



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 07:28 AM UTC

PDB ID : 7ZN2 / pdb_00007zn2
EMDB ID : EMD-14799
Title : Tail tip of siphophage T5 : full complex after interaction with its bacterial receptor FhuA
Authors : Linares, R.; Arnaud, C.A.; Effantin, G.; Darnault, C.; Epalle, N.; Boeri Erba, E.; Schoehn, G.; Breyton, C.
Deposited on : 2022-04-20
Resolution : 4.29 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

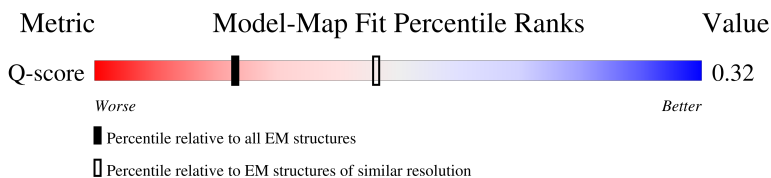
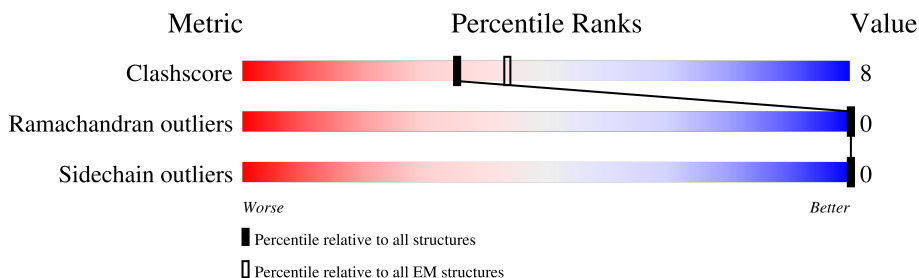
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.29 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.



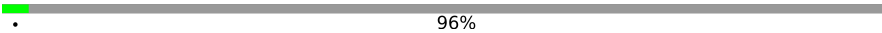
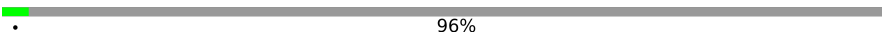
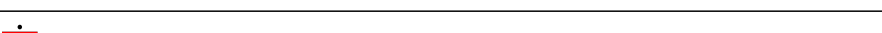
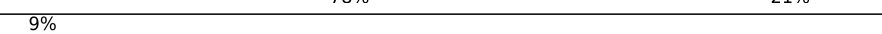
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4494 (3.79 - 4.79)

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	b	949	8% 85% 15%
1	c	949	9% 83% 17%
1	d	949	17% 85% 15%
2	h	1219	.. 96%

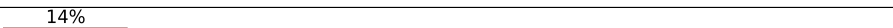
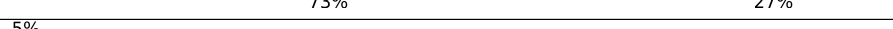
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	i	1219	 96%
2	j	1219	 96%
3	e	688	 49% 83% 14%
3	f	688	 48% 80% 17%
3	g	688	 50% 74% 12% 14%
4	J	140	 5% 75% 24%
4	K	140	 8% 79% 21%
4	L	140	 10% 81% 19%
4	M	140	 7% 74% 26%
4	N	140	 6% 76% 24%
4	O	140	 8% 79% 21%
4	P	140	 6% 80% 20%
4	Q	140	 7% 71% 29%
4	R	140	 9% 75% 24%
4	S	140	 6% 78% 21%
4	T	140	 9% 81% 19%
4	U	140	 6% 74% 26%
5	G	298	 83% 17%
5	H	298	 82% 18%
5	I	298	 84% 16%
6	V	204	 80% 20%
6	W	204	 79% 21%
6	X	204	 82% 18%
6	Y	204	 80% 20%
6	Z	204	 82% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	a	204	 80% 20%
7	A	464	 17% 73% 27%
7	B	464	 12% 72% 28%
7	C	464	 14% 73% 27%
7	D	464	 5% 78% 22%
7	E	464	 5% 79% 21%
7	F	464	 5% 80% 20%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 89393 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable baseplate hub protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	d	949	Total	C	N	O	S	0	0
			7576	4811	1274	1481	10		
1	c	949	Total	C	N	O	S	0	0
			7576	4811	1274	1481	10		
1	b	949	Total	C	N	O	S	0	0
			7576	4811	1274	1481	10		

- Molecule 2 is a protein called Pore-forming tail tip protein pb2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	j	43	Total	C	N	O	S	0	0
			328	200	60	67	1		
2	h	43	Total	C	N	O	S	0	0
			328	200	60	67	1		
2	i	43	Total	C	N	O	S	0	0
			328	200	60	67	1		

- Molecule 3 is a protein called Straight fiber protein pb4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	669	Total	C	N	O	S	0	0
			5143	3274	854	1000	15		
3	e	671	Total	C	N	O	S	0	0
			5163	3285	859	1004	15		
3	g	589	Total	C	N	O	S	0	0
			4546	2897	758	877	14		

- Molecule 4 is a protein called L-shaped tail fiber protein p132.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	139	Total	C	N	O	S	0	0
			1048	653	175	217	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	140	Total	C	N	O	S	0	0
			1056	658	176	218	4		
4	S	139	Total	C	N	O	S	0	0
			1048	653	175	217	3		
4	N	139	Total	C	N	O	S	0	0
			1048	653	175	217	3		
4	M	140	Total	C	N	O	S	0	0
			1056	658	176	218	4		
4	O	139	Total	C	N	O	S	0	0
			1048	653	175	217	3		
4	J	139	Total	C	N	O	S	0	0
			1048	653	175	217	3		
4	L	140	Total	C	N	O	S	0	0
			1056	658	176	218	4		
4	U	140	Total	C	N	O	S	0	0
			1056	658	176	218	4		
4	K	139	Total	C	N	O	S	0	0
			1048	653	175	217	3		
4	P	140	Total	C	N	O	S	0	0
			1056	658	176	218	4		
4	T	140	Total	C	N	O	S	0	0
			1056	658	176	218	4		

- Molecule 5 is a protein called Minor tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	298	Total	C	N	O	S	0	0
			2423	1551	398	464	10		
5	H	298	Total	C	N	O	S	0	0
			2423	1551	398	464	10		
5	G	298	Total	C	N	O	S	0	0
			2423	1551	398	464	10		

- Molecule 6 is a protein called Distal tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		
6	X	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		
6	Y	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		
6	V	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		
6	Z	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		

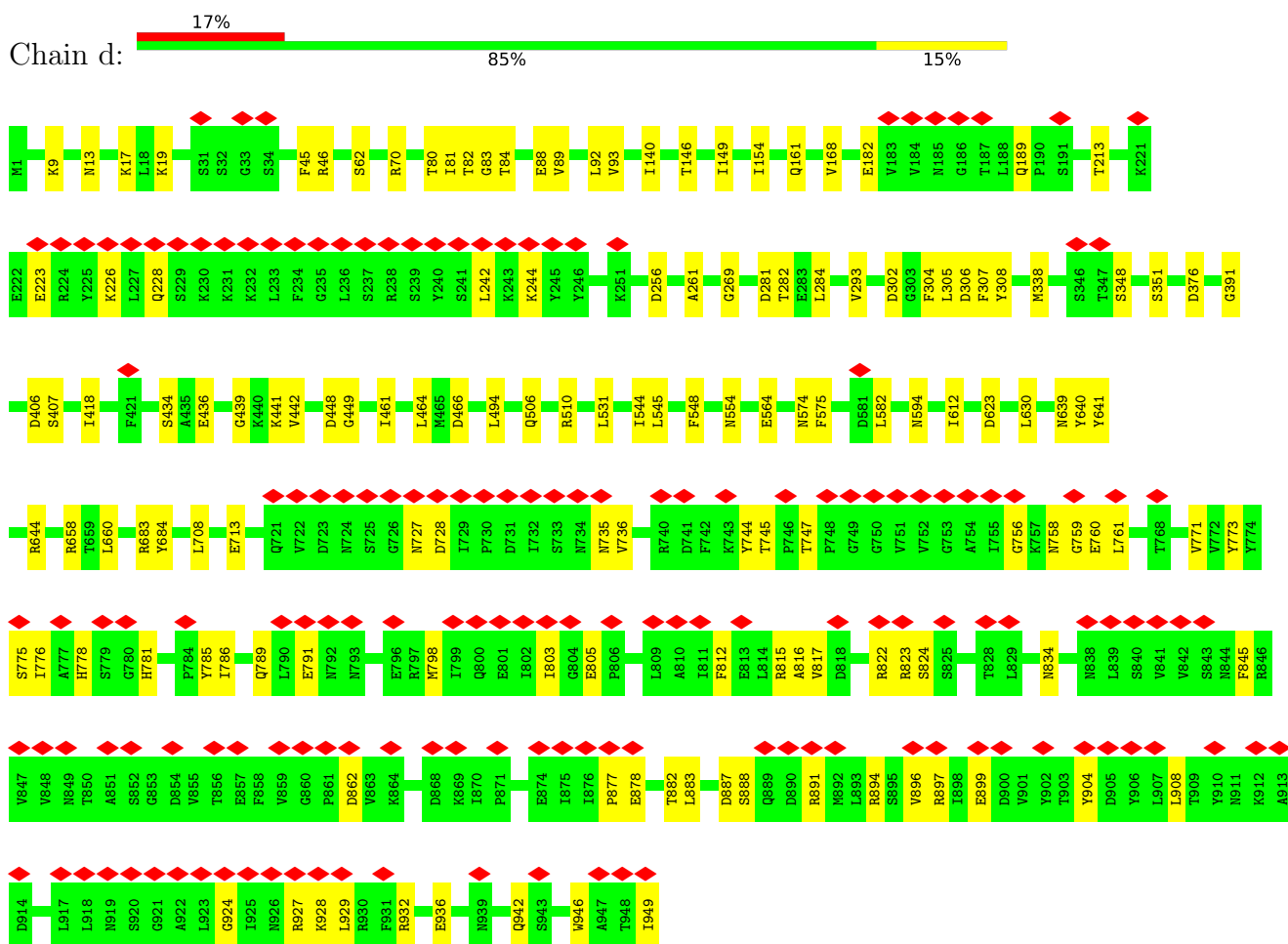
- Molecule 7 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
7	E	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
7	C	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
7	D	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
7	A	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
7	B	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		

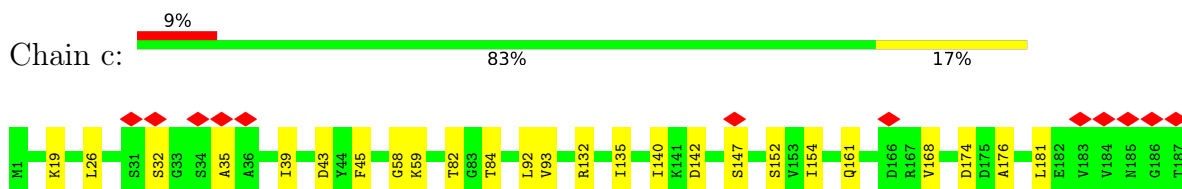
3 Residue-property plots

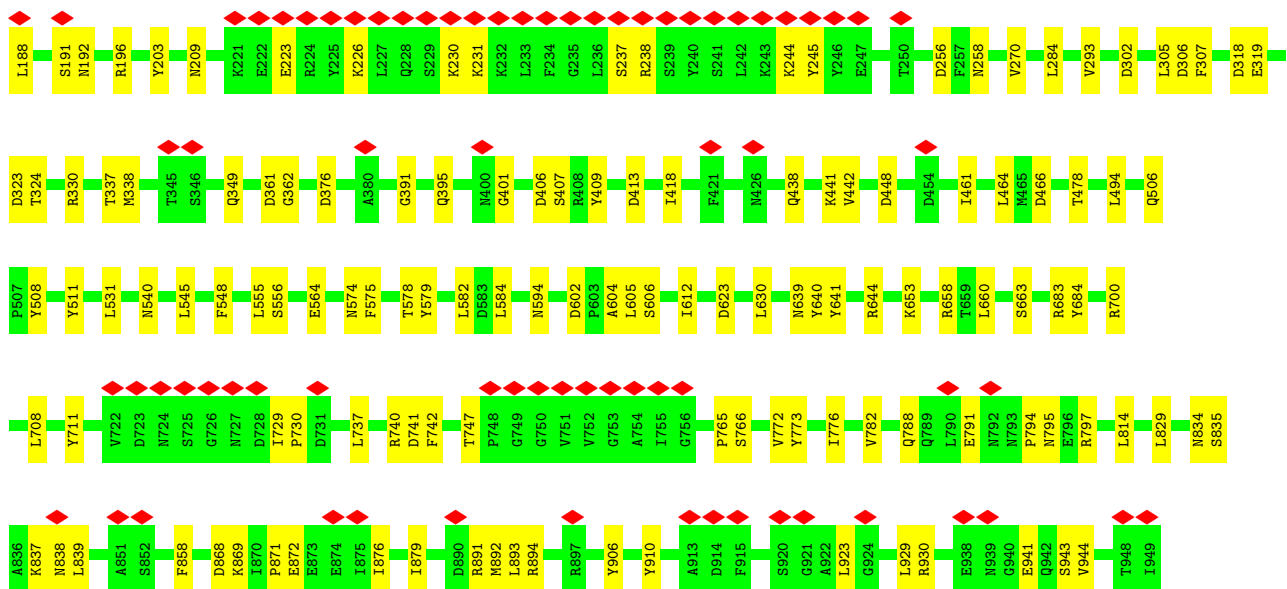
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Probable baseplate hub protein

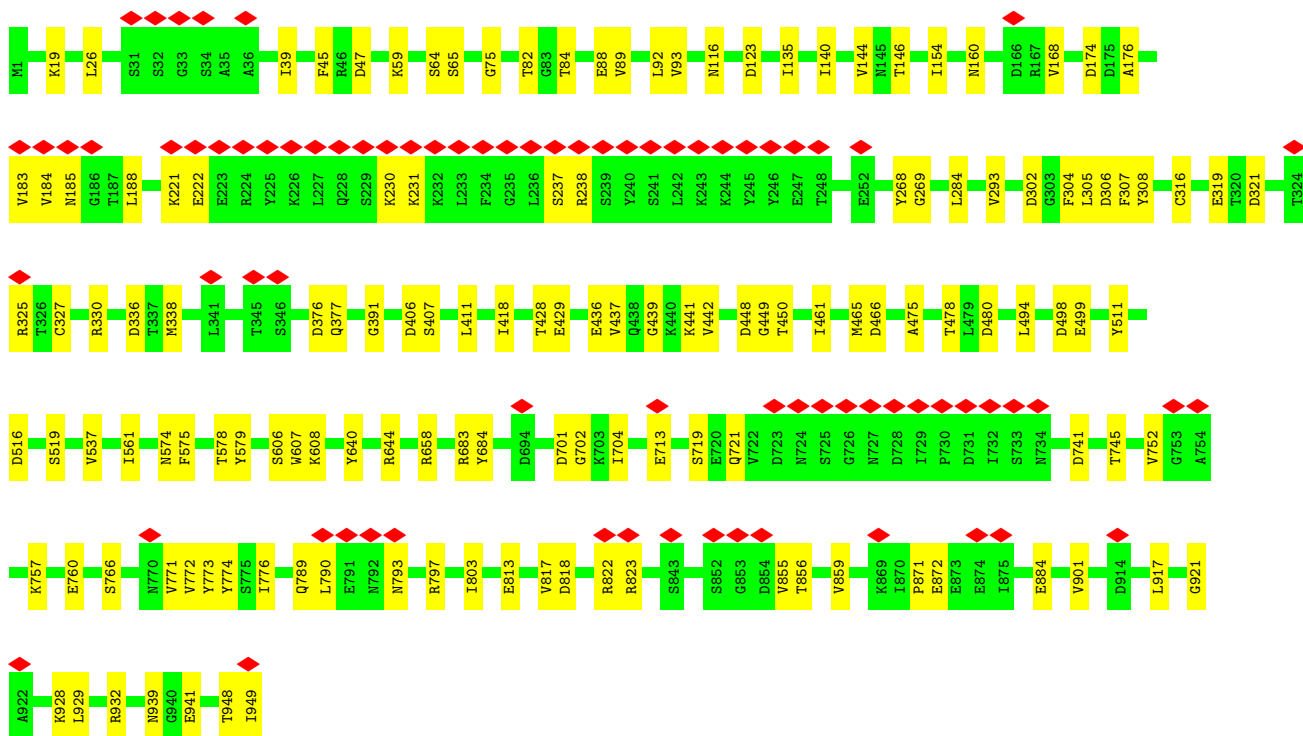
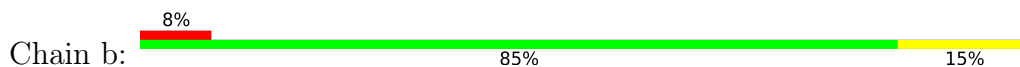


• Molecule 1: Probable baseplate hub protein





• Molecule 1: Probable baseplate hub protein



• Molecule 2: Pore-forming tail tip protein pb2

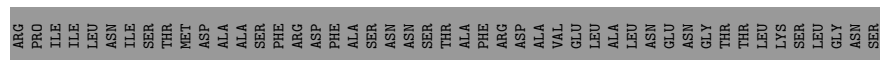
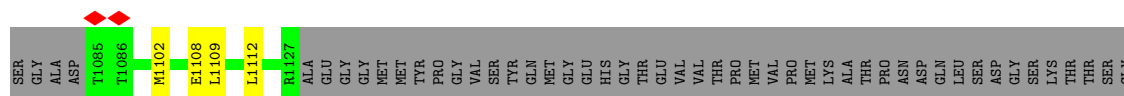


MET THR ASP LYS LEU ILE ARG GLU LEU LEU LEU ILE ASP VAL LYS GLN GLY ALA THR ARG THR LYS SER ILE GLU ASN VAL SER ASP LEU LEU ASN ALA ALA ALA ALA SER GLU LEU THR ASN GLU LEU LYS MET PRO ARG THR LEU TYR SER ILE GLU ARG ALA

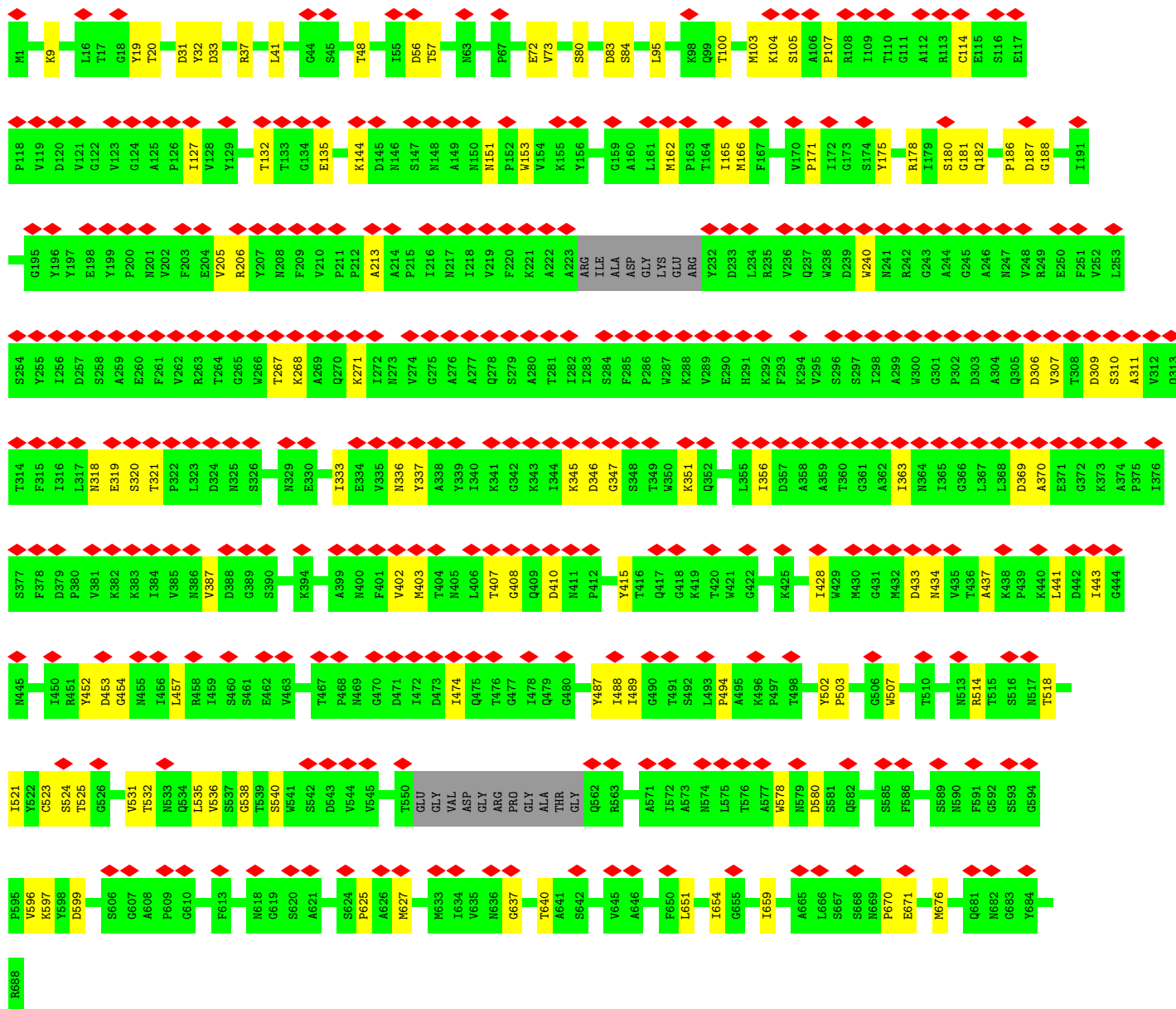
- Molecule 2: Pore-forming tail tip protein pb2

96%

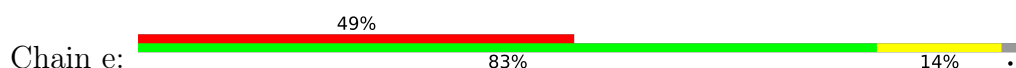
[illegible]

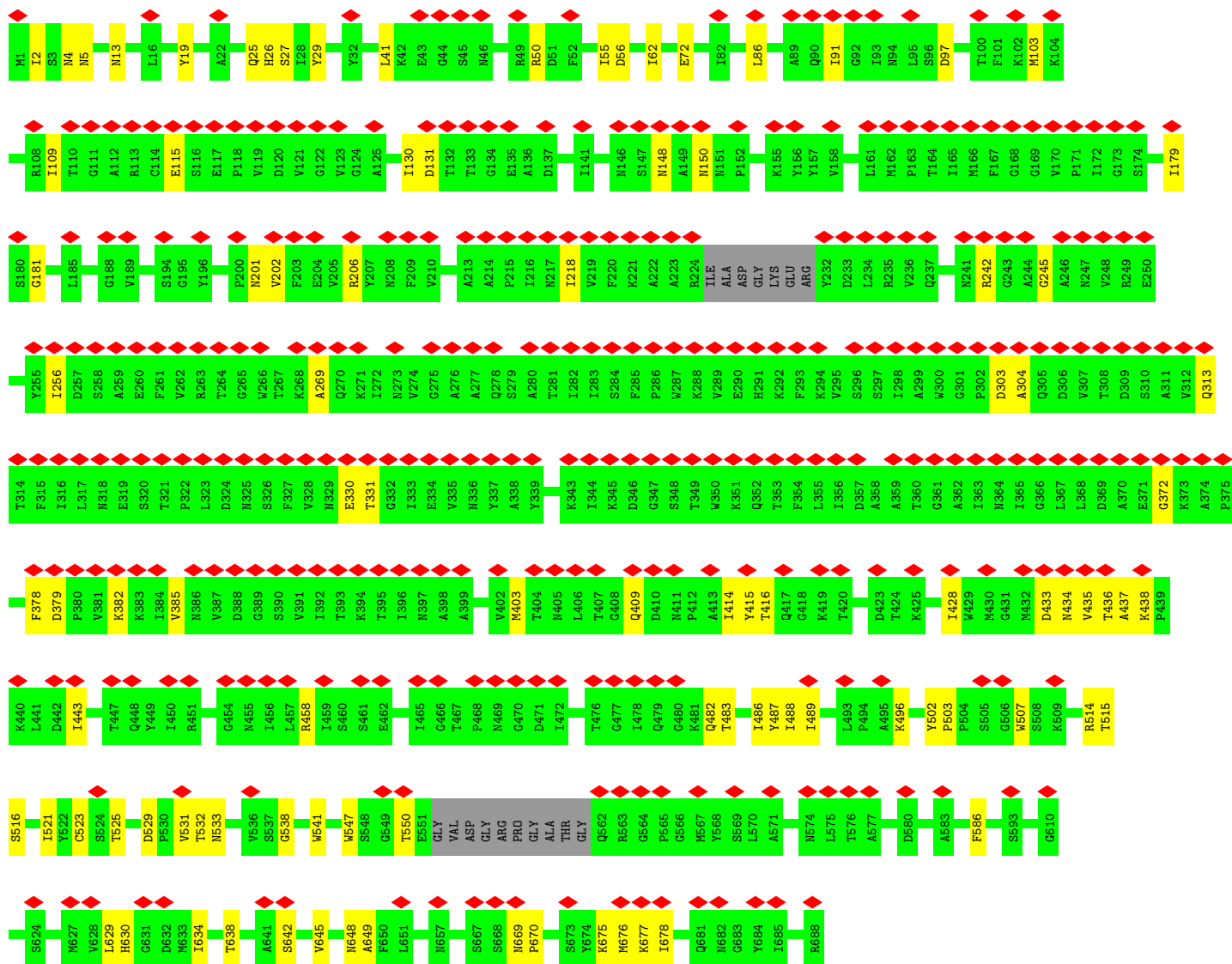


• Molecule 3: Straight fiber protein pb4

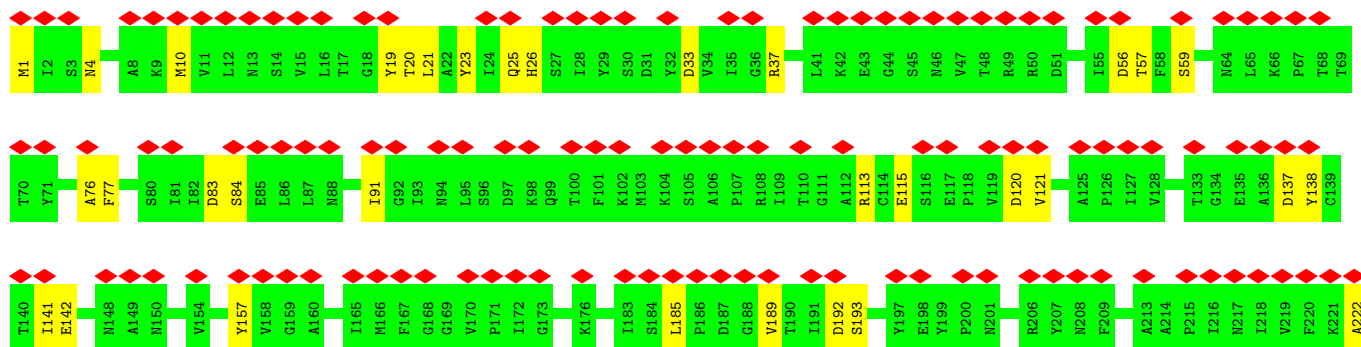
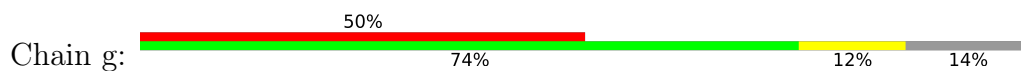


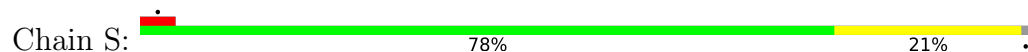
• Molecule 3: Straight fiber protein pb4

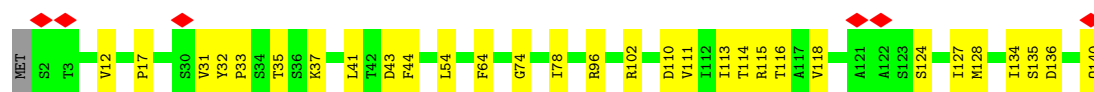




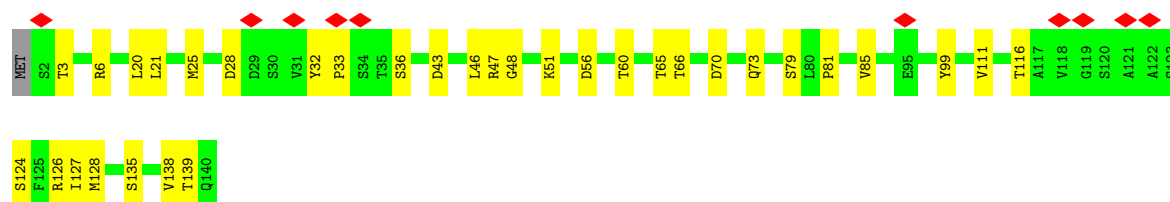
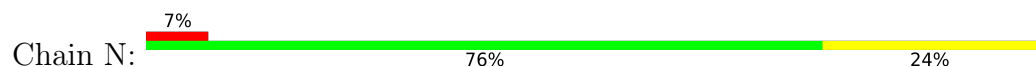
• Molecule 3: Straight fiber protein pb4



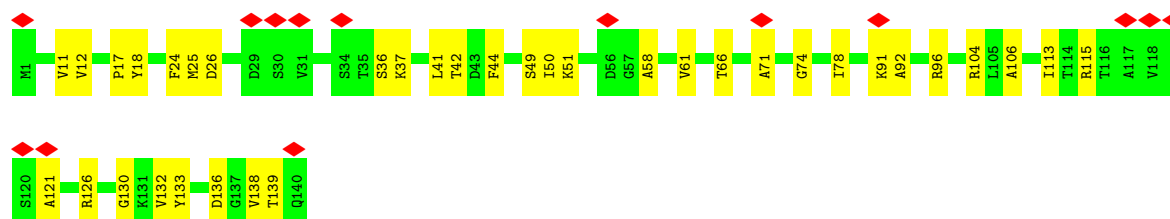
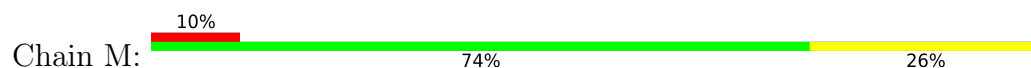




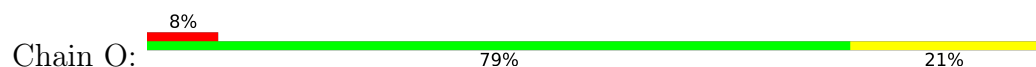
- Molecule 4: L-shaped tail fiber protein p132



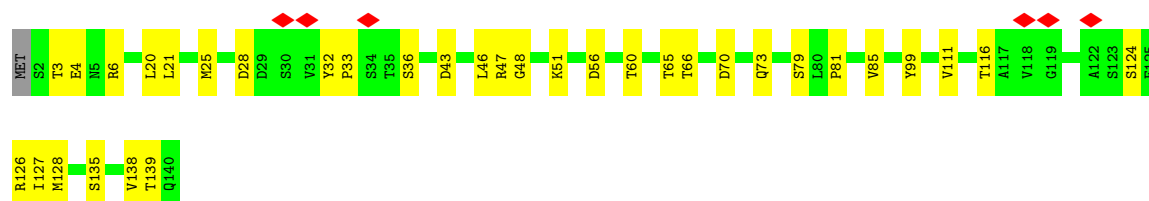
- Molecule 4: L-shaped tail fiber protein p132



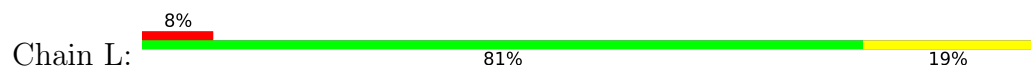
- Molecule 4: L-shaped tail fiber protein p132

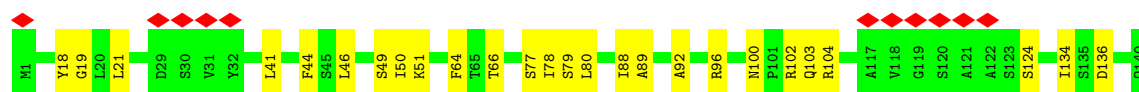


- Molecule 4: L-shaped tail fiber protein p132

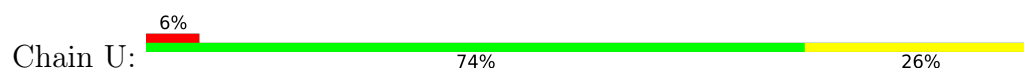


- Molecule 4: L-shaped tail fiber protein p132

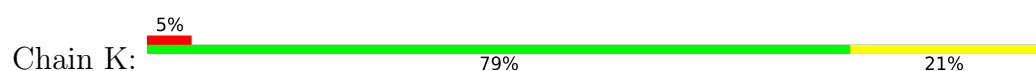




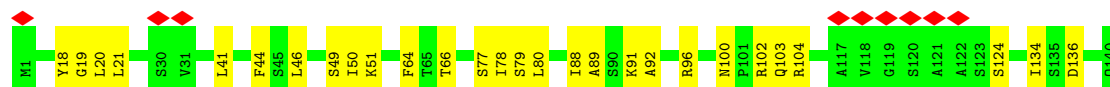
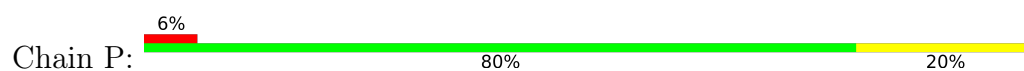
• Molecule 4: L-shaped tail fiber protein p132



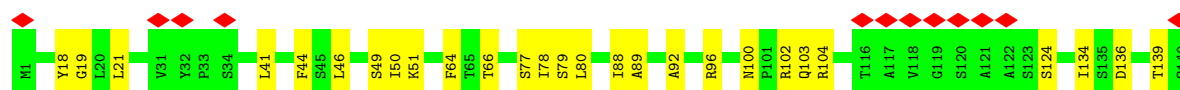
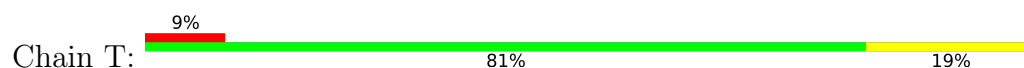
• Molecule 4: L-shaped tail fiber protein p132



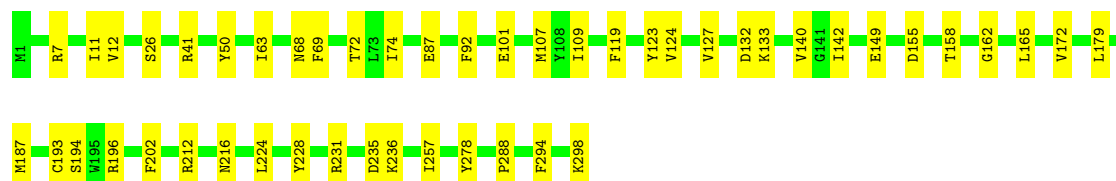
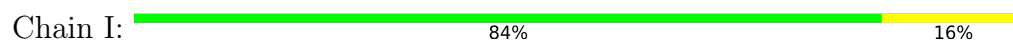
• Molecule 4: L-shaped tail fiber protein p132



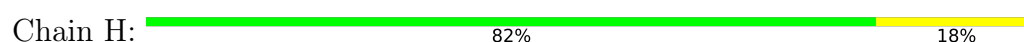
• Molecule 4: L-shaped tail fiber protein p132

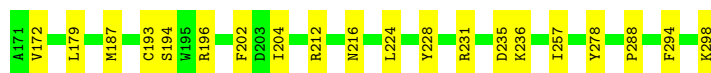


• Molecule 5: Minor tail protein

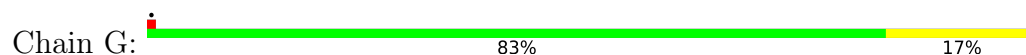


• Molecule 5: Minor tail protein

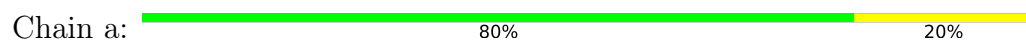




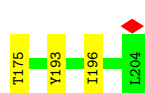
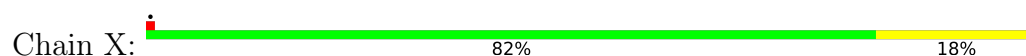
- Molecule 5: Minor tail protein



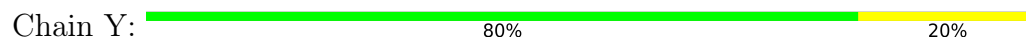
- Molecule 6: Distal tail protein



- Molecule 6: Distal tail protein

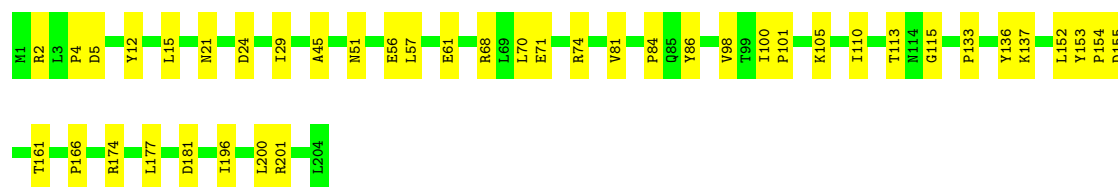


- Molecule 6: Distal tail protein



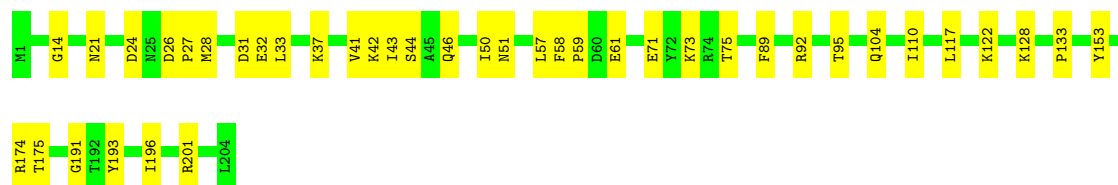
- Molecule 6: Distal tail protein

Chain W:  79% 21%



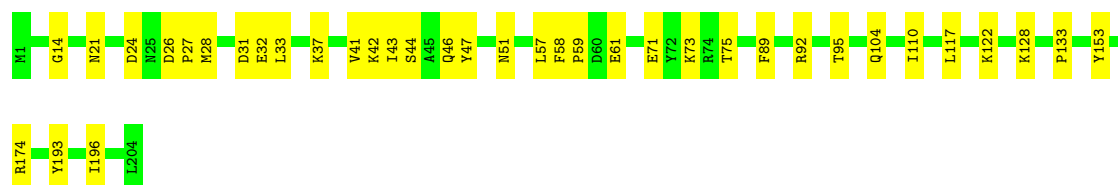
- Molecule 6: Distal tail protein

Chain V:  80% 20%



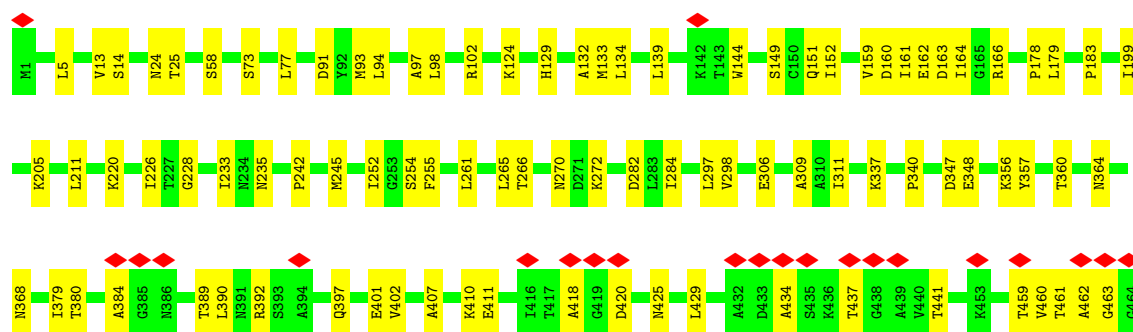
- Molecule 6: Distal tail protein

Chain Z:  82% 18%



- Molecule 7: Tail tube protein

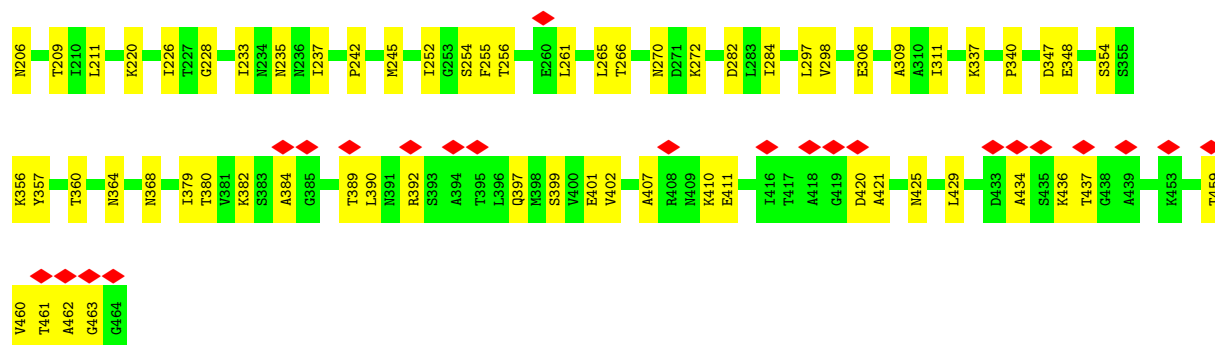
Chain F:  5% 80% 20%



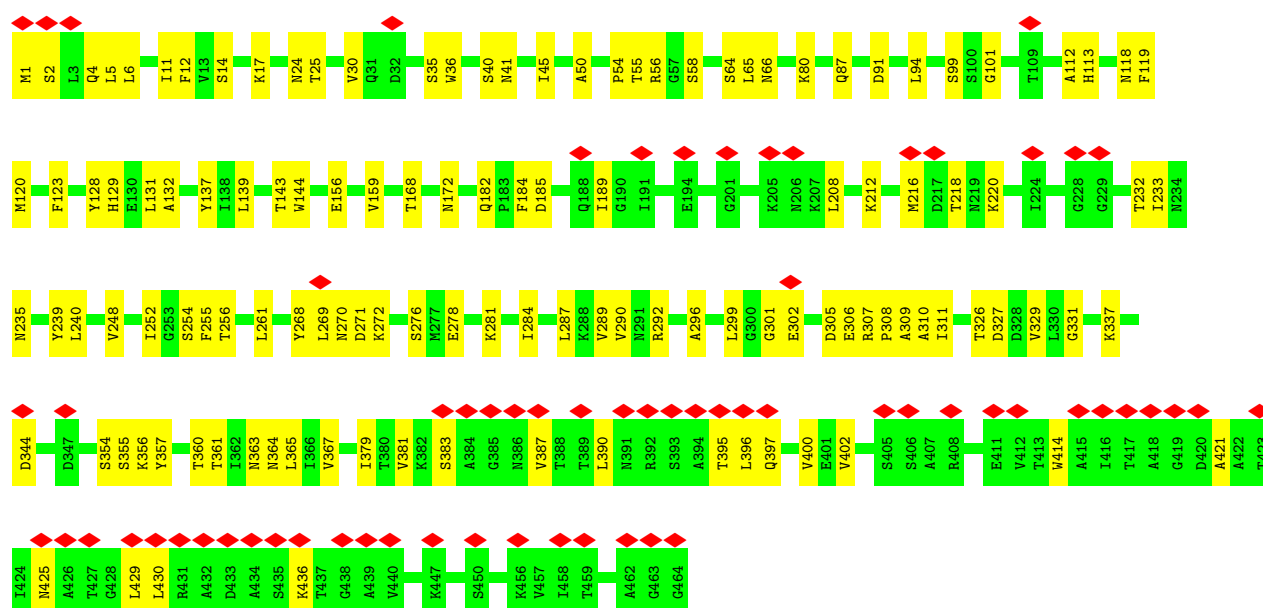
- Molecule 7: Tail tube protein

Chain E:  5% 79% 21%

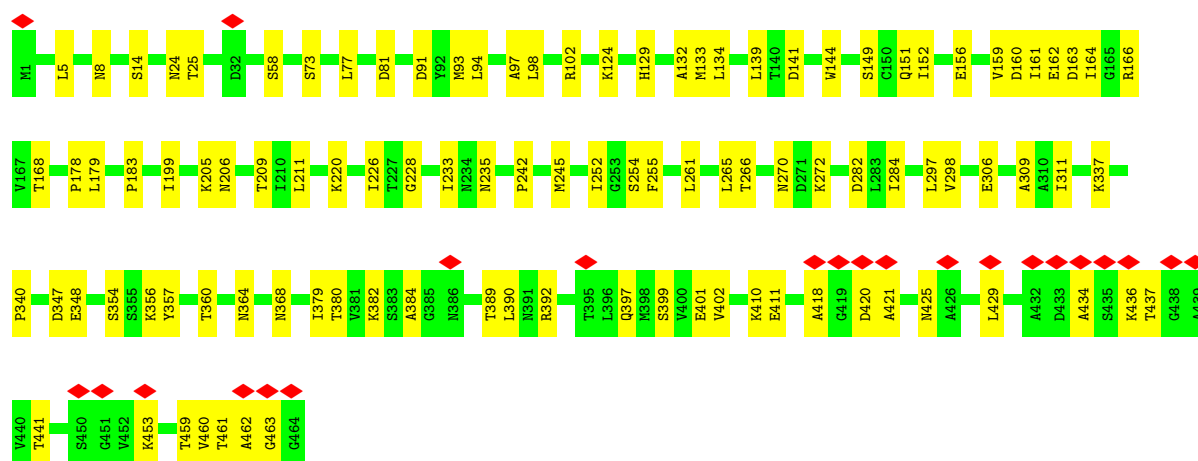
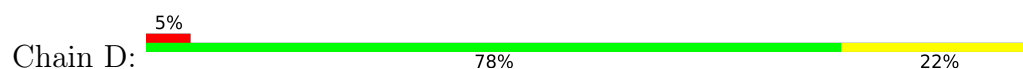




• Molecule 7: Tail tube protein



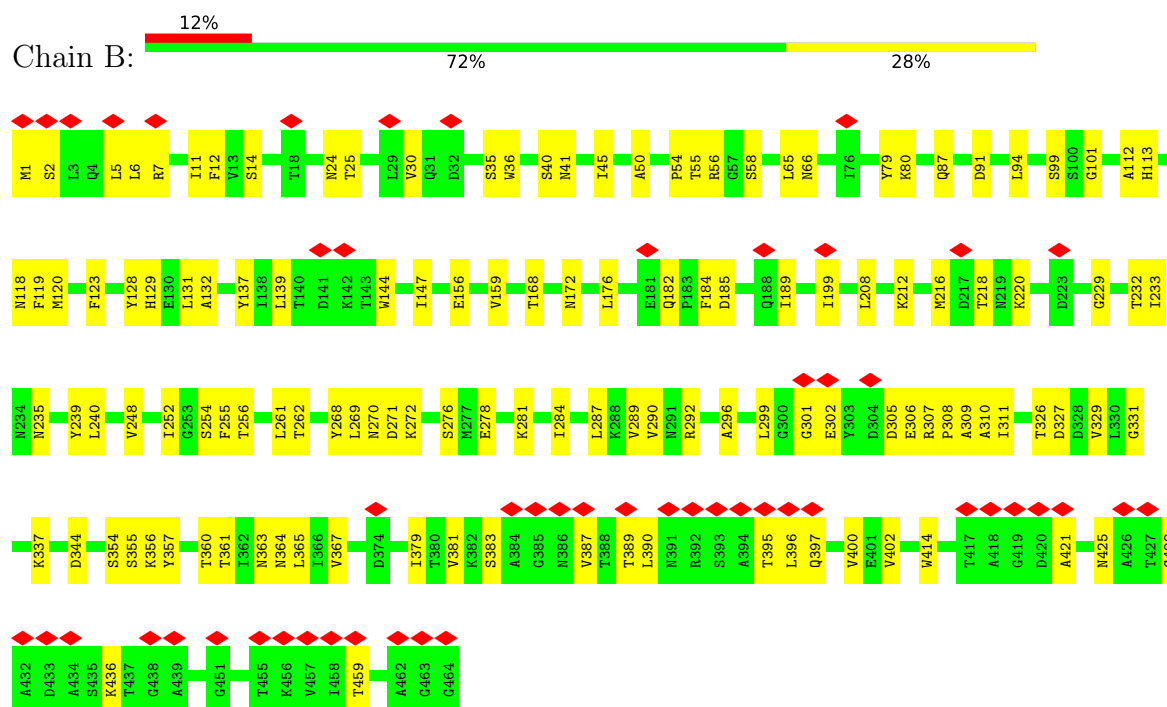
• Molecule 7: Tail tube protein



• Molecule 7: Tail tube protein



• Molecule 7: Tail tube protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25558	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0214	Depositor
Map size (Å)	459.34, 459.34, 459.34	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.351, 1.351, 1.351	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	b	0.14	0/7740	0.27	0/10500
1	c	0.14	0/7740	0.27	0/10500
1	d	0.13	0/7740	0.27	0/10500
2	h	0.13	0/331	0.27	0/444
2	i	0.12	0/331	0.26	0/444
2	j	0.13	0/331	0.24	0/444
3	e	0.13	0/5285	0.28	0/7208
3	f	0.12	0/5265	0.26	0/7182
3	g	0.12	0/4650	0.26	0/6332
4	J	0.14	0/1062	0.32	0/1443
4	K	0.14	0/1062	0.32	0/1443
4	L	0.27	0/1070	0.42	0/1453
4	M	0.14	0/1070	0.30	0/1453
4	N	0.13	0/1062	0.32	0/1443
4	O	0.14	0/1062	0.32	0/1443
4	P	0.27	0/1070	0.43	0/1453
4	Q	0.13	0/1070	0.31	0/1453
4	R	0.13	0/1062	0.32	0/1443
4	S	0.14	0/1062	0.31	0/1443
4	T	0.27	0/1070	0.43	0/1453
4	U	0.13	0/1070	0.30	0/1453
5	G	0.15	0/2483	0.27	0/3370
5	H	0.15	0/2483	0.27	0/3370
5	I	0.14	0/2483	0.28	0/3370
6	V	0.21	0/1649	0.31	0/2239
6	W	0.14	0/1649	0.27	0/2239
6	X	0.21	0/1649	0.31	0/2239
6	Y	0.14	0/1649	0.26	0/2239
6	Z	0.21	0/1649	0.31	0/2239
6	a	0.14	0/1649	0.26	0/2239
7	A	0.18	0/3604	0.35	0/4904
7	B	0.18	0/3604	0.35	0/4904
7	C	0.18	0/3604	0.35	0/4904
7	D	0.14	0/3604	0.30	0/4904

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	E	0.14	0/3604	0.30	0/4904
7	F	0.14	0/3604	0.30	0/4904
All	All	0.15	0/91172	0.30	0/123898

There are no bond length outliers.

There are no bond angle outliers.

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	b	7576	0	7410	98	0
1	c	7576	0	7410	122	0
1	d	7576	0	7410	113	0
2	h	328	0	322	9	0
2	i	328	0	322	5	0
2	j	328	0	322	6	0
3	e	5163	0	5058	74	0
3	f	5143	0	5039	81	0
3	g	4546	0	4462	59	0
4	J	1048	0	1041	23	0
4	K	1048	0	1041	21	0
4	L	1056	0	1053	22	0
4	M	1056	0	1053	25	0
4	N	1048	0	1041	22	0
4	O	1048	0	1041	21	0
4	P	1056	0	1053	26	0
4	Q	1056	0	1053	28	0
4	R	1048	0	1041	24	0
4	S	1048	0	1041	22	0
4	T	1056	0	1053	24	0
4	U	1056	0	1053	25	0
5	G	2423	0	2349	35	0
5	H	2423	0	2349	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	2423	0	2349	35	0
6	V	1610	0	1590	30	0
6	W	1610	0	1590	31	0
6	X	1610	0	1590	28	0
6	Y	1610	0	1590	35	0
6	Z	1610	0	1590	30	0
6	a	1610	0	1590	33	0
7	A	3546	0	3509	108	0
7	B	3546	0	3509	109	0
7	C	3546	0	3509	106	0
7	D	3546	0	3509	64	0
7	E	3546	0	3509	63	0
7	F	3546	0	3509	60	0
All	All	89393	0	87960	1406	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1406) 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:d:84:THR:HG23	6:V:41:VAL:HG23	1.27	1.13
1:d:683:ARG:HD3	6:Z:43:ILE:HD11	1.22	1.11
1:c:84:THR:HG23	6:Z:41:VAL:HG23	1.43	0.96
1:c:683:ARG:HD3	6:X:43:ILE:HD11	1.47	0.95
1:b:84:THR:HG23	6:X:41:VAL:HG23	1.51	0.91
1:d:683:ARG:CD	6:Z:43:ILE:HD11	2.02	0.89
4:L:100:ASN:HB3	5:G:231:ARG:HH22	1.40	0.87
5:I:231:ARG:HH22	4:T:100:ASN:HB3	1.41	0.86
1:c:302:ASP:OD1	1:c:441:LYS:NZ	2.08	0.86
7:C:5:LEU:HD13	7:B:329:VAL:HG22	1.59	0.85
5:H:231:ARG:HH22	4:P:100:ASN:HB3	1.40	0.84
7:C:329:VAL:HG22	7:A:5:LEU:HD13	1.59	0.84
1:d:932:ARG:NH2	1:d:946:TRP:O	2.09	0.83
3:e:242:ARG:NH1	3:e:245:GLY:O	2.11	0.83
1:b:230:LYS:O	1:b:238:ARG:NH1	2.11	0.83
1:d:84:THR:CG2	6:V:41:VAL:HG23	2.08	0.83
3:g:673:SER:OG	3:g:676:MET:SD	2.37	0.82
3:f:114:CYS:SG	3:f:206:ARG:NH1	2.52	0.82
7:A:329:VAL:HG22	7:B:5:LEU:HD13	1.60	0.82
3:f:514:ARG:NE	3:f:518:THR:O	2.14	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:929:LEU:O	1:c:930:ARG:NH1	2.12	0.81
1:d:84:THR:HG23	6:V:41:VAL:CG2	2.09	0.81
1:d:815:ARG:NH2	1:d:824:SER:O	2.14	0.80
4:L:88:ILE:HG22	4:L:134:ILE:HD11	1.63	0.80
4:P:88:ILE:HG22	4:P:134:ILE:HD11	1.63	0.80
1:d:644:ARG:NH2	2:i:1102:MET:O	2.15	0.80
1:b:771:VAL:O	1:b:789:GLN:NE2	2.15	0.80
4:T:88:ILE:HG22	4:T:134:ILE:HD11	1.63	0.80
1:c:582:LEU:HD11	1:c:660:LEU:HD11	1.63	0.79
4:S:54:LEU:HD21	4:T:102:ARG:HD3	1.64	0.79
3:e:428:ILE:HG22	3:e:443:ILE:HG13	1.64	0.79
7:F:163:ASP:OD1	7:F:164:ILE:N	2.16	0.79
4:O:54:LEU:HD21	4:P:102:ARG:HD3	1.64	0.79
7:D:163:ASP:OD1	7:D:164:ILE:N	2.16	0.78
7:E:163:ASP:OD1	7:E:164:ILE:N	2.16	0.78
4:L:102:ARG:HD3	4:K:54:LEU:HD21	1.64	0.78
1:d:83:GLY:O	1:b:683:ARG:NH2	2.17	0.78
1:d:582:LEU:HD11	1:d:660:LEU:HD11	1.65	0.78
1:b:790:LEU:N	1:b:793:ASN:OD1	2.16	0.77
1:c:306:ASP:OD1	1:c:307:PHE:N	2.17	0.77
1:b:719:SER:O	1:b:721:GLN:NE2	2.18	0.77
1:c:923:LEU:HD23	1:c:923:LEU:O	1.85	0.77
3:f:271:LYS:NZ	3:g:370:ALA:O	2.19	0.76
1:d:302:ASP:OD1	1:d:441:LYS:NZ	2.17	0.76
2:h:1102:MET:O	1:c:644:ARG:NH2	2.19	0.76
3:e:482:GLN:NE2	3:e:483:THR:O	2.19	0.75
7:A:1:MET:HA	7:A:1:MET:HE2	1.68	0.75
7:C:1:MET:HE2	7:C:1:MET:HA	1.69	0.75
1:d:758:ASN:OD1	1:d:805:GLU:N	2.20	0.74
2:j:1102:MET:O	1:b:644:ARG:NH2	2.21	0.73
7:C:272:LYS:HB3	7:A:1:MET:HG2	1.69	0.73
7:B:1:MET:HE2	7:B:1:MET:HA	1.69	0.73
1:d:897:ARG:NH2	1:d:899:GLU:OE1	2.21	0.73
1:b:855:VAL:O	1:b:856:THR:OG1	2.06	0.73
1:c:337:THR:OG1	1:c:349:GLN:O	2.05	0.73
4:Q:61:VAL:HG12	4:Q:91:LYS:HE3	1.71	0.72
4:U:61:VAL:HG12	4:U:91:LYS:HE3	1.71	0.72
1:c:230:LYS:O	1:c:238:ARG:NH1	2.22	0.72
7:B:216:MET:HE3	7:B:292:ARG:HB3	1.72	0.72
7:C:216:MET:HE3	7:C:292:ARG:HB3	1.72	0.72
4:M:61:VAL:HG12	4:M:91:LYS:HE3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:91:ASP:HB3	7:B:94:LEU:HD12	1.72	0.72
3:f:180:SER:O	3:f:182:GLN:NE2	2.23	0.71
7:C:91:ASP:HB3	7:C:94:LEU:HD12	1.72	0.71
1:c:683:ARG:CD	6:X:43:ILE:HD11	2.20	0.71
7:C:1:MET:HG2	7:B:272:LYS:HB3	1.72	0.71
1:d:304:PHE:N	1:d:351:SER:OG	2.23	0.71
1:c:84:THR:CG2	6:Z:41:VAL:HG23	2.19	0.71
7:A:91:ASP:HB3	7:A:94:LEU:HD12	1.72	0.70
7:A:272:LYS:HB3	7:B:1:MET:HG2	1.72	0.70
7:A:216:MET:HE3	7:A:292:ARG:HB3	1.72	0.70
7:C:239:TYR:HD1	7:C:254:SER:HB3	1.57	0.70
1:d:735:ASN:OD1	1:d:822:ARG:NH1	2.25	0.69
4:L:18:TYR:O	4:L:79:SER:HB2	1.92	0.69
5:G:63:ILE:HG21	5:G:107:MET:HE1	1.74	0.69
1:c:834:ASN:ND2	1:c:941:GLU:OE2	2.25	0.69
1:b:461:ILE:HG12	1:b:494:LEU:HD12	1.73	0.69
1:b:745:THR:OG1	1:b:760:GLU:OE2	2.10	0.69
7:B:239:TYR:HD1	7:B:254:SER:HB3	1.56	0.69
1:c:555:LEU:O	1:c:556:SER:OG	2.08	0.69
3:f:535:LEU:HD21	3:f:540:SER:HA	1.75	0.69
3:g:20:THR:O	3:g:21:LEU:HD22	1.93	0.69
1:b:284:LEU:N	1:b:391:GLY:O	2.25	0.69
4:T:18:TYR:O	4:T:79:SER:HB2	1.92	0.69
7:A:239:TYR:CD1	7:A:254:SER:HB3	2.28	0.69
1:d:92:LEU:HD22	1:d:154:ILE:HG23	1.74	0.69
7:C:239:TYR:CD1	7:C:254:SER:HB3	2.28	0.69
1:b:26:LEU:HD11	1:b:135:ILE:HD11	1.75	0.68
7:C:344:ASP:HB3	7:A:55:THR:HG23	1.75	0.68
7:A:239:TYR:HD1	7:A:254:SER:HB3	1.56	0.68
3:g:4:ASN:ND2	3:g:33:ASP:OD2	2.26	0.68
5:I:63:ILE:HG21	5:I:107:MET:HE1	1.74	0.68
7:B:239:TYR:CD1	7:B:254:SER:HB3	2.28	0.68
3:g:21:LEU:HD23	3:g:192:ASP:OD1	1.94	0.68
4:P:18:TYR:O	4:P:79:SER:HB2	1.92	0.68
5:H:63:ILE:HG21	5:H:107:MET:HE1	1.74	0.67
7:A:156:GLU:HB3	7:A:168:THR:HB	1.77	0.67
4:Q:17:PRO:HD2	4:P:124:SER:HB2	1.75	0.67
1:d:745:THR:OG1	1:d:760:GLU:OE2	2.12	0.67
1:c:579:TYR:HE1	6:Y:33:LEU:HD21	1.58	0.67
1:b:231:LYS:NZ	1:b:237:SER:O	2.26	0.67
1:b:308:TYR:OH	1:b:436:GLU:OE2	2.08	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:55:THR:HG23	7:B:344:ASP:HB3	1.77	0.67
4:U:138:VAL:HB	4:T:51:LYS:HE2	1.77	0.67
7:A:212:LYS:HB2	7:A:296:ALA:HB3	1.77	0.67
7:E:91:ASP:HB2	7:E:94:LEU:HD12	1.77	0.67
1:d:506:GLN:NE2	1:d:639:ASN:OD1	2.27	0.66
7:A:344:ASP:HB3	7:B:55:THR:HG23	1.77	0.66
7:B:212:LYS:HB2	7:B:296:ALA:HB3	1.77	0.66
4:K:41:LEU:HD23	4:K:74:GLY:HA2	1.77	0.66
4:S:41:LEU:HD23	4:S:74:GLY:HA2	1.77	0.66
7:B:156:GLU:HB3	7:B:168:THR:HB	1.77	0.66
1:d:406:ASP:OD1	1:d:407:SER:N	2.28	0.66
7:F:91:ASP:HB2	7:F:94:LEU:HD12	1.77	0.66
7:D:91:ASP:HB2	7:D:94:LEU:HD12	1.77	0.66
3:e:372:GLY:O	3:g:273:ASN:ND2	2.28	0.66
3:g:399:ALA:O	3:g:400:ASN:ND2	2.29	0.66
1:b:302:ASP:OD1	1:b:441:LYS:NZ	2.29	0.66
4:M:92:ALA:HB3	4:M:104:ARG:HH21	1.61	0.66
7:C:212:LYS:HB2	7:C:296:ALA:HB3	1.77	0.66
4:M:17:PRO:HD2	4:L:124:SER:HB2	1.76	0.66
4:O:41:LEU:HD23	4:O:74:GLY:HA2	1.77	0.66
7:C:156:GLU:HB3	7:C:168:THR:HB	1.77	0.66
4:U:17:PRO:HD2	4:T:124:SER:HB2	1.76	0.66
1:c:84:THR:HG23	6:Z:41:VAL:CG2	2.22	0.65
3:f:132:THR:OG1	3:f:162:MET:O	2.13	0.65
4:Q:96:ARG:NH1	4:Q:136:ASP:OD2	2.26	0.65
1:d:887:ASP:N	1:d:891:ARG:O	2.29	0.65
3:f:410:ASP:O	3:f:434:ASN:ND2	2.29	0.65
3:e:638:THR:HG22	3:g:643:LYS:CG	2.26	0.65
4:K:64:PHE:HB3	4:K:78:ILE:HD11	1.79	0.65
3:g:453:ASP:OD1	3:g:454:GLY:N	2.30	0.65
4:U:92:ALA:HB3	4:U:104:ARG:HH21	1.61	0.65
1:c:461:ILE:HG12	1:c:494:LEU:HD12	1.78	0.65
4:Q:92:ALA:HB3	4:Q:104:ARG:HH21	1.61	0.65
3:g:120:ASP:OD1	3:g:121:VAL:N	2.30	0.64
3:e:29:TYR:CE1	3:e:55:ILE:HD12	2.32	0.64
3:e:148:ASN:ND2	3:e:150:ASN:O	2.31	0.64
4:Q:139:THR:HA	4:P:49:SER:HB3	1.79	0.64
3:g:137:ASP:OD1	3:g:138:TYR:N	2.29	0.64
4:M:139:THR:HA	4:L:49:SER:HB3	1.79	0.64
4:U:139:THR:HA	4:T:49:SER:HB3	1.78	0.64
4:S:64:PHE:HB3	4:S:78:ILE:HD11	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:64:PHE:HB3	4:O:78:ILE:HD11	1.79	0.64
7:B:299:LEU:HB2	7:B:310:ALA:HB3	1.80	0.64
1:d:45:PHE:HZ	6:a:155:ASP:HB2	1.63	0.64
1:d:45:PHE:HB2	6:a:45:ALA:HB2	1.79	0.64
7:A:299:LEU:HB2	7:A:310:ALA:HB3	1.80	0.64
3:g:56:ASP:OD1	3:g:57:THR:N	2.31	0.64
6:Y:113:THR:HG23	6:Y:115:GLY:H	1.63	0.64
6:Z:24:ASP:OD1	6:Z:46:GLN:NE2	2.31	0.64
1:d:284:LEU:N	1:d:391:GLY:O	2.30	0.63
4:Q:138:VAL:HB	4:P:51:LYS:HE2	1.78	0.63
4:S:96:ARG:NH2	4:S:136:ASP:OD2	2.31	0.63
4:M:96:ARG:NH1	4:M:136:ASP:OD2	2.25	0.63
6:V:24:ASP:OD1	6:V:46:GLN:NE2	2.31	0.63
1:b:59:LYS:NZ	1:b:88:GLU:OE2	2.29	0.63
4:M:138:VAL:HB	4:L:51:LYS:HE2	1.78	0.63
2:h:1094:ARG:NH2	2:h:1115:ASP:O	2.31	0.63
4:K:96:ARG:NH2	4:K:136:ASP:OD2	2.31	0.63
1:c:318:ASP:OD1	1:c:508:TYR:OH	2.17	0.63
3:f:474:ILE:O	3:g:193:SER:OG	2.07	0.63
1:d:936:GLU:N	1:d:936:GLU:OE1	2.31	0.63
5:H:69:PHE:HB3	5:H:165:LEU:HD12	1.81	0.63
4:O:96:ARG:NH2	4:O:136:ASP:OD2	2.32	0.63
1:c:594:ASN:ND2	1:c:623:ASP:OD2	2.32	0.63
1:d:736:VAL:HG22	1:d:824:SER:HB3	1.79	0.63
1:c:579:TYR:CE1	6:Y:33:LEU:HD21	2.33	0.63
1:c:791:GLU:OE1	1:c:791:GLU:N	2.30	0.63
7:C:299:LEU:HB2	7:C:310:ALA:HB3	1.80	0.63
4:U:96:ARG:NH1	4:U:136:ASP:OD2	2.26	0.63
2:h:1108:GLU:OE2	1:c:644:ARG:NH1	2.31	0.62
1:c:361:ASP:OD1	1:c:362:GLY:N	2.32	0.62
1:b:701:ASP:OD1	6:W:29:ILE:HD13	1.98	0.62
7:F:205:LYS:HB3	7:A:255:PHE:HZ	1.64	0.62
6:Z:21:ASN:HB3	6:Z:51:ASN:HB2	1.82	0.62
6:X:24:ASP:OD1	6:X:46:GLN:NE2	2.31	0.62
7:D:205:LYS:HB3	7:B:255:PHE:HZ	1.64	0.62
4:P:21:LEU:HA	4:P:77:SER:HA	1.81	0.62
4:T:21:LEU:HA	4:T:77:SER:HA	1.81	0.62
4:L:21:LEU:HA	4:L:77:SER:HA	1.81	0.62
6:a:113:THR:HG23	6:a:115:GLY:H	1.64	0.62
6:W:113:THR:HG23	6:W:115:GLY:H	1.63	0.62
3:e:19:TYR:OH	3:e:181:GLY:O	2.18	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:448:ASP:OD1	1:b:449:GLY:N	2.33	0.62
5:G:69:PHE:HB3	5:G:165:LEU:HD12	1.81	0.62
7:C:354:SER:HB3	7:C:357:TYR:CE1	2.35	0.61
3:e:487:TYR:HD2	3:e:507:TRP:CE3	2.18	0.61
4:U:25:MET:HE2	4:U:36:SER:HB2	1.82	0.61
1:b:406:ASP:OD1	1:b:407:SER:N	2.32	0.61
7:E:205:LYS:HB3	7:C:255:PHE:HZ	1.64	0.61
3:g:359:ALA:O	3:g:360:THR:OG1	2.14	0.61
5:I:202:PHE:CE2	6:Y:84:PRO:HG3	2.36	0.61
7:B:354:SER:HB3	7:B:357:TYR:CE1	2.35	0.61
1:d:306:ASP:OD1	1:d:307:PHE:N	2.33	0.61
1:d:761:LEU:HD21	1:d:812:PHE:CD1	2.35	0.61
6:V:21:ASN:HB3	6:V:51:ASN:HB2	1.82	0.61
5:I:69:PHE:HB3	5:I:165:LEU:HD12	1.81	0.61
4:Q:25:MET:HE2	4:Q:36:SER:HB2	1.82	0.61
4:O:111:VAL:HG22	4:O:128:MET:HG2	1.83	0.61
4:L:66:THR:HG22	4:L:78:ILE:HD13	1.83	0.61
1:b:84:THR:HG23	6:X:41:VAL:CG2	2.30	0.61
1:d:862:ASP:OD1	1:d:908:LEU:N	2.34	0.61
7:A:354:SER:HB3	7:A:357:TYR:CE1	2.35	0.61
3:f:676:MET:HE2	3:g:679:ASP:OD1	2.01	0.60
7:C:144:TRP:HE1	7:C:182:GLN:HG2	1.66	0.60
4:J:25:MET:HE2	4:J:36:SER:HB2	1.83	0.60
7:A:12:PHE:HB2	7:A:137:TYR:HB2	1.83	0.60
4:P:66:THR:HG22	4:P:78:ILE:HD13	1.83	0.60
4:O:31:VAL:HG22	4:O:33:PRO:HD2	1.84	0.60
1:d:776:ILE:O	1:d:785:TYR:N	2.35	0.60
1:c:788:GLN:O	6:W:161:THR:HG21	2.01	0.60
4:R:47:ARG:HA	4:R:66:THR:HG21	1.84	0.60
6:X:21:ASN:HB3	6:X:51:ASN:HB2	1.81	0.60
7:B:233:ILE:HG13	7:B:261:LEU:HD13	1.83	0.60
4:T:66:THR:HG22	4:T:78:ILE:HD13	1.83	0.60
1:c:43:ASP:OD2	1:c:700:ARG:NH2	2.32	0.60
1:c:506:GLN:NE2	1:c:639:ASN:OD1	2.34	0.60
7:C:233:ILE:HG13	7:C:261:LEU:HD13	1.83	0.60
3:g:37:ARG:NH2	3:g:57:THR:O	2.34	0.60
4:S:31:VAL:HG22	4:S:33:PRO:HD2	1.84	0.60
4:K:111:VAL:HG22	4:K:128:MET:HG2	1.83	0.60
7:B:144:TRP:HE1	7:B:182:GLN:HG2	1.66	0.60
1:d:644:ARG:NH1	2:i:1108:GLU:OE2	2.35	0.60
4:N:47:ARG:HA	4:N:66:THR:HG21	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:242:PRO:HD3	7:E:252:ILE:HG12	1.84	0.60
3:f:403:MET:HE1	3:e:428:ILE:HD11	1.84	0.60
1:b:45:PHE:HB2	6:W:45:ALA:HB2	1.83	0.60
1:d:761:LEU:HD21	1:d:812:PHE:CE1	2.36	0.60
7:A:80:LYS:HB3	7:A:87:GLN:HE21	1.67	0.60
5:H:202:PHE:CE2	6:W:84:PRO:HG3	2.36	0.60
4:R:25:MET:HE2	4:R:36:SER:HB2	1.83	0.60
4:N:25:MET:HE2	4:N:36:SER:HB2	1.83	0.60
6:Y:2:ARG:NH2	6:Y:5:ASP:OD2	2.35	0.60
4:M:25:MET:HE2	4:M:36:SER:HB2	1.82	0.60
6:W:2:ARG:NH2	6:W:5:ASP:OD2	2.35	0.60
1:d:45:PHE:CZ	6:a:155:ASP:HB2	2.37	0.59
1:d:93:VAL:O	1:b:658:ARG:NH1	2.33	0.59
7:B:12:PHE:HB2	7:B:137:TYR:HB2	1.83	0.59
1:c:92:LEU:HD22	1:c:154:ILE:HG23	1.84	0.59
1:c:406:ASP:OD1	1:c:407:SER:N	2.34	0.59
7:B:80:LYS:HB3	7:B:87:GLN:HE21	1.67	0.59
1:d:62:SER:HG	1:d:80:THR:HG1	1.50	0.59
1:c:305:LEU:O	1:c:338:MET:N	2.35	0.59
3:f:494:PRO:HD3	3:f:521:ILE:HD13	1.85	0.59
3:g:113:ARG:NE	3:g:115:GLU:OE2	2.34	0.59
4:K:31:VAL:HG22	4:K:33:PRO:HD2	1.84	0.59
7:C:12:PHE:HB2	7:C:137:TYR:HB2	1.83	0.59
7:C:390:LEU:HD13	7:C:396:LEU:HD22	1.85	0.59
3:e:256:ILE:HG22	3:e:269:ALA:HA	1.84	0.59
7:D:242:PRO:HD3	7:D:252:ILE:HG12	1.84	0.59
7:A:390:LEU:HD13	7:A:396:LEU:HD22	1.85	0.59
6:a:84:PRO:HG3	5:G:202:PHE:CE2	2.37	0.59
6:Y:98:VAL:HG23	6:Y:113:THR:HA	1.85	0.59
4:O:115:ARG:HD3	4:O:118:VAL:HG11	1.85	0.59
7:B:421:ALA:HB1	7:B:436:LYS:HB3	1.85	0.59
7:D:379:ILE:HG12	7:D:402:VAL:HG12	1.85	0.59
1:c:284:LEU:N	1:c:391:GLY:O	2.36	0.59
1:c:730:PRO:HB3	1:b:901:VAL:HG23	1.85	0.59
6:a:2:ARG:NH2	6:a:5:ASP:OD2	2.35	0.59
4:Q:44:PHE:HB3	4:Q:113:ILE:HD11	1.85	0.59
4:S:111:VAL:HG22	4:S:128:MET:HG2	1.83	0.59
4:M:44:PHE:HB3	4:M:113:ILE:HD11	1.85	0.59
4:J:47:ARG:HA	4:J:66:THR:HG21	1.84	0.59
7:A:144:TRP:HE1	7:A:182:GLN:HG2	1.66	0.59
1:d:269:GLY:O	1:d:439:GLY:N	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:181:LEU:HD13	1:c:188:LEU:HD21	1.85	0.59
3:g:10:MET:HE1	3:g:76:ALA:CA	2.33	0.59
7:A:233:ILE:HG13	7:A:261:LEU:HD13	1.83	0.59
1:c:45:PHE:HB2	6:Y:45:ALA:HB2	1.85	0.58
1:b:123:ASP:O	1:b:823:ARG:NH1	2.36	0.58
7:F:379:ILE:HG12	7:F:402:VAL:HG12	1.85	0.58
7:C:80:LYS:HB3	7:C:87:GLN:HE21	1.67	0.58
4:U:24:PHE:N	4:U:74:GLY:O	2.36	0.58
4:K:115:ARG:HD3	4:K:118:VAL:HG11	1.85	0.58
7:E:379:ILE:HG12	7:E:402:VAL:HG12	1.85	0.58
1:b:269:GLY:O	1:b:439:GLY:N	2.36	0.58
7:F:242:PRO:HD3	7:F:252:ILE:HG12	1.84	0.58
4:T:50:ILE:HD11	4:T:64:PHE:CZ	2.38	0.58
6:a:98:VAL:HG23	6:a:113:THR:HA	1.85	0.58
7:C:212:LYS:NZ	7:C:302:GLU:OE2	2.36	0.58
7:B:212:LYS:NZ	7:B:302:GLU:OE2	2.36	0.58
3:g:25:GLN:NE2	3:g:26:HIS:O	2.37	0.58
4:P:50:ILE:HD11	4:P:64:PHE:CZ	2.39	0.58
1:d:882:THR:OG1	1:d:936:GLU:OE2	2.14	0.58
2:j:1108:GLU:OE2	1:b:644:ARG:NH1	2.37	0.58
4:U:44:PHE:HB3	4:U:113:ILE:HD11	1.85	0.58
7:F:77:LEU:HB3	7:F:199:ILE:HG23	1.85	0.58
5:G:26:SER:OG	5:G:68:ASN:ND2	2.35	0.58
7:A:421:ALA:HB1	7:A:436:LYS:HB3	1.85	0.57
1:d:461:ILE:HG12	1:d:494:LEU:HD12	1.86	0.57
4:L:50:ILE:HD11	4:L:64:PHE:CZ	2.39	0.57
7:A:212:LYS:NZ	7:A:302:GLU:OE2	2.36	0.57
1:d:442:VAL:HG23	1:d:466:ASP:HB2	1.87	0.57
3:f:531:VAL:HG13	3:f:532:THR:HG23	1.87	0.57
7:C:421:ALA:HB1	7:C:436:LYS:HB3	1.85	0.57
3:e:458:ARG:NH2	3:g:612:ALA:O	2.37	0.57
7:D:77:LEU:HB3	7:D:199:ILE:HG23	1.85	0.57
7:A:240:LEU:HD22	7:A:255:PHE:HE2	1.70	0.57
7:B:390:LEU:HD13	7:B:396:LEU:HD22	1.85	0.57
1:b:304:PHE:CD2	1:b:437:VAL:HG12	2.40	0.57
5:I:26:SER:OG	5:I:68:ASN:ND2	2.35	0.57
1:c:45:PHE:CB	6:Y:45:ALA:HB2	2.35	0.57
1:c:579:TYR:CE1	6:Y:33:LEU:CD2	2.86	0.57
4:S:115:ARG:HD3	4:S:118:VAL:HG11	1.85	0.57
6:W:98:VAL:HG23	6:W:113:THR:HA	1.85	0.57
4:Q:24:PHE:N	4:Q:74:GLY:O	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:77:LEU:HB3	7:E:199:ILE:HG23	1.85	0.57
7:C:240:LEU:HD22	7:C:255:PHE:HE2	1.70	0.57
4:U:51:LYS:HD3	4:U:58:ALA:HB3	1.87	0.57
7:A:139:LEU:HD13	7:A:144:TRP:CE2	2.40	0.57
7:B:172:ASN:O	7:B:239:TYR:OH	2.23	0.57
3:f:536:VAL:HG12	3:f:538:GLY:H	1.68	0.56
7:C:172:ASN:O	7:C:239:TYR:OH	2.23	0.56
4:U:42:THR:HG22	4:U:71:ALA:HB1	1.87	0.56
1:c:741:ASP:OD2	1:c:797:ARG:NH1	2.38	0.56
1:d:161:GLN:OE1	1:d:554:ASN:ND2	2.38	0.56
1:b:92:LEU:HD22	1:b:154:ILE:HG23	1.87	0.56
1:b:757:LYS:HG3	1:b:803:ILE:HG22	1.87	0.56
4:M:42:THR:HG22	4:M:71:ALA:HB1	1.87	0.56
7:E:309:ALA:HB3	7:E:357:TYR:HD2	1.70	0.56
7:C:139:LEU:HD13	7:C:144:TRP:CE2	2.40	0.56
3:e:645:VAL:HG12	3:g:650:PHE:HB2	1.86	0.56
7:A:172:ASN:O	7:A:239:TYR:OH	2.23	0.56
4:L:89:ALA:HA	4:L:134:ILE:HD13	1.88	0.56
7:C:218:THR:HG22	7:C:220:LYS:HG3	1.88	0.56
1:d:894:ARG:NH2	1:d:904:TYR:OH	2.37	0.56
7:C:329:VAL:HG22	7:A:5:LEU:CD1	2.34	0.56
4:P:89:ALA:HA	4:P:134:ILE:HD13	1.88	0.56
3:e:488:ILE:HG21	3:e:521:ILE:HB	1.88	0.56
3:g:1:MET:HE2	3:g:1:MET:HA	1.87	0.56
4:M:24:PHE:N	4:M:74:GLY:O	2.36	0.56
7:E:437:THR:HG22	7:E:462:ALA:HB2	1.88	0.56
7:D:133:MET:HE1	7:D:149:SER:HB2	1.88	0.56
7:A:309:ALA:HB3	7:A:357:TYR:HD2	1.71	0.56
3:g:10:MET:HE1	3:g:76:ALA:HA	1.88	0.56
7:F:14:SER:HB2	7:F:25:THR:HG22	1.88	0.56
7:C:397:GLN:HA	7:C:429:LEU:HA	1.88	0.56
7:D:14:SER:HB2	7:D:25:THR:HG22	1.88	0.56
7:B:139:LEU:HD13	7:B:144:TRP:CE2	2.40	0.56
7:B:240:LEU:HD22	7:B:255:PHE:HE2	1.70	0.56
1:d:744:TYR:OH	1:d:834:ASN:OD1	2.23	0.55
1:d:781:HIS:ND1	1:d:785:TYR:OH	2.33	0.55
7:F:309:ALA:HB3	7:F:357:TYR:HD2	1.70	0.55
7:E:161:ILE:O	7:E:162:GLU:HG2	2.07	0.55
7:A:397:GLN:HA	7:A:429:LEU:HA	1.88	0.55
7:B:309:ALA:HB3	7:B:357:TYR:HD2	1.71	0.55
4:O:54:LEU:HB2	4:P:96:ARG:HH12	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:147:SER:HB3	6:Z:47:TYR:OH	2.05	0.55
4:Q:42:THR:HG22	4:Q:71:ALA:HB1	1.87	0.55
4:M:51:LYS:HD3	4:M:58:ALA:HB3	1.87	0.55
7:D:161:ILE:O	7:D:162:GLU:HG2	2.07	0.55
7:D:309:ALA:HB3	7:D:357:TYR:HD2	1.70	0.55
7:F:437:THR:HG22	7:F:462:ALA:HB2	1.88	0.55
3:e:531:VAL:HG23	3:e:532:THR:HG23	1.87	0.55
1:c:305:LEU:HD11	1:c:438:GLN:HG3	1.87	0.55
3:f:187:ASP:OD1	3:f:188:GLY:N	2.38	0.55
3:g:578:TRP:NE1	3:g:580:ASP:OD1	2.40	0.55
1:b:45:PHE:CZ	6:W:155:ASP:HB2	2.42	0.55
1:b:268:TYR:OH	1:b:466:ASP:OD2	2.20	0.55
7:D:437:THR:HG22	7:D:462:ALA:HB2	1.88	0.55
1:c:660:LEU:O	1:c:708:LEU:N	2.39	0.55
7:E:133:MET:HE1	7:E:149:SER:HB2	1.88	0.55
4:T:89:ALA:HA	4:T:134:ILE:HD13	1.88	0.55
4:Q:51:LYS:HD3	4:Q:58:ALA:HB3	1.87	0.55
7:C:309:ALA:HB3	7:C:357:TYR:HD2	1.71	0.55
1:d:213:THR:HG22	1:d:256:ASP:OD1	2.07	0.55
1:b:478:THR:OG1	1:b:480:ASP:OD1	2.25	0.55
1:b:45:PHE:CB	6:W:45:ALA:HB2	2.37	0.54
7:D:139:LEU:HD13	7:D:144:TRP:CE2	2.42	0.54
7:D:298:VAL:HG13	7:D:311:ILE:HG12	1.90	0.54
7:B:218:THR:HG22	7:B:220:LYS:HG3	1.88	0.54
1:c:196:ARG:NH1	1:c:413:ASP:OD2	2.39	0.54
3:f:9:LYS:NZ	3:f:95:LEU:O	2.34	0.54
4:S:54:LEU:HB2	4:T:96:ARG:HH12	1.71	0.54
7:D:220:LYS:NZ	7:D:282:ASP:OD2	2.38	0.54
2:h:1120:ASN:OD1	2:h:1121:ALA:N	2.38	0.54
3:e:218:ILE:HD11	3:e:313:GLN:CD	2.32	0.54
4:M:104:ARG:NH1	4:M:136:ASP:OD1	2.41	0.54
4:O:54:LEU:HD23	4:P:136:ASP:HB2	1.89	0.54
7:B:397:GLN:HA	7:B:429:LEU:HA	1.88	0.54
4:R:43:ASP:OD1	4:R:116:THR:OG1	2.25	0.54
7:F:139:LEU:HD13	7:F:144:TRP:CE2	2.42	0.54
7:F:161:ILE:O	7:F:162:GLU:HG2	2.07	0.54
5:G:127:VAL:HG22	5:G:140:VAL:HG12	1.89	0.54
1:d:281:ASP:OD1	1:d:282:THR:N	2.37	0.54
1:b:683:ARG:HD3	6:V:43:ILE:HD11	1.88	0.54
4:S:54:LEU:HD23	4:T:136:ASP:HB2	1.89	0.54
7:E:14:SER:HB2	7:E:25:THR:HG22	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:96:ARG:HH12	4:K:54:LEU:HB2	1.72	0.54
1:d:594:ASN:ND2	1:d:623:ASP:OD2	2.40	0.54
3:f:83:ASP:OD1	3:f:84:SER:N	2.35	0.54
7:C:5:LEU:CD1	7:B:329:VAL:HG22	2.35	0.54
7:F:133:MET:HE1	7:F:149:SER:HB2	1.89	0.54
7:A:218:THR:HG22	7:A:220:LYS:HG3	1.88	0.54
1:c:579:TYR:CD1	6:Y:33:LEU:CD2	2.90	0.54
4:Q:104:ARG:NH1	4:Q:136:ASP:OD1	2.41	0.54
6:X:133:PRO:HG3	6:X:174:ARG:NH1	2.23	0.54
7:E:139:LEU:HD13	7:E:144:TRP:CE2	2.43	0.54
6:a:201:ARG:NE	6:V:32:GLU:OE1	2.41	0.54
7:C:159:VAL:HG22	7:C:299:LEU:HD21	1.90	0.54
4:U:104:ARG:NH1	4:U:136:ASP:OD1	2.41	0.54
1:d:683:ARG:HD2	6:Z:41:VAL:HG11	1.89	0.54
1:c:834:ASN:OD1	1:c:835:SER:N	2.41	0.54
3:g:433:ASP:O	3:g:437:ALA:N	2.38	0.54
3:g:445:ASN:OD1	3:g:448:GLN:N	2.36	0.54
7:E:228:GLY:O	7:E:266:THR:OG1	2.26	0.54
7:D:389:THR:OG1	7:D:459:THR:O	2.26	0.54
1:d:81:ILE:HG21	1:d:88:GLU:HG2	1.90	0.53
1:c:564:GLU:OE1	1:c:711:TYR:OH	2.20	0.53
7:C:326:THR:HG21	7:A:35:SER:HA	1.90	0.53
7:B:159:VAL:HG22	7:B:299:LEU:HD21	1.90	0.53
6:V:133:PRO:HG3	6:V:174:ARG:NH1	2.23	0.53
1:d:17:LYS:NZ	6:a:28:MET:HE1	2.22	0.53
4:N:43:ASP:OD1	4:N:116:THR:OG1	2.25	0.53
4:N:138:VAL:HB	4:M:51:LYS:HD2	1.90	0.53
4:L:136:ASP:HB2	4:K:54:LEU:HD23	1.89	0.53
7:B:112:ALA:HB1	7:B:119:PHE:HZ	1.74	0.53
1:c:442:VAL:HG23	1:c:466:ASP:HB2	1.90	0.53
4:R:138:VAL:HB	4:Q:51:LYS:HD2	1.90	0.53
7:F:298:VAL:HG13	7:F:311:ILE:HG12	1.90	0.53
6:Z:133:PRO:HG3	6:Z:174:ARG:NH1	2.23	0.53
5:I:124:VAL:HA	5:I:142:ILE:HG22	1.91	0.53
1:c:564:GLU:OE2	1:c:653:LYS:NZ	2.42	0.53
5:I:127:VAL:HG22	5:I:140:VAL:HG12	1.90	0.53
4:J:138:VAL:HB	4:U:51:LYS:HD2	1.90	0.53
1:d:845:PHE:CE2	1:d:949:ILE:HD12	2.44	0.53
1:c:176:ALA:HA	1:c:181:LEU:HD12	1.91	0.53
1:c:605:LEU:HD12	1:c:606:SER:O	2.08	0.53
3:e:529:ASP:O	3:e:533:ASN:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:389:THR:OG1	7:F:459:THR:O	2.26	0.53
7:D:390:LEU:HB3	7:D:460:VAL:HG22	1.91	0.53
7:A:112:ALA:HB1	7:A:119:PHE:HZ	1.74	0.53
7:A:360:THR:O	7:A:364:ASN:ND2	2.42	0.53
7:E:402:VAL:HG21	7:E:410:LYS:HD2	1.91	0.53
7:B:270:ASN:HB3	7:B:272:LYS:HG2	1.91	0.53
1:d:574:ASN:OD1	1:d:575:PHE:N	2.39	0.53
1:d:942:GLN:N	1:d:942:GLN:OE1	2.42	0.53
7:F:402:VAL:HG21	7:F:410:LYS:HD2	1.91	0.53
7:B:360:THR:O	7:B:364:ASN:ND2	2.42	0.53
7:B:379:ILE:HG12	7:B:402:VAL:HG12	1.90	0.53
7:E:298:VAL:HG13	7:E:311:ILE:HG12	1.89	0.52
7:E:390:LEU:HB3	7:E:460:VAL:HG22	1.91	0.52
7:C:35:SER:HA	7:B:326:THR:HG21	1.92	0.52
7:C:112:ALA:HB1	7:C:119:PHE:HZ	1.74	0.52
7:C:270:ASN:HB3	7:C:272:LYS:HG2	1.91	0.52
5:G:124:VAL:HA	5:G:142:ILE:HG22	1.91	0.52
1:d:293:VAL:HG22	1:d:418:ILE:HG12	1.91	0.52
1:d:727:ASN:OD1	1:d:728:ASP:N	2.42	0.52
3:f:651:LEU:HD12	3:f:654:ILE:HD11	1.91	0.52
3:g:19:TYR:O	3:g:20:THR:HG22	2.09	0.52
4:R:139:THR:HA	4:Q:49:SER:HB3	1.90	0.52
7:D:228:GLY:O	7:D:266:THR:OG1	2.26	0.52
1:c:323:ASP:OD1	1:c:324:THR:N	2.42	0.52
5:G:72:THR:HG22	5:G:162:GLY:H	1.75	0.52
7:A:379:ILE:HG12	7:A:402:VAL:HG12	1.90	0.52
1:c:395:GLN:NE2	1:c:401:GLY:O	2.41	0.52
3:f:318:ASN:OD1	3:f:319:GLU:N	2.42	0.52
3:f:345:LYS:NZ	3:f:347:GLY:O	2.42	0.52
3:e:638:THR:HG22	3:g:643:LYS:HG2	1.90	0.52
5:I:72:THR:HG22	5:I:162:GLY:H	1.75	0.52
5:H:26:SER:OG	5:H:68:ASN:ND2	2.35	0.52
6:Y:86:TYR:OH	6:Y:137:LYS:NZ	2.34	0.52
3:f:127:ILE:HD11	3:f:166:MET:HB2	1.91	0.52
3:e:676:MET:C	3:e:677:LYS:HZ3	2.18	0.52
1:b:293:VAL:HG22	1:b:418:ILE:HG12	1.90	0.52
4:N:139:THR:HA	4:M:49:SER:HB3	1.91	0.52
5:H:72:THR:HG22	5:H:162:GLY:H	1.75	0.52
7:C:56:ARG:NH2	7:B:235:ASN:OD1	2.38	0.52
7:C:156:GLU:HA	7:C:232:THR:HG22	1.91	0.52
7:C:360:THR:O	7:C:364:ASN:ND2	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:235:ASN:OD1	7:B:56:ARG:NH2	2.37	0.52
1:d:771:VAL:HG23	1:d:817:VAL:O	2.10	0.52
7:E:389:THR:OG1	7:E:459:THR:O	2.26	0.52
7:A:270:ASN:HB3	7:A:272:LYS:HG2	1.91	0.52
1:d:9:LYS:O	1:d:13:ASN:ND2	2.43	0.52
3:e:13:ASN:N	3:e:25:GLN:O	2.43	0.52
7:F:390:LEU:HB3	7:F:460:VAL:HG22	1.91	0.52
5:H:18:ARG:HH21	5:H:20:TYR:HH	1.58	0.52
5:H:124:VAL:HA	5:H:142:ILE:HG22	1.91	0.52
7:D:402:VAL:HG21	7:D:410:LYS:HD2	1.91	0.52
7:B:240:LEU:HD22	7:B:255:PHE:CE2	2.45	0.52
1:c:132:ARG:N	1:c:161:GLN:OE1	2.43	0.52
1:c:226:LYS:HB2	1:c:245:TYR:HB3	1.91	0.52
3:f:640:THR:HG22	3:e:645:VAL:HG22	1.91	0.52
7:C:379:ILE:HG12	7:C:402:VAL:HG12	1.90	0.52
7:B:381:VAL:HA	7:B:400:VAL:HG23	1.92	0.52
4:R:47:ARG:NH2	4:S:140:GLN:OE1	2.43	0.52
5:H:127:VAL:HG22	5:H:140:VAL:HG12	1.90	0.52
7:E:220:LYS:NZ	7:E:282:ASP:OD2	2.38	0.52
3:f:105:SER:N	3:f:135:GLU:OE1	2.42	0.52
3:f:625:PRO:HG3	3:e:634:ILE:HD12	1.92	0.52
3:f:637:GLY:O	3:e:642:SER:OG	2.25	0.52
5:I:101:GLU:OE2	5:I:212:ARG:NH2	2.38	0.52
4:J:139:THR:HA	4:U:49:SER:HB3	1.91	0.52
1:c:174:ASP:OD1	1:c:209:ASN:ND2	2.43	0.51
4:O:43:ASP:OD2	4:O:116:THR:N	2.43	0.51
7:A:159:VAL:HG22	7:A:299:LEU:HD21	1.90	0.51
7:A:329:VAL:HG22	7:B:5:LEU:CD1	2.36	0.51
7:B:156:GLU:HA	7:B:232:THR:HG22	1.91	0.51
1:c:45:PHE:CZ	6:Y:155:ASP:HB2	2.45	0.51
1:b:516:ASP:OD2	1:b:519:SER:N	2.36	0.51
6:Y:201:ARG:NE	6:Z:32:GLU:OE1	2.42	0.51
7:C:278:GLU:HA	7:C:281:LYS:HE2	1.92	0.51
6:W:86:TYR:OH	6:W:137:LYS:NZ	2.34	0.51
3:g:189:VAL:HG23	3:g:189:VAL:O	2.10	0.51
1:b:306:ASP:OD2	1:b:307:PHE:N	2.44	0.51
5:H:224:LEU:HB2	5:H:278:TYR:HB2	1.93	0.51
4:O:32:TYR:HB3	4:O:33:PRO:HD3	1.93	0.51
7:E:211:LEU:HD11	7:E:265:LEU:HD13	1.93	0.51
5:I:224:LEU:HB2	5:I:278:TYR:HB2	1.93	0.51
4:S:43:ASP:OD2	4:S:116:THR:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:228:GLY:O	7:F:266:THR:OG1	2.26	0.51
4:J:135:SER:HB3	4:U:126:ARG:HH22	1.76	0.51
7:A:278:GLU:HA	7:A:281:LYS:HE2	1.92	0.51
7:B:278:GLU:HA	7:B:281:LYS:HE2	1.92	0.51
6:Z:26:ASP:HB3	6:Z:46:GLN:HG3	1.93	0.51
3:g:10:MET:HE3	3:g:77:PHE:CD2	2.46	0.51
1:b:183:VAL:O	1:b:185:ASN:ND2	2.44	0.51
7:C:235:ASN:OD1	7:A:56:ARG:NH2	2.40	0.51
4:J:47:ARG:NH2	4:K:140:GLN:OE1	2.43	0.51
7:A:326:THR:HG21	7:B:35:SER:HA	1.91	0.51
3:f:171:PRO:O	3:f:175:TYR:OH	2.28	0.51
3:f:213:ALA:O	3:f:240:TRP:NE1	2.40	0.51
3:f:502:TYR:HB3	3:f:503:PRO:HD3	1.92	0.51
3:e:409:GLN:N	3:e:409:GLN:OE1	2.43	0.51
6:a:100:ILE:HD11	6:a:166:PRO:HD3	1.92	0.51
4:N:135:SER:HB3	4:M:126:ARG:HH22	1.76	0.51
4:O:113:ILE:HB	4:O:127:ILE:HD11	1.93	0.51
4:L:41:LEU:HG	4:L:44:PHE:HD2	1.76	0.51
6:W:100:ILE:HD11	6:W:166:PRO:HD3	1.92	0.51
7:A:240:LEU:HD22	7:A:255:PHE:CE2	2.45	0.51
7:A:381:VAL:HA	7:A:400:VAL:HG23	1.92	0.51
3:e:678:ILE:O	3:e:678:ILE:HG23	2.11	0.51
1:b:773:TYR:CZ	1:b:817:VAL:HG21	2.46	0.51
4:R:99:TYR:HB2	5:I:162:GLY:HA2	1.93	0.51
6:Y:136:TYR:CD2	6:Y:152:LEU:HD13	2.46	0.51
7:C:308:PRO:HA	7:C:355:SER:HA	1.93	0.51
5:G:224:LEU:HB2	5:G:278:TYR:HB2	1.92	0.51
7:D:233:ILE:HG13	7:D:261:LEU:HD13	1.93	0.51
1:c:256:ASP:OD1	1:c:258:ASN:ND2	2.44	0.51
4:N:47:ARG:NH2	4:O:140:GLN:OE1	2.43	0.51
6:W:136:TYR:CD2	6:W:152:LEU:HD13	2.46	0.51
7:A:156:GLU:HA	7:A:232:THR:HG22	1.91	0.51
1:b:64:SER:OG	1:b:65:SER:N	2.42	0.51
4:S:113:ILE:HB	4:S:127:ILE:HD11	1.93	0.51
6:X:26:ASP:HB3	6:X:46:GLN:HG3	1.93	0.51
3:f:403:MET:CE	3:e:428:ILE:HD11	2.40	0.50
6:Y:81:VAL:HG21	6:Y:200:LEU:HD13	1.93	0.50
4:J:43:ASP:OD1	4:J:116:THR:OG1	2.25	0.50
4:R:135:SER:HB3	4:Q:126:ARG:HH22	1.75	0.50
4:N:99:TYR:HB2	5:H:162:GLY:HA2	1.93	0.50
7:C:240:LEU:HD22	7:C:255:PHE:CE2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:211:LEU:HD11	7:D:265:LEU:HD13	1.93	0.50
3:f:19:TYR:O	3:f:20:THR:OG1	2.22	0.50
1:b:741:ASP:O	1:b:797:ARG:NH2	2.44	0.50
1:b:855:VAL:HG22	1:b:856:THR:HG23	1.91	0.50
4:J:99:TYR:HB2	5:G:162:GLY:HA2	1.93	0.50
4:K:43:ASP:OD2	4:K:116:THR:N	2.43	0.50
6:V:26:ASP:HB3	6:V:46:GLN:HG3	1.93	0.50
3:f:369:ASP:OD1	3:f:370:ALA:N	2.43	0.50
3:f:415:TYR:O	3:g:403:MET:N	2.41	0.50
1:b:884:GLU:OE2	1:b:932:ARG:NE	2.43	0.50
4:R:51:LYS:HG2	4:R:60:THR:HA	1.94	0.50
7:B:306:GLU:HB3	7:B:356:LYS:HA	1.93	0.50
4:N:51:LYS:HG2	4:N:60:THR:HA	1.94	0.50
6:Y:100:ILE:HD11	6:Y:166:PRO:HD3	1.92	0.50
3:f:31:ASP:OD1	3:f:32:TYR:N	2.44	0.50
6:a:81:VAL:HG21	6:a:200:LEU:HD13	1.93	0.50
6:a:136:TYR:CD2	6:a:152:LEU:HD13	2.46	0.50
7:F:337:LYS:HZ1	7:D:58:SER:HB2	1.76	0.50
4:N:70:ASP:HB3	4:N:73:GLN:HB3	1.93	0.50
4:J:70:ASP:HB3	4:J:73:GLN:HB3	1.93	0.50
1:c:448:ASP:N	1:c:448:ASP:OD1	2.45	0.50
3:f:318:ASN:ND2	3:f:320:SER:OG	2.45	0.50
1:b:174:ASP:OD1	1:b:176:ALA:N	2.44	0.50
4:S:32:TYR:HB3	4:S:33:PRO:HD3	1.93	0.50
1:d:658:ARG:NH1	1:c:93:VAL:O	2.44	0.50
1:c:142:ASP:OD1	1:c:152:SER:OG	2.23	0.50
1:c:270:VAL:HG11	1:c:511:TYR:HA	1.93	0.50
1:c:683:ARG:HD2	6:X:41:VAL:HG11	1.93	0.50
7:C:118:ASN:HD21	7:C:365:LEU:HD13	1.77	0.50
4:K:32:TYR:HB3	4:K:33:PRO:HD3	1.92	0.50
4:K:113:ILE:HB	4:K:127:ILE:HD11	1.93	0.50
7:B:252:ILE:HG13	7:B:252:ILE:O	2.12	0.50
3:f:33:ASP:HA	3:e:550:THR:HG21	1.94	0.50
3:f:402:VAL:HG22	3:e:415:TYR:CZ	2.47	0.50
3:f:452:TYR:HB2	3:f:457:LEU:HD13	1.93	0.50
7:C:271:ASP:OD2	7:A:2:SER:HB3	2.11	0.50
7:A:252:ILE:HG13	7:A:252:ILE:O	2.12	0.50
7:A:306:GLU:HB3	7:A:356:LYS:HA	1.93	0.49
1:d:823:ARG:NE	1:c:478:THR:OG1	2.45	0.49
1:c:168:VAL:HG13	1:c:168:VAL:O	2.12	0.49
4:O:111:VAL:HG23	4:O:127:ILE:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:118:ASN:HD21	7:A:365:LEU:HD13	1.77	0.49
7:A:337:LYS:NZ	7:B:58:SER:OG	2.34	0.49
7:A:389:THR:OG1	7:A:459:THR:O	2.23	0.49
1:c:293:VAL:HG22	1:c:418:ILE:HG12	1.95	0.49
3:f:407:THR:HG22	3:f:408:GLY:N	2.27	0.49
3:e:330:GLU:OE2	3:e:331:THR:HG23	2.12	0.49
3:e:648:ASN:OD1	3:e:649:ALA:N	2.44	0.49
1:b:305:LEU:O	1:b:338:MET:N	2.45	0.49
4:R:48:GLY:HA3	4:R:111:VAL:HG12	1.94	0.49
4:P:41:LEU:HG	4:P:44:PHE:HD2	1.76	0.49
1:d:82:THR:OG1	6:V:31:ASP:OD2	2.30	0.49
5:I:132:ASP:OD1	5:I:133:LYS:N	2.41	0.49
7:B:308:PRO:HA	7:B:355:SER:HA	1.94	0.49
4:T:41:LEU:HG	4:T:44:PHE:HD2	1.76	0.49
1:d:348:SER:OG	1:d:510:ARG:NE	2.42	0.49
1:c:741:ASP:O	1:c:797:ARG:NH2	2.46	0.49
1:b:498:ASP:OD1	1:b:499:GLU:N	2.46	0.49
7:C:272:LYS:HB3	7:A:1:MET:CG	2.42	0.49
7:C:306:GLU:HB3	7:C:356:LYS:HA	1.93	0.49
7:C:381:VAL:HA	7:C:400:VAL:HG23	1.93	0.49
5:G:187:MET:HG2	5:G:257:ILE:HD13	1.95	0.49
3:f:525:THR:OG1	3:f:535:LEU:HD13	2.13	0.49
6:a:24:ASP:OD2	6:Z:73:LYS:NZ	2.45	0.49
4:J:48:GLY:HA3	4:J:111:VAL:HG12	1.94	0.49
5:G:7:ARG:HA	7:D:245:MET:HE3	1.94	0.49
1:d:531:LEU:HD21	1:d:544:ILE:HD11	1.93	0.49
4:R:70:ASP:HB3	4:R:73:GLN:HB3	1.93	0.49
7:F:211:LEU:HD11	7:F:265:LEU:HD13	1.93	0.49
7:E:233:ILE:HG13	7:E:261:LEU:HD13	1.93	0.49
7:B:118:ASN:HD21	7:B:365:LEU:HD13	1.77	0.49
1:c:747:THR:O	1:c:838:ASN:ND2	2.46	0.49
1:c:776:ILE:HB	1:c:814:LEU:HD13	1.94	0.49
3:g:222:ALA:O	3:g:324:ASP:N	2.43	0.49
1:b:917:LEU:O	1:b:921:GLY:N	2.39	0.49
6:a:57:LEU:HD12	6:a:196:ILE:HD12	1.94	0.49
4:N:126:ARG:NH2	4:O:135:SER:OG	2.46	0.49
1:d:92:LEU:HD23	1:d:140:ILE:HB	1.94	0.49
3:e:26:HIS:ND1	3:e:27:SER:O	2.42	0.49
3:e:41:LEU:HD11	3:e:62:ILE:HG21	1.95	0.49
1:b:116:ASN:OD1	6:W:105:LYS:HE2	2.13	0.49
5:I:7:ARG:HA	7:F:245:MET:HE3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:172:VAL:HG13	5:I:179:LEU:HB2	1.95	0.49
7:F:233:ILE:HG13	7:F:261:LEU:HD13	1.93	0.49
5:H:132:ASP:OD1	5:H:133:LYS:N	2.41	0.49
7:C:6:LEU:HD13	7:B:327:ASP:O	2.13	0.49
7:C:272:LYS:HB3	7:A:1:MET:H3	1.78	0.49
1:d:45:PHE:CB	6:a:45:ALA:HB2	2.42	0.49
4:S:110:ASP:OD1	4:T:139:THR:OG1	2.29	0.49
4:O:35:THR:HG22	4:O:37:LYS:H	1.78	0.49
6:W:81:VAL:HG21	6:W:200:LEU:HD13	1.93	0.49
7:A:101:GLY:HA2	7:A:132:ALA:N	2.28	0.49
4:P:46:LEU:C	4:P:66:THR:HG21	2.38	0.49
1:d:924:GLY:HA2	3:g:91:ILE:HD12	1.95	0.48
1:c:59:LYS:HA	1:c:82:THR:HG22	1.95	0.48
3:e:303:ASP:CG	3:e:304:ALA:H	2.21	0.48
3:e:435:VAL:HG13	3:e:436:THR:HG23	1.94	0.48
4:S:35:THR:HG22	4:S:37:LYS:H	1.78	0.48
5:H:7:ARG:HA	7:E:245:MET:HE3	1.94	0.48
7:C:309:ALA:HB3	7:C:357:TYR:CD2	2.48	0.48
7:A:308:PRO:HA	7:A:355:SER:HA	1.94	0.48
7:B:101:GLY:HA2	7:B:132:ALA:N	2.28	0.48
1:c:92:LEU:HD23	1:c:140:ILE:HB	1.95	0.48
4:R:126:ARG:NH2	4:S:135:SER:OG	2.46	0.48
7:C:268:TYR:HA	7:C:331:GLY:HA2	1.95	0.48
4:J:51:LYS:HG2	4:J:60:THR:HA	1.94	0.48
5:G:172:VAL:HG13	5:G:179:LEU:HB2	1.95	0.48
7:A:268:TYR:HA	7:A:331:GLY:HA2	1.95	0.48
3:e:488:ILE:HD13	3:e:507:TRP:CZ3	2.49	0.48
7:F:220:LYS:NZ	7:F:282:ASP:OD2	2.38	0.48
6:Y:57:LEU:HD12	6:Y:196:ILE:HD12	1.94	0.48
4:M:11:VAL:HG12	4:M:133:TYR:HB2	1.95	0.48
7:C:101:GLY:HA2	7:C:132:ALA:N	2.28	0.48
7:C:252:ILE:HG13	7:C:252:ILE:O	2.12	0.48
7:C:395:THR:HB	7:C:429:LEU:HD11	1.95	0.48
6:W:57:LEU:HD12	6:W:196:ILE:HD12	1.94	0.48
1:b:436:GLU:OE2	1:b:607:TRP:NE1	2.39	0.48
1:b:928:LYS:C	1:b:929:LEU:HD12	2.38	0.48
4:S:111:VAL:HG23	4:S:127:ILE:HB	1.94	0.48
7:F:178:PRO:HG3	7:E:284:ILE:HD11	1.95	0.48
5:H:172:VAL:HG13	5:H:179:LEU:HB2	1.95	0.48
7:C:383:SER:OG	7:C:387:VAL:N	2.47	0.48
5:G:101:GLU:OE2	5:G:212:ARG:NH2	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:11:VAL:HG12	4:U:133:TYR:HB2	1.95	0.48
4:T:46:LEU:C	4:T:66:THR:HG21	2.38	0.48
1:c:464:LEU:HD22	1:c:545:LEU:HD21	1.95	0.48
5:I:187:MET:HG2	5:I:257:ILE:HD13	1.95	0.48
7:A:395:THR:HB	7:A:429:LEU:HD11	1.95	0.48
1:d:887:ASP:OD1	1:d:888:SER:N	2.43	0.48
1:b:448:ASP:OD1	1:b:450:THR:N	2.46	0.48
7:F:270:ASN:HB3	7:F:272:LYS:HG2	1.96	0.48
7:E:73:SER:HB3	7:E:166:ARG:HD2	1.96	0.48
7:E:252:ILE:O	7:E:252:ILE:HG13	2.14	0.48
7:C:54:PRO:HB3	7:B:129:HIS:CE1	2.48	0.48
7:C:278:GLU:HG3	7:C:281:LYS:HE2	1.95	0.48
4:J:126:ARG:NH2	4:K:135:SER:OG	2.46	0.48
3:e:72:GLU:N	3:e:72:GLU:OE1	2.46	0.48
3:e:109:ILE:HD12	3:e:131:ASP:O	2.13	0.48
3:g:593:SER:OG	3:g:594:GLY:N	2.47	0.48
4:Q:11:VAL:HG12	4:Q:133:TYR:HB2	1.95	0.48
4:S:114:THR:HG23	4:S:124:SER:HB3	1.96	0.48
7:D:252:ILE:O	7:D:252:ILE:HG13	2.14	0.48
7:A:383:SER:OG	7:A:387:VAL:N	2.47	0.48
7:B:278:GLU:HG3	7:B:281:LYS:HE2	1.96	0.48
1:c:930:ARG:NH1	3:e:2:ILE:O	2.38	0.48
3:f:356:ILE:HG12	3:f:363:ILE:HG22	1.96	0.48
7:F:252:ILE:O	7:F:252:ILE:HG13	2.14	0.48
6:X:128:LYS:HE3	6:X:133:PRO:HA	1.95	0.48
7:E:178:PRO:HG3	7:D:284:ILE:HD11	1.96	0.48
7:C:311:ILE:HD12	7:C:365:LEU:HD23	1.96	0.48
4:K:35:THR:HG22	4:K:37:LYS:H	1.78	0.48
7:D:425:ASN:OD1	7:D:429:LEU:N	2.47	0.48
7:B:80:LYS:HB3	7:B:87:GLN:NE2	2.29	0.48
7:B:311:ILE:HD12	7:B:365:LEU:HD23	1.96	0.48
1:d:464:LEU:HD22	1:d:545:LEU:HD21	1.96	0.48
1:c:737:LEU:O	1:c:766:SER:OG	2.21	0.48
3:f:306:ASP:OD1	3:f:307:VAL:N	2.47	0.48
7:E:58:SER:HB2	7:D:337:LYS:HZ1	1.79	0.48
4:K:111:VAL:HG23	4:K:127:ILE:HB	1.94	0.48
7:A:309:ALA:HB3	7:A:357:TYR:CD2	2.48	0.48
6:Z:71:GLU:O	6:Z:75:THR:HG22	2.14	0.48
6:Z:128:LYS:HE3	6:Z:133:PRO:HA	1.95	0.48
1:d:305:LEU:O	1:d:338:MET:N	2.45	0.48
1:b:575:PHE:HE2	6:V:43:ILE:HG21	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:73:SER:HB3	7:F:166:ARG:HD2	1.96	0.48
7:E:179:LEU:HD23	7:E:183:PRO:HG3	1.96	0.48
4:K:114:THR:HG23	4:K:124:SER:HB3	1.96	0.48
7:D:179:LEU:HD23	7:D:183:PRO:HG3	1.96	0.48
7:A:278:GLU:HG3	7:A:281:LYS:HE2	1.95	0.48
1:b:939:ASN:N	1:b:941:GLU:OE1	2.46	0.47
5:H:187:MET:HG2	5:H:257:ILE:HD13	1.95	0.47
6:X:71:GLU:O	6:X:75:THR:HG22	2.14	0.47
4:O:114:THR:HG23	4:O:124:SER:HB3	1.95	0.47
6:W:24:ASP:OD2	6:V:73:LYS:NZ	2.45	0.47
7:D:73:SER:HB3	7:D:166:ARG:HD2	1.96	0.47
7:A:425:ASN:OD1	7:A:429:LEU:N	2.43	0.47
7:B:268:TYR:HA	7:B:331:GLY:HA2	1.95	0.47
7:B:383:SER:OG	7:B:387:VAL:N	2.47	0.47
1:d:376:ASP:N	1:d:376:ASP:OD1	2.46	0.47
3:e:502:TYR:HB3	3:e:503:PRO:HD3	1.96	0.47
4:L:46:LEU:C	4:L:66:THR:HG21	2.38	0.47
7:B:281:LYS:HA	7:B:284:ILE:HG22	1.96	0.47
7:B:395:THR:HB	7:B:429:LEU:HD11	1.95	0.47
4:N:48:GLY:HA3	4:N:111:VAL:HG12	1.94	0.47
6:X:32:GLU:OE1	6:W:201:ARG:NE	2.45	0.47
7:C:50:ALA:HB2	7:D:161:ILE:HG21	1.97	0.47
7:A:281:LYS:HA	7:A:284:ILE:HG22	1.96	0.47
1:d:261:ALA:O	2:j:1095:GLN:NE2	2.39	0.47
1:d:640:TYR:CD2	2:i:1109:LEU:HD21	2.48	0.47
7:F:306:GLU:HG2	7:F:356:LYS:HB3	1.96	0.47
6:Y:71:GLU:OE2	6:Y:74:ARG:NH1	2.47	0.47
7:C:281:LYS:HA	7:C:284:ILE:HG22	1.96	0.47
6:V:71:GLU:O	6:V:75:THR:HG22	2.14	0.47
1:d:789:GLN:NE2	1:d:791:GLU:O	2.48	0.47
1:c:839:LEU:HB2	1:c:943:SER:HA	1.96	0.47
7:F:97:ALA:HA	7:F:132:ALA:HB3	1.97	0.47
7:E:392:ARG:HD2	7:E:434:ALA:HA	1.97	0.47
7:C:80:LYS:HB3	7:C:87:GLN:NE2	2.29	0.47
1:c:582:LEU:CD1	1:c:660:LEU:HD11	2.40	0.47
1:c:740:ARG:NH1	1:c:765:PRO:O	2.44	0.47
1:c:868:ASP:OD1	1:c:869:LYS:N	2.48	0.47
3:f:428:ILE:HG23	3:f:443:ILE:HG13	1.97	0.47
4:R:124:SER:HB2	4:S:17:PRO:HD2	1.97	0.47
7:F:284:ILE:HD11	7:D:178:PRO:HG3	1.96	0.47
5:H:11:ILE:HG12	5:H:109:ILE:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:97:ALA:HA	7:D:132:ALA:HB3	1.97	0.47
1:d:448:ASP:OD1	1:d:449:GLY:N	2.48	0.47
3:f:114:CYS:HB2	3:f:205:VAL:HG23	1.97	0.47
1:b:45:PHE:HZ	6:W:155:ASP:HB2	1.77	0.47
7:F:179:LEU:HD23	7:F:183:PRO:HG3	1.96	0.47
7:F:392:ARG:HD2	7:F:434:ALA:HA	1.97	0.47
4:N:124:SER:HB2	4:O:17:PRO:HD2	1.97	0.47
6:Y:153:TYR:HB3	6:Y:154:PRO:HD3	1.97	0.47
7:E:306:GLU:HG2	7:E:356:LYS:HB3	1.96	0.47
7:C:129:HIS:CE1	7:A:54:PRO:HB3	2.49	0.47
4:J:124:SER:HB2	4:K:17:PRO:HD2	1.97	0.47
5:G:11:ILE:HG12	5:G:109:ILE:HG12	1.96	0.47
5:G:235:ASP:OD1	5:G:236:LYS:N	2.48	0.47
7:D:270:ASN:HB3	7:D:272:LYS:HG2	1.96	0.47
7:D:306:GLU:HG2	7:D:356:LYS:HB3	1.96	0.47
7:A:129:HIS:CE1	7:B:54:PRO:HB3	2.49	0.47
7:A:131:LEU:HG	7:A:256:THR:HG21	1.96	0.47
7:A:327:ASP:O	7:B:6:LEU:HD13	2.14	0.47
4:P:92:ALA:HB2	4:P:134:ILE:HD12	1.97	0.47
1:d:168:VAL:HG13	1:d:168:VAL:O	2.14	0.47
1:b:574:ASN:OD1	1:b:575:PHE:N	2.47	0.47
6:a:71:GLU:OE2	6:a:74:ARG:NH1	2.48	0.47
6:a:153:TYR:HB3	6:a:154:PRO:HD3	1.97	0.47
7:E:161:ILE:HG21	7:A:50:ALA:HB2	1.97	0.47
7:C:131:LEU:HG	7:C:256:THR:HG21	1.96	0.47
7:C:327:ASP:O	7:A:6:LEU:HD13	2.15	0.47
5:H:101:GLU:OE2	5:H:212:ARG:NH2	2.38	0.47
7:E:97:ALA:HA	7:E:132:ALA:HB3	1.96	0.47
7:C:425:ASN:OD1	7:C:429:LEU:N	2.43	0.47
7:A:80:LYS:HB3	7:A:87:GLN:NE2	2.29	0.47
1:d:817:VAL:HG12	1:d:823:ARG:HG2	1.96	0.47
3:g:20:THR:C	3:g:21:LEU:HD22	2.39	0.47
5:I:11:ILE:HG12	5:I:109:ILE:HG12	1.96	0.47
5:I:228:TYR:OH	5:G:149:GLU:OE2	2.23	0.47
7:F:159:VAL:HG21	7:F:297:LEU:HD21	1.97	0.47
7:F:161:ILE:HG21	7:B:50:ALA:HB2	1.96	0.47
7:A:269:LEU:HA	7:A:276:SER:HB2	1.97	0.47
6:V:128:LYS:HE3	6:V:133:PRO:HA	1.95	0.47
1:c:45:PHE:HZ	6:Y:155:ASP:HB2	1.81	0.46
1:c:203:TYR:HB2	1:c:409:TYR:CD1	2.49	0.46
3:g:403:MET:HE1	3:g:414:ILE:HG22	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:677:LYS:HG3	3:g:685:ILE:HD13	1.95	0.46
5:I:294:PHE:HB3	5:I:298:LYS:HA	1.97	0.46
3:f:132:THR:HG21	3:f:165:ILE:HD12	1.96	0.46
6:Y:181:ASP:OD1	6:Y:181:ASP:N	2.48	0.46
7:C:396:LEU:O	7:C:430:LEU:N	2.48	0.46
4:L:92:ALA:HB2	4:L:134:ILE:HD12	1.97	0.46
4:P:96:ARG:HE	4:P:104:ARG:HD3	1.80	0.46
1:c:191:SER:OG	1:c:192:ASN:N	2.49	0.46
3:f:318:ASN:O	3:f:321:THR:OG1	2.33	0.46
5:H:235:ASP:OD1	5:H:236:LYS:N	2.48	0.46
5:G:18:ARG:HH21	5:G:20:TYR:HH	1.61	0.46
7:A:128:TYR:C	7:B:54:PRO:HG3	2.41	0.46
7:A:396:LEU:O	7:A:430:LEU:N	2.47	0.46
1:b:465:MET:HE1	1:b:561:ILE:HD12	1.98	0.46
5:I:235:ASP:OD1	5:I:236:LYS:N	2.48	0.46
7:E:270:ASN:HB3	7:E:272:LYS:HG2	1.96	0.46
7:C:54:PRO:HG3	7:B:128:TYR:C	2.40	0.46
7:B:131:LEU:HG	7:B:256:THR:HG21	1.96	0.46
7:B:309:ALA:HB3	7:B:357:TYR:CD2	2.48	0.46
4:T:96:ARG:HE	4:T:104:ARG:HD3	1.80	0.46
1:d:146:THR:HG22	1:d:146:THR:O	2.15	0.46
3:g:235:ARG:NH1	3:g:281:THR:OG1	2.49	0.46
1:b:606:SER:O	1:b:608:LYS:N	2.46	0.46
7:C:2:SER:HB3	7:B:271:ASP:OD2	2.15	0.46
5:G:132:ASP:OD1	5:G:133:LYS:N	2.42	0.46
4:U:106:ALA:HB3	4:U:132:VAL:HG12	1.98	0.46
7:D:392:ARG:HD2	7:D:434:ALA:HA	1.97	0.46
6:Z:14:GLY:HA3	6:Z:61:GLU:OE2	2.16	0.46
3:f:535:LEU:HD12	3:f:536:VAL:N	2.30	0.46
3:e:109:ILE:HD11	3:e:130:ILE:HB	1.97	0.46
3:g:83:ASP:OD1	3:g:84:SER:N	2.45	0.46
1:b:766:SER:N	1:b:774:TYR:OH	2.46	0.46
5:H:294:PHE:HB3	5:H:298:LYS:HA	1.97	0.46
6:X:28:MET:HE2	6:X:42:LYS:HE2	1.98	0.46
6:W:181:ASP:OD1	6:W:181:ASP:N	2.48	0.46
7:A:311:ILE:HD12	7:A:365:LEU:HD23	1.96	0.46
4:T:92:ALA:HB2	4:T:134:ILE:HD12	1.97	0.46
1:d:308:TYR:N	1:d:434:SER:O	2.44	0.46
1:b:144:VAL:HG13	1:b:144:VAL:O	2.16	0.46
1:b:772:VAL:HG12	1:b:817:VAL:HG23	1.98	0.46
6:a:86:TYR:OH	6:a:137:LYS:NZ	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:50:ILE:HD13	4:Q:132:VAL:HG21	1.98	0.46
7:D:151:GLN:OE1	7:D:254:SER:OG	2.34	0.46
1:d:182:GLU:OE1	1:d:189:GLN:O	2.33	0.46
1:c:231:LYS:NZ	1:c:237:SER:O	2.44	0.46
5:I:132:ASP:CG	5:I:133:LYS:H	2.24	0.46
5:H:155:ASP:OD1	5:H:155:ASP:N	2.49	0.46
4:M:50:ILE:HD13	4:M:132:VAL:HG21	1.98	0.46
7:E:411:GLU:N	7:E:411:GLU:OE1	2.49	0.46
6:W:71:GLU:OE2	6:W:74:ARG:NH1	2.48	0.46
7:A:271:ASP:OD2	7:B:2:SER:HB3	2.15	0.46
1:c:579:TYR:HD1	6:Y:33:LEU:HD22	1.81	0.46
3:e:416:THR:HG23	3:e:428:ILE:HG12	1.97	0.46
5:I:196:ARG:HD2	6:Y:56:GLU:O	2.15	0.46
6:X:73:LYS:NZ	6:Y:24:ASP:OD2	2.45	0.46
3:f:523:CYS:SG	3:f:524:SER:N	2.88	0.45
7:F:411:GLU:N	7:F:411:GLU:OE1	2.49	0.45
7:C:1:MET:H3	7:B:272:LYS:HB3	1.81	0.45
7:D:380:THR:OG1	7:D:401:GLU:OE2	2.27	0.45
7:B:269:LEU:HA	7:B:276:SER:HB2	1.97	0.45
6:Z:28:MET:HE2	6:Z:42:LYS:HE2	1.98	0.45
1:d:46:ARG:HD3	6:a:156:LEU:O	2.17	0.45
1:c:82:THR:OG1	6:Z:31:ASP:OD2	2.24	0.45
3:f:578:TRP:NE1	3:f:580:ASP:OD1	2.42	0.45
3:e:487:TYR:CE1	3:e:523:CYS:SG	3.09	0.45
3:g:596:VAL:HG12	3:g:597:LYS:N	2.31	0.45
1:b:19:LYS:NZ	6:W:155:ASP:OD2	2.49	0.45
7:E:309:ALA:HB3	7:E:357:TYR:CD2	2.51	0.45
7:D:124:LYS:HE2	7:D:347:ASP:HB3	1.99	0.45
7:D:159:VAL:HG21	7:D:297:LEU:HD21	1.97	0.45
7:D:420:ASP:N	7:D:420:ASP:OD1	2.49	0.45
3:e:50:ARG:HD2	3:e:62:ILE:HG23	1.98	0.45
7:F:124:LYS:HE2	7:F:347:ASP:HB3	1.99	0.45
5:H:158:THR:HG21	4:M:130:GLY:HA2	1.99	0.45
7:D:411:GLU:OE1	7:D:411:GLU:N	2.49	0.45
7:F:58:SER:HB2	7:E:337:LYS:HZ1	1.81	0.45
7:E:151:GLN:OE1	7:E:254:SER:OG	2.34	0.45
4:L:19:GLY:HA2	4:L:79:SER:HB3	1.99	0.45
6:W:153:TYR:HB3	6:W:154:PRO:HD3	1.97	0.45
1:d:19:LYS:NZ	6:a:155:ASP:OD2	2.50	0.45
1:c:578:THR:HG23	1:c:663:SER:O	2.17	0.45
1:c:658:ARG:NH1	1:b:93:VAL:O	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:482:GLN:NE2	3:e:525:THR:O	2.39	0.45
5:I:41:ARG:NH1	6:X:61:GLU:OE2	2.41	0.45
4:L:96:ARG:HE	4:L:104:ARG:HD3	1.80	0.45
2:h:1112:LEU:CD2	1:c:612:ILE:HD12	2.46	0.45
3:f:596:VAL:HG12	3:f:599:ASP:OD2	2.16	0.45
1:b:47:ASP:N	1:b:47:ASP:OD1	2.49	0.45
7:F:309:ALA:HB3	7:F:357:TYR:CD2	2.51	0.45
4:M:106:ALA:HB3	4:M:132:VAL:HG12	1.98	0.45
4:O:41:LEU:HA	4:O:44:PHE:HD2	1.82	0.45
7:C:58:SER:OG	7:B:337:LYS:NZ	2.36	0.45
6:V:14:GLY:HA3	6:V:61:GLU:OE2	2.16	0.45
1:c:772:VAL:HG23	1:c:773:TYR:CD2	2.51	0.45
3:g:274:VAL:O	3:g:274:VAL:HG22	2.16	0.45
1:b:752:VAL:HG23	1:b:757:LYS:HD3	1.99	0.45
5:I:109:ILE:HD12	5:I:119:PHE:HE2	1.82	0.45
7:B:99:SER:HA	7:B:123:PHE:HD1	1.82	0.45
1:c:574:ASN:OD1	1:c:575:PHE:N	2.50	0.45
4:U:12:VAL:HG12	4:U:18:TYR:CG	2.52	0.45
4:K:41:LEU:HA	4:K:44:PHE:HD2	1.82	0.45
7:A:184:PHE:CD2	7:A:189:ILE:HG13	2.52	0.45
1:d:713:GLU:HA	1:d:713:GLU:OE1	2.17	0.45
2:h:1109:LEU:HD23	1:c:641:TYR:CZ	2.52	0.45
3:e:97:ASP:N	3:e:97:ASP:OD1	2.50	0.45
7:F:5:LEU:HD22	7:A:45:ILE:HG21	1.98	0.45
6:X:14:GLY:HA3	6:X:61:GLU:OE2	2.16	0.45
7:C:184:PHE:CD2	7:C:189:ILE:HG13	2.52	0.45
7:D:5:LEU:HD22	7:B:45:ILE:HG21	1.98	0.45
4:P:96:ARG:NE	4:P:104:ARG:HD3	2.32	0.45
1:d:684:TYR:HB3	1:c:93:VAL:HG11	1.99	0.45
3:f:56:ASP:N	3:f:56:ASP:OD1	2.50	0.45
3:g:297:SER:N	3:g:308:THR:O	2.50	0.45
1:b:168:VAL:HG13	1:b:168:VAL:O	2.16	0.45
1:b:377:GLN:NE2	1:b:411:LEU:O	2.43	0.45
5:I:155:ASP:OD1	5:I:155:ASP:N	2.49	0.45
4:M:12:VAL:HG12	4:M:18:TYR:CG	2.52	0.45
7:E:5:LEU:HD22	7:C:45:ILE:HG21	1.99	0.45
7:C:400:VAL:HB	7:C:414:TRP:HH2	1.82	0.45
7:B:184:PHE:CD2	7:B:189:ILE:HG13	2.52	0.45
7:B:400:VAL:HB	7:B:414:TRP:HH2	1.82	0.45
4:R:32:TYR:CD1	4:R:33:PRO:HD2	2.52	0.44
4:Q:106:ALA:HB3	4:Q:132:VAL:HG12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:153:TYR:CG	6:W:70:LEU:HD22	2.53	0.44
5:G:109:ILE:HD12	5:G:119:PHE:HE2	1.82	0.44
5:G:294:PHE:HB3	5:G:298:LYS:HA	1.97	0.44
4:U:14:GLU:OE1	4:U:137:GLY:N	2.43	0.44
7:A:299:LEU:N	7:A:310:ALA:O	2.49	0.44
4:T:96:ARG:NE	4:T:104:ARG:HD3	2.32	0.44
6:V:57:LEU:HD12	6:V:196:ILE:HG13	1.99	0.44
2:j:1108:GLU:O	2:j:1112:LEU:HD13	2.16	0.44
1:c:730:PRO:CB	1:b:901:VAL:HG23	2.46	0.44
3:f:627:MET:HE2	3:e:629:LEU:HD13	1.97	0.44
5:I:123:TYR:CE2	5:I:193:CYS:HB2	2.52	0.44
6:a:181:ASP:OD1	6:a:181:ASP:N	2.48	0.44
7:F:384:ALA:HB2	7:F:397:GLN:O	2.17	0.44
5:H:231:ARG:HH22	4:P:100:ASN:CB	2.21	0.44
6:X:57:LEU:HD12	6:X:196:ILE:HG13	1.99	0.44
7:E:159:VAL:HG21	7:E:297:LEU:HD21	1.97	0.44
7:C:269:LEU:HA	7:C:276:SER:HB2	1.97	0.44
7:D:309:ALA:HB3	7:D:357:TYR:CD2	2.51	0.44
7:B:299:LEU:N	7:B:310:ALA:O	2.49	0.44
4:P:19:GLY:HA2	4:P:79:SER:HB3	1.99	0.44
1:d:308:TYR:OH	1:d:436:GLU:OE2	2.28	0.44
1:c:605:LEU:O	1:c:606:SER:C	2.60	0.44
1:c:630:LEU:HD23	1:c:630:LEU:H	1.82	0.44
1:c:894:ARG:HE	1:c:906:TYR:HE1	1.65	0.44
3:f:41:LEU:HD23	3:f:73:VAL:HG22	1.98	0.44
3:f:671:GLU:OE2	3:e:496:LYS:HE2	2.17	0.44
3:e:630:HIS:ND1	3:g:636:ASN:OD1	2.43	0.44
7:E:380:THR:OG1	7:E:401:GLU:OE2	2.27	0.44
4:L:96:ARG:NE	4:L:104:ARG:HD3	2.32	0.44
7:A:400:VAL:HB	7:A:414:TRP:HH2	1.83	0.44
3:g:57:THR:HG22	3:g:59:SER:H	1.82	0.44
6:a:70:LEU:HD22	6:V:153:TYR:CG	2.51	0.44
7:F:102:ARG:HG2	7:F:102:ARG:HH11	1.83	0.44
7:E:425:ASN:OD1	7:E:429:LEU:N	2.47	0.44
7:C:1:MET:CG	7:B:272:LYS:HB3	2.44	0.44
4:J:28:ASP:N	4:J:28:ASP:OD1	2.50	0.44
7:D:81:ASP:OD1	7:D:81:ASP:N	2.51	0.44
1:d:348:SER:OG	1:d:348:SER:O	2.36	0.44
2:h:1085:THR:HG22	2:h:1086:THR:N	2.32	0.44
1:c:684:TYR:HB3	1:b:93:VAL:HG11	2.00	0.44
4:N:28:ASP:OD1	4:N:28:ASP:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:124:LYS:HE2	7:E:347:ASP:HB3	1.98	0.44
7:C:11:ILE:HG13	7:C:30:VAL:HG11	2.00	0.44
4:U:50:ILE:HD13	4:U:132:VAL:HG21	1.98	0.44
7:A:139:LEU:HD13	7:A:144:TRP:CD2	2.53	0.44
7:B:7:ARG:HA	7:B:7:ARG:HD2	1.82	0.44
7:B:396:LEU:O	7:B:430:LEU:N	2.47	0.44
4:T:103:GLN:HA	4:T:134:ILE:O	2.18	0.44
1:d:17:LYS:HZ3	6:a:28:MET:HE1	1.81	0.44
3:f:267:THR:HG22	3:f:268:LYS:HG2	2.00	0.44
5:G:158:THR:HG21	4:U:130:GLY:HA2	1.99	0.44
6:Z:57:LEU:HD12	6:Z:196:ILE:HG13	1.99	0.44
2:j:1109:LEU:HD21	1:b:640:TYR:CD1	2.53	0.44
4:Q:12:VAL:HG12	4:Q:18:TYR:CG	2.52	0.44
4:J:32:TYR:CD1	4:J:33:PRO:HD2	2.52	0.44
4:U:41:LEU:HG	4:U:74:GLY:HA2	2.00	0.44
1:d:908:LEU:HD21	3:f:514:ARG:H	1.82	0.44
3:f:80:SER:OG	1:b:859:VAL:O	2.33	0.44
3:f:336:ASN:OD1	3:f:337:TYR:N	2.50	0.44
5:H:196:ARG:HD2	6:W:56:GLU:O	2.18	0.44
5:G:123:TYR:CE2	5:G:193:CYS:HB2	2.52	0.44
7:D:102:ARG:HG2	7:D:102:ARG:HH11	1.83	0.44
7:B:305:ASP:OD2	7:B:307:ARG:NH1	2.51	0.44
7:B:389:THR:OG1	7:B:459:THR:O	2.24	0.44
1:d:226:LYS:C	1:d:242:LEU:HD11	2.42	0.44
1:c:32:SER:O	1:c:35:ALA:N	2.51	0.44
1:c:871:PRO:C	1:c:872:GLU:HG3	2.43	0.44
3:f:186:PRO:O	3:e:586:PHE:HE1	2.00	0.44
4:S:41:LEU:HA	4:S:44:PHE:HD2	1.82	0.44
7:C:99:SER:HA	7:C:123:PHE:HD1	1.82	0.44
7:C:305:ASP:OD2	7:C:307:ARG:NH1	2.51	0.44
6:V:104:GLN:HE22	6:V:110:ILE:HB	1.83	0.44
6:Z:89:PHE:O	6:Z:92:ARG:NH1	2.51	0.44
3:g:288:LYS:NZ	3:g:318:ASN:OD1	2.27	0.43
5:G:132:ASP:CG	5:G:133:LYS:H	2.24	0.43
7:A:159:VAL:O	7:A:229:GLY:N	2.38	0.43
7:A:305:ASP:OD2	7:A:307:ARG:NH1	2.51	0.43
6:V:28:MET:HE2	6:V:42:LYS:HE2	1.98	0.43
6:Z:104:GLN:HE22	6:Z:110:ILE:HB	1.83	0.43
1:d:494:LEU:HD11	1:d:548:PHE:CD2	2.53	0.43
3:g:120:ASP:OD1	3:g:417:GLN:NE2	2.51	0.43
1:b:428:THR:OG1	1:b:429:GLU:OE1	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:32:TYR:CD1	4:N:33:PRO:HD2	2.52	0.43
7:C:139:LEU:HD13	7:C:144:TRP:CD2	2.53	0.43
4:L:103:GLN:HA	4:L:134:ILE:O	2.18	0.43
7:B:1:MET:HA	7:B:1:MET:CE	2.45	0.43
1:d:928:LYS:C	1:d:929:LEU:HD22	2.44	0.43
3:f:387:VAL:HG13	3:f:387:VAL:O	2.18	0.43
5:H:72:THR:HG23	5:H:74:ILE:HG12	2.00	0.43
4:M:26:ASP:N	4:M:37:LYS:O	2.42	0.43
7:E:420:ASP:OD1	7:E:420:ASP:N	2.49	0.43
4:U:66:THR:HG22	4:U:78:ILE:HG22	2.00	0.43
7:B:425:ASN:OD1	7:B:428:GLY:N	2.49	0.43
4:T:19:GLY:HA2	4:T:79:SER:HB3	1.99	0.43
6:V:89:PHE:O	6:V:92:ARG:NH1	2.51	0.43
1:c:26:LEU:HD11	1:c:135:ILE:HD11	2.00	0.43
3:f:33:ASP:N	3:f:33:ASP:OD1	2.51	0.43
1:b:146:THR:HG22	1:b:146:THR:O	2.18	0.43
4:Q:26:ASP:N	4:Q:37:LYS:O	2.42	0.43
5:H:109:ILE:HD12	5:H:119:PHE:HE2	1.82	0.43
7:C:421:ALA:HA	7:C:436:LYS:HD2	2.00	0.43
7:A:11:ILE:HG13	7:A:30:VAL:HG11	2.00	0.43
7:B:139:LEU:HD13	7:B:144:TRP:CD2	2.53	0.43
7:B:159:VAL:O	7:B:229:GLY:N	2.38	0.43
4:T:64:PHE:HB3	4:T:78:ILE:HD11	2.01	0.43
1:d:775:SER:O	1:d:815:ARG:N	2.51	0.43
1:c:39:ILE:O	1:c:39:ILE:HG23	2.18	0.43
1:c:579:TYR:CD1	6:Y:33:LEU:HD22	2.54	0.43
3:e:669:ASN:N	3:e:670:PRO:HD2	2.33	0.43
1:b:442:VAL:HG13	1:b:466:ASP:HB2	1.99	0.43
4:N:127:ILE:HG13	4:N:128:MET:HG2	2.01	0.43
7:C:128:TYR:C	7:A:54:PRO:HG3	2.43	0.43
5:G:41:ARG:NH1	6:Z:61:GLU:OE2	2.44	0.43
7:A:1:MET:HA	7:A:1:MET:CE	2.45	0.43
7:B:41:ASN:OD1	7:B:66:ASN:ND2	2.51	0.43
1:c:891:ARG:NH1	1:c:892:MET:O	2.45	0.43
1:b:316:CYS:HB3	1:b:327:CYS:HB3	1.99	0.43
5:I:158:THR:HG21	4:Q:130:GLY:HA2	1.99	0.43
6:a:56:GLU:O	5:G:196:ARG:HD2	2.19	0.43
4:Q:41:LEU:HG	4:Q:74:GLY:HA2	2.00	0.43
7:F:420:ASP:OD1	7:F:420:ASP:N	2.49	0.43
4:N:3:THR:HB	4:N:6:ARG:HB2	2.01	0.43
5:H:123:TYR:CE2	5:H:193:CYS:HB2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:104:GLN:HE22	6:X:110:ILE:HB	1.83	0.43
7:E:384:ALA:HB2	7:E:397:GLN:O	2.17	0.43
7:C:41:ASN:OD1	7:C:66:ASN:ND2	2.52	0.43
4:J:3:THR:HB	4:J:6:ARG:HB2	2.01	0.43
7:D:384:ALA:HB2	7:D:397:GLN:O	2.18	0.43
7:A:272:LYS:HB3	7:B:1:MET:CG	2.45	0.43
7:B:11:ILE:HG13	7:B:30:VAL:HG11	2.00	0.43
1:c:58:GLY:O	1:c:59:LYS:HB2	2.19	0.43
4:R:28:ASP:OD1	4:R:28:ASP:N	2.50	0.43
4:M:115:ARG:NH1	4:M:121:ALA:O	2.48	0.43
7:E:102:ARG:HH11	7:E:102:ARG:HG2	1.82	0.43
7:C:361:THR:HA	7:C:364:ASN:HD21	1.84	0.43
7:D:134:LEU:HD12	7:D:152:ILE:HD11	2.01	0.43
7:A:41:ASN:OD1	7:A:66:ASN:ND2	2.52	0.43
1:d:747:THR:HG23	1:d:759:GLY:HA2	2.01	0.43
1:c:782:VAL:HG21	1:b:813:GLU:HB2	2.01	0.43
3:f:309:ASP:OD1	3:f:309:ASP:N	2.50	0.43
1:b:89:VAL:HA	1:b:154:ILE:HD11	2.00	0.43
1:b:475:ALA:HB2	1:b:537:VAL:HG11	2.00	0.43
4:R:46:LEU:H	4:R:46:LEU:HD23	1.84	0.43
4:N:46:LEU:HD23	4:N:46:LEU:H	1.84	0.43
6:Y:4:PRO:HG3	6:Y:68:ARG:HG3	2.01	0.43
4:M:66:THR:HG22	4:M:78:ILE:HG22	2.00	0.43
4:J:56:ASP:OD1	4:J:56:ASP:N	2.52	0.43
7:D:211:LEU:HD13	7:D:226:ILE:HD11	2.01	0.43
7:A:99:SER:HA	7:A:123:PHE:HD1	1.82	0.43
7:A:269:LEU:HA	7:A:269:LEU:HD23	1.91	0.43
4:P:64:PHE:HB3	4:P:78:ILE:HD11	2.01	0.43
2:h:1096:LYS:HB3	1:c:612:ILE:HD13	2.01	0.43
1:c:223:GLU:HA	1:c:244:LYS:H	1.84	0.43
1:c:894:ARG:NH2	1:c:910:TYR:O	2.49	0.43
3:f:333:ILE:HG22	3:g:337:TYR:HA	2.01	0.43
3:e:109:ILE:HB	3:e:179:ILE:HD13	2.01	0.43
3:g:403:MET:HG2	3:g:412:PRO:HB2	2.01	0.43
1:b:948:THR:OG1	1:b:949:ILE:N	2.52	0.43
7:F:24:ASN:O	7:F:93:MET:HE1	2.19	0.43
7:F:380:THR:OG1	7:F:401:GLU:OE2	2.27	0.43
7:E:461:THR:HG23	7:E:463:GLY:H	1.84	0.43
7:D:461:THR:HG23	7:D:463:GLY:H	1.84	0.43
7:A:112:ALA:HB1	7:A:119:PHE:CZ	2.54	0.43
3:f:153:TRP:CZ3	3:f:178:ARG:HB2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:596:VAL:HG22	3:f:597:LYS:N	2.34	0.43
1:b:82:THR:OG1	6:X:31:ASP:OD2	2.33	0.43
1:b:319:GLU:HG3	1:b:330:ARG:HE	1.84	0.43
7:F:461:THR:HG23	7:F:463:GLY:H	1.84	0.43
4:M:41:LEU:HG	4:M:74:GLY:HA2	2.00	0.43
7:C:289:VAL:HG23	7:C:290:VAL:HG13	2.01	0.43
4:J:127:ILE:HG13	4:J:128:MET:HG2	2.01	0.43
7:A:421:ALA:HA	7:A:436:LYS:HD2	2.00	0.43
4:P:103:GLN:HA	4:P:134:ILE:O	2.18	0.43
1:d:789:GLN:NE2	1:d:798:MET:HE1	2.33	0.42
3:g:298:ILE:HG12	3:g:307:VAL:HG12	2.00	0.42
5:G:72:THR:HG23	5:G:74:ILE:HG12	2.00	0.42
7:A:361:THR:HA	7:A:364:ASN:HD21	1.84	0.42
7:B:289:VAL:HG23	7:B:290:VAL:HG13	2.01	0.42
6:V:122:LYS:HE2	6:V:122:LYS:HB3	1.84	0.42
1:d:82:THR:HG23	1:d:82:THR:O	2.19	0.42
1:d:927:ARG:NE	3:g:4:ASN:O	2.36	0.42
7:F:98:LEU:HD12	7:F:235:ASN:HD21	1.85	0.42
7:E:24:ASN:O	7:E:93:MET:HE1	2.19	0.42
4:L:64:PHE:HB3	4:L:78:ILE:HD11	2.01	0.42
4:P:18:TYR:HB3	4:P:80:LEU:HD21	2.01	0.42
4:P:20:LEU:O	4:P:78:ILE:N	2.46	0.42
1:d:778:HIS:HB3	1:d:781:HIS:CG	2.55	0.42
1:d:815:ARG:HE	1:d:816:ALA:H	1.66	0.42
3:e:434:ASN:N	3:e:434:ASN:OD1	2.52	0.42
3:g:23:TYR:HB2	3:g:185:LEU:HD13	2.00	0.42
5:I:50:TYR:OH	5:H:288:PRO:HA	2.19	0.42
4:Q:115:ARG:NH1	4:Q:121:ALA:O	2.48	0.42
7:F:134:LEU:HD12	7:F:152:ILE:HD11	2.01	0.42
7:F:211:LEU:HD13	7:F:226:ILE:HD11	2.01	0.42
6:Y:177:LEU:HA	6:Y:200:LEU:HD23	2.01	0.42
6:W:4:PRO:HG3	6:W:68:ARG:HG3	2.01	0.42
7:B:421:ALA:HA	7:B:436:LYS:HD2	2.00	0.42
7:B:425:ASN:OD1	7:B:429:LEU:N	2.43	0.42
2:h:1109:LEU:HD21	1:c:640:TYR:CD2	2.54	0.42
3:e:433:ASP:O	3:e:437:ALA:N	2.52	0.42
3:e:487:TYR:CD2	3:e:507:TRP:CE3	3.03	0.42
1:b:321:ASP:OD2	1:b:325:ARG:NH1	2.52	0.42
4:R:20:LEU:HD12	4:R:21:LEU:N	2.34	0.42
4:R:65:THR:N	4:R:79:SER:O	2.53	0.42
5:I:72:THR:HG23	5:I:74:ILE:HG12	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:425:ASN:OD1	7:F:429:LEU:N	2.47	0.42
4:N:20:LEU:HD12	4:N:21:LEU:N	2.34	0.42
6:Y:4:PRO:HB2	6:Y:15:LEU:HD13	2.02	0.42
6:Y:70:LEU:HD22	6:Z:153:TYR:CG	2.54	0.42
7:C:185:ASP:OD1	7:C:185:ASP:N	2.52	0.42
5:G:131:LEU:N	5:G:185:ALA:O	2.51	0.42
7:D:98:LEU:HD12	7:D:235:ASN:HD21	1.84	0.42
7:B:14:SER:HA	7:B:24:ASN:O	2.20	0.42
6:V:59:PRO:HA	6:V:193:TYR:HE1	1.84	0.42
1:d:89:VAL:HA	1:d:154:ILE:HD11	2.01	0.42
1:d:660:LEU:O	1:d:708:LEU:N	2.46	0.42
1:c:602:ASP:OD2	1:c:604:ALA:HB3	2.19	0.42
1:c:742:PHE:HD1	1:c:829:LEU:HD13	1.83	0.42
3:f:487:TYR:HB2	3:f:507:TRP:HB3	2.02	0.42
4:Q:11:VAL:HG23	4:Q:11:VAL:O	2.20	0.42
4:Q:66:THR:HG22	4:Q:78:ILE:HG22	2.00	0.42
7:F:160:ASP:O	7:F:163:ASP:HB3	2.20	0.42
4:N:65:THR:N	4:N:79:SER:O	2.53	0.42
7:C:14:SER:HA	7:C:24:ASN:O	2.20	0.42
4:J:46:LEU:HD23	4:J:46:LEU:H	1.84	0.42
4:L:18:TYR:HB3	4:L:80:LEU:HD21	2.01	0.42
7:B:113:HIS:NE2	7:B:120:MET:HE2	2.34	0.42
4:T:18:TYR:HB3	4:T:80:LEU:HD21	2.01	0.42
1:d:228:GLN:HA	1:d:244:LYS:HB2	2.02	0.42
3:f:670:PRO:HD3	3:e:538:GLY:HA2	1.99	0.42
3:e:403:MET:HE1	3:e:414:ILE:HG22	2.01	0.42
3:e:488:ILE:HB	3:e:507:TRP:HZ3	1.84	0.42
3:e:525:THR:HG23	3:e:541:TRP:CZ3	2.54	0.42
3:g:141:ILE:HG22	3:g:157:TYR:HB3	2.01	0.42
3:g:654:ILE:HG22	3:g:656:VAL:HG23	2.02	0.42
1:b:26:LEU:CD1	1:b:135:ILE:HD11	2.44	0.42
7:F:407:ALA:HB3	7:F:410:LYS:HD3	2.02	0.42
4:N:56:ASP:N	4:N:56:ASP:OD1	2.52	0.42
6:X:89:PHE:O	6:X:92:ARG:NH1	2.51	0.42
7:E:98:LEU:HD12	7:E:235:ASN:HD21	1.84	0.42
7:E:134:LEU:HD12	7:E:152:ILE:HD11	2.01	0.42
7:E:160:ASP:O	7:E:163:ASP:HB3	2.20	0.42
7:E:340:PRO:HD3	7:E:348:GLU:HG2	2.01	0.42
7:C:299:LEU:N	7:C:310:ALA:O	2.49	0.42
4:J:20:LEU:HD12	4:J:21:LEU:N	2.34	0.42
5:G:155:ASP:OD1	5:G:155:ASP:N	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:382:LYS:O	7:D:399:SER:N	2.46	0.42
1:d:223:GLU:HA	1:d:244:LYS:HA	2.01	0.42
1:d:256:ASP:N	2:j:1089:LEU:O	2.50	0.42
1:d:756:GLY:O	1:d:803:ILE:HG23	2.20	0.42
4:R:3:THR:HB	4:R:6:ARG:HB2	2.01	0.42
4:Q:94:LYS:HB3	4:Q:94:LYS:HE3	1.90	0.42
7:F:163:ASP:HA	7:A:240:LEU:HD11	2.01	0.42
5:H:132:ASP:CG	5:H:133:LYS:H	2.24	0.42
6:Y:12:TYR:HB3	6:Y:61:GLU:HG2	2.02	0.42
7:C:337:LYS:NZ	7:A:58:SER:OG	2.37	0.42
4:U:111:VAL:HB	4:U:128:MET:HB2	2.02	0.42
7:A:287:LEU:HB3	7:B:248:VAL:HG21	2.01	0.42
7:B:185:ASP:OD1	7:B:185:ASP:N	2.52	0.42
7:B:361:THR:HA	7:B:364:ASN:HD21	1.84	0.42
3:e:201:ASN:OD1	3:e:202:VAL:N	2.52	0.42
3:e:378:PHE:CD1	3:e:385:VAL:HG13	2.54	0.42
3:g:345:LYS:HD3	3:g:350:TRP:CD2	2.55	0.42
4:R:127:ILE:HG13	4:R:128:MET:HG2	2.01	0.42
5:I:288:PRO:HA	5:G:50:TYR:OH	2.20	0.42
6:X:27:PRO:HB2	6:X:44:SER:HB3	2.02	0.42
6:X:95:THR:HG22	6:X:117:LEU:HD11	2.02	0.42
7:E:382:LYS:O	7:E:399:SER:N	2.46	0.42
7:A:113:HIS:NE2	7:A:120:MET:HE2	2.35	0.42
1:d:146:THR:HG21	6:V:201:ARG:NH2	2.35	0.42
1:d:149:ILE:HD11	6:a:181:ASP:OD2	2.20	0.42
1:c:876:ILE:HG21	1:c:879:ILE:CG1	2.50	0.42
1:b:376:ASP:OD1	1:b:376:ASP:N	2.51	0.42
6:a:4:PRO:HG3	6:a:68:ARG:HG3	2.01	0.42
7:E:211:LEU:HD13	7:E:226:ILE:HD11	2.01	0.42
7:C:113:HIS:NE2	7:C:120:MET:HE2	2.35	0.42
4:J:65:THR:N	4:J:79:SER:O	2.53	0.42
4:K:12:VAL:HG23	4:K:134:ILE:HD12	2.02	0.42
7:D:24:ASN:O	7:D:93:MET:HE1	2.19	0.42
7:A:289:VAL:HG23	7:A:290:VAL:HG13	2.01	0.42
4:P:91:LYS:HE3	4:P:91:LYS:HB3	1.80	0.42
6:Z:33:LEU:HD12	6:Z:37:LYS:HB2	2.02	0.42
6:Z:58:PHE:HB2	6:Z:61:GLU:OE1	2.20	0.42
1:d:883:LEU:O	1:d:896:VAL:N	2.41	0.42
3:e:56:ASP:OD1	3:e:56:ASP:N	2.52	0.42
3:e:486:ILE:HD13	3:e:547:TRP:CD2	2.55	0.42
5:H:50:TYR:OH	5:G:288:PRO:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:364:ASN:O	7:E:368:ASN:HB2	2.20	0.42
6:W:133:PRO:HG3	6:W:174:ARG:NH1	2.35	0.42
6:Z:95:THR:HG22	6:Z:117:LEU:HD11	2.02	0.42
1:c:584:LEU:HB3	1:b:140:ILE:HG22	2.01	0.41
3:f:144:LYS:NZ	3:f:151:ASN:O	2.47	0.41
1:b:776:ILE:HA	1:b:813:GLU:O	2.20	0.41
4:Q:111:VAL:HB	4:Q:128:MET:HB2	2.02	0.41
4:S:102:ARG:NH1	4:S:136:ASP:O	2.53	0.41
7:F:151:GLN:OE1	7:F:254:SER:OG	2.34	0.41
5:H:179:LEU:HD23	5:H:179:LEU:HA	1.87	0.41
6:X:58:PHE:HB2	6:X:61:GLU:OE1	2.20	0.41
6:Y:21:ASN:HB3	6:Y:51:ASN:HB2	2.02	0.41
7:E:407:ALA:HB3	7:E:410:LYS:HD3	2.02	0.41
7:C:1:MET:HA	7:C:1:MET:CE	2.45	0.41
7:C:4:GLN:OE1	7:C:143:THR:OG1	2.28	0.41
7:D:453:LYS:HD3	7:D:453:LYS:HA	1.91	0.41
1:d:641:TYR:CZ	2:i:1109:LEU:HD23	2.55	0.41
1:c:729:ILE:O	1:c:729:ILE:HG23	2.20	0.41
1:c:892:MET:HE3	1:c:893:LEU:H	1.85	0.41
3:f:487:TYR:CD2	3:f:488:ILE:HB	2.55	0.41
3:f:659:ILE:HD12	3:g:654:ILE:HB	2.03	0.41
1:b:305:LEU:N	1:b:436:GLU:O	2.52	0.41
6:a:12:TYR:HB3	6:a:61:GLU:HG2	2.02	0.41
6:a:177:LEU:HA	6:a:200:LEU:HD23	2.02	0.41
7:F:364:ASN:O	7:F:368:ASN:HB2	2.20	0.41
6:X:59:PRO:HA	6:X:193:TYR:HE1	1.84	0.41
6:Y:133:PRO:HG3	6:Y:174:ARG:NH1	2.35	0.41
4:M:11:VAL:HG23	4:M:11:VAL:O	2.20	0.41
7:E:163:ASP:HA	7:C:240:LEU:HD11	2.01	0.41
7:E:206:ASN:O	7:E:209:THR:OG1	2.32	0.41
7:A:40:SER:HB3	7:A:65:LEU:HD23	2.02	0.41
7:B:14:SER:HB2	7:B:25:THR:HG22	2.02	0.41
1:d:877:PRO:O	1:d:878:GLU:C	2.64	0.41
3:f:37:ARG:NH1	3:f:57:THR:O	2.53	0.41
3:e:4:ASN:OD1	3:e:5:ASN:N	2.53	0.41
1:b:75:GLY:N	1:b:160:ASN:OD1	2.52	0.41
5:H:194:SER:HB2	5:H:216:ASN:HD21	1.86	0.41
4:O:12:VAL:HG23	4:O:134:ILE:HD12	2.02	0.41
7:C:14:SER:HB2	7:C:25:THR:HG22	2.02	0.41
5:G:194:SER:HB2	5:G:216:ASN:HD21	1.85	0.41
7:D:129:HIS:HB2	7:D:255:PHE:CD1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:340:PRO:HD3	7:D:348:GLU:HG2	2.01	0.41
6:V:58:PHE:HB2	6:V:61:GLU:OE1	2.20	0.41
4:R:56:ASP:OD1	4:R:56:ASP:N	2.52	0.41
4:N:81:PRO:O	4:N:85:VAL:HG23	2.20	0.41
4:O:102:ARG:NH1	4:O:136:ASP:O	2.53	0.41
4:K:102:ARG:NH1	4:K:136:ASP:O	2.53	0.41
7:D:206:ASN:O	7:D:209:THR:OG1	2.32	0.41
7:A:14:SER:HA	7:A:24:ASN:O	2.20	0.41
7:B:147:ILE:HG12	7:B:176:LEU:HD13	2.02	0.41
1:d:17:LYS:HE2	6:a:28:MET:SD	2.61	0.41
1:c:82:THR:O	1:c:82:THR:HG23	2.19	0.41
1:c:147:SER:HB3	6:Z:47:TYR:HH	1.84	0.41
1:b:818:ASP:N	1:b:822:ARG:O	2.53	0.41
6:a:7:TYR:CE1	5:G:202:PHE:HD2	2.38	0.41
7:F:211:LEU:HD12	7:F:297:LEU:HD13	2.03	0.41
7:C:112:ALA:HB1	7:C:119:PHE:CZ	2.54	0.41
6:W:4:PRO:HB2	6:W:15:LEU:HD13	2.02	0.41
7:D:160:ASP:O	7:D:163:ASP:HB3	2.20	0.41
7:D:364:ASN:O	7:D:368:ASN:HB2	2.20	0.41
6:V:50:ILE:HD12	6:V:175:THR:HG21	2.03	0.41
1:c:319:GLU:OE1	1:c:330:ARG:NH2	2.45	0.41
3:f:310:SER:OG	3:f:311:ALA:N	2.53	0.41
3:f:346:ASP:OD2	3:f:351:LYS:NZ	2.45	0.41
3:e:19:TYR:O	3:e:103:MET:HE2	2.19	0.41
1:b:39:ILE:O	1:b:39:ILE:HG23	2.20	0.41
5:I:231:ARG:HH22	4:T:100:ASN:CB	2.21	0.41
6:a:4:PRO:HB2	6:a:15:LEU:HD13	2.02	0.41
4:Q:14:GLU:OE1	4:Q:137:GLY:N	2.43	0.41
6:X:50:ILE:HD12	6:X:175:THR:HG21	2.03	0.41
7:C:248:VAL:HG21	7:B:287:LEU:HB3	2.02	0.41
6:W:101:PRO:HD2	6:W:110:ILE:O	2.21	0.41
7:D:163:ASP:HA	7:B:240:LEU:HD11	2.01	0.41
6:Z:122:LYS:HE2	6:Z:122:LYS:HB3	1.85	0.41
1:d:789:GLN:CD	1:d:798:MET:HE1	2.45	0.41
1:c:531:LEU:HD22	1:c:540:ASN:HB3	2.02	0.41
3:f:72:GLU:OE1	3:f:100:THR:HG22	2.21	0.41
3:f:107:PRO:HG2	3:f:181:GLY:HA3	2.03	0.41
3:f:433:ASP:O	3:f:437:ALA:N	2.54	0.41
3:f:489:ILE:O	3:f:489:ILE:HG22	2.20	0.41
1:b:871:PRO:O	1:b:872:GLU:HG3	2.21	0.41
6:a:133:PRO:HG3	6:a:174:ARG:NH1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:340:PRO:HD3	7:F:348:GLU:HG2	2.01	0.41
6:X:33:LEU:HD12	6:X:37:LYS:HB2	2.02	0.41
7:E:211:LEU:HD12	7:E:297:LEU:HD13	2.03	0.41
7:C:36:TRP:H	7:B:326:THR:HG21	1.85	0.41
7:C:272:LYS:HD3	7:A:1:MET:HE3	2.03	0.41
4:J:4:GLU:CD	4:J:4:GLU:H	2.29	0.41
4:U:11:VAL:O	4:U:11:VAL:HG23	2.20	0.41
7:A:326:THR:HG21	7:B:36:TRP:H	1.84	0.41
6:Z:27:PRO:HB2	6:Z:44:SER:HB3	2.02	0.41
5:I:12:VAL:HG21	5:I:155:ASP:HA	2.03	0.41
5:I:202:PHE:HD2	6:Y:7:TYR:CE1	2.38	0.41
4:S:12:VAL:HG23	4:S:134:ILE:HD12	2.02	0.41
7:F:129:HIS:HB2	7:F:255:PHE:CD1	2.56	0.41
5:H:12:VAL:HG21	5:H:155:ASP:HA	2.03	0.41
7:C:208:LEU:O	7:C:301:GLY:N	2.54	0.41
7:D:354:SER:HB3	7:D:357:TYR:CE1	2.56	0.41
7:B:40:SER:HB3	7:B:65:LEU:HD23	2.02	0.41
6:V:26:ASP:OD1	6:V:26:ASP:N	2.54	0.41
6:V:27:PRO:HB2	6:V:44:SER:HB3	2.02	0.41
1:d:70:ARG:NH1	1:d:564:GLU:OE2	2.53	0.41
1:d:612:ILE:HD12	2:i:1112:LEU:CD2	2.51	0.41
1:d:630:LEU:HD23	1:d:630:LEU:H	1.84	0.41
1:c:19:LYS:NZ	6:Y:155:ASP:OD2	2.54	0.41
1:c:132:ARG:O	1:c:161:GLN:OE1	2.38	0.41
1:c:494:LEU:HD11	1:c:548:PHE:CD2	2.56	0.41
1:c:776:ILE:O	1:c:776:ILE:HG23	2.21	0.41
1:c:794:PRO:O	1:c:795:ASN:HB3	2.21	0.41
3:e:86:LEU:HD11	3:e:91:ILE:HB	2.03	0.41
3:e:379:ASP:OD2	3:e:382:LYS:NZ	2.49	0.41
3:e:435:VAL:HG13	3:e:436:THR:N	2.36	0.41
3:g:369:ASP:OD1	3:g:369:ASP:O	2.39	0.41
1:b:336:ASP:O	1:b:511:TYR:OH	2.37	0.41
4:R:81:PRO:O	4:R:85:VAL:HG23	2.20	0.41
7:F:133:MET:CE	7:F:149:SER:HB2	2.50	0.41
5:H:204:ILE:HD13	6:V:191:GLY:HA2	2.03	0.41
7:C:17:LYS:HA	7:C:17:LYS:HD2	1.91	0.41
7:C:363:ASN:O	7:C:367:VAL:HG12	2.21	0.41
4:J:81:PRO:O	4:J:85:VAL:HG23	2.21	0.41
6:W:21:ASN:HB3	6:W:51:ASN:HB2	2.02	0.41
6:V:33:LEU:HD12	6:V:37:LYS:HB2	2.02	0.41
6:V:95:THR:HG22	6:V:117:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:59:PRO:HA	6:Z:193:TYR:HE1	1.84	0.41
3:f:407:THR:HG22	3:f:408:GLY:H	1.85	0.41
3:e:515:THR:HG22	3:e:516:SER:N	2.36	0.41
3:g:142:GLU:OE1	3:g:142:GLU:N	2.53	0.41
3:g:416:THR:HG23	3:g:428:ILE:HG22	2.02	0.41
5:I:149:GLU:OE2	5:H:228:TYR:OH	2.26	0.41
7:F:360:THR:O	7:F:364:ASN:ND2	2.53	0.41
6:X:26:ASP:OD1	6:X:26:ASP:N	2.54	0.41
7:E:129:HIS:HB2	7:E:255:PHE:CD1	2.56	0.41
7:E:237:ILE:HG12	7:E:256:THR:HA	2.03	0.41
7:E:360:THR:O	7:E:364:ASN:ND2	2.53	0.41
7:B:208:LEU:O	7:B:301:GLY:N	2.54	0.41
1:d:773:TYR:HB2	1:d:786:ILE:HG23	2.02	0.40
1:d:775:SER:HB2	1:d:815:ARG:HB3	2.03	0.40
3:f:41:LEU:N	3:f:48:THR:O	2.53	0.40
3:e:489:ILE:HD12	3:e:514:ARG:HB3	2.03	0.40
1:b:702:GLY:O	1:b:704:ILE:HD12	2.22	0.40
5:I:194:SER:HB2	5:I:216:ASN:HD21	1.86	0.40
5:H:87:GLU:HB2	5:H:92:PHE:HE1	1.86	0.40
7:E:354:SER:HB3	7:E:357:TYR:CE1	2.56	0.40
7:C:289:VAL:HA	7:A:62:ASN:HB2	2.03	0.40
7:D:156:GLU:HB3	7:D:168:THR:HB	2.03	0.40
7:D:360:THR:O	7:D:364:ASN:ND2	2.53	0.40
7:A:185:ASP:N	7:A:185:ASP:OD1	2.53	0.40
1:c:837:LYS:NZ	1:c:944:VAL:HA	2.37	0.40
3:f:186:PRO:O	3:e:586:PHE:CE1	2.74	0.40
3:e:675:LYS:O	3:e:675:LYS:HG3	2.21	0.40
4:R:4:GLU:H	4:R:4:GLU:CD	2.29	0.40
5:I:87:GLU:HB2	5:I:92:PHE:HE1	1.87	0.40
7:F:13:VAL:O	7:F:25:THR:HA	2.21	0.40
7:F:418:ALA:H	7:F:441:THR:HG1	1.69	0.40
5:H:75:GLU:HB3	5:H:161:GLN:HE22	1.86	0.40
5:H:131:LEU:HB3	5:H:170:PRO:HB3	2.04	0.40
7:E:13:VAL:O	7:E:25:THR:HA	2.21	0.40
5:G:131:LEU:HB3	5:G:170:PRO:HB3	2.04	0.40
6:W:12:TYR:HB3	6:W:61:GLU:HG2	2.02	0.40
7:D:418:ALA:H	7:D:441:THR:HG1	1.69	0.40
7:A:96:HIS:NE2	7:A:102:ARG:O	2.48	0.40
1:d:93:VAL:HG11	1:b:684:TYR:HB3	2.03	0.40
3:f:103:MET:HG3	3:f:104:LYS:N	2.36	0.40
3:f:441:LEU:HD11	3:f:443:ILE:HD11	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:184:VAL:HG22	1:b:188:LEU:HD13	2.04	0.40
1:b:578:THR:HG22	1:b:579:TYR:N	2.37	0.40
1:b:871:PRO:C	1:b:872:GLU:HG3	2.47	0.40
4:R:25:MET:HE2	4:R:36:SER:CB	2.51	0.40
7:E:421:ALA:HB1	7:E:436:LYS:HB3	2.04	0.40
7:C:40:SER:HB3	7:C:65:LEU:HD23	2.02	0.40
7:D:421:ALA:HB1	7:D:436:LYS:HB3	2.04	0.40
7:A:17:LYS:HA	7:A:17:LYS:HD2	1.91	0.40
7:A:315:LYS:HD2	7:A:315:LYS:HA	1.93	0.40
1:c:376:ASP:OD1	1:c:376:ASP:N	2.54	0.40
1:c:858:PHE:CZ	3:e:4:ASN:HB2	2.57	0.40
3:f:453:ASP:OD1	3:f:454:GLY:N	2.53	0.40
3:e:115:GLU:HA	3:e:206:ARG:HG2	2.04	0.40
1:b:713:GLU:OE1	1:b:713:GLU:HA	2.21	0.40
6:Y:132:HIS:CG	6:Y:133:PRO:HD2	2.57	0.40
5:G:12:VAL:HG21	5:G:155:ASP:HA	2.03	0.40
7:D:8:ASN:ND2	7:D:141:ASP:OD1	2.33	0.40
7:A:14:SER:HB2	7:A:25:THR:HG22	2.02	0.40
7:A:278:GLU:HA	7:A:281:LYS:HG2	2.03	0.40
7:A:425:ASN:OD1	7:A:428:GLY:N	2.49	0.40
7:B:79:TYR:CD1	7:B:199:ILE:HG12	2.56	0.40
7:B:112:ALA:HB1	7:B:119:PHE:CZ	2.54	0.40
7:B:113:HIS:CE1	7:B:120:MET:HE2	2.57	0.40
7:B:363:ASN:O	7:B:367:VAL:HG12	2.21	0.40
4:P:66:THR:HG22	4:P:78:ILE:CD1	2.50	0.40
3:e:436:THR:O	3:e:438:LYS:NZ	2.51	0.40
3:g:443:ILE:O	3:g:443:ILE:HG23	2.20	0.40
1:b:221:LYS:O	1:b:222:GLU:HB3	2.21	0.40
6:a:101:PRO:HD2	6:a:110:ILE:O	2.21	0.40
7:C:64:SER:OG	7:C:65:LEU:N	2.55	0.40
7:C:287:LEU:HB3	7:A:248:VAL:HG21	2.03	0.40
6:W:177:LEU:HA	6:W:200:LEU:HD23	2.02	0.40
7:B:262:THR:HG22	7:B:337:LYS:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	947/949 (100%)	903 (95%)	44 (5%)	0	100	100
1	c	947/949 (100%)	918 (97%)	29 (3%)	0	100	100
1	d	947/949 (100%)	898 (95%)	49 (5%)	0	100	100
2	h	41/1219 (3%)	41 (100%)	0	0	100	100
2	i	41/1219 (3%)	40 (98%)	1 (2%)	0	100	100
2	j	41/1219 (3%)	41 (100%)	0	0	100	100
3	e	665/688 (97%)	636 (96%)	29 (4%)	0	100	100
3	f	663/688 (96%)	648 (98%)	15 (2%)	0	100	100
3	g	583/688 (85%)	568 (97%)	15 (3%)	0	100	100
4	J	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	K	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	L	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
4	M	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
4	N	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	O	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	P	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
4	Q	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
4	R	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	S	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	T	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
4	U	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
5	G	296/298 (99%)	286 (97%)	10 (3%)	0	100	100
5	H	296/298 (99%)	286 (97%)	10 (3%)	0	100	100
5	I	296/298 (99%)	287 (97%)	9 (3%)	0	100	100
6	V	202/204 (99%)	198 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	W	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
6	X	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
6	Y	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
6	Z	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
6	a	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
7	A	462/464 (100%)	445 (96%)	17 (4%)	0	100	100
7	B	462/464 (100%)	445 (96%)	17 (4%)	0	100	100
7	C	462/464 (100%)	445 (96%)	17 (4%)	0	100	100
7	D	462/464 (100%)	446 (96%)	16 (4%)	0	100	100
7	E	462/464 (100%)	444 (96%)	18 (4%)	0	100	100
7	F	462/464 (100%)	446 (96%)	16 (4%)	0	100	100
All	All	11397/15150 (75%)	10997 (96%)	400 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	834/834 (100%)	834 (100%)	0	100	100
1	c	834/834 (100%)	834 (100%)	0	100	100
1	d	834/834 (100%)	834 (100%)	0	100	100
2	h	36/980 (4%)	36 (100%)	0	100	100
2	i	36/980 (4%)	36 (100%)	0	100	100
2	j	36/980 (4%)	36 (100%)	0	100	100
3	e	562/572 (98%)	562 (100%)	0	100	100
3	f	560/572 (98%)	560 (100%)	0	100	100
3	g	490/572 (86%)	490 (100%)	0	100	100
4	J	118/119 (99%)	118 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	K	118/119 (99%)	118 (100%)	0	100	100
4	L	119/119 (100%)	119 (100%)	0	100	100
4	M	119/119 (100%)	119 (100%)	0	100	100
4	N	118/119 (99%)	118 (100%)	0	100	100
4	O	118/119 (99%)	118 (100%)	0	100	100
4	P	119/119 (100%)	119 (100%)	0	100	100
4	Q	119/119 (100%)	119 (100%)	0	100	100
4	R	118/119 (99%)	118 (100%)	0	100	100
4	S	118/119 (99%)	118 (100%)	0	100	100
4	T	119/119 (100%)	119 (100%)	0	100	100
4	U	119/119 (100%)	119 (100%)	0	100	100
5	G	273/273 (100%)	273 (100%)	0	100	100
5	H	273/273 (100%)	273 (100%)	0	100	100
5	I	273/273 (100%)	273 (100%)	0	100	100
6	V	181/181 (100%)	181 (100%)	0	100	100
6	W	181/181 (100%)	181 (100%)	0	100	100
6	X	181/181 (100%)	181 (100%)	0	100	100
6	Y	181/181 (100%)	181 (100%)	0	100	100
6	Z	181/181 (100%)	181 (100%)	0	100	100
6	a	181/181 (100%)	181 (100%)	0	100	100
7	A	394/394 (100%)	394 (100%)	0	100	100
7	B	394/394 (100%)	394 (100%)	0	100	100
7	C	394/394 (100%)	394 (100%)	0	100	100
7	D	394/394 (100%)	394 (100%)	0	100	100
7	E	394/394 (100%)	394 (100%)	0	100	100
7	F	394/394 (100%)	394 (100%)	0	100	100
All	All	9913/12855 (77%)	9913 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	d	540	ASN
1	d	616	ASN
1	c	515	ASN
1	c	616	ASN
1	c	911	ASN
3	f	647	ASN
3	e	5	ASN
3	e	13	ASN
3	e	99	GLN
3	e	146	ASN
3	e	386	ASN
3	e	400	ASN
3	e	686	HIS
3	g	99	GLN
1	b	13	ASN
1	b	66	HIS
1	b	157	ASN
1	b	339	HIS
1	b	523	GLN
1	b	718	ASN
4	R	15	ASN
5	I	161	GLN
6	a	51	ASN
6	a	112	ASN
4	S	103	GLN
7	F	172	ASN
5	H	161	GLN
5	H	175	ASN
5	H	216	ASN
6	X	9	ASN
6	X	188	ASN
6	Y	51	ASN
6	Y	112	ASN
4	O	103	GLN
7	E	172	ASN
7	C	87	GLN
7	C	151	GLN
7	C	172	ASN
7	C	364	ASN
4	J	15	ASN
4	L	100	ASN
4	L	103	GLN
5	G	161	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	W	51	ASN
4	K	5	ASN
4	K	103	GLN
7	D	172	ASN
7	A	87	GLN
7	A	151	GLN
7	A	172	ASN
7	A	364	ASN
7	B	87	GLN
7	B	151	GLN
7	B	172	ASN
7	B	364	ASN
4	P	100	ASN
4	P	103	GLN
4	T	100	ASN
4	T	103	GLN
6	V	9	ASN
6	V	188	ASN
6	Z	9	ASN
6	Z	188	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14799. These allow visual inspection of the internal detail of the map and identification of artifacts.

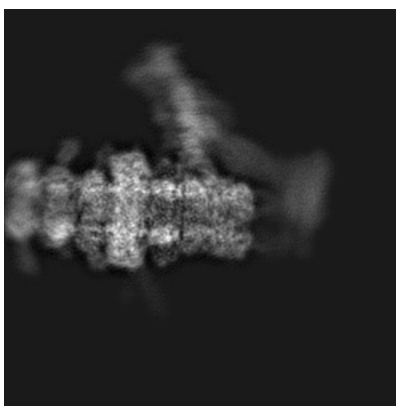
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

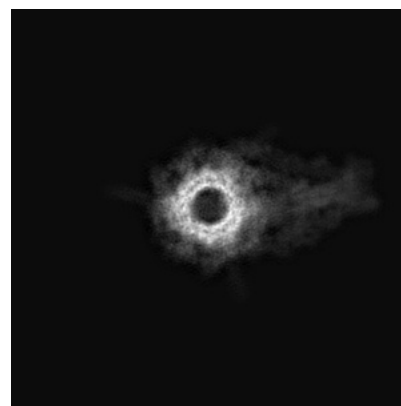
6.1.1 Primary map



X

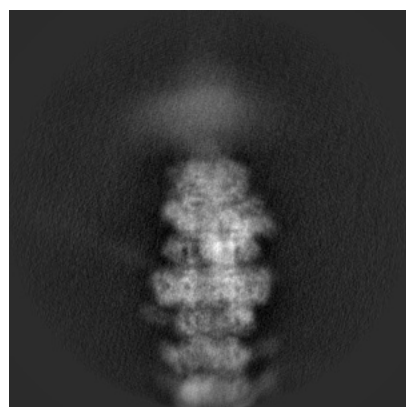


Y

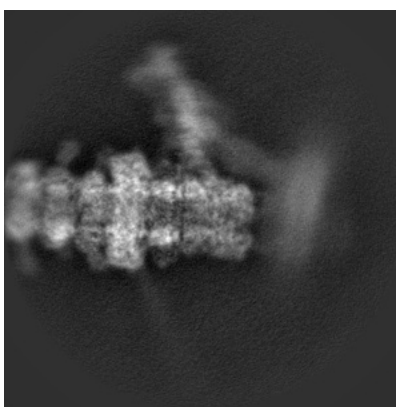


Z

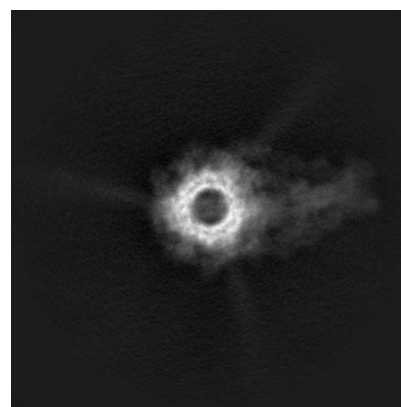
6.1.2 Raw map



X



Y

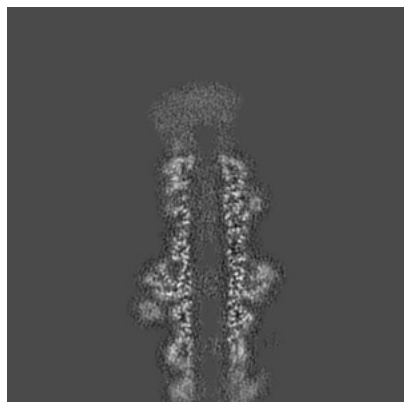


Z

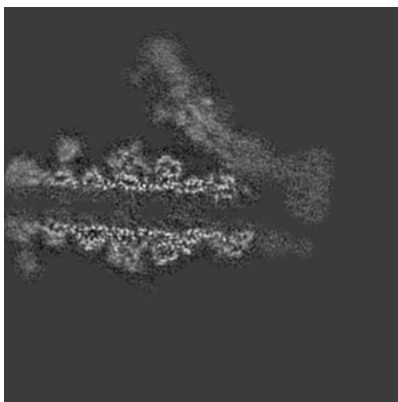
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

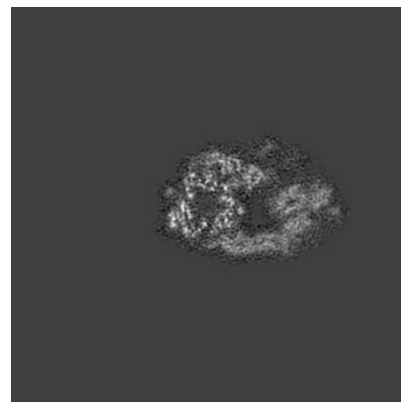
6.2.1 Primary map



X Index: 170

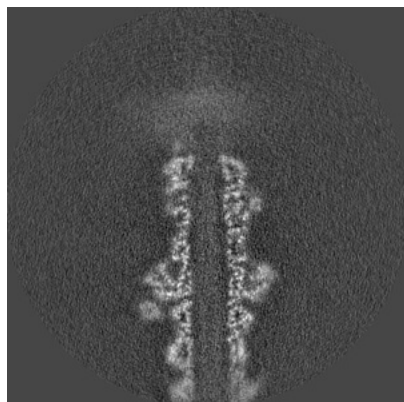


Y Index: 170

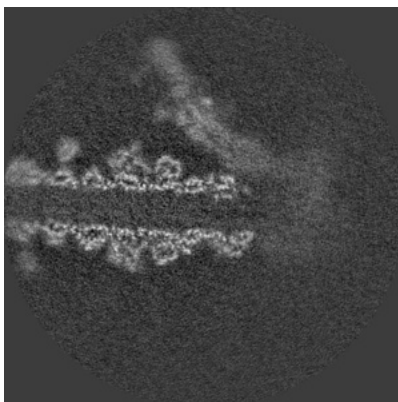


Z Index: 170

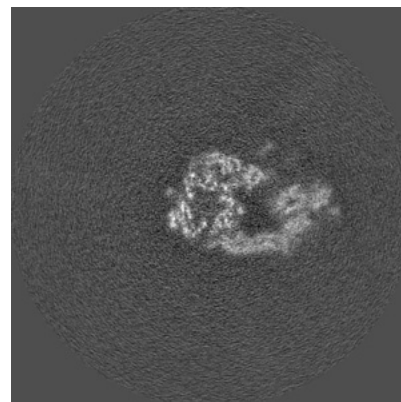
6.2.2 Raw map



X Index: 170



Y Index: 170

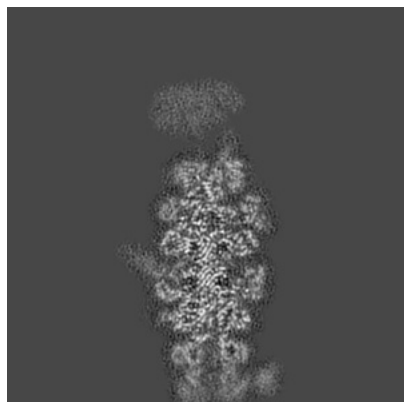


Z Index: 170

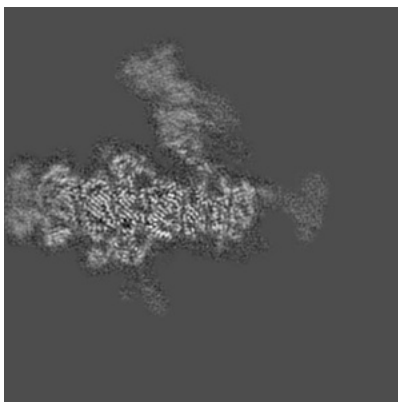
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

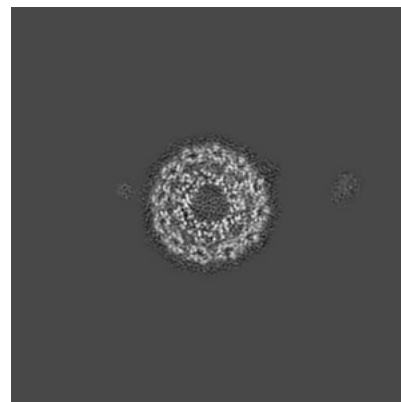
6.3.1 Primary map



X Index: 186

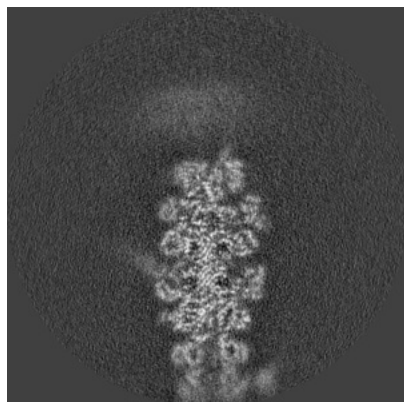


Y Index: 189

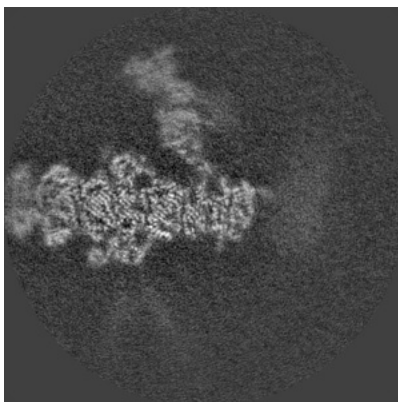


Z Index: 99

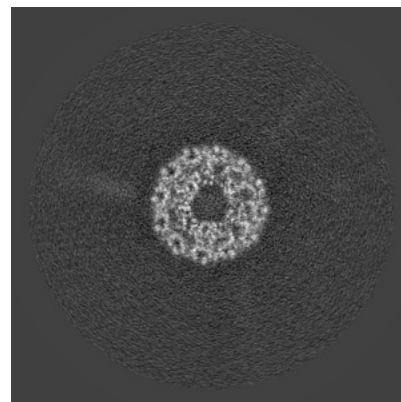
6.3.2 Raw map



X Index: 186



Y Index: 189

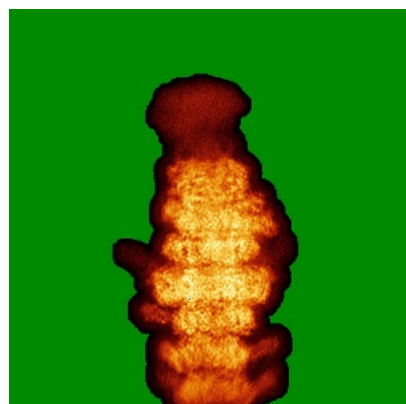


Z Index: 97

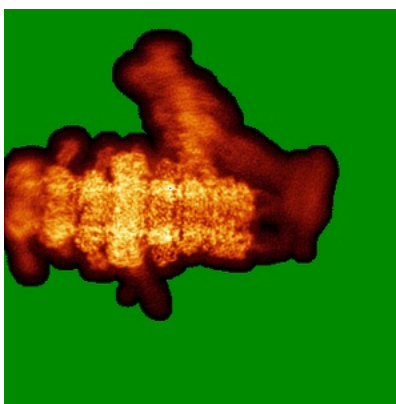
The images above show the largest variance slices of the map in three orthogonal directions.

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

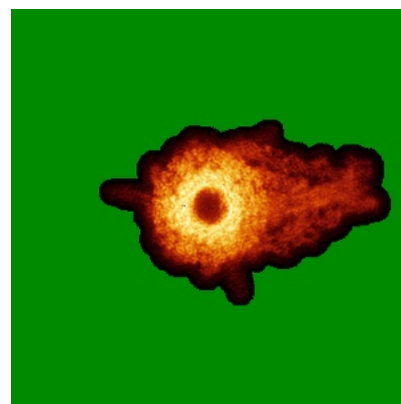
6.4.1 Primary map



X

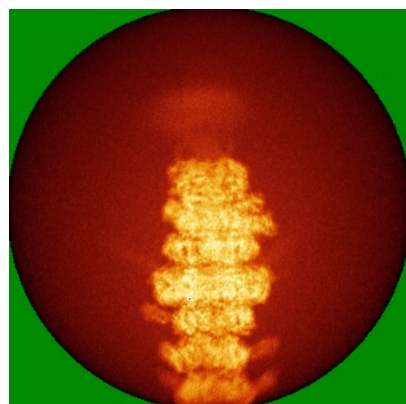


Y

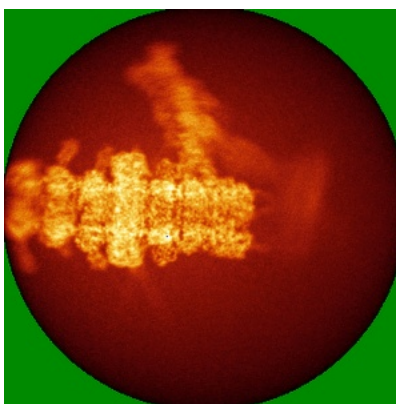


Z

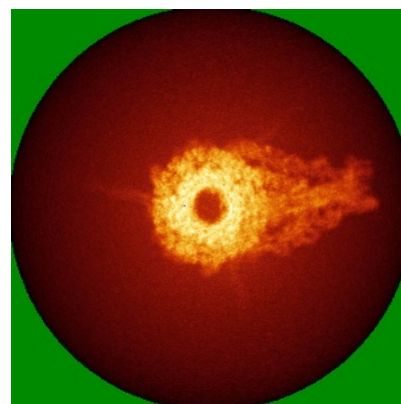
6.4.2 Raw map



X



Y

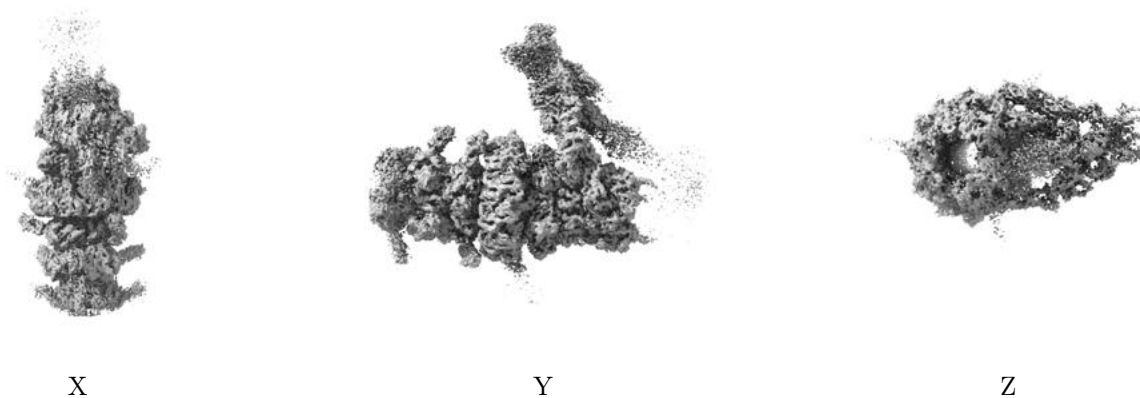


Z

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.

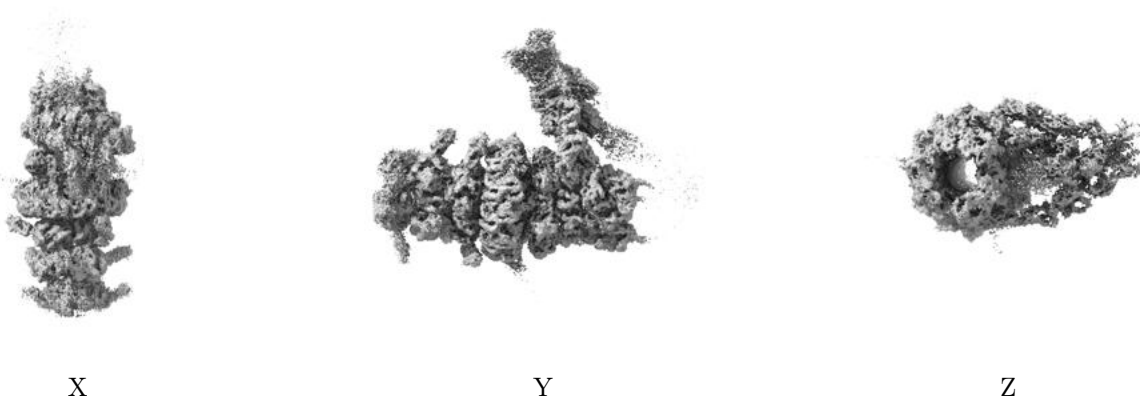
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0214. 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.

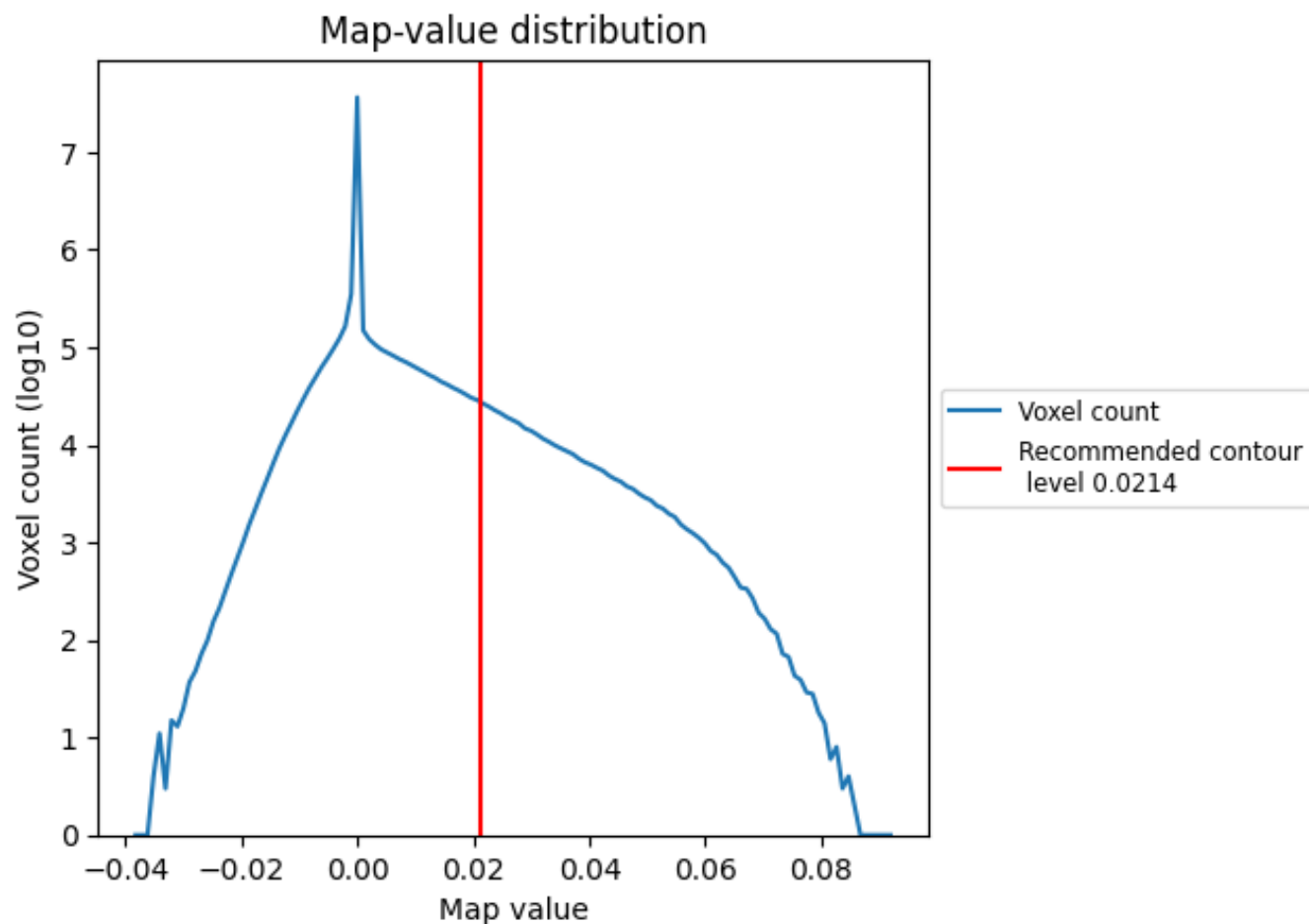
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

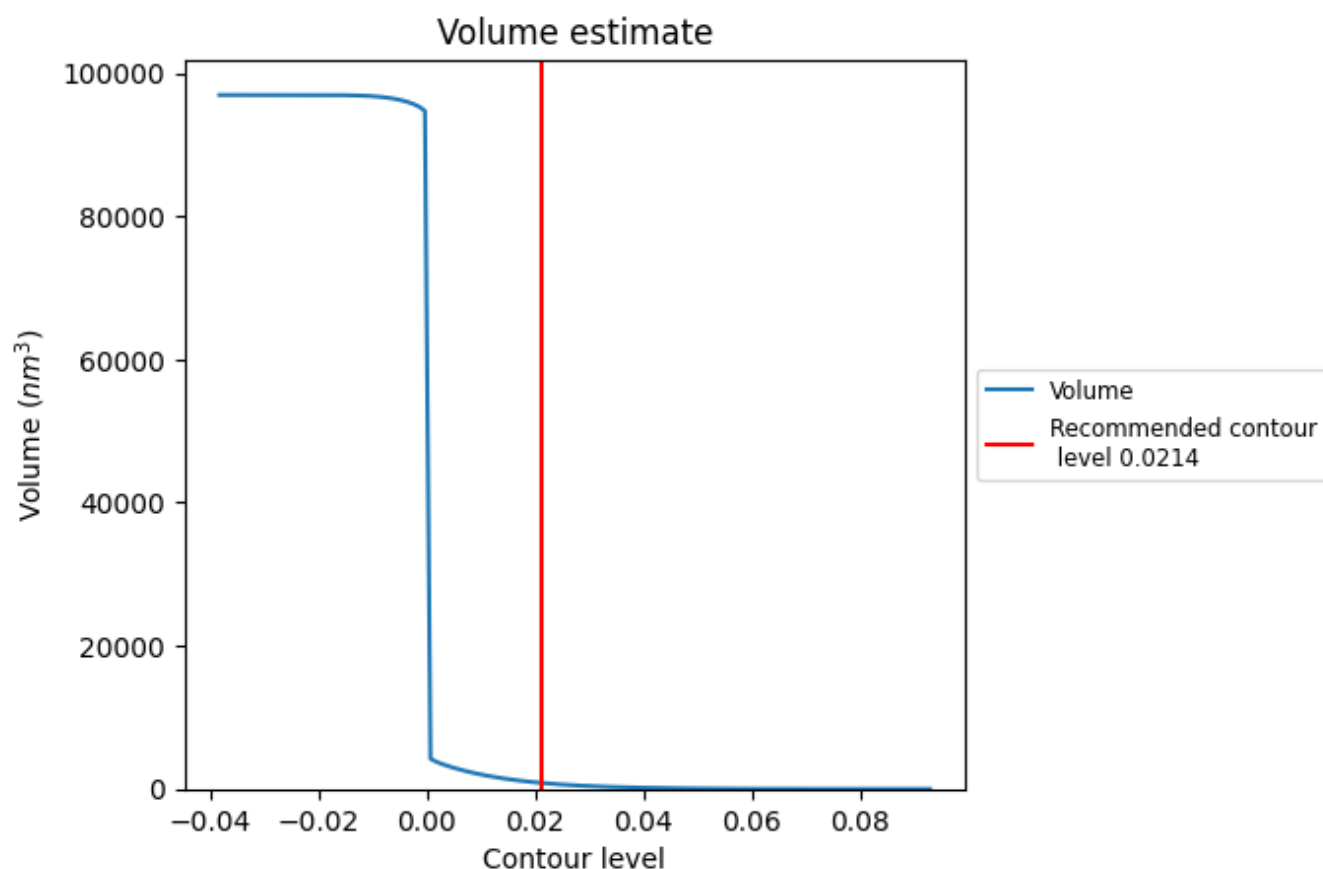
This section contains the results of statistical analysis of the map.

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.

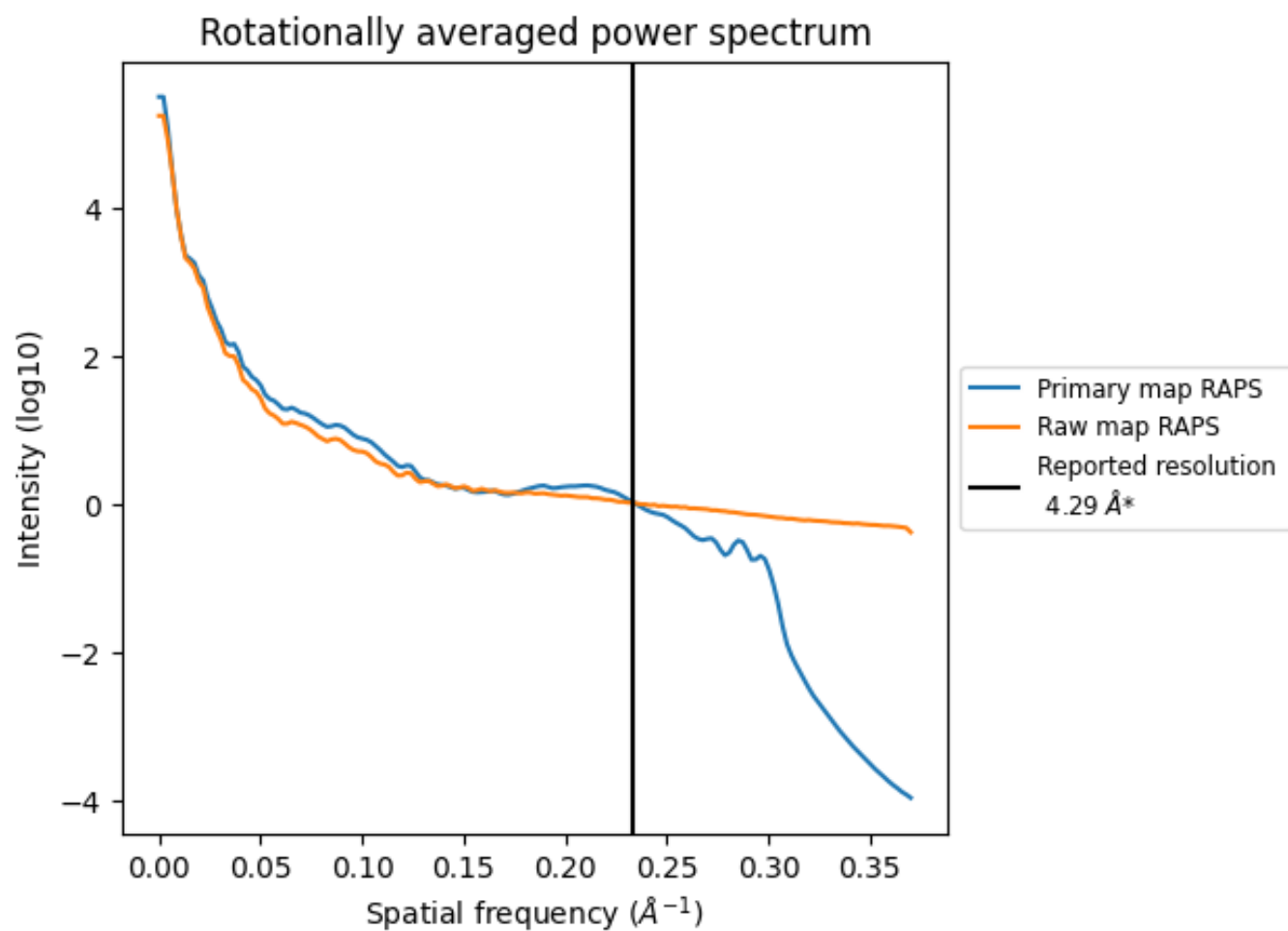
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 830 nm³; this corresponds to an approximate mass of 750 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 ⓘ

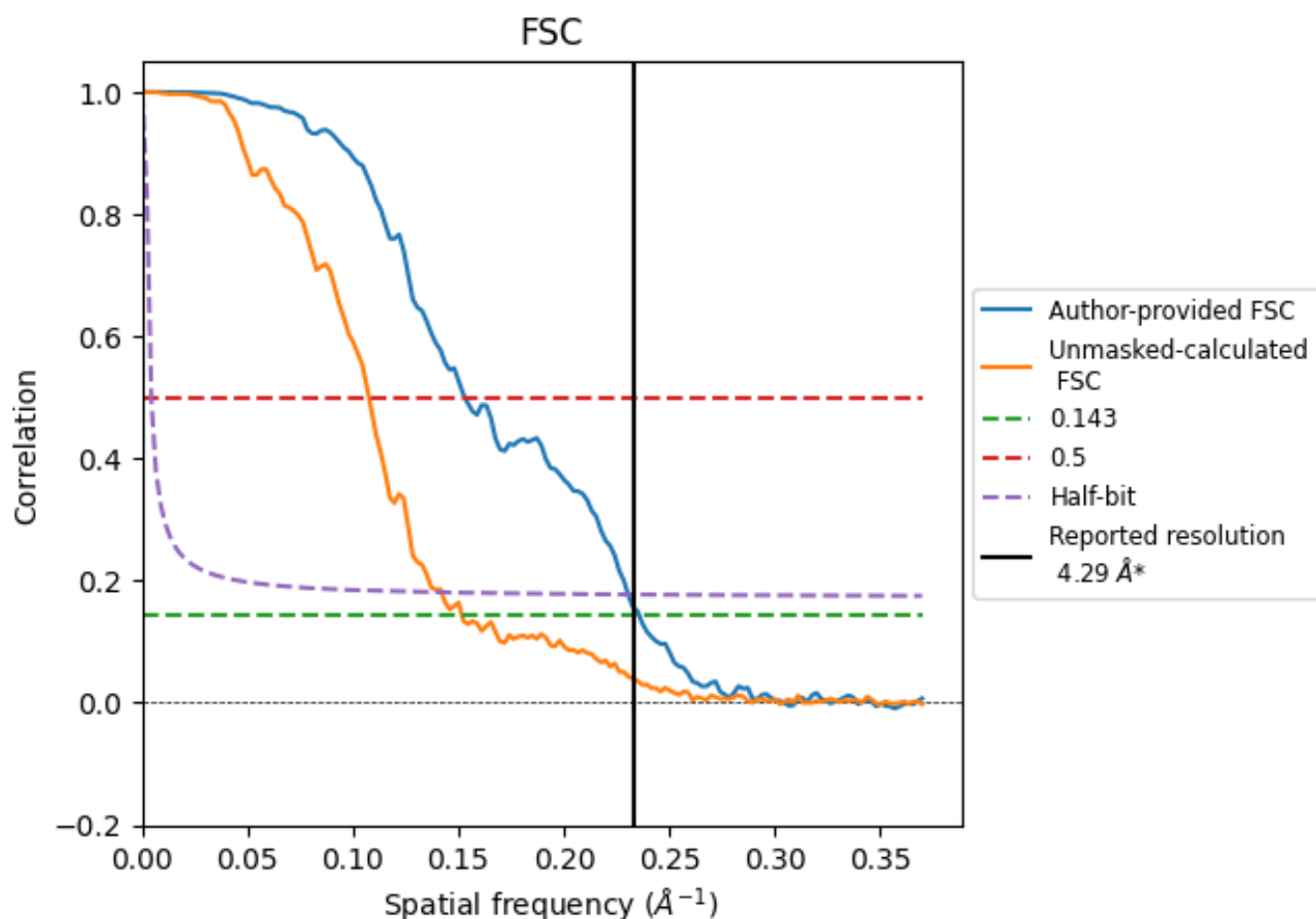


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

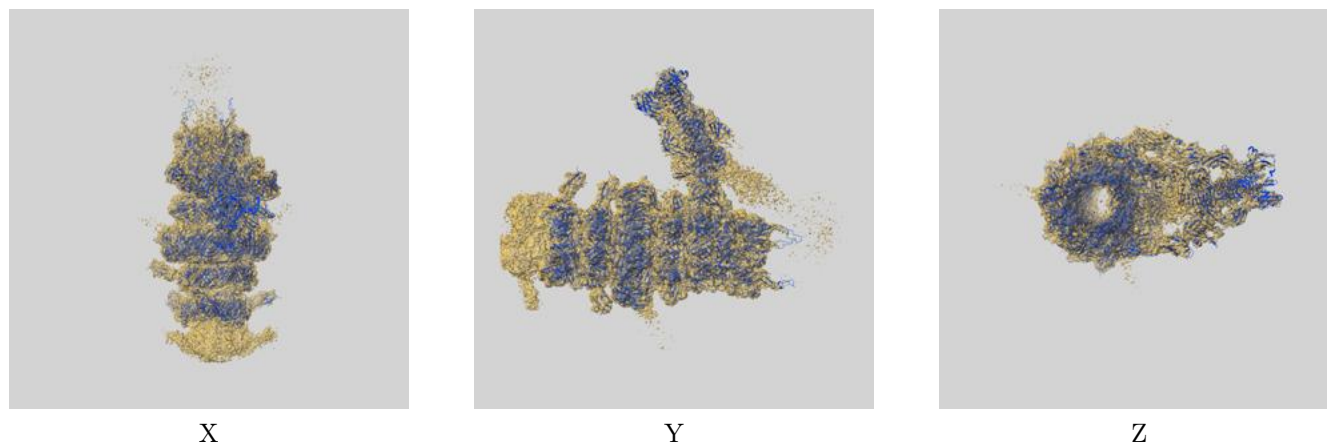
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.29	-	-
Author-provided FSC curve	4.24	6.53	4.34
Unmasked-calculated*	6.59	9.30	7.04

*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 6.59 differs from the reported value 4.29 by more than 10 %

9 Map-model fit [i](#)

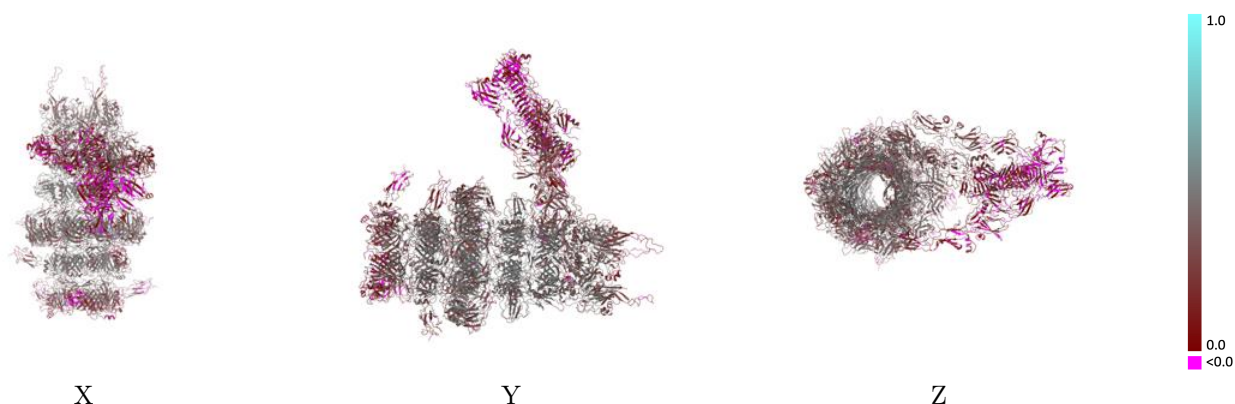
This section contains information regarding the fit between EMDB map EMD-14799 and PDB model 7ZN2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



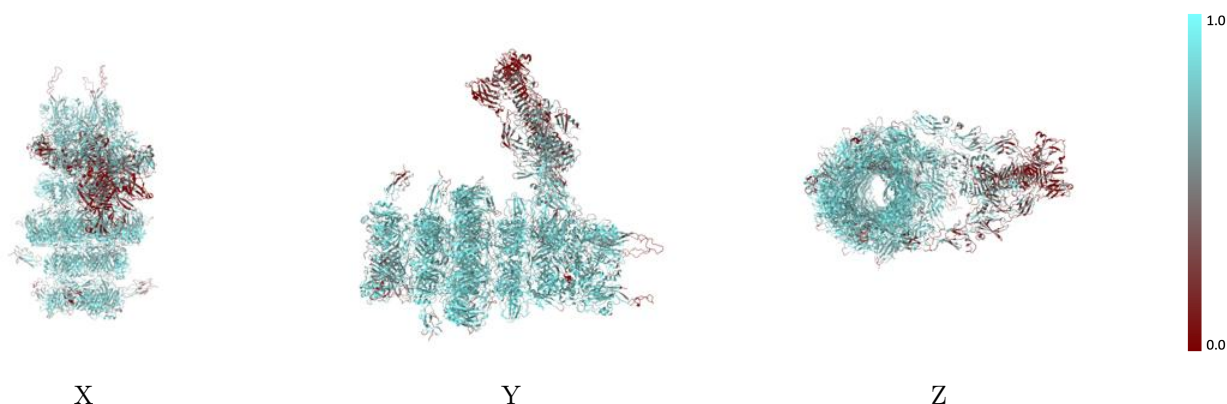
The images above show the 3D surface view of the map at the recommended contour level 0.0214 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



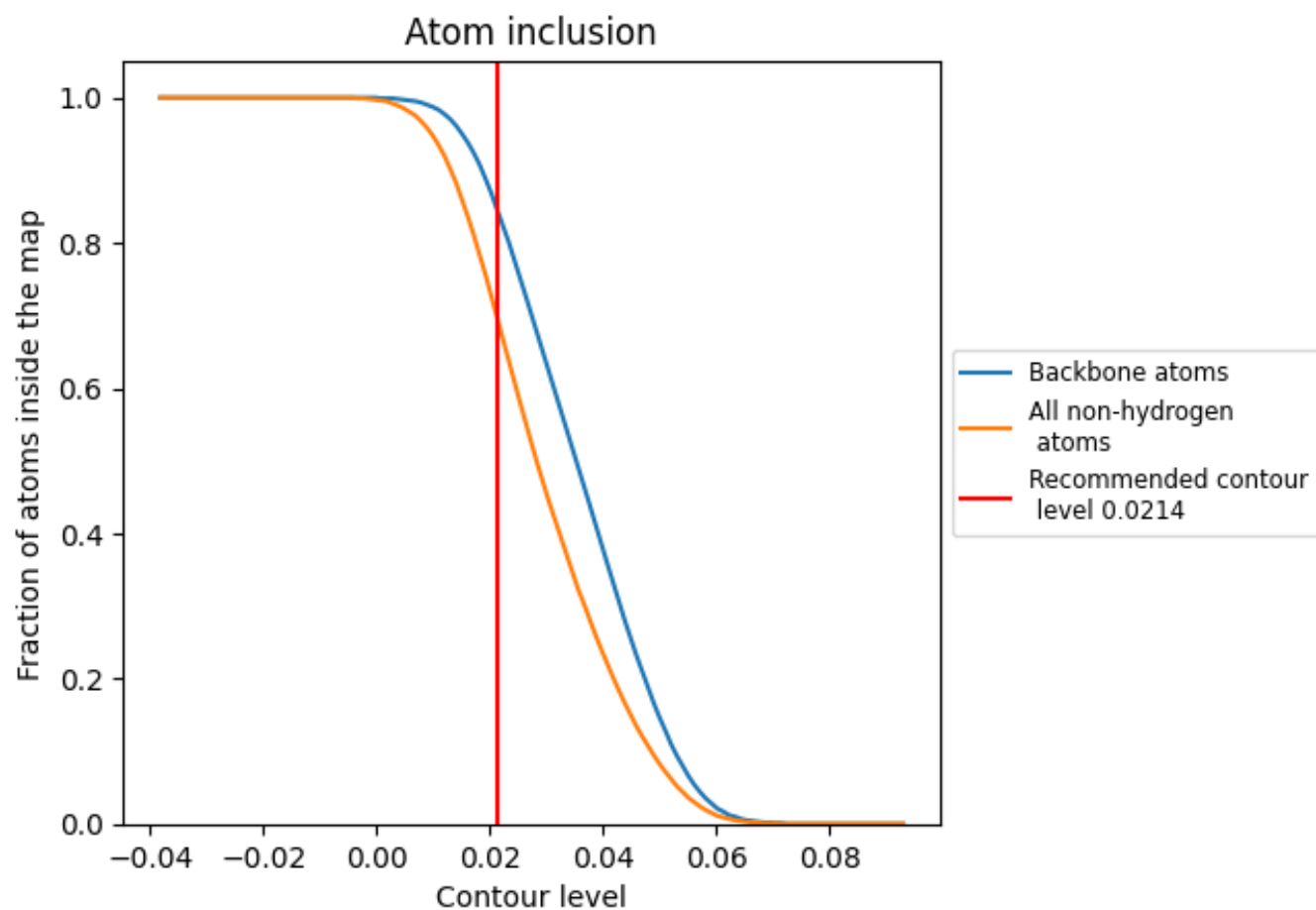
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0214).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 69% 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 (0.0214) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6930	 0.3200
A	 0.6820	 0.2530
B	 0.6860	 0.2560
C	 0.6750	 0.2500
D	 0.7840	 0.3770
E	 0.7730	 0.3780
F	 0.7840	 0.3810
G	 0.8300	 0.4530
H	 0.8350	 0.4410
I	 0.8350	 0.4490
J	 0.7690	 0.3530
K	 0.7490	 0.3230
L	 0.7280	 0.3410
M	 0.7480	 0.3490
N	 0.7560	 0.3210
O	 0.7480	 0.3280
P	 0.7500	 0.3500
Q	 0.7700	 0.3660
R	 0.7640	 0.3370
S	 0.7720	 0.3530
T	 0.7520	 0.3560
U	 0.7780	 0.3700
V	 0.8250	 0.4360
W	 0.8300	 0.4350
X	 0.8290	 0.4220
Y	 0.8430	 0.4390
Z	 0.8580	 0.4340
a	 0.8640	 0.4430
b	 0.7250	 0.3550
c	 0.7280	 0.3500
d	 0.6870	 0.3150
e	 0.4020	 0.1680
f	 0.4090	 0.1340
g	 0.3460	 0.1050
h	 0.7280	 0.3450



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.6690	 0.3240
j	 0.7590	 0.3630