:HG23	1:U:220:GLU:N	2.36	0.41
1:b:321:ASN:O	1:b:325:ILE:HG13	2.20	0.41
1:c:370:ASN:ND2	1:c:370:ASN:C	2.78	0.41
1:e:324:ASN:O	1:e:328:ASN:ND2	2.53	0.41
1:i:225:TYR:CZ	1:i:229:GLN:NE2	2.88	0.41
1:j:18:LEU:HD23	1:j:18:LEU:C	2.45	0.41
1:o:38:ILE:O	1:o:337:LYS:NZ	2.54	0.41
1:o:164:MET:HE3	1:o:164:MET:HA	2.02	0.41
1:r:332:SER:OG	1:s:73:SER:HB3	2.20	0.41
1:D:3:VAL:HG13	1:D:3:VAL:O	2.20	0.41
1:E:29:MET:O	1:E:32:LEU:HB3	2.20	0.41
1:F:106:LYS:O	1:F:110:VAL:HG23	2.21	0.41
1:G:153:ASN:OD1	1:G:153:ASN:C	2.63	0.41
1:K:160:GLU:CD	1:K:160:GLU:C	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:22:ASN:OD1	1:P:23:SER:N	2.53	0.41
1:R:289:GLU:OE1	1:R:293:ILE:HD11	2.20	0.41
1:V:336:ILE:HD12	1:V:336:ILE:H	1.85	0.41
1:b:193:ASN:HA	1:b:262:LEU:HD13	2.02	0.41
1:d:110:VAL:O	1:d:114:GLU:HG2	2.20	0.41
1:d:157:VAL:HG12	1:d:158:MET:N	2.36	0.41
1:e:252:VAL:HG12	1:e:253:GLU:N	2.35	0.41
1:f:201:ASP:OD1	1:f:201:ASP:C	2.64	0.41
1:h:171:MET:HB3	1:h:276:VAL:HG23	2.01	0.41
1:i:163:ASP:OD1	1:i:164:MET:N	2.53	0.41
1:i:280:ASP:OD1	1:i:280:ASP:C	2.63	0.41
1:n:173:GLY:HA2	1:n:249:ASN:OD1	2.20	0.41
1:q:344:GLU:OE2	1:q:344:GLU:HA	2.21	0.41
1:w:270:GLU:CD	1:w:271:GLY:H	2.29	0.41
1:A:370:ASN:HD22	1:A:370:ASN:C	2.27	0.41
1:F:66:ARG:HG3	1:F:66:ARG:HH11	1.86	0.41
1:F:179:GLU:OE2	1:F:180:SER:OG	2.36	0.41
1:K:196:LYS:HZ2	1:K:208:GLU:CD	2.28	0.41
1:N:94:ASP:OD2	1:N:94:ASP:C	2.63	0.41
1:N:113:GLN:OE1	1:N:281:VAL:HG12	2.21	0.41
1:O:332:SER:O	1:O:336:ILE:HD12	2.20	0.41
1:S:157:VAL:HG12	1:S:158:MET:N	2.35	0.41
1:Z:298:LEU:C	1:Z:298:LEU:HD23	2.46	0.41
1:b:90:GLN:OE1	1:b:90:GLN:C	2.64	0.41
1:c:91:ARG:NE	1:c:95:LEU:HD21	2.36	0.41
1:q:332:SER:OG	1:r:73:SER:HB3	2.21	0.41
1:G:148:GLN:NE2	1:G:150:GLY:O	2.54	0.41
1:H:255:GLU:OE1	1:H:255:GLU:N	2.54	0.41
1:M:113:GLN:HB2	1:M:282:THR:HG22	2.01	0.41
1:M:122:GLU:OE2	1:M:122:GLU:HA	2.21	0.41
1:N:320:SER:O	1:N:324:ASN:OD1	2.38	0.41
1:O:201:ASP:OD2	1:O:201:ASP:C	2.64	0.41
1:Q:3:VAL:O	1:Q:3:VAL:CG2	2.68	0.41
1:Q:117:THR:O	1:Q:121:ASP:OD1	2.39	0.41
1:Q:171:MET:HB3	1:Q:276:VAL:HG23	2.03	0.41
1:T:370:ASN:OD1	1:T:370:ASN:C	2.64	0.41
1:T:370:ASN:OD1	1:T:370:ASN:O	2.38	0.41
1:V:219:ILE:HG23	1:V:220:GLU:N	2.36	0.41
1:c:37:LYS:HG2	1:c:337:LYS:O	2.21	0.41
1:d:88:ILE:HD11	1:d:122:GLU:HB2	2.03	0.41
1:e:106:LYS:O	1:e:110:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:209:ILE:HD12	1:e:209:ILE:N	2.35	0.41
1:f:88:ILE:HG23	1:f:89:LEU:N	2.36	0.41
1:g:285:GLY:O	1:g:289:GLU:HG3	2.21	0.41
1:j:173:GLY:HA2	1:j:249:ASN:OD1	2.21	0.41
1:l:256:VAL:C	1:l:257:GLU:OE1	2.64	0.41
1:n:113:GLN:OE1	1:n:281:VAL:HG22	2.20	0.41
1:n:125:ARG:HG2	1:n:125:ARG:NH1	2.35	0.41
1:p:55:ASN:OD1	1:p:56:VAL:N	2.53	0.41
1:q:4:ASN:OD1	1:q:6:ASN:N	2.54	0.41
1:q:280:ASP:OD1	1:q:281:VAL:N	2.53	0.41
1:r:219:ILE:HG23	1:r:220:GLU:N	2.35	0.41
1:D:85:THR:HG21	1:D:164:MET:CE	2.51	0.41
1:I:37:LYS:HE2	1:I:338:ASP:O	2.21	0.41
1:N:209:ILE:HD12	1:N:209:ILE:HA	1.96	0.41
1:N:367:GLN:O	1:N:368:ALA:C	2.63	0.41
1:V:327:GLU:OE2	1:g:16:ARG:HD3	2.20	0.41
1:b:194:ASP:N	1:b:194:ASP:OD1	2.54	0.41
1:e:44:ASP:OD1	1:e:44:ASP:C	2.62	0.41
1:f:105:SER:O	1:f:109:ARG:HG3	2.21	0.41
1:i:356:GLN:CD	1:i:356:GLN:C	2.89	0.41
1:s:25:GLN:C	1:s:25:GLN:CD	2.89	0.41
1:s:153:ASN:OD1	1:s:153:ASN:C	2.64	0.41
1:s:370:ASN:OD1	1:s:370:ASN:C	2.63	0.41
1:w:38:ILE:O	1:w:38:ILE:HG13	2.21	0.41
1:w:62:ASP:OD1	1:w:62:ASP:N	2.55	0.41
1:C:153:ASN:ND2	1:j:291:VAL:HB	2.36	0.40
1:G:175:SER:O	1:G:271:GLY:HA2	2.22	0.40
1:J:366:LYS:O	1:J:369:PRO:HD2	2.21	0.40
1:L:171:MET:HB3	1:L:276:VAL:HG23	2.02	0.40
1:M:299:LYS:HD2	1:M:299:LYS:O	2.20	0.40
1:P:206:GLU:CD	1:P:206:GLU:N	2.78	0.40
1:S:367:GLN:O	1:S:368:ALA:C	2.64	0.40
1:c:91:ARG:O	1:c:95:LEU:HD23	2.20	0.40
1:d:217:ASP:OD1	1:d:217:ASP:N	2.54	0.40
1:f:106:LYS:HA	1:f:109:ARG:HB2	2.04	0.40
1:g:163:ASP:OD1	1:g:164:MET:N	2.54	0.40
1:h:40:SER:OG	1:h:42:LYS:HG2	2.21	0.40
1:i:190:GLU:CD	1:i:191:GLY:N	2.79	0.40
1:i:346:THR:HG23	1:i:347:ALA:N	2.36	0.40
1:j:277:ASP:OD2	1:j:277:ASP:O	2.39	0.40
1:m:144:ALA:HB2	1:m:160:GLU:CG	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:153:ASN:OD1	1:o:153:ASN:O	2.39	0.40
1:r:159:LEU:HD12	1:r:160:GLU:N	2.36	0.40
1:s:276:VAL:O	1:s:279:ILE:HG12	2.21	0.40
1:B:173:GLY:HA2	1:B:249:ASN:OD1	2.21	0.40
1:D:201:ASP:OD2	1:D:203:TYR:HD2	2.03	0.40
1:F:108:GLU:OE2	1:P:53:ARG:NH1	2.49	0.40
1:G:361:ILE:HG23	1:o:29:MET:HG2	2.02	0.40
1:H:173:GLY:HA2	1:H:249:ASN:OD1	2.22	0.40
1:K:131:SER:HB3	1:K:136:LYS:HD2	2.04	0.40
1:O:37:LYS:HG2	1:O:337:LYS:O	2.22	0.40
1:O:50:ILE:HG13	1:O:50:ILE:H	1.77	0.40
1:O:134:GLY:O	1:O:135:ASN:C	2.65	0.40
1:P:106:LYS:HG3	1:Z:203:TYR:OH	2.21	0.40
1:Q:295:ASP:OD1	1:Q:299:LYS:NZ	2.55	0.40
1:S:73:SER:OG	1:c:335:ARG:NH2	2.52	0.40
1:U:270:GLU:CD	1:U:271:GLY:N	2.79	0.40
1:g:209:ILE:N	1:g:209:ILE:CD1	2.84	0.40
1:n:39:ASN:OD1	1:n:43:ASP:OD2	2.39	0.40
1:u:70:ASP:OD2	1:u:70:ASP:C	2.64	0.40
1:H:236:SER:HB3	1:S:153:ASN:OD1	2.21	0.40
1:H:328:ASN:OD1	1:I:76:GLN:NE2	2.52	0.40
1:O:220:GLU:OE1	1:O:220:GLU:HA	2.21	0.40
1:V:336:ILE:HD12	1:V:336:ILE:N	2.35	0.40
1:X:91:ARG:NH1	1:X:95:LEU:HG	2.36	0.40
1:g:332:SER:O	1:g:336:ILE:CD1	2.70	0.40
1:h:125:ARG:NH1	1:h:129:THR:HG21	2.37	0.40
1:i:280:ASP:OD1	1:i:282:THR:HG23	2.22	0.40
1:j:182:LYS:HD3	1:j:186:TRP:CG	2.57	0.40
1:l:9:VAL:HA	1:l:12:MET:HG3	2.03	0.40
1:n:336:ILE:HG23	1:n:337:LYS:N	2.36	0.40
1:q:218:ASP:OD1	1:q:219:ILE:N	2.49	0.40
1:s:150:GLY:HA3	1:s:155:GLU:HB2	2.03	0.40
1:s:160:GLU:OE1	1:s:161:LEU:N	2.54	0.40
1:A:373:LEU:HD12	1:A:376:LEU:HD12	2.03	0.40
1:G:341:PHE:CE1	1:R:5:VAL:HG23	2.56	0.40
1:H:184:LYS:HD3	1:S:158:MET:HG2	2.04	0.40
1:K:152:ASP:OD2	1:K:152:ASP:N	2.52	0.40
1:O:177:GLN:O	1:O:269:GLY:N	2.50	0.40
1:T:46:ALA:O	1:T:50:ILE:HG13	2.21	0.40
1:c:164:MET:O	1:c:165:ARG:C	2.63	0.40
1:d:250:ASN:O	1:d:251:LYS:HD2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:307:GLU:OE2	1:d:307:GLU:HA	2.22	0.40
1:f:124:ASN:OD1	1:f:165:ARG:NH1	2.55	0.40
1:g:52:ASN:O	1:g:56:VAL:HG23	2.22	0.40
1:i:38:ILE:O	1:i:38:ILE:HG22	2.22	0.40
1:l:219:ILE:HG23	1:l:220:GLU:N	2.36	0.40
1:s:275:THR:HG22	1:s:276:VAL:N	2.37	0.40
1:s:281:VAL:O	1:s:281:VAL:CG1	2.70	0.40
1:u:231:ASP:OD1	1:u:251:LYS:NZ	2.54	0.40
1:w:8:ASN:OD1	1:w:8:ASN:N	2.54	0.40
1:B:165:ARG:HB3	1:B:167:ASP:OD1	2.22	0.40
1:D:55:ASN:OD1	1:D:55:ASN:C	2.64	0.40
1:F:349:THR:O	1:F:353:ILE:CD1	2.69	0.40
1:G:37:LYS:HG2	1:G:337:LYS:O	2.21	0.40
1:K:18:LEU:HD23	1:K:18:LEU:O	2.22	0.40
1:L:349:THR:O	1:L:353:ILE:CD1	2.69	0.40
1:M:280:ASP:OD1	1:M:282:THR:HG23	2.22	0.40
1:N:18:LEU:HD23	1:N:18:LEU:C	2.47	0.40
1:O:250:ASN:OD1	1:O:250:ASN:C	2.64	0.40
1:Q:277:ASP:OD1	1:Q:278:THR:N	2.55	0.40
1:d:188:VAL:HG12	1:d:217:ASP:N	2.36	0.40
1:f:275:THR:O	1:f:278:THR:OG1	2.36	0.40
1:j:184:LYS:O	1:j:185:ASP:HB2	2.21	0.40
1:p:238:ASP:OD1	1:p:238:ASP:C	2.64	0.40
1:p:280:ASP:OD1	1:p:282:THR:HG23	2.21	0.40
1:p:302:ASP:OD1	1:p:302:ASP:C	2.64	0.40
1:r:50:ILE:HD12	1:r:50:ILE:HA	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/377 (99%)	368 (98%)	6 (2%)	0	100	100
1	B	374/377 (99%)	362 (97%)	12 (3%)	0	100	100
1	C	374/377 (99%)	369 (99%)	5 (1%)	0	100	100
1	D	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
1	E	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
1	F	374/377 (99%)	368 (98%)	6 (2%)	0	100	100
1	G	374/377 (99%)	368 (98%)	6 (2%)	0	100	100
1	H	374/377 (99%)	368 (98%)	6 (2%)	0	100	100
1	I	374/377 (99%)	370 (99%)	4 (1%)	0	100	100
1	J	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	K	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	L	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	M	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	N	374/377 (99%)	368 (98%)	6 (2%)	0	100	100
1	O	374/377 (99%)	360 (96%)	14 (4%)	0	100	100
1	P	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	Q	374/377 (99%)	371 (99%)	3 (1%)	0	100	100
1	R	374/377 (99%)	364 (97%)	9 (2%)	1 (0%)	36	67
1	S	374/377 (99%)	369 (99%)	5 (1%)	0	100	100
1	T	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	U	374/377 (99%)	368 (98%)	6 (2%)	0	100	100
1	V	374/377 (99%)	368 (98%)	6 (2%)	0	100	100
1	X	374/377 (99%)	363 (97%)	11 (3%)	0	100	100
1	Z	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	b	374/377 (99%)	369 (99%)	5 (1%)	0	100	100
1	c	374/377 (99%)	369 (99%)	5 (1%)	0	100	100
1	d	374/377 (99%)	365 (98%)	9 (2%)	0	100	100
1	e	374/377 (99%)	363 (97%)	10 (3%)	1 (0%)	36	67
1	f	374/377 (99%)	365 (98%)	9 (2%)	0	100	100
1	g	374/377 (99%)	370 (99%)	4 (1%)	0	100	100
1	h	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	i	374/377 (99%)	366 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	374/377 (99%)	369 (99%)	4 (1%)	1 (0%)	36	67
1	k	374/377 (99%)	367 (98%)	7 (2%)	0	100	100
1	l	374/377 (99%)	360 (96%)	14 (4%)	0	100	100
1	m	374/377 (99%)	365 (98%)	9 (2%)	0	100	100
1	n	374/377 (99%)	370 (99%)	3 (1%)	1 (0%)	36	67
1	o	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	p	374/377 (99%)	367 (98%)	6 (2%)	1 (0%)	36	67
1	q	374/377 (99%)	366 (98%)	8 (2%)	0	100	100
1	r	374/377 (99%)	369 (99%)	5 (1%)	0	100	100
1	s	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
1	u	374/377 (99%)	368 (98%)	6 (2%)	0	100	100
1	w	374/377 (99%)	369 (99%)	5 (1%)	0	100	100
All	All	16456/16588 (99%)	16132 (98%)	319 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	j	188	VAL
1	e	213	ALA
1	n	145	LYS
1	R	215	ALA
1	p	188	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	B	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	C	300/301 (100%)	297 (99%)	3 (1%)	68	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	300/301 (100%)	296 (99%)	4 (1%)	61	77
1	E	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	F	300/301 (100%)	300 (100%)	0	100	100
1	G	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	H	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	I	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	J	300/301 (100%)	300 (100%)	0	100	100
1	K	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	L	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	M	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	N	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	O	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	P	300/301 (100%)	297 (99%)	3 (1%)	68	79
1	Q	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	R	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	S	300/301 (100%)	300 (100%)	0	100	100
1	T	300/301 (100%)	300 (100%)	0	100	100
1	U	300/301 (100%)	300 (100%)	0	100	100
1	V	300/301 (100%)	295 (98%)	5 (2%)	53	74
1	X	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	Z	300/301 (100%)	295 (98%)	5 (2%)	53	74
1	b	300/301 (100%)	300 (100%)	0	100	100
1	c	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	d	300/301 (100%)	297 (99%)	3 (1%)	68	79
1	e	300/301 (100%)	300 (100%)	0	100	100
1	f	300/301 (100%)	297 (99%)	3 (1%)	68	79
1	g	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	h	300/301 (100%)	300 (100%)	0	100	100
1	i	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	j	300/301 (100%)	296 (99%)	4 (1%)	61	77
1	k	300/301 (100%)	296 (99%)	4 (1%)	61	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	l	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	m	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	n	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	o	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	p	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	q	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	r	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	s	300/301 (100%)	298 (99%)	2 (1%)	76	82
1	u	300/301 (100%)	299 (100%)	1 (0%)	86	87
1	w	300/301 (100%)	299 (100%)	1 (0%)	86	87
All	All	13200/13244 (100%)	13128 (100%)	72 (0%)	78	85

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	370	ASN
1	B	185	ASP
1	B	272	LYS
1	C	145	LYS
1	C	153	ASN
1	C	177	GLN
1	D	57	GLN
1	D	231	ASP
1	D	239	GLN
1	D	273	LYS
1	E	25	GLN
1	E	32	LEU
1	G	94	ASP
1	H	184	LYS
1	I	94	ASP
1	K	152	ASP
1	L	6	ASN
1	M	6	ASN
1	M	210	ASN
1	N	101	ASN
1	N	182	LYS
1	O	242	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	299	LYS
1	P	32	LEU
1	P	76	GLN
1	P	251	LYS
1	Q	376	LEU
1	R	142	HIS
1	V	184	LYS
1	V	185	ASP
1	V	187	ASN
1	V	208	GLU
1	V	307	GLU
1	X	152	ASP
1	Z	20	ASN
1	Z	93	ARG
1	Z	95	LEU
1	Z	97	LEU
1	Z	289	GLU
1	c	375	LEU
1	d	123	LEU
1	d	162	LYS
1	d	193	ASN
1	f	138	LEU
1	f	142	HIS
1	f	362	LEU
1	g	87	ASN
1	i	79	GLU
1	i	304	HIS
1	j	22	ASN
1	j	152	ASP
1	j	240	ASP
1	j	348	MET
1	k	29	MET
1	k	184	LYS
1	k	273	LYS
1	k	343	LYS
1	l	32	LEU
1	m	275	THR
1	m	376	LEU
1	n	52	ASN
1	n	145	LYS
1	o	55	ASN
1	p	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	p	352	GLN
1	q	145	LYS
1	r	18	LEU
1	s	161	LEU
1	s	240	ASP
1	u	108	GLU
1	w	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (185) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	55	ASN
1	A	198	ASN
1	A	249	ASN
1	A	328	ASN
1	B	15	GLN
1	B	76	GLN
1	C	193	ASN
1	C	229	GLN
1	C	239	GLN
1	C	249	ASN
1	C	304	HIS
1	C	356	GLN
1	D	76	GLN
1	D	120	ASN
1	D	124	ASN
1	D	324	ASN
1	D	326	ASN
1	D	370	ASN
1	E	101	ASN
1	E	142	HIS
1	E	177	GLN
1	E	198	ASN
1	E	317	HIS
1	F	22	ASN
1	F	76	GLN
1	F	142	HIS
1	F	229	GLN
1	G	69	ASN
1	G	120	ASN
1	G	124	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	244	GLN
1	G	288	GLN
1	G	304	HIS
1	G	316	ASN
1	H	15	GLN
1	H	205	GLN
1	I	22	ASN
1	I	142	HIS
1	I	328	ASN
1	I	364	GLN
1	J	304	HIS
1	J	321	ASN
1	K	49	GLN
1	K	120	ASN
1	K	229	GLN
1	K	244	GLN
1	K	304	HIS
1	K	356	GLN
1	M	76	GLN
1	M	250	ASN
1	M	326	ASN
1	M	352	GLN
1	O	142	HIS
1	O	239	GLN
1	O	352	GLN
1	O	364	GLN
1	P	20	ASN
1	P	76	GLN
1	P	187	ASN
1	P	304	HIS
1	P	352	GLN
1	Q	120	ASN
1	Q	239	GLN
1	Q	304	HIS
1	Q	330	ASN
1	R	4	ASN
1	R	120	ASN
1	R	142	HIS
1	R	249	ASN
1	R	326	ASN
1	S	76	GLN
1	S	87	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	101	ASN
1	S	207	GLN
1	S	304	HIS
1	S	317	HIS
1	T	120	ASN
1	U	120	ASN
1	U	124	ASN
1	V	321	ASN
1	V	370	ASN
1	X	22	ASN
1	X	135	ASN
1	X	205	GLN
1	Z	352	GLN
1	b	25	GLN
1	b	55	ASN
1	b	367	GLN
1	c	15	GLN
1	c	76	GLN
1	c	187	ASN
1	c	207	GLN
1	c	324	ASN
1	c	328	ASN
1	c	370	ASN
1	d	69	ASN
1	d	87	ASN
1	d	205	GLN
1	d	326	ASN
1	d	330	ASN
1	e	22	ASN
1	e	25	GLN
1	e	39	ASN
1	e	187	ASN
1	e	205	GLN
1	e	304	HIS
1	f	120	ASN
1	f	142	HIS
1	g	26	GLN
1	g	90	GLN
1	g	321	ASN
1	g	352	GLN
1	h	90	GLN
1	i	69	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	i	142	HIS
1	i	205	GLN
1	i	326	ASN
1	j	6	ASN
1	j	87	ASN
1	j	244	GLN
1	j	326	ASN
1	k	120	ASN
1	k	288	GLN
1	k	321	ASN
1	k	356	GLN
1	l	25	GLN
1	l	148	GLN
1	l	207	GLN
1	l	317	HIS
1	l	330	ASN
1	l	352	GLN
1	m	25	GLN
1	m	76	GLN
1	m	288	GLN
1	m	304	HIS
1	m	312	GLN
1	m	367	GLN
1	m	370	ASN
1	n	15	GLN
1	n	20	ASN
1	n	135	ASN
1	n	142	HIS
1	n	198	ASN
1	n	229	GLN
1	n	244	GLN
1	o	8	ASN
1	o	55	ASN
1	o	87	ASN
1	o	153	ASN
1	o	187	ASN
1	o	239	GLN
1	o	304	HIS
1	o	352	GLN
1	o	364	GLN
1	p	76	GLN
1	p	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	p	312	GLN
1	p	324	ASN
1	q	39	ASN
1	q	120	ASN
1	q	198	ASN
1	q	244	GLN
1	q	321	ASN
1	r	142	HIS
1	r	239	GLN
1	r	304	HIS
1	r	312	GLN
1	r	364	GLN
1	s	6	ASN
1	s	26	GLN
1	s	101	ASN
1	s	142	HIS
1	s	205	GLN
1	s	312	GLN
1	u	19	ASN
1	u	25	GLN
1	u	142	HIS
1	u	239	GLN
1	u	324	ASN
1	w	39	ASN
1	w	76	GLN
1	w	101	ASN
1	w	205	GLN
1	w	356	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

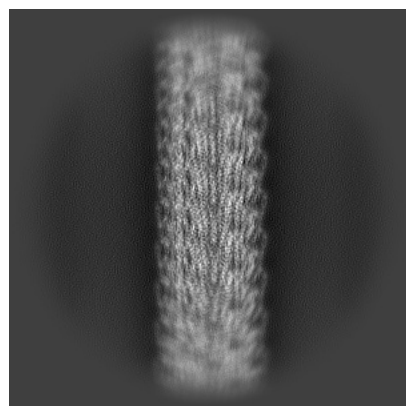
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53912. These allow visual inspection of the internal detail of the map and identification of artifacts.

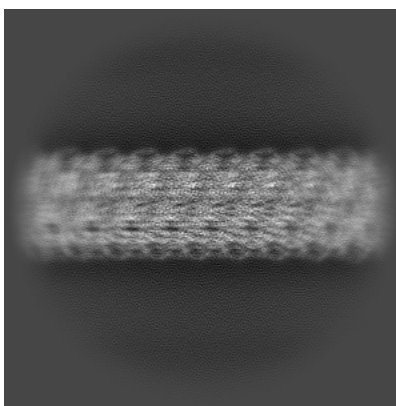
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

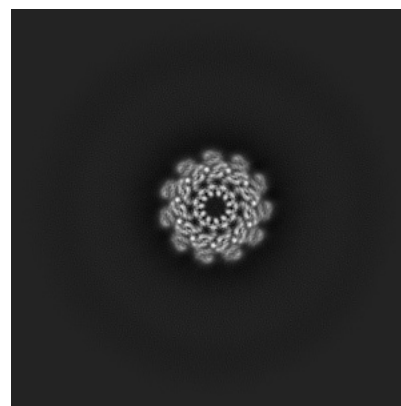
6.1.1 Primary map



X

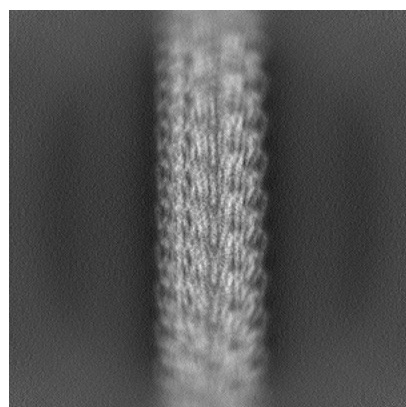


Y

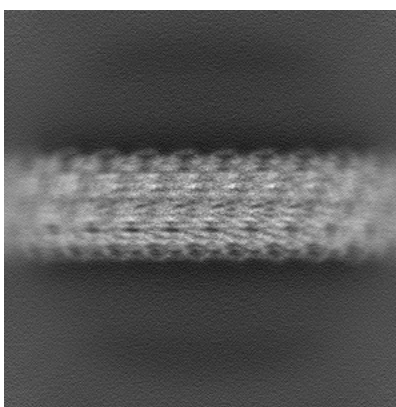


Z

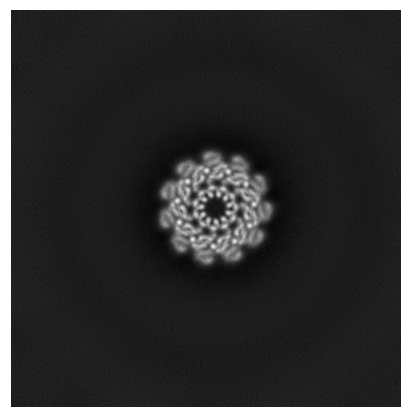
6.1.2 Raw map



X



Y

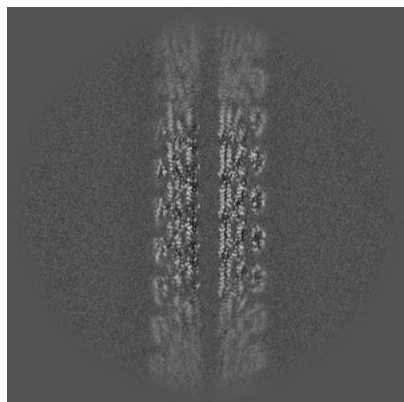


Z

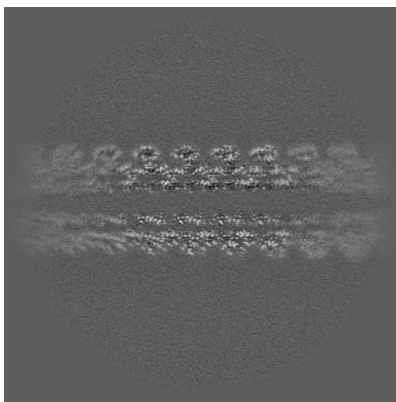
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

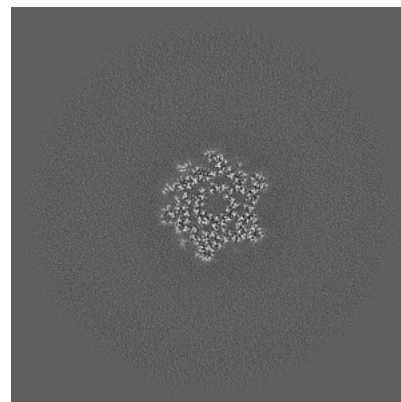
6.2.1 Primary map



X Index: 250

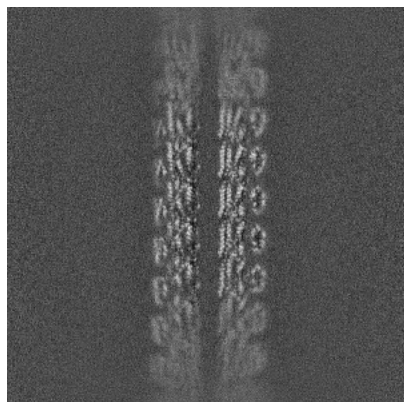


Y Index: 250

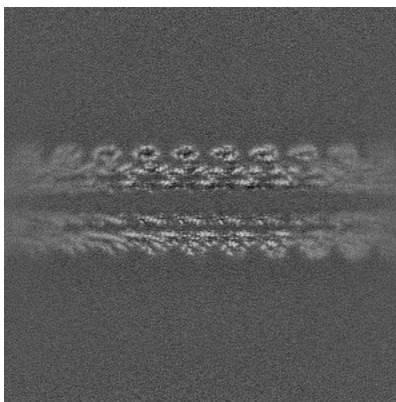


Z Index: 250

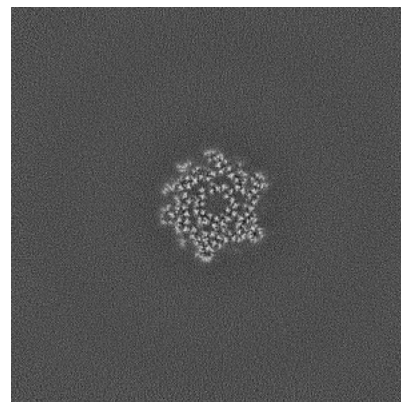
6.2.2 Raw map



X Index: 250



Y Index: 250

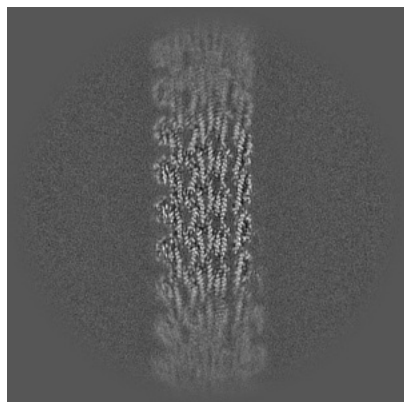


Z Index: 250

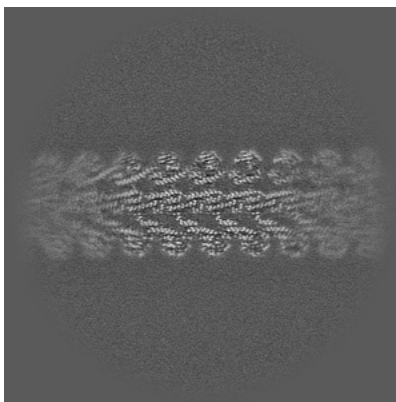
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

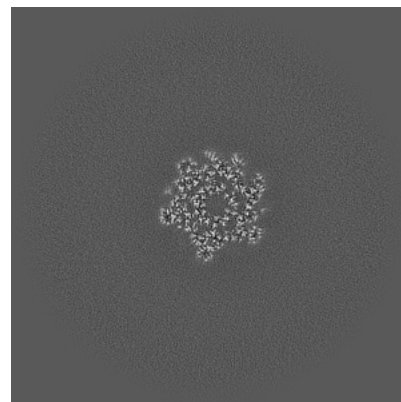
6.3.1 Primary map



X Index: 238

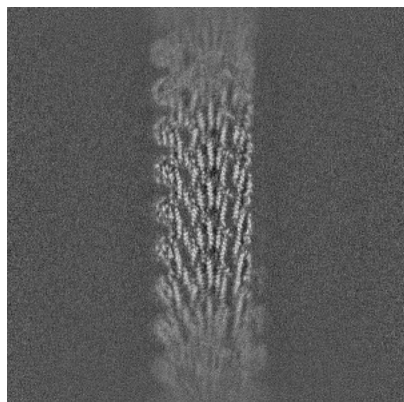


Y Index: 275

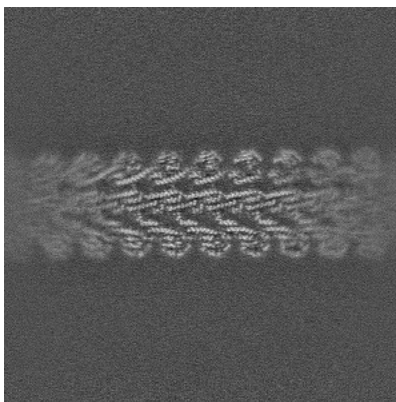


Z Index: 245

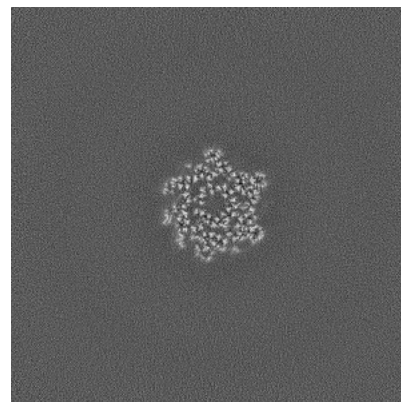
6.3.2 Raw map



X Index: 237



Y Index: 275

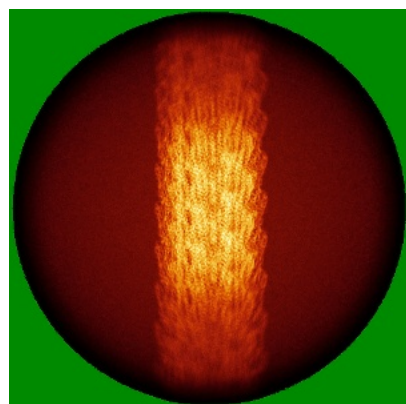


Z Index: 254

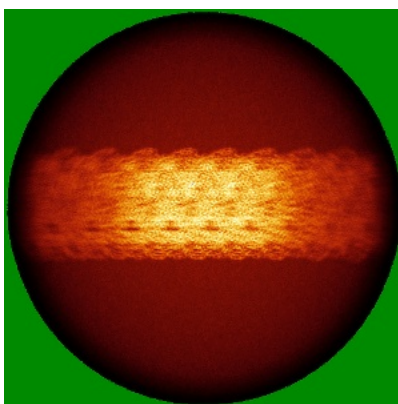
The images above show the largest variance slices of the map in three orthogonal directions.

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

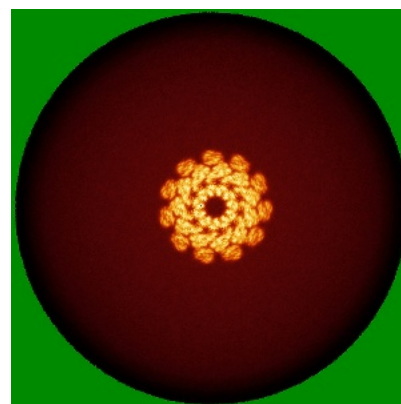
6.4.1 Primary map



X

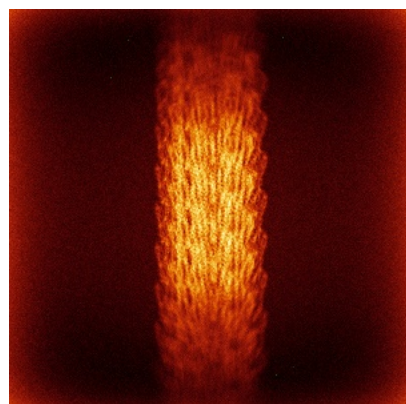


Y

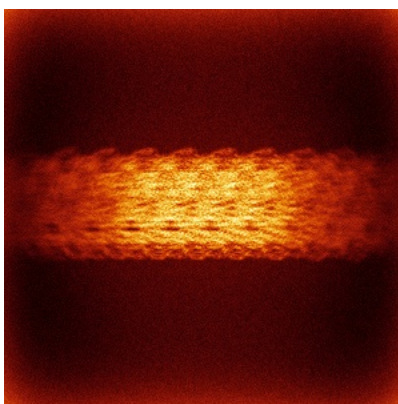


Z

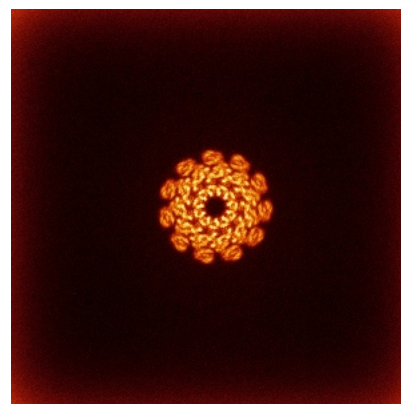
6.4.2 Raw map



X



Y

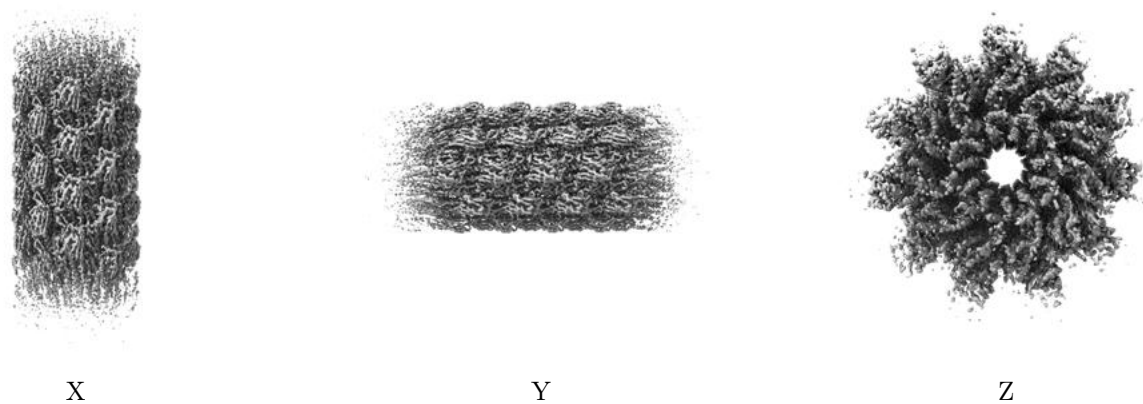


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

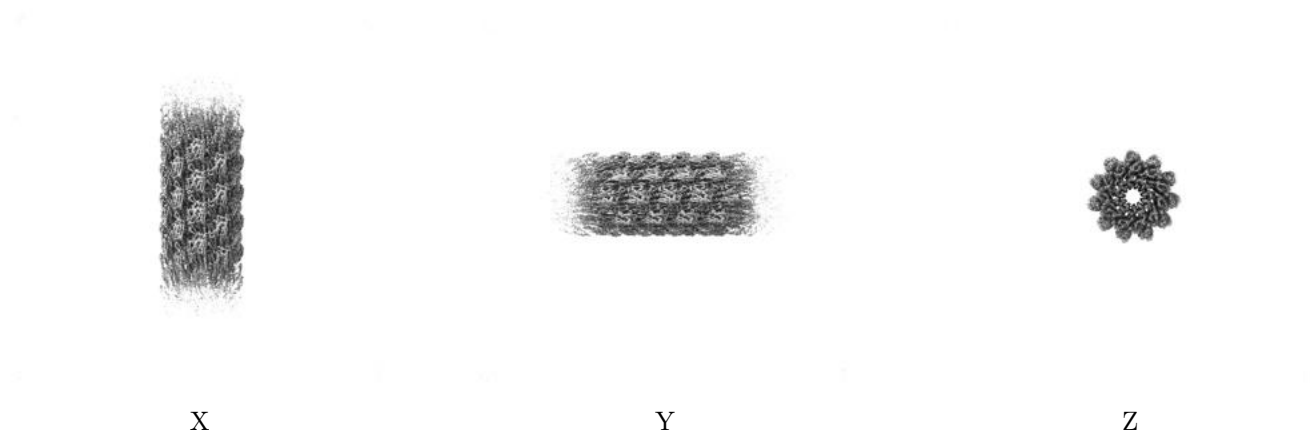
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

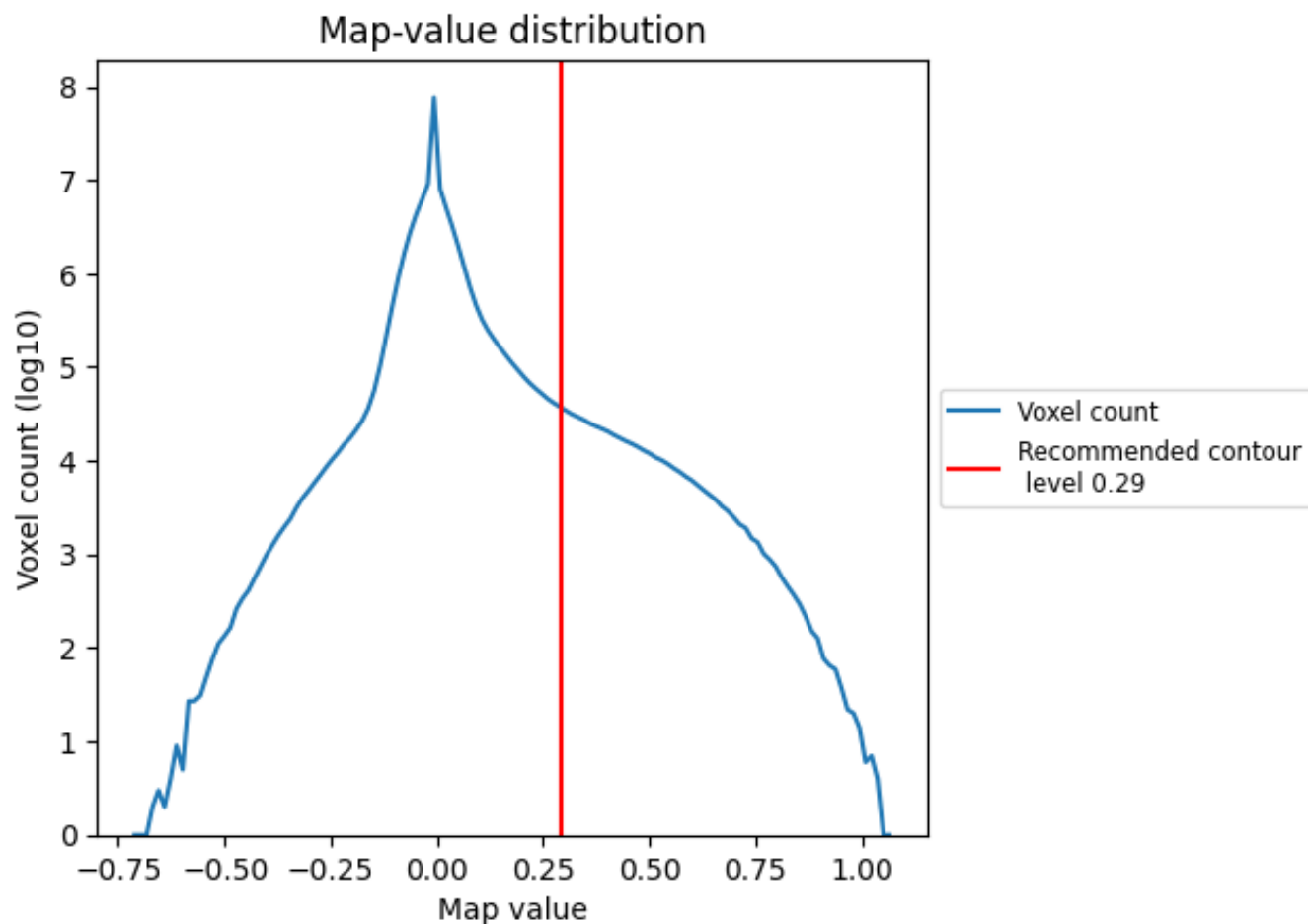
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

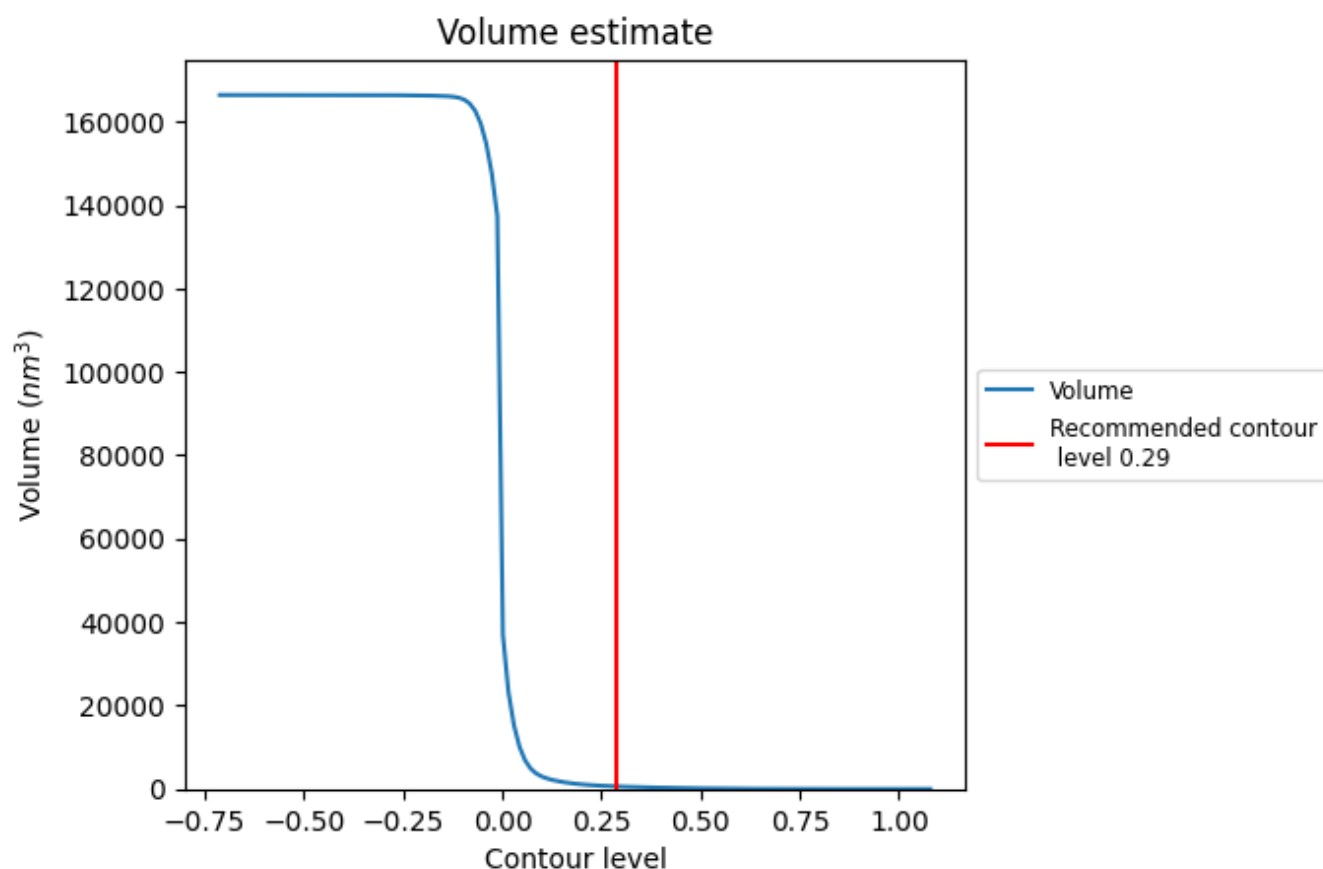
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

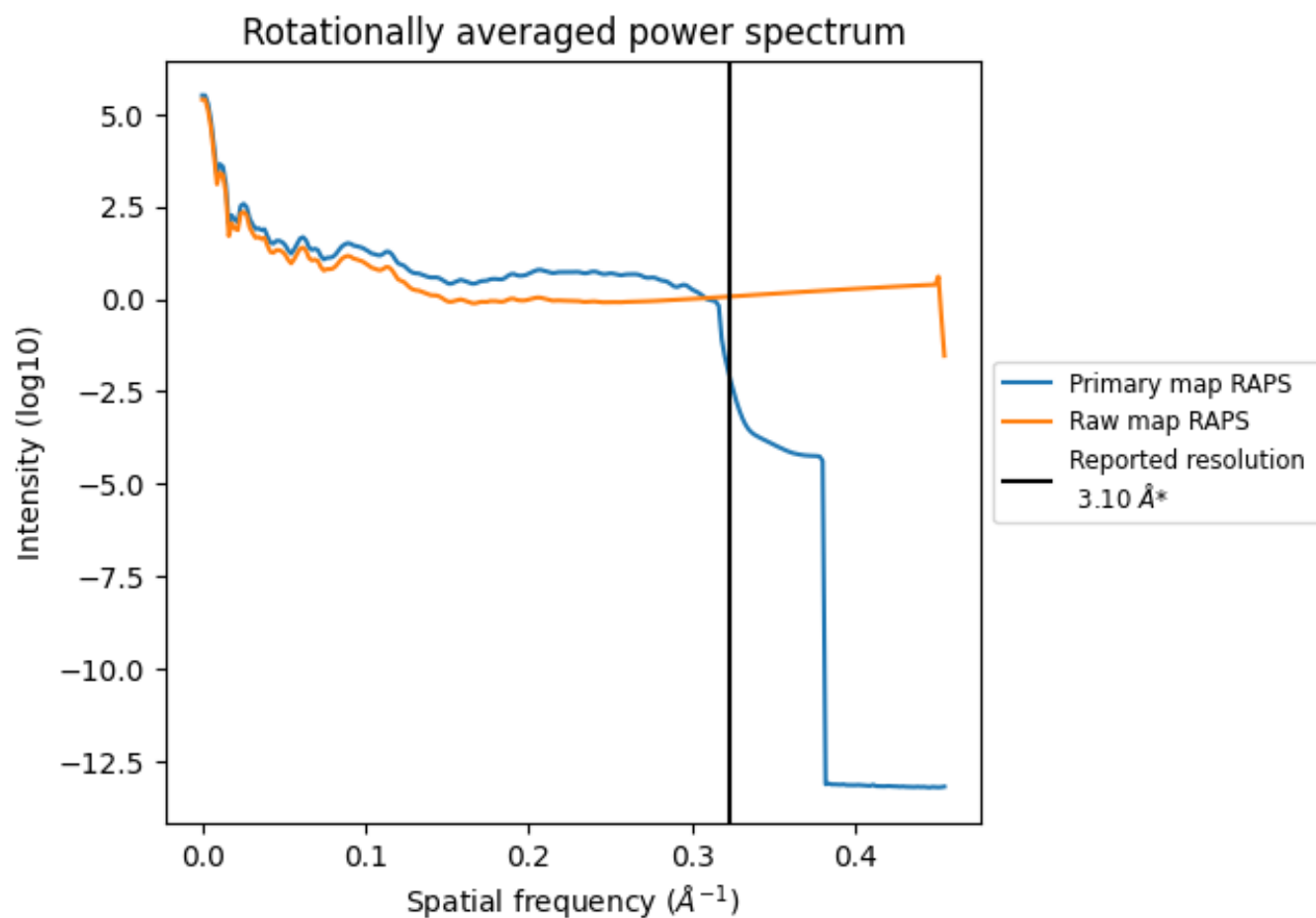
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 605 nm³; this corresponds to an approximate mass of 546 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 ⓘ

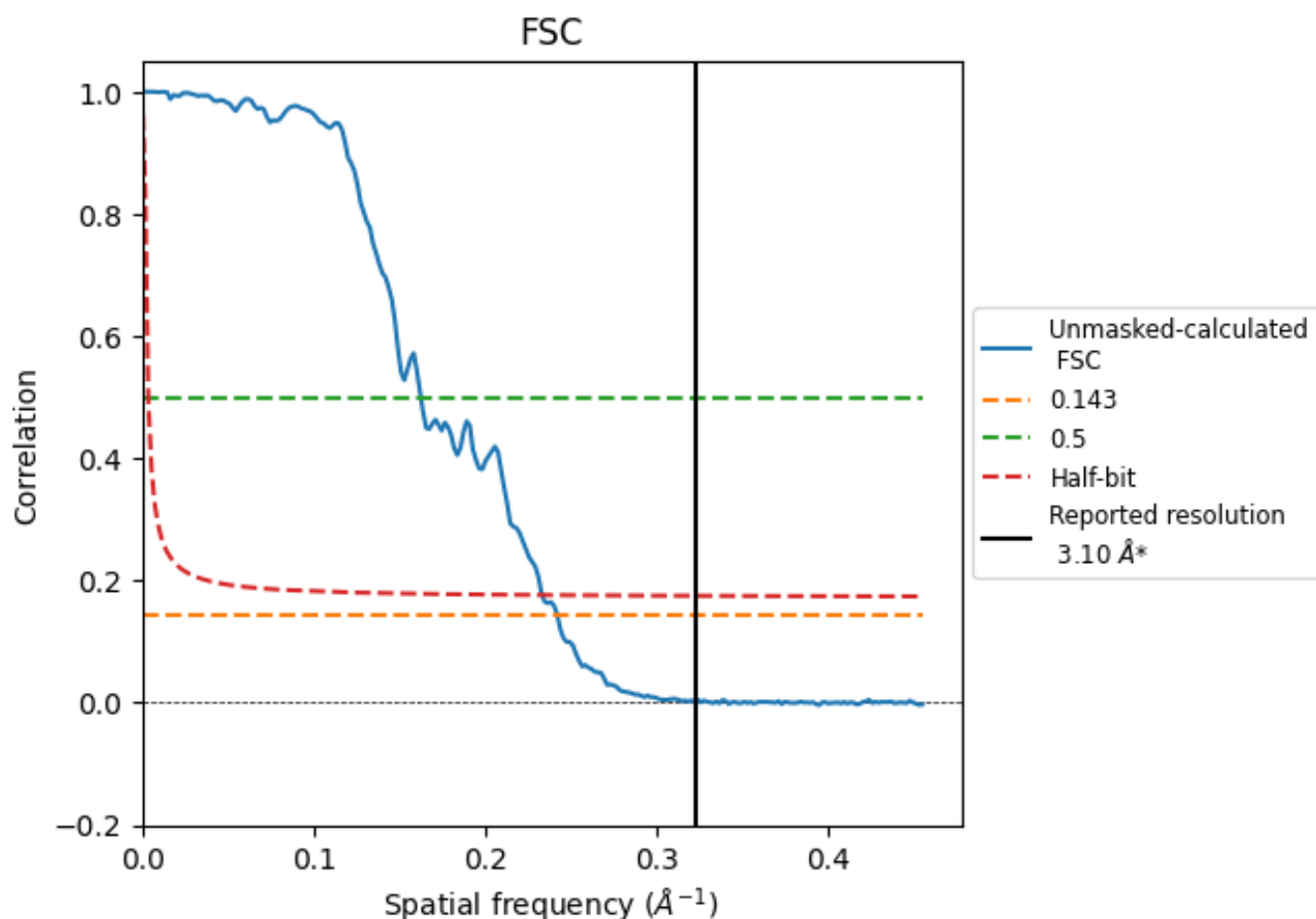


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

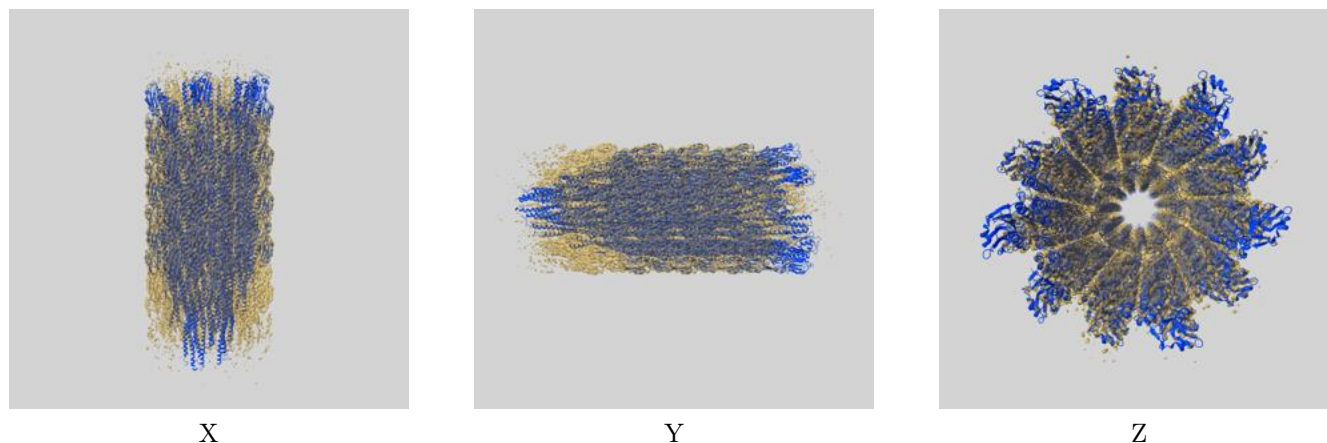
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	6.16	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

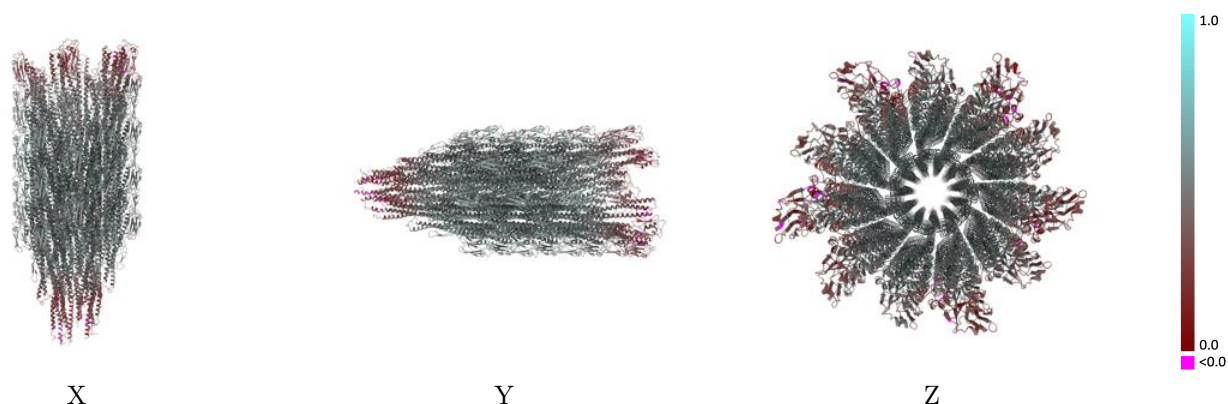
This section contains information regarding the fit between EMDB map EMD-53912 and PDB model 9RCB. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



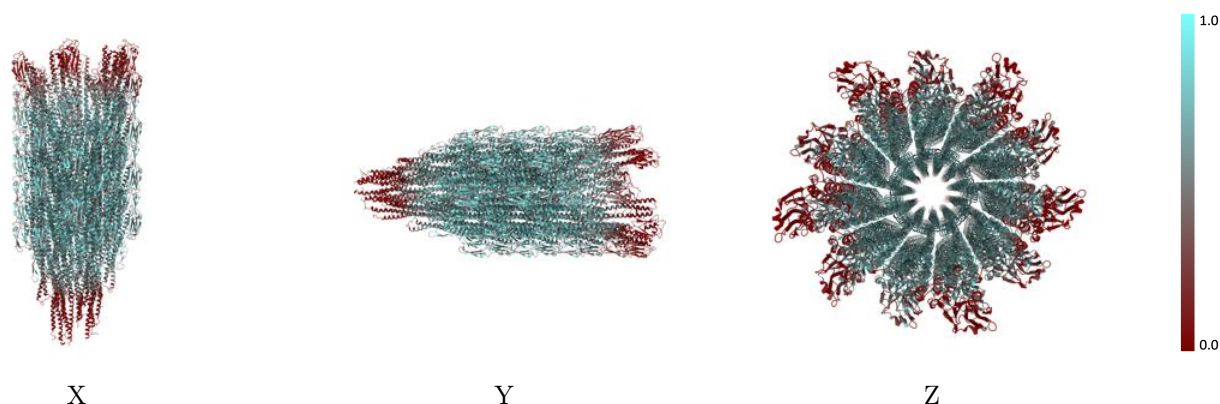
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



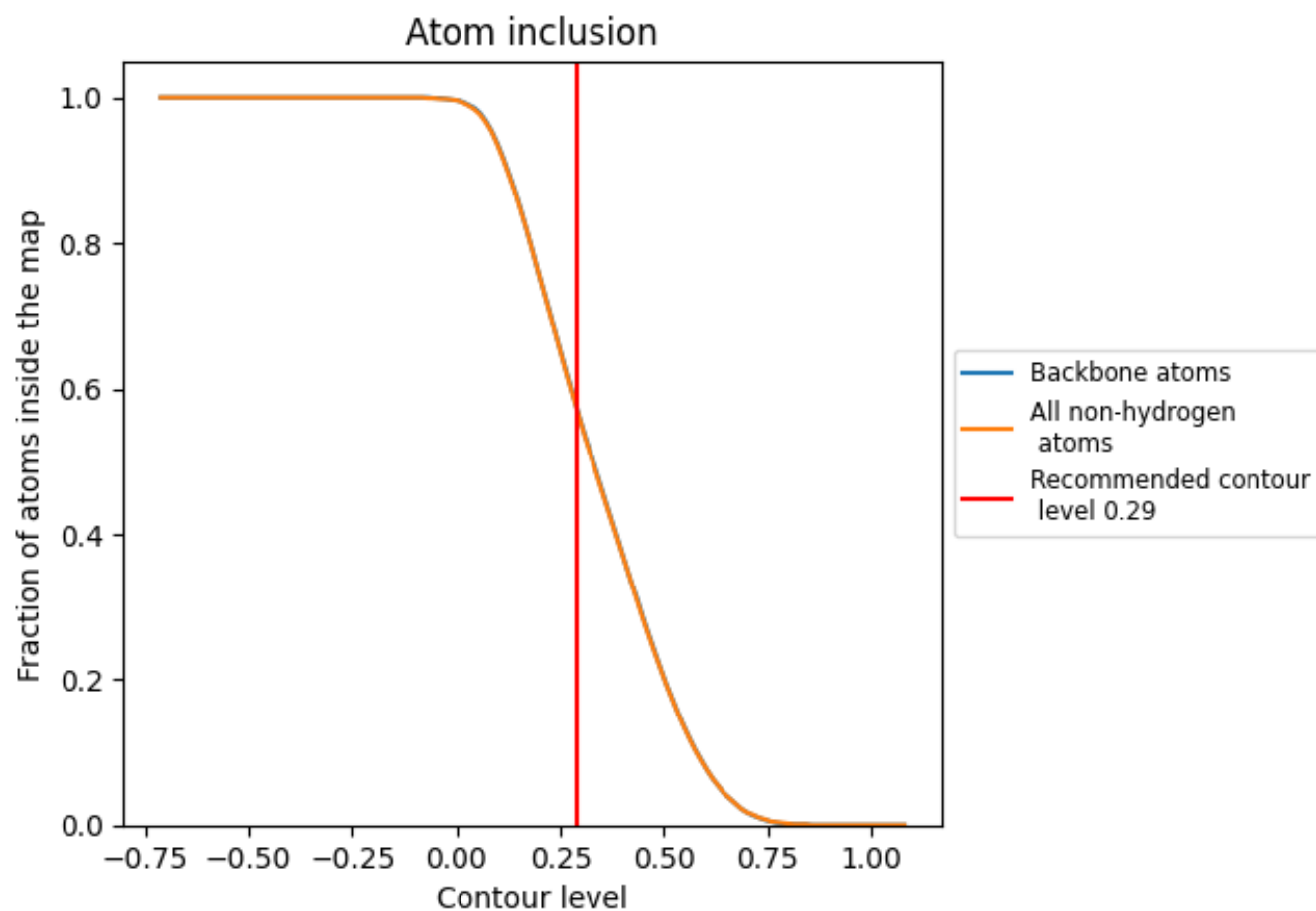
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.29).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 57% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5710	 0.4790
A	 0.6850	 0.5220
B	 0.6750	 0.5180
C	 0.6690	 0.5160
D	 0.6720	 0.5110
E	 0.6740	 0.5050
F	 0.6840	 0.5190
G	 0.6680	 0.5190
H	 0.6970	 0.5310
I	 0.6860	 0.5270
J	 0.6930	 0.5270
K	 0.6860	 0.5210
L	 0.5770	 0.4840
M	 0.6550	 0.5000
N	 0.5290	 0.4690
O	 0.6510	 0.4970
P	 0.5150	 0.4540
Q	 0.6460	 0.5050
R	 0.6830	 0.5250
S	 0.6400	 0.5120
T	 0.6840	 0.5330
U	 0.6240	 0.5000
V	 0.6770	 0.5170
X	 0.3870	 0.4120
Z	 0.3550	 0.3940
b	 0.3450	 0.3890
c	 0.5110	 0.4650
d	 0.3310	 0.3850
e	 0.4850	 0.4600
f	 0.3040	 0.3820
g	 0.4380	 0.4360
h	 0.6380	 0.5050
i	 0.5490	 0.4630
j	 0.6340	 0.5010
k	 0.5720	 0.4660



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
l	 0.6460	 0.4940
m	 0.5890	 0.4800
n	 0.5100	 0.4420
o	 0.6230	 0.5010
p	 0.5400	 0.4630
q	 0.6360	 0.5080
r	 0.5520	 0.4660
s	 0.4290	 0.4170
u	 0.4440	 0.4210
w	 0.4650	 0.4240