



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:38 AM UTC

PDB ID : 9JYZ / pdb_00009jyz
EMDB ID : EMD-61910
Title : portal-tail complex of mature T7
Authors : Liu, H.R.; Chen, W.Y.
Deposited on : 2024-10-13
Resolution : 2.70 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:

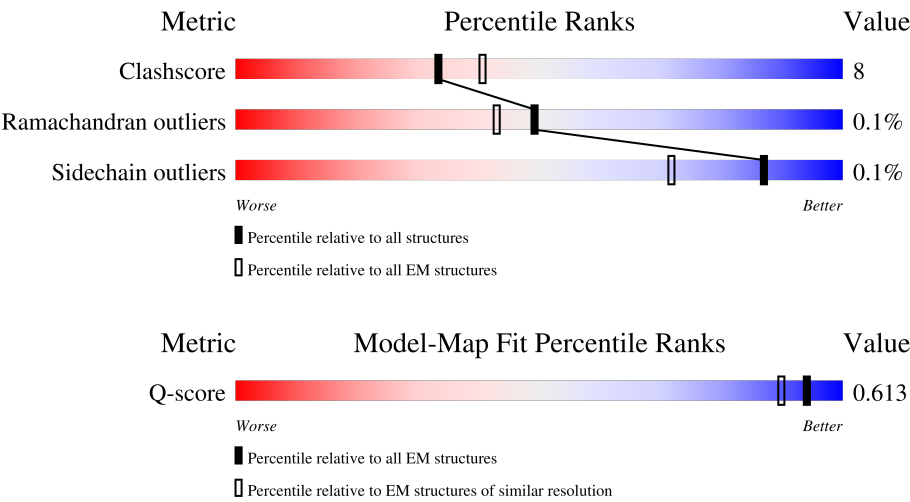
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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.



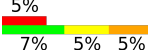
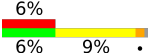
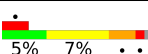
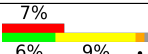
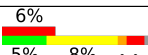
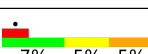
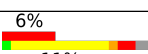
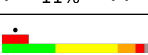
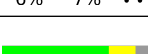
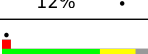
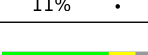
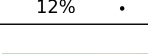
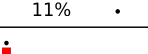
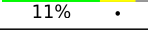
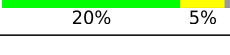
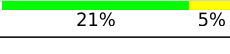
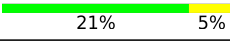
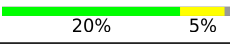
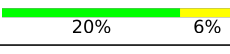
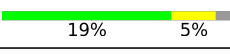
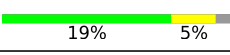
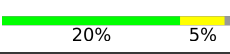
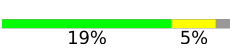
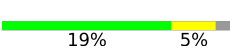
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	0	88	5% 8% . 84%
1	3	88	5% 8% . 5% 84%
1	4	88	5% . 10% . 84%
1	5	88	7% 6% . 84%

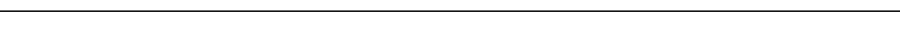
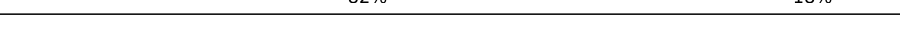
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	6	88		84%
1	7	88		84%
1	8	88		84%
1	9	88		84%
1	AA	88		84%
1	AB	88		84%
1	AC	88		84%
1	AD	88		84%
2	1	99		85%
2	2	99		85%
2	v	99		85%
2	w	99		85%
2	y	99		85%
2	z	99		85%
3	A	553		75%
3	B	553		75%
3	C	553		75%
3	D	553		75%
3	E	553		75%
3	F	553		76%
3	G	553		76%
3	H	553		76%
3	I	553		76%
3	J	553		76%
3	K	553		75%

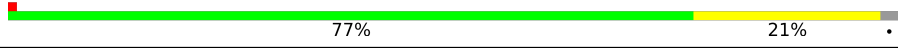
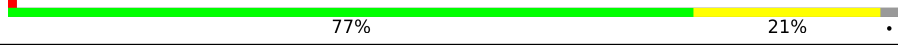
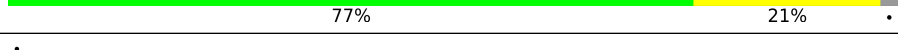
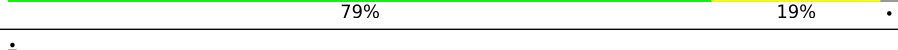
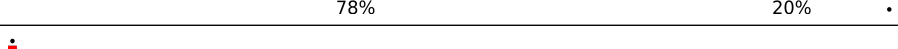
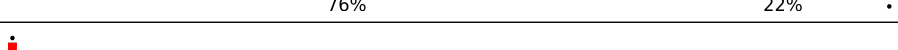
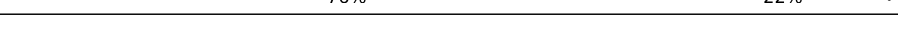
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	553	
3	M	553	
3	N	553	
3	O	553	
3	a	553	
3	b	553	
3	c	553	
4	P	794	
4	Q	794	
4	R	794	
4	S	794	
4	T	794	
4	x	794	
5	U	196	
5	V	196	
5	W	196	
5	X	196	
5	Y	196	
5	Z	196	
5	d	196	
5	e	196	
5	f	196	
5	g	196	
5	h	196	
5	i	196	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
6	j	536		.
6	k	536		.
6	l	536		.
6	m	536		.
6	n	536		.
6	o	536		.
6	p	536		.
6	q	536		.
6	r	536		.
6	s	536		.
6	t	536		.
6	u	536		.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 126948 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 Protein 6.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	3	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	4	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	5	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	6	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	7	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	8	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	9	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	AA	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	AB	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	AC	14	Total 110	C 70	N 18	O 20	S 2	0	0
1	AD	14	Total 110	C 70	N 18	O 20	S 2	0	0

- Molecule 2 is a protein called Protein 7.3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	15	Total 101	C 60	N 21	O 20	0	0
2	2	15	Total 101	C 60	N 21	O 20	0	0
2	v	15	Total 101	C 60	N 21	O 20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
2	w	15	Total	C	N	O	0	0
			101	60	21	20		
2	y	15	Total	C	N	O	0	0
			101	60	21	20		
2	z	15	Total	C	N	O	0	0
			101	60	21	20		

- Molecule 3 is a protein called Tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	141	Total	C	N	O	S	0	0
			1115	698	201	215	1		
3	B	141	Total	C	N	O	S	0	0
			1115	698	201	215	1		
3	C	141	Total	C	N	O	S	0	0
			1115	698	201	215	1		
3	D	141	Total	C	N	O	S	0	0
			1115	698	201	215	1		
3	E	141	Total	C	N	O	S	0	0
			1115	698	201	215	1		
3	F	134	Total	C	N	O	S	0	0
			1067	668	192	206	1		
3	G	134	Total	C	N	O	S	0	0
			1067	668	192	206	1		
3	H	134	Total	C	N	O	S	0	0
			1067	668	192	206	1		
3	I	134	Total	C	N	O	S	0	0
			1067	668	192	206	1		
3	J	134	Total	C	N	O	S	0	0
			1067	668	192	206	1		
3	K	136	Total	C	N	O	S	0	0
			1080	675	195	209	1		
3	L	136	Total	C	N	O	S	0	0
			1080	675	195	209	1		
3	M	136	Total	C	N	O	S	0	0
			1080	675	195	209	1		
3	N	136	Total	C	N	O	S	0	0
			1080	675	195	209	1		
3	O	136	Total	C	N	O	S	0	0
			1080	675	195	209	1		
3	a	141	Total	C	N	O	S	0	0
			1115	698	201	215	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	134	Total	C	N	O	S	0	0
			1067	668	192	206	1		
3	c	136	Total	C	N	O	S	0	0
			1080	675	195	209	1		

- Molecule 4 is a protein called Tail tubular protein gp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	793	Total	C	N	O	S	0	0
			6313	4003	1087	1208	15		
4	Q	793	Total	C	N	O	S	0	0
			6313	4003	1087	1208	15		
4	R	793	Total	C	N	O	S	0	0
			6313	4003	1087	1208	15		
4	S	793	Total	C	N	O	S	0	0
			6313	4003	1087	1208	15		
4	T	793	Total	C	N	O	S	0	0
			6313	4003	1087	1208	15		
4	x	793	Total	C	N	O	S	0	0
			6313	4003	1087	1208	15		

- Molecule 5 is a protein called Tail tubular protein gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
5	V	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
5	W	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
5	X	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
5	Y	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
5	Z	195	Total	C	N	O	S	0	0
			1557	966	266	317	8		
5	d	195	Total	C	N	O	S	0	0
			1557	966	266	317	8		
5	e	195	Total	C	N	O	S	0	0
			1557	966	266	317	8		
5	f	195	Total	C	N	O	S	0	0
			1557	966	266	317	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	195	Total	C	N	O	S	0	0
			1557	966	266	317	8		
5	h	196	Total	C	N	O	S	0	0
			1565	971	267	318	9		
5	i	195	Total	C	N	O	S	0	0
			1557	966	266	317	8		

- Molecule 6 is a protein called Portal protein.

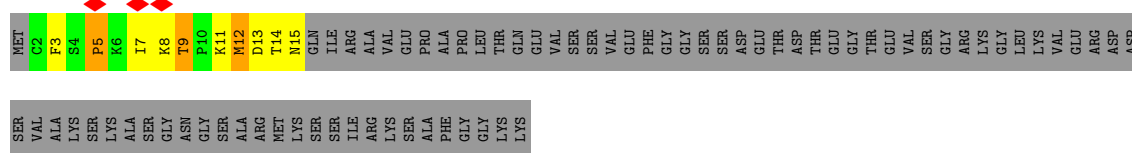
Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	k	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	l	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	m	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	n	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	o	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	p	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	q	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	r	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	s	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	t	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		
6	u	526	Total	C	N	O	S	0	0
			4070	2549	692	806	23		

3 Residue-property plots [i](#)

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

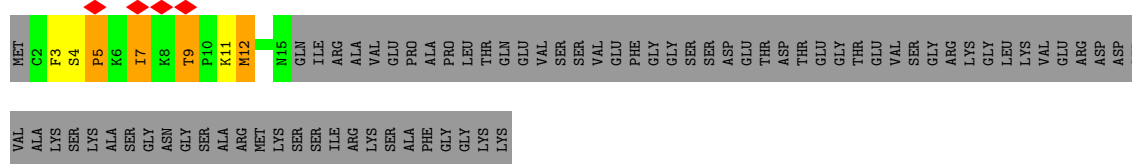
• Molecule 1: Protein 6.7

Chain 0: 84%



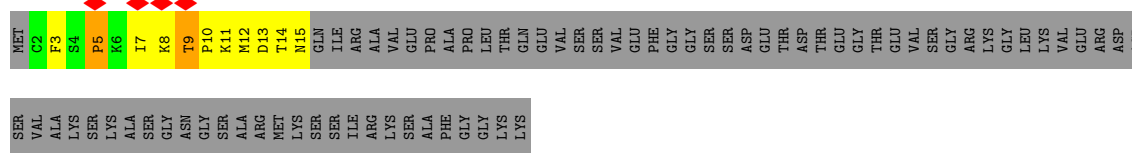
• Molecule 1: Protein 6.7

Chain 3: 84%



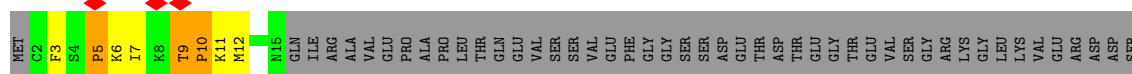
• Molecule 1: Protein 6.7

Chain 4: 84%



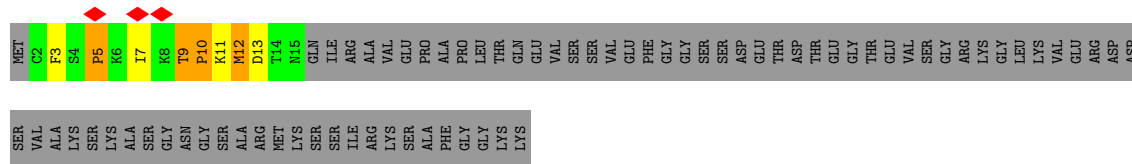
• Molecule 1: Protein 6.7

Chain 5: 84%



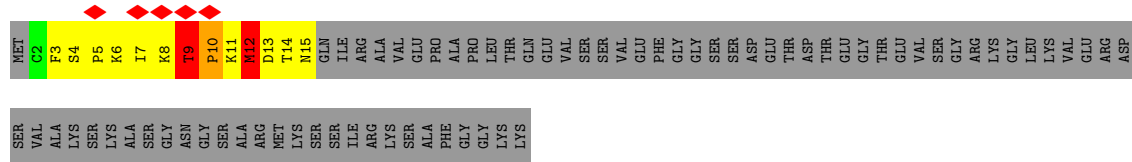
- Molecule 1: Protein 6.7

Chain AB:  84%



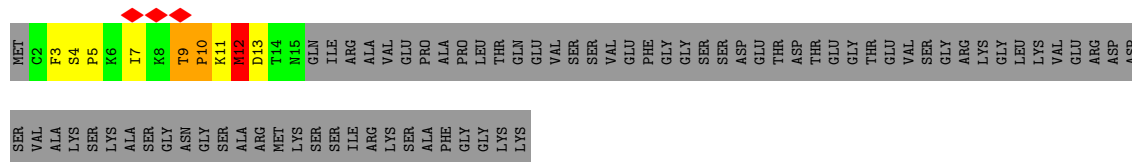
- Molecule 1: Protein 6.7

Chain AC:  84%



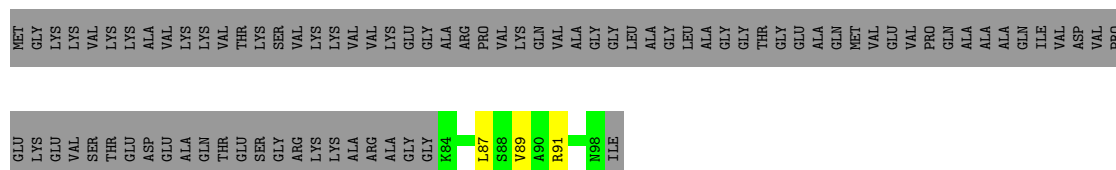
- Molecule 1: Protein 6.7

Chain AD:  84%



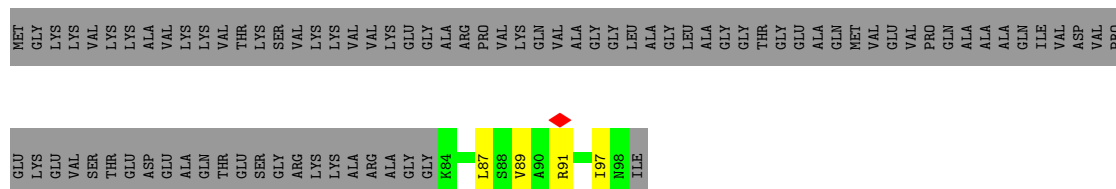
- Molecule 2: Protein 7.3

Chain 1:  85%



- Molecule 2: Protein 7.3

Chain 2:  85%



- Molecule 2: Protein 7.3

GLU	LYS	GLU	VAL	THR	GLU	ASP	ALA	GLN	THR	GLU	SER	GLY	ARG	LYS	LYS	ALA	VAL	GLU	GLY	ALA	ARG	VAL	LYS	GLN	VAL	GLY	LEU	GLY	ALA	GLY	LEU	GLY	GLY	THR	GLY	GLU	GLN	VAL	VAL	GLU	VAL	GLN	ALA	ALA	ALA	GLN	ASP	VAL	PRO
Met	Gly	Lys	Val	Lys	Lys	Ala	Val	Lys	Val	Thr	Ser	Gly	Arg	Lys	Lys	Ala	Val	Glu	Gly	Ala	Arg	Val	Lys	Gln	Val	Gly	Leu	Gly	Ala	Gly	Leu	Gly	Gly	Thr	Gly	Glu	Gln	Val	Val	Glu	Val	Gln	Ala	Ala	Ala	Gln	Asp	Val	Pro

[illegible]

GLU	LYS	GLU	GLU	VAL	SER	THR	GLU	ASP	ALA	GLU	ALA	GLN	THR	GLY	GLU	LEU	ALA	GLY	LEU	ALA	GLY	GLY	GLY	GLY	GLY	THR	GLY	GLU	ALA	GLN	MET	VAL	GLU	VAL	PRO	GLN	ALA	ALA	GLN	ILE	VAL	ASP	VAL	PRO		
884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930

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

[illegible]

[illegible]

- Molecule 3: Tail fiber protein

[illegible]

- Molecule 3: Tail fiber protein



LEU	GLY	LYS	PHE	MET
MET	LEU	ARG	GLY	ALA
TYR	ALA	PHE	GLN	ASP
GLN	GLY	LYS	LEU	VAL
VAL	ALA	ASN	LYS	ILE
ARG	ILE	THR	THR	ASP
ARG	ASP	ALA	ALA	GLY
GLU	LYS	GLY	ASN	GLN
TRP	VAL	GLN	GLN	THR
THR	ASP	TYR	ASN	THR
THR	GLY	ALA	SER	THR
ALA	ALA	THR	THR	ALA
ILE	ASN	SER	GLN	P23
GLY	VAL	ALA	ALA	P24
GLY	TYR	GLY	ARG	E25
GLY	TRP	ASN	ASN	Y26
ILE	LYS	SER	GLU	L27
GLN	GLY	ALA	ALA	I37
LEU	ASN	SER	LEU	I68
VAL	ILE	ALA	GLN	S59
VAL	HIS	ALA	PHE	LE0
GLY	ASN	HIS	ARG	LE0
GLY	GLN	GLN	ASN	I73
ILE	GLY	SER	GLU	E74
ILE	ARG	GLU	ALA	L75
TRP	LEU	VAL	THR	R76
THR	TYR	ASN	GLU	R77
GLN	MET	ALA	PHE	THR
GLY	THR	GLU	ARG	T81
GLY	THR	ASN	ASN	R95
ALA	ASN	SER	GLN	L99
MET	GLY	GLY	GLU	L99
THR	PHE	ASP	ALA	I104
GLN	CYS	SER	PHE	E111
LEU	GLY	ALA	LYS	D115
LYS	GLN	ASN	ASN	L116
LEU	TYR	SER	GLU	T117
LEU	GLN	ALA	SER	T120
GLN	GLN	THR	THR	I121
LEU	VAL	GLN	ASN	D130
LEU	THR	ALA	THR	R134
GLU	ASN	ASP	LYS	A140
SER	ARG	ARG	GLN	V143
ALA	TYR	ARG	GLN	ASP
SER	VAL	GLU	TRP	ASP
ASP	VAL	ARG	ARG	ASP
LYS	MET	GLU	GLU	ALA
LYS	GLU	ALA	THR	VAL
HIS	TRP	ASP	LYS	VAL
TYR	GLY	LYS	GLY	ASP
ILE	ASP	LEU	PHE	ARG
LEU	GLU	GLU	ARG	ASP
SER	ASN	ASN	ASP	ALA
LYS	GLY	TYR	GLU	VAL
TRP	TRP	ASN	ALA	TRP

[illegible]

- Molecule 3: Tail fiber protein

[illegible]

- Molecule 3: Tail fiber protein

[illegible]

PHE	PHE	THR	GLY	PRO	ASP	GLY	ASP	PHE	ILE	ALA	SER	GLY	TRP	LEU	ARG	GLN	HIS	SER	ASN	GLY	LEU	GLY	PHE	LYS	ASN	GLY	ALA	ASP	SER	VAL	PRO	ASN	ALA	ILE	VAL	GLU	ASN	GLU							
THR	THR	THR	LYS	GLY	GLY	LYS	TRP	LEU	ALA	TTR	LEU	ASP	PHE	VAL	ALA	LYS	LYS	ALA	TRP	THR	GLN	VAL	TRP	SER	GLY	LYS	GLY	VAL	VAL	SER	THR	VAL	SER	PHE	ARG	ASN	ILE	ILE	ILE	CYS	ALA	ASN	SER	TRP	ASP

- Molecule 3: Tail fiber protein

[illegible]

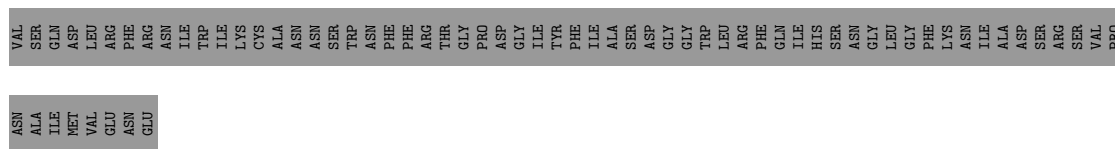
- Molecule 3: Tail fiber protein



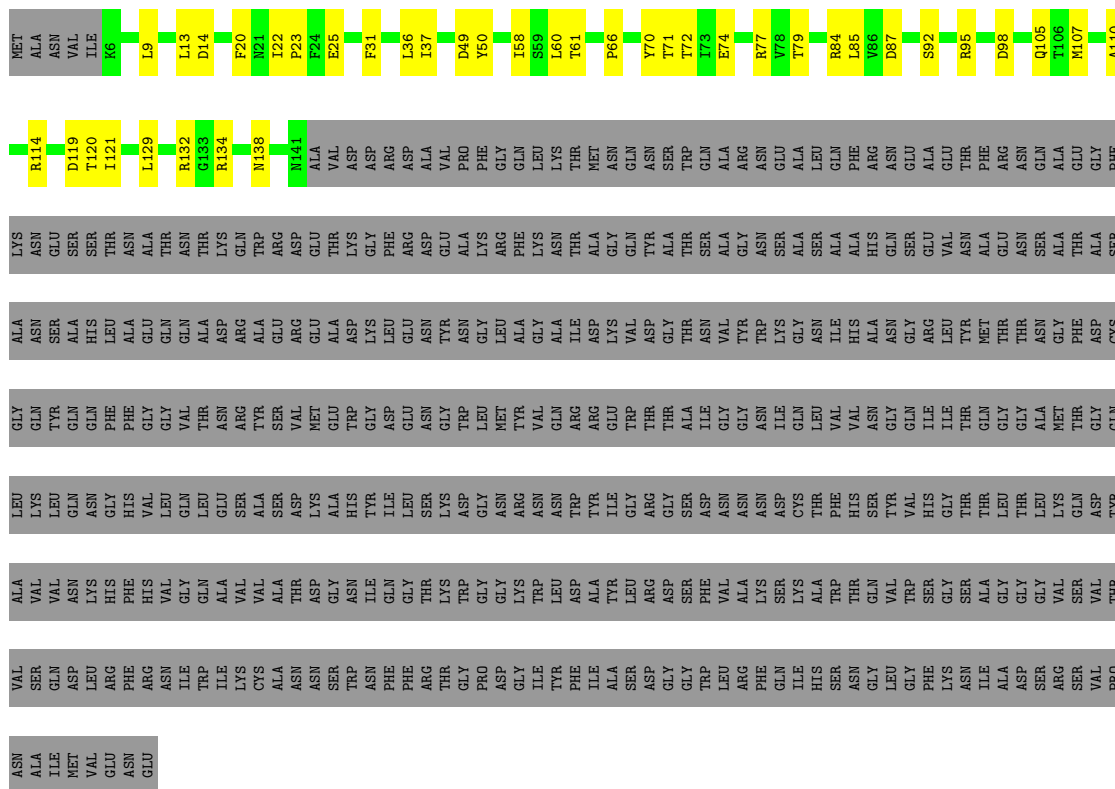
VAL	ALA	TYP	ALA	TRP	ALA	LEU	MET
THR	SER	SER	GLU	ARG	GLU	ASN	ALA
ASP	ASP	VAL	ASP	ASP	GLU	ASN	ALA
GLY	LYS	MET	ALA	THR	ALA	VAL	I5
ASN	HIS	TRP	ASP	LYS	LYS	ASP	V8
ILE	TYR	GLY	LEU	GLY	PHE	ARG	Q12
GLN	ILE	ASP	LEU	PHE	ARG		L13
THR	SER	GLU	GLU	ASP	ASP	ALA	L13
THR	SER	ASN	ASN	ASP	ASP	ALA	I22
TRP	LYS	GLY	TYR	GLU	VAL	VAL	L36
ASP	ASP	TRP	ASN	ALA	PRO	ALA	I37
GLY	GLY	LEU	GLY	LYS	PHE	PHE	R41
GLY	ASN	MET	LEU	ARG	GLY	GLY	L44
LYS	ARG	TYR	ALA	PHE	GLN	GLN	T45
TRP	VAL	VAL	GLY	LYS	LEU	LEU	I46
LEU	ASN	GLN	ALA	ASN	LYS	LYS	N47
ASP	TRP	ARG	ILE	THR	THR	THR	T48
SER	TRP	ARG	ASP	ALA	ASN	TRP	D49
PHE	ASP	ILE	ASN	SER	SER	GLN	Y50
VAL	ASN	GLY	VAL	ALA	ALA	ALA	A53
ALA	ASN	GLY	TRP	GLY	GLY	ARG	T54
LYS	ASN	ASN	TRP	ASN	ASN	GLU	T57
SER	ASP	ILE	LYS	SER	LYS	ASN	I58
LYS	CYS	GLN	GLY	ALA	ALA	ALA	S59
ALA	THR	LEU	ASN	SER	ALA	GLN	L60
THR	PHE	VAL	ILE	ALA	ILE	PHE	M64
GLN	HIS	VAL	ASN	HIS	ALA	ARG	T72
THR	SER	ASN	ALA	HIS	ALA	ARG	R76
VAL	TYR	GLY	ASN	GLN	ASN	ASN	T81
TRP	VAL	GLN	GLY	SER	GLY	GLU	R84
SER	HIS	ILE	ARG	SER	ASN	ASN	V101
GLY	GLY	ILE	ARG	GLU	GLN	GLN	L116
SER	THR	THR	LEU	VAL	GLY	ALA	T120
SER	THR	THR	THR	ASN	THR	GLY	I121
GLY	THR	GLN	ASP	ALA	ALA	GLY	N124
GLY	LEU	GLY	GLN	SER	CYS	PHE	H128
THR	ALA	LEU	GLY	ALA	GLY	LYS	L129
SER	VAL	LYS	GLN	ASN	THR	ASN	D130
GLP	ASN	GLN	GLN	ALA	GLU	ALA	W135
ASP	ASN	GLN	THR	SER	THR	THR	T136
LEU	LYS	ASN	THR	HIS	GLY	THR	T137
LEU	HIS	GLY	PHE	ALA	PHE	ASN	N124
ARG	PHE	VAL	GLY	GLU	GLY	ALA	H128
PHE	HIS	VAL	GLY	GLN	GLY	THR	L129
ARG	ASN	VAL	ILE	GLN	THR	ASN	D130
ILE	VAL	GLN	THR	ALA	THR	THR	W135
TRP	VAL	GLY	ASN	ASP	ASP	GLN	T136
ILE	ALA	THR	THR	THR	THR	THR	T137
THR	THR	THR	THR	THR	THR	THR	T138
THR	THR	THR	THR	THR	THR	THR	T139
THR	THR	THR	THR	THR	THR	THR	T140
THR	THR	THR	THR	THR	THR	THR	T141
THR	THR	THR	THR	THR	THR	THR	T142
THR	THR	THR	THR	THR	THR	THR	T143
THR	THR	THR	THR	THR	THR	THR	T144
THR	THR	THR	THR	THR	THR	THR	T145
THR	THR	THR	THR	THR	THR	THR	T146
THR	THR	THR	THR	THR	THR	THR	T147
THR	THR	THR	THR	THR	THR	THR	T148
THR	THR	THR	THR	THR	THR	THR	T149
THR	THR	THR	THR	THR	THR	THR	T150
THR	THR	THR	THR	THR	THR	THR	T151
THR	THR	THR	THR	THR	THR	THR	T152
THR	THR	THR	THR	THR	THR	THR	T153
THR	THR	THR	THR	THR	THR	THR	T154
THR	THR	THR	THR	THR	THR	THR	T155
THR	THR	THR	THR	THR	THR	THR	T156
THR	THR	THR	THR	THR	THR	THR	T157
THR	THR	THR	THR	THR	THR	THR	T158
THR	THR	THR	THR	THR	THR	THR	T159
THR	THR	THR	THR	THR	THR	THR	T160
THR	THR	THR	THR	THR	THR	THR	T161
THR	THR	THR	THR	THR	THR	THR	T162
THR	THR	THR	THR	THR	THR	THR	T163
THR	THR	THR	THR	THR	THR	THR	T164
THR	THR	THR	THR	THR	THR	THR	T165
THR	THR	THR	THR	THR	THR	THR	T166
THR	THR	THR	THR	THR	THR	THR	T167
THR	THR	THR	THR	THR	THR	THR	T168
THR	THR	THR	THR	THR	THR	THR	T169
THR	THR	THR	THR	THR	THR	THR	T170
THR	THR	THR	THR	THR	THR	THR	T171
THR	THR	THR	THR	THR	THR	THR	T172
THR	THR	THR	THR	THR	THR	THR	T173
THR	THR	THR	THR	THR	THR	THR	T174
THR	THR	THR	THR	THR	THR	THR	T175
THR	THR	THR	THR	THR	THR	THR	T176
THR	THR	THR	THR	THR	THR	THR	T177
THR	THR	THR	THR	THR	THR	THR	T178
THR	THR	THR	THR	THR	THR	THR	T179
THR	THR	THR	THR	THR	THR	THR	T180
THR	THR	THR	THR	THR	THR	THR	T181
THR	THR	THR	THR	THR	THR	THR	T182
THR	THR	THR	THR	THR	THR	THR	T183
THR	THR	THR	THR	THR	THR	THR	T184
THR	THR	THR	THR	THR	THR	THR	T185
THR	THR	THR	THR	THR	THR	THR	T186
THR	THR	THR	THR	THR	THR	THR	T187
THR	THR	THR	THR	THR	THR	THR	T188
THR	THR	THR	THR	THR	THR	THR	T189
THR	THR	THR	THR	THR	THR	THR	T190
THR	THR	THR	THR	THR	THR	THR	T191
THR	THR	THR	THR	THR	THR	THR	T192
THR	THR	THR	THR	THR	THR	THR	T193
THR	THR	THR	THR	THR	THR	THR	T194
THR	THR	THR	THR	THR	THR	THR	T195
THR	THR	THR	THR	THR	THR	THR	T196
THR	THR	THR	THR	THR	THR	THR	T197
THR	THR	THR	THR	THR	THR	THR	T198
THR	THR	THR	THR	THR	THR	THR	T199
THR	THR	THR	THR	THR	THR	THR	T200

- Molecule 3: Tail fiber protein

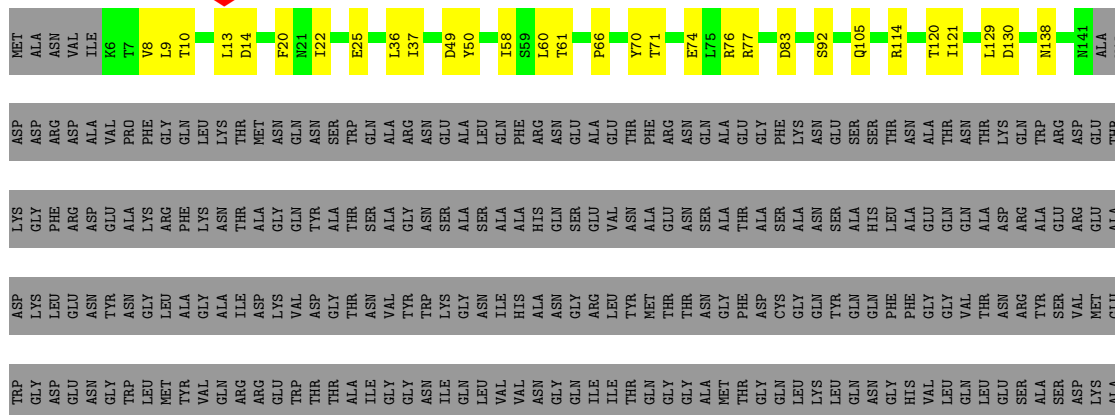
ALA	LEU	GLY	ALA	LYS	ALA10	MET
VAL	LYS	GLN	ASN	ASN	R114	ALA
VAL	LEU	TYR	SER	GLU	SER	ASN
ASN	GLN	GLN	ALA	SER	N124	VAL
LYS	ASN	PHE	LEU	SER		ILE
HIS	GLY			THR		R6
PHE	HIS	PHE	GLU	ASN	L129	T7
HIS	VAL	GLY	ALA	ALA	D130	V8
VAL	LEU	GLY	GLN	THR	R131	L9
GLY	GLN	VAL	GLN	ASN	R132	
GLN	LEU	THR	ALA	THR	G133	L13
ALA	GLU	ASN	ASP	LYS	R134	D14
VAL	SER	ARG	ARG	GLN		
VAL	ALA	TYR	ALA	TRP	N138	
VAL	SER	SER	GLU	ARG		W21
THR	ASP	VAL	ARG	ASP	R141	F20
ASP	LYS	MET	GLU	GLU	ALA	I22
GLY	ALA	GLU	ALA	THR	VAL	P23
ASN	HIS	TRP	ASP	LYS	ASP	F24
ILE	TYR	GLY	LYS	GLY		
GLN	ILE	ASP	LEU	PHE	F31	V32
GLY	LEU	GLU	GLU	ARG	ASP	
THR	SER	ASN	ASN	ASP	ALA	L36
LYS	LYS	GLY	TYR	GLU	VAL	I37
ASP	ASP	TRP	ASN	GLU	PRO	
GLY	ASN	LEU	GLY	LYS	PHE	L44
GLY	ASN	MET	GLY	ARG	GLY	
ARG	ARG	VAL	ALA	PHE	GLN	D49
TRP	ASN	VAL	GLY	LYS	LEU	Y50
LEU	ASN	GLN	ALA	ASN	LYS	
ASP	TRP	ARG	ILE	THR	THR	T56
ALA	TYR	ARG	ASP	ALA	MET	
ILE	ILE	GLU	LYS	GLY	ASN	L60
LEU	TRP	TRP	VAL	GLN	GLN	T61
ARG	ARG	THR	ASP	TYR	ASN	
ASP	GLY	THR	GLY	ALA	SER	P66
SER	SER	ALA	THR	THR	TRP	
PHE	ASP	ILE	ASN	SER	GLN	Y70
VAL	ASN	GLY	VAL	ALA	ALA	T71
ASN	ASN	ASN	GLY	TYR	ARG	
LYS	ASN	ASN	TRP	ASN	ASN	
SER	ASP	ILE	LYS	SER	GLU	E74
LYS	CYS	GLN	GLY	ALA	ALA	L75
ALA	THR	LEU	ASN	SER	LEU	R76
TRP	PHE	VAL	ILE	ALA	GLN	
THR	HIS	VAL	HIS	ALA	PHE	T79
SER	SER	ASN	ALA	HIS	ARG	
GLN	VAL	GLY	ASN	GLN	ASN	R84
TRP	TYR	GLN	GLY	SER	GLU	D87
VAL	VAL	ILE	ARG	GLU	ALA	
SER	HIS	ILE	LEU	VAL	GLU	S92
GLY	GLY	THR	TYR	ASN	THR	
THR	THR	GLN	MET	ALA	PHE	R95
LEU	LEU	GLY	THR	GLU	ARG	
THR	THR	GLY	THR	ASN	ASN	D98
GLY	GLY	ALA	ASN	SER	GLN	
GLY	LEU	MET	GLY	ALA	GLU	Q105
VAL	LYS	THR	PHE	THR	GLU	T106
SER	SER	THR	PHE	THR	GLY	M107
VAL	THR	GLN	ASP	SER	PHE	
PHE	ASP	GLY	CYS	ALA	THR	
VAL	TYR	GLN		SER	DHF	



- Molecule 3: Tail fiber protein



- Molecule 3: Tail fiber protein



[illegible]

- Molecule 3: Tail fiber protein

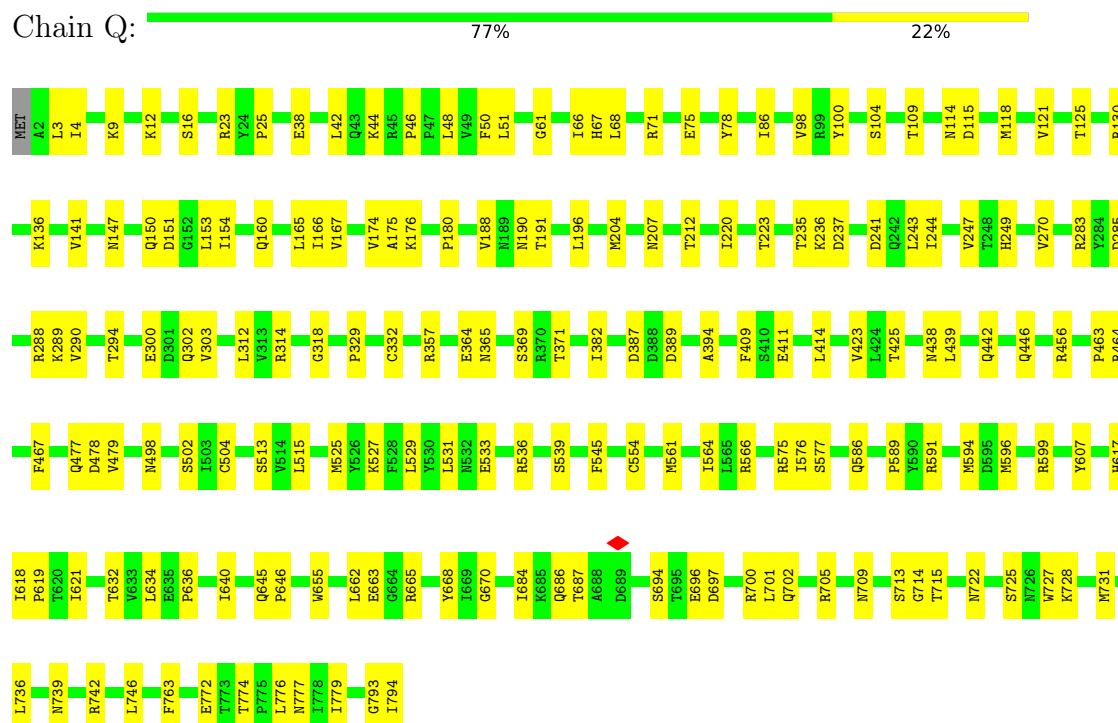


Tyr	Leu	Asn	Gln	Ala	Asn	Lys	Met
Phe	Asp	Trp	Arg	Ile	Thr	Thr	Ala
Ile	Ala	Tyr	Arg	Tyr	Ala	Met	N3
Ala	Leu	Ile	Glu	Lys	Gln	Asn	V4
Ser	Leu	Gly	Trp	Val	Gln	Gln	
Asp	Arg	Arg	Thr	Asp	Tyr	Asn	V8
Gly	Asp	Gly	Thr	Gly	Ala	Ser	L9
Gly	Ser	Ser	Ala	Thr	Thr	Trp	T10
Trp	Phe	Asp	Ile	Gly	Ser	Gln	
Leu	Val	Asn	Gly	Val	Ala	Ala	L13
Arg	Ala	Asn	Asn	Tyr	Gly	Arg	
Phe	Lys	Asn	Gly	Trp	Gly	Asn	I22
Gln	Ser	Asp	Ile	Lys	Ser	Asn	P23
Ile	Lys	Cys	Gln	Gly	Ser	Glu	F24
His	Ala	Thr	Leu	Asn	Ala	Ala	E25
Ser	Ala	Phe	Val	Ile	Ala	Gln	
Asn	Trp	His	Val	His	Ala	Phe	L36
Asn	Gln	Ser	Asn	Ala	His	Arg	
Gly	Gln	Tyr	Gly	Ala	Gln	Asn	R85
Leu	Val	Trp	Gln	Gly	Ser	Glu	
Gly	Trp	Val	Gln	Arg	Ser	Glu	I58
Phe	Ser	His	Ile	Arg	Glu	Ala	S89
Lys	Gly	Gly	Ile	Arg	Val	Ala	L60
Asn	Ser	Ser	Thr	Tyr	Asn	Thr	
Ile	Ala	Thr	Gln	Met	Ala	Phe	I73
Ala	Gly	Leu	Gly	Gly	Glu	Arg	
Asp	Gly	Thr	Gly	Thr	Asn	Asn	R76
Ser	Gly	Leu	Ala	Gly	Ser	Gln	R77
Arg	Val	Lys	Met	Phe	Ala	Ala	
Ser	Ser	Gln	Thr	Gly	Thr	Glu	L94
Val	Val	Asp	Gly	Asp	Ala	Gly	
Pro	Thr	Tyr	Gln	Cys	Ser	Phe	L99
Asn	Val	Ala	Leu	Gly	Ser	Lys	
Ala	Ser	Val	Lys	Gln	Asn	Asn	
Ile	Gln	Val	Lys	Gln	Ser	Glu	T106
Met	Asp	Asn	Gln	Gln	Ala	Ser	M107
Val	Leu	Lys	Asn	Gln	His	Ser	
Glu	Arg	His	Gly	Phe	Leu	Thr	E111
Asn	Phe	Phe	His	Phe	Asn	Asn	
Glu	Arg	His	Val	Gly	Glu	Ala	T117
Asn	Asn	Val	Leu	Gly	Gln	Thr	T118
	Ile	Gly	Gln	Val	Gln	Asn	D119
Trp	Trp	Gln	Leu	Thr	Ala	Thr	T120
Ile	Ile	Ala	Glu	Asn	Arg	Lys	
	Lys	Val	Ser	Tyr	Asp	Gln	L129
	Cys	Val	Ser	Trp	Ala	Trp	D130
Ala	Ala	Ala	Ser	Ser	Glu	Arg	
Asn	Asn	Thr	Asp	Val	Arg	Asp	
Asn	Asn	Asp	Lys	Met	Glu	Glu	A140
Ser	Ser	Gly	Ala	Glu	Ala	Thr	
Trp	Trp	Asn	His	Thr	Asp	Lys	V143
Asn	Ile	Asn	Tyr	Trp	Lys	Gly	Asp
Asn	Gln	Gln	Ile	Asp	Leu	Phe	Arg
Phe	Phe	Gly	Leu	Glu	Glu	Arg	Asp
Arg	Arg	Thr	Ser	Asn	Asn	Asp	Ala
Thr	Thr	Lys	Lys	Trp	Tyr	Glu	Val
Gly	Gly	Trp	Asp	Gly	Asn	Ala	Pro
Pro	Pro	Gly	Gly	Leu	Gly	Lys	Phe
Asp	Asp	Gly	Asn	Met	Leu	Arg	Gly
Gly	Gly	Lys	Arg	Tyr	Ala	Phe	Gln
Ile	Thr	Trp	Asn	Val	Gly	Lys	Gln

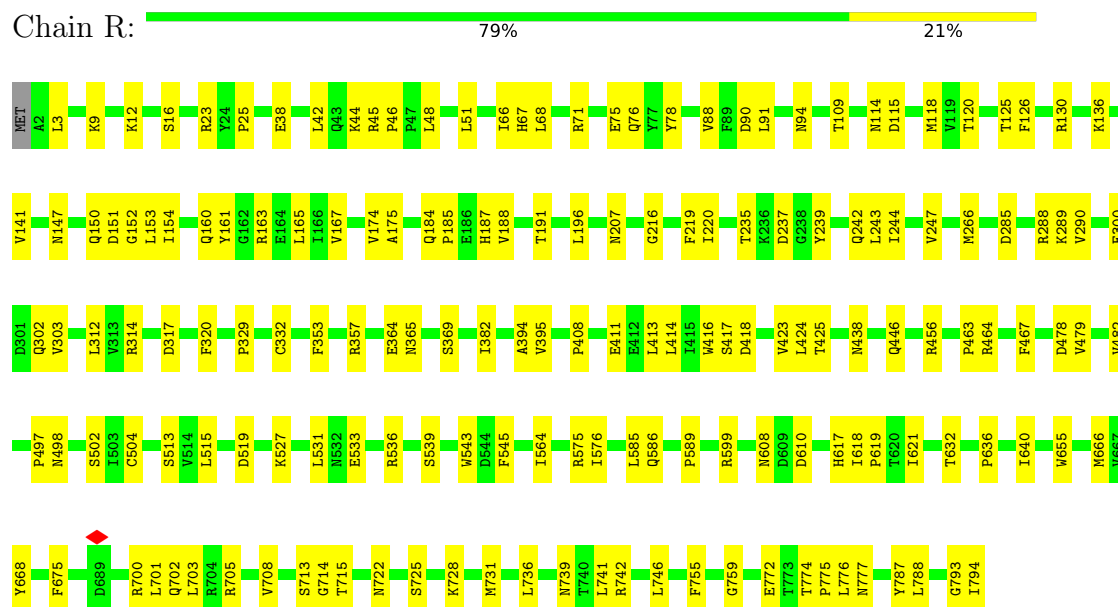
- Molecule 3: Tail fiber protein

[illegible]

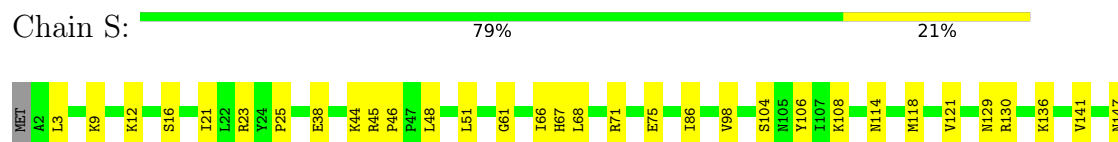
- Molecule 4: Tail tubular protein gp12

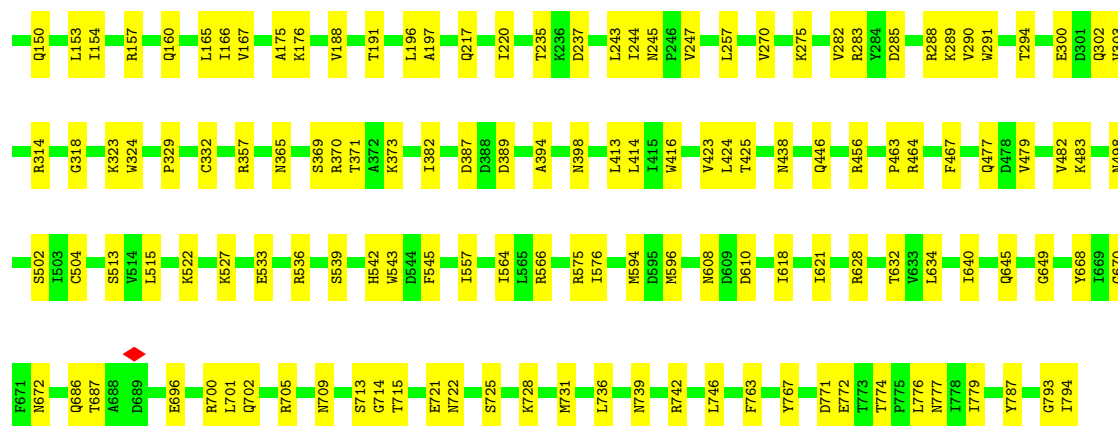


- Molecule 4: Tail tubular protein gp12



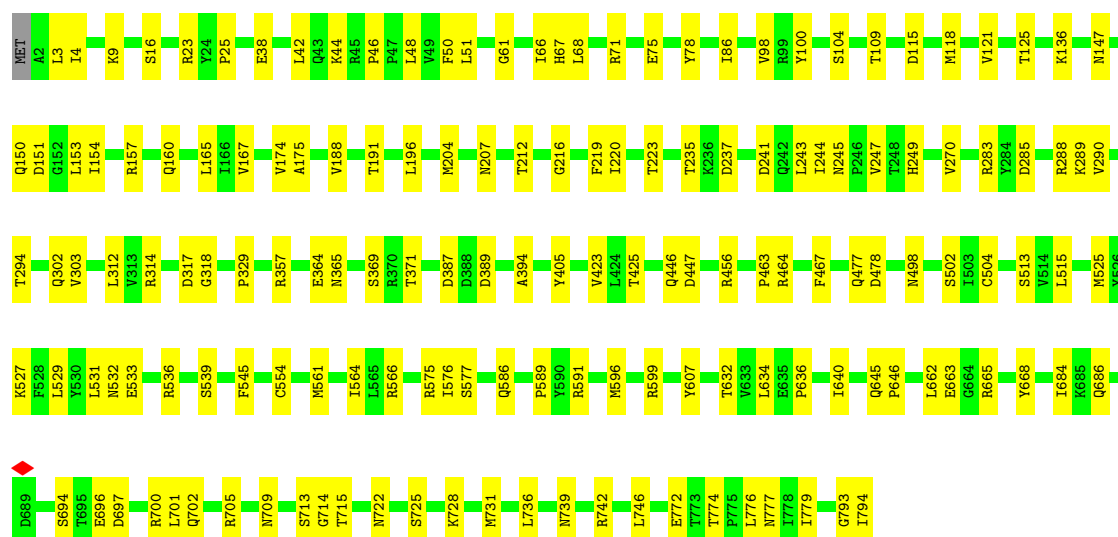
- Molecule 4: Tail tubular protein gp12





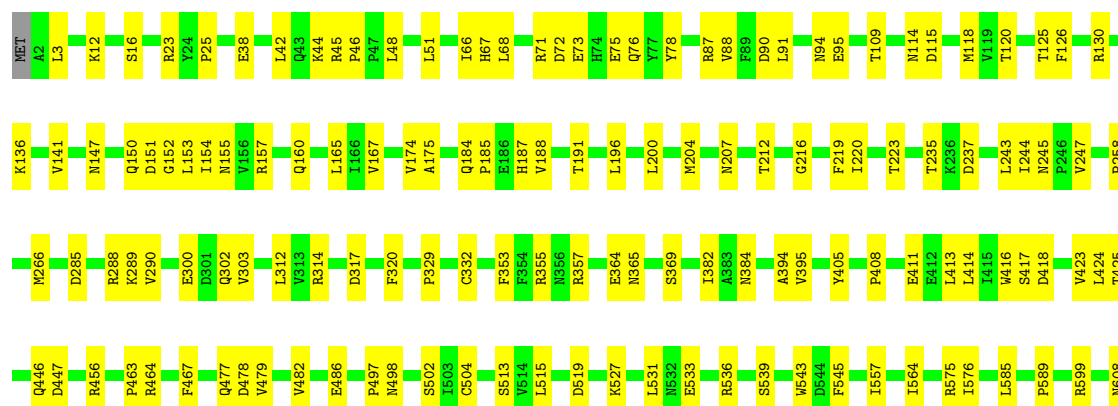
• Molecule 4: Tail tubular protein gp12

Chain T: 80% 20%



• Molecule 4: Tail tubular protein gp12

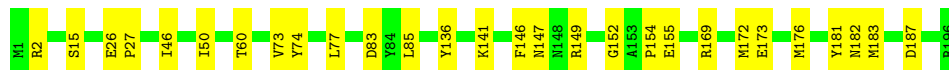
Chain x: 78% 22%





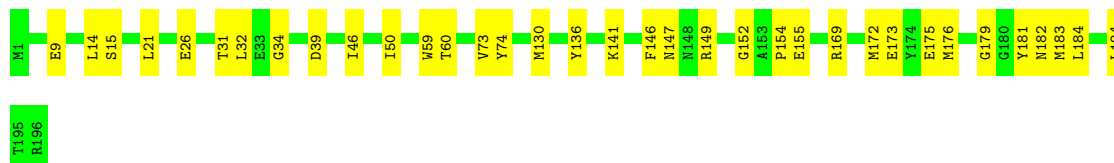
- Molecule 5: Tail tubular protein gp11

Chain U: 86% 14%



- Molecule 5: Tail tubular protein gp11

Chain V: 82% 18%



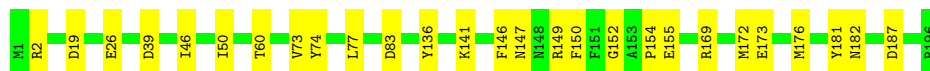
- Molecule 5: Tail tubular protein gp11

Chain W: 85% 15%



- Molecule 5: Tail tubular protein gp11

Chain X: 86% 14%



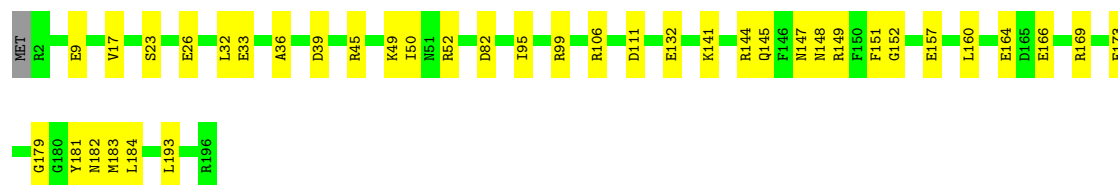
- Molecule 5: Tail tubular protein gp11

Chain Y: 88% 12%



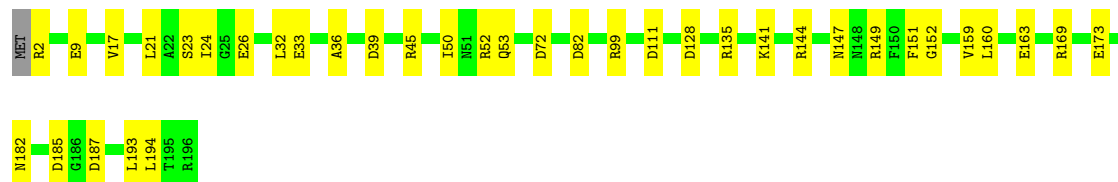
- Molecule 5: Tail tubular protein gp11

Chain Z: 80% 19%



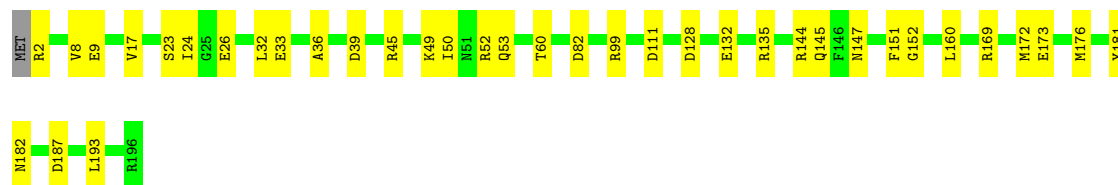
- Molecule 5: Tail tubular protein gp11

Chain d: 81% 19% .



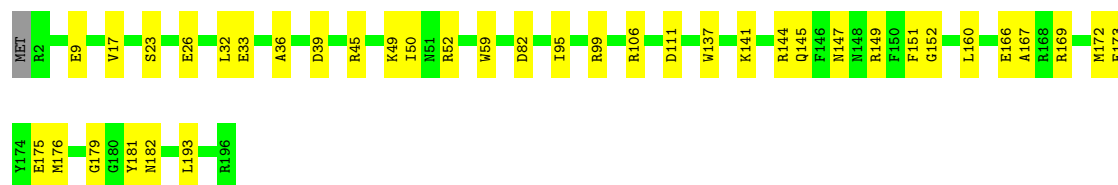
- Molecule 5: Tail tubular protein gp11

Chain e: 81% 19% .



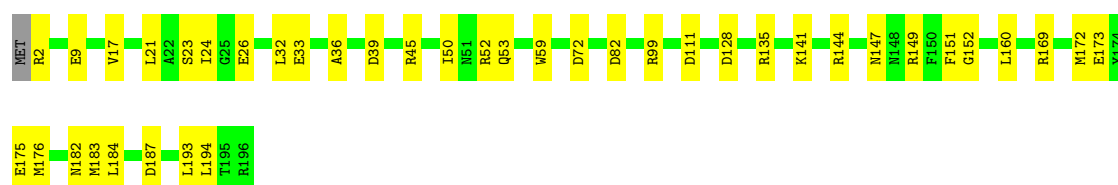
- Molecule 5: Tail tubular protein gp11

Chain f: 80% 19% .



- Molecule 5: Tail tubular protein gp11

Chain g: 79% 20% .



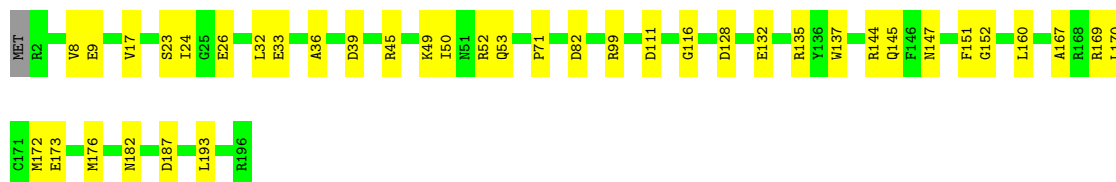
- Molecule 5: Tail tubular protein gp11

Chain h: 85% 15% .



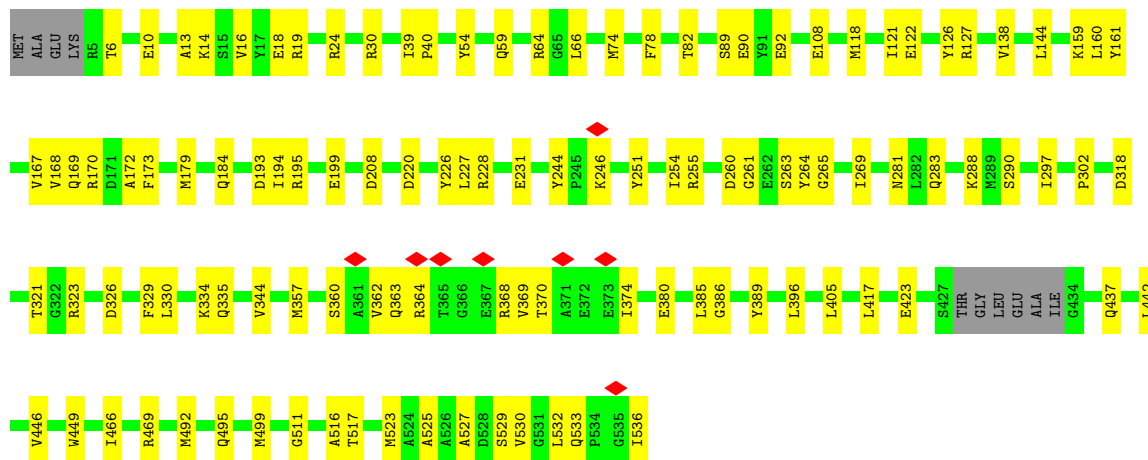
• Molecule 5: Tail tubular protein gp11

Chain i: 80% 20%



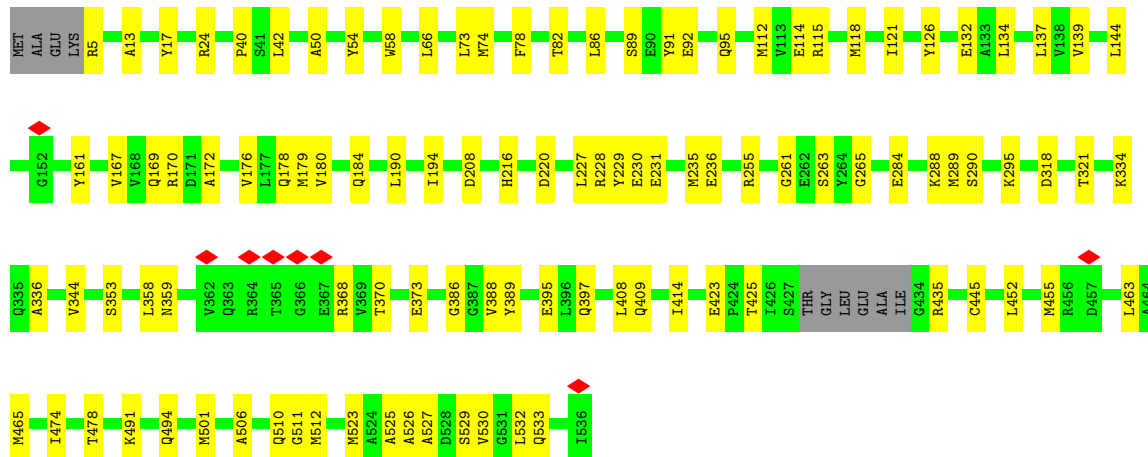
• Molecule 6: Portal protein

Chain j: 77% 21%

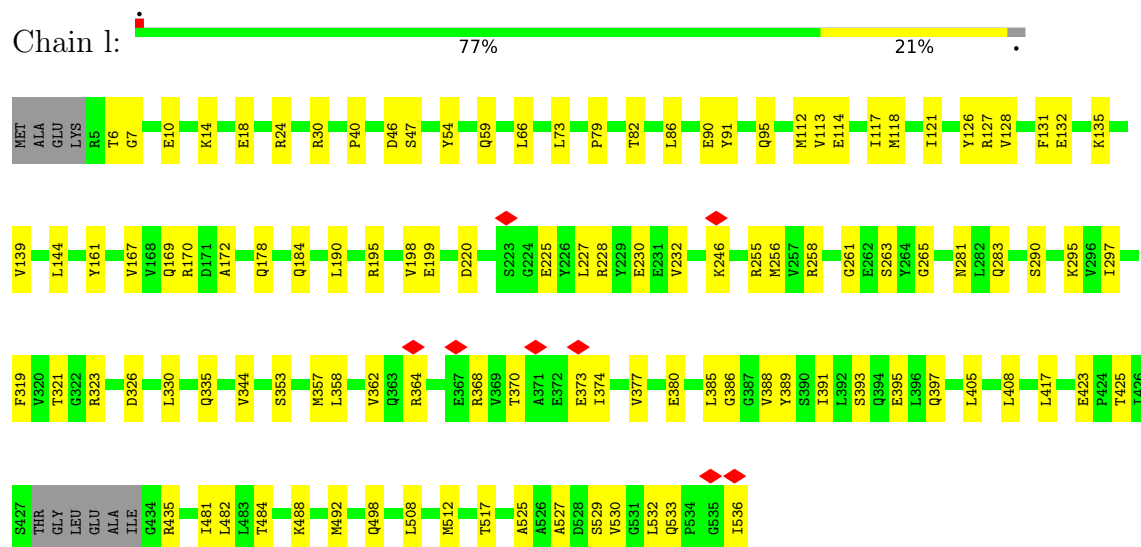


• Molecule 6: Portal protein

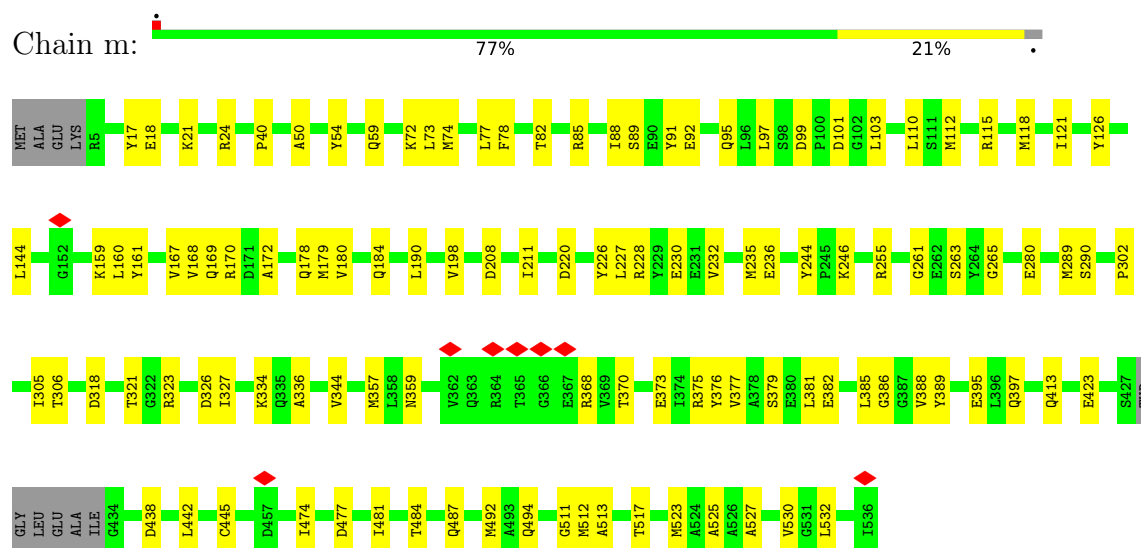
Chain k: 79% 20%



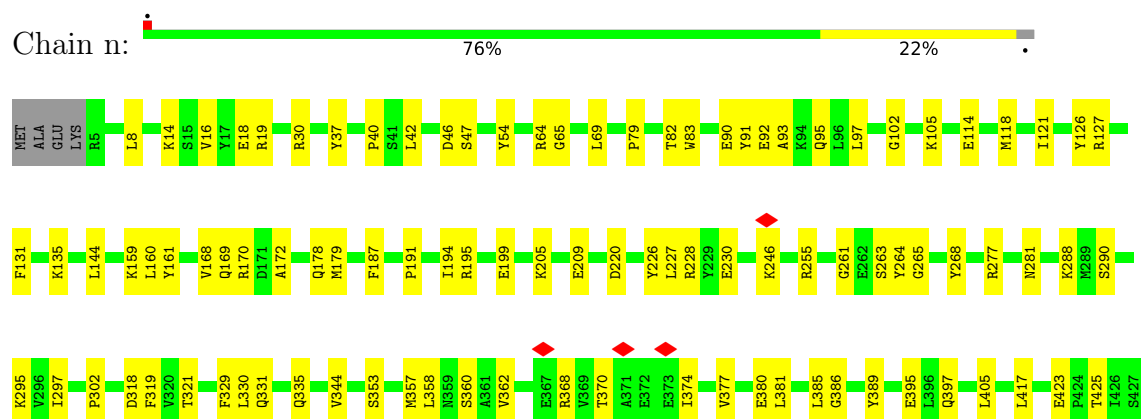
• Molecule 6: Portal protein



• Molecule 6: Portal protein



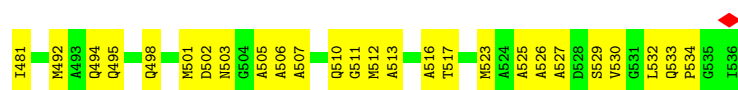
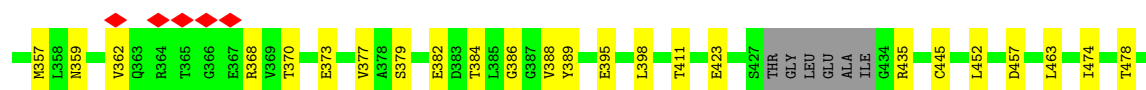
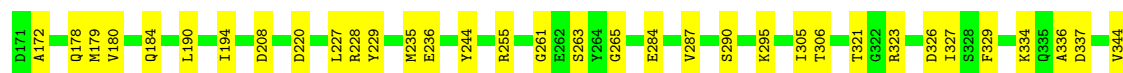
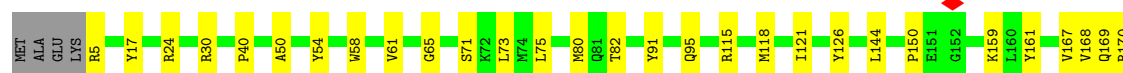
• Molecule 6: Portal protein





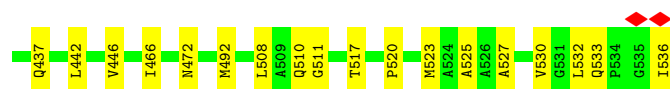
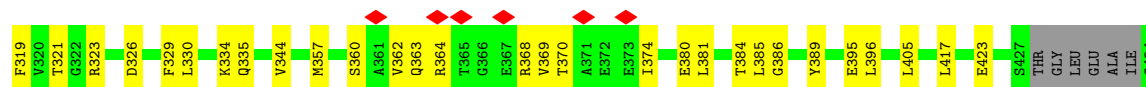
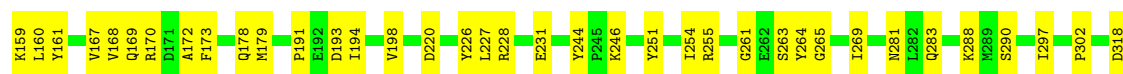
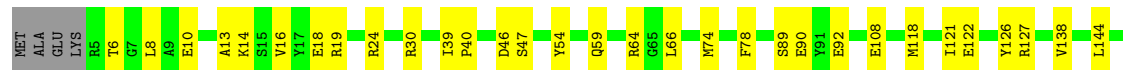
• Molecule 6: Portal protein

Chain o: 77% 21%



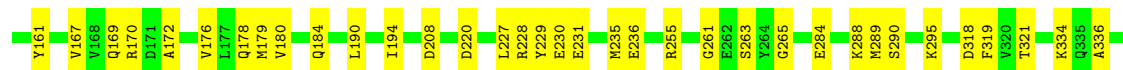
• Molecule 6: Portal protein

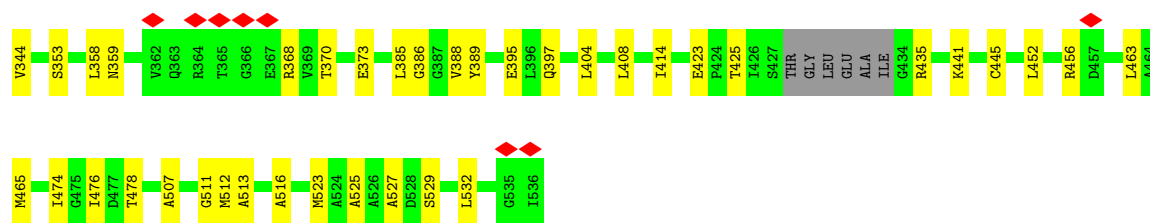
Chain p: 77% 21%



• Molecule 6: Portal protein

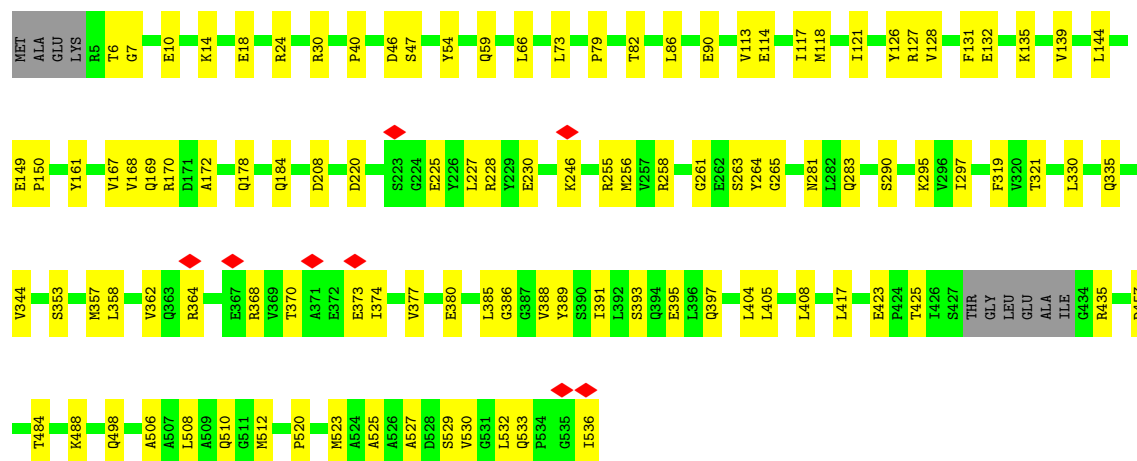
Chain q: 79% 19%





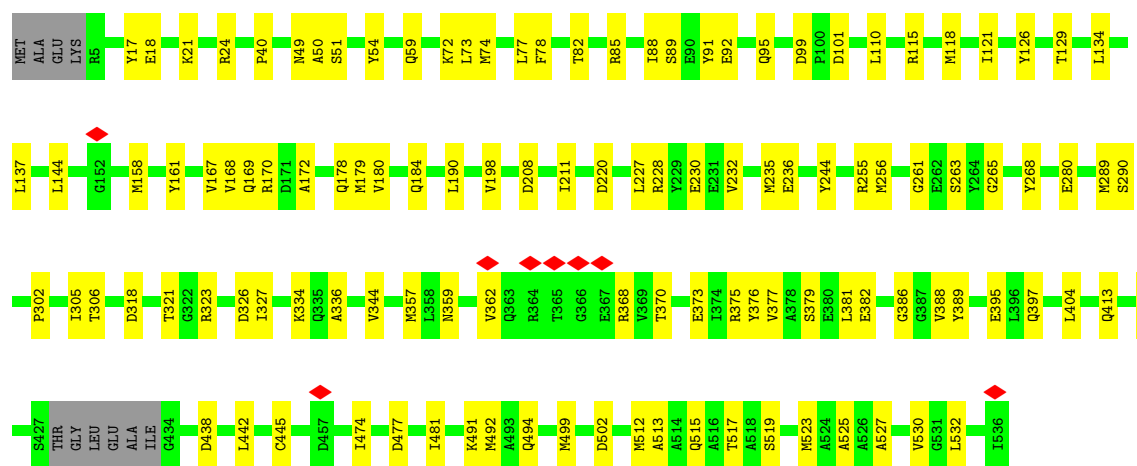
• Molecule 6: Portal protein

Chain r: 78% 20%



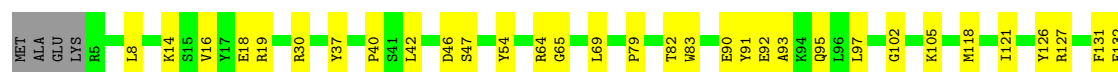
• Molecule 6: Portal protein

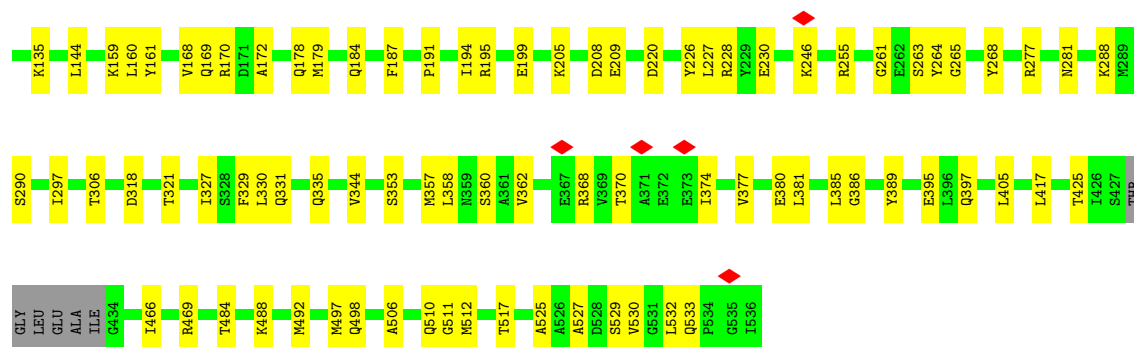
Chain s: 76% 22%



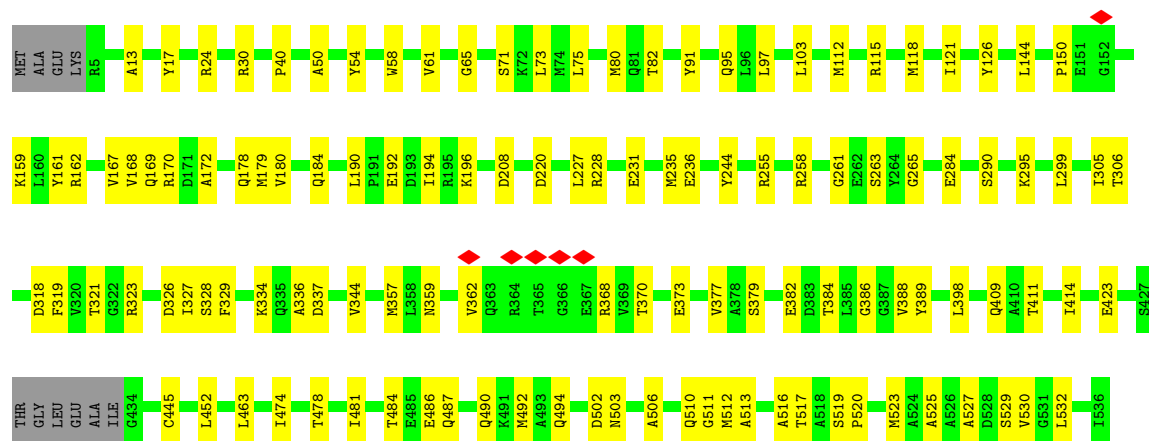
• Molecule 6: Portal protein

Chain t: 77% 21%





• Molecule 6: Portal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65620	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	57.231	Depositor
Minimum map value	-33.541	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	2.152	Depositor
Recommended contour level	2	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0	0.61	0/112	1.38	2/149 (1.3%)
1	3	0.55	0/112	1.44	2/149 (1.3%)
1	4	0.60	0/112	1.40	3/149 (2.0%)
1	5	0.55	0/112	1.45	3/149 (2.0%)
1	6	0.63	0/112	1.40	4/149 (2.7%)
1	7	0.55	0/112	1.54	2/149 (1.3%)
1	8	0.58	0/112	1.41	5/149 (3.4%)
1	9	0.23	0/112	0.63	0/149
1	AA	0.53	0/112	1.47	4/149 (2.7%)
1	AB	0.63	0/112	1.39	4/149 (2.7%)
1	AC	0.52	0/112	1.50	4/149 (2.7%)
1	AD	0.58	0/112	1.32	3/149 (2.0%)
2	1	0.12	0/100	0.30	0/130
2	2	0.13	0/100	0.31	0/130
2	v	0.13	0/100	0.32	0/130
2	w	0.12	0/100	0.30	0/130
2	y	0.13	0/100	0.32	0/130
2	z	0.14	0/100	0.32	0/130
3	A	0.13	0/1130	0.30	0/1538
3	B	0.13	0/1130	0.28	0/1538
3	C	0.13	0/1130	0.28	0/1538
3	D	0.13	0/1130	0.30	0/1538
3	E	0.13	0/1130	0.30	0/1538
3	F	0.12	0/1082	0.30	0/1471
3	G	0.13	0/1082	0.31	0/1471
3	H	0.13	0/1082	0.30	0/1471
3	I	0.13	0/1082	0.32	0/1471
3	J	0.12	0/1082	0.29	0/1471
3	K	0.14	0/1095	0.38	0/1489
3	L	0.14	0/1095	0.38	0/1489
3	M	0.13	0/1095	0.37	0/1489
3	N	0.14	0/1095	0.37	0/1489
3	O	0.13	0/1095	0.38	0/1489
3	a	0.14	0/1130	0.30	0/1538

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	b	0.13	0/1082	0.32	0/1471
3	c	0.14	0/1095	0.37	0/1489
4	P	0.16	0/6473	0.31	0/8804
4	Q	0.15	0/6473	0.31	0/8804
4	R	0.15	0/6473	0.32	0/8804
4	S	0.16	0/6473	0.32	0/8804
4	T	0.15	0/6473	0.31	0/8804
4	x	0.15	0/6473	0.32	0/8804
5	U	0.16	0/1592	0.31	0/2153
5	V	0.17	0/1592	0.30	0/2153
5	W	0.15	0/1592	0.29	0/2153
5	X	0.15	0/1592	0.30	0/2153
5	Y	0.17	0/1592	0.32	0/2153
5	Z	0.17	0/1584	0.32	0/2143
5	d	0.16	0/1584	0.33	0/2143
5	e	0.16	0/1584	0.33	0/2143
5	f	0.16	0/1584	0.31	0/2143
5	g	0.16	0/1584	0.32	0/2143
5	h	0.15	0/1592	0.28	0/2153
5	i	0.16	0/1584	0.34	0/2143
6	j	0.14	0/4131	0.32	0/5590
6	k	0.14	0/4131	0.31	0/5590
6	l	0.14	0/4131	0.31	0/5590
6	m	0.15	0/4131	0.31	0/5590
6	n	0.15	0/4131	0.33	0/5590
6	o	0.14	0/4131	0.31	0/5590
6	p	0.14	0/4131	0.32	0/5590
6	q	0.14	0/4131	0.31	0/5590
6	r	0.14	0/4131	0.32	0/5590
6	s	0.15	0/4131	0.32	0/5590
6	t	0.15	0/4131	0.33	0/5590
6	u	0.16	0/4131	0.32	0/5590
All	All	0.16	0/129252	0.34	36/175236 (0.0%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AC	14	THR	N-CA-C	8.22	120.25	111.28
1	7	14	THR	N-CA-C	7.26	119.19	111.28
1	AD	10	PRO	N-CA-C	7.16	123.71	113.47
1	4	5	PRO	N-CA-C	6.67	122.33	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	5	PRO	N-CA-C	6.64	122.75	113.53
1	0	5	PRO	N-CA-C	6.41	121.99	113.40
1	3	9	THR	N-CA-C	6.35	123.84	109.81
1	3	5	PRO	N-CA-C	6.34	121.89	113.40
1	AA	9	THR	N-CA-C	6.32	123.77	109.81
1	6	5	PRO	N-CA-C	6.31	121.85	113.40
1	AA	5	PRO	N-CA-C	6.22	122.17	113.53
1	5	9	THR	N-CA-C	6.09	123.27	109.81
1	AD	9	THR	N-CA-C	6.06	123.20	109.81
1	8	12	MET	N-CA-C	6.03	118.97	110.23
1	AB	9	THR	N-CA-C	6.02	123.11	109.81
1	6	9	THR	N-CA-C	5.99	123.05	109.81
1	AC	9	THR	N-CA-C	5.94	122.95	109.81
1	0	9	THR	N-CA-C	5.93	122.92	109.81
1	8	5	PRO	N-CA-C	5.86	121.68	113.53
1	AB	5	PRO	N-CA-C	5.86	121.67	113.53
1	AC	10	PRO	N-CA-C	5.86	121.67	113.53
1	5	10	PRO	N-CA-C	5.83	121.81	113.47
1	AC	12	MET	N-CA-C	5.78	118.64	110.50
1	4	9	THR	N-CA-C	5.70	122.40	109.81
1	7	9	THR	N-CA-C	5.60	122.20	109.81
1	6	10	PRO	N-CA-C	5.60	121.31	113.53
1	8	10	PRO	N-CA-C	5.58	121.29	113.53
1	4	10	PRO	N-CA-C	5.49	121.32	113.47
1	8	9	THR	N-CA-C	5.44	121.83	109.81
1	AB	12	MET	N-CA-C	5.43	118.11	110.23
1	AA	14	THR	N-CA-C	5.39	117.16	111.28
1	AD	12	MET	N-CA-C	5.36	117.64	110.35
1	8	6	LYS	N-CA-C	5.35	117.59	110.53
1	AB	10	PRO	N-CA-C	5.33	121.10	113.47
1	AA	12	MET	N-CA-C	5.14	117.75	110.50
1	6	12	MET	N-CA-C	5.03	117.52	110.23

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	0	110	0	115	13	0
1	3	110	0	115	11	0
1	4	110	0	115	17	0
1	5	110	0	115	10	0
1	6	110	0	115	11	0
1	7	110	0	115	12	0
1	8	110	0	115	11	0
1	9	110	0	115	13	0
1	AA	110	0	115	11	0
1	AB	110	0	115	12	0
1	AC	110	0	115	14	0
1	AD	110	0	115	11	0
2	1	101	0	109	5	0
2	2	101	0	109	5	0
2	v	101	0	109	4	0
2	w	101	0	109	5	0
2	y	101	0	109	6	0
2	z	101	0	109	5	0
3	A	1115	0	1122	26	0
3	B	1115	0	1122	21	0
3	C	1115	0	1122	21	0
3	D	1115	0	1122	25	0
3	E	1115	0	1122	25	0
3	F	1067	0	1071	20	0
3	G	1067	0	1071	21	0
3	H	1067	0	1071	18	0
3	I	1067	0	1071	23	0
3	J	1067	0	1071	19	0
3	K	1080	0	1082	24	0
3	L	1080	0	1082	24	0
3	M	1080	0	1082	26	0
3	N	1080	0	1082	23	0
3	O	1080	0	1082	19	0
3	a	1115	0	1122	22	0
3	b	1067	0	1071	22	0
3	c	1080	0	1082	19	0
4	P	6313	0	6075	114	0
4	Q	6313	0	6075	122	0
4	R	6313	0	6075	111	0
4	S	6313	0	6075	108	0
4	T	6313	0	6075	110	0
4	x	6313	0	6075	119	0
5	U	1565	0	1485	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	1565	0	1485	28	0
5	W	1565	0	1485	26	0
5	X	1565	0	1485	25	0
5	Y	1565	0	1485	22	0
5	Z	1557	0	1473	33	0
5	d	1557	0	1473	28	0
5	e	1557	0	1473	29	0
5	f	1557	0	1473	31	0
5	g	1557	0	1473	31	0
5	h	1565	0	1485	25	0
5	i	1557	0	1473	30	0
6	j	4070	0	4060	80	0
6	k	4070	0	4060	76	0
6	l	4070	0	4060	84	0
6	m	4070	0	4060	85	0
6	n	4070	0	4060	95	0
6	o	4070	0	4060	83	0
6	p	4070	0	4060	84	0
6	q	4070	0	4060	73	0
6	r	4070	0	4060	81	0
6	s	4070	0	4060	89	0
6	t	4070	0	4060	91	0
6	u	4070	0	4060	87	0
All	All	126948	0	124602	2088	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 (2088) 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)
1:0:7:ILE:HA	6:n:530:VAL:HG21	1.39	1.01
1:4:7:ILE:HA	6:t:530:VAL:HG21	1.45	0.99
1:6:7:ILE:HA	6:r:530:VAL:HG21	1.46	0.97
1:AB:7:ILE:HA	6:l:530:VAL:HG21	1.49	0.93
1:AD:7:ILE:HA	6:j:530:VAL:HG21	1.51	0.90
1:5:5:PRO:HB2	6:s:512:MET:HE3	1.55	0.89
1:4:5:PRO:HG3	6:s:523:MET:HE1	1.52	0.88
1:AA:12:MET:HB2	6:m:532:LEU:HD12	1.55	0.88
1:AC:12:MET:HB2	6:k:532:LEU:HD12	1.56	0.88
1:AA:5:PRO:HB2	6:m:512:MET:HE3	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:7:ILE:HA	6:p:530:VAL:HG21	1.57	0.85
1:7:12:MET:HB2	6:q:532:LEU:HD12	1.57	0.84
5:f:173:GLU:HA	6:k:321:THR:HG21	1.61	0.82
6:j:82:THR:HA	6:j:118:MET:HE2	1.60	0.81
5:g:173:GLU:HA	6:u:321:THR:HG21	1.62	0.80
5:Z:173:GLU:HA	6:q:321:THR:HG21	1.63	0.80
4:x:504:CYS:HG	4:x:513:SER:HG	1.26	0.80
4:R:120:THR:HG23	4:R:125:THR:HG22	1.63	0.79
4:R:456:ARG:HH12	4:R:533:GLU:HG3	1.47	0.79
5:d:173:GLU:HA	6:o:321:THR:HG21	1.63	0.79
4:x:456:ARG:HH12	4:x:533:GLU:HG3	1.47	0.79
3:L:14:ASP:HA	3:L:66:PRO:HD2	1.65	0.78
4:S:645:GLN:HE21	4:S:649:GLY:HA2	1.47	0.78
6:l:357:MET:HE1	6:l:385:LEU:HD12	1.65	0.78
4:x:120:THR:HG23	4:x:125:THR:HG22	1.65	0.78
1:3:5:PRO:HB2	6:u:512:MET:HE3	1.66	0.77
1:AA:11:LYS:HD3	6:n:529:SER:HB3	1.65	0.77
6:n:357:MET:HE1	6:n:385:LEU:HD12	1.66	0.77
4:T:456:ARG:HH12	4:T:533:GLU:HG3	1.49	0.77
3:L:22:ILE:HG22	3:L:75:LEU:HD13	1.66	0.77
4:S:25:PRO:HG3	2:y:91:ARG:HH12	1.50	0.77
1:9:8:LYS:HE3	6:p:508:LEU:HD11	1.67	0.77
3:K:50:TYR:HB3	3:K:60:LEU:HD12	1.67	0.77
6:r:357:MET:HE1	6:r:385:LEU:HD12	1.65	0.77
3:O:50:TYR:HB3	3:O:60:LEU:HD12	1.67	0.77
3:C:8:VAL:HG22	3:C:76:ARG:HG3	1.67	0.76
3:O:14:ASP:HA	3:O:66:PRO:HD2	1.68	0.76
6:t:357:MET:HE1	6:t:385:LEU:HD12	1.66	0.76
3:M:14:ASP:HA	3:M:66:PRO:HD2	1.67	0.76
6:p:362:VAL:HB	6:p:374:ILE:HD12	1.67	0.76
2:2:91:ARG:HH12	4:P:25:PRO:HG3	1.50	0.76
4:S:456:ARG:HH12	4:S:533:GLU:HG3	1.51	0.76
4:Q:456:ARG:HH12	4:Q:533:GLU:HG3	1.50	0.75
5:Y:173:GLU:HA	6:t:321:THR:HG21	1.66	0.75
6:u:478:THR:HA	6:u:481:ILE:HD12	1.69	0.75
6:u:82:THR:HA	6:u:118:MET:HE2	1.67	0.75
6:j:362:VAL:HB	6:j:374:ILE:HD12	1.68	0.75
3:a:8:VAL:HG22	3:a:76:ARG:HG3	1.69	0.75
3:K:14:ASP:HA	3:K:66:PRO:HD2	1.67	0.74
1:0:5:PRO:HD3	6:m:523:MET:HE1	1.69	0.74
1:4:5:PRO:HB2	6:t:512:MET:HE3	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:662:LEU:HD22	4:Q:665:ARG:HE	1.52	0.74
3:B:8:VAL:HG22	3:B:76:ARG:HG3	1.67	0.74
3:M:50:TYR:HB3	3:M:60:LEU:HD12	1.69	0.74
3:D:8:VAL:HG22	3:D:76:ARG:HG3	1.69	0.74
3:N:50:TYR:HB3	3:N:60:LEU:HD12	1.69	0.74
4:T:283:ARG:HE	4:T:294:THR:HG21	1.52	0.74
4:T:147:ASN:HB3	4:T:150:GLN:HB2	1.69	0.74
1:O:11:LYS:HD2	6:o:529:SER:HB3	1.71	0.73
4:P:504:CYS:SG	4:P:513:SER:OG	2.45	0.73
6:o:478:THR:HA	6:o:481:ILE:HD12	1.69	0.73
6:p:78:PHE:O	6:p:127:ARG:NH2	2.21	0.73
5:V:173:GLU:HA	6:n:321:THR:HG21	1.69	0.73
3:c:50:TYR:HB3	3:c:60:LEU:HD12	1.69	0.73
3:E:8:VAL:HG22	3:E:76:ARG:HG3	1.70	0.73
4:T:662:LEU:HD22	4:T:665:ARG:HE	1.52	0.73
3:A:8:VAL:HG22	3:A:76:ARG:HG3	1.69	0.73
4:P:456:ARG:HH12	4:P:533:GLU:HG3	1.53	0.73
4:Q:71:ARG:NH1	4:Q:121:VAL:O	2.21	0.73
6:j:78:PHE:O	6:j:127:ARG:NH2	2.22	0.73
4:S:283:ARG:HE	4:S:294:THR:HG21	1.54	0.73
2:v:91:ARG:HH12	4:x:25:PRO:HG3	1.53	0.73
4:Q:12:LYS:NZ	4:Q:536:ARG:O	2.20	0.72
4:Q:283:ARG:HE	4:Q:294:THR:HG21	1.52	0.72
3:N:14:ASP:HA	3:N:66:PRO:HD2	1.71	0.72
3:c:14:ASP:HA	3:c:66:PRO:HD2	1.72	0.72
1:6:5:PRO:O	1:7:11:LYS:HG2	1.88	0.72
5:V:149:ARG:HG2	5:d:23:SER:HA	1.71	0.72
6:o:82:THR:HA	6:o:118:MET:HE2	1.70	0.72
1:3:11:LYS:HD3	6:j:529:SER:HB3	1.70	0.72
4:R:147:ASN:HB3	4:R:150:GLN:HB2	1.69	0.72
5:Y:149:ARG:HG2	5:g:23:SER:HA	1.71	0.72
4:x:413:LEU:HD23	4:x:424:LEU:HD23	1.72	0.72
4:R:25:PRO:HG3	2:z:91:ARG:HH12	1.53	0.72
3:H:8:VAL:HG22	3:H:76:ARG:HG3	1.69	0.72
3:I:124:ASN:HD22	3:I:128:HIS:HB2	1.55	0.72
6:l:82:THR:HA	6:l:118:MET:HE2	1.70	0.72
4:x:12:LYS:NZ	4:x:536:ARG:O	2.22	0.72
3:G:8:VAL:HG22	3:G:76:ARG:HG3	1.71	0.72
4:T:25:PRO:HG3	2:w:91:ARG:HH12	1.55	0.72
3:L:50:TYR:HB3	3:L:60:LEU:HD12	1.70	0.71
6:q:50:ALA:O	6:r:30:ARG:NH2	2.21	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:r:82:THR:HA	6:r:118:MET:HE2	1.70	0.71
6:s:82:THR:HA	6:s:118:MET:HE2	1.72	0.71
4:x:147:ASN:HB3	4:x:150:GLN:HB2	1.70	0.71
3:M:22:ILE:HG22	3:M:75:LEU:HD13	1.71	0.71
4:P:147:ASN:HB3	4:P:150:GLN:HB2	1.73	0.71
4:Q:147:ASN:HB3	4:Q:150:GLN:HB2	1.72	0.71
4:S:71:ARG:NH1	4:S:121:VAL:O	2.23	0.71
3:b:124:ASN:HD22	3:b:128:HIS:HB2	1.55	0.71
1:AA:10:PRO:HD2	6:n:512:MET:HE1	1.72	0.71
4:S:504:CYS:HG	4:S:513:SER:HG	1.34	0.71
4:P:504:CYS:HG	4:P:513:SER:HG	1.35	0.70
4:S:504:CYS:SG	4:S:513:SER:OG	2.45	0.70
4:Q:527:LYS:HB3	4:Q:539:SER:HB3	1.74	0.70
3:C:117:THR:HG23	3:H:116:LEU:HD23	1.74	0.70
6:j:30:ARG:NH2	6:u:50:ALA:O	2.22	0.70
6:m:82:THR:HA	6:m:118:MET:HE2	1.72	0.70
5:U:173:GLU:HA	6:p:321:THR:HG21	1.74	0.70
5:V:182:ASN:ND2	6:n:318:ASP:OD1	2.24	0.70
5:X:2:ARG:NH1	5:X:83:ASP:OD2	2.25	0.70
6:k:50:ALA:O	6:l:30:ARG:NH2	2.21	0.70
4:S:147:ASN:HB3	4:S:150:GLN:HB2	1.73	0.69
6:o:50:ALA:O	6:p:30:ARG:NH2	2.21	0.69
5:f:59:TRP:HE3	5:f:175:GLU:HG3	1.57	0.69
4:P:71:ARG:NH1	4:P:121:VAL:O	2.24	0.69
4:R:12:LYS:NZ	4:R:536:ARG:O	2.22	0.69
1:AC:10:PRO:HD2	6:l:512:MET:HE1	1.75	0.69
3:a:107:MET:HG3	3:b:81:THR:HG23	1.74	0.69
6:k:170:ARG:HB3	6:k:263:SER:HA	1.74	0.69
1:AD:11:LYS:HD3	6:k:529:SER:HB3	1.74	0.69
3:E:107:MET:HE1	3:J:105:GLN:HG2	1.75	0.69
5:e:182:ASN:ND2	6:m:318:ASP:OD1	2.26	0.69
2:1:91:ARG:HH12	4:Q:25:PRO:HG3	1.58	0.69
5:U:2:ARG:NH1	5:U:83:ASP:OD2	2.25	0.69
4:R:413:LEU:HD23	4:R:424:LEU:HD23	1.75	0.69
3:H:36:LEU:HG	3:H:44:LEU:HD11	1.74	0.68
6:k:228:ARG:HH12	6:k:230:GLU:HG3	1.58	0.68
6:s:170:ARG:HB3	6:s:263:SER:HA	1.75	0.68
4:R:167:VAL:HG23	4:R:235:THR:HG22	1.75	0.68
5:i:182:ASN:ND2	6:s:318:ASP:OD1	2.26	0.68
3:C:22:ILE:HD11	3:C:58:ILE:HG13	1.75	0.68
6:m:170:ARG:HB3	6:m:263:SER:HA	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:132:GLU:OE2	6:l:258:ARG:NH2	2.26	0.68
6:t:335:GLN:HE22	6:u:336:ALA:HB1	1.59	0.68
6:q:172:ALA:HA	6:q:261:GLY:HA2	1.75	0.68
3:B:117:THR:HG23	3:G:116:LEU:HD23	1.75	0.68
3:K:71:THR:HG23	3:K:72:THR:H	1.59	0.68
3:K:124:ASN:HD22	3:K:130:ASP:HB2	1.58	0.68
6:l:362:VAL:HB	6:l:374:ILE:HD12	1.76	0.68
6:q:170:ARG:HB3	6:q:263:SER:HA	1.74	0.68
3:N:71:THR:HG23	3:N:72:THR:H	1.59	0.68
4:T:527:LYS:HB3	4:T:539:SER:HB3	1.74	0.68
5:X:173:GLU:HA	6:j:321:THR:HG21	1.75	0.68
5:Y:182:ASN:ND2	6:t:318:ASP:OD1	2.25	0.68
1:AC:11:LYS:HD3	6:l:529:SER:HB3	1.75	0.68
3:D:107:MET:HG3	3:I:81:THR:HG23	1.74	0.68
3:J:22:ILE:HD11	3:J:58:ILE:HG13	1.76	0.68
5:f:39:ASP:OD1	4:x:705:ARG:NH2	2.24	0.68
2:1:87:LEU:HD11	4:S:794:ILE:HD12	1.76	0.67
5:h:173:GLU:HA	6:r:321:THR:HG21	1.76	0.67
6:q:132:GLU:OE1	6:r:258:ARG:NH2	2.26	0.67
3:c:71:THR:HG23	3:c:72:THR:H	1.59	0.67
6:j:357:MET:HE1	6:j:385:LEU:HD12	1.75	0.67
6:l:40:PRO:HB2	6:l:54:TYR:HB3	1.76	0.67
6:r:362:VAL:HB	6:r:374:ILE:HD12	1.76	0.67
4:T:71:ARG:NH1	4:T:121:VAL:O	2.26	0.67
6:r:40:PRO:HB2	6:r:54:TYR:HB3	1.76	0.67
5:i:173:GLU:HA	6:s:321:THR:HG21	1.76	0.67
1:4:11:LYS:HG3	6:u:530:VAL:HG22	1.76	0.67
5:W:173:GLU:HA	6:l:321:THR:HG21	1.75	0.67
6:k:172:ALA:HA	6:k:261:GLY:HA2	1.75	0.67
3:F:22:ILE:HD11	3:F:58:ILE:HG13	1.77	0.67
3:I:130:ASP:OD1	3:N:138:ASN:ND2	2.28	0.67
4:T:464:ARG:O	4:T:498:ASN:ND2	2.24	0.67
4:S:167:VAL:HG23	4:S:235:THR:HG22	1.76	0.67
4:S:705:ARG:NH2	5:d:39:ASP:OD2	2.24	0.67
5:X:149:ARG:HG2	5:f:23:SER:HA	1.76	0.67
5:e:176:MET:HG3	6:m:321:THR:HG23	1.76	0.67
4:T:167:VAL:HG23	4:T:235:THR:HG22	1.78	0.67
5:U:182:ASN:ND2	6:p:318:ASP:OD1	2.27	0.67
5:W:149:ARG:HG2	5:e:23:SER:HA	1.76	0.67
3:b:130:ASP:OD2	3:c:138:ASN:ND2	2.28	0.67
1:0:8:LYS:HB3	1:0:12:MET:HG3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:107:MET:HE1	3:F:105:GLN:HG2	1.75	0.66
5:Z:45:ARG:NH2	5:h:19:ASP:OD1	2.28	0.66
3:B:22:ILE:HD11	3:B:58:ILE:HG13	1.75	0.66
3:G:36:LEU:HG	3:G:44:LEU:HD11	1.76	0.66
3:J:45:THR:HB	3:J:48:THR:HG22	1.77	0.66
3:J:130:ASP:OD1	3:O:138:ASN:ND2	2.29	0.66
4:x:608:ASN:ND2	4:x:610:ASP:OD1	2.28	0.66
3:D:22:ILE:HD11	3:D:58:ILE:HG13	1.77	0.66
6:n:335:GLN:HE22	6:o:336:ALA:HB1	1.59	0.66
4:P:167:VAL:HG23	4:P:235:THR:HG22	1.76	0.66
6:o:481:ILE:HG23	6:p:466:ILE:HD11	1.77	0.66
1:5:11:LYS:HD3	6:t:529:SER:HB3	1.78	0.66
5:h:149:ARG:HG2	5:i:23:SER:HA	1.77	0.66
3:F:45:THR:HB	3:F:48:THR:HG22	1.77	0.66
6:j:466:ILE:HD11	6:u:481:ILE:HG23	1.77	0.66
3:a:22:ILE:HD11	3:a:58:ILE:HG13	1.77	0.66
3:G:13:LEU:HD11	3:G:36:LEU:HD22	1.76	0.65
4:P:38:GLU:OE2	4:P:527:LYS:NZ	2.28	0.65
5:U:149:ARG:HG2	5:Z:23:SER:HA	1.77	0.65
6:o:172:ALA:HA	6:o:261:GLY:HA2	1.77	0.65
4:Q:464:ARG:O	4:Q:498:ASN:ND2	2.24	0.65
5:W:19:ASP:OD1	5:f:45:ARG:NH2	2.29	0.65
5:X:182:ASN:ND2	6:j:318:ASP:OD1	2.26	0.65
4:P:477:GLN:NE2	4:Q:478:ASP:OD2	2.29	0.65
6:n:170:ARG:HB3	6:n:263:SER:HA	1.78	0.65
6:r:170:ARG:HB3	6:r:263:SER:HA	1.79	0.65
1:AB:5:PRO:O	1:AC:11:LYS:HG2	1.96	0.65
4:S:527:LYS:HB3	4:S:539:SER:HB3	1.78	0.65
4:T:165:LEU:HD11	4:T:196:LEU:HD13	1.79	0.65
6:n:362:VAL:HB	6:n:374:ILE:HD12	1.79	0.65
6:s:499:MET:HA	6:s:502:ASP:HB2	1.79	0.65
6:t:40:PRO:HB2	6:t:54:TYR:HB3	1.79	0.65
6:u:170:ARG:HB3	6:u:263:SER:HA	1.78	0.65
4:P:527:LYS:HB3	4:P:539:SER:HB3	1.78	0.65
3:K:8:VAL:HG22	3:K:76:ARG:HG3	1.79	0.65
6:l:170:ARG:HB3	6:l:263:SER:HA	1.79	0.65
6:m:494:GLN:NE2	6:n:492:MET:SD	2.70	0.65
6:n:40:PRO:HB2	6:n:54:TYR:HB3	1.79	0.65
5:e:173:GLU:HA	6:m:321:THR:HG21	1.79	0.64
6:o:494:GLN:NE2	6:p:492:MET:SD	2.70	0.64
6:p:357:MET:HE1	6:p:385:LEU:HD12	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:t:362:VAL:HB	6:t:374:ILE:HD12	1.78	0.64
3:F:130:ASP:OD1	3:K:138:ASN:ND2	2.30	0.64
3:N:22:ILE:HD11	3:N:58:ILE:HG13	1.79	0.64
3:c:37:ILE:HD11	3:c:74:GLU:HB2	1.80	0.64
6:s:88:ILE:HG12	6:s:110:LEU:HD11	1.78	0.64
6:u:172:ALA:HA	6:u:261:GLY:HA2	1.78	0.64
4:Q:739:ASN:OD1	4:Q:742:ARG:NH2	2.30	0.64
4:S:446:GLN:HB2	4:S:463:PRO:HD3	1.78	0.64
4:T:722:ASN:OD1	4:T:725:SER:N	2.28	0.64
4:T:739:ASN:OD1	4:T:742:ARG:NH2	2.30	0.64
3:a:130:ASP:OD1	3:b:138:ASN:ND2	2.30	0.64
6:m:88:ILE:HG12	6:m:110:LEU:HD11	1.78	0.64
1:9:4:SER:HB2	6:o:526:ALA:HB2	1.78	0.64
6:p:335:GLN:HE22	6:q:336:ALA:HB1	1.63	0.64
4:S:477:GLN:NE2	4:T:478:ASP:OD2	2.30	0.64
4:x:167:VAL:HG23	4:x:235:THR:HG22	1.79	0.64
3:F:8:VAL:HG22	3:F:76:ARG:HG3	1.80	0.64
4:R:446:GLN:HB2	4:R:463:PRO:HD3	1.80	0.64
6:r:121:ILE:HG23	6:r:126:TYR:HB2	1.80	0.64
6:t:170:ARG:HB3	6:t:263:SER:HA	1.78	0.64
1:0:15:ASN:HB2	6:n:533:GLN:HB2	1.80	0.64
4:P:794:ILE:HD12	2:w:87:LEU:HD11	1.78	0.64
4:S:12:LYS:NZ	4:S:536:ARG:O	2.27	0.64
6:s:72:LYS:HZ3	6:s:357:MET:HE2	1.63	0.64
4:S:38:GLU:OE2	4:S:527:LYS:NZ	2.28	0.64
6:r:520:PRO:HD3	6:s:515:GLN:HE21	1.63	0.64
4:x:423:VAL:HG12	4:x:425:THR:HG23	1.80	0.64
1:8:10:PRO:HD2	6:q:512:MET:HE1	1.79	0.64
1:AD:3:PHE:HA	6:j:525:ALA:HB1	1.80	0.64
3:L:36:LEU:HB3	3:L:70:TYR:HB3	1.80	0.64
6:n:517:THR:HG21	6:o:511:GLY:HA3	1.79	0.64
3:E:22:ILE:HD11	3:E:58:ILE:HG13	1.80	0.63
3:O:8:VAL:HG22	3:O:76:ARG:HG3	1.80	0.63
4:R:705:ARG:NH2	5:Z:39:ASP:OD2	2.24	0.63
6:o:170:ARG:HB3	6:o:263:SER:HA	1.79	0.63
3:H:13:LEU:HD11	3:H:36:LEU:HD22	1.79	0.63
4:P:446:GLN:HB2	4:P:463:PRO:HD3	1.78	0.63
4:Q:167:VAL:HG23	4:Q:235:THR:HG22	1.80	0.63
6:q:40:PRO:HB2	6:q:54:TYR:HB3	1.80	0.63
4:Q:165:LEU:HD11	4:Q:196:LEU:HD13	1.79	0.63
6:m:18:GLU:HA	6:m:21:LYS:HD3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:5:PRO:HA	1:AD:11:LYS:HG2	1.80	0.63
4:Q:446:GLN:HB2	4:Q:463:PRO:HD3	1.81	0.63
3:c:22:ILE:HD11	3:c:58:ILE:HG13	1.80	0.63
3:c:36:LEU:HB3	3:c:70:TYR:HB3	1.80	0.63
4:x:446:GLN:HB2	4:x:463:PRO:HD3	1.79	0.63
3:J:8:VAL:HG22	3:J:76:ARG:HG3	1.80	0.63
4:Q:477:GLN:HG2	4:R:478:ASP:HB2	1.79	0.63
4:P:166:ILE:HG12	4:P:176:LYS:HG3	1.80	0.63
6:m:50:ALA:O	6:n:30:ARG:NH2	2.22	0.63
1:4:15:ASN:HB2	6:t:533:GLN:HB2	1.80	0.63
3:M:36:LEU:HB3	3:M:70:TYR:HB3	1.80	0.63
4:P:628:ARG:HG3	4:P:645:GLN:HE22	1.64	0.63
4:S:423:VAL:HG12	4:S:425:THR:HG23	1.81	0.63
6:j:335:GLN:HE22	6:k:336:ALA:HB1	1.63	0.63
3:L:37:ILE:HD11	3:L:74:GLU:HB2	1.79	0.62
6:m:172:ALA:HA	6:m:261:GLY:HA2	1.80	0.62
3:D:130:ASP:OD1	3:I:138:ASN:ND2	2.30	0.62
6:s:494:GLN:NE2	6:t:492:MET:SD	2.71	0.62
4:x:464:ARG:O	4:x:498:ASN:ND2	2.29	0.62
1:0:5:PRO:HB2	6:n:512:MET:HE3	1.81	0.62
3:N:37:ILE:HD11	3:N:74:GLU:HB2	1.82	0.62
4:P:478:ASP:HB2	4:x:477:GLN:HG2	1.81	0.62
5:f:182:ASN:ND2	6:k:318:ASP:OD2	2.26	0.62
5:g:59:TRP:HE3	5:g:175:GLU:HG3	1.63	0.62
6:t:121:ILE:HG23	6:t:126:TYR:HB2	1.82	0.62
1:7:11:LYS:HE3	1:7:12:MET:HG2	1.82	0.62
4:Q:154:ILE:HB	4:Q:220:ILE:HB	1.82	0.62
4:Q:700:ARG:NH2	5:Y:26:GLU:OE2	2.33	0.62
4:T:38:GLU:HG2	4:T:529:LEU:HD13	1.80	0.62
6:u:121:ILE:HG23	6:u:126:TYR:HB2	1.81	0.62
3:A:95:ARG:NH1	5:V:34:GLY:O	2.33	0.62
1:AD:12:MET:HB2	6:j:532:LEU:HD12	1.80	0.62
3:H:130:ASP:OD1	3:M:138:ASN:ND2	2.33	0.62
6:n:121:ILE:HG23	6:n:126:TYR:HB2	1.81	0.62
4:P:423:VAL:HG12	4:P:425:THR:HG23	1.81	0.62
3:a:111:GLU:HB2	3:b:81:THR:HG21	1.81	0.62
6:o:121:ILE:HG23	6:o:126:TYR:HB2	1.82	0.62
6:l:121:ILE:HG23	6:l:126:TYR:HB2	1.81	0.62
6:s:172:ALA:HA	6:s:261:GLY:HA2	1.82	0.62
3:G:130:ASP:OD1	3:L:138:ASN:ND2	2.33	0.61
5:U:2:ARG:HE	3:a:55:ARG:NH2	1.98	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:22:ILE:HD11	3:A:58:ILE:HG13	1.80	0.61
3:D:111:GLU:HB2	3:I:81:THR:HG21	1.83	0.61
3:N:36:LEU:HB3	3:N:70:TYR:HB3	1.81	0.61
4:T:446:GLN:HB2	4:T:463:PRO:HD3	1.81	0.61
3:a:117:THR:HA	3:a:120:THR:HG22	1.82	0.61
1:0:13:ASP:HB3	6:n:533:GLN:HB3	1.82	0.61
5:i:52:ARG:NH2	5:i:82:ASP:O	2.32	0.61
1:6:13:ASP:HB2	6:r:536:ILE:HG22	1.82	0.61
4:R:423:VAL:HG12	4:R:425:THR:HG23	1.82	0.61
4:S:166:ILE:HG12	4:S:176:LYS:HG3	1.81	0.61
5:d:17:VAL:HG11	5:d:32:LEU:HD21	1.82	0.61
3:M:37:ILE:HD11	3:M:74:GLU:HB2	1.81	0.61
6:r:335:GLN:HE22	6:s:336:ALA:HB1	1.65	0.61
1:5:10:PRO:HD2	6:t:512:MET:HE1	1.83	0.61
1:AD:10:PRO:HD2	6:k:512:MET:HE1	1.82	0.61
6:k:184:GLN:HB2	6:l:172:ALA:HB3	1.83	0.61
6:m:228:ARG:HH12	6:m:230:GLU:HG3	1.65	0.61
6:s:121:ILE:HG23	6:s:126:TYR:HB2	1.83	0.61
6:t:65:GLY:HA2	6:t:358:LEU:HD21	1.82	0.61
4:Q:38:GLU:HG2	4:Q:529:LEU:HD13	1.82	0.61
4:R:722:ASN:OD1	4:R:725:SER:N	2.31	0.61
6:o:517:THR:HG21	6:p:511:GLY:HA3	1.83	0.61
1:0:11:LYS:HG3	6:o:530:VAL:HG22	1.83	0.60
3:D:55:ARG:NH2	5:X:2:ARG:HE	1.98	0.60
4:T:302:GLN:HG2	4:T:329:PRO:HB3	1.83	0.60
6:j:90:GLU:OE2	6:u:115:ARG:NH1	2.35	0.60
6:p:121:ILE:HG23	6:p:126:TYR:HB2	1.84	0.60
5:f:49:LYS:NZ	5:f:145:GLN:OE1	2.35	0.60
6:m:517:THR:HG21	6:n:511:GLY:HA3	1.84	0.60
4:Q:302:GLN:HG2	4:Q:329:PRO:HB3	1.84	0.60
4:R:739:ASN:OD1	4:R:742:ARG:NH2	2.35	0.60
6:s:50:ALA:O	6:t:30:ARG:NH2	2.22	0.60
1:AC:3:PHE:HA	6:k:525:ALA:HB1	1.83	0.60
4:Q:713:SER:HB3	4:Q:777:ASN:H	1.67	0.60
5:Z:49:LYS:NZ	5:Z:145:GLN:OE1	2.34	0.60
5:g:17:VAL:HG11	5:g:32:LEU:HD21	1.82	0.60
6:k:40:PRO:HB2	6:k:54:TYR:HB3	1.82	0.60
6:t:397:GLN:HB3	6:t:425:THR:HG21	1.83	0.60
4:R:174:VAL:O	4:R:207:ASN:ND2	2.35	0.60
4:S:634:LEU:HB3	4:S:668:TYR:HB2	1.84	0.60
6:n:220:ASP:HB2	6:n:227:LEU:HG	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:x:527:LYS:HB3	4:x:539:SER:HB3	1.84	0.60
4:Q:409:PHE:HB3	4:Q:414:LEU:HD13	1.84	0.59
6:q:184:GLN:HB2	6:r:172:ALA:HB3	1.83	0.59
4:x:174:VAL:O	4:x:207:ASN:ND2	2.35	0.59
4:T:713:SER:HB3	4:T:777:ASN:H	1.67	0.59
5:e:17:VAL:HG11	5:e:32:LEU:HD21	1.83	0.59
5:i:128:ASP:O	5:i:135:ARG:NH2	2.28	0.59
6:p:193:ASP:OD1	6:p:194:ILE:N	2.36	0.59
6:u:168:VAL:HG22	6:u:179:MET:HG2	1.84	0.59
6:u:527:ALA:O	6:u:532:LEU:N	2.34	0.59
3:M:8:VAL:HG22	3:M:76:ARG:HG3	1.84	0.59
4:P:157:ARG:NH2	4:P:245:ASN:OD1	2.31	0.59
5:i:17:VAL:HG11	5:i:32:LEU:HD21	1.84	0.59
6:m:121:ILE:HG23	6:m:126:TYR:HB2	1.83	0.59
6:s:256:MET:HE2	6:s:268:TYR:HB2	1.83	0.59
6:t:220:ASP:HB2	6:t:227:LEU:HG	1.83	0.59
6:u:486:GLU:OE2	6:u:490:GLN:NE2	2.35	0.59
1:3:12:MET:HB2	6:u:532:LEU:HD12	1.84	0.59
5:f:52:ARG:NH2	5:f:82:ASP:O	2.31	0.59
4:P:136:LYS:HA	4:P:303:VAL:HA	1.85	0.59
6:j:121:ILE:HG23	6:j:126:TYR:HB2	1.84	0.59
6:j:172:ALA:HB3	6:u:184:GLN:HB2	1.85	0.59
1:7:5:PRO:HA	1:8:11:LYS:HG2	1.85	0.59
1:AA:7:ILE:HA	6:m:530:VAL:HG21	1.83	0.59
4:R:76:GLN:HB3	4:R:91:LEU:HG	1.84	0.59
3:K:36:LEU:HB3	3:K:70:TYR:HB3	1.85	0.59
3:b:8:VAL:HG22	3:b:76:ARG:HG3	1.85	0.59
3:L:8:VAL:HG22	3:L:76:ARG:HG3	1.84	0.58
4:R:527:LYS:HB3	4:R:539:SER:HB3	1.84	0.58
5:d:182:ASN:ND2	5:d:185:ASP:OD1	2.36	0.58
6:o:168:VAL:HG22	6:o:179:MET:HG2	1.85	0.58
4:Q:237:ASP:HB3	4:Q:244:ILE:HG12	1.85	0.58
4:S:314:ARG:HE	4:S:318:GLY:HA2	1.68	0.58
6:l:79:PRO:O	6:l:127:ARG:NH2	2.35	0.58
5:Z:52:ARG:NH2	5:Z:82:ASP:O	2.31	0.58
6:p:40:PRO:HB2	6:p:54:TYR:HB3	1.86	0.58
4:x:76:GLN:HB3	4:x:91:LEU:HG	1.84	0.58
4:P:705:ARG:NH2	5:g:39:ASP:OD2	2.26	0.58
4:R:608:ASN:ND2	4:R:610:ASP:OD1	2.36	0.58
4:S:136:LYS:HA	4:S:303:VAL:HA	1.84	0.58
6:n:168:VAL:HG23	6:n:179:MET:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:x:109:THR:OG1	4:x:115:ASP:OD2	2.21	0.58
4:x:794:ILE:HD11	2:y:87:LEU:HD21	1.84	0.58
3:I:8:VAL:HG22	3:I:76:ARG:HG3	1.85	0.58
4:Q:38:GLU:OE2	4:Q:527:LYS:NZ	2.37	0.58
4:Q:71:ARG:HB2	4:Q:75:GLU:HB2	1.85	0.58
4:Q:153:LEU:HB2	4:Q:247:VAL:HB	1.86	0.58
6:r:117:ILE:HD13	6:r:408:LEU:HD12	1.86	0.58
4:Q:645:GLN:HG2	4:Q:646:PRO:O	2.04	0.58
5:W:136:TYR:HE1	5:f:49:LYS:HE2	1.68	0.58
3:I:22:ILE:HD11	3:I:58:ILE:HG13	1.86	0.57
4:S:237:ASP:HB3	4:S:244:ILE:HG12	1.85	0.57
4:S:608:ASN:ND2	4:S:610:ASP:OD1	2.37	0.57
4:T:154:ILE:HB	4:T:220:ILE:HB	1.86	0.57
6:o:184:GLN:HB2	6:p:172:ALA:HB3	1.85	0.57
6:q:121:ILE:HG23	6:q:126:TYR:HB2	1.86	0.57
4:R:408:PRO:HD3	4:S:398:ASN:HD21	1.69	0.57
6:j:40:PRO:HB2	6:j:54:TYR:HB3	1.86	0.57
6:o:190:LEU:HD13	6:o:194:ILE:HG22	1.86	0.57
6:o:40:PRO:HB2	6:o:54:TYR:HB3	1.87	0.57
6:r:386:GLY:HA2	6:r:389:TYR:CE1	2.40	0.57
4:x:136:LYS:HA	4:x:303:VAL:HA	1.86	0.57
4:R:464:ARG:O	4:R:498:ASN:ND2	2.29	0.57
3:b:22:ILE:HD11	3:b:58:ILE:HG13	1.87	0.57
5:i:176:MET:HG3	6:s:321:THR:HG23	1.86	0.57
6:u:40:PRO:HB2	6:u:54:TYR:HB3	1.87	0.57
1:8:13:ASP:HB3	6:p:533:GLN:HB3	1.87	0.57
4:P:370:ARG:HD2	4:P:373:LYS:HG3	1.87	0.57
4:R:125:THR:OG1	4:R:312:LEU:O	2.23	0.57
4:T:174:VAL:O	4:T:207:ASN:ND2	2.38	0.57
6:k:121:ILE:HG23	6:k:126:TYR:HB2	1.87	0.57
6:k:169:GLN:OE1	6:k:178:GLN:NE2	2.35	0.57
1:5:7:ILE:HA	6:s:530:VAL:HG21	1.87	0.57
4:P:608:ASN:ND2	4:P:610:ASP:OD1	2.37	0.57
4:Q:166:ILE:HG12	4:Q:176:LYS:HG3	1.86	0.57
6:o:370:THR:OG1	6:o:373:GLU:OE1	2.21	0.57
6:t:517:THR:HG21	6:u:511:GLY:HA3	1.85	0.57
4:R:136:LYS:HA	4:R:303:VAL:HA	1.86	0.57
4:R:154:ILE:HB	4:R:220:ILE:HB	1.85	0.57
4:S:370:ARG:HD2	4:S:373:LYS:HG3	1.85	0.57
6:s:306:THR:HG22	6:s:326:ASP:HB2	1.86	0.57
5:Y:162:GLU:OE1	5:i:144:ARG:NH2	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:49:LYS:HE2	5:h:136:TYR:HE1	1.69	0.57
6:p:144:LEU:HB3	6:p:161:TYR:HB2	1.86	0.57
3:N:84:ARG:NH2	3:N:87:ASP:OD1	2.36	0.57
3:O:92:SER:HA	4:P:640:ILE:HD12	1.86	0.57
4:S:68:LEU:HD21	4:S:557:ILE:HD11	1.86	0.57
4:T:504:CYS:SG	4:T:513:SER:OG	2.50	0.57
4:T:645:GLN:HG2	4:T:646:PRO:O	2.05	0.57
5:f:50:ILE:HG23	5:f:141:LYS:HD3	1.87	0.57
6:l:386:GLY:HA2	6:l:389:TYR:CE1	2.40	0.57
6:t:144:LEU:HB3	6:t:161:TYR:HB2	1.86	0.57
4:x:739:ASN:OD1	4:x:742:ARG:NH2	2.37	0.57
3:K:92:SER:HA	4:S:640:ILE:HD12	1.87	0.57
3:c:119:ASP:O	3:c:132:ARG:NH1	2.37	0.57
3:E:95:ARG:NH1	5:Y:34:GLY:O	2.38	0.56
4:P:479:VAL:HG11	4:P:482:VAL:HG23	1.87	0.56
3:c:9:LEU:HD22	3:c:23:PRO:HG3	1.87	0.56
5:e:60:THR:HG1	5:e:181:TYR:HH	1.53	0.56
6:s:235:MET:HE3	6:s:236:GLU:H	1.70	0.56
1:6:5:PRO:HB2	6:r:512:MET:HE3	1.86	0.56
5:e:147:ASN:O	5:e:152:GLY:N	2.34	0.56
6:m:306:THR:HG22	6:m:326:ASP:HB2	1.88	0.56
6:n:255:ARG:H	6:n:395:GLU:HG2	1.70	0.56
6:p:220:ASP:HB2	6:p:227:LEU:HG	1.86	0.56
1:9:9:THR:H	1:9:10:PRO:HD2	1.69	0.56
3:G:12:GLN:CD	3:G:12:GLN:H	2.13	0.56
3:N:119:ASP:O	3:N:132:ARG:NH1	2.38	0.56
4:P:398:ASN:HD21	4:x:408:PRO:HD3	1.70	0.56
4:Q:174:VAL:O	4:Q:207:ASN:ND2	2.38	0.56
4:R:599:ARG:NH2	4:R:666:MET:HE1	2.20	0.56
5:V:46:ILE:HD12	5:V:146:PHE:HD1	1.70	0.56
6:j:437:GLN:NE2	6:u:80:MET:SD	2.78	0.56
6:o:80:MET:SD	6:p:437:GLN:NE2	2.78	0.56
6:s:73:LEU:HD21	6:s:388:VAL:HG23	1.87	0.56
3:H:12:GLN:H	3:H:12:GLN:CD	2.13	0.56
4:P:237:ASP:HB3	4:P:244:ILE:HG12	1.86	0.56
4:Q:66:ILE:HD13	4:Q:564:ILE:HD12	1.87	0.56
4:S:160:GLN:HG2	4:S:243:LEU:HD21	1.88	0.56
6:m:72:LYS:HZ3	6:m:357:MET:HE2	1.71	0.56
6:r:172:ALA:HA	6:r:261:GLY:HA2	1.87	0.56
4:P:314:ARG:HE	4:P:318:GLY:HA2	1.68	0.56
5:Z:17:VAL:HG11	5:Z:32:LEU:HD21	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:128:ASP:O	5:e:135:ARG:NH2	2.28	0.56
6:j:228:ARG:HD2	6:j:244:TYR:CE2	2.40	0.56
6:l:172:ALA:HA	6:l:261:GLY:HA2	1.87	0.56
6:n:228:ARG:NH2	6:n:230:GLU:OE2	2.38	0.56
6:p:228:ARG:HD2	6:p:244:TYR:CE2	2.40	0.56
4:x:599:ARG:NH2	4:x:666:MET:HE1	2.21	0.56
1:AD:13:ASP:HB2	6:j:536:ILE:HG22	1.87	0.56
4:R:44:LYS:NZ	4:R:772:GLU:O	2.39	0.56
4:T:38:GLU:OE2	4:T:527:LYS:NZ	2.37	0.56
6:t:255:ARG:H	6:t:395:GLU:HG2	1.71	0.56
3:O:36:LEU:HB3	3:O:70:TYR:HB3	1.88	0.56
5:h:9:GLU:OE2	5:h:31:THR:OG1	2.21	0.56
6:j:220:ASP:HB2	6:j:227:LEU:HG	1.88	0.56
6:t:102:GLY:HA2	6:t:105:LYS:HE3	1.87	0.56
1:5:11:LYS:HE3	1:5:12:MET:HG3	1.88	0.56
4:R:713:SER:HB3	4:R:777:ASN:H	1.70	0.56
6:n:397:GLN:HB3	6:n:425:THR:HG21	1.88	0.56
6:q:235:MET:HE3	6:q:236:GLU:H	1.71	0.56
6:u:169:GLN:OE1	6:u:178:GLN:NE2	2.35	0.56
3:C:117:THR:HA	3:C:120:THR:HG22	1.88	0.56
4:P:413:LEU:HD23	4:P:424:LEU:HD23	1.87	0.56
4:R:504:CYS:SG	4:R:513:SER:OG	2.51	0.56
6:j:517:THR:HG21	6:k:511:GLY:HA3	1.88	0.56
4:x:78:TYR:CD2	4:x:564:ILE:HD11	2.41	0.56
4:x:722:ASN:OD1	4:x:725:SER:N	2.31	0.56
3:D:10:THR:HG23	5:X:73:VAL:HG22	1.88	0.56
4:R:78:TYR:CD2	4:R:564:ILE:HD11	2.41	0.56
4:S:502:SER:HB3	4:S:515:LEU:HB2	1.88	0.56
5:Y:46:ILE:HD12	5:Y:146:PHE:HD1	1.70	0.56
5:d:99:ARG:NH2	5:d:111:ASP:OD2	2.37	0.56
6:t:79:PRO:O	6:t:127:ARG:NH2	2.39	0.56
1:9:5:PRO:HB2	6:o:512:MET:HE3	1.88	0.55
3:K:110:ALA:O	3:K:114:ARG:HG2	2.06	0.55
4:S:302:GLN:HG2	4:S:329:PRO:HB3	1.88	0.55
3:b:120:THR:HG22	3:b:121:ILE:H	1.71	0.55
6:r:405:LEU:HD22	6:r:417:LEU:HD11	1.88	0.55
1:8:13:ASP:HB2	6:p:536:ILE:HG22	1.88	0.55
3:A:117:THR:HG23	3:F:116:LEU:HD23	1.88	0.55
6:t:228:ARG:NH2	6:t:230:GLU:OE2	2.37	0.55
3:K:37:ILE:HD11	3:K:74:GLU:HB2	1.88	0.55
4:P:68:LEU:HD21	4:P:557:ILE:HD11	1.86	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:714:GLY:HA3	4:P:774:THR:HB	1.89	0.55
4:R:109:THR:OG1	4:R:115:ASP:OD2	2.21	0.55
5:d:52:ARG:NH2	5:d:82:ASP:O	2.35	0.55
6:m:169:GLN:OE1	6:m:178:GLN:NE2	2.37	0.55
6:n:144:LEU:HB3	6:n:161:TYR:HB2	1.87	0.55
4:x:44:LYS:NZ	4:x:772:GLU:O	2.39	0.55
1:8:5:PRO:HB3	6:o:523:MET:SD	2.45	0.55
3:D:117:THR:HA	3:D:120:THR:HG22	1.88	0.55
3:E:138:ASN:ND2	3:O:130:ASP:OD2	2.37	0.55
3:F:124:ASN:HD22	3:F:128:HIS:HB2	1.72	0.55
4:P:160:GLN:HG2	4:P:243:LEU:HD21	1.88	0.55
4:S:413:LEU:HD23	4:S:424:LEU:HD23	1.88	0.55
5:Z:50:ILE:HG23	5:Z:141:LYS:HD3	1.88	0.55
6:s:85:ARG:NH1	6:s:438:ASP:OD2	2.38	0.55
6:u:502:ASP:OD1	6:u:503:ASN:N	2.39	0.55
1:4:5:PRO:O	1:5:11:LYS:HG2	2.06	0.55
4:T:66:ILE:HD13	4:T:564:ILE:HD12	1.88	0.55
5:U:46:ILE:HD12	5:U:146:PHE:HD1	1.71	0.55
5:U:73:VAL:HG22	3:a:10:THR:HG23	1.88	0.55
5:W:46:ILE:HD12	5:W:146:PHE:HD1	1.72	0.55
5:i:147:ASN:O	5:i:152:GLY:N	2.33	0.55
6:r:86:LEU:HD23	6:r:114:GLU:HG2	1.88	0.55
4:x:125:THR:OG1	4:x:312:LEU:O	2.23	0.55
5:f:17:VAL:HG11	5:f:32:LEU:HD21	1.88	0.55
6:n:102:GLY:HA2	6:n:105:LYS:HE3	1.86	0.55
3:O:37:ILE:HD11	3:O:74:GLU:HB2	1.87	0.55
6:l:228:ARG:NH2	6:l:230:GLU:OE2	2.36	0.55
6:n:79:PRO:O	6:n:127:ARG:NH2	2.39	0.55
6:u:17:TYR:HB2	6:u:180:VAL:HG11	1.88	0.55
3:I:120:THR:HG22	3:I:121:ILE:H	1.72	0.55
4:S:714:GLY:HA3	4:S:774:THR:HB	1.89	0.55
6:l:220:ASP:HB2	6:l:227:LEU:HG	1.89	0.55
6:l:527:ALA:O	6:l:532:LEU:N	2.40	0.55
6:m:235:MET:HE3	6:m:236:GLU:H	1.71	0.55
3:N:9:LEU:HD22	3:N:23:PRO:HG3	1.87	0.55
5:V:59:TRP:HE3	5:V:175:GLU:HG3	1.72	0.55
5:g:99:ARG:NH2	5:g:111:ASP:OD2	2.37	0.55
6:t:386:GLY:HA2	6:t:389:TYR:CE1	2.42	0.55
6:t:386:GLY:HA2	6:t:389:TYR:HE1	1.72	0.55
4:T:237:ASP:HB3	4:T:244:ILE:HG12	1.89	0.55
5:V:147:ASN:O	5:V:152:GLY:N	2.33	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:x:160:GLN:HG2	4:x:243:LEU:HD21	1.89	0.55
3:F:120:THR:HG22	3:F:121:ILE:H	1.72	0.54
4:S:46:PRO:HB2	4:S:576:ILE:HG23	1.90	0.54
4:S:157:ARG:NH2	4:S:245:ASN:OD1	2.32	0.54
4:S:479:VAL:HG11	4:S:482:VAL:HG23	1.89	0.54
6:s:305:ILE:HD11	6:s:323:ARG:HG3	1.88	0.54
4:x:151:ASP:OD1	4:x:152:GLY:N	2.40	0.54
4:x:237:ASP:HB3	4:x:244:ILE:HG12	1.89	0.54
5:X:46:ILE:HD12	5:X:146:PHE:HD1	1.72	0.54
5:Y:147:ASN:O	5:Y:152:GLY:N	2.32	0.54
5:e:52:ARG:NH2	5:e:82:ASP:O	2.34	0.54
6:n:386:GLY:HA2	6:n:389:TYR:HE1	1.72	0.54
3:A:116:LEU:HD11	3:K:114:ARG:HD2	1.90	0.54
3:E:5:ILE:H	3:E:5:ILE:HD12	1.71	0.54
4:P:302:GLN:HG2	4:P:329:PRO:HB3	1.88	0.54
5:g:169:ARG:HG2	6:j:302:PRO:HB2	1.89	0.54
6:m:484:THR:OG1	6:m:487:GLN:HG3	2.07	0.54
6:r:79:PRO:O	6:r:127:ARG:NH2	2.35	0.54
6:s:184:GLN:HB2	6:t:172:ALA:HB3	1.89	0.54
3:C:95:ARG:NH1	5:W:34:GLY:O	2.40	0.54
4:R:302:GLN:HG2	4:R:329:PRO:HB3	1.90	0.54
6:n:497:MET:HA	6:n:497:MET:HE3	1.89	0.54
6:o:452:LEU:HD12	6:o:463:LEU:HD22	1.88	0.54
6:r:144:LEU:HB3	6:r:161:TYR:HB2	1.89	0.54
5:Z:182:ASN:ND2	6:q:318:ASP:OD2	2.29	0.54
6:j:323:ARG:HB2	6:j:326:ASP:OD2	2.08	0.54
6:k:501:MET:HE1	6:l:492:MET:HE3	1.89	0.54
6:o:17:TYR:HB2	6:o:180:VAL:HG11	1.88	0.54
6:o:498:GLN:HB2	6:p:492:MET:HE3	1.89	0.54
6:u:190:LEU:HD13	6:u:194:ILE:HG22	1.89	0.54
1:9:3:PHE:HA	6:o:525:ALA:HB1	1.89	0.54
4:P:502:SER:HB3	4:P:515:LEU:HB2	1.88	0.54
5:g:52:ARG:NH2	5:g:82:ASP:O	2.35	0.54
6:m:184:GLN:HB2	6:n:172:ALA:HB3	1.89	0.54
6:o:169:GLN:OE1	6:o:178:GLN:NE2	2.35	0.54
4:x:414:LEU:HD13	4:x:416:TRP:HE1	1.71	0.54
1:AC:6:LYS:HB3	6:l:508:LEU:HD13	1.90	0.54
4:P:446:GLN:HE21	4:P:463:PRO:HG3	1.73	0.54
4:Q:71:ARG:HH22	4:Q:125:THR:HG23	1.72	0.54
4:Q:125:THR:OG1	4:Q:312:LEU:O	2.26	0.54
4:T:634:LEU:HB3	4:T:668:TYR:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:170:ARG:HB3	6:j:263:SER:HA	1.89	0.54
6:p:172:ALA:HA	6:p:261:GLY:HA2	1.90	0.54
6:s:255:ARG:HB3	6:s:265:GLY:HA3	1.90	0.54
6:t:497:MET:HA	6:t:497:MET:HE3	1.89	0.54
1:4:13:ASP:HB3	6:t:533:GLN:HB3	1.89	0.54
3:M:84:ARG:NH2	3:M:87:ASP:OD1	2.41	0.54
4:R:153:LEU:HB2	4:R:247:VAL:HB	1.89	0.54
4:S:722:ASN:OD1	4:S:725:SER:N	2.39	0.54
4:T:46:PRO:HB2	4:T:576:ILE:HG23	1.90	0.54
5:h:46:ILE:HD12	5:h:146:PHE:HD1	1.71	0.54
4:R:414:LEU:HD13	4:R:416:TRP:HE1	1.72	0.54
4:S:153:LEU:HB2	4:S:247:VAL:HB	1.90	0.54
6:r:220:ASP:HB2	6:r:227:LEU:HG	1.89	0.54
4:x:302:GLN:HG2	4:x:329:PRO:HB3	1.89	0.54
3:J:120:THR:HG22	3:J:121:ILE:H	1.73	0.53
5:d:169:ARG:HG2	6:p:302:PRO:HB2	1.90	0.53
6:l:114:GLU:OE1	6:l:435:ARG:NH1	2.41	0.53
6:o:502:ASP:OD1	6:o:503:ASN:N	2.40	0.53
6:p:170:ARG:HB3	6:p:263:SER:HA	1.89	0.53
1:9:9:THR:H	1:9:10:PRO:CD	2.21	0.53
4:S:713:SER:HB3	4:S:777:ASN:H	1.73	0.53
4:T:477:GLN:HG2	4:x:478:ASP:HB2	1.90	0.53
5:Z:99:ARG:NH2	5:Z:111:ASP:OD2	2.41	0.53
6:j:108:GLU:OE1	6:k:478:THR:OG1	2.26	0.53
6:j:195:ARG:O	6:j:199:GLU:HG3	2.08	0.53
6:r:114:GLU:OE1	6:r:435:ARG:NH1	2.41	0.53
6:u:517:THR:HA	6:u:523:MET:HG3	1.90	0.53
4:P:153:LEU:HB2	4:P:247:VAL:HB	1.91	0.53
4:P:634:LEU:HB3	4:P:668:TYR:HB2	1.89	0.53
4:Q:632:THR:HG23	4:Q:640:ILE:HG23	1.91	0.53
4:S:446:GLN:HE21	4:S:463:PRO:HG3	1.73	0.53
6:l:144:LEU:HB3	6:l:161:TYR:HB2	1.90	0.53
6:l:255:ARG:H	6:l:395:GLU:HG2	1.73	0.53
4:x:713:SER:HB3	4:x:777:ASN:H	1.71	0.53
3:H:22:ILE:HD11	3:H:58:ILE:HG13	1.90	0.53
4:P:141:VAL:HG22	4:P:300:GLU:HG2	1.90	0.53
4:R:44:LYS:HG3	4:R:776:LEU:HG	1.90	0.53
5:f:99:ARG:NH2	5:f:111:ASP:OD2	2.41	0.53
6:l:86:LEU:HD23	6:l:114:GLU:HG2	1.90	0.53
6:r:255:ARG:H	6:r:395:GLU:HG2	1.73	0.53
6:u:452:LEU:HD22	6:u:463:LEU:HD22	1.88	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:GLU:HG3	3:H:81:THR:HG21	1.91	0.53
3:L:66:PRO:HG3	3:L:71:THR:HG23	1.90	0.53
3:N:120:THR:HG23	3:N:121:ILE:HG22	1.90	0.53
4:T:714:GLY:HA3	4:T:774:THR:HB	1.91	0.53
6:q:115:ARG:NH1	6:r:90:GLU:OE2	2.41	0.53
4:T:157:ARG:HH22	4:T:245:ASN:CG	2.16	0.53
6:j:511:GLY:HA3	6:u:517:THR:HG21	1.90	0.53
4:P:713:SER:HB3	4:P:777:ASN:H	1.73	0.53
6:j:144:LEU:HB3	6:j:161:TYR:HB2	1.90	0.53
6:j:193:ASP:OD1	6:j:194:ILE:N	2.41	0.53
3:B:27:LEU:HD23	3:B:108:HIS:CD2	2.44	0.53
4:P:627:GLY:O	4:P:645:GLN:NE2	2.42	0.53
4:T:502:SER:HB3	4:T:515:LEU:HB2	1.90	0.53
5:X:19:ASP:OD1	5:g:45:ARG:NH2	2.41	0.53
6:s:442:LEU:HD11	6:t:469:ARG:HB3	1.89	0.53
4:x:200:LEU:O	4:x:204:MET:HG3	2.09	0.53
4:x:365:ASN:HA	4:x:394:ALA:HA	1.91	0.53
1:7:3:PHE:HE2	1:8:12:MET:HE1	1.74	0.53
4:R:38:GLU:OE2	4:R:527:LYS:NZ	2.37	0.53
4:T:118:MET:HE3	4:T:125:THR:HB	1.90	0.53
5:X:176:MET:HG3	6:j:321:THR:HG23	1.91	0.53
6:j:527:ALA:O	6:j:532:LEU:N	2.41	0.53
6:k:115:ARG:NH1	6:l:90:GLU:OE2	2.41	0.53
6:n:386:GLY:HA2	6:n:389:TYR:CE1	2.43	0.53
6:r:353:SER:HA	6:r:358:LEU:HD12	1.91	0.53
3:L:92:SER:HA	4:Q:640:ILE:HD12	1.91	0.53
4:Q:46:PRO:HB2	4:Q:576:ILE:HG23	1.90	0.53
4:Q:160:GLN:HG2	4:Q:243:LEU:HD21	1.90	0.53
4:Q:634:LEU:HB3	4:Q:668:TYR:HB2	1.90	0.53
4:Q:714:GLY:HA3	4:Q:774:THR:HB	1.91	0.53
4:R:151:ASP:OD1	4:R:152:GLY:N	2.42	0.53
5:d:24:ILE:HG13	5:d:26:GLU:HG2	1.91	0.53
5:g:24:ILE:HG13	5:g:26:GLU:HG2	1.91	0.53
5:h:147:ASN:O	5:h:152:GLY:N	2.33	0.53
6:p:517:THR:HG21	6:q:511:GLY:HA3	1.91	0.53
1:5:3:PHE:HA	6:s:525:ALA:HB1	1.91	0.52
3:H:84:ARG:NH2	5:e:9:GLU:O	2.42	0.52
3:L:13:LEU:HD12	3:L:20:PHE:HE1	1.74	0.52
3:L:84:ARG:NH2	3:L:87:ASP:OD1	2.42	0.52
3:O:9:LEU:HD23	3:O:10:THR:N	2.25	0.52
4:R:160:GLN:HG2	4:R:243:LEU:HD21	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:290:SER:HB3	6:m:344:VAL:HG21	1.92	0.52
6:q:169:GLN:OE1	6:q:178:GLN:NE2	2.35	0.52
6:q:208:ASP:HB2	6:r:169:GLN:HE22	1.75	0.52
6:r:6:THR:HA	6:r:10:GLU:HG2	1.92	0.52
1:0:5:PRO:CD	6:m:523:MET:HE1	2.38	0.52
3:l:84:ARG:NH2	5:f:9:GLU:O	2.41	0.52
3:j:124:ASN:HD22	3:j:128:HIS:HB2	1.73	0.52
4:r:237:ASP:HB3	4:r:244:ILE:HG12	1.90	0.52
4:r:632:THR:HG23	4:r:640:ILE:HG23	1.91	0.52
5:v:32:LEU:O	5:d:2:ARG:NH2	2.42	0.52
5:g:194:LEU:HD22	6:k:288:LYS:HG2	1.91	0.52
4:x:364:GLU:HB2	4:x:395:VAL:HG12	1.91	0.52
4:r:51:LEU:HD11	4:r:575:ARG:HB2	1.91	0.52
4:s:141:VAL:HG22	4:s:300:GLU:HG2	1.91	0.52
4:t:109:THR:OG1	4:t:115:ASP:OD2	2.26	0.52
5:z:9:GLU:O	3:b:84:ARG:NH2	2.42	0.52
6:l:113:VAL:O	6:l:117:ILE:HG12	2.09	0.52
6:u:235:MET:HE3	6:u:236:GLU:H	1.74	0.52
6:l:14:LYS:O	6:l:18:GLU:HG2	2.10	0.52
4:r:365:ASN:HA	4:r:394:ALA:HA	1.92	0.52
4:s:71:ARG:HB2	4:s:75:GLU:HB2	1.91	0.52
6:j:368:ARG:HH22	6:j:370:THR:HB	1.74	0.52
6:k:208:ASP:HB2	6:l:169:GLN:HE22	1.75	0.52
6:o:115:ARG:NH1	6:p:90:GLU:OE2	2.43	0.52
6:u:220:ASP:HB2	6:u:227:LEU:HG	1.92	0.52
4:x:51:LEU:HD11	4:x:575:ARG:HB2	1.91	0.52
3:g:22:ILE:HD11	3:g:58:ILE:HG13	1.91	0.52
3:k:9:LEU:HD23	3:k:10:THR:N	2.25	0.52
4:s:686:GLN:NE2	4:s:696:GLU:OE2	2.42	0.52
5:v:9:GLU:OE1	5:v:31:THR:OG1	2.21	0.52
6:l:6:THR:HA	6:l:10:GLU:HG2	1.92	0.52
6:r:228:ARG:NH2	6:r:230:GLU:OE2	2.41	0.52
3:c:37:ILE:HD11	3:c:74:GLU:HB2	1.91	0.52
3:m:95:ARG:NH2	3:m:98:ASP:OD1	2.43	0.52
4:r:479:VAL:HG11	4:r:482:VAL:HG23	1.92	0.52
4:t:160:GLN:HG2	4:t:243:LEU:HD21	1.91	0.52
6:l:353:SER:HA	6:l:358:LEU:HD12	1.90	0.52
6:r:290:SER:HB3	6:s:344:VAL:HG21	1.91	0.52
6:t:64:ARG:NH2	6:t:360:SER:OG	2.41	0.52
4:x:44:LYS:HG3	4:x:776:LEU:HG	1.91	0.52
3:e:10:THR:HG23	5:y:73:VAL:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:194:LEU:HD22	6:q:288:LYS:HG2	1.91	0.52
6:m:85:ARG:NH1	6:m:438:ASP:OD2	2.38	0.52
6:n:255:ARG:HB3	6:n:265:GLY:HA3	1.92	0.52
1:7:3:PHE:HA	6:q:525:ALA:HB1	1.91	0.52
4:S:44:LYS:HG3	4:S:776:LEU:HG	1.91	0.52
5:g:182:ASN:ND2	6:u:318:ASP:OD1	2.30	0.52
6:p:368:ARG:HH22	6:p:370:THR:HB	1.75	0.52
4:x:504:CYS:SG	4:x:513:SER:OG	2.51	0.52
4:Q:118:MET:HE3	4:Q:125:THR:HB	1.92	0.51
4:R:16:SER:HB3	4:R:23:ARG:HD3	1.92	0.51
6:p:527:ALA:O	6:p:532:LEU:N	2.42	0.51
6:r:113:VAL:O	6:r:117:ILE:HG12	2.10	0.51
6:r:527:ALA:O	6:r:532:LEU:N	2.41	0.51
6:s:357:MET:HE3	6:s:381:LEU:HB3	1.92	0.51
6:t:195:ARG:O	6:t:199:GLU:HG3	2.10	0.51
3:A:76:ARG:NH2	3:A:119:ASP:OD2	2.43	0.51
4:P:167:VAL:HG12	4:P:175:ALA:HB3	1.92	0.51
4:Q:531:LEU:HD12	4:Q:536:ARG:HG3	1.93	0.51
5:Y:194:LEU:HD22	6:j:288:LYS:HG2	1.92	0.51
6:r:14:LYS:O	6:r:18:GLU:HG2	2.10	0.51
3:M:66:PRO:HG3	3:M:71:THR:HG23	1.93	0.51
4:Q:502:SER:HB3	4:Q:515:LEU:HB2	1.91	0.51
4:T:554:CYS:HB2	4:T:561:MET:HE2	1.92	0.51
5:f:147:ASN:O	5:f:152:GLY:N	2.36	0.51
6:m:370:THR:OG1	6:m:373:GLU:OE1	2.20	0.51
3:L:95:ARG:NH2	3:L:98:ASP:OD1	2.43	0.51
4:T:51:LEU:HD11	4:T:575:ARG:HB2	1.92	0.51
3:b:53:ALA:HB3	3:b:57:THR:HG23	1.92	0.51
3:c:13:LEU:HD12	3:c:20:PHE:HE1	1.75	0.51
6:m:168:VAL:HG22	6:m:179:MET:HB3	1.93	0.51
6:p:108:GLU:OE1	6:q:478:THR:OG1	2.25	0.51
4:x:16:SER:HB3	4:x:23:ARG:HD3	1.92	0.51
4:x:502:SER:HB3	4:x:515:LEU:HB2	1.92	0.51
4:x:632:THR:HG23	4:x:640:ILE:HG23	1.92	0.51
2:2:87:LEU:HD21	4:R:794:ILE:HD11	1.91	0.51
3:D:99:LEU:HD12	4:x:736:LEU:HD11	1.93	0.51
4:P:632:THR:HG23	4:P:640:ILE:HG23	1.93	0.51
4:T:365:ASN:HA	4:T:394:ALA:HA	1.93	0.51
6:p:323:ARG:HB2	6:p:326:ASP:OD2	2.10	0.51
6:r:520:PRO:HD3	6:s:515:GLN:NE2	2.24	0.51
3:K:120:THR:HG23	3:K:121:ILE:HG22	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:13:LEU:HD12	3:M:20:PHE:HE1	1.75	0.51
4:P:50:PHE:HD1	4:P:596:MET:HE3	1.76	0.51
4:P:71:ARG:HB2	4:P:75:GLU:HB2	1.92	0.51
4:P:288:ARG:HB3	4:P:290:VAL:HG22	1.92	0.51
4:Q:51:LEU:HD11	4:Q:575:ARG:HB2	1.92	0.51
4:Q:504:CYS:SG	4:Q:513:SER:OG	2.50	0.51
4:T:632:THR:HG23	4:T:640:ILE:HG23	1.91	0.51
3:B:111:GLU:HG3	3:G:81:THR:HG21	1.91	0.51
3:E:99:LEU:HD12	4:P:736:LEU:HD11	1.93	0.51
3:G:84:ARG:NH2	5:i:9:GLU:O	2.44	0.51
3:M:92:SER:HA	4:T:640:ILE:HD12	1.93	0.51
3:N:95:ARG:NH2	3:N:98:ASP:OD1	2.43	0.51
4:P:645:GLN:HE21	4:P:649:GLY:HA2	1.73	0.51
4:Q:365:ASN:HA	4:Q:394:ALA:HA	1.93	0.51
4:S:739:ASN:OD1	4:S:742:ARG:NH2	2.44	0.51
4:T:4:ILE:HD11	4:T:701:LEU:HD13	1.93	0.51
5:e:99:ARG:NH2	5:e:111:ASP:OD2	2.39	0.51
6:j:344:VAL:HG21	6:u:290:SER:HB3	1.93	0.51
6:o:235:MET:HE3	6:o:236:GLU:H	1.74	0.51
3:B:37:ILE:HD11	3:B:74:GLU:HB2	1.91	0.51
4:Q:554:CYS:HB2	4:Q:561:MET:HE2	1.93	0.51
4:S:167:VAL:HG12	4:S:175:ALA:HB3	1.93	0.51
6:m:73:LEU:HD21	6:m:388:VAL:HG23	1.91	0.51
6:s:169:GLN:OE1	6:s:178:GLN:NE2	2.37	0.51
3:A:99:LEU:HD12	4:S:736:LEU:HD11	1.92	0.51
3:O:66:PRO:HG3	3:O:71:THR:HG23	1.93	0.51
4:P:46:PRO:HB2	4:P:576:ILE:HG23	1.91	0.51
6:p:423:GLU:OE1	6:p:423:GLU:N	2.44	0.51
3:A:138:ASN:ND2	3:K:130:ASP:OD2	2.42	0.51
3:K:22:ILE:HD11	3:K:58:ILE:HG13	1.92	0.51
3:K:25:GLU:O	3:K:77:ARG:NH1	2.43	0.51
4:Q:136:LYS:HA	4:Q:303:VAL:HA	1.93	0.51
4:Q:794:ILE:HD12	2:v:87:LEU:HD11	1.93	0.51
5:Z:193:LEU:HG	6:t:281:ASN:HB3	1.93	0.51
5:e:169:ARG:HG2	6:n:302:PRO:HB2	1.93	0.51
5:i:144:ARG:HA	5:i:160:LEU:HD13	1.92	0.51
6:s:168:VAL:HG22	6:s:179:MET:HB3	1.93	0.51
4:x:167:VAL:HG12	4:x:175:ALA:HB3	1.93	0.51
1:7:5:PRO:HG3	6:p:523:MET:SD	2.51	0.50
3:I:53:ALA:HB3	3:I:57:THR:HG23	1.92	0.50
3:N:25:GLU:O	3:N:77:ARG:NH1	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:44:LYS:HG3	4:P:776:LEU:HG	1.92	0.50
4:T:423:VAL:HG12	4:T:425:THR:HG23	1.93	0.50
5:g:147:ASN:O	5:g:152:GLY:N	2.36	0.50
6:l:335:GLN:HE22	6:m:336:ALA:HB1	1.75	0.50
6:p:255:ARG:H	6:p:395:GLU:HG2	1.76	0.50
3:A:129:LEU:HD13	3:F:121:ILE:HG12	1.91	0.50
4:P:739:ASN:OD1	4:P:742:ARG:NH2	2.44	0.50
4:R:502:SER:HB3	4:R:515:LEU:HB2	1.92	0.50
5:W:162:GLU:OE2	5:f:144:ARG:NH2	2.43	0.50
6:m:289:MET:HE2	6:m:334:LYS:HZ3	1.75	0.50
6:t:168:VAL:HG23	6:t:179:MET:HB3	1.93	0.50
1:8:3:PHE:HA	6:p:525:ALA:HB1	1.93	0.50
4:P:51:LEU:HD11	4:P:575:ARG:HB2	1.93	0.50
6:r:73:LEU:HD21	6:r:388:VAL:HG23	1.93	0.50
4:x:46:PRO:HB2	4:x:576:ILE:HG23	1.93	0.50
1:AC:5:PRO:CD	6:j:523:MET:HE3	2.41	0.50
3:M:9:LEU:HD13	3:M:23:PRO:HG3	1.93	0.50
3:O:22:ILE:HD11	3:O:58:ILE:HG13	1.92	0.50
4:Q:109:THR:OG1	4:Q:115:ASP:OD2	2.26	0.50
4:R:46:PRO:HB2	4:R:576:ILE:HG23	1.93	0.50
4:T:531:LEU:HD12	4:T:536:ARG:HG3	1.92	0.50
3:c:95:ARG:NH2	3:c:98:ASP:OD1	2.43	0.50
6:l:405:LEU:HD22	6:l:417:LEU:HD11	1.92	0.50
6:o:220:ASP:HB2	6:o:227:LEU:HG	1.94	0.50
6:q:368:ARG:NH2	6:q:370:THR:OG1	2.45	0.50
6:s:290:SER:HB3	6:t:344:VAL:HG21	1.93	0.50
6:u:386:GLY:HA2	6:u:389:TYR:CE1	2.47	0.50
4:S:365:ASN:HA	4:S:394:ALA:HA	1.94	0.50
6:j:169:GLN:HE22	6:u:208:ASP:HB2	1.76	0.50
6:l:184:GLN:HB2	6:m:172:ALA:HB3	1.94	0.50
6:n:510:GLN:HG2	6:o:507:ALA:HB2	1.94	0.50
6:p:64:ARG:NH1	6:p:360:SER:OG	2.43	0.50
6:s:137:LEU:HB3	6:s:256:MET:HB2	1.93	0.50
6:t:255:ARG:HB3	6:t:265:GLY:HA3	1.93	0.50
3:A:10:THR:HG23	5:V:73:VAL:HG22	1.91	0.50
3:N:13:LEU:HD12	3:N:20:PHE:HE1	1.76	0.50
4:Q:44:LYS:HG3	4:Q:776:LEU:HG	1.92	0.50
4:R:364:GLU:HB2	4:R:395:VAL:HG12	1.93	0.50
5:V:194:LEU:HD22	6:p:288:LYS:HG2	1.93	0.50
6:j:64:ARG:NH1	6:j:360:SER:OG	2.43	0.50
6:s:228:ARG:HH12	6:s:230:GLU:HG3	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:t:184:GLN:HB2	6:u:172:ALA:HB3	1.94	0.50
1:AC:4:SER:HB2	6:k:526:ALA:HB2	1.93	0.50
3:C:10:THR:HG23	5:W:73:VAL:HG22	1.93	0.50
3:F:12:GLN:HA	3:F:72:THR:HG22	1.93	0.50
3:G:120:THR:HG22	3:G:121:ILE:H	1.77	0.50
4:Q:44:LYS:NZ	4:Q:772:GLU:O	2.45	0.50
4:T:686:GLN:O	4:T:694:SER:N	2.45	0.50
6:n:527:ALA:O	6:n:532:LEU:N	2.45	0.50
6:p:118:MET:O	6:p:122:GLU:HG3	2.11	0.50
6:s:370:THR:OG1	6:s:373:GLU:OE1	2.20	0.50
4:x:184:GLN:HB2	4:x:187:HIS:CD2	2.47	0.50
4:Q:4:ILE:HD11	4:Q:701:LEU:HD13	1.94	0.50
4:T:44:LYS:HG3	4:T:776:LEU:HG	1.93	0.50
4:T:67:HIS:CG	4:T:118:MET:HG2	2.47	0.50
5:X:155:GLU:H	5:X:155:GLU:CD	2.20	0.50
6:n:205:LYS:HD2	6:n:209:GLU:HG2	1.94	0.50
6:t:527:ALA:O	6:t:532:LEU:N	2.45	0.50
1:5:5:PRO:HG3	6:r:523:MET:HE1	1.94	0.50
1:AB:3:PHE:HA	6:l:525:ALA:HB1	1.94	0.50
4:R:736:LEU:HD11	3:a:99:LEU:HD12	1.93	0.50
4:S:154:ILE:HB	4:S:220:ILE:HB	1.93	0.50
4:T:136:LYS:HA	4:T:303:VAL:HA	1.93	0.50
5:U:176:MET:HG3	6:p:321:THR:HG23	1.93	0.50
6:j:208:ASP:HB2	6:k:169:GLN:HE22	1.77	0.50
6:s:40:PRO:HB2	6:s:54:TYR:HB3	1.94	0.50
4:x:285:ASP:O	4:x:289:LYS:N	2.45	0.50
3:B:95:ARG:NH1	5:h:34:GLY:O	2.45	0.49
3:B:99:LEU:HD12	4:Q:736:LEU:HD11	1.93	0.49
6:m:40:PRO:HB2	6:m:54:TYR:HB3	1.94	0.49
6:n:65:GLY:HA2	6:n:358:LEU:HD21	1.94	0.49
6:o:290:SER:HB3	6:p:344:VAL:HG21	1.93	0.49
6:o:501:MET:HE1	6:p:492:MET:HE2	1.94	0.49
6:r:506:ALA:O	6:r:510:GLN:HG3	2.12	0.49
4:x:599:ARG:HH21	4:x:666:MET:HE1	1.76	0.49
1:4:5:PRO:CG	6:s:523:MET:HE1	2.33	0.49
4:Q:288:ARG:HB3	4:Q:290:VAL:HG22	1.94	0.49
4:Q:357:ARG:NH2	4:Q:387:ASP:O	2.45	0.49
4:Q:586:GLN:OE1	4:Q:599:ARG:NH2	2.45	0.49
5:W:147:ASN:O	5:W:152:GLY:N	2.33	0.49
5:W:194:LEU:HD22	6:n:288:LYS:HG2	1.93	0.49
6:k:289:MET:HE2	6:k:334:LYS:NZ	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:m:442:LEU:HD11	6:n:469:ARG:HB3	1.94	0.49
1:AC:15:ASN:HB2	6:k:533:GLN:OE1	2.12	0.49
3:B:27:LEU:HD23	3:B:108:HIS:HD2	1.76	0.49
3:G:12:GLN:HA	3:G:72:THR:HG22	1.94	0.49
4:S:728:LYS:H	5:d:36:ALA:HB1	1.77	0.49
4:T:44:LYS:NZ	4:T:772:GLU:O	2.45	0.49
6:l:117:ILE:HD13	6:l:408:LEU:HD12	1.94	0.49
6:n:506:ALA:HB1	6:o:503:ASN:HD22	1.77	0.49
6:o:386:GLY:HA2	6:o:389:TYR:CE1	2.47	0.49
6:r:368:ARG:HH22	6:r:370:THR:HB	1.77	0.49
1:AB:5:PRO:HB2	6:l:512:MET:HE3	1.95	0.49
3:B:10:THR:HG23	5:h:73:VAL:HG22	1.93	0.49
3:K:13:LEU:HD12	3:K:20:PHE:HE1	1.77	0.49
5:U:155:GLU:H	5:U:155:GLU:CD	2.20	0.49
5:f:193:LEU:HG	6:n:281:ASN:HB3	1.93	0.49
6:j:386:GLY:HA2	6:j:389:TYR:CE1	2.47	0.49
6:k:368:ARG:NH2	6:k:370:THR:OG1	2.45	0.49
6:l:255:ARG:HB3	6:l:265:GLY:HA3	1.95	0.49
6:r:184:GLN:HB2	6:s:172:ALA:HB3	1.95	0.49
1:7:5:PRO:HD3	6:p:523:MET:HE3	1.94	0.49
1:AB:13:ASP:HB3	6:l:533:GLN:HB3	1.94	0.49
3:O:120:THR:HG23	3:O:121:ILE:HG22	1.93	0.49
4:R:165:LEU:HD11	4:R:196:LEU:HD13	1.94	0.49
4:S:44:LYS:NZ	4:S:772:GLU:O	2.46	0.49
6:j:14:LYS:O	6:j:18:GLU:HG3	2.13	0.49
6:o:208:ASP:HB2	6:p:169:GLN:HE22	1.77	0.49
6:t:484:THR:O	6:t:488:LYS:HG3	2.13	0.49
3:C:99:LEU:HD12	4:T:736:LEU:HD11	1.93	0.49
4:P:154:ILE:HB	4:P:220:ILE:HB	1.93	0.49
4:S:721:GLU:OE2	4:S:767:TYR:OH	2.26	0.49
4:T:586:GLN:OE1	4:T:599:ARG:NH2	2.45	0.49
3:a:107:MET:HE1	3:b:105:GLN:HG2	1.93	0.49
5:e:144:ARG:HA	5:e:160:LEU:HD13	1.93	0.49
6:p:14:LYS:O	6:p:18:GLU:HG3	2.13	0.49
6:u:370:THR:OG1	6:u:373:GLU:OE1	2.21	0.49
4:x:38:GLU:OE2	4:x:527:LYS:NZ	2.37	0.49
1:4:12:MET:HB3	6:t:532:LEU:HB3	1.95	0.49
4:S:16:SER:HB3	4:S:23:ARG:HD3	1.95	0.49
6:m:115:ARG:NH1	6:n:90:GLU:OE2	2.46	0.49
6:m:386:GLY:HA2	6:m:389:TYR:CE2	2.47	0.49
6:q:527:ALA:O	6:q:532:LEU:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:t:69:LEU:HD21	6:t:268:TYR:CD2	2.47	0.49
6:t:405:LEU:HD22	6:t:417:LEU:HD11	1.94	0.49
1:3:7:ILE:HA	6:u:530:VAL:HG21	1.94	0.49
1:6:10:PRO:HD2	6:s:512:MET:HE1	1.95	0.49
3:O:13:LEU:HD12	3:O:20:PHE:HE1	1.77	0.49
4:P:728:LYS:H	5:g:36:ALA:HB1	1.77	0.49
4:T:125:THR:OG1	4:T:312:LEU:O	2.28	0.49
5:i:193:LEU:HG	6:j:281:ASN:HB3	1.95	0.49
6:p:386:GLY:HA2	6:p:389:TYR:CE1	2.47	0.49
3:D:107:MET:HE1	3:I:105:GLN:HG2	1.94	0.49
4:P:44:LYS:NZ	4:P:772:GLU:O	2.46	0.49
4:T:71:ARG:HH22	4:T:125:THR:HG23	1.77	0.49
5:V:14:LEU:HA	5:V:32:LEU:HD11	1.94	0.49
5:e:193:LEU:HG	6:p:281:ASN:HB3	1.95	0.49
6:j:290:SER:HB3	6:k:344:VAL:HG21	1.95	0.49
6:l:368:ARG:HH22	6:l:370:THR:HB	1.77	0.49
6:n:69:LEU:HD21	6:n:268:TYR:CD2	2.47	0.49
4:x:165:LEU:HD11	4:x:196:LEU:HD13	1.94	0.49
1:0:5:PRO:O	1:AA:11:LYS:HG2	2.13	0.49
3:A:25:GLU:HG2	5:d:9:GLU:HG2	1.93	0.49
4:Q:423:VAL:HG12	4:Q:425:THR:HG23	1.95	0.49
4:S:632:THR:HG23	4:S:640:ILE:HG23	1.94	0.49
6:n:195:ARG:O	6:n:199:GLU:HG3	2.11	0.49
3:M:110:ALA:O	3:M:114:ARG:HG2	2.13	0.48
4:P:16:SER:HB3	4:P:23:ARG:HD3	1.95	0.48
4:P:645:GLN:HG2	4:P:646:PRO:O	2.12	0.48
4:Q:67:HIS:CG	4:Q:118:MET:HG2	2.47	0.48
4:R:184:GLN:HB2	4:R:187:HIS:CD2	2.47	0.48
5:X:154:PRO:HG2	5:X:155:GLU:OE1	2.12	0.48
5:e:169:ARG:O	5:e:173:GLU:HG3	2.13	0.48
6:j:423:GLU:OE1	6:j:423:GLU:N	2.45	0.48
6:m:290:SER:HB3	6:n:344:VAL:HG21	1.95	0.48
6:q:289:MET:HE2	6:q:334:LYS:NZ	2.28	0.48
6:t:172:ALA:HA	6:t:261:GLY:HA2	1.95	0.48
6:u:24:ARG:HD3	6:u:167:VAL:HG12	1.95	0.48
1:3:4:SER:HB3	6:u:516:ALA:HA	1.95	0.48
1:6:3:PHE:HA	6:r:525:ALA:HB1	1.95	0.48
4:S:51:LEU:HD11	4:S:575:ARG:HB2	1.94	0.48
5:V:130:MET:HE2	5:V:130:MET:HA	1.95	0.48
6:l:73:LEU:HD21	6:l:388:VAL:HG23	1.94	0.48
6:s:144:LEU:HB3	6:s:161:TYR:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:12:GLN:HA	3:I:72:THR:HG22	1.94	0.48
4:R:285:ASP:O	4:R:289:LYS:N	2.45	0.48
5:U:147:ASN:O	5:U:152:GLY:N	2.38	0.48
3:b:12:GLN:HA	3:b:72:THR:HG22	1.94	0.48
3:C:130:ASP:OD1	3:H:138:ASN:ND2	2.42	0.48
3:J:12:GLN:HA	3:J:72:THR:HG22	1.95	0.48
4:P:715:THR:HA	4:P:731:MET:O	2.13	0.48
6:k:86:LEU:HD23	6:k:423:GLU:HB3	1.94	0.48
6:p:39:ILE:HD12	6:p:66:LEU:HD23	1.94	0.48
6:t:132:GLU:OE1	6:u:258:ARG:NH2	2.46	0.48
6:u:306:THR:HG22	6:u:326:ASP:HB2	1.96	0.48
3:E:76:ARG:NH2	3:E:119:ASP:OD2	2.47	0.48
4:Q:167:VAL:HG12	4:Q:175:ALA:HB3	1.94	0.48
4:R:332:CYS:SG	4:R:382:ILE:HG12	2.54	0.48
4:T:78:TYR:HD2	4:T:564:ILE:HD11	1.79	0.48
4:T:288:ARG:HB3	4:T:290:VAL:HG22	1.94	0.48
4:T:794:ILE:HD11	2:z:87:LEU:HD21	1.95	0.48
5:i:24:ILE:HG13	5:i:26:GLU:HG2	1.96	0.48
6:n:172:ALA:HA	6:n:261:GLY:HA2	1.95	0.48
6:s:517:THR:HG21	6:t:511:GLY:HA3	1.95	0.48
3:L:110:ALA:O	3:L:114:ARG:HG2	2.13	0.48
3:N:92:SER:HA	4:x:640:ILE:HD12	1.96	0.48
4:Q:68:LEU:HD13	4:Q:78:TYR:HE1	1.78	0.48
4:S:700:ARG:NH2	5:U:26:GLU:OE2	2.47	0.48
4:S:715:THR:HA	4:S:731:MET:O	2.14	0.48
6:j:172:ALA:HA	6:j:261:GLY:HA2	1.94	0.48
6:o:306:THR:HG22	6:o:326:ASP:HB2	1.96	0.48
6:o:423:GLU:HG2	6:o:423:GLU:O	2.14	0.48
6:o:506:ALA:O	6:o:510:GLN:HG3	2.14	0.48
6:t:498:GLN:OE1	6:u:492:MET:HG3	2.14	0.48
6:u:423:GLU:HG2	6:u:423:GLU:O	2.14	0.48
4:x:66:ILE:HD13	4:x:564:ILE:HD12	1.96	0.48
4:x:68:LEU:HD13	4:x:78:TYR:HE1	1.78	0.48
4:x:703:LEU:N	4:x:759:GLY:O	2.43	0.48
3:D:55:ARG:HH21	5:X:2:ARG:HE	1.61	0.48
5:Z:147:ASN:O	5:Z:152:GLY:N	2.32	0.48
6:n:484:THR:O	6:n:488:LYS:HG3	2.13	0.48
6:q:397:GLN:HB3	6:q:425:THR:HG21	1.96	0.48
6:s:220:ASP:HB2	6:s:227:LEU:HG	1.95	0.48
4:x:118:MET:HE3	4:x:125:THR:HB	1.96	0.48
1:AB:13:ASP:HB2	6:l:536:ILE:HG22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:109:THR:OG1	4:P:115:ASP:OD2	2.29	0.48
4:P:722:ASN:OD1	4:P:725:SER:N	2.39	0.48
4:S:464:ARG:O	4:S:498:ASN:ND2	2.34	0.48
5:d:193:LEU:HG	6:r:281:ASN:HB3	1.96	0.48
5:e:24:ILE:HG13	5:e:26:GLU:HG2	1.95	0.48
6:s:255:ARG:H	6:s:395:GLU:HG2	1.78	0.48
6:s:289:MET:HE2	6:s:334:LYS:NZ	2.29	0.48
3:L:84:ARG:HA	3:L:105:GLN:HE22	1.79	0.48
3:O:25:GLU:O	3:O:77:ARG:NH1	2.44	0.48
4:P:793:GLY:HA3	2:v:87:LEU:C	2.39	0.48
4:Q:78:TYR:HD2	4:Q:564:ILE:HD11	1.78	0.48
4:R:66:ILE:HD13	4:R:564:ILE:HD12	1.96	0.48
4:R:167:VAL:HG12	4:R:175:ALA:HB3	1.95	0.48
4:R:288:ARG:HB3	4:R:290:VAL:HG22	1.96	0.48
4:T:188:VAL:O	4:T:191:THR:HG22	2.14	0.48
4:T:314:ARG:HH11	4:T:318:GLY:HA2	1.79	0.48
5:U:187:ASP:OD1	6:r:295:LYS:NZ	2.43	0.48
6:j:39:ILE:HD12	6:j:66:LEU:HD23	1.94	0.48
6:n:14:LYS:O	6:n:18:GLU:HG3	2.13	0.48
1:3:3:PHE:HA	6:u:525:ALA:HB1	1.95	0.48
3:C:9:LEU:HG	3:C:23:PRO:HG2	1.95	0.48
4:Q:188:VAL:O	4:Q:191:THR:HG22	2.14	0.48
4:T:357:ARG:NH1	4:T:389:ASP:O	2.44	0.48
5:U:2:ARG:HE	3:a:55:ARG:HH21	1.60	0.48
3:c:25:GLU:O	3:c:77:ARG:NH1	2.41	0.48
5:g:193:LEU:HG	6:l:281:ASN:HB3	1.96	0.48
6:k:82:THR:HA	6:k:118:MET:HE2	1.96	0.48
6:m:220:ASP:HB2	6:m:227:LEU:HG	1.94	0.48
6:r:255:ARG:HB3	6:r:265:GLY:HA3	1.95	0.48
6:s:89:SER:HB3	6:s:92:GLU:HB2	1.96	0.48
4:x:154:ILE:HB	4:x:220:ILE:HB	1.95	0.48
3:C:81:THR:HG23	3:M:107:MET:HE3	1.95	0.47
3:M:124:ASN:HB3	3:M:130:ASP:HB2	1.94	0.47
4:R:118:MET:HE3	4:R:125:THR:HB	1.96	0.47
4:S:285:ASP:O	4:S:289:LYS:N	2.43	0.47
4:T:78:TYR:CD2	4:T:564:ILE:HD11	2.49	0.47
6:q:255:ARG:HB3	6:q:265:GLY:HA3	1.95	0.47
1:9:11:LYS:NZ	6:o:534:PRO:O	2.46	0.47
4:P:464:ARG:O	4:P:498:ASN:ND2	2.34	0.47
4:R:141:VAL:HG22	4:R:300:GLU:HG2	1.96	0.47
5:V:179:GLY:HA3	5:V:181:TYR:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:147:ASN:O	5:X:152:GLY:N	2.37	0.47
5:h:194:LEU:HD22	6:t:288:LYS:HG2	1.94	0.47
6:o:24:ARG:HD3	6:o:167:VAL:HG12	1.95	0.47
6:s:523:MET:HE3	6:t:512:MET:HG2	1.96	0.47
4:P:285:ASP:O	4:P:289:LYS:N	2.45	0.47
4:S:596:MET:HA	4:S:596:MET:HE2	1.96	0.47
6:l:386:GLY:HA2	6:l:389:TYR:HE1	1.78	0.47
4:x:188:VAL:O	4:x:191:THR:HG22	2.15	0.47
3:C:25:GLU:HG2	5:e:8:VAL:HA	1.97	0.47
4:R:68:LEU:HD13	4:R:78:TYR:HE1	1.78	0.47
5:U:15:SER:O	5:d:45:ARG:NH2	2.47	0.47
5:X:187:ASP:OD1	6:l:295:LYS:NZ	2.43	0.47
5:Y:130:MET:HE2	5:Y:130:MET:HA	1.95	0.47
5:i:169:ARG:O	5:i:173:GLU:HG3	2.14	0.47
6:k:255:ARG:HB3	6:k:265:GLY:HA3	1.96	0.47
6:m:77:LEU:O	6:m:397:GLN:NE2	2.48	0.47
6:p:255:ARG:HB3	6:p:265:GLY:HA3	1.94	0.47
6:r:386:GLY:HA2	6:r:389:TYR:HE1	1.78	0.47
6:s:289:MET:HE2	6:s:334:LYS:HZ3	1.80	0.47
3:B:9:LEU:HG	3:B:23:PRO:HG2	1.96	0.47
3:E:60:LEU:HD11	3:E:73:ILE:HD12	1.97	0.47
3:G:45:THR:HB	3:G:48:THR:HG22	1.95	0.47
6:p:290:SER:HB3	6:q:344:VAL:HG21	1.95	0.47
6:q:13:ALA:N	6:q:231:GLU:OE1	2.45	0.47
3:A:60:LEU:HD11	3:A:73:ILE:HD12	1.95	0.47
3:H:120:THR:HG22	3:H:121:ILE:H	1.80	0.47
6:p:405:LEU:HD22	6:p:417:LEU:HD11	1.97	0.47
1:AC:13:ASP:HB3	6:k:533:GLN:NE2	2.30	0.47
3:C:25:GLU:O	3:C:77:ARG:HD3	2.15	0.47
4:Q:577:SER:O	4:Q:591:ARG:NH2	2.48	0.47
4:Q:684:ILE:HB	4:Q:696:GLU:HB2	1.95	0.47
4:T:68:LEU:HD13	4:T:78:TYR:HE1	1.79	0.47
4:T:167:VAL:HG12	4:T:175:ALA:HB3	1.96	0.47
5:Y:154:PRO:HG2	5:Y:155:GLU:OE1	2.15	0.47
3:b:54:THR:OG1	3:b:57:THR:HG22	2.15	0.47
5:f:169:ARG:O	5:f:173:GLU:HG3	2.14	0.47
6:k:17:TYR:HB2	6:k:180:VAL:HG11	1.97	0.47
6:l:195:ARG:O	6:l:199:GLU:HG2	2.14	0.47
6:m:477:ASP:HB3	6:n:469:ARG:HH22	1.79	0.47
6:n:357:MET:HE3	6:n:381:LEU:O	2.15	0.47
6:n:405:LEU:HD22	6:n:417:LEU:HD11	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:n:498:GLN:OE1	6:o:492:MET:HG3	2.15	0.47
6:s:481:ILE:HG23	6:t:466:ILE:HD11	1.96	0.47
6:t:255:ARG:NH1	6:t:395:GLU:OE1	2.47	0.47
4:x:700:ARG:NE	4:x:702:GLN:OE1	2.48	0.47
1:AA:5:PRO:O	1:AB:11:LYS:HG2	2.14	0.47
3:B:81:THR:HG23	3:L:107:MET:HE3	1.96	0.47
4:R:188:VAL:O	4:R:191:THR:HG22	2.15	0.47
4:T:684:ILE:HB	4:T:696:GLU:HB2	1.97	0.47
5:Z:144:ARG:NH2	5:h:162:GLU:OE1	2.47	0.47
3:a:25:GLU:O	3:a:77:ARG:HD3	2.15	0.47
3:b:137:VAL:HG23	3:b:138:ASN:ND2	2.30	0.47
6:j:255:ARG:HB3	6:j:265:GLY:HA3	1.96	0.47
6:q:17:TYR:HB2	6:q:180:VAL:HG11	1.97	0.47
6:q:353:SER:HA	6:q:358:LEU:HD12	1.97	0.47
6:t:205:LYS:HD2	6:t:209:GLU:HG2	1.95	0.47
4:x:479:VAL:HG11	4:x:482:VAL:HG23	1.96	0.47
4:x:714:GLY:HA3	4:x:774:THR:HB	1.97	0.47
1:AA:3:PHE:HA	6:m:525:ALA:HB1	1.97	0.47
4:Q:314:ARG:HH11	4:Q:318:GLY:HA2	1.79	0.47
4:R:700:ARG:NE	4:R:702:GLN:OE1	2.48	0.47
4:T:16:SER:HB3	4:T:23:ARG:HD3	1.96	0.47
6:j:118:MET:O	6:j:122:GLU:HG3	2.15	0.47
6:k:290:SER:HB3	6:l:344:VAL:HG21	1.97	0.47
6:m:289:MET:HE2	6:m:334:LYS:NZ	2.29	0.47
6:s:306:THR:HG21	6:s:327:ILE:HG12	1.97	0.47
6:t:290:SER:HB3	6:u:344:VAL:HG21	1.97	0.47
6:t:357:MET:HE1	6:t:385:LEU:HB2	1.96	0.47
6:u:144:LEU:HB3	6:u:161:TYR:HB2	1.97	0.47
4:x:317:ASP:OD2	4:x:317:ASP:N	2.47	0.47
1:AD:13:ASP:HB3	6:j:533:GLN:HB3	1.96	0.47
3:O:83:ASP:O	3:O:105:GLN:NE2	2.48	0.47
4:P:700:ARG:NH2	5:X:26:GLU:OE1	2.47	0.47
4:Q:67:HIS:CD2	4:Q:118:MET:HG2	2.50	0.47
5:Z:141:LYS:HG3	5:Z:164:GLU:OE2	2.15	0.47
5:d:187:ASP:OD1	6:q:295:LYS:NZ	2.45	0.47
5:f:36:ALA:HB1	4:x:728:LYS:H	1.80	0.47
5:i:169:ARG:HG3	5:i:170:LEU:HD22	1.96	0.47
6:o:435:ARG:NH2	6:p:472:ASN:OD1	2.47	0.47
4:x:617:HIS:CE1	4:x:619:PRO:HD2	2.50	0.47
1:6:12:MET:HB3	6:r:532:LEU:HB3	1.97	0.46
1:9:4:SER:HB3	6:o:516:ALA:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:60:LEU:HD11	3:B:73:ILE:HD12	1.97	0.46
3:E:10:THR:HG21	5:Y:74:TYR:CE2	2.50	0.46
3:I:137:VAL:HG23	3:I:138:ASN:ND2	2.29	0.46
4:P:357:ARG:HG2	4:P:371:THR:HA	1.97	0.46
4:T:728:LYS:H	5:e:36:ALA:HB1	1.80	0.46
6:k:397:GLN:HB3	6:k:425:THR:HG21	1.96	0.46
6:m:255:ARG:HB3	6:m:265:GLY:HA3	1.95	0.46
6:m:481:ILE:HG23	6:n:466:ILE:HD11	1.96	0.46
6:n:297:ILE:HD12	6:n:330:LEU:HD23	1.97	0.46
6:o:305:ILE:HD11	6:o:323:ARG:HG3	1.97	0.46
6:q:527:ALA:HA	6:q:532:LEU:HB2	1.97	0.46
6:t:306:THR:HG21	6:t:327:ILE:HG12	1.97	0.46
4:x:288:ARG:HB3	4:x:290:VAL:HG22	1.96	0.46
1:3:3:PHE:HE2	1:4:12:MET:HE1	1.80	0.46
4:R:585:LEU:HD22	4:R:599:ARG:HB2	1.98	0.46
5:i:99:ARG:NH2	5:i:111:ASP:OD2	2.39	0.46
5:i:137:TRP:HA	5:i:167:ALA:HB1	1.98	0.46
6:j:260:ASP:OD2	6:u:162:ARG:HD3	2.15	0.46
6:j:405:LEU:HD22	6:j:417:LEU:HD11	1.96	0.46
6:m:144:LEU:HB3	6:m:161:TYR:HB2	1.95	0.46
6:q:74:MET:HE3	6:q:78:PHE:HB2	1.98	0.46
6:q:513:ALA:HB1	6:r:508:LEU:HA	1.96	0.46
6:t:187:PHE:HZ	6:t:199:GLU:HG2	1.80	0.46
3:I:54:THR:OG1	3:I:57:THR:HG22	2.15	0.46
4:Q:16:SER:HB3	4:Q:23:ARG:HD3	1.96	0.46
4:R:75:GLU:HG3	4:R:314:ARG:NH1	2.30	0.46
4:R:317:ASP:OD1	4:R:317:ASP:N	2.47	0.46
4:T:577:SER:O	4:T:591:ARG:NH2	2.48	0.46
5:Y:136:TYR:HE1	5:i:49:LYS:HE3	1.81	0.46
6:j:492:MET:HE1	6:u:494:GLN:NE2	2.30	0.46
6:q:255:ARG:H	6:q:395:GLU:HG2	1.81	0.46
4:x:141:VAL:HG22	4:x:300:GLU:HG2	1.96	0.46
1:AA:12:MET:H	1:AA:12:MET:HG2	1.42	0.46
3:D:76:ARG:NH2	3:D:119:ASP:OD2	2.49	0.46
4:P:188:VAL:O	4:P:191:THR:HG22	2.15	0.46
4:P:365:ASN:HA	4:P:394:ALA:HA	1.98	0.46
4:P:479:VAL:HG22	4:x:477:GLN:O	2.15	0.46
4:R:714:GLY:HA3	4:R:774:THR:HB	1.97	0.46
4:S:197:ALA:HA	4:S:220:ILE:HD11	1.97	0.46
3:a:60:LEU:HD11	3:a:73:ILE:HD12	1.97	0.46
6:k:494:GLN:NE2	6:l:492:MET:SD	2.89	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:n:357:MET:HE1	6:n:385:LEU:HB2	1.97	0.46
6:p:89:SER:OG	6:p:92:GLU:HB2	2.15	0.46
6:p:297:ILE:HD12	6:p:330:LEU:HD23	1.96	0.46
6:q:73:LEU:HD21	6:q:388:VAL:HG23	1.98	0.46
6:q:86:LEU:HD23	6:q:423:GLU:HB3	1.98	0.46
6:s:198:VAL:HG22	6:s:232:VAL:HG11	1.97	0.46
6:u:97:LEU:HD11	6:u:103:LEU:HB2	1.97	0.46
2:1:87:LEU:C	4:R:793:GLY:HA3	2.41	0.46
3:B:25:GLU:O	3:B:77:ARG:HD3	2.16	0.46
3:C:60:LEU:HD11	3:C:73:ILE:HD12	1.96	0.46
3:G:107:MET:HE1	3:L:105:GLN:HG2	1.97	0.46
4:P:414:LEU:HD23	4:P:416:TRP:HE1	1.81	0.46
4:Q:589:PRO:HD3	4:Q:636:PRO:HA	1.97	0.46
6:j:89:SER:OG	6:j:92:GLU:HB2	2.16	0.46
6:o:73:LEU:HD22	6:o:389:TYR:HB3	1.98	0.46
6:o:287:VAL:O	6:o:290:SER:OG	2.29	0.46
6:u:305:ILE:HD11	6:u:323:ARG:HG3	1.97	0.46
1:9:13:ASP:HB3	6:o:533:GLN:NE2	2.30	0.46
3:E:25:GLU:HG2	5:g:9:GLU:HG2	1.97	0.46
3:E:121:ILE:HG13	3:O:129:LEU:HD13	1.97	0.46
3:F:62:LYS:HE3	5:d:72:ASP:HA	1.97	0.46
4:T:357:ARG:NH2	4:T:387:ASP:O	2.49	0.46
5:W:187:ASP:OD1	6:n:295:LYS:NZ	2.48	0.46
6:k:386:GLY:HA2	6:k:389:TYR:CE1	2.50	0.46
6:s:517:THR:HA	6:s:523:MET:HG2	1.97	0.46
6:t:357:MET:HE3	6:t:381:LEU:O	2.16	0.46
2:w:87:LEU:C	4:x:793:GLY:HA3	2.41	0.46
4:x:746:LEU:HD11	4:x:774:THR:HG22	1.98	0.46
3:C:27:LEU:HD21	3:C:104:ILE:HG22	1.98	0.46
3:M:84:ARG:HA	3:M:105:GLN:HE22	1.80	0.46
4:P:464:ARG:HB2	4:P:467:PHE:O	2.16	0.46
4:P:746:LEU:HD11	4:P:774:THR:HG22	1.97	0.46
4:Q:78:TYR:CD2	4:Q:564:ILE:HD11	2.49	0.46
4:Q:617:HIS:CE1	4:Q:619:PRO:HD2	2.50	0.46
4:R:9:LYS:HD2	4:S:21:ILE:HD12	1.98	0.46
4:R:67:HIS:CG	4:R:118:MET:HG2	2.50	0.46
4:S:48:LEU:HD22	4:S:545:PHE:CD1	2.50	0.46
4:S:357:ARG:HG2	4:S:371:THR:HA	1.98	0.46
4:T:477:GLN:O	4:x:479:VAL:HG22	2.15	0.46
3:a:76:ARG:NH2	3:a:119:ASP:OD2	2.48	0.46
3:b:132:ARG:HB2	3:b:134:ARG:NH1	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:73:LEU:HD21	6:k:388:VAL:HG23	1.97	0.46
6:k:144:LEU:HB3	6:k:161:TYR:HB2	1.97	0.46
6:m:517:THR:HA	6:m:523:MET:HG2	1.97	0.46
6:r:24:ARG:HD3	6:r:167:VAL:HG12	1.98	0.46
6:t:14:LYS:O	6:t:18:GLU:HG3	2.16	0.46
6:u:506:ALA:O	6:u:510:GLN:HG3	2.16	0.46
2:2:87:LEU:C	4:Q:793:GLY:HA3	2.41	0.46
1:7:11:LYS:HD3	6:r:529:SER:HB3	1.98	0.46
4:Q:686:GLN:O	4:Q:694:SER:N	2.49	0.46
4:Q:700:ARG:NE	4:Q:702:GLN:OE1	2.49	0.46
4:S:628:ARG:HH11	4:S:645:GLN:HE22	1.64	0.46
5:V:154:PRO:HG2	5:V:155:GLU:OE1	2.15	0.46
6:k:89:SER:HB3	6:k:92:GLU:HB2	1.98	0.46
6:m:306:THR:HG21	6:m:327:ILE:HG12	1.98	0.46
3:A:117:THR:HA	3:A:120:THR:HG22	1.97	0.46
3:I:124:ASN:ND2	3:I:130:ASP:HB2	2.31	0.46
4:P:3:LEU:HD21	5:g:151:PHE:O	2.16	0.46
4:P:438:ASN:HB3	4:x:411:GLU:HA	1.97	0.46
4:S:188:VAL:O	4:S:191:THR:HG22	2.15	0.46
5:f:179:GLY:HA3	5:f:181:TYR:CE2	2.51	0.46
6:k:13:ALA:N	6:k:231:GLU:OE1	2.43	0.46
6:m:89:SER:HB3	6:m:92:GLU:HB2	1.97	0.46
6:o:306:THR:HG21	6:o:327:ILE:HG12	1.98	0.46
6:p:363:GLN:HA	6:q:373:GLU:OE2	2.16	0.46
6:u:357:MET:HE1	6:u:384:THR:OG1	2.15	0.46
4:x:464:ARG:HB2	4:x:467:PHE:O	2.16	0.46
4:S:701:LEU:HD13	4:S:787:TYR:HB2	1.97	0.46
4:T:700:ARG:NE	4:T:702:GLN:OE1	2.47	0.46
5:U:154:PRO:HG2	5:U:155:GLU:OE2	2.16	0.46
5:U:183:MET:HE2	6:p:319:PHE:CZ	2.51	0.46
5:g:187:ASP:OD1	6:k:295:LYS:NZ	2.44	0.46
5:i:50:ILE:HD11	5:i:145:GLN:OE1	2.16	0.46
6:j:297:ILE:HD12	6:j:330:LEU:HD23	1.98	0.46
6:o:144:LEU:HB3	6:o:161:TYR:HB2	1.96	0.46
6:p:46:ASP:OD1	6:p:47:SER:N	2.48	0.46
6:q:144:LEU:HB3	6:q:161:TYR:HB2	1.97	0.46
6:q:386:GLY:HA2	6:q:389:TYR:CE1	2.50	0.46
6:r:397:GLN:HB3	6:r:425:THR:HG21	1.98	0.46
6:s:24:ARG:HD3	6:s:167:VAL:HG12	1.98	0.46
6:u:445:CYS:SG	6:u:474:ILE:HG13	2.56	0.46
4:x:67:HIS:CG	4:x:118:MET:HG2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:97:ILE:HG23	4:x:531:LEU:HD21	1.98	0.45
3:D:25:GLU:O	3:D:77:ARG:HD3	2.15	0.45
4:Q:285:ASP:O	4:Q:289:LYS:N	2.49	0.45
4:R:589:PRO:HD3	4:R:636:PRO:HA	1.98	0.45
5:V:155:GLU:CD	5:V:155:GLU:H	2.24	0.45
5:Y:155:GLU:CD	5:Y:155:GLU:H	2.24	0.45
6:k:255:ARG:H	6:k:395:GLU:HG2	1.81	0.45
6:m:159:LYS:NZ	6:m:160:LEU:O	2.48	0.45
6:m:255:ARG:H	6:m:395:GLU:HG2	1.81	0.45
6:n:353:SER:HB3	6:n:358:LEU:HB2	1.99	0.45
4:S:464:ARG:HB2	4:S:467:PHE:O	2.16	0.45
4:T:48:LEU:HD22	4:T:545:PHE:CD1	2.52	0.45
3:c:49:ASP:O	3:c:61:THR:N	2.49	0.45
5:g:17:VAL:O	5:g:21:LEU:HG	2.17	0.45
6:j:363:GLN:HA	6:k:373:GLU:OE2	2.16	0.45
6:l:24:ARG:HD3	6:l:167:VAL:HG12	1.98	0.45
6:l:397:GLN:HB3	6:l:425:THR:HG21	1.98	0.45
6:n:290:SER:HB3	6:o:344:VAL:HG21	1.98	0.45
4:x:357:ARG:HD3	4:x:369:SER:O	2.17	0.45
4:x:715:THR:HA	4:x:731:MET:O	2.16	0.45
1:5:5:PRO:O	1:6:11:LYS:HG2	2.16	0.45
3:A:10:THR:HG21	5:V:74:TYR:CE2	2.51	0.45
3:I:132:ARG:HB2	3:I:134:ARG:NH1	2.31	0.45
3:J:62:LYS:HE3	5:g:72:ASP:HA	1.97	0.45
3:M:24:PHE:HE1	3:M:32:VAL:HG22	1.82	0.45
4:P:165:LEU:HD22	4:P:196:LEU:HD22	1.98	0.45
4:P:332:CYS:SG	4:P:382:ILE:HG12	2.57	0.45
4:Q:357:ARG:HD3	4:Q:369:SER:O	2.16	0.45
4:R:266:MET:HE3	4:R:266:MET:HB3	1.79	0.45
4:S:332:CYS:SG	4:S:382:ILE:HG12	2.56	0.45
4:T:71:ARG:HB2	4:T:75:GLU:HB2	1.98	0.45
5:V:172:MET:O	5:V:176:MET:HG2	2.17	0.45
5:Y:15:SER:O	5:i:45:ARG:NH2	2.50	0.45
6:k:74:MET:HE3	6:k:78:PHE:HB2	1.98	0.45
6:q:66:LEU:HD11	6:q:139:VAL:HB	1.99	0.45
6:t:169:GLN:OE1	6:t:178:GLN:NE2	2.43	0.45
6:u:73:LEU:HD21	6:u:388:VAL:HG23	1.98	0.45
4:x:708:VAL:HG23	4:x:755:PHE:HE1	1.81	0.45
3:F:132:ARG:HH11	3:F:134:ARG:HH22	1.64	0.45
4:Q:728:LYS:H	5:i:36:ALA:HB1	1.81	0.45
4:S:3:LEU:HD21	5:d:151:PHE:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:67:HIS:CD2	4:T:118:MET:HG2	2.51	0.45
5:Z:179:GLY:HA3	5:Z:181:TYR:CE2	2.51	0.45
3:a:129:LEU:HD13	3:b:121:ILE:HG12	1.98	0.45
6:o:73:LEU:HD21	6:o:388:VAL:HG23	1.97	0.45
6:o:445:CYS:SG	6:o:474:ILE:HG13	2.56	0.45
6:p:385:LEU:HD23	6:p:389:TYR:CE1	2.52	0.45
6:q:220:ASP:HB2	6:q:227:LEU:HG	1.98	0.45
6:u:73:LEU:HD22	6:u:389:TYR:HB3	1.98	0.45
4:x:332:CYS:SG	4:x:382:ILE:HG12	2.56	0.45
1:AB:10:PRO:HD2	6:m:512:MET:HE1	1.98	0.45
3:B:25:GLU:HG2	5:i:8:VAL:HA	1.98	0.45
4:R:640:ILE:HD12	3:c:92:SER:HA	1.97	0.45
4:T:589:PRO:HD3	4:T:636:PRO:HA	1.97	0.45
5:W:85:LEU:HD22	5:e:132:GLU:HG2	1.99	0.45
5:W:176:MET:HG3	6:l:321:THR:HG23	1.98	0.45
3:a:13:LEU:HD11	3:a:36:LEU:HD22	1.98	0.45
3:b:124:ASN:ND2	3:b:130:ASP:HB2	2.30	0.45
6:j:380:GLU:HB2	6:u:359:ASN:ND2	2.32	0.45
6:o:362:VAL:HG12	6:o:377:VAL:HG23	1.98	0.45
3:C:4:VAL:HG11	5:W:77:LEU:HD12	1.99	0.45
3:D:129:LEU:HD13	3:I:121:ILE:HG12	1.99	0.45
3:E:133:GLY:H	3:J:138:ASN:HB3	1.81	0.45
4:P:197:ALA:HA	4:P:220:ILE:HD11	1.97	0.45
4:R:90:ASP:OD1	4:R:94:ASN:N	2.46	0.45
4:R:617:HIS:CE1	4:R:619:PRO:HD2	2.51	0.45
4:S:257:LEU:HD11	4:S:282:VAL:HG21	1.99	0.45
4:S:522:LYS:HE3	4:S:542:HIS:CE1	2.52	0.45
4:T:357:ARG:HD3	4:T:369:SER:O	2.16	0.45
4:T:793:GLY:HA3	2:y:87:LEU:C	2.41	0.45
5:Z:148:ASN:ND2	5:Z:157:GLU:OE1	2.50	0.45
5:Z:169:ARG:O	5:Z:173:GLU:HG3	2.16	0.45
5:e:50:ILE:HD11	5:e:145:GLN:OE1	2.17	0.45
5:h:176:MET:HG3	6:r:321:THR:HG23	1.99	0.45
6:k:66:LEU:HD11	6:k:139:VAL:HB	1.99	0.45
6:k:353:SER:HA	6:k:358:LEU:HD12	1.97	0.45
6:q:289:MET:HE2	6:q:334:LYS:HZ3	1.82	0.45
6:t:353:SER:HB3	6:t:358:LEU:HB2	1.98	0.45
1:4:11:LYS:HD2	6:u:529:SER:HB3	1.97	0.45
1:AB:12:MET:HB3	6:l:532:LEU:HB3	1.99	0.45
3:D:10:THR:HG21	5:X:74:TYR:CE2	2.52	0.45
4:P:270:VAL:HG21	4:x:290:VAL:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:212:THR:HB	4:T:223:THR:HB	1.99	0.45
4:T:665:ARG:HH11	4:T:665:ARG:HG3	1.82	0.45
6:m:527:ALA:O	6:m:532:LEU:N	2.50	0.45
6:n:169:GLN:OE1	6:n:178:GLN:NE2	2.43	0.45
6:t:297:ILE:HD12	6:t:330:LEU:HD23	1.98	0.45
6:u:255:ARG:HB3	6:u:265:GLY:HA3	1.98	0.45
3:D:60:LEU:HD11	3:D:73:ILE:HD12	1.97	0.45
3:E:25:GLU:O	3:E:77:ARG:HD3	2.17	0.45
3:G:54:THR:OG1	3:G:57:THR:HG22	2.17	0.45
4:P:290:VAL:HG21	4:Q:270:VAL:HG21	1.99	0.45
4:P:686:GLN:O	4:P:694:SER:N	2.49	0.45
4:S:217:GLN:NE2	4:T:241:ASP:OD1	2.49	0.45
4:S:357:ARG:HD3	4:S:369:SER:O	2.17	0.45
4:S:696:GLU:HG3	2:z:87:LEU:HD22	1.99	0.45
4:T:285:ASP:O	4:T:289:LYS:N	2.49	0.45
6:m:357:MET:SD	6:m:385:LEU:HB2	2.57	0.45
6:n:64:ARG:NH2	6:n:360:SER:OG	2.45	0.45
6:n:255:ARG:NH1	6:n:395:GLU:OE1	2.50	0.45
6:o:359:ASN:ND2	6:p:380:GLU:HB2	2.32	0.45
6:p:510:GLN:HG2	6:q:507:ALA:HB2	1.99	0.45
6:s:190:LEU:HD11	6:s:211:ILE:HG13	1.99	0.45
6:u:362:VAL:HG12	6:u:377:VAL:HG23	1.98	0.45
4:x:414:LEU:HB3	4:x:416:TRP:HE1	1.82	0.45
1:6:5:PRO:HB2	6:r:512:MET:HG2	1.99	0.45
3:D:13:LEU:HD11	3:D:36:LEU:HD22	1.98	0.45
3:I:45:THR:HB	3:I:48:THR:HG22	1.98	0.45
4:P:709:ASN:O	4:P:779:ILE:N	2.48	0.45
4:R:357:ARG:HD3	4:R:369:SER:O	2.16	0.45
4:R:715:THR:HA	4:R:731:MET:O	2.16	0.45
4:R:728:LYS:H	5:Z:36:ALA:HB1	1.81	0.45
4:R:746:LEU:HD11	4:R:774:THR:HG22	1.99	0.45
5:g:50:ILE:HD12	5:g:141:LYS:HE3	1.98	0.45
6:l:131:PHE:CE2	6:l:135:LYS:HD2	2.52	0.45
6:m:24:ARG:HD3	6:m:167:VAL:HG12	1.98	0.45
6:m:77:LEU:HD21	6:m:389:TYR:HB2	1.99	0.45
6:s:49:ASN:OD1	6:s:51:SER:OG	2.30	0.45
6:s:77:LEU:O	6:s:397:GLN:NE2	2.50	0.45
3:A:25:GLU:O	3:A:77:ARG:HD3	2.17	0.45
3:E:116:LEU:HD11	3:O:114:ARG:HD3	1.99	0.45
4:P:357:ARG:HD3	4:P:369:SER:O	2.17	0.45
4:P:357:ARG:NH1	4:P:389:ASP:O	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:531:LEU:HD21	2:y:97:ILE:HG23	1.99	0.45
4:S:414:LEU:HD23	4:S:416:TRP:HE1	1.81	0.45
4:T:607:TYR:HB3	4:T:663:GLU:OE1	2.17	0.45
4:T:700:ARG:NH2	5:V:26:GLU:OE2	2.50	0.45
3:b:45:THR:HB	3:b:48:THR:HG22	1.99	0.45
6:j:16:VAL:HG22	6:j:19:ARG:HH21	1.82	0.45
6:j:226:TYR:CE2	6:j:246:LYS:HD2	2.52	0.45
3:F:101:VAL:HG11	5:d:33:GLU:OE2	2.18	0.44
4:P:701:LEU:HD13	4:P:787:TYR:HB2	1.98	0.44
4:Q:48:LEU:HD22	4:Q:545:PHE:CD1	2.52	0.44
4:S:288:ARG:HB3	4:S:290:VAL:HG22	1.98	0.44
4:S:746:LEU:HD11	4:S:774:THR:HG22	1.98	0.44
4:T:536:ARG:HA	4:T:536:ARG:HD2	1.75	0.44
5:h:60:THR:OG1	5:h:181:TYR:OH	2.25	0.44
6:k:134:LEU:HD23	6:k:137:LEU:HD12	1.99	0.44
6:m:357:MET:HE3	6:m:381:LEU:HB3	1.99	0.44
6:p:16:VAL:HG22	6:p:19:ARG:HH21	1.82	0.44
6:q:134:LEU:HD23	6:q:137:LEU:HD12	2.00	0.44
6:s:73:LEU:HD22	6:s:389:TYR:HB3	1.99	0.44
6:s:208:ASP:HB2	6:t:169:GLN:HE22	1.82	0.44
6:u:255:ARG:NH2	6:u:258:ARG:HB3	2.32	0.44
3:J:101:VAL:HG11	5:g:33:GLU:OE2	2.18	0.44
3:M:74:GLU:OE2	3:M:76:ARG:NH1	2.51	0.44
4:Q:71:ARG:NH2	4:Q:125:THR:HG23	2.33	0.44
4:Q:665:ARG:HH11	4:Q:665:ARG:HG3	1.82	0.44
4:R:414:LEU:HB3	4:R:416:TRP:HE1	1.83	0.44
4:S:414:LEU:HD11	4:S:483:LYS:HE2	1.98	0.44
6:j:329:PHE:HB3	6:k:334:LYS:HD3	1.99	0.44
6:j:449:TRP:HB3	6:k:455:MET:SD	2.56	0.44
6:n:187:PHE:HZ	6:n:199:GLU:HG2	1.82	0.44
6:o:61:VAL:O	6:o:65:GLY:N	2.44	0.44
6:o:357:MET:HE1	6:o:384:THR:OG1	2.16	0.44
6:q:290:SER:HB3	6:r:344:VAL:HG21	1.98	0.44
4:P:522:LYS:HE3	4:P:542:HIS:CE1	2.52	0.44
4:Q:536:ARG:HA	4:Q:536:ARG:HD2	1.74	0.44
4:R:464:ARG:HB2	4:R:467:PHE:O	2.16	0.44
5:U:74:TYR:CE2	3:a:10:THR:HG21	2.52	0.44
5:U:169:ARG:O	5:U:173:GLU:HG3	2.17	0.44
5:V:136:TYR:CE1	5:e:53:GLN:HG3	2.52	0.44
5:V:136:TYR:HE1	5:e:49:LYS:HE3	1.81	0.44
6:m:513:ALA:O	6:m:517:THR:HG22	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:r:131:PHE:CE2	6:r:135:LYS:HD2	2.52	0.44
6:t:82:THR:HA	6:t:118:MET:HE2	2.00	0.44
6:u:306:THR:HG21	6:u:327:ILE:HG12	1.98	0.44
6:u:398:LEU:HD23	6:u:398:LEU:HA	1.83	0.44
4:Q:607:TYR:HB3	4:Q:663:GLU:OE1	2.16	0.44
4:R:216:GLY:HA3	4:R:219:PHE:CZ	2.53	0.44
4:R:714:GLY:N	4:R:775:PRO:O	2.28	0.44
4:S:44:LYS:HE3	4:S:776:LEU:HD23	1.99	0.44
4:S:793:GLY:HA3	2:z:87:LEU:C	2.41	0.44
5:e:187:ASP:OD1	6:o:295:LYS:NZ	2.43	0.44
6:k:359:ASN:ND2	6:l:380:GLU:HB2	2.33	0.44
6:l:323:ARG:HB2	6:l:326:ASP:OD2	2.18	0.44
6:n:131:PHE:CE2	6:n:135:LYS:HD2	2.53	0.44
6:q:359:ASN:ND2	6:r:380:GLU:HB2	2.33	0.44
6:s:413:GLN:HA	6:t:92:GLU:OE2	2.17	0.44
6:u:71:SER:O	6:u:75:LEU:HG	2.17	0.44
4:x:589:PRO:HD3	4:x:636:PRO:HA	1.99	0.44
1:AC:7:ILE:HA	6:k:530:VAL:HG21	1.99	0.44
3:D:106:THR:HG23	3:N:107:MET:HG2	2.00	0.44
3:H:54:THR:OG1	3:H:57:THR:HG22	2.17	0.44
3:N:85:LEU:H	3:N:105:GLN:NE2	2.15	0.44
3:O:49:ASP:O	3:O:61:THR:N	2.50	0.44
4:R:741:LEU:HG	3:a:94:LEU:HB2	2.00	0.44
4:T:42:LEU:HD12	4:T:42:LEU:HA	1.89	0.44
5:Y:136:TYR:CE1	5:i:53:GLN:HG3	2.52	0.44
5:d:169:ARG:O	5:d:173:GLU:HG3	2.17	0.44
6:k:289:MET:HE2	6:k:334:LYS:HZ3	1.82	0.44
4:x:88:VAL:HG11	4:x:320:PHE:CE1	2.53	0.44
4:Q:212:THR:HB	4:Q:223:THR:HB	1.99	0.44
4:S:290:VAL:HG21	4:T:270:VAL:HG21	1.99	0.44
4:T:525:MET:HE3	4:T:525:MET:HB3	1.86	0.44
5:V:15:SER:O	5:e:45:ARG:NH2	2.50	0.44
5:d:17:VAL:O	5:d:21:LEU:HG	2.17	0.44
6:m:413:GLN:HA	6:n:92:GLU:OE2	2.17	0.44
6:u:228:ARG:HD2	6:u:244:TYR:CE2	2.53	0.44
4:x:266:MET:HE3	4:x:266:MET:HB3	1.79	0.44
1:4:11:LYS:HG2	1:4:11:LYS:O	2.17	0.44
3:F:46:ILE:HD12	3:F:50:TYR:CE2	2.53	0.44
3:I:84:ARG:HA	3:I:105:GLN:HE22	1.82	0.44
4:S:323:LYS:HG3	4:S:324:TRP:O	2.17	0.44
5:X:169:ARG:O	5:X:173:GLU:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:144:ARG:HA	5:Z:160:LEU:HD13	2.00	0.44
5:d:144:ARG:HA	5:d:160:LEU:HD13	1.99	0.44
6:n:8:LEU:HD13	6:n:178:GLN:HB3	2.00	0.44
6:o:71:SER:O	6:o:75:LEU:HG	2.17	0.44
6:s:445:CYS:SG	6:s:474:ILE:HG13	2.58	0.44
6:t:46:ASP:OD1	6:t:47:SER:N	2.50	0.44
6:t:91:TYR:O	6:t:95:GLN:HG2	2.18	0.44
6:u:61:VAL:O	6:u:65:GLY:N	2.42	0.44
4:x:153:LEU:HB2	4:x:247:VAL:HB	1.98	0.44
3:D:9:LEU:HG	3:D:23:PRO:HG2	1.99	0.44
4:R:78:TYR:HD2	4:R:564:ILE:HD11	1.82	0.44
4:S:66:ILE:HD13	4:S:564:ILE:HD12	2.00	0.44
4:T:464:ARG:HB2	4:T:467:PHE:O	2.18	0.44
5:g:169:ARG:O	5:g:173:GLU:HG3	2.18	0.44
6:j:74:MET:HE3	6:j:78:PHE:HB2	2.00	0.44
6:l:198:VAL:HG22	6:l:232:VAL:HG11	1.98	0.44
6:m:208:ASP:HB2	6:n:169:GLN:HE22	1.82	0.44
6:n:42:LEU:HD12	6:n:42:LEU:HA	1.81	0.44
6:t:374:ILE:HA	6:t:377:VAL:HG22	2.00	0.44
6:u:150:PRO:HB2	6:u:411:THR:HG21	2.00	0.44
1:6:13:ASP:HB3	6:r:533:GLN:HB3	1.99	0.44
3:B:4:VAL:HG11	5:h:77:LEU:HD12	1.99	0.44
3:B:117:THR:HA	3:B:120:THR:HG22	2.00	0.44
3:J:132:ARG:HH11	3:J:134:ARG:HH22	1.65	0.44
4:P:436:GLU:HG2	4:x:355:ARG:NE	2.32	0.44
4:T:61:GLY:O	4:T:566:ARG:NH1	2.51	0.44
4:T:364:GLU:H	4:T:364:GLU:CD	2.25	0.44
3:a:9:LEU:HG	3:a:23:PRO:HG2	1.99	0.44
3:c:85:LEU:H	3:c:105:GLN:NE2	2.16	0.44
5:d:147:ASN:O	5:d:152:GLY:N	2.36	0.44
5:d:149:ARG:HH11	5:d:149:ARG:HG3	1.82	0.44
5:h:59:TRP:HD1	5:h:62:ASN:HD21	1.66	0.44
5:i:187:ASP:OD1	6:u:295:LYS:NZ	2.43	0.44
6:j:385:LEU:HD23	6:j:389:TYR:CE1	2.52	0.44
6:k:220:ASP:HB2	6:k:227:LEU:HG	1.99	0.44
6:o:513:ALA:O	6:o:517:THR:HG22	2.18	0.44
6:p:442:LEU:O	6:p:446:VAL:HG23	2.18	0.44
6:q:445:CYS:SG	6:q:474:ILE:HG13	2.58	0.44
6:r:423:GLU:OE1	6:r:423:GLU:N	2.51	0.44
4:x:44:LYS:HE3	4:x:776:LEU:HD23	2.00	0.44
2:z:89:VAL:O	2:z:91:ARG:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:7:ILE:O	1:9:7:ILE:HG13	2.18	0.43
1:AC:8:LYS:HD3	1:AC:8:LYS:HA	1.77	0.43
3:B:10:THR:HG21	5:h:74:TYR:CE2	2.53	0.43
4:P:44:LYS:HE3	4:P:776:LEU:HD23	1.99	0.43
4:Q:439:LEU:HD21	4:Q:442:GLN:HG3	2.00	0.43
4:R:290:VAL:HG21	4:S:270:VAL:HG21	1.99	0.43
4:R:703:LEU:N	4:R:759:GLY:O	2.47	0.43
4:S:86:ILE:HB	4:S:98:VAL:HG11	2.00	0.43
5:U:60:THR:OG1	5:U:181:TYR:OH	2.22	0.43
5:g:149:ARG:HH11	5:g:149:ARG:HG3	1.82	0.43
5:h:85:LEU:HD22	5:i:132:GLU:HG2	1.99	0.43
6:k:506:ALA:O	6:k:510:GLN:HG3	2.18	0.43
6:n:329:PHE:HB3	6:o:334:LYS:HD3	2.00	0.43
6:n:374:ILE:HA	6:n:377:VAL:HG22	2.00	0.43
6:p:329:PHE:HB3	6:q:334:LYS:HD3	1.99	0.43
1:7:5:PRO:HB2	6:q:512:MET:HE3	1.99	0.43
1:7:8:LYS:NZ	6:q:523:MET:HG2	2.33	0.43
3:F:54:THR:OG1	3:F:57:THR:HG22	2.18	0.43
4:Q:166:ILE:HB	4:Q:236:LYS:HB2	2.00	0.43
4:Q:180:PRO:HG2	4:Q:190:ASN:HD22	1.84	0.43
4:Q:364:GLU:H	4:Q:364:GLU:CD	2.25	0.43
4:S:357:ARG:NH1	4:S:389:ASP:O	2.47	0.43
6:j:138:VAL:HG12	6:j:269:ILE:HG12	2.00	0.43
6:m:21:LYS:HB3	6:m:21:LYS:HE3	1.92	0.43
6:m:97:LEU:HD11	6:m:103:LEU:HB2	2.00	0.43
6:n:69:LEU:HD21	6:n:268:TYR:HD2	1.83	0.43
6:o:527:ALA:O	6:o:532:LEU:N	2.51	0.43
6:p:159:LYS:NZ	6:p:160:LEU:O	2.46	0.43
6:t:131:PHE:CE2	6:t:135:LYS:HD2	2.53	0.43
6:t:506:ALA:O	6:t:510:GLN:HG3	2.18	0.43
6:u:13:ALA:HB3	6:u:231:GLU:HB3	2.00	0.43
3:C:10:THR:HG21	5:W:74:TYR:CE2	2.53	0.43
3:E:117:THR:HG23	3:J:116:LEU:HD23	2.00	0.43
3:G:37:ILE:HG12	3:G:41:ARG:HE	1.83	0.43
3:H:53:ALA:HB3	3:H:57:THR:HG23	1.99	0.43
3:H:60:LEU:HD13	3:H:64:TRP:HD1	1.83	0.43
3:J:53:ALA:HB3	3:J:57:THR:HG23	2.00	0.43
3:J:54:THR:OG1	3:J:57:THR:HG22	2.18	0.43
4:P:21:ILE:HG13	4:P:22:LEU:HD22	1.99	0.43
5:Z:9:GLU:HG2	3:a:25:GLU:HG2	2.00	0.43
3:c:110:ALA:O	3:c:114:ARG:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:172:MET:O	5:i:176:MET:HG2	2.17	0.43
6:l:66:LEU:HD11	6:l:139:VAL:HB	2.00	0.43
6:l:256:MET:O	6:l:391:ILE:HD11	2.18	0.43
6:n:362:VAL:HB	6:n:374:ILE:HG23	1.99	0.43
6:r:169:GLN:OE1	6:r:178:GLN:NE2	2.46	0.43
6:r:256:MET:O	6:r:391:ILE:HD11	2.18	0.43
6:u:513:ALA:O	6:u:517:THR:HG22	2.19	0.43
3:G:53:ALA:HB3	3:G:57:THR:HG23	1.99	0.43
4:P:479:VAL:HG11	4:P:482:VAL:CG2	2.48	0.43
6:m:445:CYS:SG	6:m:474:ILE:HG13	2.58	0.43
6:n:46:ASP:OD1	6:n:47:SER:N	2.50	0.43
6:o:379:SER:HA	6:o:382:GLU:HG2	2.01	0.43
6:q:465:MET:HA	6:q:465:MET:HE3	2.01	0.43
6:t:362:VAL:HB	6:t:374:ILE:HG23	1.99	0.43
6:t:506:ALA:HB1	6:u:503:ASN:HD22	1.82	0.43
3:H:46:ILE:HD12	3:H:50:TYR:CE2	2.53	0.43
4:Q:357:ARG:NH1	4:Q:389:ASP:O	2.47	0.43
5:Z:50:ILE:HG21	5:Z:141:LYS:HB3	2.00	0.43
6:k:452:LEU:HD22	6:k:463:LEU:HD22	2.00	0.43
6:o:150:PRO:HB2	6:o:411:THR:HG21	2.00	0.43
6:t:69:LEU:HD21	6:t:268:TYR:HD2	1.83	0.43
4:x:78:TYR:HD2	4:x:564:ILE:HD11	1.81	0.43
4:x:157:ARG:HH22	4:x:245:ASN:CG	2.26	0.43
1:0:11:LYS:O	1:0:11:LYS:HG2	2.17	0.43
1:4:3:PHE:HA	6:t:525:ALA:HB1	2.01	0.43
1:8:8:LYS:HD3	1:8:8:LYS:HA	1.85	0.43
3:A:9:LEU:HG	3:A:23:PRO:HG2	1.99	0.43
3:A:29:ARG:HH11	3:A:52:PHE:HB2	1.84	0.43
3:G:60:LEU:HD13	3:G:64:TRP:HD1	1.83	0.43
4:P:672:ASN:ND2	4:P:771:ASP:O	2.51	0.43
4:T:532:ASN:N	4:x:486:GLU:OE2	2.45	0.43
5:W:172:MET:O	5:W:176:MET:HG2	2.18	0.43
5:X:172:MET:O	5:X:176:MET:HG2	2.19	0.43
5:g:184:LEU:HD23	5:g:184:LEU:HA	1.90	0.43
6:o:359:ASN:O	6:o:362:VAL:HG22	2.19	0.43
6:q:176:VAL:HG11	6:q:179:MET:HE2	2.01	0.43
6:s:386:GLY:HA2	6:s:389:TYR:CE2	2.53	0.43
3:C:5:ILE:HG23	3:C:115:ASP:HB3	1.98	0.43
3:K:83:ASP:O	3:K:105:GLN:NE2	2.49	0.43
4:Q:464:ARG:HB2	4:Q:467:PHE:O	2.18	0.43
4:S:709:ASN:O	4:S:779:ILE:N	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:715:THR:HA	4:T:731:MET:O	2.19	0.43
5:Y:169:ARG:O	5:Y:173:GLU:HG3	2.18	0.43
6:l:423:GLU:OE1	6:l:423:GLU:N	2.51	0.43
6:n:226:TYR:CE2	6:n:246:LYS:HD2	2.54	0.43
6:p:6:THR:HA	6:p:10:GLU:HG2	2.01	0.43
6:r:374:ILE:HA	6:r:377:VAL:HG22	2.01	0.43
6:u:359:ASN:O	6:u:362:VAL:HG22	2.18	0.43
2:w:89:VAL:O	2:w:91:ARG:HG3	2.19	0.43
1:4:11:LYS:HE2	1:4:11:LYS:HB3	1.66	0.43
3:A:120:THR:OG1	3:K:121:ILE:HG23	2.18	0.43
3:E:9:LEU:HG	3:E:23:PRO:HG2	2.00	0.43
3:L:124:ASN:HB3	3:L:130:ASP:HB2	1.99	0.43
4:Q:9:LYS:HD3	4:Q:9:LYS:HA	1.72	0.43
4:Q:411:GLU:HA	4:R:438:ASN:HB3	2.00	0.43
4:Q:746:LEU:HD11	4:Q:774:THR:HG22	2.00	0.43
5:V:169:ARG:O	5:V:173:GLU:HG3	2.18	0.43
5:V:184:LEU:HD23	5:V:184:LEU:HA	1.84	0.43
5:W:17:VAL:HG11	5:W:32:LEU:HD21	2.00	0.43
5:Y:32:LEU:O	5:g:2:ARG:NH2	2.51	0.43
3:a:106:THR:HG23	3:c:107:MET:HG2	2.01	0.43
5:h:169:ARG:O	5:h:173:GLU:HG3	2.19	0.43
6:k:235:MET:HE3	6:k:236:GLU:H	1.82	0.43
6:k:465:MET:HA	6:k:465:MET:HE3	2.01	0.43
6:l:374:ILE:HA	6:l:377:VAL:HG22	2.01	0.43
6:o:398:LEU:HD23	6:o:398:LEU:HA	1.83	0.43
6:q:228:ARG:HH12	6:q:230:GLU:HG3	1.83	0.43
6:r:66:LEU:HD11	6:r:139:VAL:HB	2.00	0.43
6:s:115:ARG:NH1	6:t:90:GLU:OE2	2.52	0.43
6:s:491:LYS:HE2	6:s:491:LYS:HB3	1.86	0.43
3:E:26:TYR:OH	3:E:55:ARG:O	2.33	0.43
4:P:257:LEU:HD11	4:P:282:VAL:HG21	2.00	0.43
4:R:497:PRO:HG3	4:R:519:ASP:HB2	2.00	0.43
4:S:446:GLN:NE2	4:S:463:PRO:HG3	2.34	0.43
6:m:198:VAL:HG22	6:m:232:VAL:HG11	2.01	0.43
6:s:359:ASN:ND2	6:t:380:GLU:HB2	2.34	0.43
6:s:519:SER:O	6:s:523:MET:HG3	2.19	0.43
6:u:484:THR:OG1	6:u:487:GLN:HG3	2.17	0.43
2:v:89:VAL:O	2:v:91:ARG:HG3	2.19	0.43
4:x:497:PRO:HG3	4:x:519:ASP:HB2	2.00	0.43
2:2:89:VAL:O	2:2:91:ARG:HG3	2.19	0.43
1:AC:5:PRO:HG2	6:k:512:MET:HE3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:46:ILE:HD12	3:G:50:TYR:CE2	2.54	0.43
4:P:217:GLN:NE2	4:Q:241:ASP:OD1	2.52	0.43
4:Q:141:VAL:HG22	4:Q:300:GLU:HG2	2.00	0.43
4:Q:618:ILE:HA	4:Q:621:ILE:HD12	2.00	0.43
4:R:44:LYS:HE3	4:R:776:LEU:HD23	2.00	0.43
4:T:3:LEU:HD21	5:e:151:PHE:O	2.19	0.43
6:m:74:MET:HE3	6:m:78:PHE:HB2	2.01	0.43
6:q:82:THR:HA	6:q:118:MET:HE2	2.01	0.43
6:q:456:ARG:NH1	6:r:457:ASP:OD2	2.52	0.43
1:0:3:PHE:HA	6:n:525:ALA:HB1	2.00	0.42
3:D:25:GLU:HG2	5:f:9:GLU:HG2	2.00	0.42
3:H:12:GLN:HA	3:H:72:THR:HG22	2.01	0.42
3:K:31:PHE:CE2	3:K:79:THR:HG23	2.54	0.42
4:P:86:ILE:HB	4:P:98:VAL:HG11	2.00	0.42
4:R:617:HIS:HD2	4:R:655:TRP:CZ2	2.37	0.42
5:f:50:ILE:HG21	5:f:141:LYS:HB3	2.00	0.42
6:j:159:LYS:NZ	6:j:160:LEU:O	2.46	0.42
6:l:393:SER:HA	6:l:397:GLN:HB2	2.01	0.42
6:n:82:THR:HA	6:n:118:MET:HE2	2.01	0.42
6:n:93:ALA:O	6:n:97:LEU:HG	2.19	0.42
6:q:441:LYS:HE3	6:q:476:ILE:HG22	2.01	0.42
6:s:477:ASP:O	6:t:469:ARG:NH2	2.52	0.42
6:t:226:TYR:CE2	6:t:246:LYS:HD2	2.54	0.42
4:x:67:HIS:CD2	4:x:118:MET:HG2	2.54	0.42
3:A:116:LEU:HD21	3:K:114:ARG:CZ	2.49	0.42
3:F:53:ALA:HB3	3:F:57:THR:HG23	2.00	0.42
3:L:74:GLU:OE2	3:L:76:ARG:NH1	2.52	0.42
3:M:22:ILE:HG12	3:M:56:THR:O	2.19	0.42
5:f:26:GLU:HG3	4:x:705:ARG:NH2	2.34	0.42
6:j:6:THR:HA	6:j:10:GLU:HG2	2.01	0.42
6:m:359:ASN:ND2	6:n:380:GLU:HB2	2.34	0.42
6:n:159:LYS:HD2	6:n:160:LEU:N	2.34	0.42
6:o:255:ARG:H	6:o:395:GLU:HG2	1.85	0.42
6:r:225:GLU:OE2	6:r:246:LYS:N	2.52	0.42
6:r:393:SER:HA	6:r:397:GLN:HB2	2.00	0.42
6:s:92:GLU:HA	6:s:92:GLU:OE1	2.19	0.42
6:t:37:TYR:CZ	6:t:277:ARG:HG2	2.54	0.42
6:t:159:LYS:HD2	6:t:160:LEU:N	2.34	0.42
6:t:208:ASP:HB2	6:u:169:GLN:HE22	1.85	0.42
4:x:75:GLU:HG3	4:x:314:ARG:NH1	2.34	0.42
4:x:126:PHE:CE2	4:x:353:PHE:HZ	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:x:216:GLY:HA3	4:x:219:PHE:CZ	2.54	0.42
2:1:91:ARG:HD2	4:Q:687:THR:HG23	2.02	0.42
3:E:29:ARG:HH11	3:E:52:PHE:HB2	1.84	0.42
3:N:110:ALA:O	3:N:114:ARG:HG2	2.19	0.42
4:S:594:MET:HB3	4:S:670:GLY:HA3	2.01	0.42
4:T:357:ARG:HG2	4:T:371:THR:HA	2.01	0.42
5:V:21:LEU:HB3	5:V:26:GLU:HB2	2.00	0.42
5:W:8:VAL:HG12	5:e:2:ARG:O	2.19	0.42
5:h:172:MET:O	5:h:176:MET:HG2	2.18	0.42
6:j:59:GLN:HB3	6:j:283:GLN:HG3	2.02	0.42
6:l:225:GLU:OE2	6:l:246:LYS:N	2.52	0.42
6:p:226:TYR:CE2	6:p:246:LYS:HD2	2.54	0.42
6:r:297:ILE:HD12	6:r:330:LEU:HD23	2.00	0.42
6:u:379:SER:HA	6:u:382:GLU:HG2	2.01	0.42
2:w:86:SER:O	4:x:793:GLY:N	2.52	0.42
4:x:212:THR:HB	4:x:223:THR:HB	2.02	0.42
3:D:94:LEU:HB2	4:x:741:LEU:HG	2.00	0.42
3:J:46:ILE:HD12	3:J:50:TYR:CE2	2.53	0.42
4:P:66:ILE:HD13	4:P:564:ILE:HD12	2.00	0.42
4:P:446:GLN:NE2	4:P:463:PRO:HG3	2.34	0.42
4:R:167:VAL:HG13	4:R:174:VAL:HG23	2.01	0.42
4:T:705:ARG:HH22	5:e:39:ASP:CG	2.27	0.42
5:Z:184:LEU:HD23	5:Z:184:LEU:HA	1.89	0.42
5:f:144:ARG:HA	5:f:160:LEU:HD13	2.01	0.42
6:k:24:ARG:HD3	6:k:167:VAL:HG12	2.01	0.42
6:k:91:TYR:O	6:k:95:GLN:HG2	2.20	0.42
6:l:297:ILE:HD12	6:l:330:LEU:HD23	2.01	0.42
6:l:368:ARG:HH11	6:m:368:ARG:NH2	2.18	0.42
6:s:74:MET:HE3	6:s:78:PHE:HB2	2.01	0.42
6:s:379:SER:HA	6:s:382:GLU:HG2	2.01	0.42
6:t:329:PHE:HB3	6:u:334:LYS:HD3	2.00	0.42
1:5:6:LYS:HD3	1:5:6:LYS:HA	1.88	0.42
1:8:12:MET:HB3	6:p:532:LEU:HB3	2.01	0.42
3:D:4:VAL:HG11	5:X:77:LEU:HD12	2.02	0.42
3:I:101:VAL:HG11	5:f:33:GLU:OE2	2.19	0.42
3:L:24:PHE:HE1	3:L:32:VAL:HG22	1.84	0.42
4:Q:709:ASN:O	4:Q:779:ILE:N	2.50	0.42
4:R:126:PHE:CE2	4:R:353:PHE:HZ	2.37	0.42
4:R:788:LEU:HD22	5:h:153:ALA:HA	2.02	0.42
4:S:3:LEU:HD23	4:S:3:LEU:HA	1.83	0.42
5:U:172:MET:O	5:U:176:MET:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:m:228:ARG:HD2	6:m:244:TYR:CE2	2.54	0.42
6:n:37:TYR:CZ	6:n:277:ARG:HG2	2.55	0.42
1:0:12:MET:SD	6:n:527:ALA:HB2	2.59	0.42
1:AB:5:PRO:HG3	6:k:523:MET:SD	2.60	0.42
4:P:257:LEU:HD13	4:P:291:TRP:CD2	2.55	0.42
4:Q:174:VAL:HG23	4:Q:204:MET:HG2	2.02	0.42
4:R:45:ARG:HD3	4:R:543:TRP:CD2	2.55	0.42
4:T:50:PHE:HD1	4:T:596:MET:HE3	1.84	0.42
5:V:183:MET:HB3	6:n:319:PHE:CE2	2.54	0.42
5:X:46:ILE:HD11	5:X:150:PHE:HE2	1.85	0.42
5:X:60:THR:OG1	5:X:181:TYR:OH	2.23	0.42
5:Z:33:GLU:OE2	3:b:101:VAL:HG11	2.20	0.42
6:l:364:ARG:NH2	6:l:373:GLU:OE1	2.52	0.42
6:m:190:LEU:HD11	6:m:211:ILE:HG13	1.99	0.42
6:m:379:SER:HA	6:m:382:GLU:HG2	2.01	0.42
6:n:498:GLN:NE2	6:o:495:GLN:OE1	2.52	0.42
6:p:13:ALA:N	6:p:231:GLU:OE2	2.50	0.42
6:r:364:ARG:NH2	6:r:373:GLU:OE1	2.52	0.42
6:t:368:ARG:HH11	6:u:368:ARG:NH2	2.17	0.42
4:x:417:SER:OG	4:x:418:ASP:N	2.53	0.42
3:E:120:THR:OG1	3:O:121:ILE:HG23	2.18	0.42
4:P:48:LEU:HD22	4:P:545:PHE:CD1	2.54	0.42
4:Q:525:MET:HE3	4:Q:525:MET:HB3	1.86	0.42
4:Q:715:THR:HA	4:Q:731:MET:O	2.19	0.42
5:W:23:SER:HA	5:f:149:ARG:HG2	2.02	0.42
5:W:183:MET:HB3	6:l:319:PHE:CE2	2.55	0.42
5:h:169:ARG:HG3	6:s:302:PRO:HB2	2.01	0.42
6:j:442:LEU:O	6:j:446:VAL:HG23	2.20	0.42
6:m:92:GLU:OE1	6:m:92:GLU:HA	2.19	0.42
6:m:99:ASP:OD1	6:m:101:ASP:HB3	2.19	0.42
6:n:91:TYR:O	6:n:95:GLN:HG2	2.19	0.42
6:q:91:TYR:O	6:q:95:GLN:HG2	2.20	0.42
6:q:114:GLU:OE2	6:q:435:ARG:HD2	2.19	0.42
6:s:423:GLU:O	6:s:423:GLU:HG2	2.20	0.42
6:t:79:PRO:HD2	6:t:83:TRP:HB3	2.02	0.42
4:x:90:ASP:OD1	4:x:94:ASN:N	2.47	0.42
3:A:5:ILE:HG22	3:A:8:VAL:H	1.84	0.42
3:J:13:LEU:HD23	3:J:13:LEU:HA	1.95	0.42
3:L:9:LEU:HD23	3:L:10:THR:N	2.35	0.42
3:N:31:PHE:CE2	3:N:79:THR:HG23	2.55	0.42
4:P:721:GLU:OE2	4:P:767:TYR:OH	2.26	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:599:ARG:HH21	4:R:666:MET:HE1	1.83	0.42
5:f:26:GLU:HG3	4:x:705:ARG:CZ	2.50	0.42
6:j:184:GLN:HB2	6:k:172:ALA:HB3	2.02	0.42
6:k:445:CYS:SG	6:k:474:ILE:HG13	2.59	0.42
6:l:517:THR:HG21	6:m:511:GLY:HA3	2.02	0.42
6:m:373:GLU:O	6:m:377:VAL:HG22	2.20	0.42
6:n:16:VAL:HG22	6:n:19:ARG:HH21	1.85	0.42
6:o:255:ARG:HB3	6:o:265:GLY:HA3	2.00	0.42
6:p:74:MET:HE3	6:p:78:PHE:HB2	2.00	0.42
6:q:58:TRP:CE2	6:q:284:GLU:HG3	2.55	0.42
6:u:91:TYR:O	6:u:95:GLN:HG2	2.20	0.42
2:y:89:VAL:O	2:y:91:ARG:HG3	2.20	0.42
1:8:11:LYS:HD3	6:q:529:SER:HB3	2.02	0.42
3:A:133:GLY:H	3:F:138:ASN:HB3	1.85	0.42
1:AB:11:LYS:O	6:l:536:ILE:HG21	2.19	0.42
3:C:121:ILE:HG13	3:M:129:LEU:HD13	2.01	0.42
4:P:120:THR:HG23	4:P:125:THR:HG22	2.01	0.42
4:Q:285:ASP:HB3	4:Q:288:ARG:HB2	2.02	0.42
4:R:48:LEU:HD22	4:R:545:PHE:CD1	2.54	0.42
4:R:705:ARG:CZ	5:Z:26:GLU:HG3	2.50	0.42
4:T:216:GLY:HA3	4:T:219:PHE:CZ	2.55	0.42
4:T:405:TYR:OH	4:T:447:ASP:O	2.29	0.42
4:T:746:LEU:HD11	4:T:774:THR:HG22	2.00	0.42
5:W:153:ALA:HA	4:x:788:LEU:HD22	2.02	0.42
6:j:24:ARG:HD3	6:j:167:VAL:HG12	2.02	0.42
6:j:364:ARG:HD2	6:j:369:VAL:HG22	2.01	0.42
6:k:114:GLU:OE2	6:k:435:ARG:HD2	2.20	0.42
6:l:484:THR:O	6:l:488:LYS:HG3	2.20	0.42
6:p:59:GLN:HB3	6:p:283:GLN:HG3	2.02	0.42
6:q:190:LEU:HD13	6:q:194:ILE:HG22	2.02	0.42
6:t:331:GLN:HA	6:u:337:ASP:OD2	2.20	0.42
3:E:117:THR:HA	3:E:120:THR:HG22	2.01	0.42
3:G:37:ILE:HD11	3:G:41:ARG:HH21	1.85	0.42
3:G:101:VAL:HG11	5:i:33:GLU:OE2	2.20	0.42
3:L:19:ASP:OD1	3:L:59:SER:OG	2.29	0.42
4:P:411:GLU:HA	4:Q:438:ASN:HB3	2.02	0.42
4:Q:705:ARG:HH22	5:i:39:ASP:CG	2.28	0.42
4:R:67:HIS:CD2	4:R:118:MET:HG2	2.55	0.42
4:R:705:ARG:NH2	5:Z:26:GLU:HG3	2.34	0.42
4:T:174:VAL:HG23	4:T:204:MET:HG2	2.02	0.42
4:T:700:ARG:NH2	5:V:39:ASP:OD1	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:155:GLU:H	5:W:155:GLU:CD	2.28	0.42
3:b:84:ARG:HA	3:b:105:GLN:HE22	1.85	0.42
6:l:169:GLN:OE1	6:l:178:GLN:NE2	2.47	0.42
1:3:7:ILE:H	1:3:7:ILE:HG12	1.57	0.41
4:P:700:ARG:HH22	5:X:39:ASP:CG	2.28	0.41
4:R:411:GLU:HA	4:S:438:ASN:HB3	2.01	0.41
5:W:60:THR:OG1	5:W:181:TYR:OH	2.21	0.41
3:c:132:ARG:HB2	3:c:134:ARG:NE	2.35	0.41
6:k:13:ALA:HB2	6:k:216:HIS:HB2	2.02	0.41
6:k:58:TRP:CE2	6:k:284:GLU:HG3	2.55	0.41
6:k:491:LYS:HE2	6:k:491:LYS:HB3	1.96	0.41
6:l:46:ASP:OD1	6:l:47:SER:N	2.53	0.41
6:l:255:ARG:NH1	6:l:395:GLU:OE1	2.53	0.41
6:l:498:GLN:OE1	6:m:492:MET:HG3	2.19	0.41
6:m:91:TYR:O	6:m:95:GLN:HG2	2.20	0.41
6:n:331:GLN:HA	6:o:337:ASP:OD2	2.20	0.41
6:u:192:GLU:O	6:u:196:LYS:HG3	2.19	0.41
1:9:8:LYS:NZ	6:o:516:ALA:HB1	2.35	0.41
3:B:5:ILE:HG23	3:B:115:ASP:HB3	2.00	0.41
3:M:44:LEU:HD23	3:M:60:LEU:HD11	2.02	0.41
4:P:477:GLN:HA	4:Q:479:VAL:HG22	2.02	0.41
4:Q:160:GLN:HA	4:Q:160:GLN:OE1	2.20	0.41
4:S:106:TYR:O	4:S:129:ASN:ND2	2.46	0.41
4:S:165:LEU:HD22	4:S:196:LEU:HD22	2.01	0.41
4:S:357:ARG:NH2	4:S:387:ASP:O	2.53	0.41
4:T:446:GLN:HE21	4:T:463:PRO:HG3	1.85	0.41
5:W:169:ARG:HG3	6:m:302:PRO:HB2	2.01	0.41
5:Z:166:GLU:HA	5:Z:169:ARG:HG2	2.01	0.41
6:j:173:PHE:CE1	6:u:159:LYS:HE3	2.55	0.41
6:l:59:GLN:HB3	6:l:283:GLN:HG3	2.03	0.41
6:p:179:MET:HE3	6:p:251:TYR:HB2	2.01	0.41
6:r:149:GLU:HA	6:r:150:PRO:HD3	1.93	0.41
6:s:373:GLU:O	6:s:377:VAL:HG22	2.20	0.41
6:t:191:PRO:HD2	6:t:194:ILE:HD12	2.02	0.41
6:u:520:PRO:HA	6:u:523:MET:HE3	2.02	0.41
4:x:45:ARG:HD3	4:x:543:TRP:CD2	2.55	0.41
4:x:48:LEU:HD22	4:x:545:PHE:CD1	2.54	0.41
2:1:89:VAL:O	2:1:91:ARG:HG3	2.20	0.41
1:AB:5:PRO:HB2	6:l:512:MET:HG2	2.03	0.41
4:P:9:LYS:HE3	4:Q:697:ASP:OD1	2.20	0.41
4:Q:332:CYS:SG	4:Q:382:ILE:HG12	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:617:HIS:HD2	4:Q:655:TRP:CZ2	2.38	0.41
4:R:701:LEU:HD13	4:R:787:TYR:HB2	2.02	0.41
5:U:26:GLU:OE1	5:U:27:PRO:HD2	2.20	0.41
5:W:169:ARG:O	5:W:173:GLU:HG3	2.19	0.41
6:l:7:GLY:O	6:l:10:GLU:HG3	2.20	0.41
6:n:168:VAL:HG12	6:n:264:TYR:CE2	2.55	0.41
6:p:191:PRO:HD2	6:p:194:ILE:HD12	2.02	0.41
6:p:364:ARG:HD2	6:p:369:VAL:HG22	2.02	0.41
6:p:381:LEU:HA	6:p:384:THR:HG22	2.02	0.41
6:r:255:ARG:NH1	6:r:395:GLU:OE1	2.53	0.41
6:r:368:ARG:HH11	6:s:368:ARG:NH2	2.18	0.41
6:s:134:LEU:HD23	6:s:134:LEU:HA	1.92	0.41
6:s:375:ARG:HH21	6:s:376:TYR:HB2	1.85	0.41
6:s:404:LEU:HD23	6:s:404:LEU:HA	1.92	0.41
6:s:527:ALA:O	6:s:532:LEU:N	2.53	0.41
6:t:42:LEU:HD12	6:t:42:LEU:HA	1.81	0.41
4:x:42:LEU:HD12	4:x:42:LEU:HA	1.88	0.41
4:x:617:HIS:HD2	4:x:655:TRP:CZ2	2.38	0.41
1:9:5:PRO:HG3	6:n:523:MET:SD	2.60	0.41
3:D:120:THR:OG1	3:N:121:ILE:HG23	2.19	0.41
3:L:44:LEU:HD23	3:L:60:LEU:HD11	2.03	0.41
4:P:357:ARG:NH2	4:P:387:ASP:O	2.53	0.41
4:P:700:ARG:NE	4:P:702:GLN:OE1	2.53	0.41
5:d:50:ILE:HD12	5:d:141:LYS:HE3	2.01	0.41
5:h:50:ILE:HG21	5:h:141:LYS:HB3	2.02	0.41
5:h:183:MET:HB3	6:r:319:PHE:CE2	2.55	0.41
6:k:176:VAL:HG11	6:k:179:MET:HE2	2.02	0.41
6:l:128:VAL:O	6:l:132:GLU:HG2	2.21	0.41
6:l:362:VAL:HB	6:l:374:ILE:HG23	2.03	0.41
6:o:501:MET:O	6:o:505:ALA:N	2.34	0.41
6:p:138:VAL:HG12	6:p:269:ILE:HG12	2.01	0.41
6:q:408:LEU:HB3	6:q:414:ILE:HG23	2.02	0.41
6:s:99:ASP:OD1	6:s:101:ASP:HB3	2.20	0.41
6:s:323:ARG:HB2	6:s:326:ASP:OD2	2.20	0.41
6:u:409:GLN:HG3	6:u:414:ILE:HD11	2.01	0.41
4:x:618:ILE:HA	4:x:621:ILE:HD12	2.01	0.41
1:3:3:PHE:HD2	1:4:11:LYS:NZ	2.18	0.41
1:3:3:PHE:HD2	1:4:11:LYS:HZ1	1.68	0.41
3:A:40:ASP:OD2	3:A:40:ASP:N	2.53	0.41
3:H:101:VAL:HG11	5:e:33:GLU:OE2	2.21	0.41
3:M:49:ASP:O	3:M:61:THR:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:67:HIS:CG	4:P:118:MET:HG2	2.55	0.41
4:Q:42:LEU:HD12	4:Q:42:LEU:HA	1.90	0.41
4:S:67:HIS:CG	4:S:118:MET:HG2	2.55	0.41
4:T:285:ASP:HB3	4:T:288:ARG:HB2	2.02	0.41
4:T:317:ASP:OD1	4:T:317:ASP:N	2.53	0.41
4:T:709:ASN:O	4:T:779:ILE:N	2.50	0.41
5:U:77:LEU:HD12	3:a:4:VAL:HG11	2.02	0.41
6:k:5:ARG:HH12	6:k:229:TYR:HB3	1.85	0.41
6:n:368:ARG:HH11	6:o:368:ARG:NH2	2.17	0.41
6:o:91:TYR:O	6:o:95:GLN:HG2	2.21	0.41
6:r:59:GLN:HB3	6:r:283:GLN:HG3	2.02	0.41
1:3:11:LYS:HG2	1:AD:5:PRO:O	2.20	0.41
3:E:46:ILE:HD12	3:E:50:TYR:CE1	2.56	0.41
3:K:49:ASP:O	3:K:61:THR:N	2.50	0.41
3:N:49:ASP:O	3:N:61:THR:N	2.49	0.41
4:P:525:MET:HE3	4:P:525:MET:HB3	1.89	0.41
4:Q:50:PHE:HD1	4:Q:596:MET:HE3	1.84	0.41
4:Q:357:ARG:HG2	4:Q:371:THR:HA	2.03	0.41
4:R:161:TYR:O	4:R:163:ARG:NH1	2.54	0.41
4:R:531:LEU:HB2	4:R:536:ARG:CG	2.51	0.41
4:S:157:ARG:HH22	4:S:245:ASN:CG	2.24	0.41
4:S:672:ASN:ND2	4:S:771:ASP:O	2.51	0.41
4:S:687:THR:HG23	2:y:91:ARG:HD2	2.02	0.41
4:T:71:ARG:NH2	4:T:125:THR:HG23	2.35	0.41
4:T:160:GLN:HA	4:T:160:GLN:OE1	2.20	0.41
4:T:446:GLN:NE2	4:T:463:PRO:HG3	2.36	0.41
5:f:172:MET:O	5:f:176:MET:HG2	2.21	0.41
5:g:172:MET:O	5:g:176:MET:HG2	2.21	0.41
6:j:13:ALA:N	6:j:231:GLU:OE2	2.50	0.41
6:j:179:MET:HE3	6:j:251:TYR:HB2	2.01	0.41
6:j:334:LYS:HD3	6:u:329:PHE:HB3	2.02	0.41
6:n:79:PRO:HD2	6:n:83:TRP:HB3	2.02	0.41
6:n:357:MET:CE	6:n:385:LEU:HB2	2.50	0.41
6:p:168:VAL:HG12	6:p:264:TYR:CE2	2.56	0.41
6:p:193:ASP:OD1	6:p:194:ILE:HG13	2.20	0.41
6:s:513:ALA:O	6:s:517:THR:HG22	2.21	0.41
4:x:585:LEU:HD22	4:x:599:ARG:HB2	2.03	0.41
3:A:46:ILE:HD12	3:A:50:TYR:CE1	2.55	0.41
3:D:5:ILE:HG23	3:D:115:ASP:HB3	2.03	0.41
4:P:61:GLY:O	4:P:566:ARG:NH1	2.54	0.41
4:Q:3:LEU:HD21	5:i:151:PHE:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:61:GLY:O	4:Q:566:ARG:NH1	2.54	0.41
4:S:257:LEU:HD13	4:S:291:TRP:CD2	2.55	0.41
4:S:700:ARG:NE	4:S:702:GLN:OE1	2.53	0.41
4:T:9:LYS:HD3	4:T:9:LYS:HA	1.71	0.41
5:U:85:LEU:HD22	5:Z:132:GLU:HG2	2.02	0.41
5:Z:95:ILE:O	5:Z:106:ARG:HG2	2.21	0.41
5:e:172:MET:O	5:e:176:MET:HG2	2.19	0.41
5:f:166:GLU:HA	5:f:169:ARG:HG2	2.02	0.41
6:p:24:ARG:HD3	6:p:167:VAL:HG12	2.01	0.41
6:q:5:ARG:HH12	6:q:229:TYR:HB3	1.85	0.41
6:s:18:GLU:HA	6:s:21:LYS:HD3	2.02	0.41
6:s:228:ARG:HD2	6:s:244:TYR:CE2	2.56	0.41
4:x:405:TYR:OH	4:x:447:ASP:O	2.37	0.41
4:x:675:PHE:CD1	4:x:776:LEU:HD21	2.56	0.41
1:AD:12:MET:HB2	6:j:532:LEU:HB3	2.03	0.41
3:F:13:LEU:HD11	3:F:36:LEU:HD22	2.03	0.41
3:G:124:ASN:HD22	3:G:128:HIS:HB2	1.85	0.41
3:K:124:ASN:ND2	3:K:128:HIS:O	2.54	0.41
4:P:285:ASP:HB3	4:P:288:ARG:HB2	2.03	0.41
4:P:628:ARG:HA	4:P:645:GLN:NE2	2.35	0.41
4:Q:68:LEU:HD13	4:Q:78:TYR:CE1	2.56	0.41
4:Q:446:GLN:HE21	4:Q:463:PRO:HG3	1.85	0.41
5:d:159:VAL:O	5:d:163:GLU:HG3	2.21	0.41
5:g:144:ARG:HA	5:g:160:LEU:HD13	2.01	0.41
6:k:112:MET:HE2	6:k:112:MET:HB3	1.99	0.41
6:q:69:LEU:HD23	6:q:69:LEU:HA	1.94	0.41
6:q:452:LEU:HD22	6:q:463:LEU:HD22	2.01	0.41
6:r:46:ASP:OD1	6:r:47:SER:N	2.53	0.41
6:r:362:VAL:HB	6:r:374:ILE:HG23	2.03	0.41
6:t:357:MET:CE	6:t:385:LEU:HB2	2.51	0.41
6:t:368:ARG:HH22	6:t:370:THR:HB	1.86	0.41
4:x:87:ARG:NE	4:x:95:GLU:OE1	2.45	0.41
1:AA:8:LYS:HB3	1:AA:12:MET:HG3	2.01	0.41
1:AD:4:SER:HB3	6:j:516:ALA:HA	2.02	0.41
3:B:27:LEU:HD21	3:B:104:ILE:HG22	2.03	0.41
3:E:40:ASP:OD2	3:E:40:ASP:N	2.53	0.41
3:I:13:LEU:HB2	3:I:71:THR:C	2.46	0.41
3:I:120:THR:HG22	3:I:121:ILE:N	2.35	0.41
3:L:31:PHE:CE2	3:L:79:THR:HG23	2.56	0.41
4:P:492:VAL:HB	4:P:495:TYR:HB2	2.03	0.41
4:P:721:GLU:HG2	4:P:726:ASN:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:239:TYR:O	4:R:242:GLN:HG3	2.21	0.41
4:S:9:LYS:HE3	4:T:697:ASP:OD1	2.21	0.41
4:S:114:ASN:O	4:S:130:ARG:NH1	2.54	0.41
4:T:86:ILE:HB	4:T:98:VAL:HG11	2.03	0.41
5:U:50:ILE:HG21	5:U:141:LYS:HB3	2.03	0.41
5:X:136:TYR:CE1	5:g:53:GLN:HG3	2.56	0.41
5:Z:149:ARG:HG2	5:h:23:SER:HA	2.03	0.41
5:f:137:TRP:HA	5:f:167:ALA:HB1	2.03	0.41
6:j:168:VAL:HG12	6:j:264:TYR:CE2	2.55	0.41
6:j:469:ARG:HH22	6:u:481:ILE:HD11	1.86	0.41
6:k:408:LEU:HB3	6:k:414:ILE:HG23	2.03	0.41
6:l:190:LEU:HD23	6:l:190:LEU:HA	1.94	0.41
6:m:59:GLN:HG3	6:m:280:GLU:OE1	2.21	0.41
6:o:58:TRP:CE2	6:o:284:GLU:HG3	2.56	0.41
6:o:228:ARG:HD2	6:o:244:TYR:CE2	2.55	0.41
6:p:194:ILE:O	6:p:198:VAL:HG23	2.20	0.41
6:q:404:LEU:HD23	6:q:404:LEU:HA	1.94	0.41
6:r:484:THR:O	6:r:488:LYS:HG3	2.21	0.41
6:t:93:ALA:O	6:t:97:LEU:HG	2.21	0.41
6:t:168:VAL:HG12	6:t:264:TYR:CE2	2.56	0.41
6:u:58:TRP:CE2	6:u:284:GLU:HG3	2.56	0.41
6:u:112:MET:HE2	6:u:112:MET:HB3	1.99	0.41
6:u:299:LEU:N	6:u:328:SER:O	2.53	0.41
4:x:72:ASP:CG	4:x:73:GLU:H	2.29	0.41
4:x:185:PRO:O	4:x:188:VAL:HG12	2.20	0.41
1:7:4:SER:HB3	6:q:516:ALA:HA	2.03	0.41
3:A:35:THR:HG23	3:A:74:GLU:HB3	2.02	0.41
3:D:121:ILE:HG13	3:N:129:LEU:HD13	2.03	0.41
3:E:35:THR:HG23	3:E:74:GLU:HB3	2.03	0.41
3:J:13:LEU:HD11	3:J:36:LEU:HD22	2.03	0.41
4:P:722:ASN:HA	4:P:763:PHE:O	2.21	0.41
4:Q:151:ASP:HB3	4:Q:249:HIS:NE2	2.36	0.41
4:Q:700:ARG:HH22	5:Y:39:ASP:CG	2.29	0.41
4:R:708:VAL:HG23	4:R:755:PHE:HE1	1.85	0.41
4:S:61:GLY:O	4:S:566:ARG:NH1	2.53	0.41
5:Y:50:ILE:HG21	5:Y:141:LYS:HB3	2.03	0.41
5:f:151:PHE:O	4:x:3:LEU:HD21	2.21	0.41
5:h:155:GLU:H	5:h:155:GLU:CD	2.29	0.41
6:m:375:ARG:HH21	6:m:376:TYR:HB2	1.85	0.41
6:n:513:ALA:O	6:n:517:THR:HG22	2.21	0.41
6:o:159:LYS:HE3	6:p:173:PHE:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:r:7:GLY:O	6:r:10:GLU:HG3	2.20	0.41
6:r:208:ASP:OD1	6:r:208:ASP:N	2.42	0.41
4:x:114:ASN:O	4:x:130:ARG:NH1	2.54	0.41
3:J:50:TYR:HA	3:J:60:LEU:HA	2.03	0.40
4:P:276:SER:HA	4:x:384:ASN:HD22	1.86	0.40
4:P:618:ILE:HA	4:P:621:ILE:HD12	2.03	0.40
4:R:42:LEU:HD12	4:R:42:LEU:HA	1.87	0.40
4:R:88:VAL:HG11	4:R:320:PHE:CE1	2.56	0.40
4:R:114:ASN:O	4:R:130:ARG:NH1	2.53	0.40
4:R:618:ILE:HA	4:R:621:ILE:HD12	2.02	0.40
5:U:169:ARG:NH1	5:U:173:GLU:OE2	2.53	0.40
5:V:50:ILE:HG21	5:V:141:LYS:HB3	2.03	0.40
5:g:183:MET:HB3	6:u:319:PHE:CE2	2.56	0.40
5:i:71:PRO:HD3	5:i:116:GLY:HA2	2.03	0.40
6:k:190:LEU:HD13	6:k:194:ILE:HG22	2.03	0.40
6:k:527:ALA:O	6:k:532:LEU:N	2.54	0.40
6:m:305:ILE:HD11	6:m:323:ARG:HG3	2.03	0.40
6:m:423:GLU:HG2	6:m:423:GLU:O	2.20	0.40
6:o:457:ASP:OD1	6:o:457:ASP:N	2.50	0.40
6:p:8:LEU:HD13	6:p:178:GLN:HB3	2.04	0.40
6:q:42:LEU:HD12	6:q:42:LEU:HA	1.90	0.40
6:s:59:GLN:HG3	6:s:280:GLU:OE1	2.21	0.40
6:s:255:ARG:HH11	6:s:255:ARG:HG3	1.86	0.40
4:x:155:ASN:HD21	4:x:258:PRO:HB3	1.86	0.40
1:AA:6:LYS:HB3	6:n:508:LEU:HD22	2.03	0.40
3:B:120:THR:OG1	3:L:121:ILE:HG23	2.21	0.40
3:F:13:LEU:HD23	3:F:13:LEU:HA	1.95	0.40
4:Q:86:ILE:HB	4:Q:98:VAL:HG11	2.03	0.40
4:Q:114:ASN:O	4:Q:130:ARG:NH1	2.55	0.40
4:R:185:PRO:O	4:R:188:VAL:HG12	2.21	0.40
4:R:417:SER:OG	4:R:418:ASP:N	2.53	0.40
4:R:675:PHE:CD1	4:R:776:LEU:HD21	2.56	0.40
4:T:100:TYR:CD1	4:T:104:SER:HB3	2.56	0.40
4:T:151:ASP:HB3	4:T:249:HIS:NE2	2.36	0.40
5:U:136:TYR:CE1	5:d:53:GLN:HG3	2.55	0.40
5:X:50:ILE:HG21	5:X:141:LYS:HB3	2.03	0.40
3:b:13:LEU:HB2	3:b:71:THR:C	2.46	0.40
3:b:120:THR:HG22	3:b:121:ILE:N	2.35	0.40
3:c:62:LYS:HE3	3:c:62:LYS:HB2	1.84	0.40
5:d:128:ASP:O	5:d:135:ARG:NH2	2.54	0.40
6:k:42:LEU:HD12	6:k:42:LEU:HA	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:m:226:TYR:CE2	6:m:246:LYS:HD2	2.56	0.40
6:m:359:ASN:HD22	6:n:380:GLU:HB2	1.85	0.40
6:n:114:GLU:OE2	6:n:435:ARG:HD2	2.22	0.40
6:r:368:ARG:NH2	6:r:370:THR:HB	2.35	0.40
6:s:129:THR:HG21	6:s:158:MET:HG3	2.04	0.40
1:9:8:LYS:HZ2	6:o:516:ALA:HB1	1.87	0.40
3:A:121:ILE:HG13	3:K:129:LEU:HD13	2.03	0.40
3:N:132:ARG:HB2	3:N:134:ARG:NE	2.36	0.40
4:P:126:PHE:CE2	4:P:353:PHE:HZ	2.40	0.40
4:Q:100:TYR:CD1	4:Q:104:SER:HB3	2.57	0.40
4:R:586:GLN:O	4:R:668:TYR:OH	2.37	0.40
4:S:45:ARG:HD3	4:S:543:TRP:CD2	2.56	0.40
4:S:275:LYS:HE2	4:S:275:LYS:HB3	1.91	0.40
5:W:50:ILE:HG21	5:W:141:LYS:HB3	2.02	0.40
5:X:169:ARG:NH1	5:X:173:GLU:OE2	2.53	0.40
5:f:95:ILE:O	5:f:106:ARG:HG2	2.21	0.40
5:g:128:ASP:O	5:g:135:ARG:NH2	2.54	0.40
6:j:254:ILE:HG12	6:j:396:LEU:HB2	2.03	0.40
6:j:495:GLN:O	6:j:499:MET:HE3	2.21	0.40
6:l:91:TYR:O	6:l:95:GLN:HG2	2.21	0.40
6:n:191:PRO:HD2	6:n:194:ILE:HD12	2.03	0.40
6:r:498:GLN:OE1	6:s:492:MET:HG3	2.21	0.40
6:s:91:TYR:O	6:s:95:GLN:HG2	2.21	0.40
6:t:8:LEU:HD13	6:t:178:GLN:HB3	2.03	0.40
3:F:120:THR:HG22	3:F:121:ILE:N	2.36	0.40
3:I:50:TYR:HA	3:I:60:LEU:HA	2.04	0.40
3:M:31:PHE:CE2	3:M:79:THR:HG23	2.56	0.40
3:M:132:ARG:HB2	3:M:134:ARG:NE	2.36	0.40
4:P:45:ARG:HD3	4:P:543:TRP:CD2	2.56	0.40
4:P:414:LEU:HB3	4:P:416:TRP:HE1	1.87	0.40
4:Q:594:MET:HB3	4:Q:670:GLY:HA3	2.04	0.40
4:Q:722:ASN:HA	4:Q:763:PHE:O	2.21	0.40
4:S:104:SER:O	4:S:108:LYS:HG3	2.22	0.40
4:S:722:ASN:HA	4:S:763:PHE:O	2.22	0.40
4:T:68:LEU:HD13	4:T:78:TYR:CE1	2.57	0.40
5:Y:26:GLU:OE1	5:Y:26:GLU:HA	2.22	0.40
6:m:255:ARG:HH11	6:m:255:ARG:HG3	1.86	0.40
6:n:368:ARG:HH22	6:n:370:THR:HB	1.86	0.40
6:p:254:ILE:HG12	6:p:396:LEU:HB2	2.03	0.40
6:p:520:PRO:HA	6:p:523:MET:HB3	2.03	0.40
6:q:24:ARG:HD3	6:q:167:VAL:HG12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:q:385:LEU:HG	6:q:389:TYR:HE1	1.86	0.40
6:r:128:VAL:O	6:r:132:GLU:HG2	2.22	0.40
6:s:17:TYR:HB2	6:s:180:VAL:HG11	2.04	0.40
4:x:91:LEU:HD11	4:x:557:ILE:HD12	2.03	0.40
4:x:155:ASN:HB2	4:x:245:ASN:OD1	2.22	0.40
1:4:8:LYS:HA	1:4:8:LYS:HD3	1.92	0.40
1:6:5:PRO:HG3	6:q:523:MET:SD	2.62	0.40
3:C:134:ARG:HG3	3:M:129:LEU:HG	2.03	0.40
3:H:45:THR:HB	3:H:48:THR:HG22	2.03	0.40
4:Q:446:GLN:NE2	4:Q:463:PRO:HG3	2.36	0.40
4:Q:725:SER:HB2	4:Q:727:TRP:CH2	2.56	0.40
4:R:3:LEU:HD21	5:Z:151:PHE:O	2.21	0.40
4:S:618:ILE:HA	4:S:621:ILE:HD12	2.03	0.40
4:T:153:LEU:HB2	4:T:247:VAL:HB	2.03	0.40
5:Z:183:MET:HB3	6:q:319:PHE:CE2	2.56	0.40
6:k:409:GLN:HG3	6:k:414:ILE:HD11	2.04	0.40
6:l:112:MET:HE2	6:l:112:MET:HB3	1.86	0.40
6:l:368:ARG:NH2	6:l:370:THR:HB	2.35	0.40
6:l:481:ILE:HG13	6:l:482:LEU:HD22	2.04	0.40
6:m:17:TYR:HB2	6:m:180:VAL:HG11	2.04	0.40
6:m:112:MET:HE2	6:m:112:MET:HB3	2.00	0.40
6:o:5:ARG:HH12	6:o:229:TYR:HB3	1.86	0.40
6:o:329:PHE:HB3	6:p:334:LYS:HD3	2.02	0.40
6:q:77:LEU:HD21	6:q:389:TYR:HB2	2.04	0.40
6:r:168:VAL:HG12	6:r:264:TYR:CE2	2.57	0.40
6:r:404:LEU:HD23	6:r:404:LEU:HA	1.96	0.40
6:s:359:ASN:O	6:s:362:VAL:HG22	2.22	0.40
6:t:16:VAL:HG22	6:t:19:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	12/88 (14%)	11 (92%)	0	1 (8%)	0	1
1	3	12/88 (14%)	11 (92%)	0	1 (8%)	0	1
1	4	12/88 (14%)	11 (92%)	0	1 (8%)	0	1
1	5	12/88 (14%)	11 (92%)	0	1 (8%)	0	1
1	6	12/88 (14%)	11 (92%)	0	1 (8%)	0	1
1	7	12/88 (14%)	10 (83%)	1 (8%)	1 (8%)	0	1
1	8	12/88 (14%)	11 (92%)	0	1 (8%)	0	1
1	9	12/88 (14%)	10 (83%)	1 (8%)	1 (8%)	0	1
1	AA	12/88 (14%)	11 (92%)	0	1 (8%)	0	1
1	AB	12/88 (14%)	11 (92%)	0	1 (8%)	0	1
1	AC	12/88 (14%)	11 (92%)	0	1 (8%)	0	1
1	AD	12/88 (14%)	10 (83%)	1 (8%)	1 (8%)	0	1
2	1	13/99 (13%)	12 (92%)	1 (8%)	0	100	100
2	2	13/99 (13%)	12 (92%)	1 (8%)	0	100	100
2	v	13/99 (13%)	12 (92%)	1 (8%)	0	100	100
2	w	13/99 (13%)	12 (92%)	1 (8%)	0	100	100
2	y	13/99 (13%)	12 (92%)	1 (8%)	0	100	100
2	z	13/99 (13%)	12 (92%)	1 (8%)	0	100	100
3	A	139/553 (25%)	135 (97%)	4 (3%)	0	100	100
3	B	139/553 (25%)	134 (96%)	5 (4%)	0	100	100
3	C	139/553 (25%)	134 (96%)	5 (4%)	0	100	100
3	D	139/553 (25%)	134 (96%)	5 (4%)	0	100	100
3	E	139/553 (25%)	135 (97%)	4 (3%)	0	100	100
3	F	132/553 (24%)	128 (97%)	4 (3%)	0	100	100
3	G	132/553 (24%)	129 (98%)	3 (2%)	0	100	100
3	H	132/553 (24%)	129 (98%)	3 (2%)	0	100	100
3	I	132/553 (24%)	128 (97%)	4 (3%)	0	100	100
3	J	132/553 (24%)	129 (98%)	3 (2%)	0	100	100
3	K	134/553 (24%)	127 (95%)	7 (5%)	0	100	100
3	L	134/553 (24%)	127 (95%)	7 (5%)	0	100	100
3	M	134/553 (24%)	127 (95%)	7 (5%)	0	100	100
3	N	134/553 (24%)	127 (95%)	7 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	134/553 (24%)	127 (95%)	7 (5%)	0	100	100
3	a	139/553 (25%)	134 (96%)	5 (4%)	0	100	100
3	b	132/553 (24%)	128 (97%)	4 (3%)	0	100	100
3	c	134/553 (24%)	127 (95%)	7 (5%)	0	100	100
4	P	791/794 (100%)	773 (98%)	18 (2%)	0	100	100
4	Q	791/794 (100%)	775 (98%)	16 (2%)	0	100	100
4	R	791/794 (100%)	776 (98%)	15 (2%)	0	100	100
4	S	791/794 (100%)	774 (98%)	17 (2%)	0	100	100
4	T	791/794 (100%)	775 (98%)	16 (2%)	0	100	100
4	x	791/794 (100%)	774 (98%)	17 (2%)	0	100	100
5	U	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
5	V	194/196 (99%)	192 (99%)	2 (1%)	0	100	100
5	W	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
5	X	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
5	Y	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
5	Z	193/196 (98%)	191 (99%)	2 (1%)	0	100	100
5	d	193/196 (98%)	191 (99%)	2 (1%)	0	100	100
5	e	193/196 (98%)	191 (99%)	2 (1%)	0	100	100
5	f	193/196 (98%)	191 (99%)	2 (1%)	0	100	100
5	g	193/196 (98%)	191 (99%)	2 (1%)	0	100	100
5	h	194/196 (99%)	192 (99%)	2 (1%)	0	100	100
5	i	193/196 (98%)	191 (99%)	2 (1%)	0	100	100
6	j	522/536 (97%)	514 (98%)	8 (2%)	0	100	100
6	k	522/536 (97%)	513 (98%)	9 (2%)	0	100	100
6	l	522/536 (97%)	515 (99%)	7 (1%)	0	100	100
6	m	522/536 (97%)	515 (99%)	7 (1%)	0	100	100
6	n	522/536 (97%)	515 (99%)	7 (1%)	0	100	100
6	o	522/536 (97%)	513 (98%)	9 (2%)	0	100	100
6	p	522/536 (97%)	514 (98%)	8 (2%)	0	100	100
6	q	522/536 (97%)	515 (99%)	7 (1%)	0	100	100
6	r	522/536 (97%)	515 (99%)	7 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	s	522/536 (97%)	514 (98%)	8 (2%)	0	100	100
6	t	522/536 (97%)	514 (98%)	8 (2%)	0	100	100
6	u	522/536 (97%)	514 (98%)	8 (2%)	0	100	100
All	All	15984/25152 (64%)	15660 (98%)	312 (2%)	12 (0%)	49	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	9	9	THR
1	0	9	THR
1	6	9	THR
1	AB	9	THR
1	AC	9	THR
1	5	9	THR
1	8	9	THR
1	AA	9	THR
1	4	9	THR
1	AD	9	THR
1	3	9	THR
1	7	9	THR

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	0	14/73 (19%)	12 (86%)	2 (14%)	3	8
1	3	14/73 (19%)	12 (86%)	2 (14%)	3	8
1	4	14/73 (19%)	13 (93%)	1 (7%)	13	33
1	5	14/73 (19%)	14 (100%)	0	100	100
1	6	14/73 (19%)	14 (100%)	0	100	100
1	7	14/73 (19%)	13 (93%)	1 (7%)	13	33
1	8	14/73 (19%)	13 (93%)	1 (7%)	13	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9	14/73 (19%)	14 (100%)	0	100	100
1	AA	14/73 (19%)	12 (86%)	2 (14%)	3	8
1	AB	14/73 (19%)	14 (100%)	0	100	100
1	AC	14/73 (19%)	12 (86%)	2 (14%)	3	8
1	AD	14/73 (19%)	13 (93%)	1 (7%)	13	33
2	1	11/72 (15%)	11 (100%)	0	100	100
2	2	11/72 (15%)	11 (100%)	0	100	100
2	v	11/72 (15%)	11 (100%)	0	100	100
2	w	11/72 (15%)	11 (100%)	0	100	100
2	y	11/72 (15%)	11 (100%)	0	100	100
2	z	11/72 (15%)	11 (100%)	0	100	100
3	A	122/451 (27%)	122 (100%)	0	100	100
3	B	122/451 (27%)	122 (100%)	0	100	100
3	C	122/451 (27%)	122 (100%)	0	100	100
3	D	122/451 (27%)	122 (100%)	0	100	100
3	E	122/451 (27%)	122 (100%)	0	100	100
3	F	117/451 (26%)	117 (100%)	0	100	100
3	G	117/451 (26%)	117 (100%)	0	100	100
3	H	117/451 (26%)	117 (100%)	0	100	100
3	I	117/451 (26%)	117 (100%)	0	100	100
3	J	117/451 (26%)	117 (100%)	0	100	100
3	K	118/451 (26%)	118 (100%)	0	100	100
3	L	118/451 (26%)	118 (100%)	0	100	100
3	M	118/451 (26%)	118 (100%)	0	100	100
3	N	118/451 (26%)	118 (100%)	0	100	100
3	O	118/451 (26%)	118 (100%)	0	100	100
3	a	122/451 (27%)	122 (100%)	0	100	100
3	b	117/451 (26%)	117 (100%)	0	100	100
3	c	118/451 (26%)	118 (100%)	0	100	100
4	P	687/688 (100%)	687 (100%)	0	100	100
4	Q	687/688 (100%)	687 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	687/688 (100%)	686 (100%)	1 (0%)	88	96
4	S	687/688 (100%)	687 (100%)	0	100	100
4	T	687/688 (100%)	687 (100%)	0	100	100
4	x	687/688 (100%)	686 (100%)	1 (0%)	88	96
5	U	169/169 (100%)	169 (100%)	0	100	100
5	V	169/169 (100%)	168 (99%)	1 (1%)	78	91
5	W	169/169 (100%)	169 (100%)	0	100	100
5	X	169/169 (100%)	169 (100%)	0	100	100
5	Y	169/169 (100%)	169 (100%)	0	100	100
5	Z	168/169 (99%)	168 (100%)	0	100	100
5	d	168/169 (99%)	168 (100%)	0	100	100
5	e	168/169 (99%)	168 (100%)	0	100	100
5	f	168/169 (99%)	168 (100%)	0	100	100
5	g	168/169 (99%)	168 (100%)	0	100	100
5	h	169/169 (100%)	169 (100%)	0	100	100
5	i	168/169 (99%)	168 (100%)	0	100	100
6	j	435/442 (98%)	435 (100%)	0	100	100
6	k	435/442 (98%)	435 (100%)	0	100	100
6	l	435/442 (98%)	435 (100%)	0	100	100
6	m	435/442 (98%)	435 (100%)	0	100	100
6	n	435/442 (98%)	434 (100%)	1 (0%)	87	95
6	o	435/442 (98%)	434 (100%)	1 (0%)	87	95
6	p	435/442 (98%)	435 (100%)	0	100	100
6	q	435/442 (98%)	435 (100%)	0	100	100
6	r	435/442 (98%)	435 (100%)	0	100	100
6	s	435/442 (98%)	435 (100%)	0	100	100
6	t	435/442 (98%)	435 (100%)	0	100	100
6	u	435/442 (98%)	433 (100%)	2 (0%)	81	92
All	All	13740/20886 (66%)	13721 (100%)	19 (0%)	87	96

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	12	MET
1	0	14	THR
1	3	7	ILE
1	3	12	MET
1	4	14	THR
1	7	7	ILE
1	8	9	THR
1	AA	9	THR
1	AA	12	MET
1	AC	9	THR
1	AC	12	MET
1	AD	12	MET
4	R	71	ARG
5	V	60	THR
6	n	423	GLU
6	o	30	ARG
6	u	30	ARG
6	u	519	SER
4	x	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	98	ASN
2	2	98	ASN
3	B	47	ASN
3	B	138	ASN
3	C	47	ASN
3	C	138	ASN
3	D	138	ASN
3	F	124	ASN
3	I	124	ASN
3	J	124	ASN
3	L	47	ASN
4	P	10	ASN
4	P	214	ASN
4	P	217	GLN
4	P	228	GLN
4	P	398	ASN
4	P	477	GLN
4	P	542	HIS
4	P	645	GLN
4	Q	190	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Q	207	ASN
4	Q	242	GLN
4	Q	686	GLN
4	Q	709	ASN
4	Q	723	GLN
4	Q	752	GLN
4	R	10	ASN
4	R	207	ASN
4	S	10	ASN
4	S	477	GLN
4	S	542	HIS
4	T	207	ASN
4	T	242	GLN
4	T	661	ASN
4	T	709	ASN
4	T	752	GLN
5	U	93	GLN
5	U	147	ASN
5	V	93	GLN
5	V	147	ASN
5	W	93	GLN
5	W	147	ASN
5	X	93	GLN
5	X	147	ASN
5	Y	93	GLN
5	Y	147	ASN
5	Z	93	GLN
3	a	138	ASN
3	b	124	ASN
3	c	105	GLN
5	d	37	ASN
5	d	93	GLN
5	e	93	GLN
5	f	93	GLN
5	f	109	GLN
5	g	37	ASN
5	g	93	GLN
5	h	93	GLN
5	h	147	ASN
5	i	93	GLN
6	j	36	GLN
6	j	95	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	j	335	GLN
6	j	397	GLN
6	j	498	GLN
6	j	503	ASN
6	k	68	ASN
6	k	95	GLN
6	k	175	ASN
6	k	413	GLN
6	k	462	ASN
6	k	487	GLN
6	k	498	GLN
6	k	503	ASN
6	k	515	GLN
6	l	331	GLN
6	l	335	GLN
6	m	413	GLN
6	n	335	GLN
6	n	359	ASN
6	n	363	GLN
6	n	397	GLN
6	n	495	GLN
6	n	498	GLN
6	o	95	GLN
6	o	437	GLN
6	o	462	ASN
6	o	498	GLN
6	o	503	ASN
6	p	36	GLN
6	p	95	GLN
6	p	335	GLN
6	p	397	GLN
6	p	503	ASN
6	q	68	ASN
6	q	95	GLN
6	q	175	ASN
6	q	413	GLN
6	q	462	ASN
6	q	472	ASN
6	q	494	GLN
6	q	498	GLN
6	q	503	ASN
6	q	515	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	r	335	GLN
6	r	363	GLN
6	r	503	ASN
6	s	413	GLN
6	s	503	ASN
6	t	335	GLN
6	t	359	ASN
6	t	363	GLN
6	t	397	GLN
6	t	495	GLN
6	u	95	GLN
6	u	359	ASN
6	u	462	ASN
6	u	487	GLN
6	u	498	GLN
6	u	533	GLN
2	w	98	ASN
4	x	10	ASN
4	x	207	ASN
4	x	548	ASN
4	x	764	ASN
2	y	98	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-61910. These allow visual inspection of the internal detail of the map and identification of artifacts.

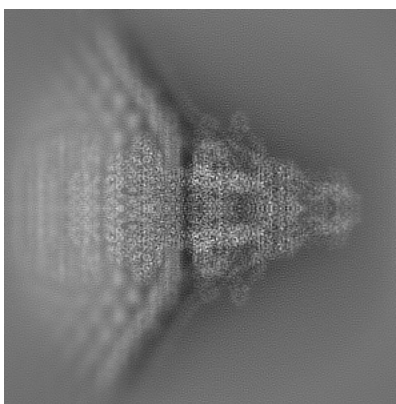
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

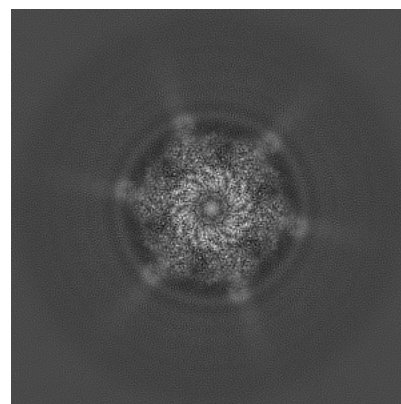
6.1.1 Primary map



X

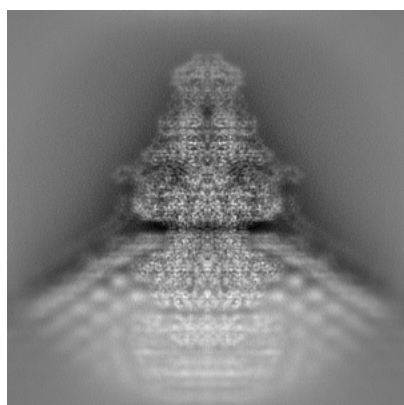


Y

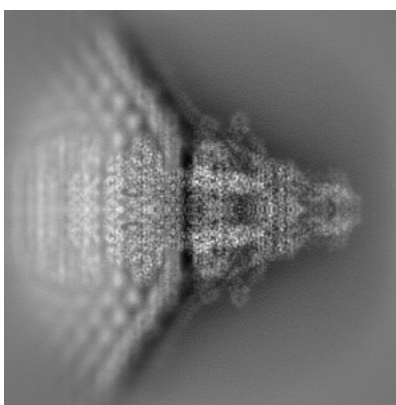


Z

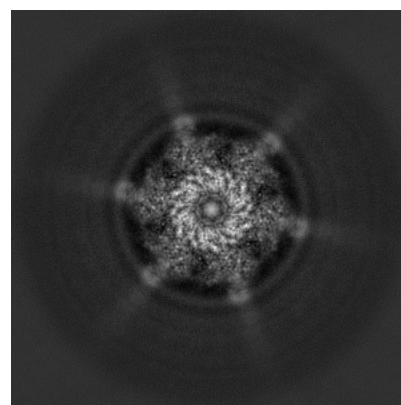
6.1.2 Raw map



X



Y

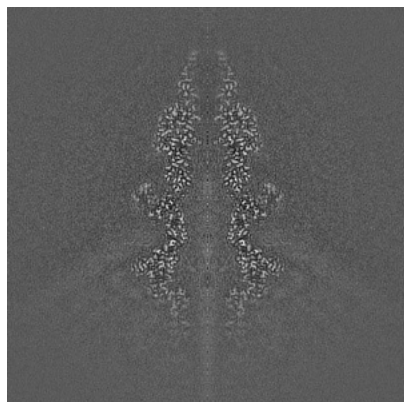


Z

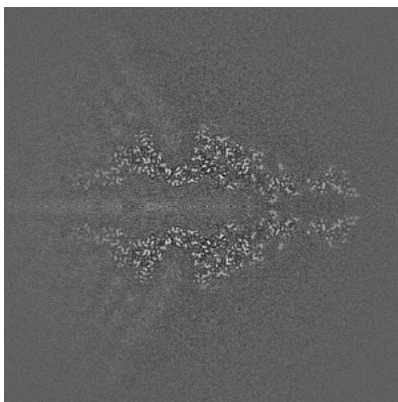
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

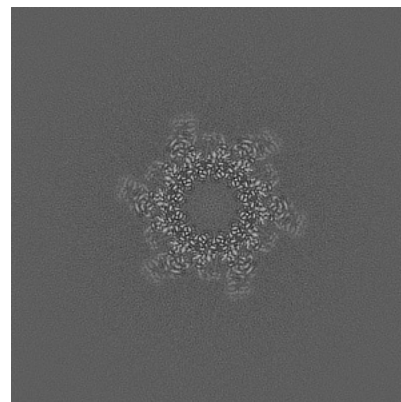
6.2.1 Primary map



X Index: 200

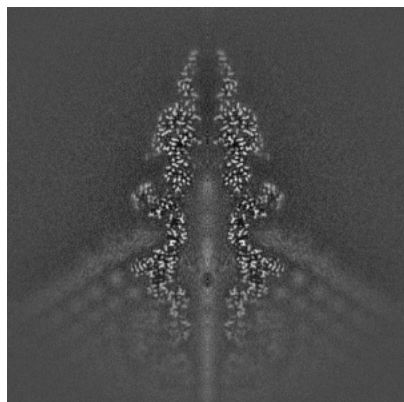


Y Index: 200

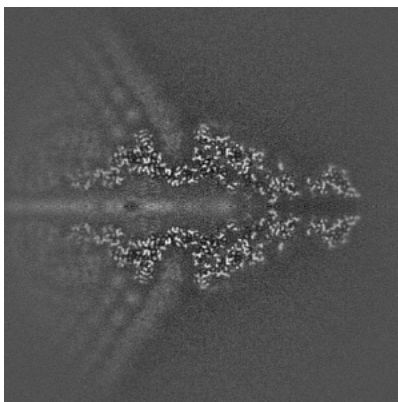


Z Index: 200

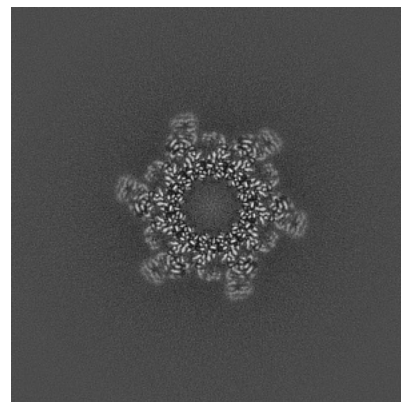
6.2.2 Raw map



X Index: 200



Y Index: 200

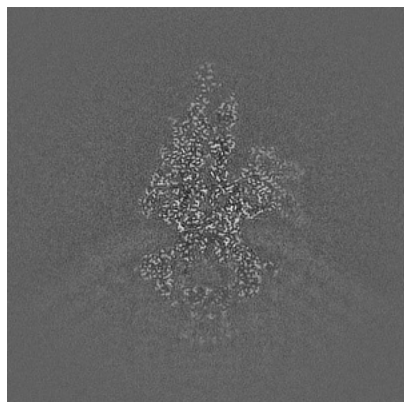


Z Index: 200

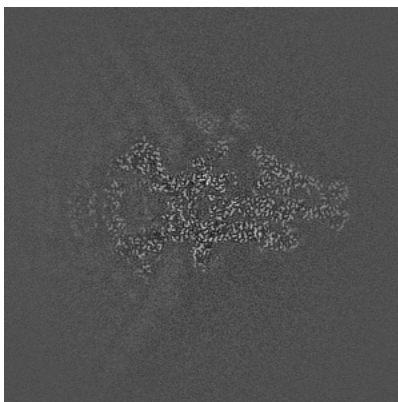
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

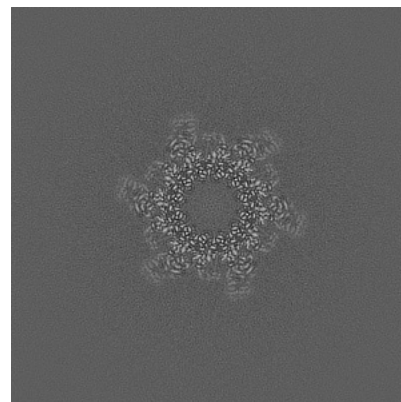
6.3.1 Primary map



X Index: 173

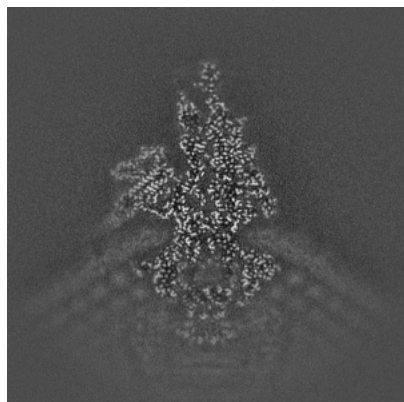


Y Index: 176

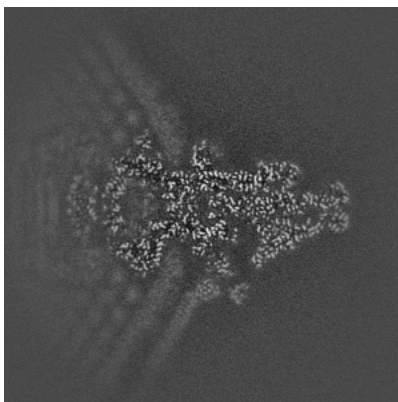


Z Index: 200

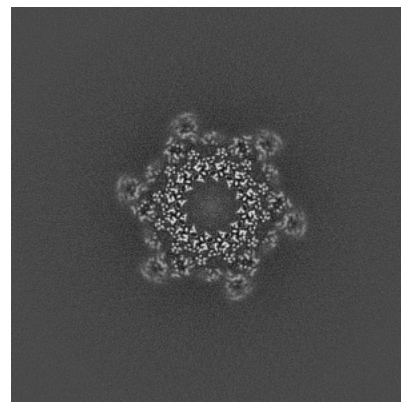
6.3.2 Raw map



X Index: 227



Y Index: 224

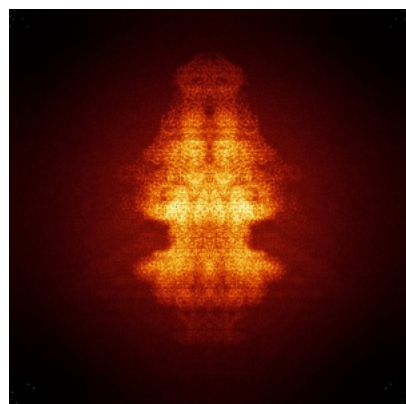


Z Index: 202

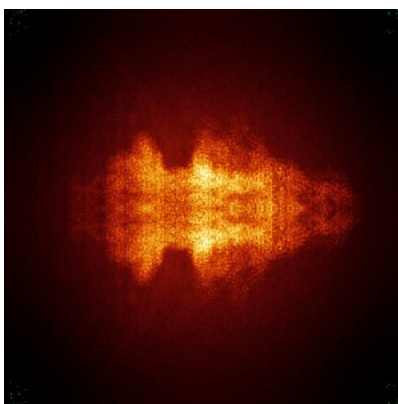
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

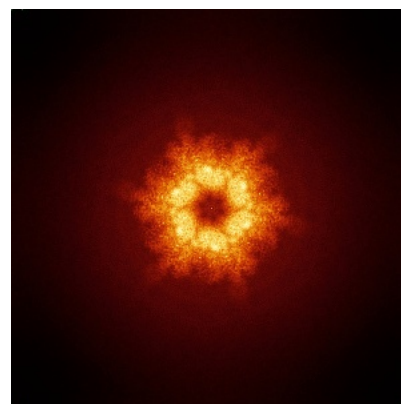
6.4.1 Primary map



X

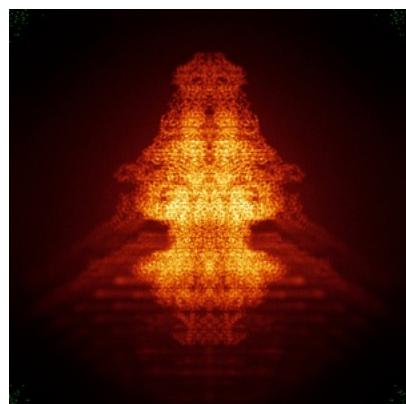


Y

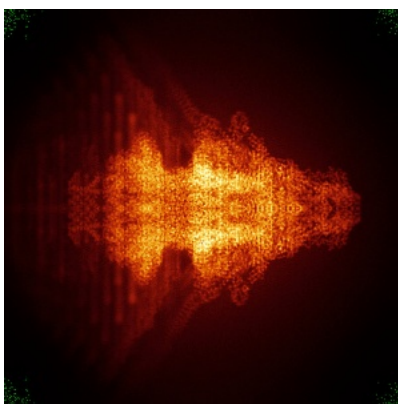


Z

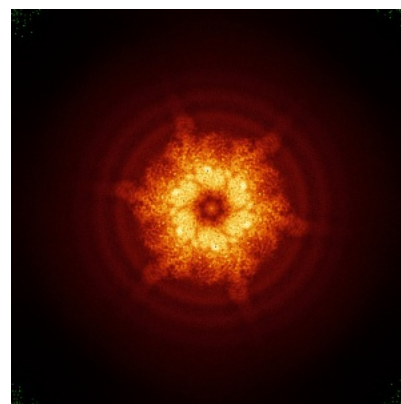
6.4.2 Raw map



X



Y

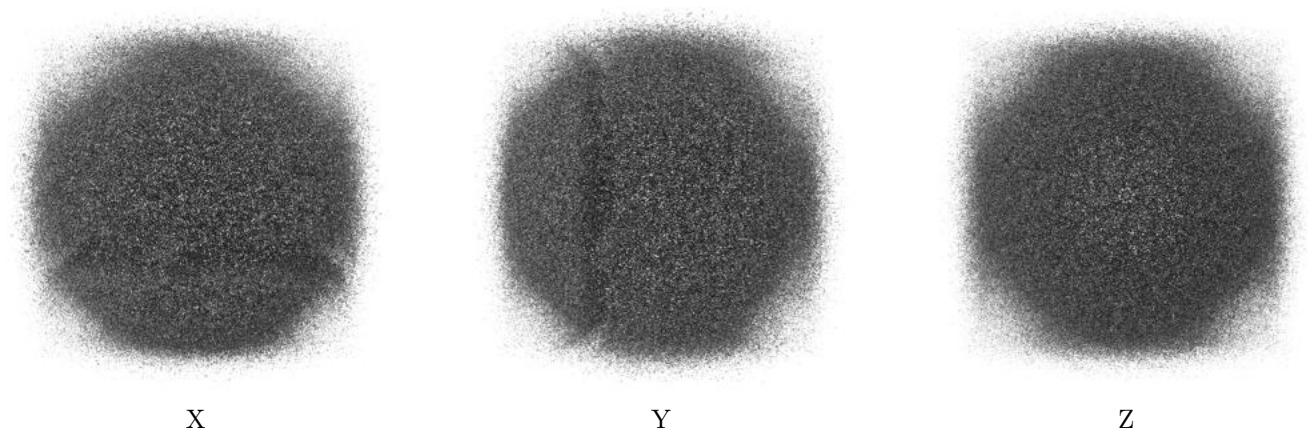


Z

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

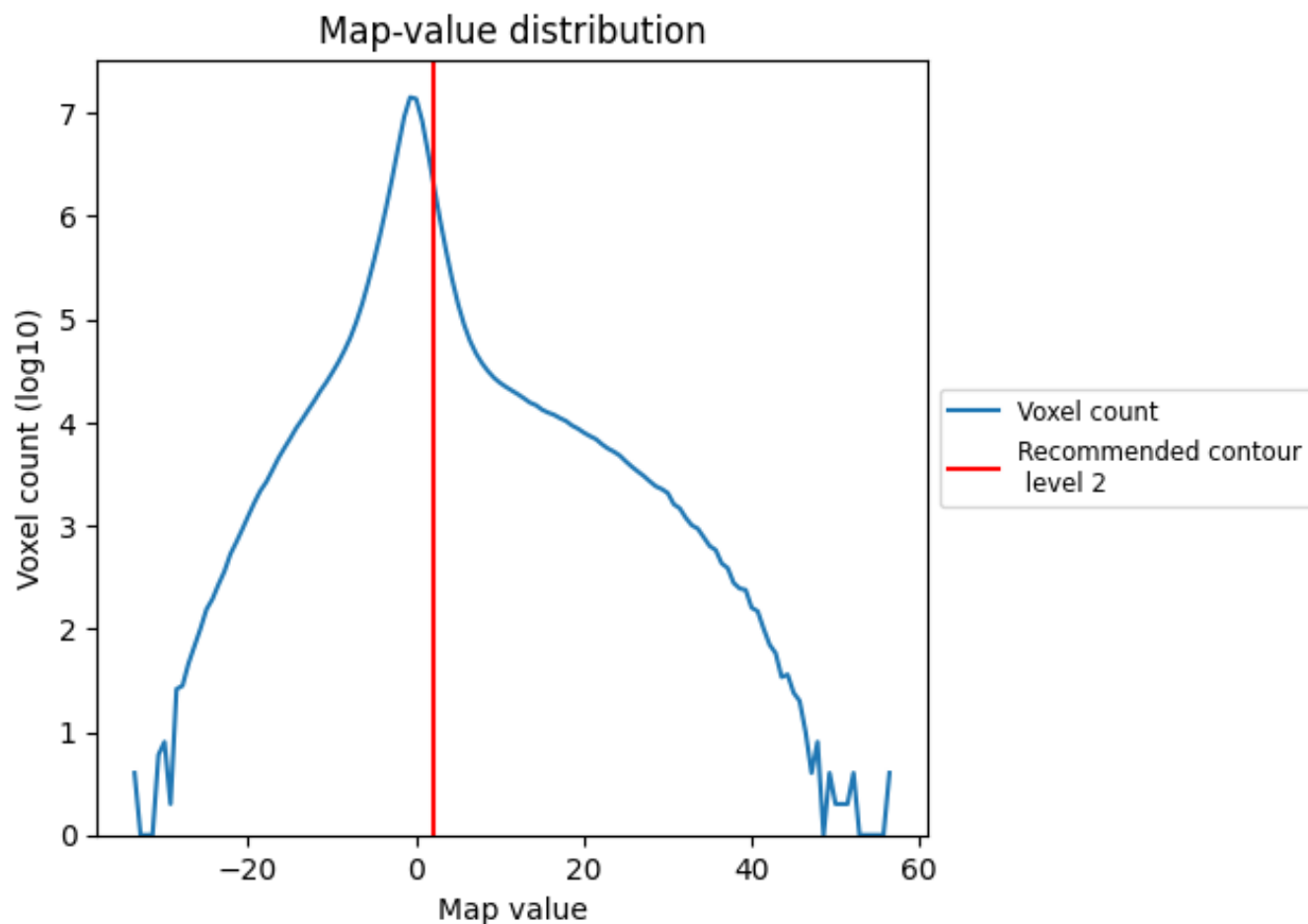
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

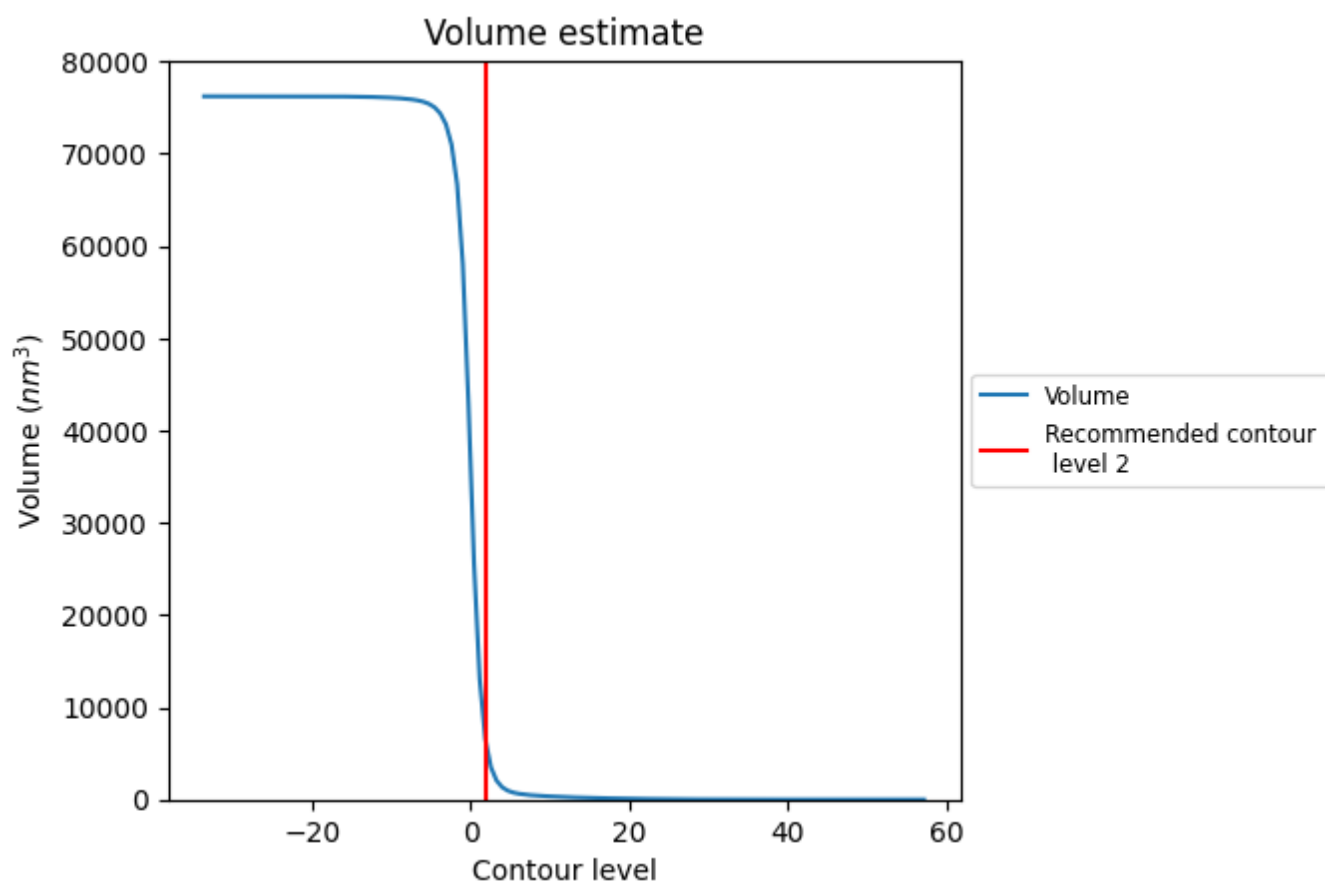
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

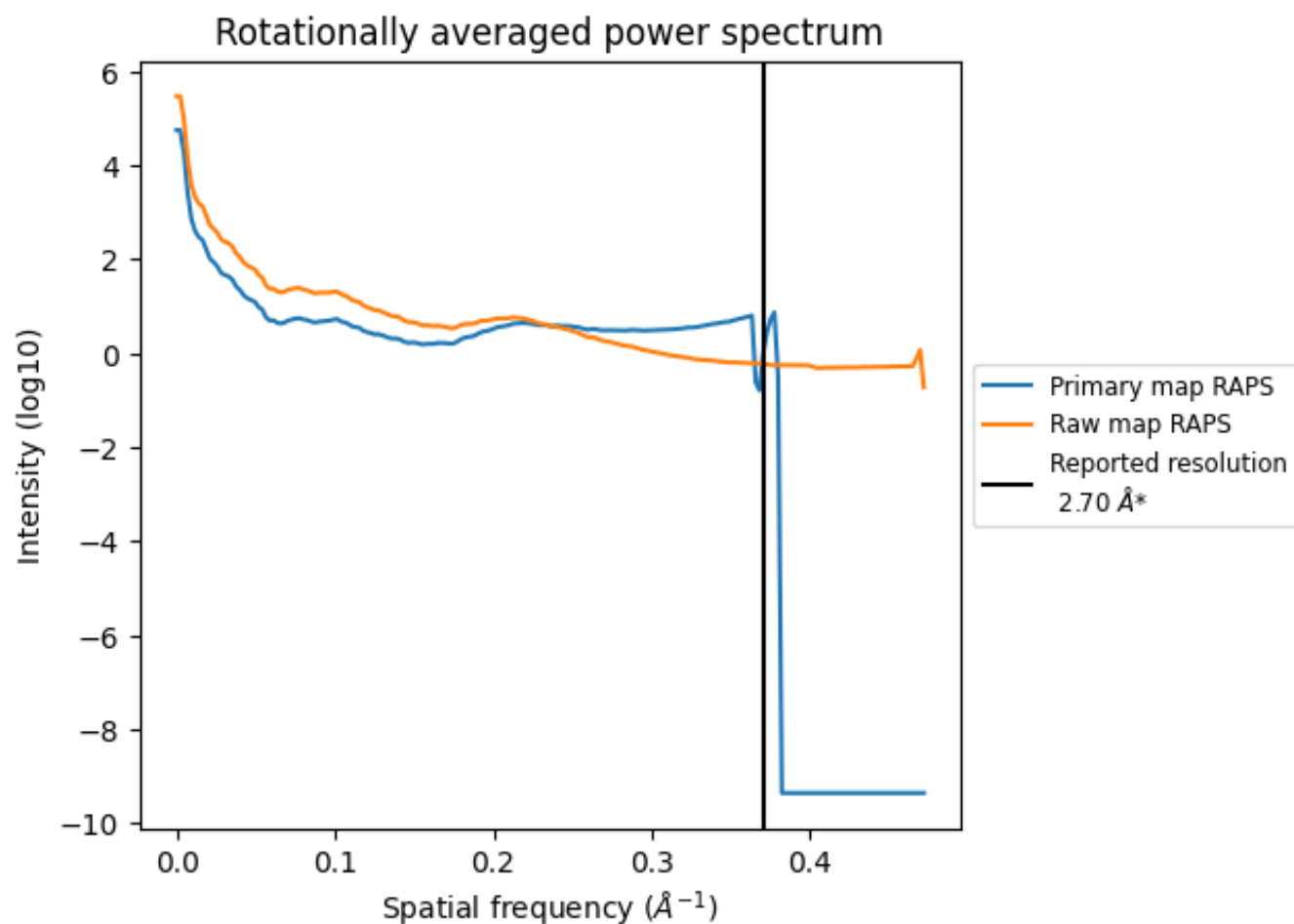
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6205 nm³; this corresponds to an approximate mass of 5605 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 ⓘ

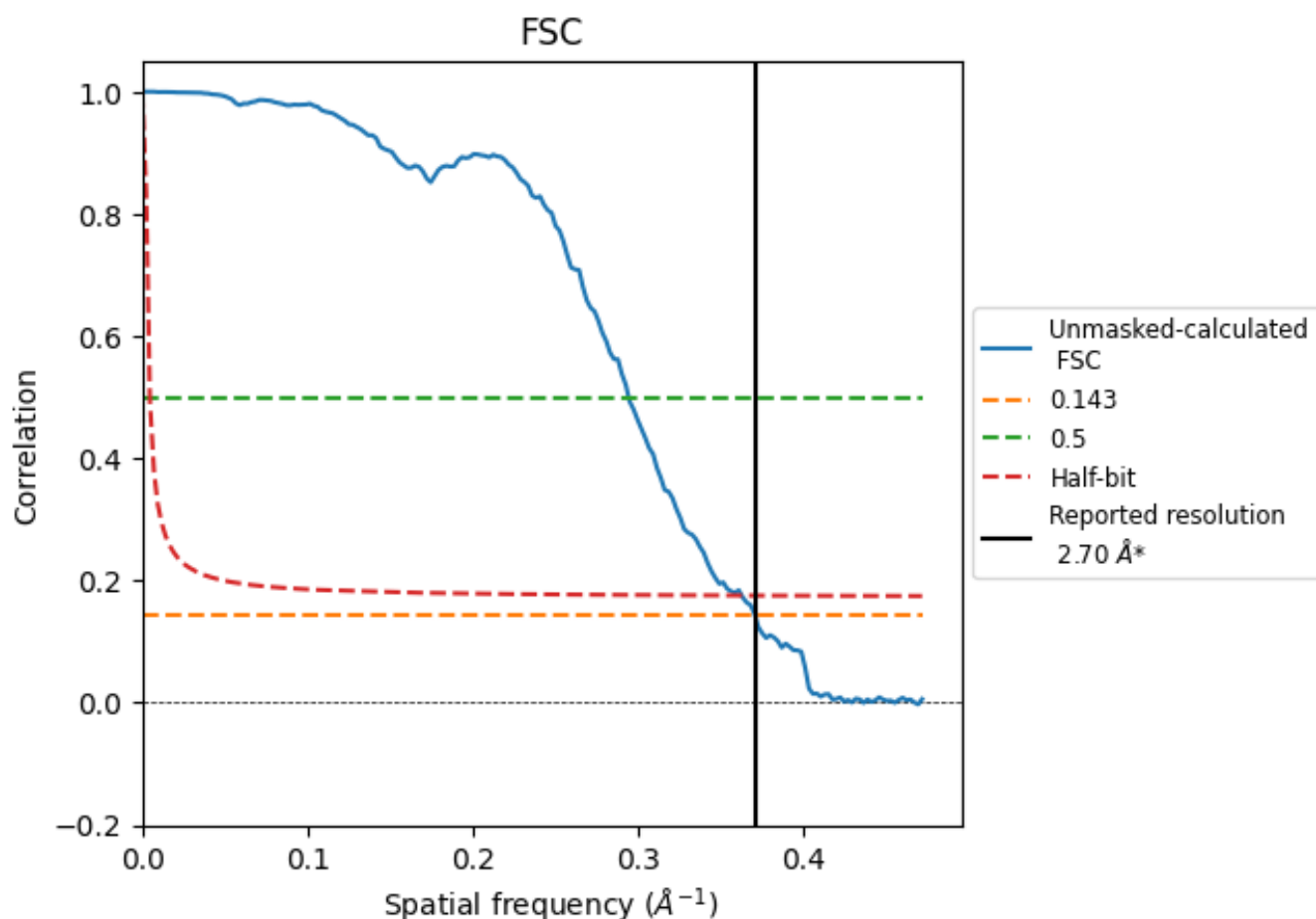


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

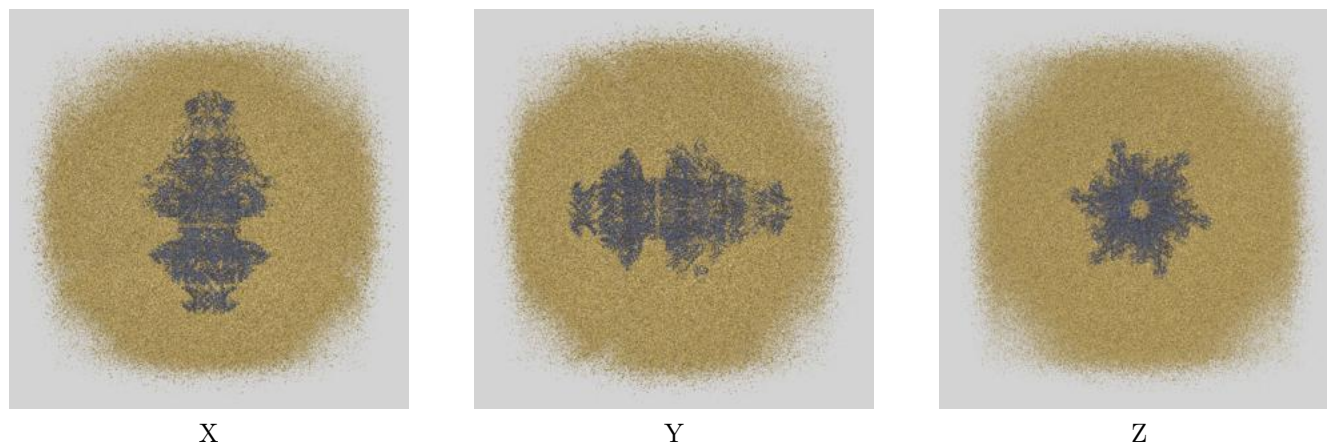
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.70	3.40	2.76

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

9 Map-model fit [i](#)

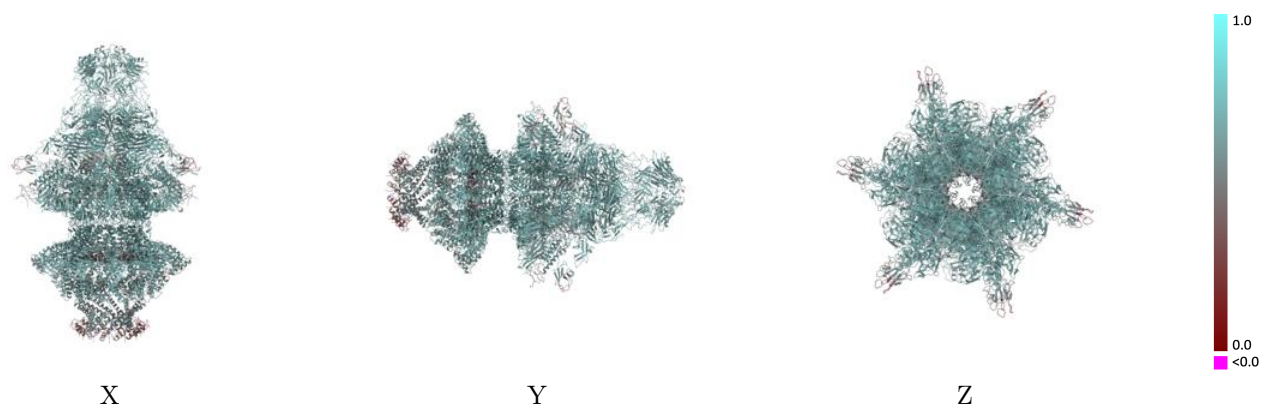
This section contains information regarding the fit between EMDB map EMD-61910 and PDB model 9JYZ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



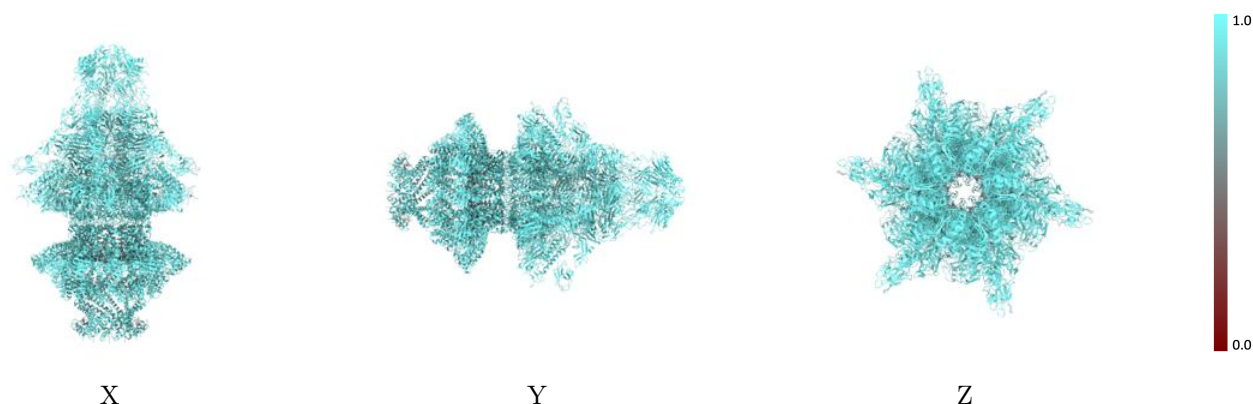
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



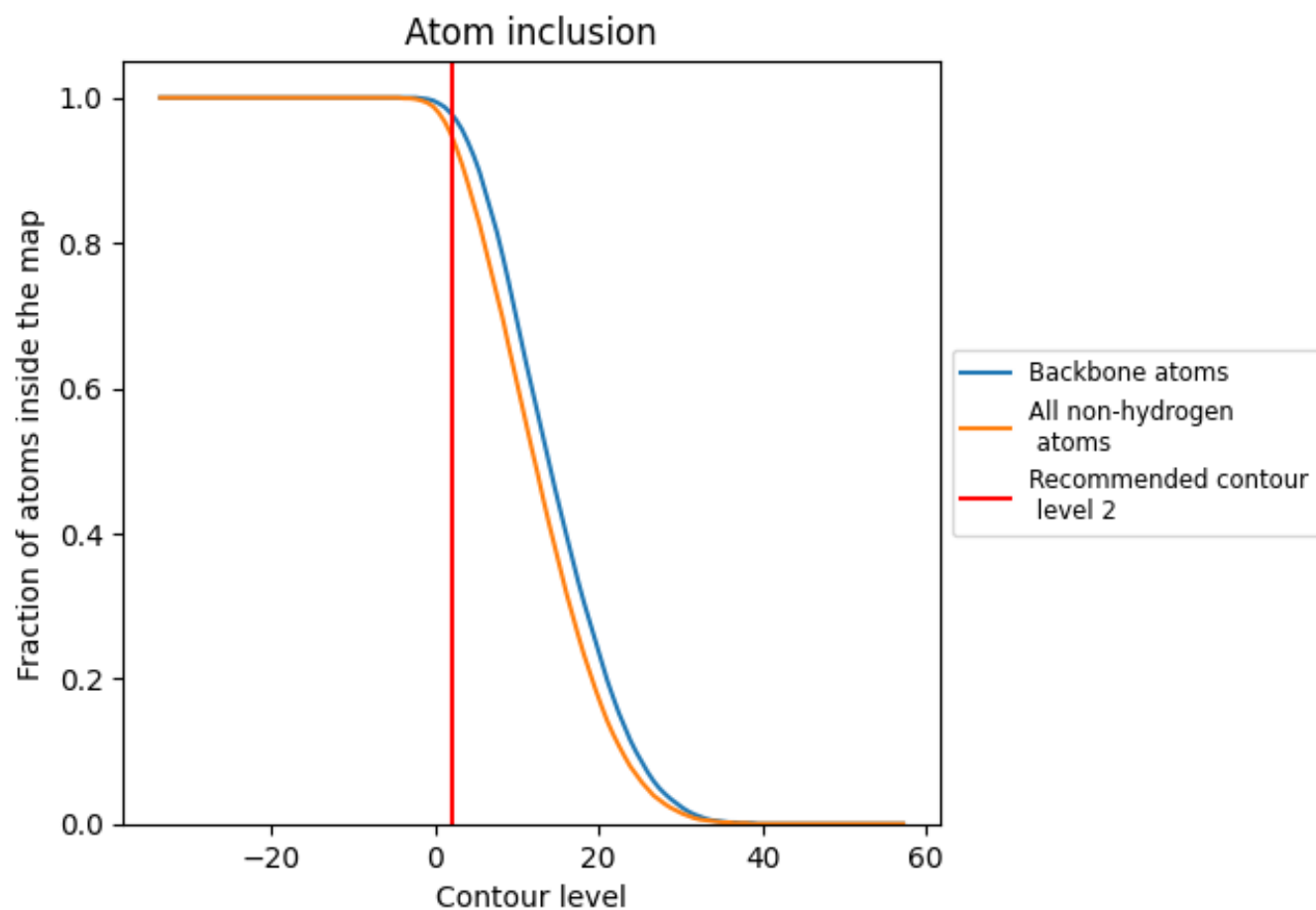
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.6130
0	 0.6000	 0.3620
1	 0.7170	 0.4660
2	 0.7370	 0.4670
3	 0.4820	 0.2770
4	 0.6000	 0.3440
5	 0.5450	 0.3070
6	 0.5820	 0.3550
7	 0.5090	 0.2810
8	 0.5820	 0.3480
9	 0.4640	 0.2300
A	 0.9680	 0.6220
AA	 0.5180	 0.3240
AB	 0.5730	 0.3570
AC	 0.4820	 0.3260
AD	 0.6000	 0.3260
B	 0.9690	 0.6240
C	 0.9670	 0.6250
D	 0.9700	 0.6230
E	 0.9670	 0.6220
F	 0.9680	 0.6060
G	 0.9630	 0.6100
H	 0.9630	 0.6060
I	 0.9690	 0.6040
J	 0.9680	 0.6090
K	 0.9260	 0.5230
L	 0.9280	 0.5230
M	 0.9290	 0.5180
N	 0.9340	 0.5210
O	 0.9250	 0.5200
P	 0.9760	 0.6410
Q	 0.9770	 0.6420
R	 0.9770	 0.6410
S	 0.9760	 0.6410
T	 0.9780	 0.6430



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
U	 0.9780	 0.6600
V	 0.9760	 0.6640
W	 0.9730	 0.6610
X	 0.9780	 0.6610
Y	 0.9760	 0.6660
Z	 0.9770	 0.6600
a	 0.9700	 0.6230
b	 0.9700	 0.6030
c	 0.9350	 0.5220
d	 0.9740	 0.6560
e	 0.9780	 0.6600
f	 0.9780	 0.6580
g	 0.9730	 0.6550
h	 0.9760	 0.6630
i	 0.9780	 0.6610
j	 0.9270	 0.5900
k	 0.9310	 0.6000
l	 0.9290	 0.5910
m	 0.9290	 0.5970
n	 0.9280	 0.5910
o	 0.9320	 0.5960
p	 0.9270	 0.5900
q	 0.9290	 0.5980
r	 0.9290	 0.5910
s	 0.9300	 0.5960
t	 0.9290	 0.5910
u	 0.9330	 0.5970
v	 0.7580	 0.4670
w	 0.6970	 0.4620
x	 0.9760	 0.6410
y	 0.7480	 0.4770
z	 0.7480	 0.4670