



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:09 PM UTC

PDB ID : 6Q15 / pdb_00006q15
EMDB ID : EMD-20312
Title : Structure of the Salmonella SPI-1 injectisome needle complex
Authors : Hu, J.; Worrall, L.J.; Strynadka, N.C.J.
Deposited on : 2019-08-02
Resolution : 5.15 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

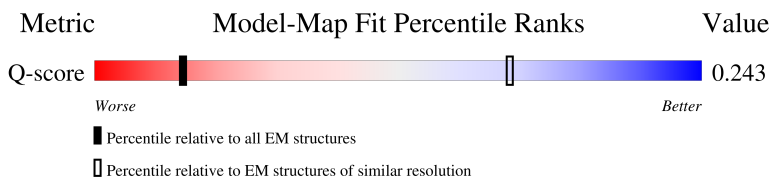
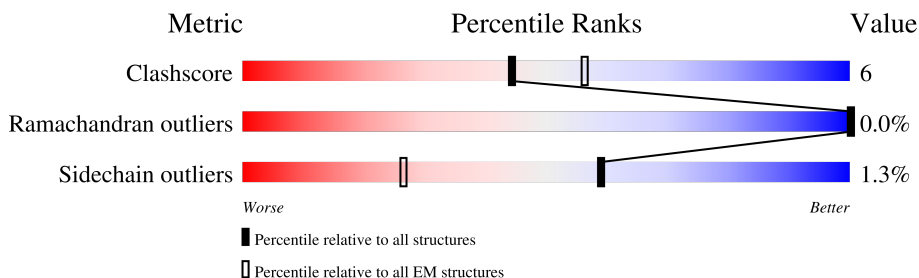
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.15 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	694 (4.65 - 5.65)

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	AA	252	12% 63% 10% 27%
1	AB	252	10% 63% 10% 27%
1	AC	252	12% 60% 13% 27%
1	AD	252	12% 62% 11% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AE	252	9% 62% 12% 27%
1	AF	252	11% 61% 12% 27%
1	AG	252	11% 62% 12% 27%
1	AH	252	12% 62% 11% 27%
1	AI	252	12% 60% 13% 27%
1	AJ	252	13% 60% 13% 27%
1	AK	252	11% 64% 8% 27%
1	AL	252	11% 58% 14% 27%
1	o	252	13% 60% 13% 27%
1	p	252	13% 60% 13% 27%
1	q	252	16% 60% 13% 27%
1	r	252	10% 59% 13% 27%
1	s	252	15% 58% 15% 27%
1	t	252	12% 60% 12% 27%
1	u	252	13% 62% 12% 27%
1	v	252	17% 56% 17% 27%
1	w	252	17% 60% 13% 27%
1	x	252	12% 67% 6% 27%
1	y	252	12% 61% 12% 27%
1	z	252	11% 59% 14% 27%
2	E	392	9% 47% 9% 43%
2	R	392	7% 49% 7% 44%
2	S	392	6% 45% 12% 43%
2	T	392	9% 47% 9% 43%
2	U	392	7% 47% 9% 44%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	V	392	
2	W	392	
2	X	392	
2	Y	392	
2	Z	392	
2	a	392	
2	b	392	
2	c	392	
2	d	392	
2	e	392	
2	f	392	
2	g	392	
2	h	392	
2	i	392	
2	j	392	
2	k	392	
2	l	392	
2	m	392	
2	n	392	
3	A	562	
3	B	562	
3	C	562	
3	D	562	
3	F	562	
3	G	562	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	562	
3	I	562	
3	J	562	
3	K	562	
3	L	562	
3	M	562	
3	N	562	
3	O	562	
3	P	562	
3	Q	562	
4	0	224	
4	1	224	
4	2	224	
4	3	224	
4	4	224	
5	5	263	
6	6	86	
6	7	86	
6	8	86	
6	9	86	
7	AM	101	
7	AN	101	
7	AO	101	
7	AP	101	
7	AQ	101	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	AR	101	
8	AS	80	
8	AT	80	
8	AU	80	
8	AV	80	
8	AW	80	
8	AX	80	
8	AY	80	
8	AZ	80	
8	BA	80	
8	BB	80	
8	BC	80	
8	BD	80	
8	BE	80	
8	BF	80	
8	BG	80	
8	BH	80	
8	BI	80	
8	BJ	80	
8	BK	80	
8	BL	80	
8	BM	80	
8	BN	80	
8	BO	80	
8	BP	80	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	BQ	80	81% 15%
8	BR	80	90% 11%
8	BS	80	92% 10%
8	BT	80	88% 15%
8	BU	80	95% 15%
8	BU	80	81% 18%
8	BV	80	80% 98%
8	BV	80	88% 10%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 170801 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 Lipoprotein PrgK.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AB	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AC	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AD	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AE	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AF	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AG	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AH	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AI	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	AL	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	o	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	p	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	q	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	r	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	s	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	t	184	Total 1431	C 901	N 250	O 277	S 3	0	0
1	u	184	Total 1431	C 901	N 250	O 277	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	v	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	w	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	x	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	y	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	z	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AJ	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
1	AK	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		

- Molecule 2 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	R	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	S	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
2	T	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	U	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	V	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
2	W	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	X	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	Y	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
2	Z	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	a	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	b	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	d	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	e	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
2	f	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	g	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	h	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
2	i	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	j	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	k	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		
2	l	222	Total	C	N	O	S	0	0
			1836	1170	326	335	5		
2	m	221	Total	C	N	O	S	0	0
			1827	1164	325	333	5		
2	n	222	Total	C	N	O	S	0	0
			1831	1167	326	333	5		

- Molecule 3 is a protein called Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	144	Total	C	N	O	S	1	0
			1154	741	198	209	6		
3	A	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	B	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		
3	C	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	D	502	Total	C	N	O	S	0	0
			3876	2454	670	739	13		
3	F	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	G	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	I	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		
3	J	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	K	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		
3	L	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	M	502	Total	C	N	O	S	0	0
			3876	2454	670	739	13		
3	N	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		
3	O	502	Total	C	N	O	S	1	0
			3884	2459	673	739	13		
3	P	497	Total	C	N	O	S	0	0
			3838	2428	664	733	13		

- Molecule 4 is a protein called Surface presentation of antigens protein SpaP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	199	Total	C	N	O	S	0	0
			1562	1041	231	279	11		
4	1	199	Total	C	N	O	S	0	0
			1569	1047	232	279	11		
4	2	197	Total	C	N	O	S	0	0
			1553	1037	230	275	11		
4	3	204	Total	C	N	O	S	0	0
			1606	1071	238	286	11		
4	4	221	Total	C	N	O	S	1	0
			1758	1163	266	318	11		

- Molecule 5 is a protein called Surface presentation of antigens protein SpaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	247	Total	C	N	O	S	0	0
			1885	1252	300	320	13		

- Molecule 6 is a protein called Surface presentation of antigens protein SpaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	53	Total	C	N	O	S	0	0
			405	276	61	67	1		
6	7	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
6	8	84	Total	C	N	O	S	0	0
			644	436	97	109	2		
6	9	84	Total	C	N	O	S	0	0
			647	438	97	109	3		

- Molecule 7 is a protein called Protein PrgJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AM	39	Total	C	N	O	S	0	0
			298	187	49	60	2		
7	AN	78	Total	C	N	O	S	7	0
			644	396	116	130	2		
7	AO	88	Total	C	N	O	S	0	0
			667	410	114	140	3		
7	AP	88	Total	C	N	O	S	0	0
			667	410	114	140	3		
7	AQ	88	Total	C	N	O	S	0	0
			667	410	114	140	3		
7	AR	88	Total	C	N	O	S	0	0
			667	410	114	140	3		

- Molecule 8 is a protein called Protein PrgI.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AS	59	Total	C	N	O	0	0
			466	294	80	92		
8	AT	59	Total	C	N	O	0	0
			466	294	80	92		
8	AU	59	Total	C	N	O	0	0
			466	294	80	92		
8	AV	59	Total	C	N	O	0	0
			466	294	80	92		
8	AW	59	Total	C	N	O	0	0
			466	294	80	92		
8	AX	73	Total	C	N	O	0	0
			574	362	95	117		
8	AY	78	Total	C	N	O	0	0
			612	387	101	124		
8	AZ	78	Total	C	N	O	0	0
			612	387	101	124		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
8	BB	78	Total 612	C 387	N 101	O 124	0	0
8	BD	78	Total 612	C 387	N 101	O 124	0	0
8	BE	78	Total 612	C 387	N 101	O 124	0	0
8	BJ	78	Total 612	C 387	N 101	O 124	0	0
8	BK	78	Total 612	C 387	N 101	O 124	0	0
8	BF	78	Total 612	C 387	N 101	O 124	0	0
8	BL	78	Total 612	C 387	N 101	O 124	0	0
8	BG	78	Total 612	C 387	N 101	O 124	0	0
8	BM	78	Total 612	C 387	N 101	O 124	0	0
8	BH	78	Total 612	C 387	N 101	O 124	0	0
8	BN	78	Total 612	C 387	N 101	O 124	0	0
8	BI	78	Total 612	C 387	N 101	O 124	0	0
8	BO	78	Total 612	C 387	N 101	O 124	0	0
8	BP	78	Total 612	C 387	N 101	O 124	0	0
8	BQ	78	Total 612	C 387	N 101	O 124	0	0
8	BC	78	Total 612	C 387	N 101	O 124	0	0
8	BA	78	Total 612	C 387	N 101	O 124	0	0
8	BV	78	Total 612	C 387	N 101	O 124	0	0
8	BU	78	Total 612	C 387	N 101	O 124	0	0
8	BT	78	Total 612	C 387	N 101	O 124	0	0
8	BS	78	Total 612	C 387	N 101	O 124	0	0

Continued on next page...

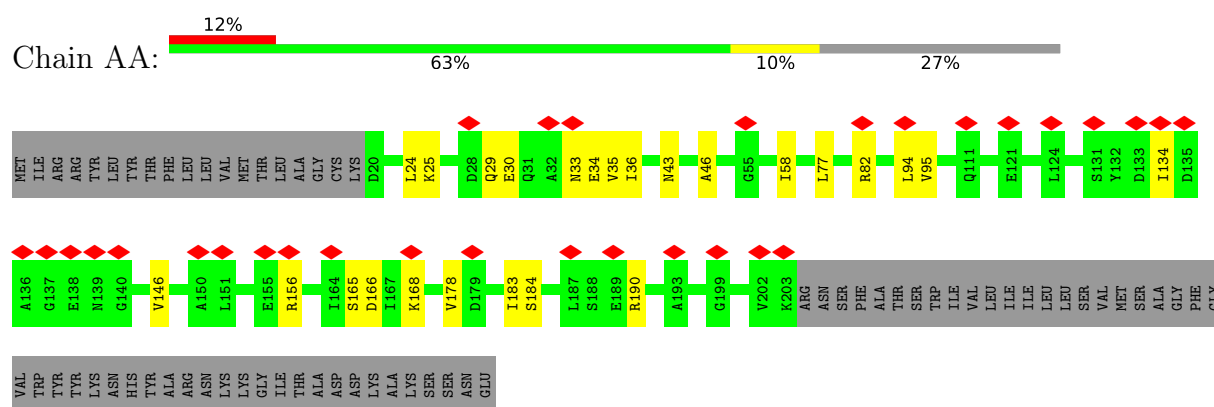
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
8	BR	78	Total	C	N	O	0	0
			612	387	101	124		

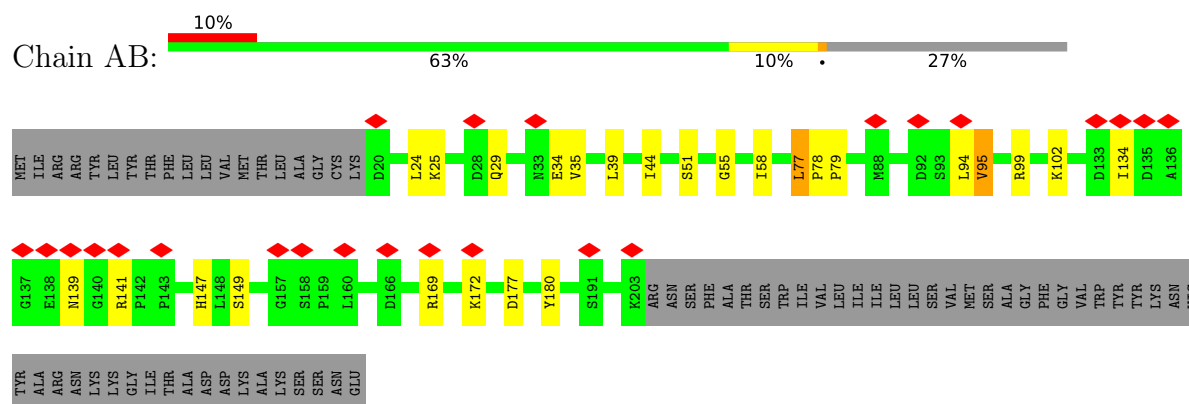
3 Residue-property plots

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

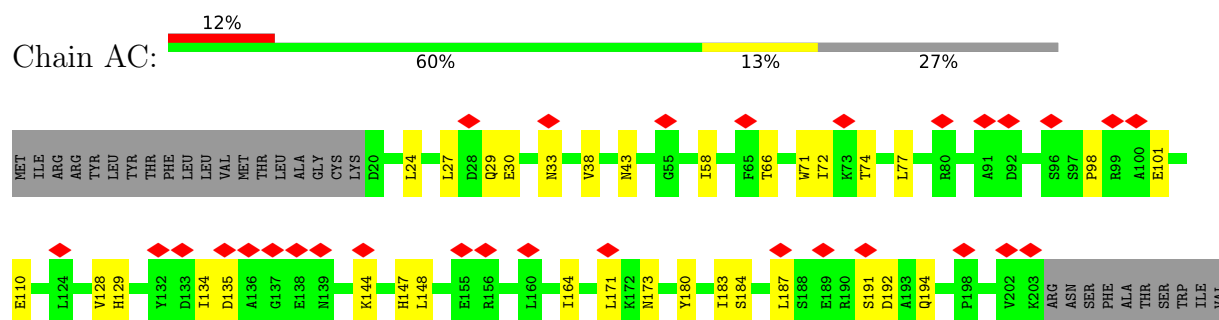
• Molecule 1: Lipoprotein PrgK



• Molecule 1: Lipoprotein PrgK



• Molecule 1: Lipoprotein PrgK



LEU
ILE
ILE
LEU
LEU
SER
VAL
MET
SER
GLY
PHE
GLY
VAL
TRP
TYR
TYR
LYS
ASN
HIS
TYR
ALA
ALA
ASN
LYS
LYS
GLY
ILE
THR
ALA
ASP
ASP
LYS
ALA
LYS
SER
SER
ASN
GLU

• Molecule 1: Lipoprotein PrgK

Chain AD: 

MET
ILE
ARG
ARG
TYR
LEU
TYR
THR
PHE
LEU
LEU
ALA
PHE
MET
THR
LEU
ALA
GLY
CYS
LYS
D20
L24
L27
Q31
A32
V35
I36
A37
K53
L54
V60
P63
D64
W71
T74
Y75
Q76
L77
P78
P79
I85
D92
S93
L94
V95
A100
E101
K102
A103

VAL
LEU
ILE
ILE
LEU
SER
VAL
MET
SER
SER
GLY
PHE
GLY
VAL
TRP
GLY
TYR
TYR
LYS
ASN
HIS
TYR
ALA
ASN
LYS
LYS
GLY
ILE
THR
ALA
ASP
ASP
LYS
ALA
LYS
SER
SER
ASN
GLU

• Molecule 1: Lipoprotein PrgK

Chain AE: 

MET
ILE
ARG
ARG
TYR
LEU
TYR
THR
PHE
LEU
LEU
VAL
MET
THR
LEU
ALA
CYS
LYS
D20
K21
D22
L23
G26
A32
V35
I36
A37
V38
L39
I44
N47
G52
K53
Y56
Y75
Q76
L77
D92
S93
L94
V95
P98
R99
L105
Y106
S107
E110

PHE
GLY
VAL
TRP
TYR
TYR
LYS
ASN
HIS
TYR
TYR
ALA
ARG
ASN
LYS
LYS
GLY
ILE
THR
ALA
ASP
ASP
LYS
ALA
SER
SER
ASN
GLU

• Molecule 1: Lipoprotein PrgK

Chain AF: 

MET
ILE
ARG
ARG
TYR
LEU
TYR
TYR
PHE
LEU
LEU
VAL
MET
THR
LEU
ALA
CYS
LYS
D20
L23
Q29
E30
N33
E34
V35
I36
L39
N43
I44
K48
K53
F62
V69
R82
A91
D92
V95
S96
R99
K102
L117
M120
E121

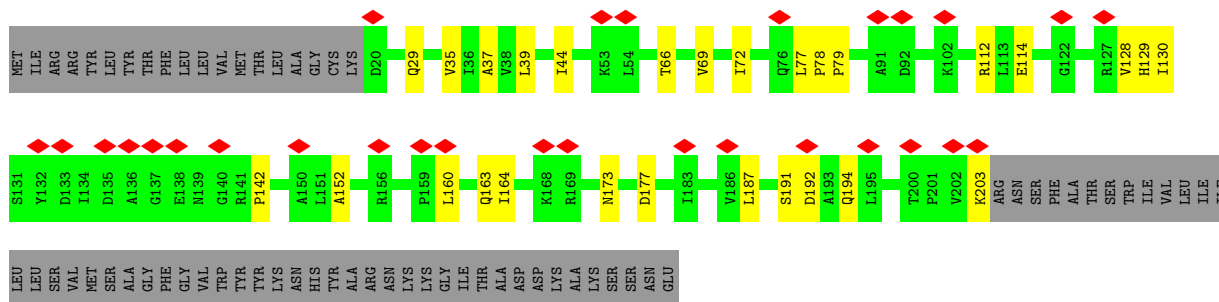
SER
ALA
GLY
PHE
GLY
VAL
TYR
TYR
PHE
LEU
LEU
ASN
HIS
TYR
ALA
ALA
ASN
LYS
LYS
GLY
ILE
THR
ASP
ASP
LYS
ALA
LYS
SER
SER
SER
ASN
GLU

• Molecule 1: Lipoprotein PrgK

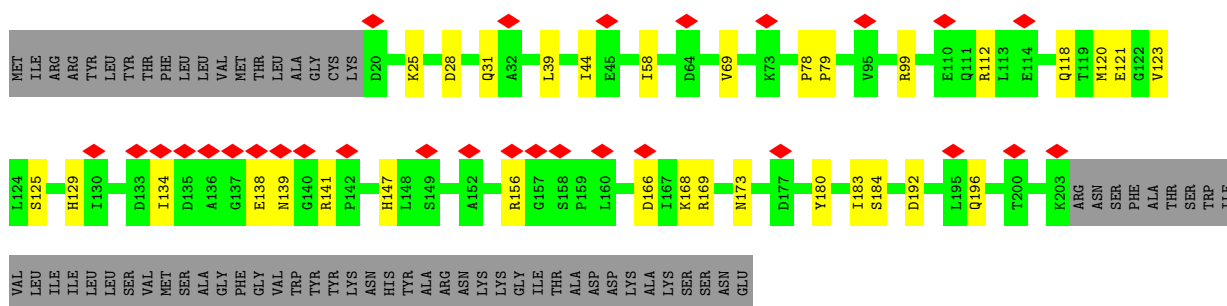
Chain AG: 

MET
ILE
ARG
ARG
TYR
LEU
TYR
TYR
PHE
LEU
LEU
VAL
MET
THR
LEU
ALA
CYS
LYS
D20
K21
D28
I36
A37
V38
L39
Q40
M41
I44
E45
A46
S51
L54
E84
D92
S93
L94
V95
S96
E101
K102
Y106
R112
L117
V123
L124
H129

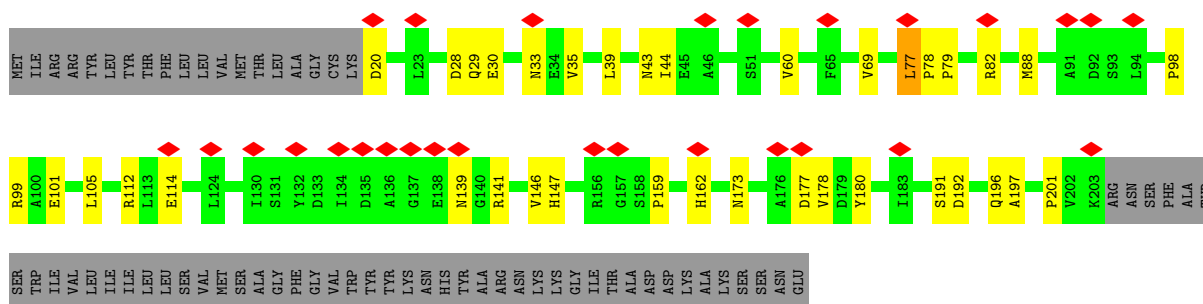
- Molecule 1: Lipoprotein PrgK



- Molecule 1: Lipoprotein PrgK

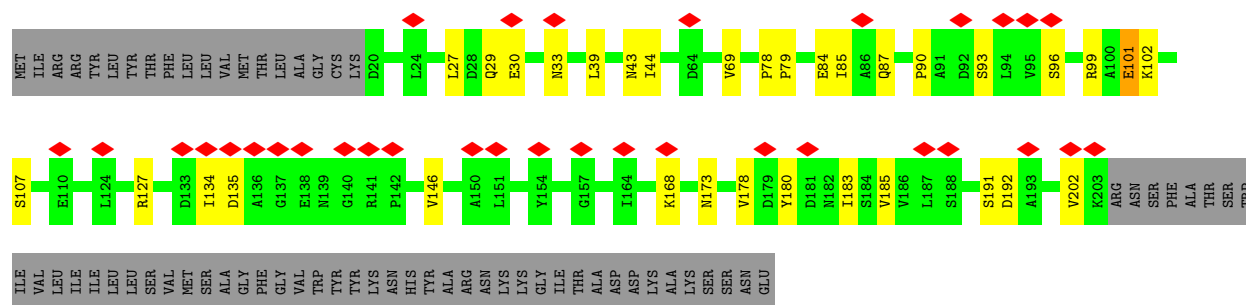


- Molecule 1: Lipoprotein PrgK

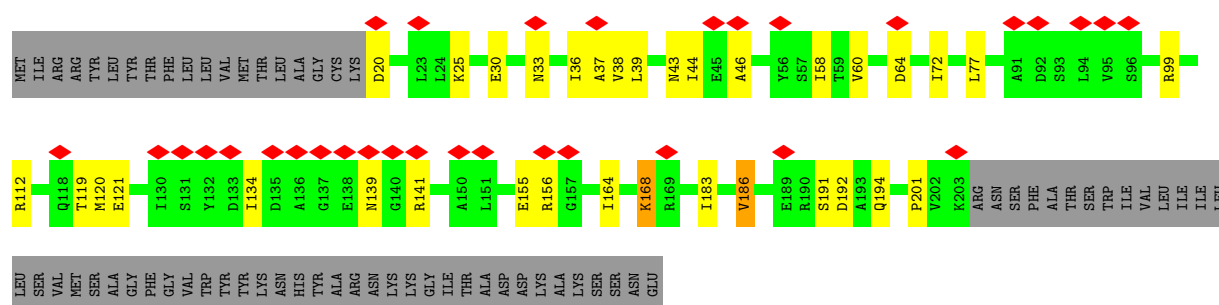


- Molecule 1: Lipoprotein PrgK

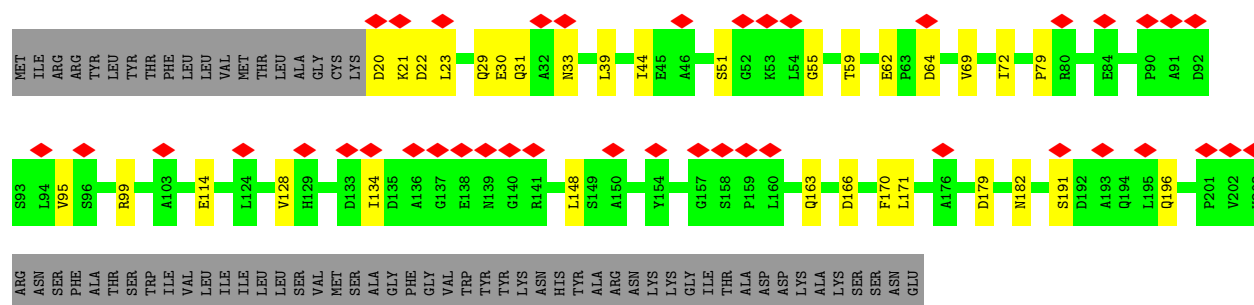




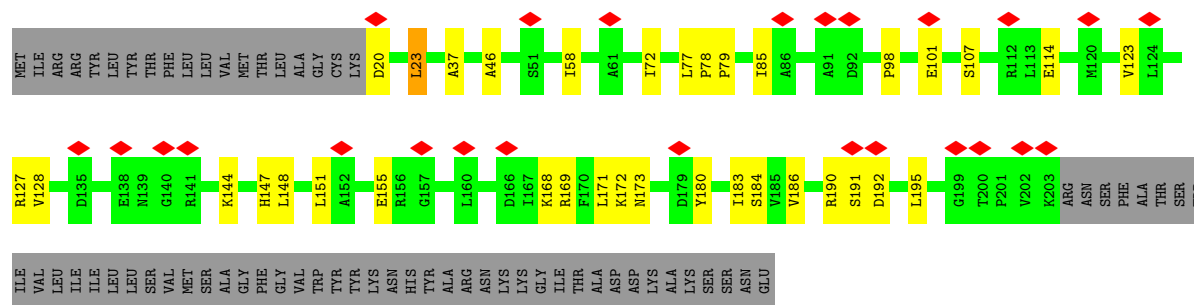
• Molecule 1: Lipoprotein PrgK

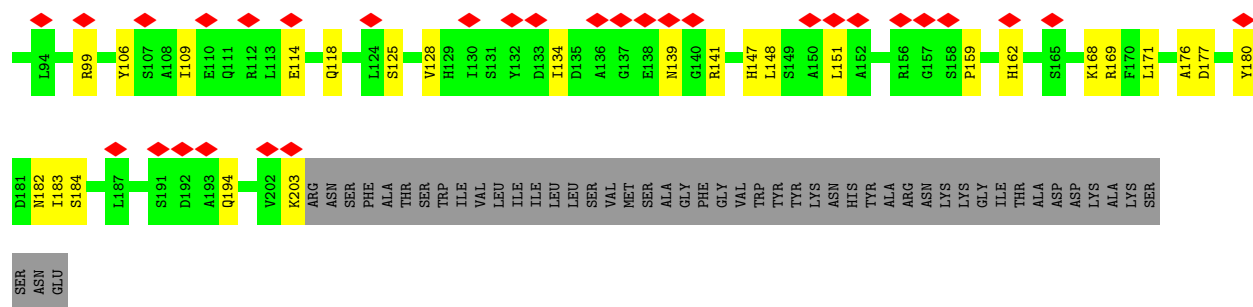


• Molecule 1: Lipoprotein PrgK

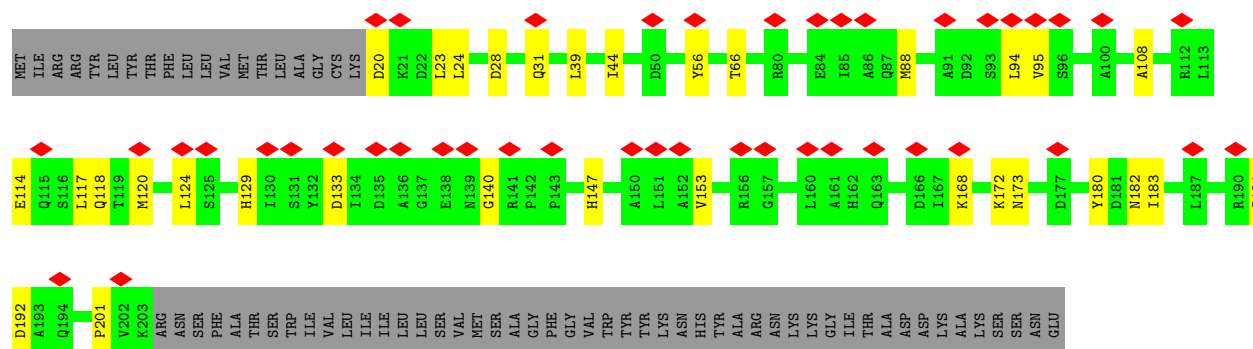


• Molecule 1: Lipoprotein PrgK

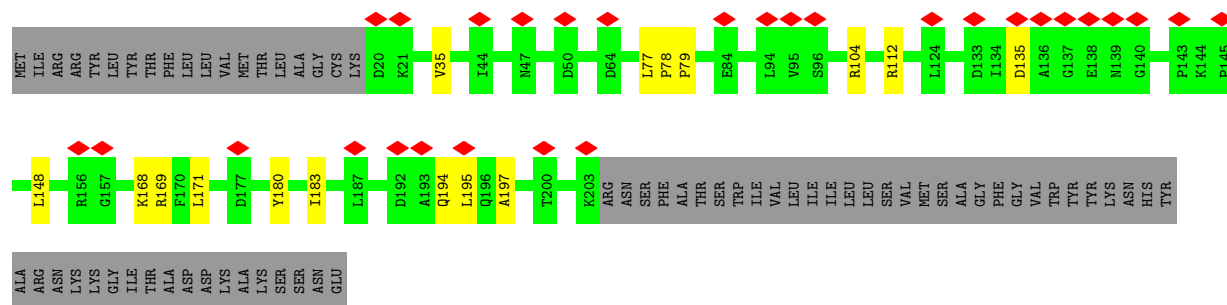




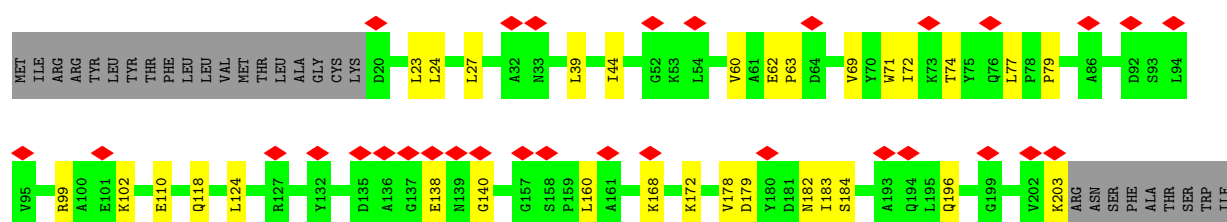
• Molecule 1: Lipoprotein PrgK

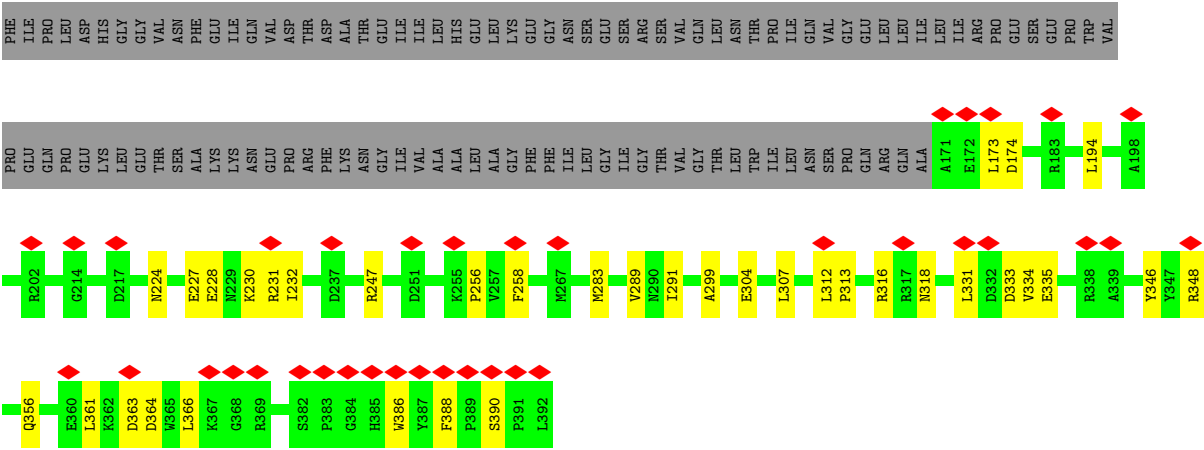


• Molecule 1: Lipoprotein PrgK

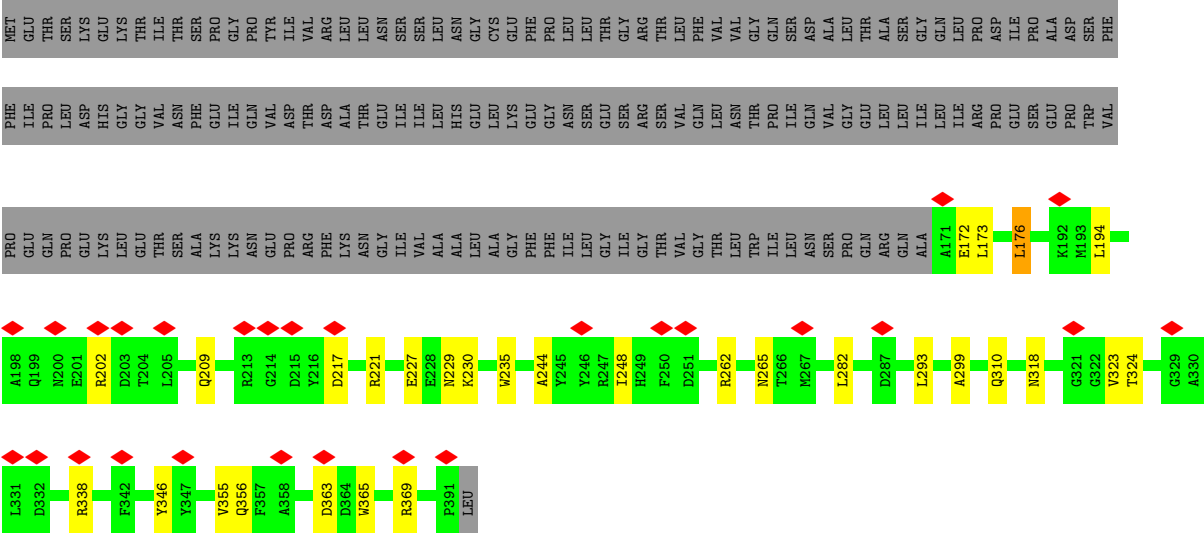


• Molecule 1: Lipoprotein PrgK

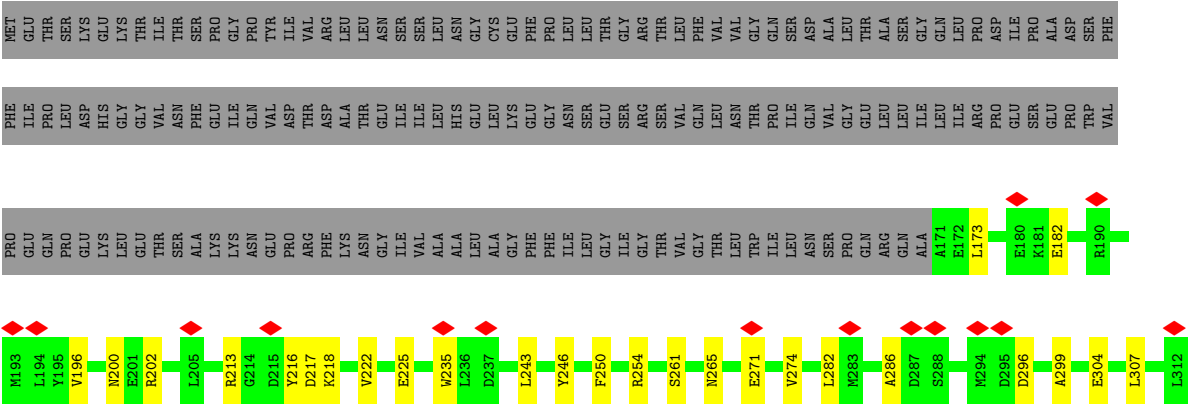


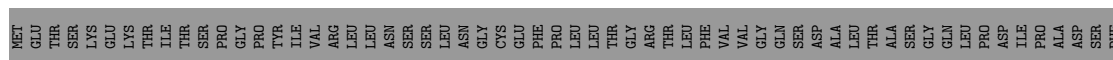


• Molecule 2: Protein PrgH

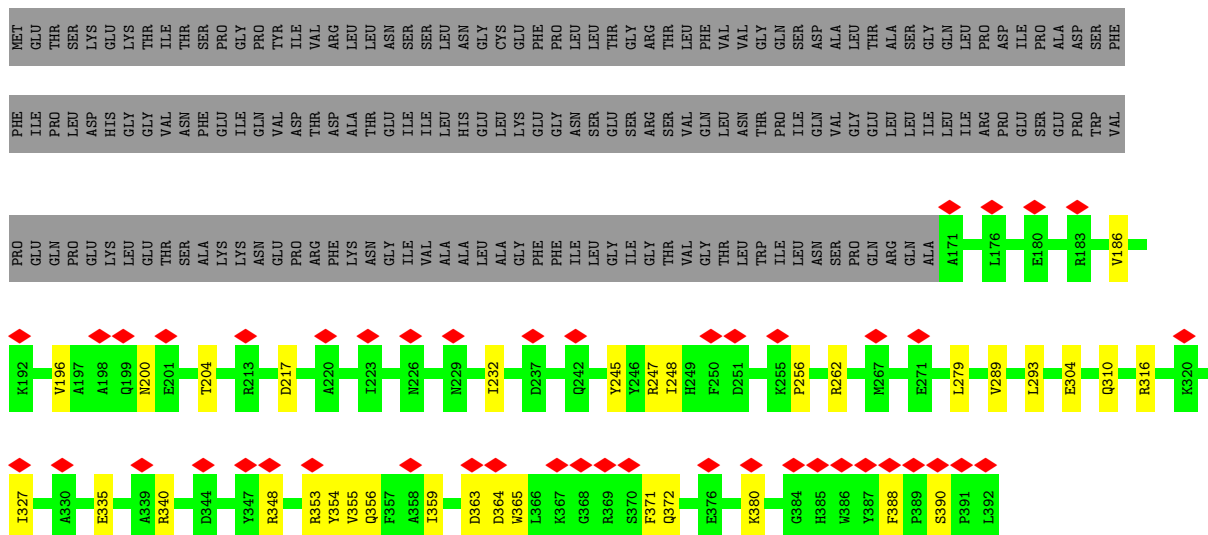


• Molecule 2: Protein PrgH

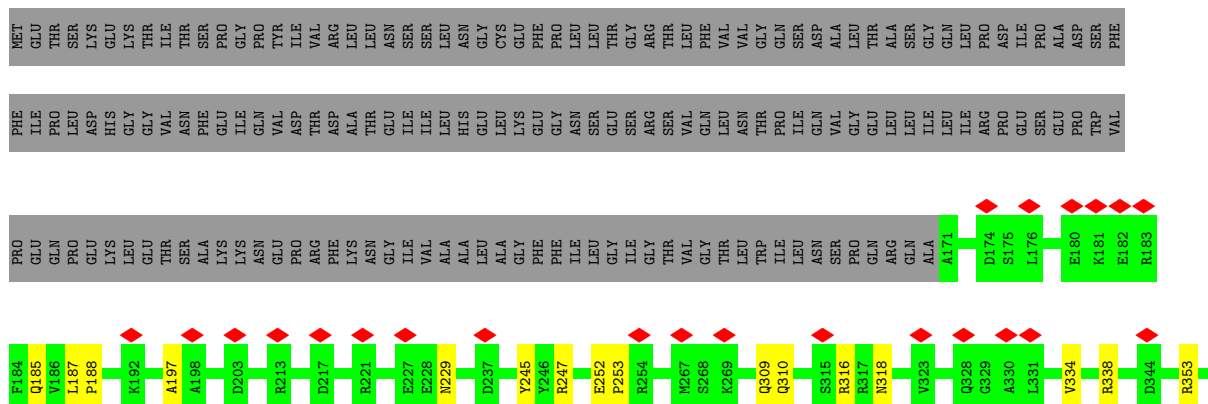


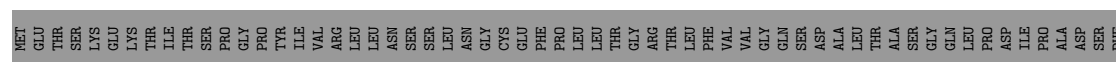


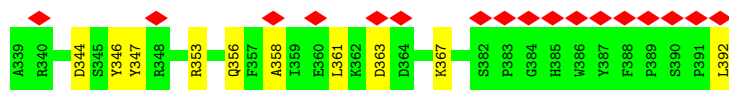
- Molecule 2: Protein PrgH



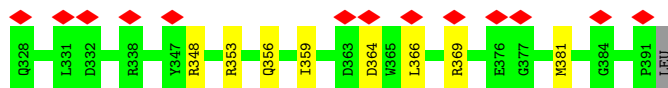
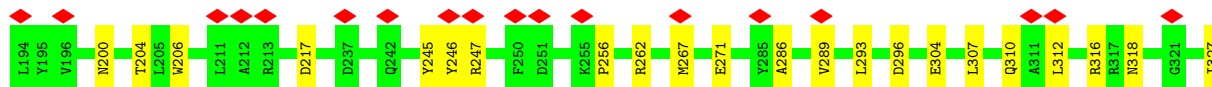
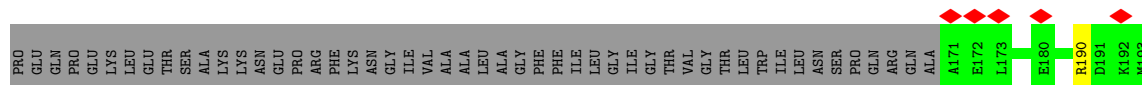
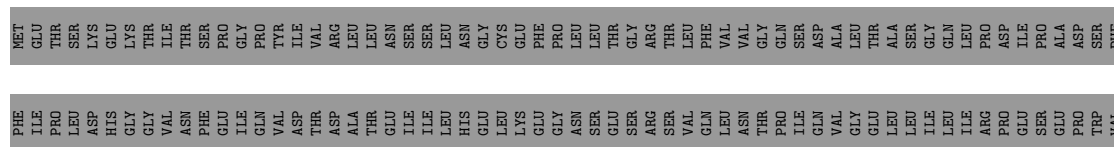
- Molecule 2: Protein PrgH



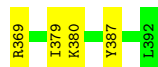
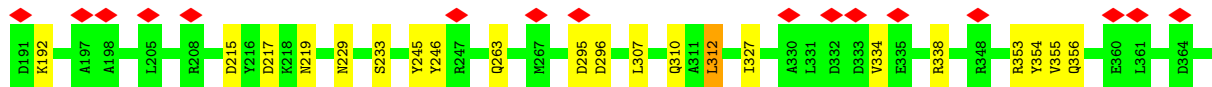
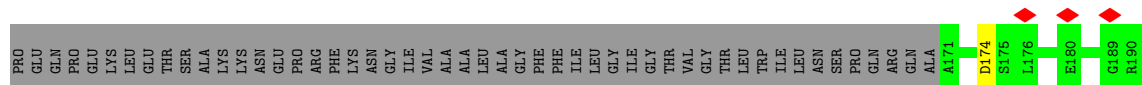
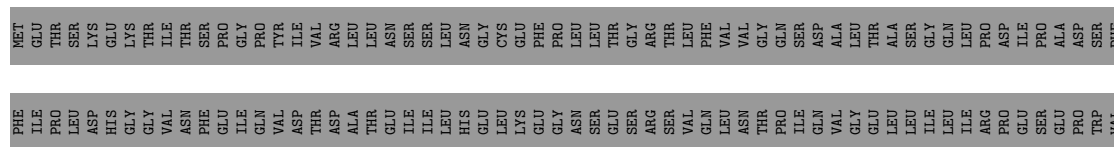




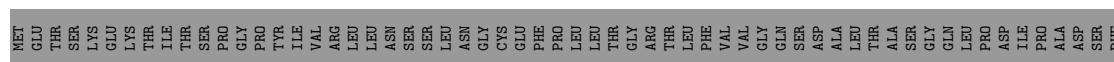
• Molecule 2: Protein PrgH

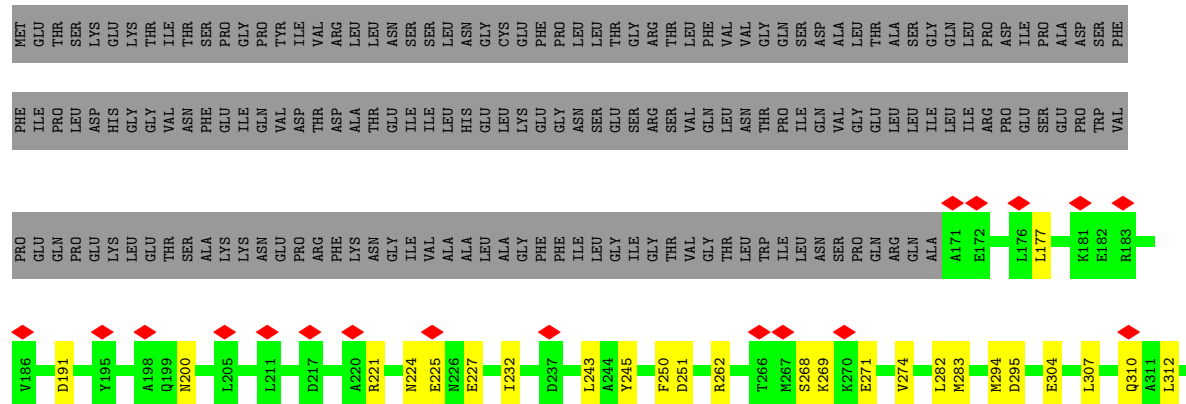


• Molecule 2: Protein PrgH

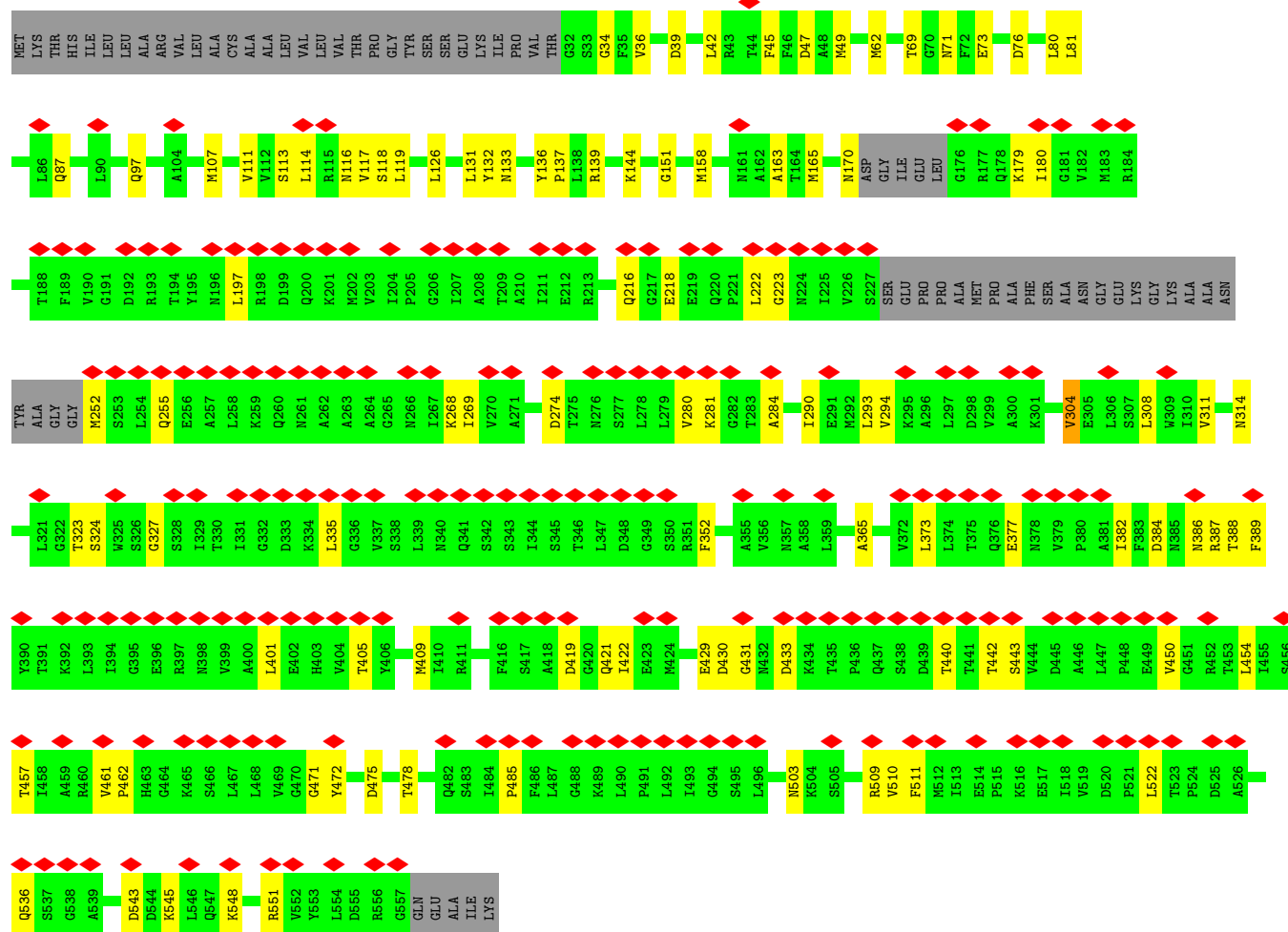


• Molecule 2: Protein PrgH

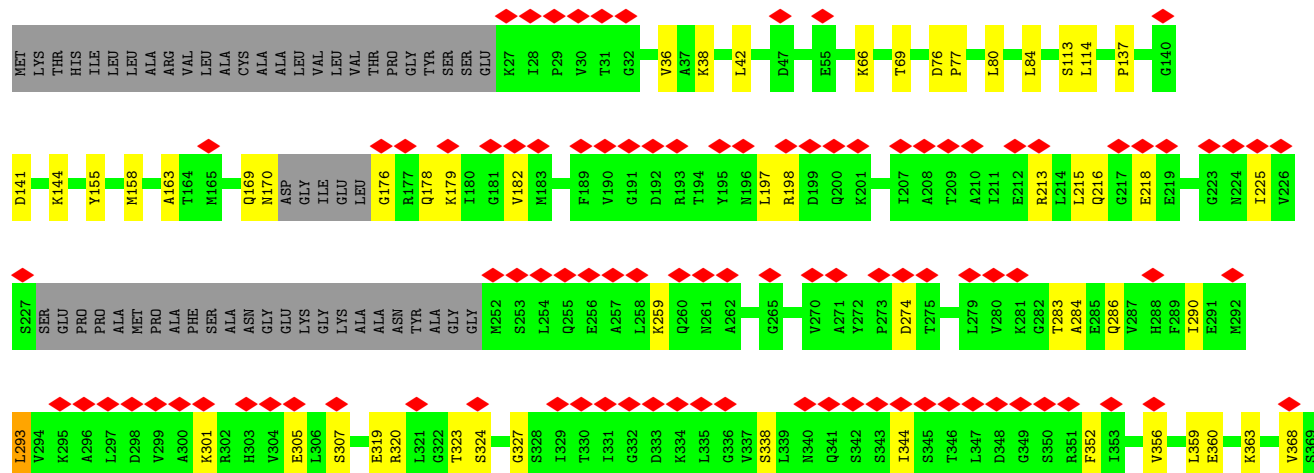


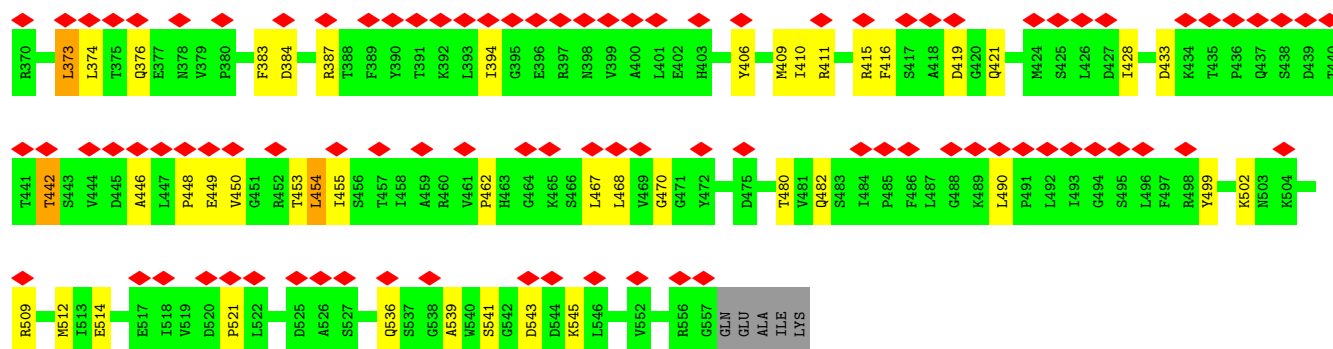




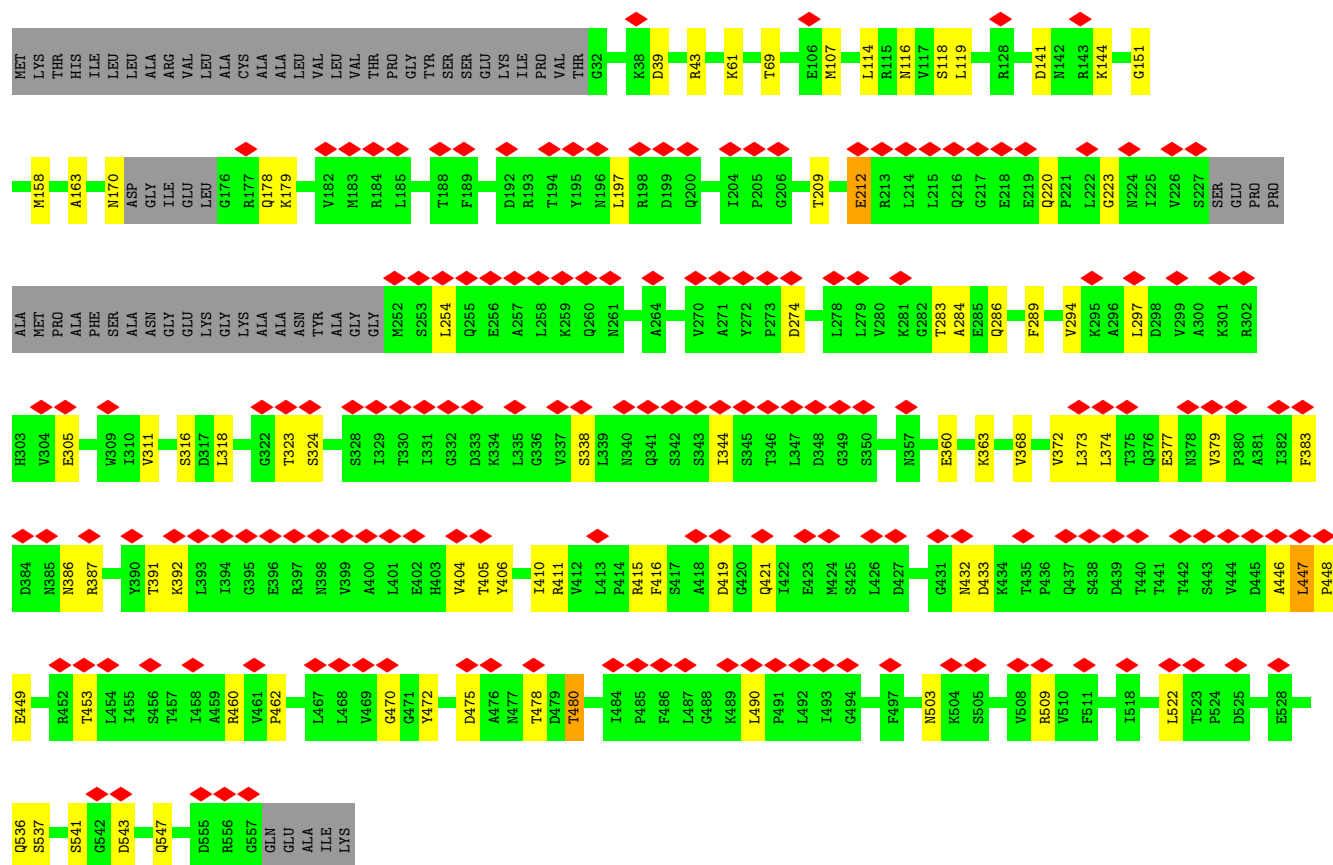


• Molecule 3: Protein InvG

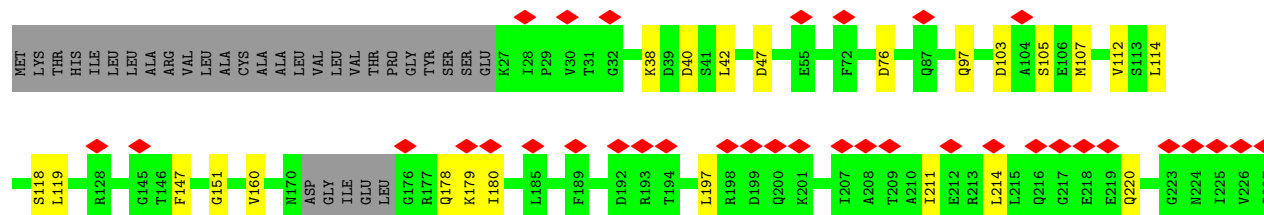
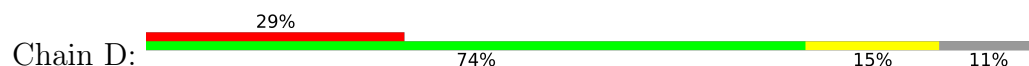


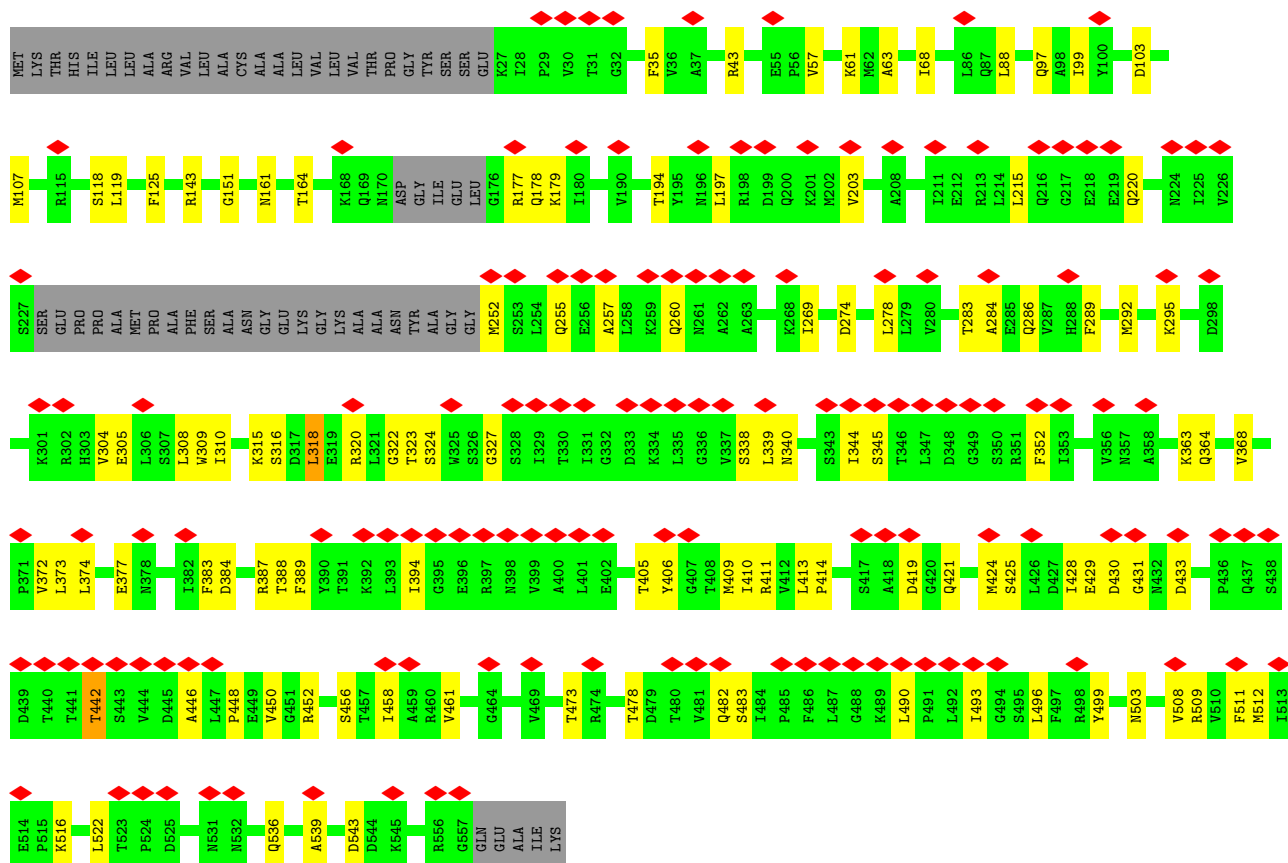


• Molecule 3: Protein InvG

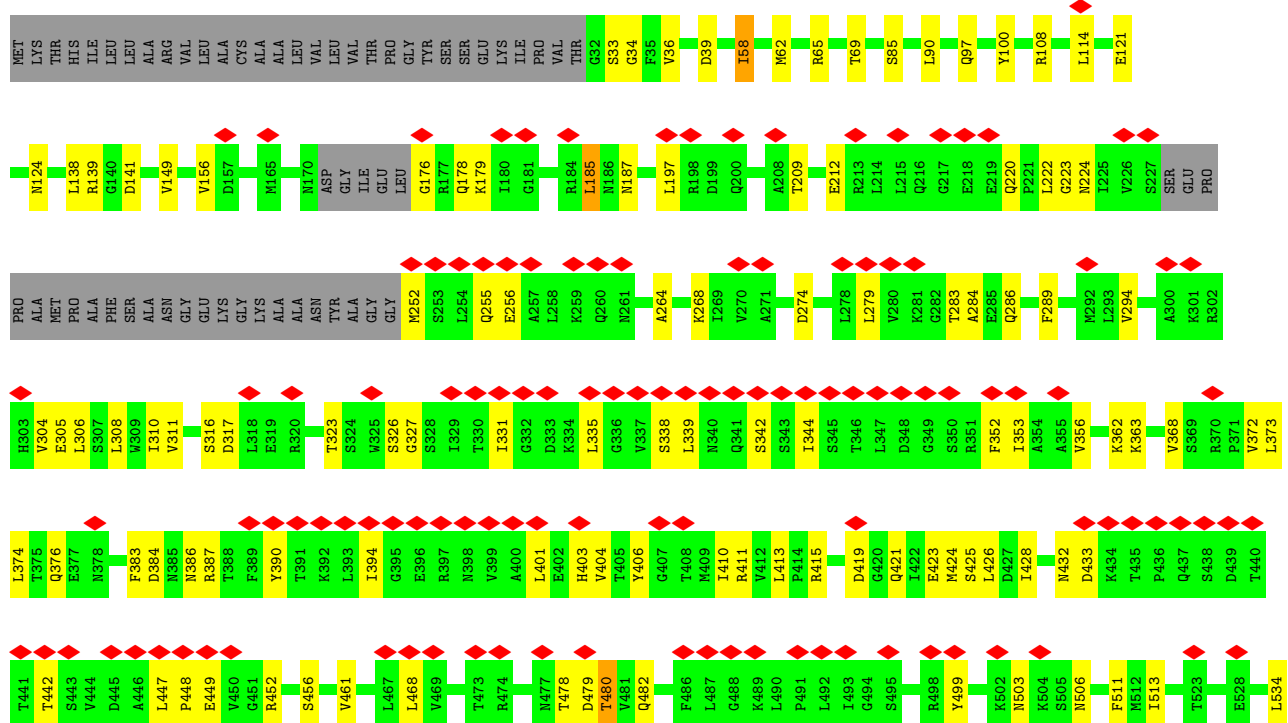


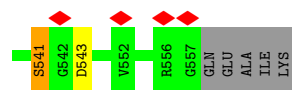
• Molecule 3: Protein InvG



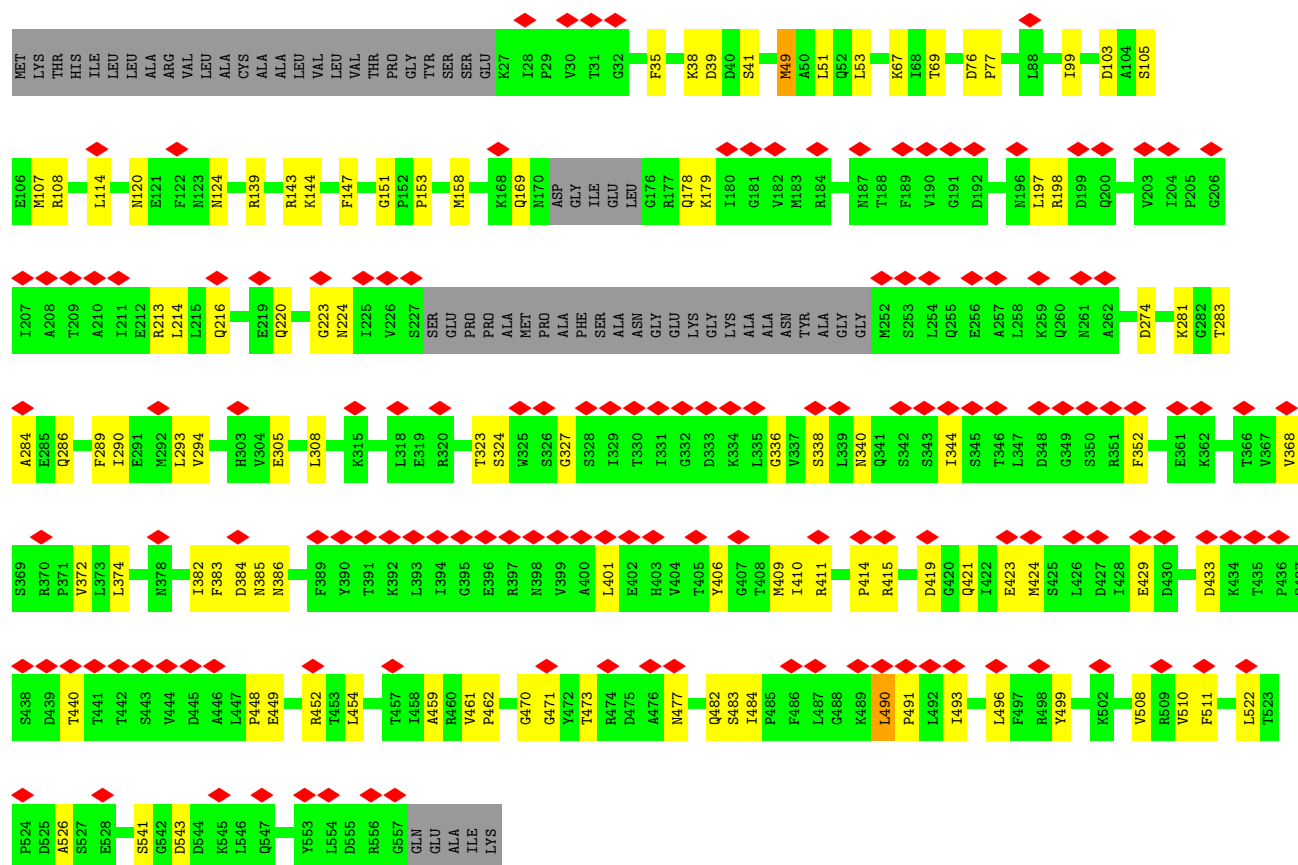


• Molecule 3: Protein InvG

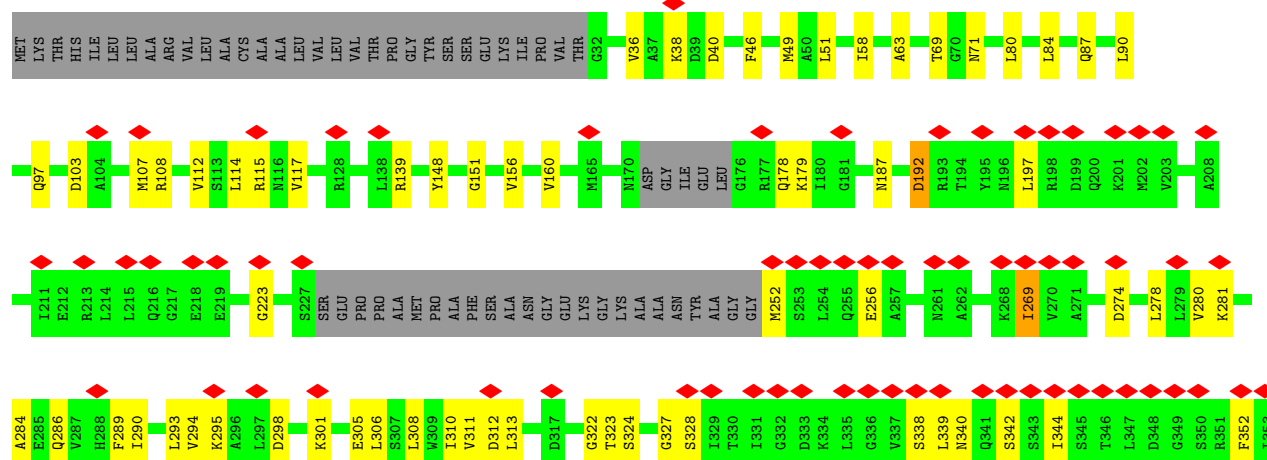


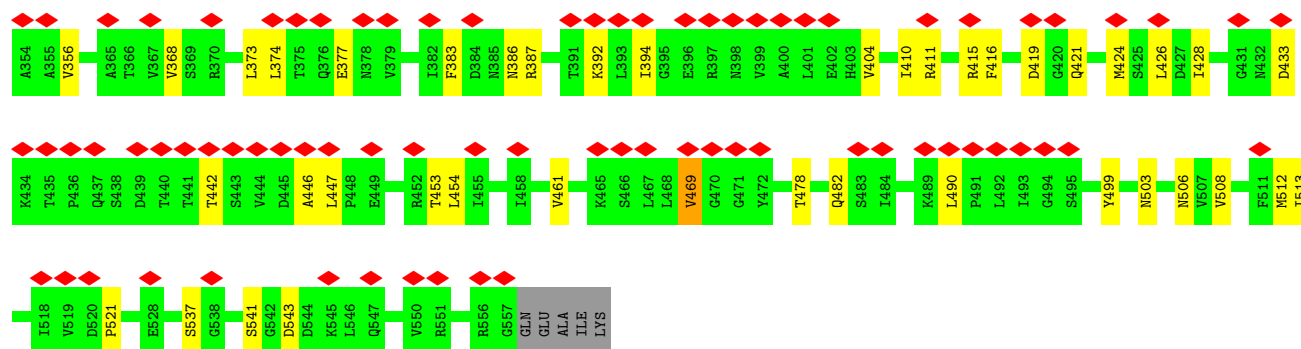


• Molecule 3: Protein InvG

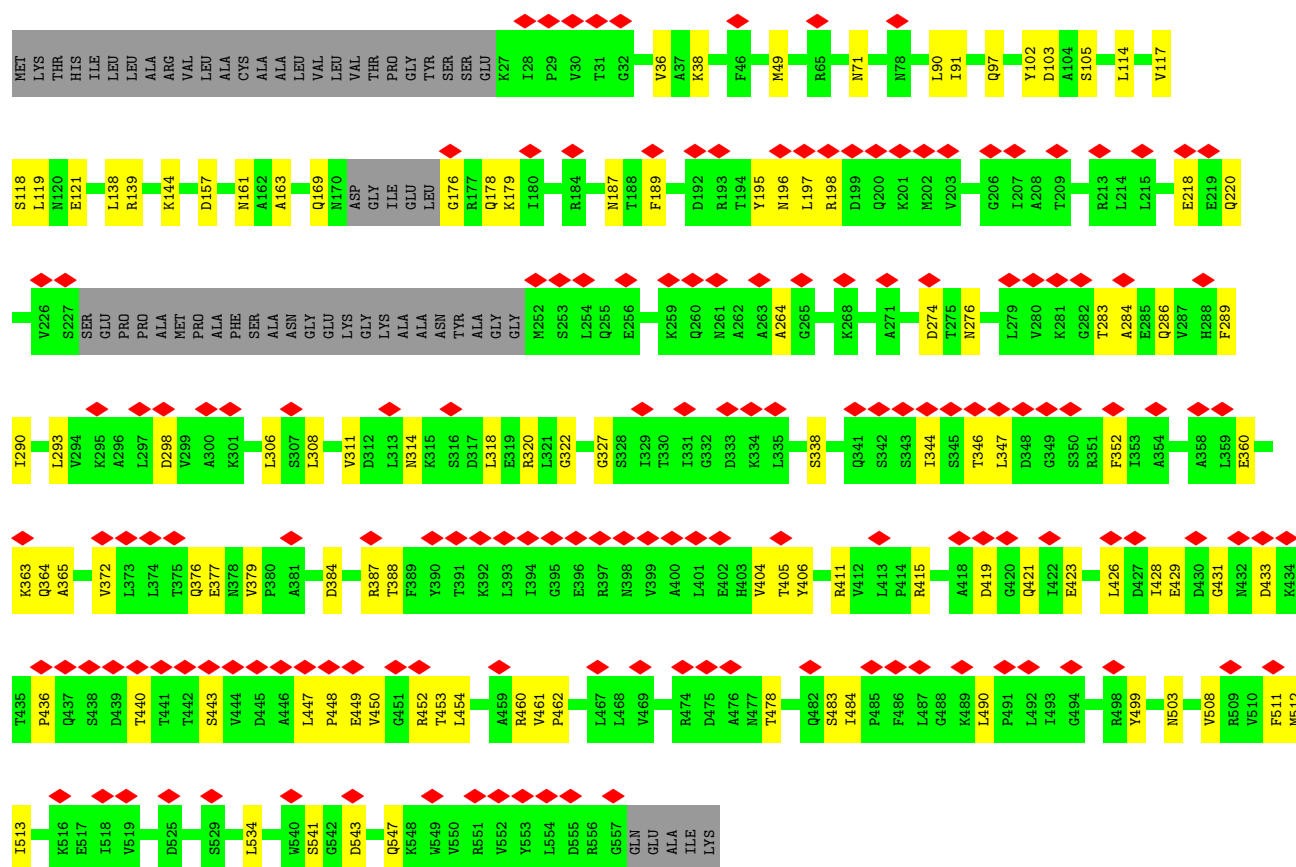


• Molecule 3: Protein InvG

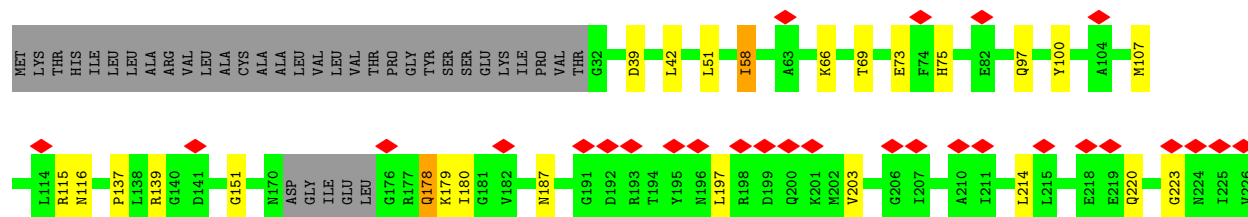


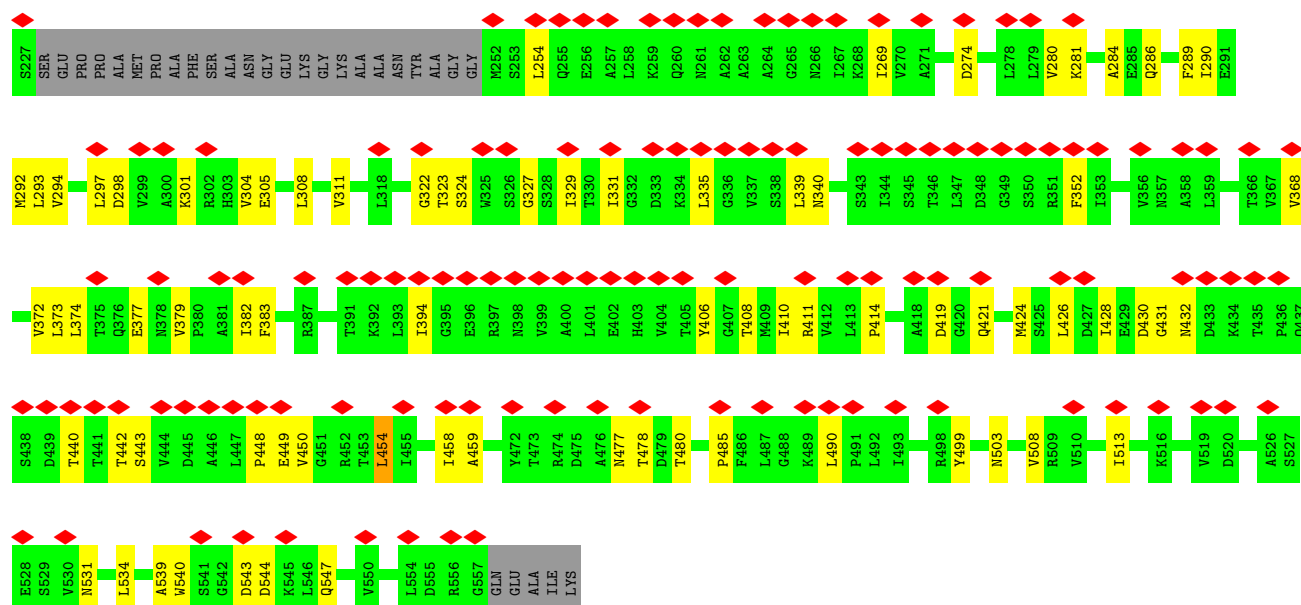


• Molecule 3: Protein InvG

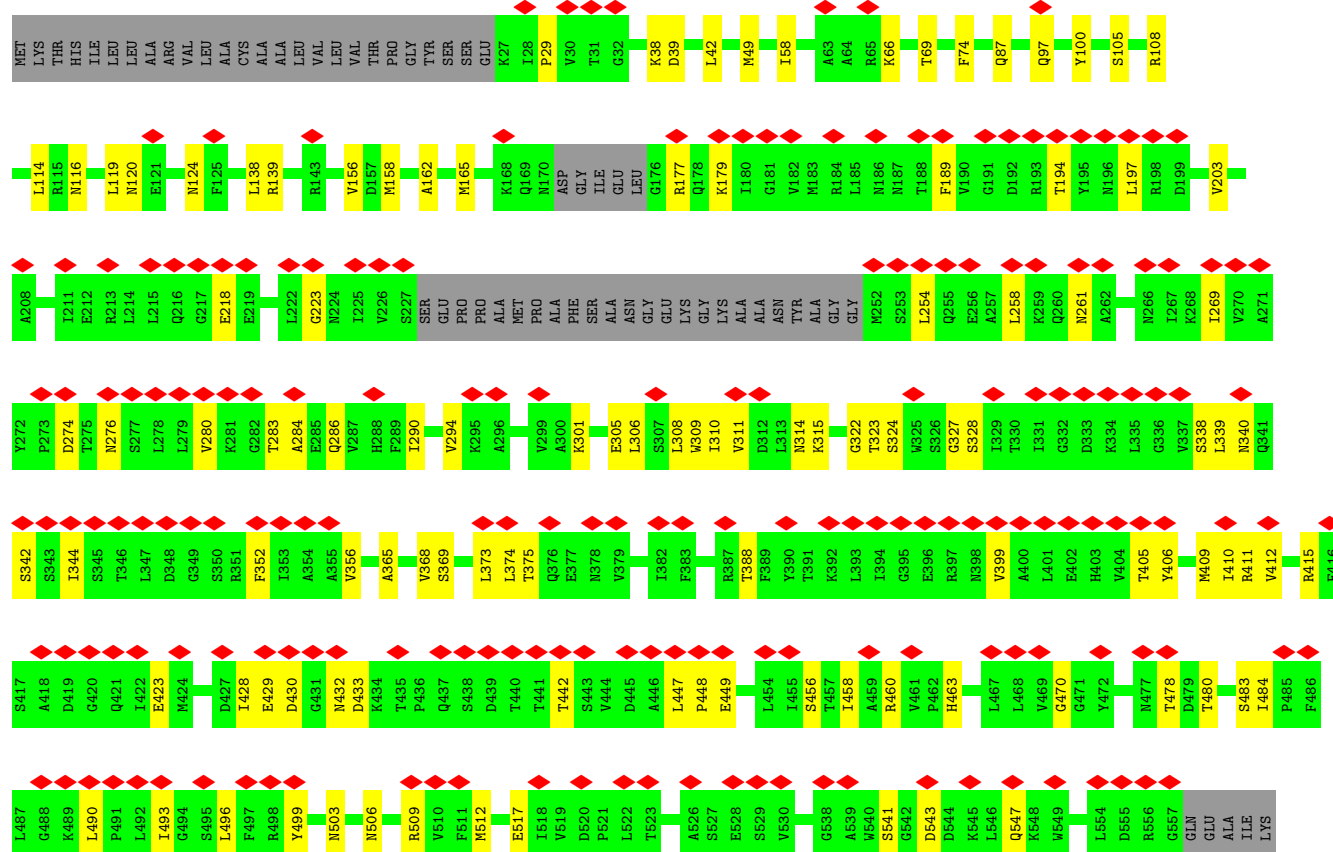


• Molecule 3: Protein InvG





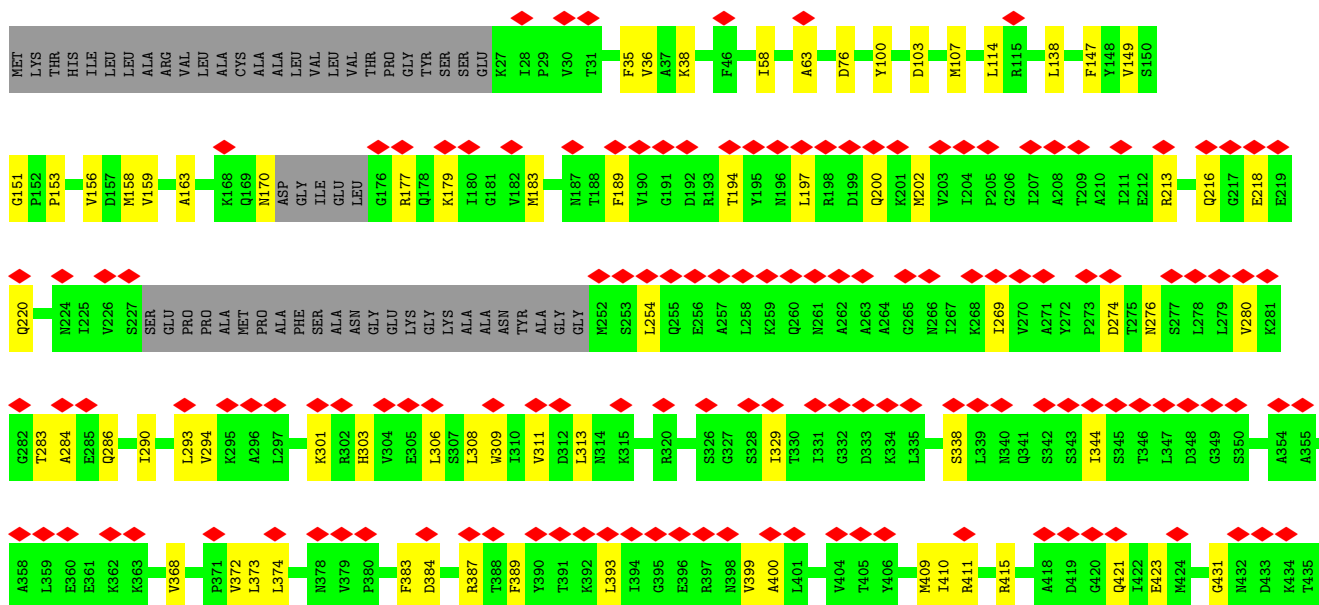
• Molecule 3: Protein InvG

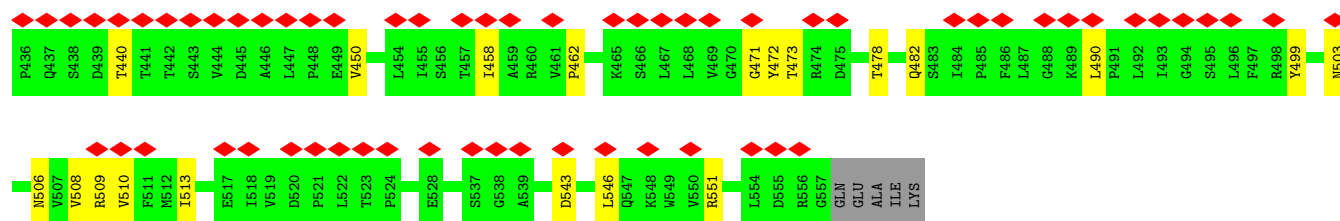


• Molecule 3: Protein InvG

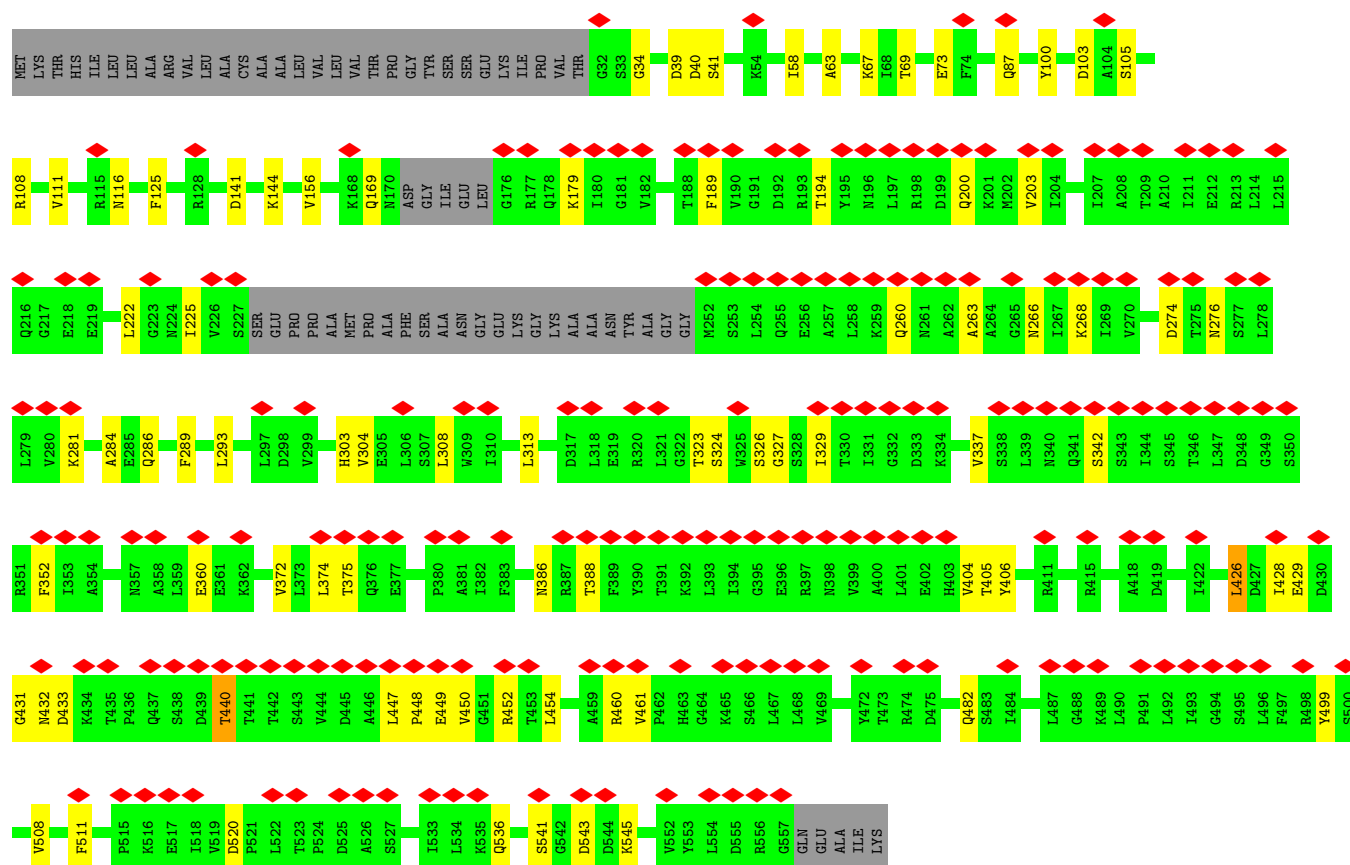


- Molecule 3: Protein InvG

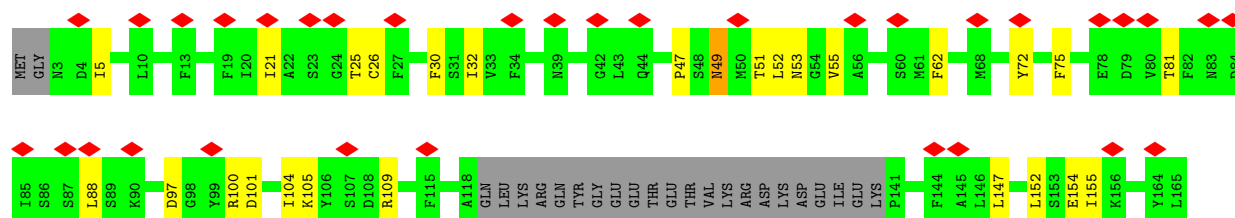


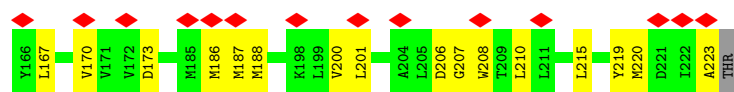


• Molecule 3: Protein InvG

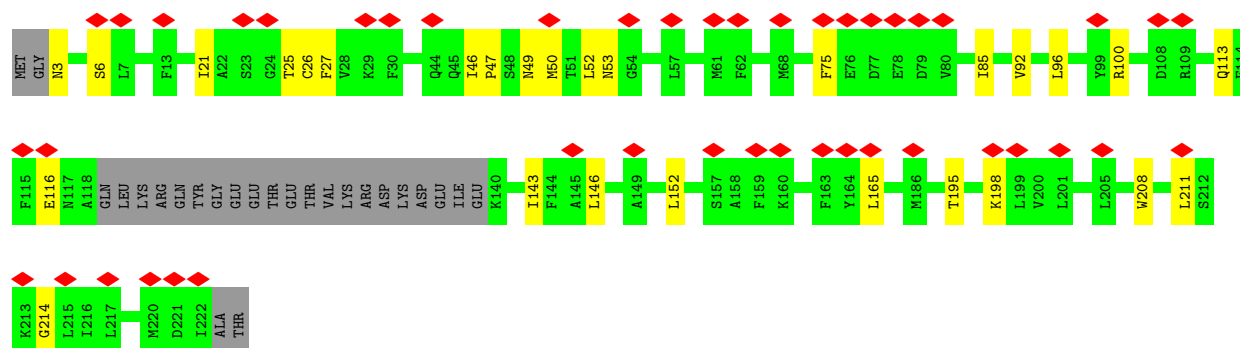
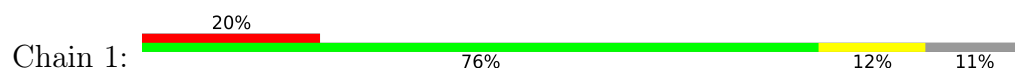


• Molecule 4: Surface presentation of antigens protein SpaP

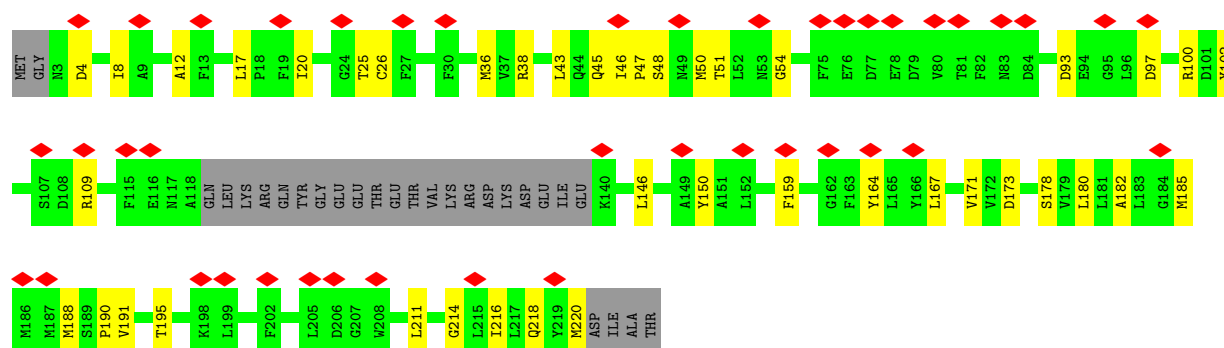




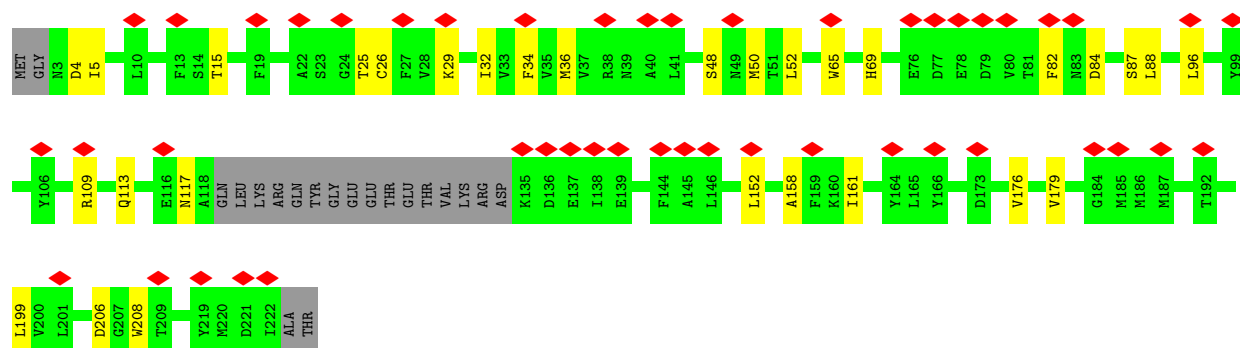
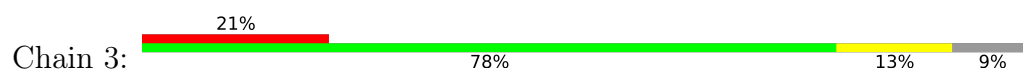
- Molecule 4: Surface presentation of antigens protein SpaP



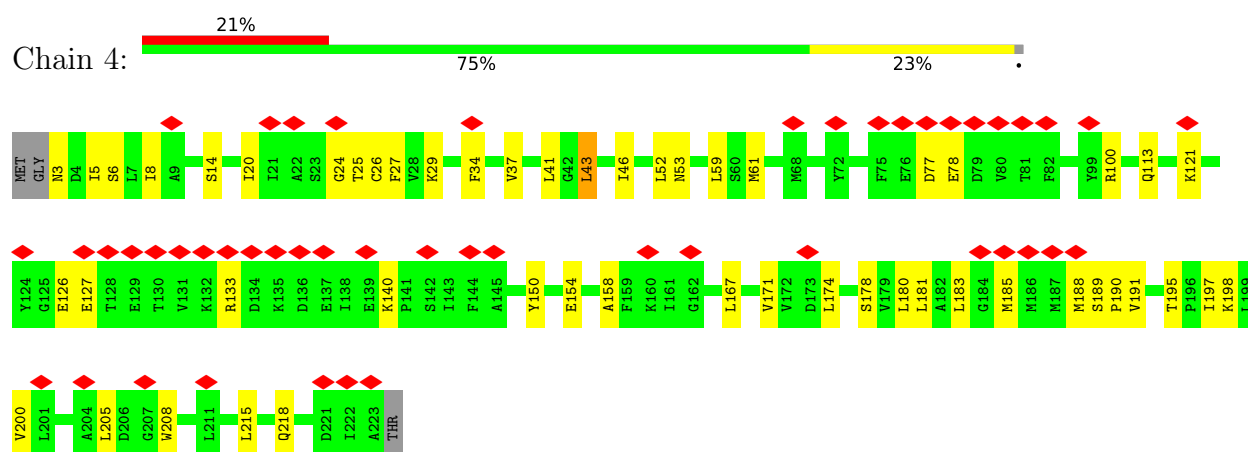
- Molecule 4: Surface presentation of antigens protein SpaP



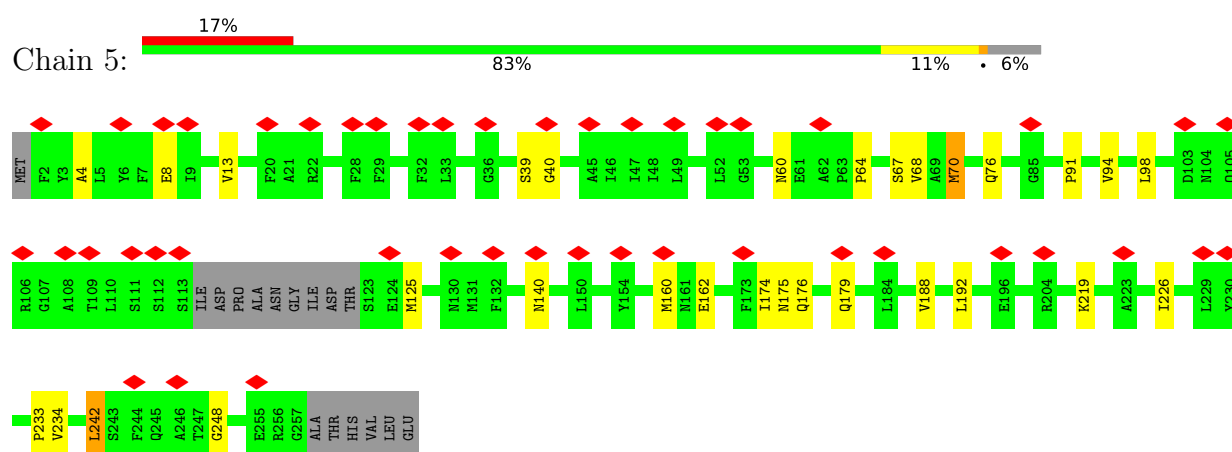
- Molecule 4: Surface presentation of antigens protein SpaP



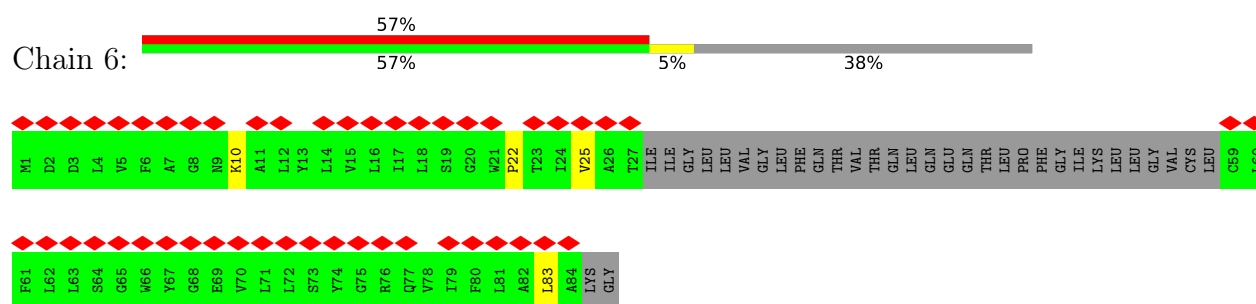
- Molecule 4: Surface presentation of antigens protein SpaP



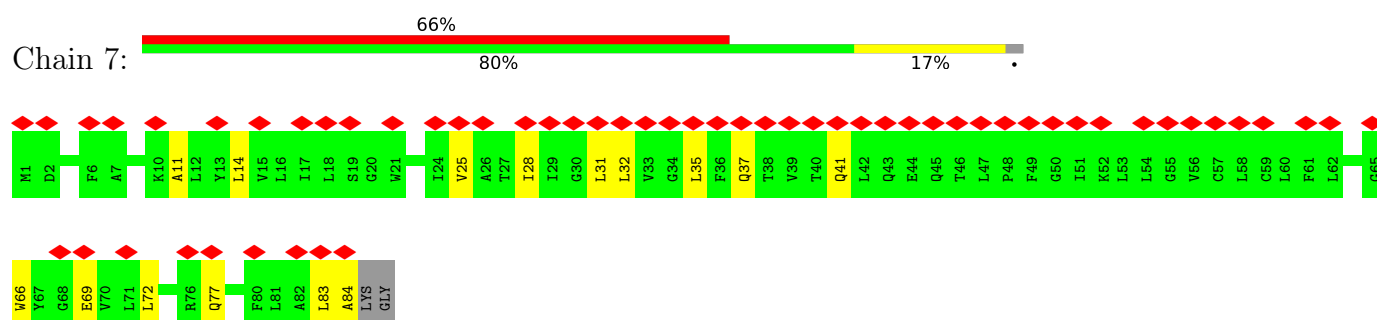
• Molecule 5: Surface presentation of antigens protein SpaR



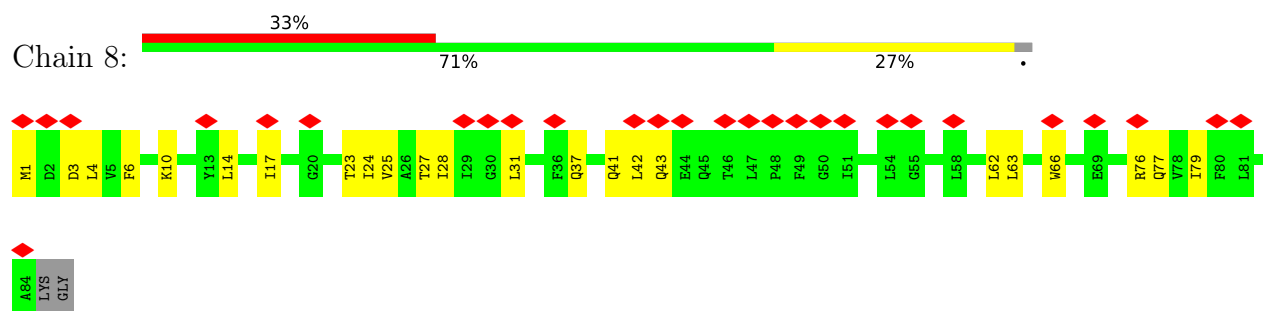
• Molecule 6: Surface presentation of antigens protein SpaQ



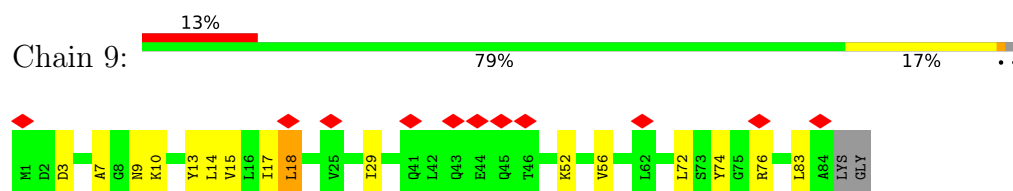
• Molecule 6: Surface presentation of antigens protein SpaQ



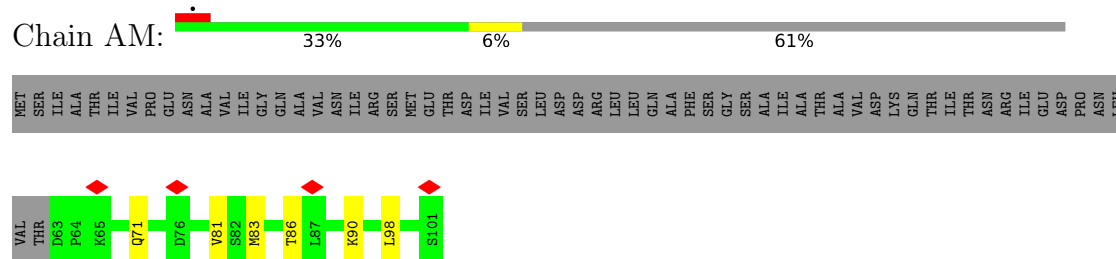
- Molecule 6: Surface presentation of antigens protein SpaQ



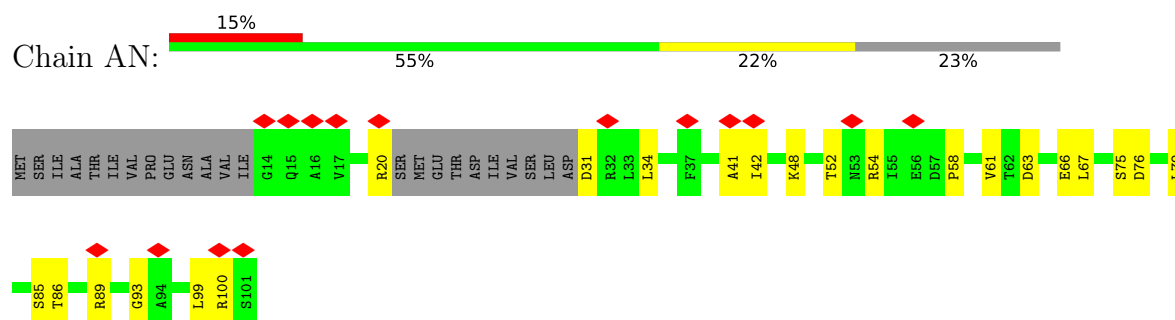
- Molecule 6: Surface presentation of antigens protein SpaQ



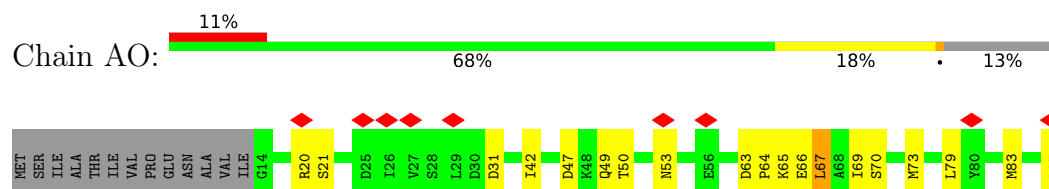
- Molecule 7: Protein PrgJ



- Molecule 7: Protein PrgJ

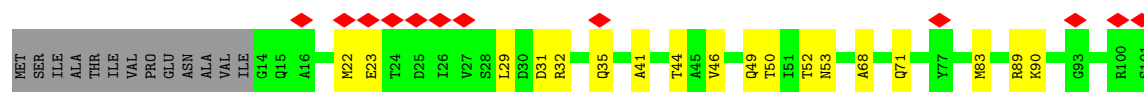


- Molecule 7: Protein PrgJ

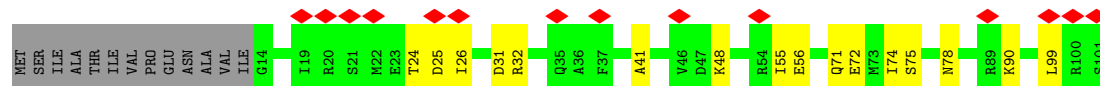
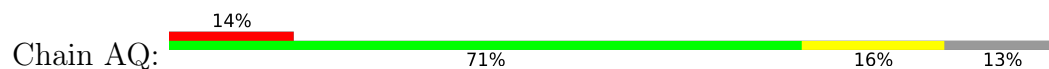


- Molecule 7: Protein PrgJ

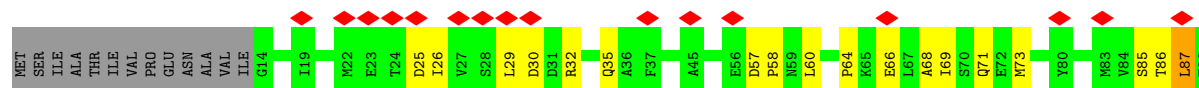




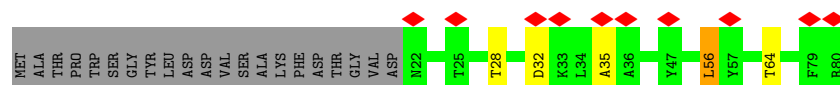
• Molecule 7: Protein PrgJ



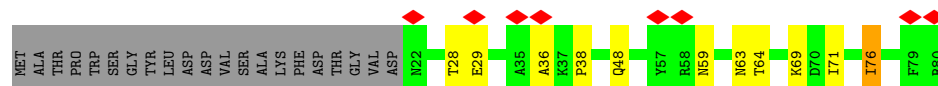
• Molecule 7: Protein PrgJ



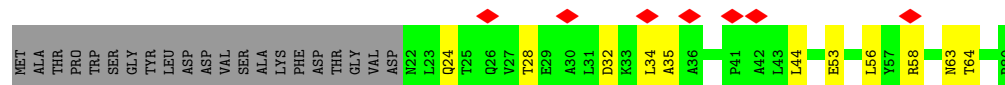
• Molecule 8: Protein PrgI



• Molecule 8: Protein PrgI

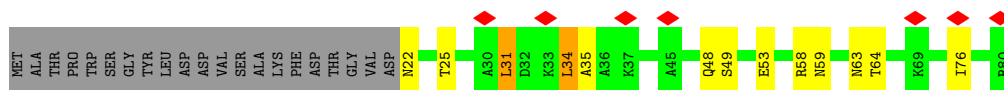


• Molecule 8: Protein PrgI



• Molecule 8: Protein PrgI

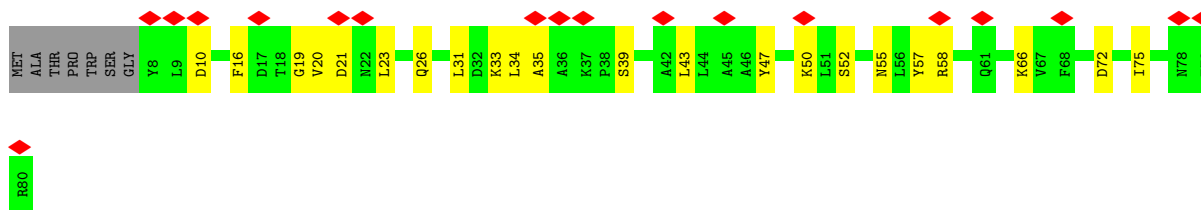




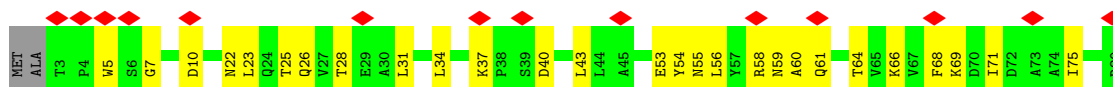
● Molecule 8: Protein PrgI



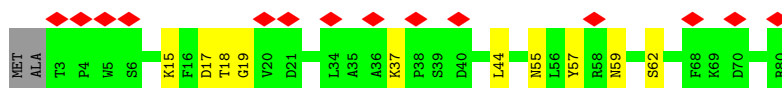
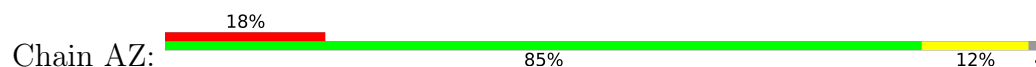
● Molecule 8: Protein PrgI



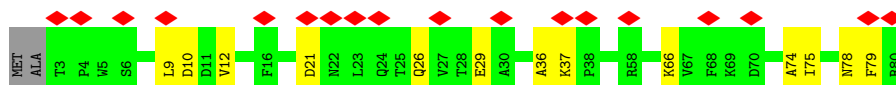
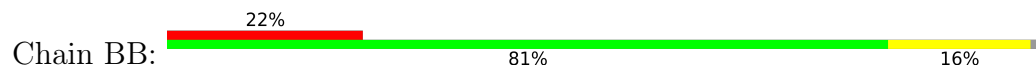
● Molecule 8: Protein PrgI



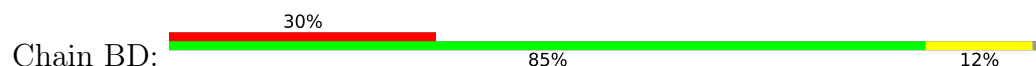
● Molecule 8: Protein PrgI

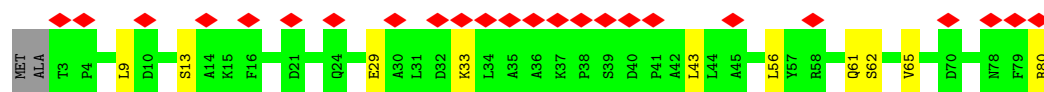


● Molecule 8: Protein PrgI

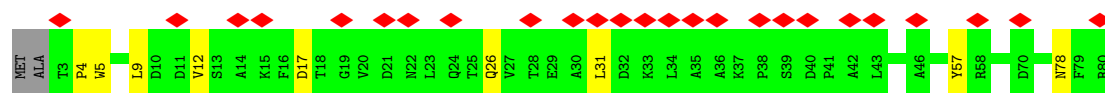
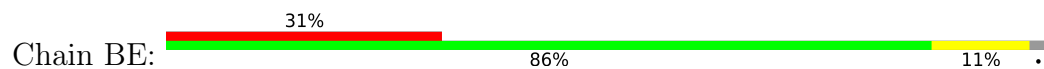


● Molecule 8: Protein PrgI

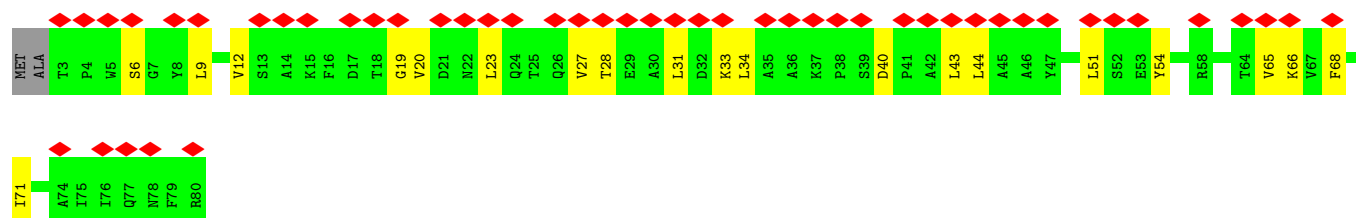
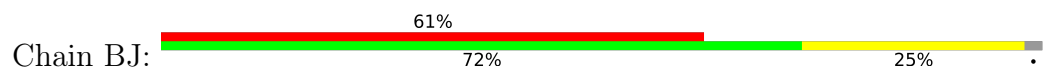




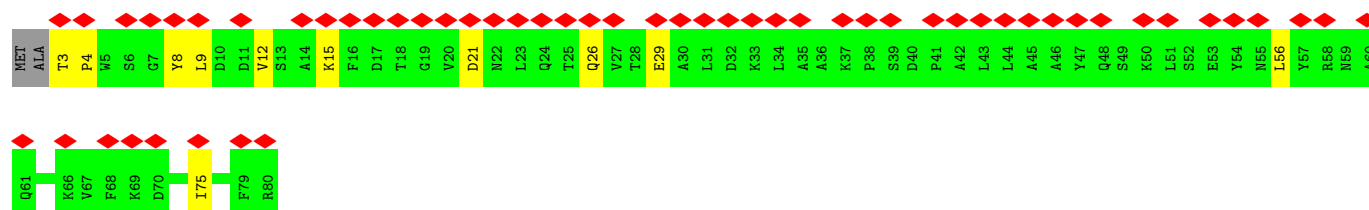
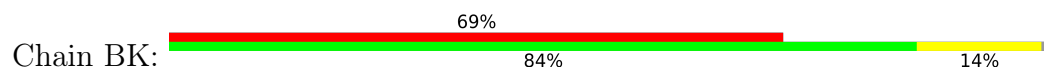
• Molecule 8: Protein PrgI



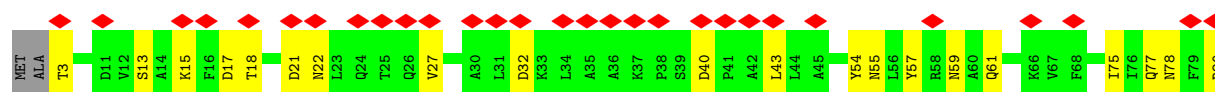
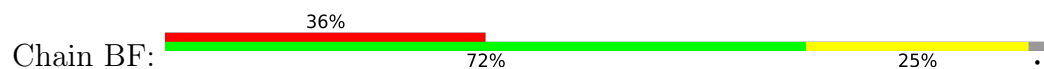
• Molecule 8: Protein PrgI



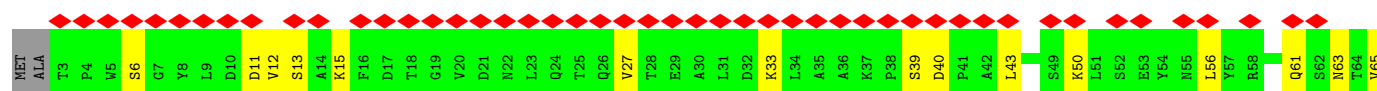
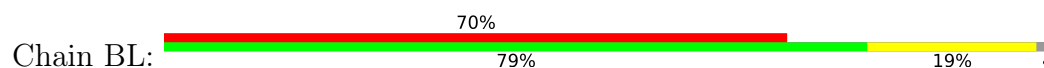
• Molecule 8: Protein PrgI

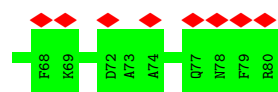


• Molecule 8: Protein PrgI

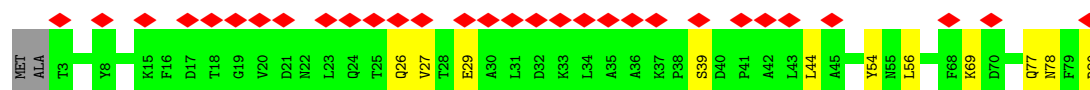
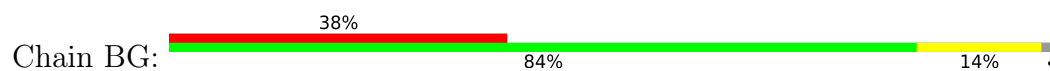


• Molecule 8: Protein PrgI

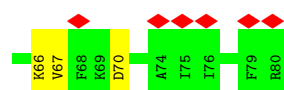
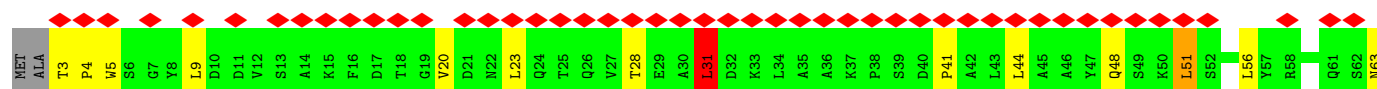
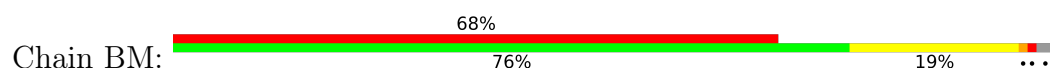




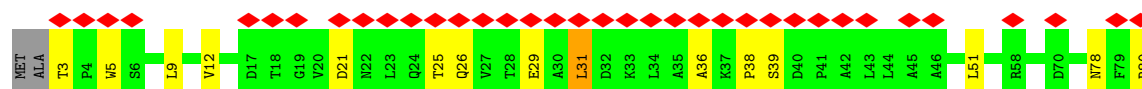
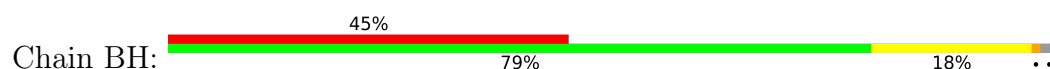
• Molecule 8: Protein PrgI



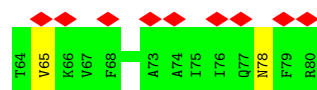
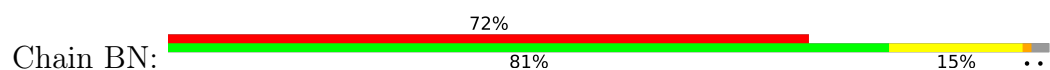
• Molecule 8: Protein PrgI



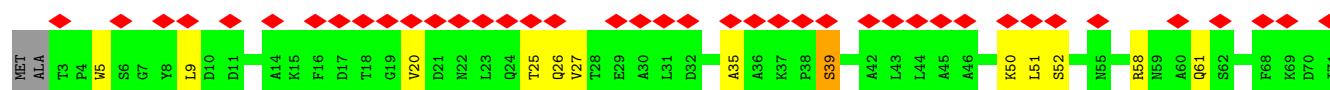
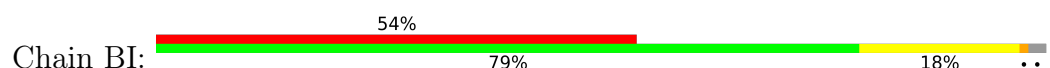
• Molecule 8: Protein PrgI

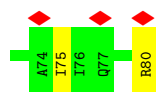


• Molecule 8: Protein PrgI

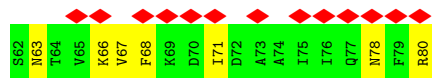
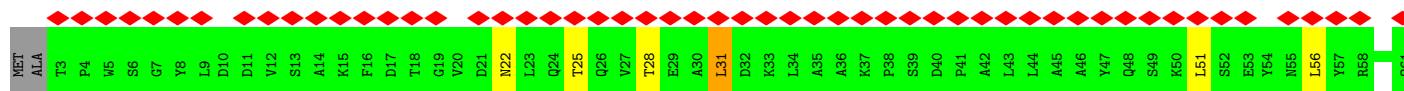
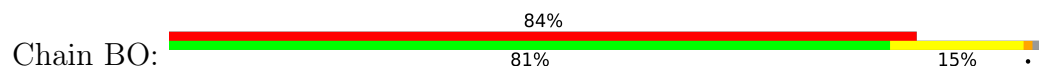


• Molecule 8: Protein PrgI

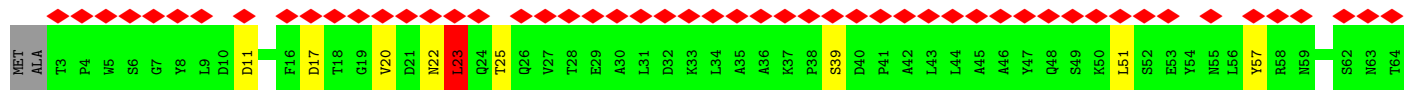
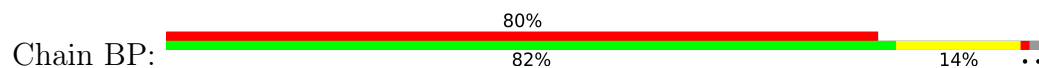




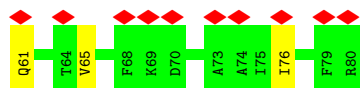
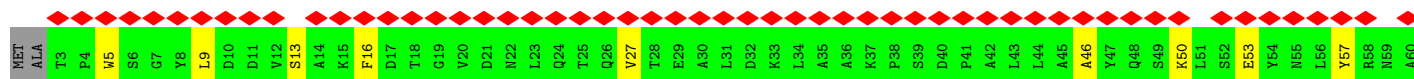
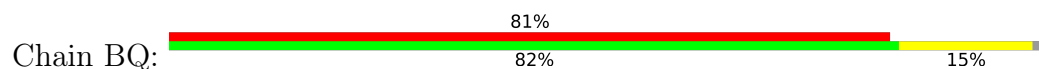
- Molecule 8: Protein PrgI



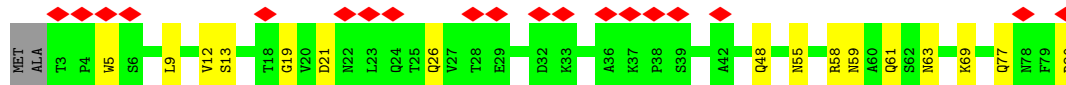
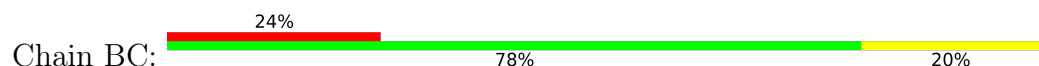
- Molecule 8: Protein PrgI



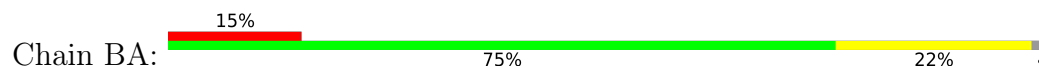
- Molecule 8: Protein PrgI

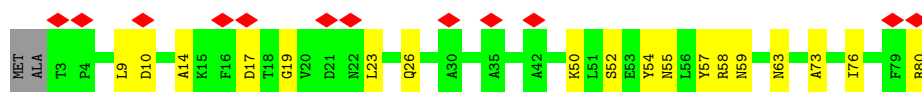


- Molecule 8: Protein PrgI

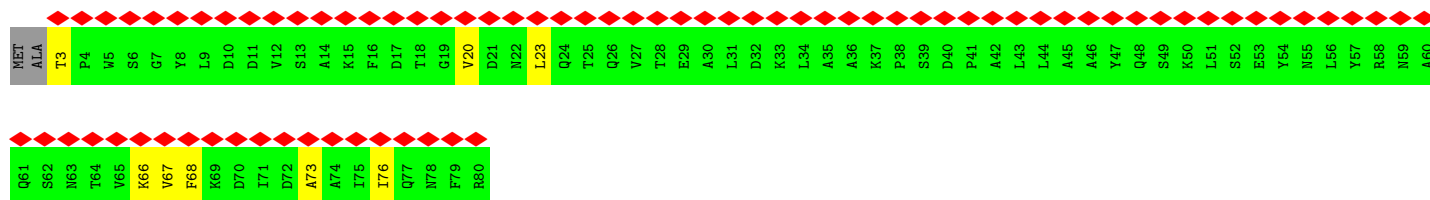
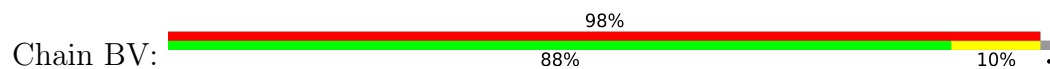


- Molecule 8: Protein PrgI

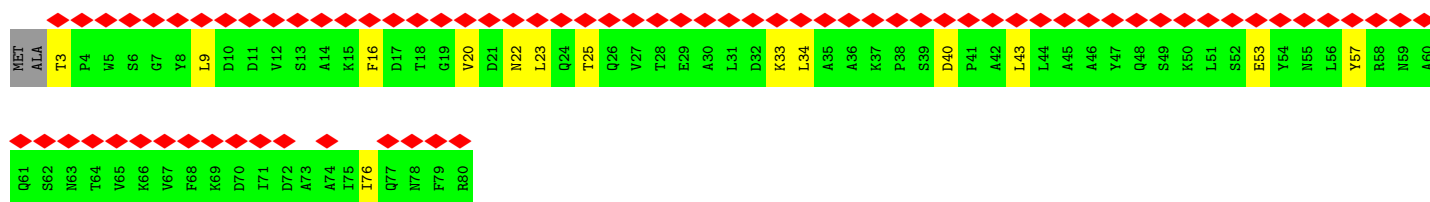
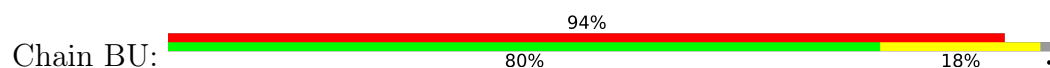




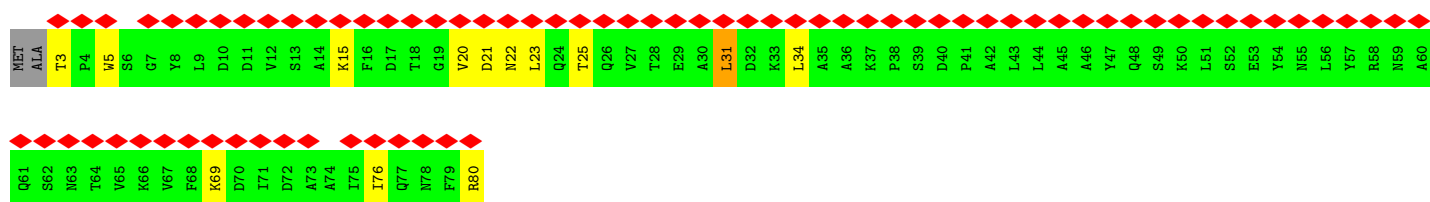
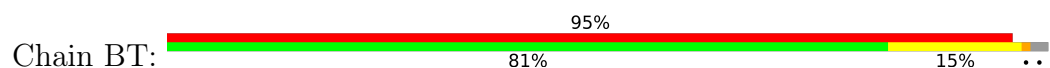
• Molecule 8: Protein PrgI



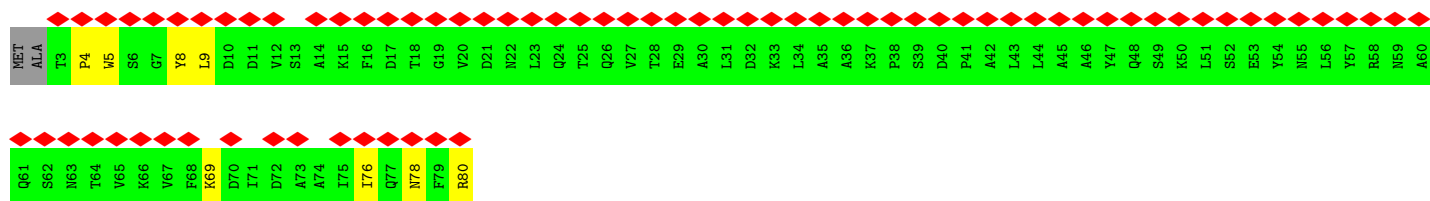
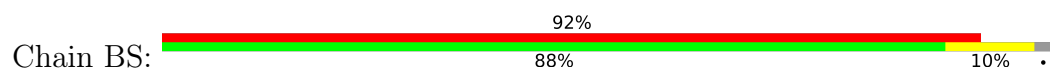
• Molecule 8: Protein PrgI



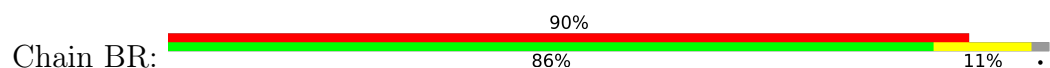
• Molecule 8: Protein PrgI

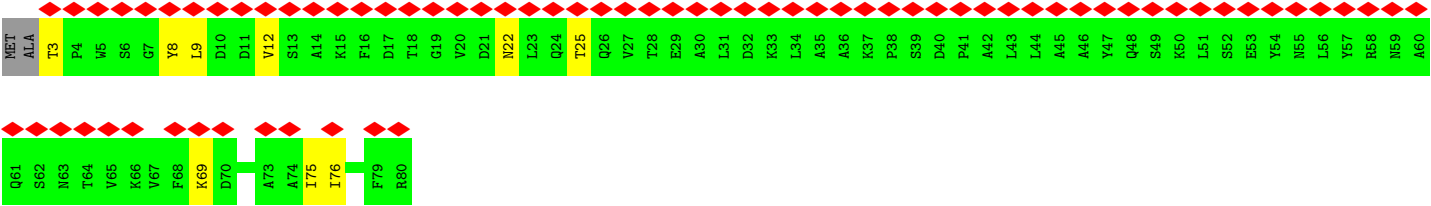


• Molecule 8: Protein PrgI



• Molecule 8: Protein PrgI





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.108	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	427.5, 427.5, 427.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.71, 1.71, 1.71	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	AA	0.29	0/1458	0.63	0/1979
1	AB	0.28	0/1458	0.60	1/1979 (0.1%)
1	AC	0.29	0/1458	0.64	0/1979
1	AD	0.29	0/1458	0.62	0/1979
1	AE	0.30	0/1458	0.63	0/1979
1	AF	0.30	0/1458	0.67	0/1979
1	AG	0.30	0/1458	0.60	0/1979
1	AH	0.27	0/1458	0.62	0/1979
1	AI	0.30	0/1458	0.64	0/1979
1	AJ	0.31	0/1458	0.64	0/1979
1	AK	0.29	0/1458	0.64	0/1979
1	AL	0.31	0/1458	0.65	1/1979 (0.1%)
1	o	0.29	0/1458	0.61	0/1979
1	p	0.31	0/1458	0.69	1/1979 (0.1%)
1	q	0.30	0/1458	0.63	0/1979
1	r	0.28	0/1458	0.63	0/1979
1	s	0.27	0/1458	0.60	0/1979
1	t	0.29	0/1458	0.63	0/1979
1	u	0.31	0/1458	0.69	0/1979
1	v	0.28	0/1458	0.59	0/1979
1	w	0.29	0/1458	0.62	0/1979
1	x	0.28	0/1458	0.63	0/1979
1	y	0.31	0/1458	0.68	0/1979
1	z	0.29	0/1458	0.64	0/1979
2	E	0.27	0/1881	0.60	0/2541
2	R	0.27	0/1872	0.63	0/2530
2	S	0.28	0/1876	0.65	0/2536
2	T	0.26	0/1881	0.62	0/2541
2	U	0.27	0/1872	0.62	0/2530
2	V	0.25	0/1876	0.62	0/2536
2	W	0.26	0/1881	0.61	0/2541
2	X	0.27	0/1872	0.63	0/2530
2	Y	0.27	0/1876	0.63	0/2536
2	Z	0.25	0/1881	0.58	0/2541

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	a	0.26	0/1872	0.61	1/2530 (0.0%)
2	b	0.27	0/1876	0.66	0/2536
2	c	0.27	0/1881	0.62	2/2541 (0.1%)
2	d	0.28	0/1872	0.62	0/2530
2	e	0.28	0/1876	0.63	0/2536
2	f	0.27	0/1881	0.64	0/2541
2	g	0.28	0/1872	0.63	0/2530
2	h	0.29	0/1876	0.65	0/2536
2	i	0.26	0/1881	0.57	0/2541
2	j	0.27	0/1872	0.64	0/2530
2	k	0.27	0/1876	0.64	0/2536
2	l	0.26	0/1881	0.59	0/2541
2	m	0.26	0/1872	0.61	0/2530
2	n	0.27	0/1876	0.63	0/2536
3	A	0.27	0/3901	0.67	0/5284
3	B	0.28	0/3951	0.69	0/5352
3	C	0.28	0/3901	0.68	1/5284 (0.0%)
3	D	0.27	0/3940	0.68	1/5338 (0.0%)
3	F	0.28	0/3901	0.66	0/5284
3	G	0.29	0/3951	0.72	1/5352 (0.0%)
3	H	0.28	0/3901	0.70	0/5284
3	I	0.28	0/3951	0.70	2/5352 (0.0%)
3	J	0.27	0/3901	0.65	0/5284
3	K	0.27	0/3951	0.68	0/5352
3	L	0.27	0/3901	0.68	1/5284 (0.0%)
3	M	0.27	0/3940	0.68	0/5338
3	N	0.27	0/3901	0.69	0/5284
3	O	0.29	0/3951	0.72	0/5352
3	P	0.27	0/3901	0.68	0/5284
3	Q	0.31	0/1181	0.65	0/1593
4	0	0.29	0/1598	0.67	0/2172
4	1	0.30	0/1605	0.70	0/2181
4	2	0.29	0/1589	0.66	0/2159
4	3	0.30	0/1642	0.69	2/2230 (0.1%)
4	4	0.31	0/1799	0.74	0/2441
5	5	0.31	0/1935	0.70	0/2647
6	6	0.23	0/414	0.62	0/565
6	7	0.29	0/657	0.76	0/897
6	8	0.27	0/657	0.74	0/897
6	9	0.28	0/660	0.65	0/900
7	AM	0.35	0/300	0.70	0/403
7	AN	0.30	0/646	0.64	0/870
7	AO	0.29	0/671	0.64	0/908

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
7	AP	0.31	0/671	0.64	0/908
7	AQ	0.28	0/671	0.66	0/908
7	AR	0.30	0/671	0.71	1/908 (0.1%)
8	AS	0.32	0/472	0.64	0/638
8	AT	0.28	0/472	0.54	0/638
8	AU	0.32	0/472	0.66	0/638
8	AV	0.31	0/472	0.76	1/638 (0.2%)
8	AW	0.30	0/472	0.58	0/638
8	AX	0.35	0/582	0.69	0/788
8	AY	0.33	0/623	0.75	0/846
8	AZ	0.29	0/623	0.68	0/846
8	BA	0.30	0/623	0.69	0/846
8	BB	0.28	0/623	0.61	0/846
8	BC	0.29	0/623	0.59	0/846
8	BD	0.29	0/623	0.59	0/846
8	BE	0.27	0/623	0.66	0/846
8	BF	0.27	0/623	0.60	0/846
8	BG	0.29	0/623	0.59	0/846
8	BH	0.29	0/623	0.68	1/846 (0.1%)
8	BI	0.28	0/623	0.64	0/846
8	BJ	0.29	0/623	0.72	0/846
8	BK	0.26	0/623	0.69	0/846
8	BL	0.26	0/623	0.59	0/846
8	BM	0.25	0/623	0.66	1/846 (0.1%)
8	BN	0.26	0/623	0.68	0/846
8	BO	0.30	0/623	0.67	1/846 (0.1%)
8	BP	0.28	0/623	0.74	1/846 (0.1%)
8	BQ	0.27	0/623	0.64	0/846
8	BR	0.28	0/623	0.69	0/846
8	BS	0.29	0/623	0.72	0/846
8	BT	0.28	0/623	0.76	0/846
8	BU	0.26	0/623	0.70	0/846
8	BV	0.24	0/623	0.58	0/846
All	All	0.28	0/174128	0.66	20/235929 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
6	8	0	1
All	All	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	49	MET	CB-CG-SD	7.13	134.08	112.70
8	AV	34	LEU	CA-CB-CG	6.21	138.05	116.30
3	L	178	GLN	CA-CB-CG	5.95	125.99	114.10
1	p	168	LYS	CB-CG-CD	5.73	124.48	111.30
2	c	283	MET	CB-CA-C	5.56	116.43	110.65
3	D	348	ASP	N-CA-C	-5.56	107.50	114.56
3	C	212	GLU	CA-CB-CG	5.49	125.08	114.10
8	BM	31	LEU	CA-CB-CG	5.45	135.38	116.30
2	c	283	MET	CA-CB-CG	5.37	124.84	114.10
4	3	206	ASP	CA-CB-CG	5.36	117.96	112.60
1	AB	77	LEU	CA-CB-CG	5.36	135.04	116.30
3	G	339	LEU	CA-CB-CG	5.31	134.89	116.30
8	BO	31	LEU	CA-CB-CG	5.31	134.88	116.30
1	AL	77	LEU	CA-CB-CG	5.29	134.80	116.30
8	BH	31	LEU	CA-CB-CG	5.29	134.80	116.30
7	AR	87	LEU	CA-CB-CG	5.24	134.63	116.30
4	3	96	LEU	CA-CB-CG	5.15	134.32	116.30
3	I	143	ARG	CA-CB-CG	5.14	124.38	114.10
2	a	382	SER	N-CA-C	-5.13	103.51	108.07
8	BP	23	LEU	CA-CB-CG	5.06	134.00	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	8	41	GLN	Peptide
2	b	366	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1431	0	1424	19	0
1	AB	1431	0	1424	18	0
1	AC	1431	0	1424	30	0
1	AD	1431	0	1424	19	0
1	AE	1431	0	1424	20	0
1	AF	1431	0	1424	23	0
1	AG	1431	0	1424	19	0
1	AH	1431	0	1424	24	0
1	AI	1431	0	1424	25	0
1	AJ	1431	0	1424	25	0
1	AK	1431	0	1424	17	0
1	AL	1431	0	1424	30	0
1	o	1431	0	1424	27	0
1	p	1431	0	1424	26	0
1	q	1431	0	1424	22	0
1	r	1431	0	1424	21	0
1	s	1431	0	1424	29	0
1	t	1431	0	1424	23	0
1	u	1431	0	1424	24	0
1	v	1431	0	1424	32	0
1	w	1431	0	1424	24	0
1	x	1431	0	1424	13	0
1	y	1431	0	1424	22	0
1	z	1431	0	1424	25	0
2	E	1836	0	1800	27	0
2	R	1827	0	1789	22	0
2	S	1831	0	1788	34	0
2	T	1836	0	1800	26	0
2	U	1827	0	1789	27	0
2	V	1831	0	1788	23	0
2	W	1836	0	1800	22	0
2	X	1827	0	1789	17	0
2	Y	1831	0	1788	19	0
2	Z	1836	0	1800	12	0
2	a	1827	0	1789	26	0
2	b	1831	0	1788	24	0
2	c	1836	0	1800	23	0
2	d	1827	0	1789	20	0
2	e	1831	0	1788	20	0
2	f	1836	0	1800	22	0
2	g	1827	0	1789	19	0
2	h	1831	0	1788	24	0
2	i	1836	0	1800	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	j	1827	0	1789	26	0
2	k	1831	0	1788	17	0
2	l	1836	0	1800	26	0
2	m	1827	0	1789	26	0
2	n	1831	0	1788	15	0
3	A	3838	0	3858	74	0
3	B	3884	0	3918	67	0
3	C	3838	0	3858	55	0
3	D	3876	0	3905	57	0
3	F	3838	0	3858	60	0
3	G	3884	0	3918	70	0
3	H	3838	0	3858	76	0
3	I	3884	0	3918	72	0
3	J	3838	0	3858	69	0
3	K	3884	0	3918	71	0
3	L	3838	0	3858	66	0
3	M	3876	0	3905	71	0
3	N	3838	0	3858	65	0
3	O	3884	0	3918	57	0
3	P	3838	0	3858	52	0
3	Q	1154	0	1163	22	0
4	0	1562	0	1597	32	0
4	1	1569	0	1613	20	0
4	2	1553	0	1598	28	0
4	3	1606	0	1649	20	0
4	4	1758	0	1806	37	0
5	5	1885	0	1931	21	0
6	6	405	0	418	4	0
6	7	644	0	685	13	0
6	8	644	0	685	13	0
6	9	647	0	692	13	0
7	AM	298	0	307	6	0
7	AN	644	0	654	16	0
7	AO	667	0	672	13	0
7	AP	667	0	672	13	0
7	AQ	667	0	672	14	0
7	AR	667	0	672	13	0
8	AS	466	0	470	3	0
8	AT	466	0	470	7	0
8	AU	466	0	470	7	0
8	AV	466	0	470	9	0
8	AW	466	0	470	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AX	574	0	566	17	0
8	AY	612	0	598	16	0
8	AZ	612	0	598	7	0
8	BA	612	0	598	13	0
8	BB	612	0	598	13	0
8	BC	612	0	598	13	0
8	BD	612	0	598	6	0
8	BE	612	0	598	10	0
8	BF	612	0	598	15	0
8	BG	612	0	598	12	0
8	BH	612	0	598	14	0
8	BI	612	0	598	10	0
8	BJ	612	0	598	16	0
8	BK	612	0	598	10	0
8	BL	612	0	598	10	0
8	BM	612	0	598	15	0
8	BN	612	0	598	11	0
8	BO	612	0	598	9	0
8	BP	612	0	598	6	0
8	BQ	612	0	598	8	0
8	BR	612	0	598	8	0
8	BS	612	0	598	9	0
8	BT	612	0	598	10	0
8	BU	612	0	598	12	0
8	BV	612	0	598	5	0
All	All	170801	0	170210	2194	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (2194) 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)
2:S:369:ARG:HB3	2:S:379:ILE:HD11	1.60	0.84
8:BN:26:GLN:HE22	8:BT:5:TRP:H	1.35	0.73
1:x:148:LEU:HB2	1:x:183:ILE:HG22	1.69	0.73
3:J:478:THR:HB	3:J:503:ASN:HB3	1.70	0.73
3:Q:165:MET:HE3	3:A:113:SER:HB2	1.73	0.71
3:Q:97:GLN:HE21	3:A:137:PRO:HD2	1.56	0.71
3:H:478:THR:HB	3:H:503:ASN:HB2	1.72	0.71
3:A:179:LYS:HD3	3:A:284:ALA:HA	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:139:ASN:HD21	1:v:141:ARG:HE	1.39	0.70
3:C:478:THR:HB	3:C:503:ASN:HB3	1.73	0.69
8:BI:5:TRP:H	8:BC:26:GLN:HE22	1.39	0.69
2:Z:224:ASN:HB2	2:Z:227:GLU:HG2	1.72	0.69
8:BQ:50:LYS:HA	8:BQ:53:GLU:HG2	1.75	0.69
3:Q:39:ASP:H	3:Q:69:THR:HG22	1.56	0.68
1:AJ:46:ALA:HB1	1:AJ:58:ILE:HD11	1.75	0.68
3:H:179:LYS:HD3	3:H:284:ALA:HA	1.76	0.68
7:AN:67:LEU:HB3	8:AY:75:ILE:HG21	1.75	0.68
3:G:478:THR:HB	3:G:503:ASN:HB3	1.74	0.67
1:AD:35:VAL:HG12	1:AD:77:LEU:HD13	1.77	0.67
3:H:317:ASP:HB3	3:H:362:LYS:HD2	1.77	0.67
1:u:62:GLU:HG2	1:u:63:PRO:HD3	1.76	0.67
3:M:179:LYS:HD3	3:M:284:ALA:HA	1.75	0.67
2:S:381:MET:HE1	2:T:391:PRO:HG2	1.77	0.67
3:O:478:THR:HB	3:O:503:ASN:HB3	1.75	0.67
3:J:38:LYS:HA	3:J:69:THR:HG23	1.76	0.67
2:U:336:ILE:HD11	1:s:165:SER:HB2	1.75	0.66
7:AR:32:ARG:HD2	7:AR:35:GLN:HE21	1.59	0.66
1:AI:139:ASN:HB3	1:AI:141:ARG:HG2	1.78	0.66
2:m:363:ASP:OD1	2:m:363:ASP:N	2.29	0.66
4:2:214:GLY:HA3	6:7:83:LEU:HD13	1.78	0.66
3:A:478:THR:HB	3:A:503:ASN:HB3	1.78	0.66
5:5:76:GLN:HE22	5:5:162:GLU:HG2	1.61	0.65
3:D:179:LYS:HD3	3:D:284:ALA:HA	1.79	0.65
2:b:341:GLN:HE22	1:y:160:LEU:HD21	1.62	0.65
1:z:158:SER:HB3	1:z:163:GLN:HE22	1.61	0.65
3:K:388:THR:HG22	3:K:405:THR:HG22	1.78	0.65
3:L:178:GLN:HE22	3:L:180:ILE:HG13	1.60	0.65
3:O:179:LYS:HD3	3:O:284:ALA:HA	1.77	0.64
2:E:173:LEU:HD12	2:E:194:LEU:HD23	1.79	0.64
4:4:121:LYS:HD2	4:4:126:GLU:HA	1.78	0.64
3:N:432:ASN:HD21	3:N:449:GLU:HG2	1.62	0.64
2:j:367:LYS:O	3:I:38:LYS:NZ	2.30	0.64
7:AQ:55:ILE:HG12	8:AV:64:THR:HG21	1.80	0.64
2:S:213:ARG:HD3	1:p:201:PRO:HB3	1.78	0.64
1:t:136:ALA:O	4:0:109:ARG:NH1	2.31	0.64
8:AS:32:ASP:OD1	8:AS:32:ASP:N	2.30	0.64
8:AY:58:ARG:HH11	8:AY:61:GLN:HE22	1.45	0.64
3:J:290:ILE:HA	3:J:293:LEU:HD23	1.78	0.63
3:M:258:LEU:HD23	3:M:261:ASN:HD22	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:197:LEU:O	3:H:411:ARG:NH1	2.30	0.63
3:K:478:THR:HB	3:K:503:ASN:HB3	1.80	0.63
3:L:187:ASN:HB2	3:L:298:ASP:HB2	1.81	0.63
3:L:290:ILE:HA	3:L:293:LEU:HD23	1.81	0.63
3:L:373:LEU:HD23	3:M:470:GLY:HA3	1.80	0.63
6:8:1:MET:HA	6:8:4:LEU:HD23	1.80	0.63
3:H:404:VAL:HG22	3:H:447:LEU:HD13	1.80	0.63
3:H:541:SER:OG	3:J:506:ASN:ND2	2.31	0.63
2:Y:261:SER:O	2:Y:265:ASN:ND2	2.31	0.63
3:F:478:THR:HB	3:F:503:ASN:HB3	1.81	0.63
3:G:68:ILE:HD11	3:G:88:LEU:HD21	1.80	0.63
3:L:327:GLY:HA3	3:L:352:PHE:HA	1.79	0.63
3:M:405:THR:HG21	8:BR:3:THR:HA	1.81	0.63
3:O:107:MET:HE2	3:O:151:GLY:HA2	1.80	0.63
2:V:267:MET:HG3	2:V:271:GLU:HG3	1.81	0.63
2:T:202:ARG:NH1	1:q:191:SER:OG	2.32	0.63
8:AV:48:GLN:NE2	8:BG:78:ASN:O	2.31	0.63
3:M:373:LEU:HD23	3:N:470:GLY:HA3	1.81	0.63
8:BL:40:ASP:HB3	8:BL:43:LEU:HB2	1.80	0.63
1:AI:99:ARG:HG3	1:AI:134:ILE:HG21	1.80	0.63
4:O:206:ASP:OD1	5:5:175:ASN:ND2	2.32	0.63
1:AC:148:LEU:HB2	1:AC:183:ILE:HG22	1.81	0.62
3:H:252:MET:HG3	3:H:256:GLU:HG2	1.82	0.62
1:s:135:ASP:O	1:s:139:ASN:ND2	2.32	0.62
3:I:327:GLY:HA3	3:I:352:PHE:HA	1.82	0.62
1:AA:35:VAL:HG12	1:AA:77:LEU:HD13	1.81	0.62
2:V:340:ARG:HH21	1:t:163:GLN:HE21	1.46	0.62
2:d:316:ARG:HH21	2:d:318:ASN:HD21	1.46	0.62
3:F:39:ASP:H	3:F:69:THR:HB	1.63	0.62
8:AY:37:LYS:NZ	8:BJ:6:SER:O	2.32	0.62
3:A:39:ASP:H	3:A:69:THR:HG22	1.64	0.62
3:C:178:GLN:HG2	3:D:220:GLN:HE21	1.64	0.62
1:AI:168:LYS:HE2	1:AI:183:ILE:HG23	1.80	0.62
4:1:214:GLY:HA3	6:6:83:LEU:HD13	1.81	0.62
7:AO:65:LYS:HD3	8:AU:24:GLN:HG3	1.80	0.62
8:AY:53:GLU:HB3	8:BE:9:LEU:HD21	1.81	0.62
1:AE:99:ARG:NH1	1:o:101:GLU:OE1	2.33	0.62
5:5:13:VAL:HG13	7:AM:81:VAL:HG21	1.80	0.62
2:h:282:LEU:HD12	2:h:283:MET:HG3	1.81	0.62
5:5:176:GLN:OE1	5:5:179:GLN:NE2	2.33	0.62
3:B:179:LYS:HD3	3:B:284:ALA:HA	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:139:ASN:HD22	1:AB:141:ARG:HE	1.47	0.61
3:G:97:GLN:HE22	3:H:139:ARG:HE	1.46	0.61
3:K:49:MET:N	3:K:49:MET:SD	2.73	0.61
1:AI:28:ASP:HB3	1:AI:31:GLN:HG2	1.82	0.61
4:2:218:GLN:NE2	6:7:83:LEU:O	2.33	0.61
3:G:179:LYS:HD3	3:G:284:ALA:HA	1.82	0.61
3:P:39:ASP:H	3:P:69:THR:HG22	1.66	0.61
8:BE:26:GLN:HE22	8:BK:4:PRO:HA	1.64	0.61
1:p:99:ARG:HE	1:p:134:ILE:HB	1.66	0.61
3:D:311:VAL:HG22	3:D:368:VAL:HG22	1.82	0.61
3:I:338:SER:HB3	3:I:344:ILE:HD11	1.82	0.61
2:c:247:ARG:NH1	2:c:347:TYR:O	2.32	0.61
3:B:176:GLY:HA2	3:B:259:LYS:HE2	1.82	0.61
3:G:305:GLU:HA	3:G:374:LEU:HA	1.81	0.61
3:J:327:GLY:HA3	3:J:352:PHE:HA	1.82	0.61
3:J:114:LEU:HD13	3:J:117:VAL:HB	1.82	0.61
3:M:309:TRP:HB2	3:M:512:MET:HB2	1.82	0.61
4:0:53:ASN:ND2	7:AM:98:LEU:O	2.34	0.61
7:AO:20:ARG:NH1	7:AO:21:SER:O	2.34	0.61
3:I:473:THR:HG22	3:I:508:VAL:HG23	1.83	0.61
2:a:187:LEU:HD12	2:a:188:PRO:HD2	1.81	0.61
1:r:168:LYS:NZ	1:r:183:ILE:O	2.34	0.61
3:J:179:LYS:HD3	3:J:284:ALA:HA	1.83	0.61
3:O:213:ARG:HA	3:O:216:GLN:HG2	1.83	0.61
2:W:372:GLN:NE2	2:X:373:TYR:OH	2.33	0.61
1:p:20:ASP:N	1:p:60:VAL:O	2.34	0.61
2:k:323:VAL:HG12	2:k:355:VAL:HG12	1.83	0.60
2:l:333:ASP:OD2	1:AK:168:LYS:NZ	2.34	0.60
1:r:46:ALA:HB1	1:r:58:ILE:HD11	1.82	0.60
3:A:62:MET:N	3:A:62:MET:SD	2.74	0.60
1:AA:94:LEU:HG	1:AA:95:VAL:HG23	1.83	0.60
2:S:379:ILE:HG23	2:S:387:TYR:HB3	1.83	0.60
3:J:426:LEU:HD21	3:J:428:ILE:HG12	1.83	0.60
2:X:187:LEU:HD12	2:X:188:PRO:HD2	1.83	0.60
2:c:224:ASN:HB3	2:c:227:GLU:HG2	1.82	0.60
3:K:195:TYR:O	8:BM:3:THR:N	2.34	0.60
3:A:373:LEU:HD23	3:B:470:GLY:HA3	1.83	0.60
3:N:274:ASP:N	3:N:274:ASP:OD1	2.34	0.60
2:V:263:GLN:NE2	2:V:295:ASP:OD2	2.34	0.60
2:f:327:ILE:HB	2:f:359:ILE:HA	1.82	0.60
2:k:187:LEU:HD12	2:k:188:PRO:HD2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:169:GLN:HE22	3:J:115:ARG:HA	1.66	0.60
3:N:323:THR:HB	3:N:356:VAL:HG22	1.83	0.60
8:BJ:66:LYS:NZ	8:BO:80:ARG:O	2.33	0.60
8:BH:21:ASP:HB2	8:BN:5:TRP:HB2	1.83	0.60
2:l:391:PRO:HG3	3:K:38:LYS:HE2	1.82	0.60
3:L:322:GLY:HA3	3:L:499:TYR:HA	1.83	0.60
2:c:283:MET:HE2	2:c:286:ALA:HB2	1.84	0.60
2:d:327:ILE:HD12	2:d:359:ILE:HG12	1.82	0.60
3:M:373:LEU:HD21	3:N:455:ILE:HD12	1.84	0.60
8:BM:56:LEU:HD11	8:BS:69:LYS:HA	1.83	0.60
1:w:94:LEU:HG	1:w:95:VAL:HG23	1.82	0.60
1:x:148:LEU:HD22	1:x:171:LEU:HD13	1.83	0.60
3:G:473:THR:HG22	3:G:508:VAL:HG23	1.84	0.60
3:H:58:ILE:HD13	3:I:105:SER:HA	1.84	0.60
2:f:263:GLN:HE22	2:f:297:VAL:HG23	1.67	0.60
1:p:120:MET:HE3	1:p:121:GLU:HG2	1.84	0.60
3:B:198:ARG:NH1	8:BJ:19:GLY:O	2.32	0.60
3:I:197:LEU:HA	3:I:382:ILE:HD11	1.83	0.60
3:O:63:ALA:HB2	3:O:103:ASP:HB3	1.83	0.60
1:AE:164:ILE:HD11	2:E:334:VAL:HG22	1.84	0.60
2:E:232:ILE:HD12	2:E:283:MET:HE2	1.83	0.60
1:s:35:VAL:HG12	1:s:77:LEU:HD13	1.84	0.60
8:AV:59:ASN:O	8:AV:63:ASN:ND2	2.34	0.60
3:I:179:LYS:HD3	3:I:284:ALA:HA	1.83	0.60
3:M:388:THR:HG22	3:M:405:THR:HG22	1.83	0.60
3:O:473:THR:HG22	3:O:508:VAL:HG23	1.83	0.60
1:AA:43:ASN:ND2	2:d:206:TRP:O	2.33	0.59
1:v:147:HIS:HB3	1:w:173:ASN:HB2	1.82	0.59
4:4:41:LEU:HD13	4:4:198:LYS:HG2	1.84	0.59
3:H:403:HIS:O	8:BT:3:THR:N	2.35	0.59
8:BU:34:LEU:HA	8:BU:43:LEU:HD21	1.83	0.59
3:D:393:LEU:HD23	3:D:400:ALA:HB3	1.82	0.59
3:M:39:ASP:H	3:M:69:THR:HB	1.66	0.59
4:3:34:PHE:HB3	4:3:52:LEU:HD22	1.84	0.59
3:L:478:THR:HB	3:L:503:ASN:HB3	1.84	0.59
3:N:65:ARG:O	3:N:67:LYS:NZ	2.34	0.59
3:N:436:PRO:O	8:BL:33:LYS:NZ	2.36	0.59
3:D:461:VAL:HG22	3:D:467:LEU:HD12	1.84	0.59
3:G:197:LEU:O	3:G:411:ARG:NH1	2.35	0.59
8:BD:29:GLU:OE2	8:BD:33:LYS:NZ	2.35	0.59
8:BF:78:ASN:ND2	8:BA:63:ASN:OD1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:475:ASP:OD1	3:O:551:ARG:NH2	2.36	0.59
1:y:179:ASP:OD1	1:y:179:ASP:N	2.35	0.59
8:BP:22:ASN:HB2	8:BP:25:THR:HG22	1.83	0.59
1:AE:164:ILE:HG22	1:AE:187:LEU:HD21	1.85	0.59
2:W:256:PRO:HG2	2:W:289:VAL:HG12	1.85	0.59
2:b:304:GLU:HG2	2:b:308:LYS:HE2	1.84	0.59
1:AK:72:ILE:HD13	1:AK:77:LEU:HD13	1.84	0.59
3:D:314:ASN:HB3	3:D:365:ALA:HB3	1.85	0.59
3:N:179:LYS:HD3	3:N:284:ALA:HA	1.84	0.59
3:G:292:MET:HA	3:G:295:LYS:HE3	1.84	0.59
1:t:25:LYS:O	1:u:29:GLN:NE2	2.36	0.59
3:A:485:PRO:HG3	3:P:360:GLU:HB2	1.85	0.59
3:C:197:LEU:O	3:C:411:ARG:NH1	2.35	0.59
3:C:547:GLN:HE21	3:F:508:VAL:HG13	1.68	0.59
3:G:283:THR:H	3:G:286:GLN:HE21	1.50	0.59
2:Y:304:GLU:OE1	2:Y:316:ARG:NH1	2.36	0.58
1:q:29:GLN:O	1:q:33:ASN:ND2	2.36	0.58
1:s:102:LYS:HA	1:s:105:LEU:HG	1.84	0.58
3:J:308:LEU:HG	3:J:513:ILE:HG22	1.84	0.58
8:BF:13:SER:HB2	8:BF:61:GLN:HE21	1.69	0.58
3:K:169:GLN:HE22	3:L:115:ARG:HA	1.67	0.58
7:AN:75:SER:HB2	8:AT:69:LYS:HD3	1.85	0.58
3:O:338:SER:HB3	3:O:344:ILE:HD11	1.85	0.58
1:AI:118:GLN:HE21	1:AI:125:SER:HA	1.68	0.58
7:AP:49:GLN:O	7:AP:53:ASN:ND2	2.35	0.58
2:b:187:LEU:HD21	2:b:253:PRO:HB2	1.85	0.58
4:3:4:ASP:OD2	7:AQ:48:LYS:NZ	2.36	0.58
3:O:290:ILE:HA	3:O:293:LEU:HD13	1.85	0.58
2:V:235:TRP:HE3	2:V:236:LEU:HD22	1.69	0.58
7:AM:86:THR:OG1	7:AM:90:LYS:NZ	2.36	0.58
3:F:107:MET:HE2	3:F:151:GLY:HA2	1.86	0.58
3:M:447:LEU:HD12	3:M:448:PRO:HD2	1.86	0.58
3:M:274:ASP:OD1	3:M:274:ASP:N	2.37	0.58
8:AT:48:GLN:NE2	8:BE:78:ASN:O	2.37	0.58
3:F:274:ASP:N	3:F:274:ASP:OD1	2.36	0.58
3:H:338:SER:HB3	3:H:344:ILE:HD11	1.85	0.58
3:J:404:VAL:HG22	3:J:447:LEU:HD13	1.86	0.58
8:BB:37:LYS:HA	8:BM:5:TRP:HZ2	1.69	0.58
1:AL:201:PRO:HB3	2:g:213:ARG:HD3	1.86	0.58
2:i:190:ARG:NH2	2:i:280:ARG:O	2.37	0.58
3:L:406:TYR:OH	3:L:448:PRO:O	2.20	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:173:ASN:HB2	1:AI:147:HIS:HB3	1.86	0.57
1:AF:120:MET:SD	1:AF:121:GLU:N	2.75	0.57
2:R:369:ARG:O	3:M:38:LYS:NZ	2.37	0.57
7:AM:71:GLN:NE2	8:AX:75:ILE:O	2.38	0.57
3:A:388:THR:HG22	3:A:405:THR:HG22	1.85	0.57
3:I:120:ASN:O	3:I:124:ASN:ND2	2.36	0.57
3:I:409:MET:HB3	3:I:429:GLU:HG3	1.85	0.57
3:J:305:GLU:HA	3:J:374:LEU:HA	1.86	0.57
3:L:269:ILE:HG12	3:L:280:VAL:HG23	1.86	0.57
3:L:274:ASP:N	3:L:274:ASP:OD1	2.36	0.57
2:e:369:ARG:HB3	2:e:379:ILE:HD11	1.87	0.57
2:f:190:ARG:NH1	2:f:286:ALA:O	2.35	0.57
2:l:173:LEU:HD12	2:l:194:LEU:HD23	1.87	0.57
3:D:274:ASP:N	3:D:274:ASP:OD1	2.36	0.57
3:L:58:ILE:HD13	3:M:105:SER:HA	1.86	0.57
8:BH:78:ASN:OD1	8:BI:80:ARG:NH1	2.35	0.57
1:AA:29:GLN:O	1:AA:33:ASN:ND2	2.38	0.57
2:k:221:ARG:HD2	2:l:182:GLU:HG2	1.85	0.57
1:w:66:THR:HG21	1:x:197:ALA:HA	1.85	0.57
3:J:394:ILE:HD11	3:L:340:ASN:HA	1.86	0.57
1:AE:35:VAL:HG12	1:AE:77:LEU:HD13	1.86	0.57
2:T:190:ARG:NH1	2:T:286:ALA:O	2.36	0.57
4:0:200:VAL:HG13	4:0:201:LEU:HD12	1.86	0.57
3:A:421:GLN:HG3	3:A:462:PRO:HA	1.86	0.57
3:B:169:GLN:OE1	3:B:170:ASN:ND2	2.38	0.57
3:F:555:ASP:O	3:G:516:LYS:NZ	2.37	0.57
2:Y:316:ARG:HE	2:Y:318:ASN:HD21	1.53	0.57
2:j:323:VAL:HG12	2:j:355:VAL:HG12	1.86	0.57
3:N:290:ILE:HA	3:N:293:LEU:HD23	1.87	0.57
3:N:453:THR:OG1	3:N:509:ARG:NH1	2.36	0.57
8:AZ:17:ASP:OD1	8:AZ:57:TYR:OH	2.22	0.57
1:AB:99:ARG:HD3	1:AB:134:ILE:HD13	1.86	0.57
2:e:245:TYR:OH	2:e:353:ARG:NH1	2.38	0.57
3:A:47:ASP:N	3:A:47:ASP:OD1	2.34	0.57
3:B:394:ILE:HD11	3:D:340:ASN:HA	1.85	0.57
3:G:327:GLY:HA3	3:G:352:PHE:HA	1.87	0.57
1:AA:156:ARG:NH2	1:AA:190:ARG:O	2.36	0.57
7:AR:66:GLU:HA	7:AR:69:ILE:HD12	1.87	0.57
8:AY:55:ASN:O	8:AY:59:ASN:ND2	2.33	0.57
3:I:213:ARG:HB3	8:BH:3:THR:HG21	1.87	0.57
3:G:482:GLN:HB3	3:G:499:TYR:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:69:VAL:HA	1:AH:72:ILE:HD12	1.86	0.57
1:o:168:LYS:HG3	1:o:183:ILE:HD13	1.87	0.57
3:D:431:GLY:HA2	3:D:450:VAL:HG23	1.87	0.57
3:H:58:ILE:HG23	3:H:100:TYR:HA	1.87	0.57
2:R:310:GLN:O	2:R:338:ARG:NH1	2.38	0.56
2:b:379:ILE:HB	2:b:387:TYR:HB3	1.87	0.56
3:B:114:LEU:HD21	3:B:163:ALA:HB1	1.87	0.56
1:AL:20:ASP:N	1:AL:60:VAL:O	2.38	0.56
1:z:69:VAL:HA	1:z:72:ILE:HD12	1.87	0.56
3:L:58:ILE:HG23	3:L:100:TYR:HA	1.87	0.56
1:AB:24:LEU:HD12	1:AB:58:ILE:HD11	1.87	0.56
3:Q:107:MET:O	7:AN:20[A]:ARG:NH1	2.38	0.56
2:a:232:ILE:HD11	2:a:248:ILE:HG21	1.87	0.56
2:m:365:TRP:O	2:m:369:ARG:NH1	2.38	0.56
1:s:148:LEU:HD11	1:s:171:LEU:HB3	1.87	0.56
4:0:30:PHE:HE1	4:0:215:LEU:HB3	1.69	0.56
3:C:39:ASP:H	3:C:69:THR:HG22	1.70	0.56
3:F:179:LYS:HD3	3:F:284:ALA:HA	1.86	0.56
3:H:279:LEU:HD13	3:I:214:LEU:HD22	1.86	0.56
3:H:426:LEU:HD21	3:H:428:ILE:HG12	1.86	0.56
3:I:107:MET:HE2	3:I:151:GLY:HA2	1.87	0.56
3:K:189:PHE:HA	3:K:276:ASN:HD21	1.69	0.56
3:K:274:ASP:N	3:K:274:ASP:OD1	2.38	0.56
3:L:305:GLU:HA	3:L:374:LEU:HA	1.88	0.56
3:M:415:ARG:NH2	3:M:423:GLU:OE2	2.35	0.56
3:N:421:GLN:HG3	3:N:462:PRO:HA	1.87	0.56
8:BJ:44:LEU:HD22	8:BU:76:ILE:HD11	1.87	0.56
1:s:29:GLN:O	1:s:33:ASN:ND2	2.39	0.56
3:I:51:LEU:HD23	3:J:87:GLN:HE22	1.71	0.56
1:AH:29:GLN:NE2	1:AI:25:LYS:O	2.39	0.56
2:b:274:VAL:HG12	2:b:278:LYS:HE2	1.88	0.56
1:q:31:GLN:NE2	1:q:79:PRO:O	2.39	0.56
4:0:186:MET:HG2	4:0:187:MET:HG3	1.87	0.56
3:L:73:GLU:OE1	3:L:75:HIS:ND1	2.34	0.56
3:O:197:LEU:O	3:O:411:ARG:NH1	2.39	0.56
3:P:179:LYS:HD3	3:P:284:ALA:HA	1.87	0.56
3:P:327:GLY:HA3	3:P:352:PHE:HA	1.87	0.56
2:a:304:GLU:OE1	2:a:316:ARG:NH1	2.39	0.56
2:c:363:ASP:OD1	2:c:363:ASP:N	2.39	0.56
2:j:316:ARG:HH21	2:j:318:ASN:HD21	1.53	0.56
2:l:364:ASP:HA	2:l:390:SER:HB2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:62:LEU:HD12	6:8:63:LEU:HG	1.88	0.56
3:A:290:ILE:HA	3:A:293:LEU:HD23	1.88	0.56
3:K:406:TYR:OH	3:K:448:PRO:O	2.23	0.56
3:O:183:MET:HE1	3:O:290:ILE:HG13	1.88	0.56
8:BO:22:ASN:HB2	8:BO:25:THR:HB	1.88	0.56
1:AI:39:LEU:HD22	1:AI:44:ILE:HD11	1.88	0.56
1:z:39:LEU:HD22	1:z:44:ILE:HD11	1.88	0.56
3:A:327:GLY:HA3	3:A:352:PHE:HA	1.87	0.56
3:A:401:LEU:N	8:BV:3:THR:OG1	2.35	0.56
2:S:389:PRO:HB2	2:T:366:LEU:HD11	1.88	0.56
2:U:321:GLY:O	2:V:309:GLN:NE2	2.39	0.56
2:W:364:ASP:N	2:W:364:ASP:OD1	2.39	0.56
2:m:245:TYR:OH	2:m:353:ARG:NH1	2.39	0.56
5:5:192:LEU:HD11	5:5:219:LYS:HB2	1.87	0.56
3:K:384:ASP:HB3	3:L:454:LEU:HD21	1.87	0.56
1:AF:197:ALA:HA	1:AJ:66:THR:HG21	1.86	0.56
2:g:187:LEU:HD12	2:g:188:PRO:HD2	1.88	0.56
2:j:379:ILE:HG23	2:j:387:TYR:HB3	1.88	0.56
2:m:202:ARG:NH1	1:AJ:192:ASP:O	2.38	0.56
2:n:332:ASP:OD2	2:n:332:ASP:N	2.38	0.56
3:K:290:ILE:HA	3:K:293:LEU:HD13	1.88	0.56
3:M:269:ILE:HG12	3:M:280:VAL:HG23	1.88	0.56
2:a:263:GLN:NE2	2:a:295:ASP:OD1	2.38	0.56
2:i:326:VAL:HA	2:i:358:ALA:HB3	1.88	0.56
7:AP:31:ASP:O	7:AP:35:GLN:NE2	2.39	0.56
3:H:362:LYS:NZ	3:H:363:LYS:O	2.38	0.56
1:AH:142:PRO:HB3	1:AI:141:ARG:HH22	1.70	0.55
3:Q:107:MET:HE2	3:Q:151:GLY:HA2	1.87	0.55
2:d:356:GLN:OE1	2:e:310:GLN:NE2	2.39	0.55
1:o:96:SER:OG	6:7:69:GLU:OE2	2.23	0.55
1:w:88:MET:O	1:x:104:ARG:NH1	2.39	0.55
3:F:197:LEU:O	3:F:411:ARG:NH1	2.33	0.55
3:L:379:VAL:HG21	3:M:458:ILE:HD11	1.89	0.55
3:P:406:TYR:OH	3:P:448:PRO:O	2.22	0.55
1:s:39:LEU:HD22	1:s:44:ILE:HD11	1.88	0.55
4:2:191:VAL:O	4:2:195:THR:OG1	2.21	0.55
6:7:37:GLN:HB3	6:7:41:GLN:HA	1.88	0.55
3:F:322:GLY:HA3	3:F:499:TYR:HA	1.87	0.55
3:G:269:ILE:HD11	3:G:278:LEU:HB3	1.89	0.55
3:H:433:ASP:OD1	3:H:433:ASP:N	2.39	0.55
2:U:373:TYR:HE1	3:O:36:VAL:HG23	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:316:ARG:NE	2:d:318:ASN:OD1	2.38	0.55
1:t:184:SER:HB2	1:u:173:ASN:HD22	1.72	0.55
3:F:423:GLU:HG3	3:F:460:ARG:HB3	1.88	0.55
3:I:471:GLY:HA3	3:I:510:VAL:HG22	1.88	0.55
1:r:20:ASP:OD1	1:r:20:ASP:N	2.40	0.55
1:v:20:ASP:N	1:v:60:VAL:O	2.39	0.55
1:z:150:ALA:HB3	1:z:185:VAL:HG12	1.88	0.55
8:AX:21:ASP:OD1	8:AX:21:ASP:N	2.39	0.55
3:P:274:ASP:OD1	3:P:274:ASP:N	2.38	0.55
3:P:429:GLU:OE1	3:P:452:ARG:NH2	2.39	0.55
4:0:47:PRO:HD2	4:0:52:LEU:HD11	1.88	0.55
3:C:114:LEU:HD21	3:C:163:ALA:HB1	1.88	0.55
8:BN:56:LEU:HD11	8:BT:69:LYS:HA	1.87	0.55
2:b:245:TYR:OH	2:b:353:ARG:NH2	2.40	0.55
1:q:69:VAL:HG22	1:r:37:ALA:HB2	1.89	0.55
1:y:140:GLY:HA3	5:5:248:GLY:HA2	1.88	0.55
8:AX:10:ASP:OD1	8:AX:10:ASP:N	2.40	0.55
3:B:319:GLU:HG2	3:B:502:LYS:HG2	1.89	0.55
3:B:545:LYS:HG3	3:C:536:GLN:HE22	1.71	0.55
3:K:379:VAL:HG11	3:L:458:ILE:HD11	1.88	0.55
3:N:213:ARG:HA	3:N:216:GLN:HG2	1.88	0.55
2:b:360:GLU:HG2	2:c:334:VAL:HG21	1.89	0.55
2:k:210:VAL:HG13	2:k:211:LEU:HD22	1.89	0.55
4:4:8:ILE:HG12	8:AW:75:ILE:HG12	1.89	0.55
3:L:331:ILE:HB	3:L:335:LEU:HB2	1.88	0.55
1:AI:166:ASP:OD1	2:h:340:ARG:NH1	2.39	0.55
1:r:85:ILE:HB	1:r:107:SER:HB3	1.89	0.55
1:t:168:LYS:HE2	1:t:183:ILE:HB	1.89	0.55
1:v:29:GLN:O	1:v:33:ASN:ND2	2.39	0.55
8:AX:26:GLN:OE1	8:AX:50:LYS:NZ	2.36	0.55
3:D:119:LEU:HD21	3:D:147:PHE:HB3	1.88	0.55
3:M:409:MET:HE3	3:M:429:GLU:HG3	1.88	0.55
3:N:187:ASN:HB2	3:N:298:ASP:HB2	1.89	0.55
3:Q:115:ARG:O	3:P:169:GLN:NE2	2.40	0.55
2:j:369:ARG:HB3	2:j:379:ILE:HD11	1.89	0.55
1:z:114:GLU:HB2	1:z:128:VAL:HG22	1.89	0.55
4:4:191:VAL:O	4:4:195:THR:OG1	2.25	0.55
3:I:197:LEU:O	3:I:411:ARG:NH1	2.39	0.55
3:J:108:ARG:HB3	3:J:156:VAL:HG21	1.87	0.55
3:N:178:GLN:HG2	3:O:220:GLN:HE21	1.73	0.55
1:AE:112:ARG:HG2	1:AF:129:HIS:HE1	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:304:GLU:OE1	2:W:316:ARG:NH1	2.40	0.54
2:Z:356:GLN:OE1	2:a:310:GLN:NE2	2.39	0.54
3:C:107:MET:HE2	3:C:151:GLY:HA2	1.89	0.54
3:L:426:LEU:HD21	3:L:428:ILE:HG12	1.90	0.54
3:N:473:THR:HG22	3:N:508:VAL:HG23	1.88	0.54
8:BQ:27:VAL:HA	8:BQ:50:LYS:HZ1	1.72	0.54
2:X:245:TYR:OH	2:X:353:ARG:NH1	2.40	0.54
1:AL:43:ASN:ND2	2:g:206:TRP:O	2.39	0.54
2:j:245:TYR:OH	2:j:353:ARG:NH1	2.41	0.54
1:o:85:ILE:HB	1:o:107:SER:HB3	1.89	0.54
1:y:184:SER:OG	1:z:169:ARG:NE	2.41	0.54
7:AP:46:VAL:O	7:AP:50:THR:N	2.40	0.54
3:A:409:MET:HB3	3:A:429:GLU:HG2	1.88	0.54
3:G:388:THR:HG22	3:G:405:THR:HG22	1.89	0.54
3:H:252:MET:HE3	3:H:255:GLN:HB2	1.89	0.54
3:H:387:ARG:NH2	3:I:449:GLU:O	2.41	0.54
3:N:379:VAL:HG11	3:O:458:ILE:HD11	1.88	0.54
8:AZ:62:SER:O	8:BE:78:ASN:ND2	2.41	0.54
8:BB:21:ASP:OD1	8:BB:21:ASP:N	2.31	0.54
3:D:394:ILE:HD11	3:G:340:ASN:HA	1.89	0.54
3:I:53:LEU:HD23	3:I:99:ILE:HD12	1.89	0.54
3:L:414:PRO:HB3	3:L:424:MET:HG2	1.90	0.54
3:M:410:ILE:HA	3:M:428:ILE:HG22	1.89	0.54
2:S:304:GLU:OE1	2:S:316:ARG:NH1	2.39	0.54
2:W:356:GLN:OE1	2:X:310:GLN:NE2	2.39	0.54
4:2:216:ILE:HG22	4:2:220:MET:HB2	1.90	0.54
3:J:80:LEU:HD23	3:J:84:LEU:HD23	1.89	0.54
2:S:213:ARG:NH2	1:p:43:ASN:O	2.40	0.54
2:U:245:TYR:OH	2:U:353:ARG:NH1	2.40	0.54
4:4:174:LEU:HD11	5:5:125:MET:HB2	1.88	0.54
6:7:25:VAL:HA	6:7:28:ILE:HG22	1.88	0.54
3:G:363:LYS:HD2	3:H:480:THR:HB	1.88	0.54
3:I:406:TYR:OH	3:I:448:PRO:O	2.25	0.54
3:J:97:GLN:HE22	3:K:139:ARG:HE	1.55	0.54
3:O:543:ASP:N	3:O:543:ASP:OD1	2.40	0.54
1:t:156:ARG:NH2	1:t:190:ARG:O	2.40	0.54
8:AX:39:SER:HB2	8:BI:9:LEU:HG	1.90	0.54
3:A:545:LYS:HD2	3:A:548:LYS:HD2	1.89	0.54
3:H:274:ASP:OD1	3:H:274:ASP:N	2.35	0.54
3:H:310:ILE:HG22	3:H:511:PHE:HD1	1.73	0.54
3:J:63:ALA:HB2	3:J:103:ASP:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:198:ARG:H	8:BM:3:THR:HA	1.72	0.54
3:K:387:ARG:NH2	3:L:449:GLU:O	2.41	0.54
3:M:432:ASN:HD21	3:M:449:GLU:HG2	1.71	0.54
8:BH:39:SER:HG	8:BS:8:TYR:H	1.56	0.54
1:AC:110:GLU:OE2	1:AL:112:ARG:NH2	2.40	0.54
1:AG:190:ARG:NH1	1:AG:191:SER:O	2.38	0.54
2:Y:310:GLN:HB2	2:Y:312:LEU:HD23	1.90	0.54
2:a:299:ALA:O	2:a:346:TYR:OH	2.23	0.54
2:f:262:ARG:NH1	2:f:295:ASP:OD1	2.41	0.54
3:B:406:TYR:OH	3:B:448:PRO:O	2.26	0.54
3:D:97:GLN:HE21	3:F:137:PRO:HD2	1.73	0.54
3:F:388:THR:HG22	3:F:405:THR:HG22	1.90	0.54
8:BC:13:SER:HB2	8:BC:61:GLN:HE21	1.72	0.54
1:AL:29:GLN:O	1:AL:33:ASN:ND2	2.41	0.54
2:a:335:GLU:OE2	2:a:338:ARG:NH2	2.41	0.54
2:c:310:GLN:O	2:c:338:ARG:NH2	2.40	0.54
2:d:190:ARG:NH1	2:d:286:ALA:O	2.40	0.54
1:u:140:GLY:HA3	4:0:105:LYS:HG3	1.90	0.54
4:2:38:ARG:NH1	4:2:48:SER:O	2.40	0.54
7:AO:64:PRO:HA	7:AO:67:LEU:HB2	1.90	0.54
3:B:373:LEU:HG	3:C:470:GLY:HA3	1.90	0.54
3:J:58:ILE:HD13	3:K:105:SER:HA	1.89	0.54
3:J:387:ARG:NH2	3:K:449:GLU:O	2.41	0.54
1:AC:43:ASN:HB3	2:f:209:GLN:HG2	1.90	0.54
2:U:190:ARG:O	2:U:192:LYS:NZ	2.40	0.54
2:b:256:PRO:HG2	2:b:289:VAL:HG12	1.90	0.54
4:2:48:SER:OG	4:2:51:THR:N	2.37	0.54
5:5:91:PRO:HB3	5:5:242:LEU:HB3	1.90	0.54
3:B:213:ARG:HA	3:B:216:GLN:HG2	1.90	0.54
3:M:305:GLU:HA	3:M:374:LEU:HA	1.89	0.54
3:N:426:LEU:HD21	3:N:428:ILE:HG12	1.90	0.54
8:BU:22:ASN:HB2	8:BU:25:THR:HB	1.89	0.54
1:AG:39:LEU:HB3	1:AG:44:ILE:HG13	1.90	0.54
2:W:200:ASN:O	2:W:204:THR:OG1	2.25	0.54
2:Y:332:ASP:OD1	2:Y:332:ASP:N	2.40	0.54
2:e:334:VAL:HG13	2:e:338:ARG:HH21	1.73	0.54
2:k:245:TYR:OH	2:k:353:ARG:NH1	2.41	0.54
3:A:131:LEU:HD13	3:A:158:MET:HE1	1.90	0.54
3:C:179:LYS:HD3	3:C:284:ALA:HA	1.90	0.54
3:F:290:ILE:HA	3:F:293:LEU:HD13	1.89	0.54
3:J:197:LEU:O	3:J:411:ARG:NH1	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:263:ALA:HB3	3:P:266:ASN:HB2	1.90	0.54
2:Y:202:ARG:HH22	1:v:194:GLN:HB2	1.74	0.53
1:t:148:LEU:HD21	1:t:171:LEU:HD13	1.90	0.53
4:0:32:ILE:HD12	4:1:46:ILE:HG23	1.90	0.53
8:BI:25:THR:OG1	8:BI:26:GLN:NE2	2.42	0.53
2:Y:196:VAL:HB	2:Y:222:VAL:HG12	1.90	0.53
2:i:173:LEU:HD12	2:i:194:LEU:HD23	1.90	0.53
1:AJ:158:SER:HB3	1:AJ:163:GLN:HE22	1.73	0.53
3:A:281:LYS:NZ	3:B:218:GLU:OE2	2.39	0.53
3:D:47:ASP:N	3:D:47:ASP:OD1	2.41	0.53
3:H:384:ASP:HB3	3:I:454:LEU:HD21	1.91	0.53
3:O:471:GLY:HA3	3:O:510:VAL:HG22	1.91	0.53
2:X:185:GLN:HB3	2:X:197:ALA:HB3	1.89	0.53
2:j:262:ARG:NH2	2:j:293:LEU:O	2.41	0.53
1:t:30:GLU:HA	1:t:33:ASN:HD21	1.72	0.53
1:AD:24:LEU:HB3	1:AD:27:LEU:HD21	1.90	0.53
2:f:326:VAL:HA	2:f:358:ALA:HB3	1.89	0.53
1:AJ:39:LEU:HD22	1:AJ:44:ILE:HD11	1.90	0.53
3:F:482:GLN:HB2	3:F:499:TYR:HB3	1.88	0.53
3:G:57:VAL:HG12	3:G:99:ILE:HB	1.88	0.53
3:J:252:MET:HG3	3:J:256:GLU:HG3	1.91	0.53
8:BJ:20:VAL:HB	8:BJ:23:LEU:HD22	1.89	0.53
8:BL:63:ASN:HD22	8:BR:76:ILE:HG22	1.72	0.53
2:m:185:GLN:HB3	2:m:197:ALA:HB3	1.91	0.53
7:AN:31:ASP:HB2	7:AN:34:LEU:HD23	1.90	0.53
7:AR:58:PRO:HB3	8:AW:23:LEU:HD11	1.91	0.53
3:O:114:LEU:HD21	3:O:163:ALA:HB1	1.91	0.53
8:BG:69:LYS:NZ	8:BA:52:SER:O	2.38	0.53
8:BG:78:ASN:OD1	8:BH:80:ARG:NH1	2.42	0.53
2:c:316:ARG:HH21	2:c:318:ASN:HD21	1.56	0.53
2:k:356:GLN:NE2	2:l:310:GLN:OE1	2.41	0.53
6:9:3:ASP:OD1	6:9:3:ASP:N	2.42	0.53
7:AO:31:ASP:N	7:AO:31:ASP:OD1	2.40	0.53
3:G:125:PHE:HD1	3:H:141:ASP:HB2	1.74	0.53
3:G:493:ILE:HG22	3:G:496:LEU:HB2	1.89	0.53
3:K:404:VAL:HG12	3:K:447:LEU:HD13	1.89	0.53
3:O:399:VAL:HG21	3:P:440:THR:HA	1.89	0.53
8:BK:15:LYS:NZ	8:BF:32:ASP:OD1	2.35	0.53
8:BL:27:VAL:HG12	8:BL:50:LYS:HG3	1.90	0.53
8:BC:21:ASP:OD1	8:BC:21:ASP:N	2.28	0.53
8:BR:22:ASN:HB3	8:BR:25:THR:HB	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:94:LEU:HD12	1:AD:95:VAL:HG13	1.90	0.53
2:E:364:ASP:HA	2:E:390:SER:HB2	1.91	0.53
2:Y:229:ASN:HD21	2:Y:248:ILE:H	1.55	0.53
1:q:179:ASP:OD1	1:q:179:ASP:N	2.34	0.53
4:0:167:LEU:HA	4:0:170:VAL:HG22	1.91	0.53
3:I:305:GLU:HA	3:I:374:LEU:HA	1.90	0.53
3:M:323:THR:HB	3:M:356:VAL:HG12	1.90	0.53
3:N:415:ARG:NH2	3:N:423:GLU:OE2	2.37	0.53
1:AC:164:ILE:HG22	1:AC:187:LEU:HD21	1.91	0.53
2:a:256:PRO:HG2	2:a:289:VAL:HG12	1.91	0.53
2:m:187:LEU:HD21	2:m:253:PRO:HB2	1.90	0.53
1:s:168:LYS:HG3	1:s:183:ILE:HD13	1.91	0.53
3:D:543:ASP:OD1	3:D:543:ASP:N	2.42	0.53
3:M:430:ASP:OD2	3:M:509:ARG:NH2	2.41	0.53
8:BO:63:ASN:HD22	8:BU:76:ILE:HG22	1.74	0.53
2:h:262:ARG:NH1	2:h:295:ASP:OD1	2.38	0.53
2:j:264:ARG:NE	2:j:296:ASP:OD1	2.42	0.53
1:o:84:GLU:OE1	1:p:112:ARG:NH1	2.38	0.53
1:u:24:LEU:HD22	1:v:29:GLN:HE21	1.74	0.53
1:w:133:ASP:OD1	1:w:133:ASP:N	2.42	0.53
6:8:10:LYS:NZ	6:8:77:GLN:OE1	2.33	0.53
3:B:327:GLY:HA3	3:B:352:PHE:HA	1.91	0.53
3:G:338:SER:HB2	3:G:344:ILE:HD11	1.91	0.53
3:M:311:VAL:HG12	3:M:368:VAL:HG22	1.90	0.53
3:C:387:ARG:NH2	3:D:449:GLU:OE2	2.42	0.53
3:F:178:GLN:HG2	3:G:220:GLN:HE21	1.74	0.53
1:AH:112:ARG:HG2	1:AI:129:HIS:HE1	1.72	0.52
2:T:356:GLN:NE2	2:U:310:GLN:OE1	2.42	0.52
2:i:174:ASP:OD2	2:i:174:ASP:N	2.40	0.52
2:k:246:TYR:OH	2:k:296:ASP:OD1	2.27	0.52
1:t:25:LYS:H	1:u:29:GLN:HE21	1.57	0.52
1:v:184:SER:HB2	1:w:173:ASN:HD21	1.74	0.52
3:B:410:ILE:HG22	3:B:428:ILE:HG22	1.91	0.52
3:P:41:SER:OG	3:P:67:LYS:NZ	2.42	0.52
8:BM:28:THR:HA	8:BM:31:LEU:HG	1.91	0.52
1:AD:37:ALA:HB2	1:AL:69:VAL:HG22	1.91	0.52
1:t:168:LYS:NZ	1:t:180:TYR:O	2.41	0.52
1:y:99:ARG:NH2	1:y:138:GLU:OE2	2.42	0.52
1:AJ:102:LYS:HE2	1:AK:134:ILE:HB	1.89	0.52
4:4:29:LYS:HD2	4:4:158:ALA:HB2	1.91	0.52
3:C:360:GLU:HB2	3:D:485:PRO:HG3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:39:ASP:H	3:I:69:THR:HB	1.72	0.52
3:J:426:LEU:HD13	3:J:469:VAL:HG21	1.90	0.52
3:P:543:ASP:OD1	3:P:543:ASP:N	2.42	0.52
8:BQ:13:SER:OG	8:BQ:61:GLN:NE2	2.41	0.52
1:AD:101:GLU:OE1	1:AL:99:ARG:NH1	2.41	0.52
1:AG:28:ASP:OD1	1:AG:28:ASP:N	2.40	0.52
2:d:245:TYR:OH	2:d:353:ARG:NH1	2.42	0.52
8:AX:31:LEU:HA	8:AX:34:LEU:HB2	1.89	0.52
3:A:36:VAL:HG22	3:A:71:ASN:HD22	1.75	0.52
3:A:274:ASP:N	3:A:274:ASP:OD1	2.38	0.52
3:C:274:ASP:N	3:C:274:ASP:OD1	2.41	0.52
3:D:211:ILE:HA	3:D:214:LEU:HB2	1.90	0.52
3:K:363:LYS:NZ	3:K:364:GLN:O	2.43	0.52
3:M:493:ILE:HG13	3:M:496:LEU:HB2	1.91	0.52
8:BA:23:LEU:HD21	8:BA:54:TYR:HA	1.91	0.52
1:AF:29:GLN:O	1:AF:33:ASN:ND2	2.43	0.52
2:T:364:ASP:N	2:T:364:ASP:OD1	2.40	0.52
1:AL:39:LEU:HD22	1:AL:44:ILE:HD11	1.92	0.52
2:c:173:LEU:HD12	2:c:194:LEU:HD23	1.91	0.52
2:i:245:TYR:OH	2:i:353:ARG:NH1	2.43	0.52
1:o:30:GLU:HA	1:o:33:ASN:HD21	1.74	0.52
4:0:5:ILE:HG21	7:AN:41:ALA:HA	1.91	0.52
4:2:25:THR:OG1	4:2:26:CYS:N	2.42	0.52
4:4:178:SER:HA	4:4:181:LEU:HG	1.91	0.52
8:AX:16:PHE:HB3	8:AX:57:TYR:HE1	1.73	0.52
3:F:379:VAL:HG11	3:G:458:ILE:HD11	1.90	0.52
3:J:192:ASP:OD1	3:J:192:ASP:N	2.32	0.52
8:BD:9:LEU:HD12	8:BD:65:VAL:HG23	1.91	0.52
1:AB:147:HIS:HB3	1:AC:173:ASN:HB2	1.91	0.52
2:f:245:TYR:OH	2:f:353:ARG:NH1	2.43	0.52
2:k:299:ALA:O	2:k:346:TYR:OH	2.27	0.52
1:s:20:ASP:N	1:s:20:ASP:OD1	2.41	0.52
8:AY:66:LYS:HA	8:AY:69:LYS:HG2	1.91	0.52
3:C:432:ASN:HD21	3:C:449:GLU:HG2	1.75	0.52
3:C:433:ASP:OD1	3:C:433:ASP:N	2.42	0.52
3:K:114:LEU:HD13	3:K:117:VAL:HB	1.92	0.52
3:K:114:LEU:HD21	3:K:163:ALA:HB1	1.90	0.52
1:AA:146:VAL:HB	1:AA:178:VAL:HG12	1.92	0.52
1:AC:134:ILE:HG23	1:AL:105:LEU:HD23	1.90	0.52
1:AH:152:ALA:HB3	1:AH:187:LEU:HD22	1.90	0.52
2:Z:185:GLN:HB3	2:Z:197:ALA:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AL:180:TYR:HD2	2:f:363:ASP:HB3	1.74	0.52
2:c:246:TYR:OH	2:c:296:ASP:OD2	2.26	0.52
2:e:263:GLN:NE2	2:e:295:ASP:OD1	2.43	0.52
2:m:310:GLN:O	2:m:338:ARG:NH1	2.42	0.52
1:r:147:HIS:HB3	1:s:173:ASN:HB2	1.92	0.52
1:t:22:ASP:HA	1:t:59:THR:HA	1.92	0.52
1:y:71:TRP:HA	1:y:74:THR:HG22	1.91	0.52
7:AR:86:THR:HA	7:AR:89:ARG:HB3	1.92	0.52
3:A:387:ARG:NH2	3:B:449:GLU:O	2.42	0.52
3:I:103:ASP:OD2	3:I:105:SER:OG	2.27	0.52
3:L:289:PHE:HA	3:L:292:MET:HE2	1.91	0.52
3:M:314:ASN:HB2	3:M:365:ALA:HB3	1.92	0.52
8:BB:66:LYS:NZ	8:BG:80:ARG:O	2.42	0.52
1:AH:194:GLN:HB2	2:j:202:ARG:HH22	1.75	0.52
1:AI:156:ARG:NH2	1:AI:192:ASP:OD1	2.42	0.52
3:Q:105:SER:HA	3:P:58:ILE:HD13	1.90	0.52
2:Y:268:SER:OG	2:Y:269:LYS:N	2.43	0.52
1:s:114:GLU:HB3	1:s:128:VAL:HG22	1.91	0.52
1:AK:22:ASP:OD1	1:AK:22:ASP:N	2.42	0.52
7:AO:63:ASP:HB3	7:AO:66:GLU:HG2	1.92	0.52
3:G:274:ASP:OD1	3:G:274:ASP:N	2.40	0.52
3:I:414:PRO:HB3	3:I:424:MET:HG2	1.92	0.52
3:G:409:MET:HB3	3:G:429:GLU:HG3	1.91	0.52
3:H:376:GLN:HE21	3:I:459:ALA:HA	1.75	0.52
3:K:187:ASN:HB2	3:K:298:ASP:HB2	1.92	0.52
2:Z:244:ALA:H	2:Z:265:ASN:HD21	1.57	0.52
2:k:196:VAL:HB	2:k:222:VAL:HG12	1.92	0.52
1:AJ:112:ARG:NH1	1:AK:110:GLU:OE2	2.43	0.52
3:A:107:MET:HE2	3:A:151:GLY:HA2	1.92	0.52
3:L:301:LYS:O	3:M:460:ARG:NH2	2.41	0.52
2:l:247:ARG:NH1	2:l:348:ARG:O	2.42	0.52
2:l:274:VAL:HG22	2:l:278:LYS:HE2	1.92	0.52
1:o:102:LYS:NZ	1:o:134:ILE:O	2.32	0.52
7:AQ:26:ILE:HD11	7:AQ:32:ARG:HB2	1.92	0.52
3:A:97:GLN:HE21	3:B:137:PRO:HD2	1.75	0.52
3:B:384:ASP:HB3	3:B:409:MET:HG3	1.91	0.52
8:BP:17:ASP:OD1	8:BP:57:TYR:OH	2.28	0.52
3:Q:138:LEU:HD22	3:Q:149:VAL:HG22	1.92	0.51
2:c:256:PRO:HG2	2:c:289:VAL:HG12	1.91	0.51
2:d:304:GLU:OE1	2:d:316:ARG:NH1	2.40	0.51
2:d:369:ARG:HG2	2:d:381:MET:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:304:GLU:OE1	2:i:316:ARG:NH1	2.41	0.51
1:AK:24:LEU:HB2	1:AK:58:ILE:HG22	1.92	0.51
3:D:387:ARG:HH12	3:F:450:VAL:HG12	1.75	0.51
3:F:57:VAL:HG22	3:F:99:ILE:HB	1.93	0.51
3:K:97:GLN:HE21	3:L:137:PRO:HD2	1.75	0.51
3:O:274:ASP:OD1	3:O:274:ASP:N	2.43	0.51
8:BO:56:LEU:HD12	8:BU:9:LEU:HD11	1.92	0.51
2:h:268:SER:OG	2:h:269:LYS:N	2.43	0.51
4:4:183:LEU:HB2	4:4:185:MET:HG3	1.92	0.51
3:B:320:ARG:HD2	3:B:359:LEU:HD11	1.92	0.51
3:B:433:ASP:N	3:B:433:ASP:OD1	2.43	0.51
3:J:90:LEU:HD12	3:J:103:ASP:HA	1.92	0.51
1:AD:20:ASP:N	1:AD:60:VAL:O	2.43	0.51
2:T:326:VAL:HA	2:T:358:ALA:HB3	1.91	0.51
2:h:224:ASN:HB2	2:h:227:GLU:HG3	1.93	0.51
2:m:173:LEU:HD23	2:m:176:LEU:HD21	1.92	0.51
1:u:39:LEU:HD22	1:u:44:ILE:HD11	1.92	0.51
1:v:148:LEU:HD12	1:v:183:ILE:HG12	1.91	0.51
1:AJ:99:ARG:NH2	1:AJ:138:GLU:OE1	2.43	0.51
4:2:185:MET:HB3	4:2:188:MET:HG3	1.93	0.51
3:K:97:GLN:HE22	3:L:139:ARG:HE	1.56	0.51
8:BG:56:LEU:HD12	8:BM:9:LEU:HD11	1.91	0.51
1:AL:196:GLN:OE1	2:g:179:GLN:N	2.43	0.51
2:a:246:TYR:OH	2:a:296:ASP:OD1	2.28	0.51
2:a:356:GLN:NE2	2:b:310:GLN:OE1	2.42	0.51
1:p:139:ASN:HB2	1:p:141:ARG:HG2	1.91	0.51
3:B:305:GLU:HA	3:B:374:LEU:HA	1.92	0.51
3:I:274:ASP:N	3:I:274:ASP:OD1	2.38	0.51
3:J:543:ASP:OD1	3:J:543:ASP:N	2.43	0.51
3:M:327:GLY:HA3	3:M:352:PHE:HA	1.91	0.51
8:BH:26:GLN:HA	8:BH:29:GLU:HG2	1.93	0.51
1:AE:37:ALA:HB2	1:AF:69:VAL:HG22	1.93	0.51
2:V:310:GLN:O	2:V:338:ARG:NH1	2.43	0.51
3:G:543:ASP:N	3:G:543:ASP:OD1	2.41	0.51
3:H:33:SER:OG	3:H:34:GLY:N	2.42	0.51
3:J:107:MET:HE2	3:J:151:GLY:HA2	1.91	0.51
2:g:344:ASP:OD2	2:g:344:ASP:N	2.44	0.51
2:l:187:LEU:HD12	2:l:188:PRO:HD2	1.93	0.51
1:s:99:ARG:NH2	1:s:138:GLU:OE2	2.44	0.51
1:t:141:ARG:NH1	1:u:141:ARG:O	2.43	0.51
1:u:156:ARG:NH2	1:u:190:ARG:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:177:ASP:OD1	1:v:177:ASP:N	2.44	0.51
4:2:17:LEU:HA	4:2:20:ILE:HB	1.93	0.51
7:AQ:71:GLN:HB2	8:BB:75:ILE:HD11	1.92	0.51
3:G:322:GLY:HA3	3:G:499:TYR:HA	1.92	0.51
3:I:543:ASP:OD1	3:I:543:ASP:N	2.43	0.51
1:AB:25:LYS:H	1:AC:29:GLN:NE2	2.08	0.51
1:AB:39:LEU:HD22	1:AB:44:ILE:HD11	1.93	0.51
2:e:174:ASP:OD1	2:e:174:ASP:N	2.38	0.51
3:B:80:LEU:HD23	3:B:84:LEU:HD23	1.93	0.51
3:K:338:SER:HB2	3:K:344:ILE:HD11	1.91	0.51
8:BA:26:GLN:HB3	8:BA:50:LYS:HD2	1.93	0.51
8:BT:22:ASN:HB2	8:BT:25:THR:HB	1.92	0.51
1:AF:171:LEU:HD11	1:AF:183:ILE:HG21	1.93	0.51
2:T:333:ASP:OD1	2:T:333:ASP:N	2.43	0.51
2:h:225:GLU:HG3	2:h:250:PHE:HD2	1.75	0.51
1:r:144:LYS:NZ	1:s:176:ALA:O	2.44	0.51
5:5:39:SER:OG	5:5:40:GLY:N	2.42	0.51
3:O:200:GLN:HE22	3:O:202:MET:HB2	1.75	0.51
2:T:310:GLN:HB2	2:T:312:LEU:HD23	1.92	0.51
2:U:256:PRO:HG2	2:U:289:VAL:HG12	1.92	0.51
2:n:260:LEU:HB2	2:n:291:ILE:HD11	1.93	0.51
3:D:482:GLN:HB3	3:D:499:TYR:HB3	1.92	0.51
3:J:46:PHE:HA	3:J:49:MET:HE3	1.93	0.51
3:P:326:SER:OG	3:P:342:SER:OG	2.29	0.51
2:V:356:GLN:NE2	2:W:310:GLN:OE1	2.40	0.51
2:Z:187:LEU:HD23	2:Z:285:TYR:HB2	1.93	0.51
1:AL:39:LEU:HB3	1:AL:44:ILE:HG13	1.93	0.51
2:d:364:ASP:OD1	2:d:364:ASP:N	2.44	0.51
1:y:69:VAL:HG22	1:z:37:ALA:HB2	1.92	0.51
4:1:75:PHE:HZ	4:1:92:VAL:HG23	1.76	0.51
3:A:118:SER:OG	3:A:119:LEU:N	2.43	0.51
3:P:189:PHE:HA	3:P:276:ASN:HD21	1.75	0.51
2:T:191:ASP:OD1	2:T:191:ASP:N	2.42	0.50
2:X:381:MET:HE2	2:X:387:TYR:HB2	1.94	0.50
2:Z:274:VAL:HG22	2:Z:278:LYS:HE2	1.93	0.50
1:AJ:64:ASP:OD2	1:AJ:64:ASP:N	2.44	0.50
3:A:440:THR:O	3:A:443:SER:OG	2.29	0.50
3:B:338:SER:HB2	3:B:344:ILE:HD11	1.93	0.50
3:D:107:MET:HE2	3:D:151:GLY:HA2	1.92	0.50
3:F:534:LEU:HD21	3:G:368:VAL:HG11	1.93	0.50
1:AC:24:LEU:HD13	1:AC:27:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AF:43:ASN:ND2	2:n:206:TRP:O	2.38	0.50
2:S:331:LEU:HG	2:S:361:LEU:HD13	1.93	0.50
3:G:309:TRP:HB2	3:G:512:MET:HB2	1.93	0.50
3:L:197:LEU:O	3:L:411:ARG:NH1	2.43	0.50
3:P:432:ASN:HD21	3:P:449:GLU:HB2	1.77	0.50
8:BB:36:ALA:O	8:BM:5:TRP:NE1	2.43	0.50
8:BH:36:ALA:O	8:BS:5:TRP:NE1	2.32	0.50
1:AH:114:GLU:HB3	1:AH:128:VAL:HG22	1.94	0.50
1:AH:177:ASP:N	1:AH:177:ASP:OD2	2.45	0.50
2:X:369:ARG:HG2	2:X:381:MET:HA	1.93	0.50
1:u:28:ASP:H	1:u:31:GLN:HB2	1.76	0.50
1:u:177:ASP:N	1:u:177:ASP:OD1	2.43	0.50
4:2:173:ASP:OD1	4:2:173:ASP:N	2.44	0.50
8:BP:20:VAL:HG11	8:BP:23:LEU:HD23	1.93	0.50
1:AD:147:HIS:HB3	1:AI:173:ASN:HB2	1.93	0.50
1:AF:148:LEU:HB2	1:AF:183:ILE:HD12	1.94	0.50
1:AG:177:ASP:N	1:AG:177:ASP:OD1	2.43	0.50
2:V:245:TYR:OH	2:V:353:ARG:NH1	2.44	0.50
1:p:191:SER:OG	1:p:192:ASP:N	2.44	0.50
4:0:173:ASP:OD1	4:0:173:ASP:N	2.43	0.50
4:4:171:VAL:HG23	6:9:15:VAL:HG13	1.94	0.50
8:AY:68:PHE:HD1	8:AY:71:ILE:HD11	1.77	0.50
3:F:387:ARG:HE	3:F:389:PHE:HE1	1.60	0.50
3:H:62:MET:SD	3:H:65:ARG:NH1	2.85	0.50
3:J:419:ASP:HB2	3:J:421:GLN:HE22	1.76	0.50
3:M:399:VAL:HG21	3:N:440:THR:HA	1.91	0.50
3:P:141:ASP:HB3	3:P:144:LYS:HB2	1.92	0.50
8:BB:26:GLN:HA	8:BB:29:GLU:HG2	1.92	0.50
1:AC:30:GLU:HA	1:AC:33:ASN:HD21	1.77	0.50
2:U:299:ALA:O	2:U:346:TYR:OH	2.30	0.50
2:Z:209:GLN:HE22	1:x:195:LEU:HD22	1.75	0.50
2:f:304:GLU:OE1	2:f:316:ARG:NH1	2.44	0.50
1:x:135:ASP:OD1	1:y:102:LYS:NZ	2.42	0.50
4:2:97:ASP:HA	4:2:100:ARG:HE	1.77	0.50
4:2:164:TYR:HA	4:2:167:LEU:HD23	1.93	0.50
3:C:379:VAL:HG11	3:D:458:ILE:HD11	1.94	0.50
3:H:138:LEU:HD22	3:H:149:VAL:HG12	1.92	0.50
3:H:327:GLY:HA3	3:H:352:PHE:HA	1.92	0.50
3:M:58:ILE:HG23	3:M:100:TYR:HA	1.94	0.50
8:BG:77:GLN:OE1	8:BH:80:ARG:NH1	2.45	0.50
8:BU:40:ASP:HB3	8:BU:43:LEU:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:202:ARG:HH22	1:p:194:GLN:HB2	1.76	0.50
2:g:372:GLN:HB2	3:G:35:PHE:HD1	1.77	0.50
1:w:114:GLU:OE1	1:w:118:GLN:NE2	2.44	0.50
8:AY:7:GLY:H	8:AY:10:ASP:HB2	1.76	0.50
3:I:522:LEU:HD12	3:J:512:MET:HE1	1.92	0.50
3:O:384:ASP:HB3	3:O:409:MET:HG3	1.94	0.50
3:P:58:ILE:HG23	3:P:100:TYR:HA	1.93	0.50
1:AG:129:HIS:HE1	1:AK:112:ARG:HG2	1.75	0.50
2:g:369:ARG:NH1	2:g:381:MET:SD	2.85	0.50
1:q:148:LEU:HD21	1:q:171:LEU:HD22	1.93	0.50
1:s:30:GLU:HA	1:s:33:ASN:HD21	1.75	0.50
7:AO:49:GLN:HG3	7:AO:53:ASN:HD21	1.76	0.50
3:C:305:GLU:HA	3:C:374:LEU:HA	1.94	0.50
3:H:305:GLU:HA	3:H:374:LEU:HA	1.93	0.50
3:J:178:GLN:OE1	3:J:281:LYS:NZ	2.45	0.50
8:BO:68:PHE:HA	8:BO:71:ILE:HD12	1.94	0.50
1:AG:168:LYS:NZ	1:AG:183:ILE:O	2.45	0.50
2:E:228:GLU:HG2	2:E:283:MET:HE1	1.93	0.50
2:U:263:GLN:NE2	2:U:295:ASP:OD1	2.44	0.50
2:Y:363:ASP:OD1	2:Y:363:ASP:N	2.44	0.50
2:i:247:ARG:NH1	2:i:347:TYR:O	2.45	0.50
2:l:364:ASP:N	2:l:364:ASP:OD1	2.45	0.50
1:s:167:ILE:HG21	1:s:185:VAL:HG11	1.94	0.50
4:O:72:TYR:HA	4:O:75:PHE:HB2	1.94	0.50
6:8:3:ASP:HA	6:8:6:PHE:HB3	1.93	0.50
3:B:421:GLN:HG3	3:B:462:PRO:HA	1.94	0.50
3:G:384:ASP:HB3	3:G:409:MET:HG3	1.92	0.50
3:H:482:GLN:HB3	3:H:499:TYR:HB3	1.92	0.50
3:H:543:ASP:OD1	3:H:543:ASP:N	2.44	0.50
3:N:326:SER:OG	3:N:342:SER:OG	2.30	0.50
2:T:229:ASN:HD21	2:T:248:ILE:H	1.60	0.50
2:a:356:GLN:HE21	2:b:338:ARG:HD2	1.77	0.50
2:e:217:ASP:OD1	2:e:217:ASP:N	2.42	0.50
2:l:363:ASP:OD1	2:l:363:ASP:N	2.41	0.50
4:4:43:LEU:HB3	4:4:46:ILE:HG13	1.93	0.50
8:AX:72:ASP:OD2	8:AX:72:ASP:N	2.45	0.50
8:AY:28:THR:HA	8:AY:31:LEU:HG	1.92	0.50
3:F:311:VAL:HG22	3:F:368:VAL:HG22	1.94	0.50
3:J:274:ASP:OD1	3:J:274:ASP:N	2.39	0.50
3:K:327:GLY:HA3	3:K:352:PHE:HA	1.94	0.50
3:M:197:LEU:O	3:M:411:ARG:NH1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:361:LEU:O	1:o:168:LYS:NZ	2.41	0.49
2:R:229:ASN:HD21	2:R:248:ILE:H	1.59	0.49
2:S:299:ALA:O	2:S:346:TYR:OH	2.28	0.49
2:U:381:MET:N	2:U:381:MET:SD	2.85	0.49
2:j:385:HIS:NE2	3:J:69:THR:OG1	2.40	0.49
1:w:147:HIS:HA	1:w:182:ASN:HB3	1.94	0.49
4:4:77:ASP:OD2	4:4:77:ASP:N	2.43	0.49
3:H:394:ILE:HD11	3:J:340:ASN:HB3	1.95	0.49
3:H:415:ARG:NH2	3:H:423:GLU:OE2	2.42	0.49
3:K:176:GLY:O	3:L:220:GLN:NE2	2.44	0.49
3:K:419:ASP:HB2	3:K:421:GLN:HE22	1.77	0.49
3:L:51:LEU:HD21	3:M:87:GLN:HG2	1.92	0.49
3:N:404:VAL:HG22	3:N:447:LEU:HD13	1.94	0.49
1:AD:190:ARG:NH1	1:AD:191:SER:O	2.44	0.49
1:AE:39:LEU:HB3	1:AE:44:ILE:HG13	1.94	0.49
2:E:312:LEU:HD12	2:E:313:PRO:HD2	1.93	0.49
2:E:361:LEU:HD23	1:o:168:LYS:HE3	1.93	0.49
2:R:173:LEU:HD12	2:R:194:LEU:HD23	1.94	0.49
2:j:197:ALA:HA	2:j:223:ILE:HG22	1.94	0.49
2:n:245:TYR:OH	2:n:353:ARG:NH2	2.44	0.49
1:o:29:GLN:O	1:o:33:ASN:ND2	2.45	0.49
3:B:545:LYS:O	3:C:536:GLN:NE2	2.45	0.49
3:C:406:TYR:OH	3:C:448:PRO:O	2.24	0.49
3:D:328:SER:OG	3:D:342:SER:OG	2.25	0.49
3:F:391:THR:HG21	3:F:446:ALA:HB1	1.94	0.49
8:BV:20:VAL:HB	8:BV:23:LEU:HD23	1.95	0.49
2:R:217:ASP:OD1	2:R:217:ASP:N	2.44	0.49
1:AJ:35:VAL:HG12	1:AJ:77:LEU:HD13	1.93	0.49
4:4:215:LEU:HD23	6:9:83:LEU:HD11	1.93	0.49
3:A:49:MET:HE1	3:A:81:LEU:HB3	1.93	0.49
1:AC:128:VAL:O	1:AL:112:ARG:NH2	2.46	0.49
1:AF:39:LEU:HD22	1:AF:44:ILE:HD11	1.94	0.49
1:AH:35:VAL:HG12	1:AH:77:LEU:HD13	1.94	0.49
3:J:338:SER:HB3	3:J:344:ILE:HD11	1.93	0.49
3:L:394:ILE:HD11	3:N:340:ASN:HB3	1.94	0.49
3:O:393:LEU:HD23	3:O:400:ALA:HB3	1.94	0.49
8:BJ:9:LEU:HD22	8:BJ:65:VAL:HG23	1.93	0.49
8:BM:63:ASN:HD22	8:BS:76:ILE:HG22	1.77	0.49
1:AL:28:ASP:OD1	1:AL:28:ASP:N	2.46	0.49
2:l:183:ARG:NH1	2:l:203:ASP:OD2	2.46	0.49
1:q:23:LEU:HD11	1:q:72:ILE:HG13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:129:HIS:HE1	1:x:112:ARG:HG2	1.77	0.49
1:z:155:GLU:OE2	1:z:190:ARG:NE	2.41	0.49
7:AQ:31:ASP:OD2	7:AQ:31:ASP:N	2.45	0.49
3:F:331:ILE:HD12	3:F:335:LEU:HD11	1.95	0.49
3:G:406:TYR:OH	3:G:448:PRO:O	2.24	0.49
3:P:404:VAL:HG12	3:P:447:LEU:HD13	1.94	0.49
8:BJ:33:LYS:NZ	8:BJ:43:LEU:O	2.45	0.49
2:R:299:ALA:O	2:R:346:TYR:OH	2.28	0.49
2:S:196:VAL:HB	2:S:222:VAL:HG12	1.94	0.49
7:AR:69:ILE:HG22	7:AR:73:MET:HE1	1.93	0.49
3:A:34:GLY:HA2	3:A:73:GLU:HA	1.94	0.49
3:A:268:LYS:HE3	3:A:281:LYS:HD3	1.93	0.49
3:B:320:ARG:HB2	3:B:359:LEU:HG	1.94	0.49
3:K:314:ASN:HB3	3:K:365:ALA:HB3	1.93	0.49
3:L:408:THR:OG1	3:L:430:ASP:OD1	2.29	0.49
3:O:383:PHE:HB3	3:O:410:ILE:HG23	1.94	0.49
3:P:433:ASP:OD1	3:P:433:ASP:N	2.41	0.49
2:R:229:ASN:ND2	2:R:248:ILE:O	2.45	0.49
1:AL:159:PRO:HB2	1:AL:162:HIS:HD2	1.78	0.49
2:d:246:TYR:OH	2:d:296:ASP:OD1	2.31	0.49
1:r:148:LEU:HD21	1:r:171:LEU:HD22	1.95	0.49
4:4:150:TYR:O	4:4:154:GLU:HG2	2.13	0.49
8:AV:53:GLU:HG2	8:BB:9:LEU:HD13	1.95	0.49
3:D:178:GLN:O	3:F:223:GLY:N	2.46	0.49
1:AB:35:VAL:HG23	1:AB:77:LEU:HD11	1.93	0.49
1:AE:26:GLY:N	1:AE:56:TYR:O	2.46	0.49
2:c:356:GLN:NE2	2:d:310:GLN:OE1	2.34	0.49
2:g:196:VAL:HB	2:g:222:VAL:HG12	1.95	0.49
1:t:94:LEU:HD12	1:t:95:VAL:HG13	1.95	0.49
1:AK:191:SER:OG	1:AK:192:ASP:N	2.44	0.49
4:2:93:ASP:OD1	4:2:93:ASP:N	2.45	0.49
3:I:384:ASP:OD1	3:I:385:ASN:N	2.46	0.49
1:AA:165:SER:HB2	2:c:361:LEU:HD13	1.94	0.49
1:AD:135:ASP:OD1	1:AD:135:ASP:N	2.45	0.49
1:AD:177:ASP:N	1:AD:177:ASP:OD1	2.44	0.49
1:AE:105:LEU:HD23	1:AE:106:TYR:HD1	1.78	0.49
2:R:323:VAL:HG12	2:R:355:VAL:HG12	1.93	0.49
2:U:369:ARG:O	3:O:38:LYS:NZ	2.34	0.49
2:W:186:VAL:HG22	2:W:196:VAL:HG12	1.95	0.49
1:p:168:LYS:NZ	1:p:183:ILE:O	2.46	0.49
1:w:140:GLY:HA2	4:0:223:ALA:HB1	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:96:LEU:HD11	4:1:100:ARG:HH21	1.78	0.49
7:AN:63:ASP:OD1	7:AN:66:GLU:N	2.44	0.49
3:J:323:THR:OG1	3:J:324:SER:N	2.45	0.49
3:K:440:THR:O	3:K:443:SER:OG	2.30	0.49
8:AZ:15:LYS:HA	8:AZ:18:THR:HG22	1.95	0.49
8:BF:27:VAL:HG11	8:BF:54:TYR:HB2	1.94	0.49
2:E:366:LEU:HB2	2:E:388:PHE:HZ	1.78	0.49
2:d:304:GLU:HA	2:d:307:LEU:HG	1.94	0.49
2:j:173:LEU:HD12	2:j:194:LEU:HD23	1.95	0.49
2:n:316:ARG:HH21	2:n:318:ASN:HD21	1.59	0.49
2:n:363:ASP:OD1	2:n:363:ASP:N	2.45	0.49
1:v:159:PRO:HB2	1:v:162:HIS:HD2	1.78	0.49
5:5:64:PRO:HB2	5:5:160:MET:HE3	1.94	0.49
3:K:197:LEU:O	3:K:411:ARG:NH1	2.38	0.49
3:O:194:THR:HG21	3:P:200:GLN:HG3	1.95	0.49
8:BK:56:LEU:HD12	8:BQ:76:ILE:HD12	1.94	0.49
1:AA:36:ILE:HG23	1:z:69:VAL:HG21	1.94	0.48
2:W:327:ILE:HD12	2:W:359:ILE:HG12	1.94	0.48
2:h:333:ASP:OD1	2:h:333:ASP:N	2.45	0.48
1:t:99:ARG:NH1	1:u:101:GLU:OE1	2.45	0.48
4:2:45:GLN:H	4:2:46:ILE:HD12	1.78	0.48
4:3:82:PHE:HD2	4:3:88:LEU:HG	1.78	0.48
6:8:37:GLN:HE21	6:8:43:GLN:HA	1.77	0.48
3:B:182:VAL:HG11	3:C:297:LEU:HD21	1.95	0.48
3:J:311:VAL:HG12	3:J:368:VAL:HG22	1.95	0.48
3:L:42:LEU:HD12	3:L:66:LYS:HB2	1.94	0.48
8:BN:9:LEU:HD12	8:BN:65:VAL:HG23	1.95	0.48
8:BI:58:ARG:NH1	8:BI:61:GLN:OE1	2.46	0.48
1:AE:94:LEU:HD11	6:7:66:TRP:HZ2	1.79	0.48
2:U:213:ARG:NE	2:U:215:ASP:OD2	2.44	0.48
2:Z:213:ARG:HD3	1:w:201:PRO:HB3	1.96	0.48
2:d:247:ARG:NH1	2:d:348:ARG:O	2.45	0.48
2:g:356:GLN:NE2	2:h:310:GLN:OE1	2.46	0.48
2:i:221:ARG:HD2	2:j:182:GLU:HG2	1.95	0.48
1:s:184:SER:HB2	1:t:173:ASN:HD22	1.78	0.48
3:A:222:LEU:HD23	3:A:223:GLY:H	1.78	0.48
3:G:394:ILE:HD11	3:I:340:ASN:HB3	1.94	0.48
3:L:116:ASN:HB3	3:L:254:LEU:HD13	1.94	0.48
3:M:108:ARG:HB2	3:M:156:VAL:HG21	1.95	0.48
3:M:308:LEU:HD11	3:M:428:ILE:HD13	1.95	0.48
8:BI:52:SER:OG	8:BO:66:LYS:NZ	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:194:GLN:OE1	2:f:202:ARG:NH2	2.46	0.48
1:AF:34:GLU:OE2	1:AJ:73:LYS:NZ	2.45	0.48
2:h:232:ILE:HG21	2:h:282:LEU:HD13	1.95	0.48
7:AR:26:ILE:HD11	7:AR:29:LEU:HD23	1.95	0.48
3:A:431:GLY:HA2	3:A:450:VAL:HG23	1.95	0.48
3:C:116:ASN:ND2	3:C:170:ASN:O	2.43	0.48
3:D:283:THR:H	3:D:286:GLN:HE21	1.61	0.48
3:F:360:GLU:OE1	3:G:483:SER:OG	2.31	0.48
3:G:315:LYS:HA	3:G:364:GLN:HA	1.95	0.48
3:O:482:GLN:HB3	3:O:499:TYR:HB3	1.95	0.48
2:X:229:ASN:HD22	2:X:247:ARG:HE	1.62	0.48
1:AL:98:PRO:HA	1:AL:101:GLU:HG2	1.94	0.48
2:b:179:GLN:N	1:y:196:GLN:OE1	2.46	0.48
2:h:221:ARG:NH1	2:i:182:GLU:OE2	2.47	0.48
1:o:99:ARG:HA	1:o:102:LYS:HE2	1.95	0.48
1:r:172:LYS:HD2	1:r:180:TYR:CZ	2.48	0.48
1:u:20:ASP:N	1:u:60:VAL:O	2.47	0.48
1:AJ:165:SER:HA	1:AJ:168:LYS:HG2	1.95	0.48
3:G:43[A]:ARG:HH22	3:G:61:LYS:HZ2	1.61	0.48
3:I:482:GLN:HB3	3:I:499:TYR:HB3	1.94	0.48
3:J:36:VAL:HA	3:J:71:ASN:HA	1.94	0.48
3:J:112:VAL:HG11	3:J:160:VAL:HG23	1.94	0.48
3:M:543:ASP:OD1	3:M:543:ASP:N	2.44	0.48
3:O:76:ASP:OD1	3:O:76:ASP:N	2.41	0.48
8:BC:58:ARG:NH1	8:BC:61:GLN:OE1	2.47	0.48
8:BA:17:ASP:OD1	8:BA:57:TYR:OH	2.32	0.48
2:S:371:PHE:HB3	2:S:379:ILE:HD13	1.94	0.48
2:f:363:ASP:OD1	2:f:363:ASP:N	2.45	0.48
4:0:47:PRO:O	4:0:51:THR:OG1	2.26	0.48
4:1:50:MET:HE1	7:AN:100:ARG:HD3	1.95	0.48
4:3:113:GLN:O	4:3:117:ASN:ND2	2.46	0.48
4:4:218:GLN:NE2	6:9:83:LEU:O	2.39	0.48
3:G:433:ASP:N	3:G:433:ASP:OD1	2.45	0.48
3:I:493:ILE:HG13	3:I:496:LEU:HB2	1.95	0.48
3:N:307:SER:OG	3:N:370:ARG:NH2	2.47	0.48
3:N:433:ASP:OD1	3:N:433:ASP:N	2.43	0.48
1:AG:147:HIS:HA	1:AG:182:ASN:HB3	1.94	0.48
2:E:364:ASP:OD1	2:E:364:ASP:N	2.47	0.48
2:V:262:ARG:HA	2:V:293:LEU:HD23	1.94	0.48
2:l:304:GLU:HA	2:l:307:LEU:HG	1.96	0.48
1:t:34:GLU:HG2	1:t:79:PRO:HG2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:114:GLU:HB3	1:v:128:VAL:HG22	1.96	0.48
3:B:543:ASP:OD1	3:B:543:ASP:N	2.43	0.48
3:F:252:MET:N	3:F:252:MET:SD	2.86	0.48
3:N:197:LEU:O	3:N:411:ARG:NH1	2.45	0.48
1:AA:134:ILE:HD12	1:AB:102:LYS:HD3	1.94	0.48
2:E:331:LEU:HG	2:E:335:GLU:HB2	1.96	0.48
2:R:202:ARG:NH1	1:o:191:SER:OG	2.46	0.48
2:b:335:GLU:OE2	2:b:338:ARG:NH2	2.45	0.48
2:d:256:PRO:HG2	2:d:289:VAL:HG12	1.96	0.48
2:g:190:ARG:NH1	2:g:286:ALA:O	2.45	0.48
1:s:114:GLU:HA	1:s:117:LEU:HB2	1.95	0.48
4:0:152:LEU:HD12	4:1:208:TRP:HB3	1.94	0.48
3:I:224:ASN:HA	3:I:289:PHE:HZ	1.78	0.48
3:N:382:ILE:HD13	3:N:411:ARG:HB2	1.96	0.48
1:AG:135:ASP:OD1	1:AG:135:ASP:N	2.45	0.48
2:l:340:ARG:HH22	1:AJ:163:GLN:HG2	1.78	0.48
1:v:168:LYS:NZ	1:v:180:TYR:O	2.38	0.48
1:w:39:LEU:HB2	1:w:44:ILE:HG13	1.96	0.48
3:F:541:SER:HB2	3:H:506:ASN:HD22	1.79	0.48
3:H:283:THR:H	3:H:286:GLN:HE21	1.62	0.48
3:H:406:TYR:OH	3:H:448:PRO:O	2.30	0.48
3:I:76:ASP:HA	3:I:77:PRO:HD3	1.77	0.48
1:AD:71:TRP:HA	1:AD:74:THR:HG22	1.96	0.48
1:AI:180:TYR:HD2	2:h:363:ASP:HB3	1.79	0.48
2:E:304:GLU:HA	2:E:307:LEU:HG	1.96	0.48
2:T:263:GLN:NE2	2:T:295:ASP:OD1	2.47	0.48
1:o:135:ASP:OD1	1:o:135:ASP:N	2.46	0.48
1:y:23:LEU:HG	1:y:24:LEU:HG	1.95	0.48
4:3:48:SER:OG	4:3:50:MET:N	2.47	0.48
3:F:323:THR:OG1	3:F:324:SER:N	2.47	0.48
3:J:281:LYS:NZ	3:K:218:GLU:OE2	2.44	0.48
3:N:522:LEU:HD23	3:N:522:LEU:HA	1.71	0.48
2:R:235:TRP:CD2	2:R:282:LEU:HD11	2.49	0.48
2:S:319:HIS:HE1	2:S:324:THR:HG23	1.79	0.48
4:4:127:GLU:OE2	3:C:43:ARG:NH2	2.47	0.48
7:AN:76:ASP:HA	7:AN:79:LEU:HG	1.96	0.48
7:AP:68:ALA:HA	7:AP:71:GLN:HB3	1.96	0.48
3:A:551:ARG:NH2	3:C:475:ASP:OD1	2.43	0.48
3:B:274:ASP:OD1	3:B:274:ASP:N	2.43	0.48
3:B:387:ARG:NH2	3:C:449:GLU:O	2.47	0.48
3:F:433:ASP:OD1	3:F:433:ASP:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:39:ASP:H	3:H:69:THR:HB	1.78	0.48
3:H:316:SER:O	3:H:362:LYS:NZ	2.41	0.48
3:N:216:GLN:HA	8:BF:3:THR:HG21	1.94	0.48
3:P:34:GLY:HA2	3:P:73:GLU:HA	1.96	0.48
2:Y:187:LEU:HD22	2:Y:285:TYR:HB2	1.96	0.47
2:b:381:MET:HE1	2:c:392:LEU:HD12	1.96	0.47
2:e:369:ARG:O	3:F:38:LYS:NZ	2.45	0.47
4:4:41:LEU:HA	4:4:198:LYS:HD3	1.96	0.47
6:8:25:VAL:HA	6:8:28:ILE:HG12	1.96	0.47
3:A:543:ASP:OD1	3:A:543:ASP:N	2.44	0.47
3:G:194:THR:HG22	3:G:203:VAL:HG22	1.94	0.47
3:K:415:ARG:NH2	3:K:423:GLU:OE2	2.44	0.47
3:N:338:SER:HB2	3:N:344:ILE:HD11	1.95	0.47
3:P:323:THR:OG1	3:P:324:SER:N	2.47	0.47
8:BF:17:ASP:OD1	8:BF:57:TYR:OH	2.29	0.47
2:b:299:ALA:O	2:b:346:TYR:OH	2.31	0.47
2:j:251:ASP:OD1	2:j:251:ASP:N	2.47	0.47
4:4:188:MET:HE3	4:4:189:SER:H	1.78	0.47
8:AX:20:VAL:HB	8:AX:23:LEU:HD22	1.95	0.47
3:C:543:ASP:OD1	3:C:543:ASP:N	2.41	0.47
3:H:185:LEU:HD23	3:H:187:ASN:H	1.79	0.47
3:H:311:VAL:HG12	3:H:368:VAL:HG22	1.95	0.47
3:H:331:ILE:HD12	3:H:335:LEU:HD11	1.96	0.47
3:K:483:SER:OG	3:K:484:ILE:N	2.47	0.47
3:K:543:ASP:OD1	3:K:543:ASP:N	2.43	0.47
3:L:432:ASN:HD21	3:L:449:GLU:HG2	1.79	0.47
3:M:541:SER:HB2	3:O:506:ASN:HD22	1.79	0.47
1:AA:36:ILE:HD13	1:AA:46:ALA:HB3	1.95	0.47
3:Q:35:PHE:HD1	2:X:372:GLN:HB2	1.78	0.47
2:S:217:ASP:N	2:S:217:ASP:OD1	2.41	0.47
2:d:217:ASP:N	2:d:217:ASP:OD2	2.43	0.47
2:h:363:ASP:OD1	2:h:363:ASP:N	2.47	0.47
2:n:327:ILE:HB	2:n:359:ILE:HA	1.96	0.47
4:0:21:ILE:HD12	4:0:25:THR:HG21	1.96	0.47
8:AY:40:ASP:HB2	8:AY:43:LEU:HB2	1.97	0.47
3:A:114:LEU:HD13	3:A:117:VAL:HG13	1.95	0.47
8:BJ:51:LEU:HD21	8:BO:67:VAL:HG21	1.96	0.47
2:R:262:ARG:HE	2:R:293:LEU:HD23	1.79	0.47
2:W:354:TYR:O	2:X:309:GLN:NE2	2.47	0.47
1:z:85:ILE:HB	1:z:107:SER:HB3	1.94	0.47
3:H:178:GLN:O	3:I:223:GLY:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:534:LEU:HD21	3:I:368:VAL:HG21	1.97	0.47
1:AA:34:GLU:OE2	1:z:73:LYS:NZ	2.48	0.47
2:R:221:ARG:NH1	2:S:182:GLU:OE2	2.47	0.47
2:Y:200:ASN:N	2:Y:200:ASN:OD1	2.48	0.47
2:i:356:GLN:NE2	2:j:310:GLN:OE1	2.43	0.47
1:v:30:GLU:HA	1:v:33:ASN:HD21	1.79	0.47
3:M:58:ILE:HD13	3:N:105:SER:HA	1.95	0.47
3:N:406:TYR:OH	3:N:448:PRO:O	2.32	0.47
3:O:303:HIS:HB3	3:O:374:LEU:HD12	1.96	0.47
8:BJ:28:THR:HA	8:BJ:31:LEU:HG	1.96	0.47
2:c:310:GLN:HB2	2:c:312:LEU:HD23	1.96	0.47
2:g:260:LEU:O	2:g:294:MET:N	2.44	0.47
2:h:191:ASP:N	2:h:191:ASP:OD1	2.45	0.47
1:p:39:LEU:HD22	1:p:44:ILE:HD11	1.96	0.47
1:y:39:LEU:HD22	1:y:44:ILE:HD11	1.95	0.47
4:1:85:ILE:HG21	7:AO:42:ILE:HD13	1.95	0.47
8:AW:32:ASP:N	8:AW:32:ASP:OD1	2.42	0.47
3:C:415:ARG:NH1	3:C:416:PHE:O	2.48	0.47
3:G:414:PRO:HA	3:G:424:MET:HA	1.97	0.47
3:K:433:ASP:OD1	3:K:433:ASP:N	2.47	0.47
3:N:323:THR:OG1	3:N:324:SER:N	2.47	0.47
3:O:415:ARG:NH2	3:O:423:GLU:OE2	2.37	0.47
1:AA:166:ASP:OD1	1:AA:166:ASP:N	2.46	0.47
1:AH:37:ALA:HB2	1:AI:69:VAL:HG22	1.96	0.47
1:AI:169:ARG:NH1	1:AI:180:TYR:OH	2.47	0.47
2:S:356:GLN:HB2	2:T:309:GLN:HE21	1.78	0.47
2:b:323:VAL:HG22	2:b:355:VAL:HG12	1.95	0.47
1:p:39:LEU:HB3	1:p:44:ILE:HG13	1.95	0.47
1:t:177:ASP:N	1:t:177:ASP:OD1	2.47	0.47
7:AP:89:ARG:NH1	7:AP:89:ARG:O	2.48	0.47
3:C:338:SER:HB2	3:C:344:ILE:HD11	1.95	0.47
3:D:327:GLY:HA3	3:D:352:PHE:HA	1.97	0.47
3:D:331:ILE:HD12	3:D:335:LEU:HD11	1.95	0.47
3:D:406:TYR:OH	3:D:448:PRO:O	2.26	0.47
3:F:543:ASP:OD1	3:F:543:ASP:N	2.42	0.47
3:G:387:ARG:HE	3:G:389:PHE:HE1	1.63	0.47
3:H:413:LEU:HB3	3:H:425:SER:HB2	1.97	0.47
3:I:383:PHE:HB3	3:I:410:ILE:HG23	1.96	0.47
3:K:118:SER:OG	3:K:119:LEU:N	2.47	0.47
3:K:322:GLY:HA3	3:K:499:TYR:HA	1.96	0.47
8:AZ:37:LYS:HD3	8:BK:8:TYR:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BG:26:GLN:HA	8:BG:29:GLU:HG2	1.96	0.47
8:BO:78:ASN:OD1	8:BP:80:ARG:NH1	2.43	0.47
2:e:310:GLN:O	2:e:338:ARG:NH1	2.48	0.47
2:j:364:ASP:OD1	2:j:364:ASP:N	2.47	0.47
1:v:151:LEU:HD13	1:w:120:MET:HE3	1.97	0.47
3:A:457:THR:HG23	3:P:375:THR:HG23	1.96	0.47
3:B:468:LEU:HD12	3:B:512:MET:HE1	1.95	0.47
3:D:180:ILE:HG13	3:F:293:LEU:HD21	1.97	0.47
3:F:60:SER:OG	3:F:61:LYS:N	2.46	0.47
3:F:179:LYS:N	3:F:282:GLY:O	2.43	0.47
3:J:301:LYS:O	3:K:460:ARG:NH2	2.36	0.47
3:O:472:TYR:N	3:O:509:ARG:O	2.48	0.47
8:BJ:40:ASP:HB3	8:BJ:43:LEU:HG	1.96	0.47
1:AC:135:ASP:OD1	1:AC:135:ASP:N	2.44	0.47
2:S:216:TYR:CZ	2:S:218:LYS:HB2	2.50	0.47
2:Y:307:LEU:HD11	2:Y:357:PHE:HE1	1.79	0.47
2:f:260:LEU:HD13	2:f:291:ILE:HG23	1.96	0.47
4:3:25:THR:OG1	4:3:26:CYS:N	2.48	0.47
4:4:14:SER:OG	7:AQ:90:LYS:NZ	2.48	0.47
4:4:25:THR:HG23	4:4:27:PHE:H	1.79	0.47
7:AO:50:THR:HA	7:AO:53:ASN:HD22	1.80	0.47
7:AR:30:ASP:OD1	7:AR:30:ASP:N	2.47	0.47
3:A:314:ASN:HB3	3:A:365:ALA:HB3	1.96	0.47
3:A:373:LEU:HD21	3:B:455:ILE:HD12	1.97	0.47
3:N:543:ASP:N	3:N:543:ASP:OD1	2.44	0.47
8:BN:63:ASN:HD22	8:BT:76:ILE:HG22	1.80	0.47
1:AC:66:THR:HG21	1:AL:197:ALA:HA	1.97	0.47
2:b:363:ASP:OD1	2:b:363:ASP:N	2.48	0.47
1:o:84:GLU:HB2	1:o:87:GLN:HG3	1.97	0.47
1:s:177:ASP:OD1	1:s:177:ASP:N	2.48	0.47
7:AO:66:GLU:HA	7:AO:69:ILE:HG12	1.97	0.47
3:F:323:THR:HB	3:F:356:VAL:HG12	1.96	0.47
3:H:220:GLN:O	3:H:264:ALA:N	2.48	0.47
3:K:198:ARG:HA	8:BM:3:THR:HG23	1.97	0.47
3:N:149:VAL:HG11	3:N:159:VAL:HG21	1.97	0.47
3:N:415:ARG:NH1	3:N:416:PHE:O	2.48	0.47
8:BL:56:LEU:HD11	8:BR:69:LYS:HA	1.97	0.47
8:BT:80:ARG:NH1	8:BS:78:ASN:OD1	2.48	0.47
1:AE:98:PRO:HD3	6:7:77:GLN:HE21	1.80	0.46
2:W:247:ARG:NH1	2:W:348:ARG:O	2.48	0.46
1:u:148:LEU:HD13	1:u:171:LEU:HD13	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:35:VAL:HG22	1:x:77:LEU:HD23	1.98	0.46
1:y:118:GLN:HE22	1:y:124:LEU:HA	1.79	0.46
3:A:384:ASP:HB3	3:B:454:LEU:HD21	1.97	0.46
3:C:537:SER:HB2	3:D:366:THR:HG21	1.97	0.46
3:G:429:GLU:OE1	3:G:452:ARG:NH2	2.48	0.46
3:J:537:SER:O	3:L:477:ASN:ND2	2.48	0.46
3:L:329:ILE:HD11	3:L:352:PHE:HD1	1.80	0.46
8:BG:69:LYS:HD3	8:BA:52:SER:HB3	1.95	0.46
8:BO:28:THR:HA	8:BO:31:LEU:HG	1.98	0.46
2:U:258:PHE:HB3	2:U:291:ILE:HG12	1.97	0.46
2:V:299:ALA:O	2:V:346:TYR:OH	2.33	0.46
2:l:206:TRP:O	1:AK:43:ASN:ND2	2.37	0.46
2:m:228:GLU:OE2	2:m:231:ARG:NH2	2.41	0.46
4:2:102:TYR:OH	4:2:150:TYR:OH	2.33	0.46
6:7:11:ALA:HA	6:7:14:LEU:HG	1.97	0.46
7:AP:22:MET:HE3	7:AP:23:GLU:H	1.79	0.46
3:H:308:LEU:HD13	3:H:513:ILE:HD12	1.96	0.46
3:H:326:SER:OG	3:H:342:SER:OG	2.33	0.46
3:H:419:ASP:HB2	3:H:421:GLN:HE22	1.80	0.46
3:I:482:GLN:O	3:I:499:TYR:N	2.48	0.46
3:J:306:LEU:HD22	3:J:424:MET:HE3	1.95	0.46
3:L:179:LYS:HD3	3:L:284:ALA:HA	1.98	0.46
8:BH:39:SER:HB2	8:BS:9:LEU:HD13	1.96	0.46
1:AB:172:LYS:HG3	1:AB:180:TYR:CZ	2.50	0.46
1:AC:38:VAL:HG11	1:AC:77:LEU:HD11	1.98	0.46
3:Q:46:PHE:HB3	3:Q:57:VAL:HG21	1.96	0.46
2:R:363:ASP:OD1	2:R:363:ASP:N	2.44	0.46
2:Y:206:TRP:O	1:v:43:ASN:ND2	2.42	0.46
2:Z:327:ILE:HD12	2:Z:359:ILE:HG12	1.96	0.46
2:e:215:ASP:N	2:e:215:ASP:OD1	2.48	0.46
3:B:42:LEU:HD11	3:B:66:LYS:HB2	1.96	0.46
3:D:197:LEU:O	3:D:411:ARG:NH1	2.49	0.46
3:G:363:LYS:NZ	3:H:479:ASP:O	2.44	0.46
3:I:429:GLU:OE2	3:I:452:ARG:NH2	2.49	0.46
3:K:179:LYS:HD3	3:K:284:ALA:HA	1.97	0.46
3:N:545:LYS:HD2	3:N:545:LYS:HA	1.69	0.46
3:O:177:ARG:NH2	3:P:222:LEU:O	2.48	0.46
2:T:310:GLN:O	2:T:338:ARG:NH2	2.48	0.46
1:AL:82:ARG:NH2	1:AL:114:GLU:OE2	2.49	0.46
2:d:369:ARG:O	3:D:38:LYS:NZ	2.43	0.46
2:k:306:GLY:O	2:k:310:GLN:NE2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:25:LYS:NZ	1:w:56:TYR:OH	2.49	0.46
1:v:64:ASP:OD1	1:v:64:ASP:N	2.32	0.46
3:B:442:THR:O	3:B:446:ALA:N	2.48	0.46
3:F:55:GLU:HG3	3:F:94:PHE:HE1	1.79	0.46
3:H:373:LEU:HD23	3:I:470:GLY:HA3	1.98	0.46
3:J:433:ASP:OD1	3:J:433:ASP:N	2.48	0.46
3:K:512:MET:N	3:K:512:MET:SD	2.89	0.46
3:L:440:THR:O	3:L:443:SER:OG	2.33	0.46
8:BG:39:SER:HB2	8:BR:8:TYR:HB3	1.97	0.46
2:E:333:ASP:OD2	2:E:333:ASP:N	2.49	0.46
2:e:312:LEU:HD23	2:e:327:ILE:HD13	1.98	0.46
2:h:307:LEU:HB2	2:h:312:LEU:HD11	1.96	0.46
2:n:299:ALA:O	2:n:346:TYR:OH	2.28	0.46
1:p:38:VAL:HG11	1:p:77:LEU:HD11	1.98	0.46
1:s:36:ILE:HD13	1:s:46:ALA:HB3	1.97	0.46
7:AR:57:ASP:OD1	7:AR:60:LEU:N	2.48	0.46
8:AT:38:PRO:HD2	8:BE:5:TRP:HZ2	1.81	0.46
8:AV:22:ASN:O	8:AV:25:THR:OG1	2.28	0.46
8:AX:66:LYS:HD3	8:BD:80:ARG:HD2	1.98	0.46
3:C:118:SER:OG	3:C:119:LEU:N	2.48	0.46
3:G:63:ALA:HB2	3:G:103:ASP:HB2	1.96	0.46
3:K:90:LEU:HA	3:K:103:ASP:HA	1.97	0.46
3:K:431:GLY:HA2	3:K:450:VAL:HG23	1.97	0.46
3:M:119:LEU:HD11	3:M:138:LEU:HD23	1.97	0.46
3:O:58:ILE:HD13	3:P:105:SER:HA	1.98	0.46
8:AZ:44:LEU:HB3	8:BK:75:ILE:HD13	1.97	0.46
8:BN:19:GLY:HA3	8:BI:35:ALA:HB1	1.97	0.46
1:AA:25:LYS:O	1:AB:29:GLN:NE2	2.49	0.46
1:AF:155:GLU:OE2	1:AF:190:ARG:NH2	2.48	0.46
1:AF:201:PRO:HB3	2:n:213:ARG:HD2	1.97	0.46
2:a:217:ASP:OD2	2:a:217:ASP:N	2.46	0.46
2:a:307:LEU:HD11	2:a:357:PHE:HE1	1.80	0.46
1:r:114:GLU:HB2	1:r:128:VAL:HG22	1.98	0.46
1:z:24:LEU:HB3	1:z:27:LEU:HD21	1.97	0.46
4:4:100:ARG:HD3	4:4:140[A]:LYS:HD3	1.96	0.46
6:9:10:LYS:HE2	6:9:74:TYR:HE1	1.81	0.46
7:AR:58:PRO:HB2	8:BC:5:TRP:CZ2	2.50	0.46
8:AV:35:ALA:HB1	8:BA:19:GLY:HA3	1.97	0.46
8:AV:58:ARG:HD3	8:AV:58:ARG:HA	1.81	0.46
3:G:107:MET:HE2	3:G:151:GLY:HA2	1.97	0.46
3:I:414:PRO:HA	3:I:424:MET:HA	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:157:ASP:O	3:K:161:ASN:ND2	2.49	0.46
3:M:177:ARG:NH2	3:N:222:LEU:O	2.48	0.46
3:O:313:LEU:HB2	3:O:508:VAL:HG12	1.97	0.46
3:P:108:ARG:HG3	3:P:156:VAL:HG21	1.97	0.46
2:R:209:GLN:HG2	1:o:43:ASN:HB3	1.96	0.46
2:U:310:GLN:O	2:U:338:ARG:NH1	2.48	0.46
2:V:316:ARG:HH21	2:V:318:ASN:HD21	1.64	0.46
5:5:70:MET:HE3	5:5:70:MET:HB3	1.75	0.46
3:B:141:ASP:HB3	3:B:144:LYS:HB2	1.96	0.46
3:G:383:PHE:HB3	3:G:410:ILE:HG23	1.98	0.46
3:K:286:GLN:HA	3:K:289:PHE:HB2	1.97	0.46
8:BJ:20:VAL:HG11	8:BJ:23:LEU:HB3	1.97	0.46
1:AH:191:SER:OG	1:AH:192:ASP:N	2.49	0.46
2:m:381:MET:N	2:m:381:MET:SD	2.88	0.46
4:1:25:THR:HG23	4:1:27:PHE:H	1.81	0.46
3:B:415:ARG:NH1	3:B:416:PHE:O	2.49	0.46
3:F:545:LYS:O	3:G:536:GLN:NE2	2.46	0.46
3:L:377:GLU:H	3:L:377:GLU:HG2	1.56	0.46
3:M:323:THR:OG1	3:M:324:SER:N	2.49	0.46
3:N:327:GLY:HA3	3:N:352:PHE:HA	1.97	0.46
8:BV:67:VAL:HG13	8:BV:68:PHE:HD1	1.81	0.46
1:AF:196:GLN:OE1	2:n:179:GLN:N	2.48	0.46
2:R:324:THR:HB	2:R:356:GLN:HE21	1.81	0.46
2:X:316:ARG:HE	2:X:318:ASN:HD21	1.62	0.46
2:Y:228:GLU:OE2	2:Y:231:ARG:NH2	2.40	0.46
1:q:21:LYS:HD2	1:q:62:GLU:HG2	1.98	0.46
1:z:39:LEU:HB3	1:z:44:ILE:HG13	1.98	0.46
4:1:211:LEU:HA	6:6:83:LEU:HD11	1.97	0.46
4:2:50:MET:O	4:2:54:GLY:N	2.49	0.46
8:AY:60:ALA:O	8:AY:64:THR:OG1	2.30	0.46
3:H:268:LYS:HZ2	3:I:213:ARG:HG3	1.80	0.46
3:I:216:GLN:HE22	8:BB:21:ASP:HB3	1.81	0.46
3:J:482:GLN:HB3	3:J:499:TYR:HB3	1.98	0.46
3:K:541:SER:OG	3:M:506:ASN:ND2	2.48	0.46
3:N:534:LEU:HD21	3:O:368:VAL:HG11	1.98	0.46
8:BL:13:SER:HB2	8:BL:61:GLN:HE21	1.79	0.46
1:AA:168:LYS:HE3	1:AA:183:ILE:HB	1.98	0.46
1:AC:129:HIS:HE1	1:AL:112:ARG:HG2	1.81	0.46
1:AD:63:PRO:HG2	1:AD:203:LYS:HD3	1.97	0.46
1:AG:194:GLN:HB2	2:k:202:ARG:HH22	1.81	0.46
2:S:340:ARG:NH1	1:q:166:ASP:OD1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:335:GLU:N	2:i:335:GLU:OE1	2.48	0.46
2:m:370:SER:HG	3:K:38:LYS:H	1.58	0.46
1:o:39:LEU:HB3	1:o:44:ILE:HG13	1.98	0.46
1:o:90:PRO:HG2	1:o:93:SER:HB3	1.99	0.46
1:r:23:LEU:HB2	1:r:58:ILE:HG23	1.98	0.46
1:u:184:SER:OG	1:v:169:ARG:NE	2.49	0.46
1:AK:53:LYS:HE3	1:AK:53:LYS:HB3	1.76	0.46
7:AO:47:ASP:HA	7:AO:50:THR:HG22	1.98	0.46
7:AQ:25:ASP:HB2	3:G:61:LYS:HE2	1.98	0.46
3:D:402:GLU:HA	8:BU:3:THR:N	2.31	0.46
3:F:40:ASP:HB3	3:F:44:THR:HG23	1.98	0.46
3:G:283:THR:H	3:G:286:GLN:NE2	2.12	0.46
3:M:456:SER:O	3:M:456:SER:OG	2.34	0.46
8:BJ:9:LEU:HA	8:BJ:12:VAL:HG12	1.97	0.46
1:AC:184:SER:HB2	1:AL:173:ASN:HD21	1.81	0.45
2:S:225:GLU:HG3	2:S:250:PHE:HD2	1.80	0.45
2:c:304:GLU:HG2	2:c:308:LYS:HE2	1.97	0.45
2:i:190:ARG:NH1	2:i:286:ALA:O	2.44	0.45
2:j:263:GLN:NE2	2:j:295:ASP:OD1	2.50	0.45
1:o:191:SER:OG	1:o:192:ASP:N	2.48	0.45
1:AK:38:VAL:HG21	1:AK:77:LEU:HD21	1.98	0.45
4:1:195:THR:HA	4:1:198:LYS:HB2	1.99	0.45
4:4:25:THR:OG1	4:4:26:CYS:N	2.49	0.45
4:4:113:GLN:HE22	4:4:133:ARG:HA	1.80	0.45
8:AX:34:LEU:HD22	8:AX:43:LEU:HG	1.98	0.45
3:A:387:ARG:HE	3:A:389:PHE:HE1	1.63	0.45
3:B:144:LYS:HD3	3:B:144:LYS:HA	1.72	0.45
3:M:478:THR:HB	3:M:503:ASN:HB3	1.98	0.45
8:BJ:34:LEU:HA	8:BJ:43:LEU:HD13	1.98	0.45
1:AD:85:ILE:HB	1:AD:107:SER:HB2	1.97	0.45
1:AE:53:LYS:HE2	1:AE:53:LYS:HB2	1.76	0.45
1:AE:147:HIS:HB3	1:o:173:ASN:HB2	1.98	0.45
2:m:192:LYS:HD3	2:m:192:LYS:HA	1.73	0.45
6:9:72:LEU:HD13	6:9:76:ARG:HH12	1.81	0.45
7:AP:49:GLN:HA	7:AP:52:THR:HG22	1.98	0.45
3:A:197:LEU:HA	3:A:382:ILE:HD11	1.97	0.45
3:D:42:LEU:HD23	3:D:42:LEU:HA	1.79	0.45
3:G:316:SER:N	3:G:363:LYS:O	2.37	0.45
3:H:323:THR:HB	3:H:356:VAL:HG22	1.97	0.45
3:J:313:LEU:HB3	3:J:508:VAL:HG23	1.98	0.45
3:J:322:GLY:HA3	3:J:499:TYR:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:421:GLN:HA	3:K:462:PRO:HA	1.98	0.45
1:AC:180:TYR:HD1	1:AC:183:ILE:HD11	1.81	0.45
1:AG:40:GLN:HE22	1:AH:66:THR:HA	1.82	0.45
2:a:364:ASP:OD1	2:a:364:ASP:N	2.43	0.45
1:o:146:VAL:HB	1:o:178:VAL:HG12	1.99	0.45
1:q:95:VAL:HG11	6:6:10:LYS:HB2	1.97	0.45
1:r:98:PRO:HA	1:r:101:GLU:HG2	1.98	0.45
1:w:23:LEU:HG	1:w:24:LEU:HG	1.99	0.45
1:AJ:177:ASP:OD2	1:AJ:177:ASP:N	2.49	0.45
4:1:21:ILE:HD12	4:1:25:THR:HG21	1.99	0.45
6:6:22:PRO:HA	6:6:25:VAL:HG22	1.98	0.45
3:A:433:ASP:N	3:A:433:ASP:OD1	2.43	0.45
3:A:545:LYS:O	3:B:536:GLN:NE2	2.49	0.45
3:C:209:THR:HA	3:C:212:GLU:HG3	1.99	0.45
3:D:112:VAL:HG11	3:D:160:VAL:HG23	1.98	0.45
3:H:383:PHE:HB3	3:H:410:ILE:HG23	1.97	0.45
3:M:97:GLN:HE21	3:N:137:PRO:HD2	1.82	0.45
3:N:308:LEU:HD11	3:N:428:ILE:HD13	1.97	0.45
8:BH:9:LEU:HA	8:BH:12:VAL:HG22	1.99	0.45
8:BP:68:PHE:HA	8:BP:71:ILE:HG12	1.98	0.45
8:BU:20:VAL:HG11	8:BU:23:LEU:HB2	1.98	0.45
1:AF:20:ASP:N	1:AF:20:ASP:OD1	2.49	0.45
2:E:224:ASN:HB3	2:E:227:GLU:HG3	1.99	0.45
4:O:186:MET:HE3	4:O:186:MET:HB3	1.89	0.45
7:AP:29:LEU:HD23	7:AP:29:LEU:HA	1.73	0.45
8:AY:23:LEU:HG	8:AY:54:TYR:HD1	1.80	0.45
3:B:363:LYS:HD3	3:C:480:THR:HB	1.98	0.45
3:D:541:SER:OG	3:D:547:GLN:OE1	2.26	0.45
3:M:116:ASN:HA	3:M:254:LEU:HD13	1.99	0.45
3:N:363:LYS:HZ2	3:N:365:ALA:HB2	1.80	0.45
3:O:431:GLY:HA2	3:O:450:VAL:HG23	1.98	0.45
3:P:194:THR:HB	8:BK:3:THR:HA	1.99	0.45
8:BL:6:SER:OG	8:BL:11:ASP:OD1	2.26	0.45
8:BR:9:LEU:HA	8:BR:12:VAL:HG22	1.98	0.45
3:Q:36:VAL:HG13	2:X:373:TYR:HE1	1.79	0.45
3:Q:166:MET:HE3	3:A:144:LYS:HE2	1.98	0.45
1:AL:146:VAL:HG13	1:AL:178:VAL:HG12	1.97	0.45
2:a:201:GLU:HA	2:a:204:THR:HG22	1.99	0.45
2:e:379:ILE:HG22	2:e:387:TYR:HB3	1.97	0.45
1:v:118:GLN:HE22	1:v:125:SER:HA	1.81	0.45
4:1:143:ILE:H	4:1:143:ILE:HD12	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:53:ASN:HD22	7:AQ:99:LEU:HA	1.81	0.45
8:AY:22:ASN:O	8:AY:26:GLN:N	2.46	0.45
3:F:149:VAL:HG21	3:F:159:VAL:HG11	1.98	0.45
3:J:187:ASN:HB2	3:J:298:ASP:HB2	1.98	0.45
3:J:383:PHE:HB3	3:J:410:ILE:HG23	1.99	0.45
3:O:269:ILE:HG23	3:O:280:VAL:HG12	1.98	0.45
8:BM:66:LYS:NZ	8:BM:70:ASP:OD2	2.48	0.45
1:AF:30:GLU:HA	1:AF:33:ASN:HD21	1.80	0.45
2:T:179:GLN:N	1:q:196:GLN:OE1	2.48	0.45
2:e:379:ILE:HD12	2:e:379:ILE:HA	1.82	0.45
2:i:173:LEU:HA	2:i:176:LEU:HD12	1.97	0.45
1:r:184:SER:HB2	1:s:173:ASN:HD21	1.81	0.45
1:v:39:LEU:HB3	1:v:44:ILE:HG13	1.98	0.45
4:1:25:THR:OG1	4:1:26:CYS:N	2.49	0.45
4:4:205:LEU:HD21	6:9:72:LEU:HA	1.99	0.45
7:AQ:71:GLN:HE22	8:BB:79:PHE:HA	1.80	0.45
3:C:387:ARG:NH2	3:D:449:GLU:O	2.50	0.45
3:K:283:THR:H	3:K:286:GLN:HE21	1.63	0.45
3:P:426:LEU:HD21	3:P:428:ILE:HG12	1.99	0.45
8:BG:39:SER:HB3	8:BR:9:LEU:HG	1.98	0.45
1:AA:25:LYS:H	1:AB:29:GLN:HE21	1.63	0.45
3:Q:141:ASP:HB3	3:Q:144:LYS:HB2	1.99	0.45
1:AL:30:GLU:HA	1:AL:33:ASN:HD21	1.82	0.45
2:h:245:TYR:OH	2:h:353:ARG:NH1	2.50	0.45
1:r:169:ARG:NH1	1:r:180:TYR:OH	2.43	0.45
4:0:152:LEU:HD13	4:0:155:ILE:HD11	1.99	0.45
4:3:36:MET:HE2	4:3:36:MET:HB3	1.80	0.45
4:3:158:ALA:HA	4:3:161:ILE:HG22	1.99	0.45
3:B:76:ASP:HA	3:B:77:PRO:HD3	1.75	0.45
3:D:433:ASP:OD1	3:D:433:ASP:N	2.47	0.45
3:D:482:GLN:O	3:D:499:TYR:N	2.50	0.45
3:F:407:GLY:N	3:F:431:GLY:O	2.49	0.45
3:H:268:LYS:NZ	3:I:213:ARG:HG3	2.32	0.45
3:K:436:PRO:HD3	8:BS:4:PRO:HB3	1.99	0.45
3:K:534:LEU:HD21	3:L:368:VAL:HG21	1.98	0.45
3:L:323:THR:OG1	3:L:324:SER:N	2.49	0.45
1:AB:177:ASP:N	1:AB:177:ASP:OD1	2.49	0.45
1:AG:202:VAL:N	2:k:215:ASP:OD2	2.50	0.45
1:AH:173:ASN:HD21	1:AI:184:SER:HB2	1.82	0.45
2:S:363:ASP:N	2:S:363:ASP:OD1	2.46	0.45
2:a:258:PHE:HB3	2:a:291:ILE:HG12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:356:GLN:NE2	2:f:310:GLN:OE1	2.48	0.45
2:k:173:LEU:HA	2:k:176:LEU:HD12	1.98	0.45
4:4:34:PHE:HB3	4:4:52:LEU:HD21	1.98	0.45
4:4:197:ILE:HA	4:4:200:VAL:HG22	1.98	0.45
8:AW:48:GLN:HA	8:AW:51:LEU:HD23	1.98	0.45
8:AX:33:LYS:HB3	8:AX:43:LEU:HD11	1.97	0.45
3:A:280:VAL:HG21	3:A:290:ILE:HD11	1.99	0.45
3:K:376:GLN:HE21	3:L:459:ALA:HA	1.81	0.45
8:BB:74:ALA:O	8:BB:78:ASN:ND2	2.50	0.45
1:AE:107:SER:O	1:AE:111:GLN:NE2	2.48	0.45
1:AF:139:ASN:HD21	1:AF:141:ARG:HB2	1.81	0.45
2:a:373:TYR:HE1	3:B:36:VAL:HG23	1.81	0.45
2:j:387:TYR:HD1	3:J:69:THR:HB	1.82	0.45
2:m:246:TYR:OH	2:m:296:ASP:OD1	2.35	0.45
1:x:169:ARG:NH1	1:x:180:TYR:OH	2.47	0.45
4:2:180:LEU:HD11	4:2:190:PRO:HB3	1.98	0.45
4:3:176:VAL:HA	4:3:179:VAL:HG12	1.98	0.45
3:F:384:ASP:HB3	3:F:409:MET:HG3	1.98	0.45
3:H:401:LEU:HD23	3:H:401:LEU:HA	1.85	0.45
3:J:269:ILE:HD13	3:J:280:VAL:HG12	1.98	0.45
3:K:346:THR:HG23	3:K:347:LEU:HG	1.98	0.45
3:L:286:GLN:HA	3:L:289:PHE:HB2	1.98	0.45
3:L:419:ASP:HB2	3:L:421:GLN:HE22	1.82	0.45
8:BH:38:PRO:HD2	8:BS:5:TRP:HZ2	1.82	0.45
8:BT:21:ASP:OD1	8:BT:21:ASP:N	2.48	0.45
1:AC:98:PRO:HA	1:AC:101:GLU:HG3	1.98	0.45
2:E:258:PHE:HB3	2:E:291:ILE:HG12	1.99	0.45
2:T:248:ILE:HG12	2:T:258:PHE:HD1	1.81	0.45
2:e:192:LYS:O	2:e:219:ASN:ND2	2.33	0.45
2:g:363:ASP:N	2:g:363:ASP:OD1	2.40	0.45
1:y:110:GLU:OE1	1:z:112:ARG:NH2	2.49	0.45
6:9:17:ILE:HG13	6:9:18:LEU:HD23	1.98	0.45
8:AX:34:LEU:HD21	8:AX:47:TYR:HB2	1.98	0.45
8:AY:22:ASN:OD1	8:AY:25:THR:OG1	2.35	0.45
3:B:176:GLY:O	3:C:220:GLN:NE2	2.49	0.45
3:I:323:THR:OG1	3:I:324:SER:N	2.50	0.45
3:K:306:LEU:HD21	3:K:513:ILE:HD11	2.00	0.45
3:M:547:GLN:HE21	3:O:508:VAL:HB	1.81	0.45
3:P:431:GLY:HA2	3:P:450:VAL:HG23	1.98	0.45
8:BN:78:ASN:O	8:BC:48:GLN:NE2	2.50	0.45
1:AC:164:ILE:HD11	2:f:334:VAL:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:114:GLU:HB3	1:AE:128:VAL:HG22	1.99	0.44
2:E:363:ASP:HB2	1:o:180:TYR:HD2	1.82	0.44
2:T:224:ASN:N	2:T:228:GLU:OE2	2.51	0.44
2:Z:356:GLN:NE2	2:a:310:GLN:OE1	2.49	0.44
2:m:265:ASN:OD1	2:m:265:ASN:N	2.50	0.44
2:m:327:ILE:HD13	2:m:359:ILE:HG12	1.98	0.44
1:t:117:LEU:HD23	1:t:117:LEU:HA	1.85	0.44
1:AJ:140:GLY:O	4:2:109:ARG:NH2	2.41	0.44
4:0:208:TRP:H	5:5:175:ASN:HD21	1.65	0.44
8:AU:63:ASN:OD1	8:BA:80:ARG:NH1	2.50	0.44
3:F:286:GLN:HA	3:F:289:PHE:HB2	1.99	0.44
3:L:178:GLN:O	3:M:223:GLY:N	2.50	0.44
3:L:539:ALA:HA	3:N:504:LYS:HD2	1.99	0.44
3:M:194:THR:HG22	3:M:203:VAL:HG22	1.99	0.44
3:O:283:THR:H	3:O:286:GLN:HE21	1.65	0.44
3:P:308:LEU:HD21	3:P:511:PHE:HB3	1.99	0.44
1:AF:168:LYS:NZ	1:AF:183:ILE:O	2.49	0.44
2:X:334:VAL:HG22	2:X:338:ARG:HE	1.83	0.44
2:c:245:TYR:OH	2:c:353:ARG:NH1	2.51	0.44
2:h:304:GLU:HA	2:h:307:LEU:HG	1.98	0.44
1:s:39:LEU:HB3	1:s:44:ILE:HG13	1.99	0.44
4:2:178:SER:O	4:2:182:ALA:N	2.50	0.44
3:D:442:THR:HB	3:F:320:ARG:HH12	1.81	0.44
3:G:257:ALA:HA	3:G:260:GLN:HG2	1.98	0.44
8:BL:12:VAL:HG13	8:BL:65:VAL:HG12	1.98	0.44
1:AD:85:ILE:HD11	1:AI:112:ARG:HH11	1.82	0.44
1:AE:110:GLU:HG3	1:AE:130:ILE:HD12	2.00	0.44
1:AF:36:ILE:HD11	1:AF:48:LYS:HB2	2.00	0.44
2:E:304:GLU:OE1	2:E:316:ARG:NH1	2.51	0.44
3:Q:141:ASP:H	3:P:125:PHE:HE1	1.65	0.44
2:U:381:MET:HE2	2:U:381:MET:HB2	1.87	0.44
2:m:316:ARG:HE	2:m:318:ASN:HD21	1.64	0.44
1:y:168:LYS:HE3	1:y:183:ILE:HB	1.99	0.44
4:2:159:PHE:HB3	4:3:199:LEU:HD12	1.99	0.44
5:5:60:ASN:OD1	5:5:60:ASN:N	2.51	0.44
7:AR:25:ASP:OD1	3:C:61:LYS:NZ	2.48	0.44
3:A:471:GLY:HA3	3:A:510:VAL:HG23	1.99	0.44
3:B:319:GLU:HB3	3:B:360:GLU:HG2	1.99	0.44
3:J:327:GLY:O	3:J:342:SER:OG	2.34	0.44
3:L:431:GLY:HA2	3:L:450:VAL:HG23	1.98	0.44
8:BN:53:GLU:OE2	8:BI:39:SER:OG	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:94:LEU:HG	1:AE:95:VAL:HG13	1.98	0.44
1:AE:190:ARG:NH1	1:AE:191:SER:O	2.45	0.44
2:E:299:ALA:O	2:E:346:TYR:OH	2.29	0.44
2:U:217:ASP:OD2	2:U:217:ASP:N	2.49	0.44
2:W:245:TYR:OH	2:W:353:ARG:NH1	2.51	0.44
2:W:340:ARG:HH12	1:u:163:GLN:HG3	1.83	0.44
2:f:246:TYR:OH	2:f:296:ASP:OD1	2.35	0.44
1:v:35:VAL:HG22	1:v:77:LEU:HD13	2.00	0.44
4:4:180:LEU:HD11	4:4:188:MET:HB3	2.00	0.44
7:AM:83:MET:HE3	7:AM:83:MET:HB3	1.82	0.44
7:AR:85:SER:HB2	8:AW:75:ILE:HD13	1.98	0.44
3:D:404:VAL:HG22	3:D:447:LEU:HD13	1.99	0.44
3:G:318:LEU:HD21	3:G:320:ARG:HE	1.82	0.44
3:K:144:LYS:HD3	3:K:144:LYS:HA	1.87	0.44
3:P:116:ASN:OD1	3:P:116:ASN:N	2.51	0.44
3:P:308:LEU:HD11	3:P:428:ILE:HD13	1.99	0.44
8:BF:21:ASP:OD2	8:BF:21:ASP:N	2.47	0.44
1:AD:146:VAL:HG23	1:AD:178:VAL:HG12	2.00	0.44
1:AD:173:ASN:HB2	1:AL:147:HIS:HB3	1.99	0.44
2:i:332:ASP:OD1	2:i:332:ASP:N	2.40	0.44
2:j:318:ASN:HA	2:j:323:VAL:HG23	2.00	0.44
2:l:299:ALA:O	2:l:346:TYR:OH	2.31	0.44
2:m:333:ASP:OD1	2:m:333:ASP:N	2.48	0.44
1:q:51:SER:OG	1:q:55:GLY:O	2.29	0.44
1:AJ:115:GLN:HE22	1:AK:83:VAL:H	1.66	0.44
7:AN:58:PRO:HG2	8:AY:5:TRP:CE2	2.53	0.44
3:F:144:LYS:HD3	3:F:144:LYS:HA	1.76	0.44
3:F:338:SER:HB2	3:F:344:ILE:HD11	2.00	0.44
3:J:521:PRO:HG3	3:K:462:PRO:HD2	2.00	0.44
1:AC:71:TRP:HA	1:AC:74:THR:HG22	1.98	0.44
2:E:247:ARG:NH1	2:E:348:ARG:O	2.51	0.44
2:h:200:ASN:OD1	2:h:200:ASN:N	2.50	0.44
2:m:323:VAL:HG22	2:m:355:VAL:HG12	2.00	0.44
1:v:38:VAL:HG11	1:v:77:LEU:HD11	1.99	0.44
1:z:21:LYS:NZ	1:z:62:GLU:OE1	2.50	0.44
4:3:84:ASP:OD1	4:3:87:SER:N	2.48	0.44
7:AN:89:ARG:O	7:AN:93:GLY:N	2.51	0.44
7:AQ:74:ILE:O	7:AQ:78:ASN:ND2	2.39	0.44
8:AW:33:LYS:HE2	8:AW:43:LEU:HD13	1.99	0.44
3:C:419:ASP:HB2	3:C:421:GLN:HE22	1.83	0.44
3:H:178:GLN:HE21	3:I:220:GLN:HE21	1.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:426:LEU:HD21	3:K:428:ILE:HG12	1.99	0.44
3:P:225:ILE:HG13	3:P:293:LEU:HG	1.98	0.44
1:AA:184:SER:OG	1:AB:169:ARG:NE	2.46	0.44
1:AF:99:ARG:HH21	1:AF:138:GLU:HG2	1.82	0.44
2:T:236:LEU:HD12	2:T:236:LEU:HA	1.82	0.44
2:T:323:VAL:HG22	2:T:355:VAL:HG12	1.99	0.44
2:a:187:LEU:O	2:a:195:TYR:N	2.45	0.44
2:c:257:VAL:HG12	2:c:290:ASN:HD22	1.82	0.44
1:v:147:HIS:HA	1:v:182:ASN:HB3	2.00	0.44
4:2:4:ASP:OD2	4:2:4:ASP:N	2.47	0.44
4:3:152:LEU:HD22	4:4:208:TRP:HB3	1.98	0.44
8:AV:49:SER:OG	8:BB:10:ASP:OD1	2.31	0.44
3:A:308:LEU:HD21	3:A:511:PHE:HB3	2.00	0.44
3:C:377:GLU:H	3:C:377:GLU:HG2	1.59	0.44
3:C:404:VAL:HG22	3:C:447:LEU:HD22	1.99	0.44
3:J:328:SER:OG	3:J:342:SER:OG	2.33	0.44
3:N:220:GLN:H	3:N:264:ALA:H	1.65	0.44
1:AA:24:LEU:HB2	1:AA:58:ILE:HD11	1.99	0.44
2:i:364:ASP:N	2:i:364:ASP:OD1	2.48	0.44
2:j:372:GLN:HB2	3:I:35:PHE:HD1	1.82	0.44
2:l:200:ASN:O	2:l:204:THR:OG1	2.29	0.44
2:l:223:ILE:HB	2:l:228:GLU:HG3	1.99	0.44
1:q:22:ASP:HA	1:q:59:THR:HA	1.98	0.44
4:1:113:GLN:HA	4:1:116:GLU:HG3	2.00	0.44
4:2:43:LEU:HD12	4:2:46:ILE:HD13	2.00	0.44
7:AQ:55:ILE:HD12	7:AQ:55:ILE:HA	1.89	0.44
3:A:472:TYR:N	3:A:509:ARG:O	2.50	0.44
3:L:116:ASN:OD1	3:L:116:ASN:N	2.49	0.44
3:L:383:PHE:HB3	3:L:410:ILE:HG23	2.00	0.44
3:N:76:ASP:N	3:N:76:ASP:OD1	2.50	0.44
3:N:90:LEU:HA	3:N:103:ASP:HA	1.99	0.44
3:N:313:LEU:HB3	3:N:508:VAL:HG12	2.00	0.44
2:U:245:TYR:HA	2:U:260:LEU:HA	1.98	0.44
2:f:174:ASP:N	2:f:174:ASP:OD1	2.50	0.44
2:n:173:LEU:HD23	2:n:173:LEU:HA	1.86	0.44
1:o:69:VAL:HG22	1:p:37:ALA:HB2	2.00	0.44
1:v:31:GLN:NE2	1:v:79:PRO:O	2.36	0.44
1:w:20:ASP:OD1	1:w:20:ASP:N	2.50	0.44
1:x:168:LYS:HE2	1:x:183:ILE:HG13	2.00	0.44
1:z:203:LYS:HA	1:z:203:LYS:HD2	1.78	0.44
4:0:25:THR:OG1	4:0:26:CYS:N	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:67:SER:HA	5:5:70:MET:HE1	2.00	0.44
6:9:7:ALA:O	6:9:74:TYR:OH	2.36	0.44
7:AO:79:LEU:O	7:AO:83:MET:HG2	2.17	0.44
8:AT:71:ILE:HD12	8:AT:71:ILE:HA	1.86	0.44
3:D:338:SER:OG	3:D:342:SER:O	2.36	0.44
3:H:121:GLU:HA	3:H:124:ASN:HB2	2.00	0.44
3:M:406:TYR:OH	3:M:448:PRO:O	2.31	0.44
8:BD:33:LYS:HD3	8:BD:43:LEU:HD22	2.00	0.44
1:AH:130:ILE:HD12	1:AH:130:ILE:HA	1.81	0.43
1:AI:120:MET:HE3	1:AI:121:GLU:H	1.82	0.43
2:W:365:TRP:HD1	2:W:390:SER:HB3	1.83	0.43
2:a:190:ARG:NH2	2:a:280:ARG:O	2.50	0.43
2:b:217:ASP:OD1	2:b:217:ASP:N	2.45	0.43
2:h:251:ASP:OD1	2:h:251:ASP:N	2.51	0.43
2:l:333:ASP:OD1	1:AJ:169:ARG:NE	2.50	0.43
1:q:20:ASP:N	1:q:20:ASP:OD1	2.51	0.43
1:q:44:ILE:HD12	1:q:64:ASP:HB3	1.99	0.43
1:u:33:ASN:OD1	1:u:33:ASN:N	2.47	0.43
1:AJ:98:PRO:HA	1:AJ:101:GLU:HB2	2.00	0.43
6:7:31:LEU:HD23	6:7:35:LEU:HD23	2.00	0.43
6:8:28:ILE:HA	6:8:31:LEU:HB2	2.00	0.43
3:F:185:LEU:HD12	3:F:185:LEU:HA	1.90	0.43
3:G:178:GLN:O	3:H:223:GLY:N	2.50	0.43
3:M:483:SER:OG	3:M:484:ILE:N	2.51	0.43
2:W:232:ILE:HG21	2:W:248:ILE:HD12	2.00	0.43
2:Y:304:GLU:HG2	2:Y:308:LYS:HE2	2.01	0.43
2:i:295:ASP:HB3	2:i:298:THR:HG22	2.00	0.43
1:v:148:LEU:HD13	1:v:171:LEU:HB3	2.00	0.43
1:w:191:SER:OG	1:w:192:ASP:N	2.51	0.43
1:AJ:20:ASP:OD1	1:AJ:20:ASP:N	2.51	0.43
8:AT:76:ILE:H	8:AT:76:ILE:HG12	1.39	0.43
8:AY:34:LEU:HA	8:AY:43:LEU:HD23	2.00	0.43
3:A:430:ASP:OD2	3:A:509:ARG:NH2	2.51	0.43
3:B:301:LYS:O	3:C:460:ARG:NH2	2.43	0.43
3:H:339:LEU:HD13	3:H:339:LEU:HA	1.90	0.43
3:I:419:ASP:HB2	3:I:421:GLN:HE22	1.83	0.43
3:K:91:ILE:HG13	3:K:102:TYR:HB2	2.00	0.43
3:K:178:GLN:O	3:L:223:GLY:N	2.51	0.43
3:K:429:GLU:OE1	3:K:452:ARG:NH2	2.51	0.43
3:L:543:ASP:N	3:L:543:ASP:OD1	2.44	0.43
3:M:328:SER:OG	3:M:342:SER:OG	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BM:20:VAL:HG11	8:BM:23:LEU:HD22	1.99	0.43
1:AH:163:GLN:HE22	2:i:340:ARG:HH22	1.67	0.43
1:AI:196:GLN:OE1	2:i:179:GLN:N	2.51	0.43
2:E:316:ARG:NE	2:E:318:ASN:OD1	2.51	0.43
2:c:194:LEU:HA	2:c:194:LEU:HD12	1.78	0.43
2:d:200:ASN:O	2:d:204:THR:OG1	2.32	0.43
2:f:177:LEU:HD23	2:f:210:VAL:HG21	2.00	0.43
2:f:371:PHE:HE1	2:f:380:LYS:HG2	1.82	0.43
1:y:77:LEU:HD12	1:y:79:PRO:HD3	2.00	0.43
3:K:308:LEU:HD21	3:K:511:PHE:HB3	2.00	0.43
3:M:177:ARG:NH1	3:N:260:GLN:OE1	2.50	0.43
3:M:433:ASP:OD1	3:M:433:ASP:N	2.46	0.43
3:N:120:ASN:OD1	3:N:120:ASN:N	2.51	0.43
8:BV:73:ALA:HA	8:BV:76:ILE:HG12	1.98	0.43
2:S:316:ARG:HH21	2:S:318:ASN:HD21	1.64	0.43
2:U:234:ILE:HG23	2:V:348:ARG:HH12	1.82	0.43
2:U:304:GLU:OE1	2:U:316:ARG:NH1	2.51	0.43
1:AL:191:SER:OG	1:AL:192:ASP:N	2.52	0.43
2:k:369:ARG:HH12	2:l:392:LEU:HG	1.83	0.43
7:AQ:24:THR:OG1	7:AQ:25:ASP:N	2.51	0.43
8:AS:35:ALA:HB1	8:AX:19:GLY:HA3	2.01	0.43
3:A:144:LYS:HD2	3:A:144:LYS:HA	1.73	0.43
3:B:283:THR:H	3:B:286:GLN:HE21	1.66	0.43
3:H:306:LEU:HD22	3:H:424:MET:HE3	1.99	0.43
3:J:482:GLN:O	3:J:499:TYR:N	2.51	0.43
3:O:149:VAL:HG11	3:O:159:VAL:HG11	2.00	0.43
8:BQ:16:PHE:HB3	8:BQ:57:TYR:CE1	2.53	0.43
1:AL:78:PRO:HA	1:AL:79:PRO:HD3	1.90	0.43
2:b:190:ARG:NH1	2:b:286:ALA:O	2.47	0.43
2:g:364:ASP:OD1	2:g:364:ASP:N	2.40	0.43
1:y:62:GLU:HG3	1:y:63:PRO:HD3	1.99	0.43
1:AJ:78:PRO:HA	1:AJ:79:PRO:HD3	1.89	0.43
3:C:392:LYS:HG3	3:D:441:THR:HG23	2.01	0.43
3:G:118:SER:OG	3:G:119:LEU:N	2.52	0.43
3:G:539:ALA:HB2	3:I:477:ASN:HD21	1.83	0.43
3:H:108:ARG:HD3	3:H:156:VAL:HG11	2.00	0.43
3:H:331:ILE:HB	3:H:335:LEU:HG	1.99	0.43
3:J:339:LEU:HD12	3:J:339:LEU:HA	1.78	0.43
3:L:534:LEU:HG	3:L:540:TRP:HB2	2.00	0.43
3:N:281:LYS:NZ	3:O:218:GLU:OE2	2.47	0.43
8:BF:40:ASP:HB2	8:BF:43:LEU:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:34:GLU:H	1:AB:34:GLU:HG2	1.69	0.43
1:AE:156:ARG:NH2	1:AE:190:ARG:O	2.35	0.43
2:S:271:GLU:HA	2:S:274:VAL:HG22	2.01	0.43
2:S:323:VAL:HG12	2:S:355:VAL:HG22	2.00	0.43
1:z:64:ASP:OD1	1:z:64:ASP:N	2.38	0.43
5:5:188:VAL:HG22	5:5:226:ILE:HG23	2.01	0.43
3:A:323:THR:OG1	3:A:324:SER:N	2.51	0.43
3:A:522:LEU:HD23	3:B:467:LEU:HD12	2.00	0.43
3:C:311:VAL:HG22	3:C:368:VAL:HG12	2.01	0.43
3:H:386:ASN:OD1	3:H:386:ASN:N	2.52	0.43
3:L:107:MET:HE2	3:L:151:GLY:HA2	2.00	0.43
1:AB:149:SER:OG	1:AC:173:ASN:OD1	2.36	0.43
1:AD:152:ALA:HB3	1:AD:187:LEU:HD22	2.01	0.43
2:W:279:LEU:HD23	2:W:279:LEU:HA	1.87	0.43
2:c:326:VAL:HA	2:c:358:ALA:HB3	2.01	0.43
2:h:294:MET:HB2	2:h:294:MET:HE3	1.68	0.43
2:j:255:LYS:HB3	2:j:255:LYS:HE3	1.85	0.43
2:l:173:LEU:HD23	2:l:173:LEU:HA	1.88	0.43
1:AK:74:THR:HG23	1:AK:75:TYR:HD1	1.83	0.43
4:3:65:TRP:CE2	7:AP:29:LEU:HD21	2.54	0.43
3:A:454:LEU:HD12	3:A:454:LEU:HA	1.82	0.43
3:G:419:ASP:HB2	3:G:421:GLN:HE22	1.84	0.43
3:J:442:THR:O	3:J:446:ALA:N	2.52	0.43
8:BM:41:PRO:HA	8:BM:44:LEU:HG	2.01	0.43
1:AE:99:ARG:HE	1:AE:134:ILE:HD12	1.84	0.43
1:AF:203:LYS:HA	1:AF:203:LYS:HD2	1.81	0.43
2:E:316:ARG:HH21	2:E:318:ASN:HD21	1.66	0.43
2:S:254:ARG:HA	2:S:286:ALA:HA	2.01	0.43
2:V:272:LEU:HD23	2:V:272:LEU:HA	1.88	0.43
1:AL:139:ASN:OD1	1:AL:141:ARG:NH1	2.52	0.43
2:a:252:GLU:HA	2:a:253:PRO:HD3	1.89	0.43
2:c:299:ALA:O	2:c:346:TYR:OH	2.37	0.43
4:3:29:LYS:HG3	4:3:158:ALA:HB2	2.00	0.43
6:9:29:ILE:HD11	6:9:52:LYS:HA	2.01	0.43
8:AS:56:LEU:HD13	8:AS:56:LEU:HA	1.90	0.43
3:H:224:ASN:HA	3:H:289:PHE:HZ	1.82	0.43
3:I:144:LYS:HD3	3:I:144:LYS:HA	1.73	0.43
3:I:308:LEU:HD21	3:I:511:PHE:HB3	2.00	0.43
3:I:483:SER:OG	3:I:484:ILE:N	2.51	0.43
3:L:280:VAL:HG21	3:L:290:ILE:HD11	2.00	0.43
3:M:283:THR:H	3:M:286:GLN:HE21	1.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:203:VAL:HG13	8:BF:22:ASN:HD22	1.84	0.43
3:N:265:GLY:O	8:BF:3:THR:N	2.52	0.43
3:O:58:ILE:HG23	3:O:100:TYR:HA	2.01	0.43
3:P:63:ALA:HB2	3:P:103:ASP:HB3	1.99	0.43
3:P:268:LYS:HD3	3:P:281:LYS:HD3	2.01	0.43
8:AZ:55:ASN:O	8:AZ:59:ASN:ND2	2.52	0.43
8:BF:55:ASN:OD1	8:BF:59:ASN:ND2	2.52	0.43
1:AH:39:LEU:HB3	1:AH:44:ILE:HG13	2.01	0.43
1:AH:164:ILE:HD11	2:j:337:LEU:HD13	2.00	0.43
2:E:256:PRO:HG2	2:E:289:VAL:HG12	2.01	0.43
2:E:386:TRP:HB2	3:M:29:PRO:HG2	2.01	0.43
2:V:204:THR:OG1	2:V:224:ASN:ND2	2.52	0.43
1:v:99:ARG:HG3	1:v:134:ILE:HB	2.00	0.43
4:0:88:LEU:HD13	7:AN:42:ILE:HD11	2.01	0.43
4:0:97:ASP:HA	4:0:100:ARG:HB3	2.00	0.43
4:3:65:TRP:O	4:3:69:HIS:N	2.51	0.43
4:4:20:ILE:O	4:4:24:GLY:N	2.31	0.43
7:AO:70:SER:HA	7:AO:73:MET:HE2	2.01	0.43
7:AR:64:PRO:O	8:AX:58:ARG:NH2	2.51	0.43
8:AU:34:LEU:HD11	8:AU:44:LEU:HA	2.01	0.43
3:G:430:ASP:OD2	3:G:509:ARG:NH2	2.52	0.43
3:H:432:ASN:C	3:H:452:ARG:HE	2.27	0.43
3:I:290:ILE:HA	3:I:293:LEU:HD13	2.01	0.43
3:I:415:ARG:NH2	3:I:423:GLU:OE2	2.50	0.43
3:O:301:LYS:O	3:P:460:ARG:NH2	2.42	0.43
3:P:144:LYS:HA	3:P:144:LYS:HD2	1.81	0.43
8:BL:15:LYS:HD2	8:BL:15:LYS:HA	1.76	0.43
8:BC:77:GLN:HA	8:BC:80:ARG:HH12	1.82	0.43
2:S:333:ASP:OD1	2:S:333:ASP:N	2.47	0.43
2:V:202:ARG:NH1	1:s:192:ASP:O	2.40	0.43
2:b:250:PHE:HE1	2:b:283:MET:HE1	1.84	0.43
2:c:344:ASP:OD1	2:c:344:ASP:N	2.51	0.43
1:x:78:PRO:HA	1:x:79:PRO:HD3	1.89	0.43
4:0:188:MET:HE2	4:0:188:MET:HB3	1.75	0.43
3:A:42:LEU:HA	3:A:45:PHE:HB3	2.00	0.43
3:B:323:THR:OG1	3:B:324:SER:N	2.52	0.43
3:C:383:PHE:HB3	3:C:410:ILE:HG23	2.01	0.43
3:C:522:LEU:HA	3:C:522:LEU:HD23	1.77	0.43
3:G:286:GLN:HA	3:G:289:PHE:HB2	2.01	0.43
3:G:323:THR:OG1	3:G:324:SER:N	2.50	0.43
3:L:308:LEU:HA	3:L:513:ILE:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:42:LEU:HD12	3:M:66:LYS:HB2	2.01	0.43
3:O:189:PHE:HA	3:O:276:ASN:HD21	1.84	0.43
8:BB:9:LEU:HA	8:BB:12:VAL:HG22	1.99	0.43
8:BK:9:LEU:HA	8:BK:12:VAL:HG22	1.99	0.43
8:BQ:9:LEU:HD12	8:BQ:65:VAL:HG13	1.99	0.43
8:BU:33:LYS:HA	8:BU:33:LYS:HD3	1.81	0.43
1:AB:78:PRO:HA	1:AB:79:PRO:HD3	1.91	0.42
1:AG:148:LEU:HD22	1:AG:171:LEU:HD21	2.01	0.42
3:Q:114:LEU:HD21	3:Q:117:VAL:HB	2.01	0.42
2:T:196:VAL:HB	2:T:222:VAL:HG12	2.01	0.42
2:W:371:PHE:CE1	2:W:380:LYS:HG2	2.54	0.42
2:c:331:LEU:HD13	2:c:367:LYS:HD3	2.01	0.42
1:w:172:LYS:HG3	1:w:180:TYR:CZ	2.54	0.42
4:2:8:ILE:O	4:2:12:ALA:N	2.48	0.42
6:8:63:LEU:HD22	6:8:66:TRP:HE3	1.84	0.42
3:B:376:GLN:HE22	3:C:460:ARG:HG2	1.84	0.42
3:H:456:SER:O	3:H:456:SER:OG	2.36	0.42
3:I:433:ASP:OD1	3:I:433:ASP:N	2.48	0.42
3:L:531:ASN:HA	3:L:534:LEU:HD22	2.00	0.42
8:BT:15:LYS:HD2	8:BT:15:LYS:HA	1.86	0.42
8:BT:20:VAL:HB	8:BT:23:LEU:HD23	2.01	0.42
1:AF:139:ASN:HA	6:7:84:ALA:HB1	2.01	0.42
1:AI:138:GLU:HB2	6:8:1:MET:N	2.35	0.42
2:E:231:ARG:NH2	2:E:283:MET:SD	2.92	0.42
2:V:224:ASN:N	2:V:227:GLU:OE1	2.52	0.42
2:V:380:LYS:HE2	2:V:380:LYS:HB3	1.85	0.42
2:Y:274:VAL:HG12	2:Y:278:LYS:HE2	2.01	0.42
2:b:200:ASN:OD1	2:b:200:ASN:N	2.49	0.42
2:g:235:TRP:CD2	2:g:282:LEU:HD11	2.54	0.42
2:g:245:TYR:OH	2:g:353:ARG:NH1	2.51	0.42
2:h:271:GLU:HA	2:h:274:VAL:HG12	2.01	0.42
1:s:117:LEU:HD23	1:s:117:LEU:HA	1.87	0.42
3:A:180:ILE:HD12	3:B:225:ILE:HD11	2.01	0.42
3:B:307:SER:OG	3:B:514:GLU:O	2.32	0.42
3:B:419:ASP:HB2	3:B:421:GLN:HE22	1.84	0.42
3:D:545:LYS:O	3:F:536:GLN:NE2	2.50	0.42
3:M:280:VAL:HG21	3:M:290:ILE:HD11	2.01	0.42
3:N:530:VAL:HG21	3:O:309:TRP:CZ3	2.54	0.42
3:O:308:LEU:HD12	3:O:513:ILE:HD12	2.00	0.42
8:BD:13:SER:OG	8:BD:61:GLN:NE2	2.40	0.42
8:BJ:68:PHE:HA	8:BJ:71:ILE:HD12	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BH:78:ASN:ND2	8:BC:63:ASN:OD1	2.52	0.42
8:BC:9:LEU:HA	8:BC:12:VAL:HG22	2.01	0.42
2:S:261:SER:O	2:S:265:ASN:ND2	2.52	0.42
2:X:252:GLU:HA	2:X:253:PRO:HD3	1.90	0.42
2:a:202:ARG:HH22	1:x:194:GLN:HB2	1.84	0.42
2:m:320:LYS:HE2	2:m:320:LYS:HB3	1.88	0.42
1:o:69:VAL:HG21	1:p:36:ILE:HG23	2.01	0.42
1:o:90:PRO:O	1:o:93:SER:OG	2.28	0.42
1:u:23:LEU:HD11	1:u:60:VAL:HG13	2.00	0.42
1:y:184:SER:HG	1:z:169:ARG:HE	1.68	0.42
3:A:377:GLU:H	3:A:377:GLU:HG2	1.57	0.42
3:C:323:THR:OG1	3:C:324:SER:N	2.52	0.42
3:D:103:ASP:OD2	3:D:105:SER:OG	2.36	0.42
3:I:490:LEU:HA	3:I:491:PRO:HD3	1.89	0.42
3:K:360:GLU:HB2	3:L:485:PRO:HG3	2.00	0.42
3:M:189:PHE:HA	3:M:276:ASN:HD21	1.83	0.42
3:N:38:LYS:HA	3:N:69:THR:HG23	2.00	0.42
3:N:263:ALA:HB3	3:N:266:ASN:HB2	2.02	0.42
3:N:387:ARG:HE	3:N:389:PHE:HE1	1.68	0.42
8:BA:73:ALA:HA	8:BA:76:ILE:HG22	2.01	0.42
1:AG:146:VAL:HB	1:AG:178:VAL:HG12	2.00	0.42
3:Q:129:SER:OG	3:Q:130:GLY:N	2.52	0.42
2:S:235:TRP:CD2	2:S:282:LEU:HD11	2.54	0.42
2:S:334:VAL:HG23	1:p:164:ILE:HG21	2.01	0.42
2:k:363:ASP:OD2	2:k:363:ASP:N	2.50	0.42
1:z:23:LEU:HD13	1:z:72:ILE:HD11	2.02	0.42
4:0:49:ASN:N	4:0:49:ASN:OD1	2.50	0.42
4:1:85:ILE:HG22	7:AO:42:ILE:HG21	2.01	0.42
8:AU:58:ARG:HA	8:AU:58:ARG:HD3	1.81	0.42
3:B:178:GLN:O	3:C:223:GLY:N	2.52	0.42
3:F:109:ASN:N	3:F:109:ASN:OD1	2.53	0.42
3:I:114:LEU:HG	3:I:147:PHE:HE1	1.85	0.42
3:J:377:GLU:H	3:J:377:GLU:HG2	1.51	0.42
8:BE:9:LEU:HA	8:BE:12:VAL:HG22	2.02	0.42
8:BE:17:ASP:OD1	8:BE:57:TYR:OH	2.37	0.42
8:BE:31:LEU:HD11	8:BJ:12:VAL:HG23	2.02	0.42
1:AA:82:ARG:H	1:AA:82:ARG:HG2	1.68	0.42
1:AB:51:SER:OG	1:AB:55:GLY:O	2.34	0.42
1:AC:29:GLN:O	1:AC:33:ASN:ND2	2.53	0.42
1:AH:160:LEU:HD12	2:j:337:LEU:HD21	2.02	0.42
2:T:173:LEU:HD12	2:T:176:LEU:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:331:LEU:HD23	2:U:361:LEU:HD13	2.00	0.42
2:e:246:TYR:OH	2:e:296:ASP:OD1	2.36	0.42
1:s:82:ARG:HA	1:t:115:GLN:HE22	1.84	0.42
1:y:39:LEU:HB3	1:y:44:ILE:HG13	2.01	0.42
1:AJ:139:ASN:HD22	1:AJ:141:ARG:NH1	2.18	0.42
5:5:140:ASN:OD1	5:5:140:ASN:N	2.53	0.42
7:AP:41:ALA:HA	7:AP:44:THR:HG22	2.01	0.42
8:AT:36:ALA:O	8:BE:5:TRP:NE1	2.32	0.42
3:C:286:GLN:HA	3:C:289:PHE:HB2	2.01	0.42
3:G:143:ARG:HG3	3:G:252:MET:N	2.34	0.42
3:J:295:LYS:HA	3:J:295:LYS:HD3	1.85	0.42
3:P:520:ASP:OD2	3:P:520:ASP:N	2.44	0.42
1:AC:191:SER:OG	1:AC:192:ASP:N	2.51	0.42
1:AG:102:LYS:HE3	1:AG:134:ILE:HA	2.02	0.42
2:R:244:ALA:HB3	2:R:265:ASN:HD21	1.85	0.42
2:g:249:HIS:HB2	2:g:257:VAL:HG22	2.01	0.42
2:m:200:ASN:OD1	2:m:200:ASN:N	2.51	0.42
1:v:39:LEU:HD22	1:v:44:ILE:HD11	2.00	0.42
1:AK:31:GLN:HG2	1:AK:79:PRO:HD2	2.02	0.42
6:7:66:TRP:HA	6:7:69:GLU:HG2	2.02	0.42
3:B:38:LYS:HA	3:B:69:THR:HG23	2.00	0.42
3:B:155:TYR:HA	3:B:158:MET:HE2	2.00	0.42
3:D:419:ASP:HB3	3:D:421:GLN:HE22	1.83	0.42
3:G:252:MET:HE3	3:G:255:GLN:HB3	2.01	0.42
3:I:386:ASN:OD1	3:I:386:ASN:N	2.53	0.42
3:N:91:ILE:HG13	3:N:102:TYR:HB2	2.01	0.42
3:N:304:VAL:HG11	3:N:422:ILE:HG21	2.02	0.42
2:V:179:GLN:N	1:s:196:GLN:OE1	2.53	0.42
2:V:381:MET:HE3	2:V:381:MET:HB3	1.78	0.42
2:k:304:GLU:OE2	2:k:314:TYR:OH	2.35	0.42
1:p:25:LYS:H	1:q:29:GLN:NE2	2.17	0.42
1:s:22:ASP:HA	1:s:59:THR:HA	2.00	0.42
1:v:203:LYS:HE3	1:v:203:LYS:HB3	1.88	0.42
1:z:168:LYS:HE2	1:z:183:ILE:HB	2.01	0.42
4:0:55:VAL:HG21	5:5:174:ILE:HD11	2.01	0.42
4:0:207:GLY:HA2	4:0:210:LEU:HD12	2.02	0.42
4:2:159:PHE:HE1	4:3:208:TRP:HE1	1.68	0.42
3:A:419:ASP:HB3	3:A:421:GLN:HE22	1.85	0.42
3:B:197:LEU:O	3:B:411:ARG:NH1	2.47	0.42
3:B:521:PRO:HG3	3:C:462:PRO:HD2	2.02	0.42
3:F:283:THR:H	3:F:286:GLN:HE21	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:386:ASN:OD1	3:F:386:ASN:N	2.51	0.42
3:G:310:ILE:HG22	3:G:511:PHE:HD1	1.85	0.42
3:G:522:LEU:HD11	3:H:468:LEU:H	1.85	0.42
3:I:526:ALA:HB2	3:J:512:MET:HE2	2.01	0.42
3:J:139:ARG:O	3:J:148:TYR:N	2.50	0.42
3:M:301:LYS:O	3:N:460:ARG:NH2	2.44	0.42
1:AD:31:GLN:NE2	1:AD:79:PRO:O	2.53	0.42
2:S:246:TYR:OH	2:S:296:ASP:OD1	2.31	0.42
2:T:235:TRP:CD2	2:T:282:LEU:HD11	2.54	0.42
2:V:364:ASP:OD1	2:V:364:ASP:N	2.49	0.42
2:Y:194:LEU:HD12	2:Y:194:LEU:HA	1.89	0.42
2:Z:267:MET:SD	2:Z:267:MET:N	2.93	0.42
2:l:363:ASP:HB3	1:AJ:180:TYR:HD2	1.85	0.42
6:8:14:LEU:HA	6:8:17:ILE:HG22	2.02	0.42
7:AP:83:MET:HE3	7:AP:83:MET:HB2	1.97	0.42
8:AU:32:ASP:OD2	8:AU:32:ASP:N	2.48	0.42
3:B:368:VAL:HG13	3:C:475:ASP:HB2	2.02	0.42
3:F:438:SER:HB2	3:F:443:SER:HB2	2.02	0.42
3:F:456:SER:O	3:F:456:SER:OG	2.37	0.42
3:I:178:GLN:O	3:J:223:GLY:N	2.52	0.42
3:M:158:MET:HE3	3:M:158:MET:HB3	1.80	0.42
3:M:338:SER:HB2	3:M:344:ILE:HD11	2.01	0.42
3:N:289:PHE:HA	3:N:292:MET:HE2	2.02	0.42
3:O:387:ARG:HE	3:O:389:PHE:HE1	1.67	0.42
3:P:482:GLN:HB3	3:P:499:TYR:HB3	2.02	0.42
8:BT:31:LEU:HA	8:BT:34:LEU:HG	2.01	0.42
1:AB:94:LEU:HG	1:AB:95:VAL:HG22	2.01	0.42
2:E:356:GLN:NE2	2:R:310:GLN:OE1	2.52	0.42
2:V:327:ILE:HG13	2:V:359:ILE:HA	2.01	0.42
2:n:235:TRP:HE3	2:n:236:LEU:HD12	1.84	0.42
2:n:271:GLU:HA	2:n:274:VAL:HG22	2.01	0.42
1:r:127:ARG:HB2	1:r:151:LEU:HD11	2.02	0.42
1:u:133:ASP:OD1	1:u:133:ASP:N	2.52	0.42
4:4:5:ILE:HG22	4:4:8:ILE:HD12	2.01	0.42
3:B:383:PHE:HB3	3:B:410:ILE:HG13	2.02	0.42
3:B:539:ALA:HA	3:D:504:LYS:HD2	2.01	0.42
3:C:141:ASP:HB3	3:C:144:LYS:HB2	2.02	0.42
3:G:345:SER:O	8:BU:22:ASN:HB3	2.20	0.42
3:G:377:GLU:H	3:G:377:GLU:HG2	1.58	0.42
3:H:85:SER:HA	3:H:90:LEU:HD13	2.01	0.42
3:H:362:LYS:HZ3	3:H:363:LYS:H	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:283:THR:H	3:I:286:GLN:HE21	1.68	0.42
3:J:187:ASN:O	3:J:301:LYS:NZ	2.52	0.42
3:J:392:LYS:O	3:K:320:ARG:NH2	2.53	0.42
3:N:144:LYS:HD2	3:N:144:LYS:HA	1.87	0.42
3:O:177:ARG:NH1	3:P:260:GLN:OE1	2.52	0.42
8:BK:21:ASP:HB3	8:BQ:5:TRP:HB2	2.02	0.42
8:BF:15:LYS:HA	8:BF:18:THR:HG22	2.02	0.42
8:BA:55:ASN:O	8:BA:59:ASN:ND2	2.53	0.42
2:R:230:LYS:HB3	2:R:230:LYS:HE2	1.85	0.42
2:T:224:ASN:HB3	2:T:227:GLU:HG2	2.02	0.42
2:W:363:ASP:OD1	2:W:363:ASP:N	2.44	0.42
2:l:217:ASP:OD1	2:l:217:ASP:N	2.40	0.42
2:m:387:TYR:HD1	3:L:69:THR:HG23	1.84	0.42
4:2:36:MET:HE3	4:2:36:MET:HB2	1.97	0.42
4:4:61:MET:HE2	4:4:61:MET:HB2	1.90	0.42
3:D:377:GLU:H	3:D:377:GLU:HG2	1.47	0.42
3:G:161:ASN:HA	3:G:164:THR:HG22	2.02	0.42
3:I:108:ARG:HH12	3:I:153:PRO:HB3	1.83	0.42
3:J:415:ARG:NH1	3:J:416:PHE:O	2.53	0.42
3:M:120:ASN:O	3:M:124:ASN:ND2	2.48	0.42
3:M:310:ILE:HG23	3:M:369:SER:HB2	2.02	0.42
8:BB:26:GLN:HE22	8:BH:5:TRP:H	1.66	0.42
1:AG:37:ALA:HB2	1:AH:69:VAL:HG22	2.02	0.41
1:AH:203:LYS:HE2	1:AH:203:LYS:HB2	1.94	0.41
3:Q:158:MET:HE3	3:Q:158:MET:HB3	1.89	0.41
2:S:243:LEU:HD12	2:S:243:LEU:HA	1.84	0.41
2:W:354:TYR:CD2	2:W:355:VAL:HG13	2.55	0.41
2:i:262:ARG:HB2	2:i:293:LEU:HB3	2.00	0.41
2:j:217:ASP:OD1	2:j:217:ASP:N	2.53	0.41
1:p:30:GLU:HA	1:p:33:ASN:HD21	1.85	0.41
1:p:64:ASP:OD2	1:p:64:ASP:N	2.34	0.41
1:r:72:ILE:HD13	1:r:77:LEU:HD23	2.02	0.41
1:r:155:GLU:CD	1:r:190:ARG:HE	2.28	0.41
1:u:117:LEU:HA	1:u:117:LEU:HD23	1.85	0.41
1:v:88:MET:HG3	1:w:108:ALA:HB2	2.01	0.41
4:0:154:GLU:OE1	4:0:219:TYR:OH	2.38	0.41
4:4:180:LEU:HD22	4:4:190:PRO:HB3	2.01	0.41
3:L:339:LEU:HG	3:L:340:ASN:OD1	2.20	0.41
3:M:306:LEU:HD12	3:M:306:LEU:HA	1.90	0.41
3:P:303:HIS:HB3	3:P:374:LEU:HD12	2.02	0.41
3:Q:97:GLN:NE2	3:A:139:ARG:HE	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:177:LEU:HD23	2:V:210:VAL:HG21	2.02	0.41
2:Y:246:TYR:OH	2:Y:296:ASP:OD1	2.35	0.41
1:t:151:LEU:HD13	1:t:186:VAL:HG23	2.02	0.41
4:0:62:PHE:HB3	4:0:220:MET:HE1	2.01	0.41
4:4:3:ASN:O	4:4:6:SER:OG	2.30	0.41
6:8:76:ARG:HA	6:8:79:ILE:HD11	2.02	0.41
8:AU:53:GLU:HG3	8:BA:9:LEU:HD12	2.02	0.41
8:AX:52:SER:HA	8:AX:55:ASN:HD21	1.85	0.41
3:C:158:MET:HE3	3:C:158:MET:HB3	1.98	0.41
3:F:541:SER:O	3:F:541:SER:OG	2.34	0.41
3:I:49:MET:HE3	3:I:77:PRO:HB3	2.02	0.41
3:K:196:ASN:HB3	8:BM:4:PRO:HD3	2.01	0.41
3:N:373:LEU:HD22	3:N:383:PHE:HB2	2.01	0.41
3:P:203:VAL:HG12	8:BK:3:THR:HG21	2.01	0.41
3:P:313:LEU:HD13	3:P:313:LEU:HA	1.89	0.41
3:P:386:ASN:OD1	3:P:386:ASN:N	2.54	0.41
8:BM:67:VAL:HG22	8:BS:80:ARG:HB3	2.01	0.41
1:AI:78:PRO:HA	1:AI:79:PRO:HD3	1.88	0.41
2:W:217:ASP:OD1	2:W:217:ASP:N	2.43	0.41
2:a:316:ARG:HH21	2:a:318:ASN:HD21	1.68	0.41
2:e:354:TYR:CD2	2:e:355:VAL:HG13	2.55	0.41
2:l:270:LYS:HD3	2:l:270:LYS:HA	1.86	0.41
1:p:155:GLU:OE2	1:p:156:ARG:N	2.52	0.41
1:p:168:LYS:NZ	1:p:183:ILE:HG23	2.34	0.41
1:q:114:GLU:HB2	1:q:128:VAL:HG22	2.02	0.41
1:AJ:136:ALA:HB1	1:AJ:143:PRO:HA	2.02	0.41
4:2:48:SER:OG	4:2:50:MET:N	2.48	0.41
4:3:5:ILE:HG21	7:AQ:41:ALA:HA	2.02	0.41
8:AW:44:LEU:HA	8:AW:47:TYR:HB3	2.02	0.41
3:D:306:LEU:HD12	3:D:513:ILE:HD11	2.02	0.41
3:H:97:GLN:HE22	3:I:139:ARG:HE	1.66	0.41
3:J:386:ASN:OD1	3:J:386:ASN:N	2.53	0.41
3:K:220:GLN:O	3:K:264:ALA:N	2.54	0.41
3:N:419:ASP:HB2	3:N:421:GLN:HE22	1.84	0.41
8:BK:26:GLN:HA	8:BK:29:GLU:HG3	2.02	0.41
3:Q:97:GLN:HE22	3:A:139:ARG:HE	1.67	0.41
3:Q:114:LEU:HD12	3:Q:115:ARG:H	1.85	0.41
2:R:318:ASN:HA	2:R:323:VAL:HG23	2.02	0.41
2:Z:217:ASP:OD1	2:Z:217:ASP:N	2.46	0.41
2:l:317:ARG:HB2	2:l:324:THR:HG23	2.01	0.41
1:w:117:LEU:HD23	1:w:117:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:74:THR:HG23	1:z:75:TYR:HD1	1.86	0.41
7:AN:54:ARG:NH1	7:AN:66:GLU:OE2	2.53	0.41
3:A:114:LEU:HD21	3:A:163:ALA:HB1	2.01	0.41
3:A:269:ILE:HG23	3:A:280:VAL:HG12	2.02	0.41
3:A:386:ASN:OD1	3:A:386:ASN:N	2.54	0.41
3:C:472:TYR:N	3:C:509:ARG:O	2.53	0.41
3:L:197:LEU:HA	3:L:382:ILE:HD11	2.02	0.41
8:BI:27:VAL:HG22	8:BI:50:LYS:HG3	2.02	0.41
8:BQ:46:ALA:O	8:BQ:50:LYS:HG2	2.20	0.41
2:R:365:TRP:O	2:R:369:ARG:NH1	2.53	0.41
2:S:340:ARG:HH21	1:q:163:GLN:HE21	1.67	0.41
2:n:354:TYR:CD2	2:n:355:VAL:HG23	2.55	0.41
1:q:99:ARG:HE	1:q:134:ILE:HD12	1.86	0.41
1:r:78:PRO:HA	1:r:79:PRO:HD3	1.93	0.41
1:s:74:THR:HG23	1:s:75:TYR:HD1	1.85	0.41
1:u:39:LEU:HB3	1:u:44:ILE:HG13	2.00	0.41
1:w:28:ASP:H	1:w:31:GLN:HB2	1.86	0.41
1:z:159:PRO:HB2	1:z:162:HIS:HD2	1.86	0.41
1:AJ:173:ASN:HB2	1:AK:147:HIS:HB3	2.03	0.41
3:A:165:MET:HB3	3:B:113:SER:HB3	2.02	0.41
3:A:536:GLN:NE2	3:P:545:LYS:O	2.52	0.41
3:C:391:THR:HG21	3:C:446:ALA:HB1	2.02	0.41
3:F:320:ARG:HB2	3:F:359:LEU:HG	2.02	0.41
3:L:39:ASP:H	3:L:69:THR:HB	1.85	0.41
3:L:97:GLN:HE22	3:M:139:ARG:HE	1.68	0.41
3:L:544:ASP:OD2	3:L:547:GLN:N	2.51	0.41
3:M:339:LEU:HG	3:M:340:ASN:OD1	2.21	0.41
8:BJ:27:VAL:HG21	8:BJ:54:TYR:HB2	2.03	0.41
8:BF:77:GLN:HE22	8:BF:80:ARG:HH22	1.68	0.41
8:BC:55:ASN:O	8:BC:59:ASN:ND2	2.54	0.41
1:AF:117:LEU:HD23	1:AF:117:LEU:HA	1.79	0.41
2:R:227:GLU:HA	2:R:230:LYS:HG2	2.03	0.41
2:S:200:ASN:OD1	2:S:200:ASN:N	2.54	0.41
2:T:187:LEU:HD22	2:T:285:TYR:HB2	2.02	0.41
2:U:320:LYS:HA	2:U:320:LYS:HD2	1.79	0.41
2:b:201:GLU:OE1	2:b:224:ASN:ND2	2.49	0.41
2:e:307:LEU:HD12	2:e:307:LEU:HA	1.94	0.41
1:r:191:SER:OG	1:r:192:ASP:N	2.53	0.41
1:u:147:HIS:NE2	1:v:176:ALA:O	2.54	0.41
1:u:156:ARG:HH21	1:u:191:SER:C	2.29	0.41
1:w:124:LEU:HB2	1:w:153:VAL:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:168:LYS:HE3	1:w:183:ILE:HB	2.02	0.41
4:3:15:THR:HG22	7:AP:90:LYS:HD2	2.03	0.41
3:D:276:ASN:HD22	3:F:378:ASN:ND2	2.18	0.41
3:H:306:LEU:HD21	3:H:513:ILE:HD11	2.02	0.41
3:K:121:GLU:N	3:K:121:GLU:OE2	2.53	0.41
8:BN:9:LEU:HA	8:BN:12:VAL:HG22	2.02	0.41
8:BN:22:ASN:OD1	8:BN:26:GLN:NE2	2.53	0.41
1:AG:36:ILE:HG22	1:AG:46:ALA:HB3	2.02	0.41
1:AH:29:GLN:HE21	1:AI:25:LYS:H	1.69	0.41
3:Q:144:LYS:HD3	3:Q:144:LYS:HA	1.91	0.41
2:T:223:ILE:HB	2:T:228:GLU:HG2	2.02	0.41
2:d:267:MET:HE2	2:d:271:GLU:HB3	2.03	0.41
2:g:270:LYS:HA	2:g:270:LYS:HD3	1.79	0.41
2:l:385:HIS:CD2	2:m:313:PRO:HB3	2.56	0.41
1:q:30:GLU:HA	1:q:33:ASN:HD21	1.85	0.41
8:AT:59:ASN:O	8:AT:63:ASN:ND2	2.45	0.41
3:B:323:THR:HB	3:B:356:VAL:HG12	2.02	0.41
3:D:399:VAL:HG21	3:F:440:THR:HA	2.02	0.41
3:F:440:THR:O	3:F:443:SER:OG	2.38	0.41
3:G:308:LEU:HD11	3:G:428:ILE:HD13	2.03	0.41
3:I:158:MET:HE3	3:I:158:MET:HB3	1.77	0.41
3:K:547:GLN:HB2	3:M:315:LYS:HZ1	1.86	0.41
3:O:170:ASN:HB3	3:O:254:LEU:HD22	2.02	0.41
1:AA:30:GLU:HA	1:AA:33:ASN:HD21	1.85	0.41
1:AC:24:LEU:HD21	1:AC:58:ILE:HD12	2.03	0.41
1:AC:171:LEU:HD23	1:AC:171:LEU:HA	1.85	0.41
1:AF:148:LEU:HD12	1:AF:171:LEU:HD13	2.02	0.41
2:E:174:ASP:OD1	2:E:174:ASP:N	2.54	0.41
2:S:173:LEU:HD11	2:S:216:TYR:CZ	2.54	0.41
2:S:202:ARG:NH2	1:p:194:GLN:HB2	2.35	0.41
2:X:376:GLU:HB3	3:A:87:GLN:HE22	1.86	0.41
2:c:334:VAL:HG12	1:z:164:ILE:HG21	2.02	0.41
2:m:380:LYS:HE3	2:m:380:LYS:HB3	1.76	0.41
1:p:72:ILE:HD13	1:p:77:LEU:HD12	2.02	0.41
1:AJ:36:ILE:HG23	1:AK:69:VAL:HG21	2.03	0.41
4:1:47:PRO:HG2	4:1:52:LEU:HD21	2.03	0.41
5:5:233:PRO:HG2	5:5:234:VAL:HG23	2.02	0.41
6:8:24:ILE:HD13	6:8:24:ILE:HA	1.90	0.41
3:A:281:LYS:HE2	3:A:281:LYS:HB2	1.86	0.41
3:I:281:LYS:HE2	3:I:281:LYS:HB2	1.89	0.41
3:K:36:VAL:HA	3:K:71:ASN:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:162:ALA:HA	3:M:165:MET:HG2	2.02	0.41
3:O:153:PRO:HA	3:O:156:VAL:HG22	2.03	0.41
3:O:482:GLN:O	3:O:499:TYR:N	2.54	0.41
8:BD:62:SER:HB3	8:BI:75:ILE:HD12	2.02	0.41
8:BL:39:SER:O	8:BL:39:SER:OG	2.32	0.41
8:BN:28:THR:HA	8:BN:31:LEU:HG	2.02	0.41
1:AG:164:ILE:HG13	1:AG:185:VAL:HB	2.03	0.41
3:Q:38:LYS:HG2	2:W:388:PHE:HE2	1.85	0.41
2:V:295:ASP:OD2	2:V:296:ASP:N	2.51	0.41
2:X:363:ASP:OD1	2:X:363:ASP:N	2.45	0.41
2:b:283:MET:HA	2:b:284:PRO:HD3	1.90	0.41
2:e:229:ASN:O	2:e:233:SER:OG	2.30	0.41
2:f:236:LEU:HD12	2:f:236:LEU:HA	1.92	0.41
2:f:272:LEU:HD23	2:f:272:LEU:HA	1.93	0.41
2:g:200:ASN:OD1	2:g:200:ASN:N	2.53	0.41
2:h:224:ASN:N	2:h:227:GLU:OE2	2.54	0.41
2:i:221:ARG:HE	2:i:221:ARG:HB3	1.57	0.41
2:m:191:ASP:OD1	2:m:191:ASP:N	2.51	0.41
2:m:209:GLN:HE22	2:m:213:ARG:NH2	2.18	0.41
1:o:127:ARG:HE	1:p:119:THR:HG21	1.86	0.41
1:t:23:LEU:HD23	1:t:24:LEU:HG	2.03	0.41
1:t:51:SER:O	1:t:51:SER:OG	2.32	0.41
1:u:135:ASP:OD1	1:u:135:ASP:N	2.41	0.41
4:0:5:ILE:HD12	4:0:5:ILE:HA	1.94	0.41
4:1:46:ILE:HA	4:1:47:PRO:HA	1.87	0.41
4:3:109:ARG:O	4:3:113:GLN:HG2	2.21	0.41
4:4:171:VAL:HG21	6:9:14:LEU:HD23	2.01	0.41
5:5:4:ALA:O	5:5:8:GLU:HG3	2.20	0.41
8:AV:31:LEU:O	8:AV:35:ALA:N	2.52	0.41
8:AW:24:GLN:O	8:AW:28:THR:OG1	2.32	0.41
3:D:76:ASP:N	3:D:76:ASP:OD2	2.54	0.41
3:D:118:SER:OG	3:D:119:LEU:N	2.53	0.41
3:G:177:ARG:NH2	3:H:222:LEU:O	2.54	0.41
3:G:456:SER:O	3:G:456:SER:OG	2.37	0.41
3:H:212:GLU:OE1	3:H:212:GLU:N	2.53	0.41
3:I:421:GLN:HG3	3:I:462:PRO:HA	2.01	0.41
3:K:377:GLU:H	3:K:377:GLU:HG2	1.63	0.41
3:L:281:LYS:NZ	3:M:218:GLU:OE2	2.54	0.41
3:L:293:LEU:O	3:L:297:LEU:HG	2.21	0.41
3:N:109:ASN:N	3:N:109:ASN:OD1	2.52	0.41
8:BM:48:GLN:HA	8:BM:51:LEU:HG	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:123:VAL:H	1:AI:123:VAL:HG22	1.70	0.41
2:U:340:ARG:HH21	1:s:163:GLN:HE21	1.67	0.41
2:W:262:ARG:HB2	2:W:293:LEU:HB3	2.03	0.41
2:X:366:LEU:HD23	2:X:366:LEU:H	1.85	0.41
2:a:245:TYR:HB3	2:a:260:LEU:HD12	2.01	0.41
2:a:271:GLU:H	2:a:271:GLU:HG2	1.73	0.41
2:d:262:ARG:HA	2:d:293:LEU:HD23	2.03	0.41
2:j:340:ARG:HH11	2:j:340:ARG:HD3	1.75	0.41
1:s:110:GLU:HB2	1:s:128:VAL:HG23	2.02	0.41
1:z:179:ASP:OD1	1:z:182:ASN:N	2.53	0.41
4:1:53:ASN:ND2	7:AN:99:LEU:O	2.54	0.41
4:2:146:LEU:O	4:2:150:TYR:N	2.53	0.41
4:2:171:VAL:HG21	6:7:14:LEU:HD12	2.02	0.41
7:AN:48:LYS:O	7:AN:52:THR:OG1	2.26	0.41
3:A:133:ASN:HD22	3:A:136:TYR:HD2	1.67	0.41
3:I:41:SER:HB3	3:I:67:LYS:HZ2	1.86	0.41
3:K:512:MET:HE2	3:K:512:MET:HB2	1.97	0.41
3:M:49:MET:HG3	3:M:74:PHE:CD1	2.56	0.41
1:AC:147:HIS:HB3	1:AL:173:ASN:HB2	2.03	0.40
1:AH:78:PRO:HA	1:AH:79:PRO:HD3	1.91	0.40
2:R:172:GLU:O	2:R:176:LEU:HD23	2.22	0.40
2:U:252:GLU:HA	2:U:253:PRO:HD3	1.95	0.40
2:U:260:LEU:HD13	2:U:291:ILE:HG23	2.03	0.40
2:U:372:GLN:HB2	3:O:35:PHE:HD1	1.85	0.40
2:a:367:LYS:O	3:B:38:LYS:NZ	2.39	0.40
2:b:214:GLY:O	1:y:203:LYS:NZ	2.54	0.40
2:j:188:PRO:HA	2:j:194:LEU:HD12	2.02	0.40
1:q:182:ASN:C	1:r:173:ASN:HD22	2.29	0.40
1:t:27:LEU:HD23	1:t:31:GLN:HB3	2.03	0.40
4:0:101:ASP:HA	4:0:104:ILE:HG22	2.03	0.40
4:1:3:ASN:O	4:1:6:SER:OG	2.33	0.40
4:4:78:GLU:H	4:4:78:GLU:HG2	1.68	0.40
6:8:23:THR:O	6:8:27:THR:OG1	2.29	0.40
7:AN:58:PRO:HA	7:AN:61:VAL:HG22	2.02	0.40
7:AQ:72:GLU:O	7:AQ:75:SER:OG	2.30	0.40
8:AU:35:ALA:HB1	8:AZ:19:GLY:HA3	2.02	0.40
8:AX:35:ALA:HB1	8:BC:19:GLY:HA3	2.02	0.40
3:A:216:GLN:O	3:P:268:LYS:NZ	2.54	0.40
3:A:218:GLU:H	8:BE:4:PRO:HD3	1.87	0.40
3:I:401:LEU:HD23	3:I:401:LEU:HA	1.91	0.40
3:O:158:MET:HE3	3:O:158:MET:HB3	1.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BF:75:ILE:HD11	8:BA:58:ARG:HB3	2.02	0.40
8:BP:39:SER:OG	8:BU:53:GLU:OE2	2.32	0.40
8:BV:66:LYS:HD3	8:BV:66:LYS:HA	1.86	0.40
1:AC:72:ILE:HD13	1:AC:77:LEU:HD12	2.02	0.40
2:E:227:GLU:HA	2:E:230:LYS:HE2	2.03	0.40
2:U:262:ARG:HA	2:U:293:LEU:HD23	2.03	0.40
2:e:380:LYS:HE3	2:e:380:LYS:HB3	1.93	0.40
2:g:252:GLU:HA	2:g:253:PRO:HD3	1.80	0.40
2:k:326:VAL:HA	2:k:358:ALA:HB3	2.03	0.40
1:o:27:LEU:HD23	1:o:27:LEU:HA	1.93	0.40
1:p:46:ALA:HB1	1:p:58:ILE:HD11	2.02	0.40
1:p:186:VAL:HG11	1:q:170:PHE:HB2	2.03	0.40
1:w:88:MET:HB3	1:w:88:MET:HE2	1.83	0.40
1:x:169:ARG:HA	1:x:169:ARG:HD2	1.83	0.40
1:y:172:LYS:NZ	1:y:178:VAL:O	2.54	0.40
1:AK:130:ILE:HD12	1:AK:130:ILE:HA	1.90	0.40
4:1:146:LEU:H	4:1:146:LEU:HG	1.77	0.40
7:AM:86:THR:O	7:AM:90:LYS:NZ	2.49	0.40
3:A:126:LEU:HB3	3:A:132:TYR:HB2	2.03	0.40
3:D:456:SER:O	3:D:456:SER:OG	2.37	0.40
3:F:116:ASN:OD1	3:F:116:ASN:N	2.51	0.40
3:G:413:LEU:HB3	3:G:425:SER:OG	2.21	0.40
3:G:431:GLY:HA2	3:G:450:VAL:HG23	2.02	0.40
3:H:176:GLY:O	3:I:220:GLN:NE2	2.46	0.40
3:H:353:ILE:HA	3:I:336:GLY:H	1.85	0.40
3:M:322:GLY:HA3	3:M:499:TYR:HA	2.03	0.40
3:O:546:LEU:HD12	3:P:536:GLN:HG2	2.02	0.40
3:P:286:GLN:HA	3:P:289:PHE:HB2	2.02	0.40
8:BG:44:LEU:HB3	8:BR:75:ILE:HD13	2.04	0.40
1:AC:27:LEU:HD12	1:AC:27:LEU:HA	1.94	0.40
1:AC:144:LYS:HZ1	1:AL:177:ASP:CG	2.29	0.40
1:AC:194:GLN:HB2	2:f:202:ARG:HH22	1.87	0.40
1:AD:104:ARG:HG2	1:AL:88:MET:HB3	2.03	0.40
1:AG:112:ARG:HG2	1:AH:129:HIS:HE1	1.86	0.40
2:U:376:GLU:HB3	3:P:87:GLN:HE22	1.87	0.40
2:h:243:LEU:HD12	2:h:243:LEU:HA	1.96	0.40
1:o:78:PRO:HA	1:o:79:PRO:HD3	1.96	0.40
1:v:106:TYR:HD1	1:v:109:ILE:HD12	1.87	0.40
1:y:179:ASP:OD1	1:y:182:ASN:ND2	2.55	0.40
4:4:183:LEU:HD21	6:9:56:VAL:HG21	2.04	0.40
6:9:9:ASN:O	6:9:13:TYR:N	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AN:85:SER:OG	7:AN:86:THR:N	2.54	0.40
7:AR:68:ALA:HA	7:AR:71:GLN:HB3	2.03	0.40
3:A:116:ASN:ND2	3:A:170:ASN:HB2	2.36	0.40
3:A:387:ARG:NH1	3:B:450:VAL:HA	2.36	0.40
3:C:316:SER:HB3	3:C:363:LYS:HE3	2.03	0.40
3:C:386:ASN:OD1	3:C:386:ASN:N	2.55	0.40
3:D:283:THR:H	3:D:286:GLN:NE2	2.19	0.40
3:F:305:GLU:HA	3:F:374:LEU:HA	2.03	0.40
3:G:442:THR:O	3:G:446:ALA:N	2.54	0.40
3:H:390:TYR:CD1	3:H:403:HIS:HB3	2.56	0.40
3:M:463:HIS:CD2	3:M:517:GLU:H	2.39	0.40
3:O:114:LEU:HD23	3:O:147:PHE:HE1	1.87	0.40
3:O:306:LEU:HD21	3:O:373:LEU:HB3	2.02	0.40
3:P:388:THR:HG22	3:P:405:THR:HG22	2.02	0.40
8:BG:27:VAL:HG11	8:BG:54:TYR:HB2	2.04	0.40
8:BC:55:ASN:OD1	8:BC:59:ASN:ND2	2.52	0.40
1:AG:117:LEU:O	1:AG:123:VAL:HG21	2.21	0.40
1:AI:58:ILE:HD13	1:AI:58:ILE:HA	1.93	0.40
1:AL:35:VAL:HB	1:AL:77:LEU:HD21	2.02	0.40
2:f:248:ILE:HG12	2:f:258:PHE:CD1	2.55	0.40
2:n:200:ASN:OD1	2:n:200:ASN:N	2.53	0.40
1:y:72:ILE:HD12	1:y:77:LEU:HD23	2.04	0.40
1:z:160:LEU:HD23	1:z:160:LEU:H	1.87	0.40
4:0:208:TRP:HB2	5:5:175:ASN:CG	2.47	0.40
4:3:69:HIS:CE1	7:AP:32:ARG:HH12	2.39	0.40
4:4:34:PHE:HA	4:4:37:VAL:HG12	2.03	0.40
5:5:94:VAL:O	5:5:98:LEU:N	2.54	0.40
6:7:28:ILE:O	6:7:32:LEU:N	2.54	0.40
8:AW:52:SER:HB2	8:BC:69:LYS:HD2	2.04	0.40
3:A:252:MET:HE3	3:A:255:GLN:HB2	2.04	0.40
3:A:304:VAL:HG21	3:A:422:ILE:HG21	2.03	0.40
3:B:290:ILE:HA	3:B:293:LEU:HD12	2.03	0.40
3:B:453:THR:OG1	3:B:509:ARG:NH1	2.44	0.40
3:B:482:GLN:O	3:B:499:TYR:N	2.55	0.40
3:D:308:LEU:HD21	3:D:511:PHE:HB3	2.03	0.40
3:D:315:LYS:HA	3:D:364:GLN:HA	2.03	0.40
3:D:376:GLN:HE21	3:F:459:ALA:HA	1.87	0.40
3:I:198:ARG:HA	8:BH:25:THR:HG21	2.03	0.40
3:J:286:GLN:HA	3:J:289:PHE:HB2	2.03	0.40
3:N:201:LYS:O	8:BF:22:ASN:ND2	2.33	0.40
3:O:421:GLN:HG3	3:O:462:PRO:HA	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BA:10:ASP:O	8:BA:14:ALA:N	2.54	0.40
2:T:209:GLN:HE22	1:r:195:LEU:HD22	1.87	0.40
2:b:193:MET:HE3	2:b:193:MET:HB2	1.94	0.40
2:h:227:GLU:HG3	2:h:227:GLU:H	1.79	0.40
2:h:349:THR:HG23	2:h:350:TRP:CD1	2.57	0.40
2:m:307:LEU:HD23	2:m:307:LEU:HA	1.92	0.40
1:v:24:LEU:HD13	1:v:27:LEU:HD21	2.04	0.40
8:AW:56:LEU:HD13	8:AW:56:LEU:HA	1.96	0.40
3:A:76:ASP:OD1	3:A:76:ASP:N	2.52	0.40
3:C:283:THR:H	3:C:286:GLN:HE21	1.70	0.40
3:J:114:LEU:HD23	3:J:114:LEU:HA	1.87	0.40
3:J:269:ILE:HD11	3:J:278:LEU:HD12	2.02	0.40
8:BU:16:PHE:HB3	8:BU:57:TYR:HE1	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	AA	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	AB	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	AC	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	AD	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AE	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	AF	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AG	182/252 (72%)	173 (95%)	9 (5%)	0	100	100
1	AH	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	AI	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	AJ	182/252 (72%)	176 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AK	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	AL	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	o	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	p	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	q	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	r	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
1	s	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	t	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	u	182/252 (72%)	178 (98%)	4 (2%)	0	100	100
1	v	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	w	182/252 (72%)	177 (97%)	5 (3%)	0	100	100
1	x	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
1	y	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
1	z	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
2	E	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
2	R	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
2	S	220/392 (56%)	208 (94%)	12 (6%)	0	100	100
2	T	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
2	U	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
2	V	220/392 (56%)	206 (94%)	14 (6%)	0	100	100
2	W	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
2	X	219/392 (56%)	211 (96%)	8 (4%)	0	100	100
2	Y	220/392 (56%)	206 (94%)	14 (6%)	0	100	100
2	Z	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
2	a	219/392 (56%)	214 (98%)	5 (2%)	0	100	100
2	b	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
2	c	220/392 (56%)	210 (96%)	10 (4%)	0	100	100
2	d	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
2	e	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
2	f	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
2	g	219/392 (56%)	213 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	220/392 (56%)	207 (94%)	13 (6%)	0	100	100
2	i	220/392 (56%)	212 (96%)	8 (4%)	0	100	100
2	j	219/392 (56%)	213 (97%)	6 (3%)	0	100	100
2	k	220/392 (56%)	206 (94%)	14 (6%)	0	100	100
2	l	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
2	m	219/392 (56%)	212 (97%)	7 (3%)	0	100	100
2	n	220/392 (56%)	209 (95%)	11 (5%)	0	100	100
3	A	491/562 (87%)	471 (96%)	20 (4%)	0	100	100
3	B	497/562 (88%)	474 (95%)	23 (5%)	0	100	100
3	C	491/562 (87%)	471 (96%)	20 (4%)	0	100	100
3	D	496/562 (88%)	473 (95%)	23 (5%)	0	100	100
3	F	491/562 (87%)	471 (96%)	20 (4%)	0	100	100
3	G	497/562 (88%)	472 (95%)	25 (5%)	0	100	100
3	H	491/562 (87%)	471 (96%)	20 (4%)	0	100	100
3	I	497/562 (88%)	477 (96%)	20 (4%)	0	100	100
3	J	491/562 (87%)	468 (95%)	23 (5%)	0	100	100
3	K	497/562 (88%)	473 (95%)	24 (5%)	0	100	100
3	L	491/562 (87%)	469 (96%)	22 (4%)	0	100	100
3	M	496/562 (88%)	472 (95%)	24 (5%)	0	100	100
3	N	491/562 (87%)	469 (96%)	22 (4%)	0	100	100
3	O	497/562 (88%)	474 (95%)	23 (5%)	0	100	100
3	P	491/562 (87%)	469 (96%)	22 (4%)	0	100	100
3	Q	143/562 (25%)	139 (97%)	4 (3%)	0	100	100
4	0	195/224 (87%)	189 (97%)	5 (3%)	1 (0%)	24	62
4	1	195/224 (87%)	188 (96%)	6 (3%)	1 (0%)	24	62
4	2	193/224 (86%)	186 (96%)	6 (3%)	1 (0%)	24	62
4	3	200/224 (89%)	195 (98%)	5 (2%)	0	100	100
4	4	220/224 (98%)	207 (94%)	13 (6%)	0	100	100
5	5	243/263 (92%)	224 (92%)	19 (8%)	0	100	100
6	6	49/86 (57%)	46 (94%)	3 (6%)	0	100	100
6	7	82/86 (95%)	80 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	8	82/86 (95%)	80 (98%)	1 (1%)	1 (1%)	10	42
6	9	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
7	AM	37/101 (37%)	37 (100%)	0	0	100	100
7	AN	79/101 (78%)	79 (100%)	0	0	100	100
7	AO	86/101 (85%)	84 (98%)	2 (2%)	0	100	100
7	AP	86/101 (85%)	86 (100%)	0	0	100	100
7	AQ	86/101 (85%)	86 (100%)	0	0	100	100
7	AR	86/101 (85%)	83 (96%)	3 (4%)	0	100	100
8	AS	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AT	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AU	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AV	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AW	57/80 (71%)	55 (96%)	2 (4%)	0	100	100
8	AX	71/80 (89%)	68 (96%)	3 (4%)	0	100	100
8	AY	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
8	AZ	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BA	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BB	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BC	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BD	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BE	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BF	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BG	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BH	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BI	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
8	BJ	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BK	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BL	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BM	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BN	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BO	76/80 (95%)	74 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BP	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BQ	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
8	BR	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
8	BS	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
8	BT	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BU	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
8	BV	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
All	All	21369/29181 (73%)	20501 (96%)	864 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	8	42	LEU
4	0	49	ASN
4	1	49	ASN
4	2	47	PRO

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	AA	155/215 (72%)	155 (100%)	0	100	100
1	AB	155/215 (72%)	154 (99%)	1 (1%)	78	81
1	AC	155/215 (72%)	155 (100%)	0	100	100
1	AD	155/215 (72%)	154 (99%)	1 (1%)	78	81
1	AE	155/215 (72%)	154 (99%)	1 (1%)	78	81
1	AF	155/215 (72%)	154 (99%)	1 (1%)	78	81
1	AG	155/215 (72%)	155 (100%)	0	100	100
1	AH	155/215 (72%)	155 (100%)	0	100	100
1	AI	155/215 (72%)	155 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AJ	155/215 (72%)	155 (100%)	0	100	100
1	AK	155/215 (72%)	154 (99%)	1 (1%)	78	81
1	AL	155/215 (72%)	155 (100%)	0	100	100
1	o	155/215 (72%)	152 (98%)	3 (2%)	50	66
1	p	155/215 (72%)	154 (99%)	1 (1%)	78	81
1	q	155/215 (72%)	154 (99%)	1 (1%)	78	81
1	r	155/215 (72%)	152 (98%)	3 (2%)	50	66
1	s	155/215 (72%)	155 (100%)	0	100	100
1	t	155/215 (72%)	154 (99%)	1 (1%)	78	81
1	u	155/215 (72%)	154 (99%)	1 (1%)	78	81
1	v	155/215 (72%)	155 (100%)	0	100	100
1	w	155/215 (72%)	155 (100%)	0	100	100
1	x	155/215 (72%)	155 (100%)	0	100	100
1	y	155/215 (72%)	153 (99%)	2 (1%)	61	73
1	z	155/215 (72%)	155 (100%)	0	100	100
2	E	190/337 (56%)	190 (100%)	0	100	100
2	R	189/337 (56%)	188 (100%)	1 (0%)	81	82
2	S	188/337 (56%)	187 (100%)	1 (0%)	81	82
2	T	190/337 (56%)	190 (100%)	0	100	100
2	U	189/337 (56%)	188 (100%)	1 (0%)	81	82
2	V	188/337 (56%)	187 (100%)	1 (0%)	81	82
2	W	190/337 (56%)	189 (100%)	1 (0%)	81	82
2	X	189/337 (56%)	188 (100%)	1 (0%)	81	82
2	Y	188/337 (56%)	188 (100%)	0	100	100
2	Z	190/337 (56%)	190 (100%)	0	100	100
2	a	189/337 (56%)	187 (99%)	2 (1%)	65	75
2	b	188/337 (56%)	187 (100%)	1 (0%)	81	82
2	c	190/337 (56%)	189 (100%)	1 (0%)	81	82
2	d	189/337 (56%)	187 (99%)	2 (1%)	65	75
2	e	188/337 (56%)	187 (100%)	1 (0%)	81	82
2	f	190/337 (56%)	190 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	g	189/337 (56%)	184 (97%)	5 (3%)	40	61
2	h	188/337 (56%)	187 (100%)	1 (0%)	81	82
2	i	190/337 (56%)	190 (100%)	0	100	100
2	j	189/337 (56%)	188 (100%)	1 (0%)	81	82
2	k	188/337 (56%)	188 (100%)	0	100	100
2	l	190/337 (56%)	190 (100%)	0	100	100
2	m	189/337 (56%)	187 (99%)	2 (1%)	65	75
2	n	188/337 (56%)	188 (100%)	0	100	100
3	A	420/477 (88%)	412 (98%)	8 (2%)	50	66
3	B	426/477 (89%)	418 (98%)	8 (2%)	50	66
3	C	420/477 (88%)	409 (97%)	11 (3%)	40	61
3	D	425/477 (89%)	415 (98%)	10 (2%)	43	63
3	F	420/477 (88%)	410 (98%)	10 (2%)	43	63
3	G	426/477 (89%)	418 (98%)	8 (2%)	50	66
3	H	420/477 (88%)	407 (97%)	13 (3%)	35	56
3	I	426/477 (89%)	420 (99%)	6 (1%)	59	72
3	J	420/477 (88%)	405 (96%)	15 (4%)	31	52
3	K	426/477 (89%)	417 (98%)	9 (2%)	47	64
3	L	420/477 (88%)	408 (97%)	12 (3%)	37	58
3	M	425/477 (89%)	418 (98%)	7 (2%)	55	69
3	N	420/477 (88%)	402 (96%)	18 (4%)	26	47
3	O	426/477 (89%)	419 (98%)	7 (2%)	55	69
3	P	420/477 (88%)	408 (97%)	12 (3%)	37	58
3	Q	125/477 (26%)	125 (100%)	0	100	100
4	0	175/199 (88%)	173 (99%)	2 (1%)	65	75
4	1	177/199 (89%)	175 (99%)	2 (1%)	65	75
4	2	175/199 (88%)	174 (99%)	1 (1%)	78	81
4	3	180/199 (90%)	179 (99%)	1 (1%)	78	81
4	4	197/199 (99%)	194 (98%)	3 (2%)	57	71
5	5	205/219 (94%)	202 (98%)	3 (2%)	57	71
6	6	41/71 (58%)	41 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	7	69/71 (97%)	68 (99%)	1 (1%)	59	72
6	8	69/71 (97%)	69 (100%)	0	100	100
6	9	70/71 (99%)	69 (99%)	1 (1%)	59	72
7	AM	34/88 (39%)	34 (100%)	0	100	100
7	AN	71/88 (81%)	71 (100%)	0	100	100
7	AO	76/88 (86%)	74 (97%)	2 (3%)	40	61
7	AP	76/88 (86%)	76 (100%)	0	100	100
7	AQ	76/88 (86%)	75 (99%)	1 (1%)	61	73
7	AR	76/88 (86%)	75 (99%)	1 (1%)	61	73
8	AS	50/67 (75%)	47 (94%)	3 (6%)	17	39
8	AT	50/67 (75%)	46 (92%)	4 (8%)	11	31
8	AU	50/67 (75%)	47 (94%)	3 (6%)	17	39
8	AV	50/67 (75%)	47 (94%)	3 (6%)	17	39
8	AW	50/67 (75%)	45 (90%)	5 (10%)	7	24
8	AX	62/67 (92%)	62 (100%)	0	100	100
8	AY	66/67 (98%)	65 (98%)	1 (2%)	57	71
8	AZ	66/67 (98%)	66 (100%)	0	100	100
8	BA	66/67 (98%)	66 (100%)	0	100	100
8	BB	66/67 (98%)	66 (100%)	0	100	100
8	BC	66/67 (98%)	66 (100%)	0	100	100
8	BD	66/67 (98%)	65 (98%)	1 (2%)	57	71
8	BE	66/67 (98%)	66 (100%)	0	100	100
8	BF	66/67 (98%)	66 (100%)	0	100	100
8	BG	66/67 (98%)	66 (100%)	0	100	100
8	BH	66/67 (98%)	64 (97%)	2 (3%)	36	57
8	BI	66/67 (98%)	63 (96%)	3 (4%)	24	46
8	BJ	66/67 (98%)	66 (100%)	0	100	100
8	BK	66/67 (98%)	66 (100%)	0	100	100
8	BL	66/67 (98%)	66 (100%)	0	100	100
8	BM	66/67 (98%)	64 (97%)	2 (3%)	36	57
8	BN	66/67 (98%)	65 (98%)	1 (2%)	57	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BO	66/67 (98%)	65 (98%)	1 (2%)	57	71
8	BP	66/67 (98%)	63 (96%)	3 (4%)	24	46
8	BQ	66/67 (98%)	66 (100%)	0	100	100
8	BR	66/67 (98%)	66 (100%)	0	100	100
8	BS	66/67 (98%)	66 (100%)	0	100	100
8	BT	66/67 (98%)	65 (98%)	1 (2%)	57	71
8	BU	66/67 (98%)	66 (100%)	0	100	100
8	BV	66/67 (98%)	66 (100%)	0	100	100
All	All	18384/24916 (74%)	18140 (99%)	244 (1%)	59	73

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	95	VAL
1	AD	60	VAL
1	AE	23	LEU
1	AF	123	VAL
2	R	176	LEU
2	S	307	LEU
2	U	366	LEU
2	V	366	LEU
2	W	335	GLU
2	X	366	LEU
2	a	332	ASP
2	a	366	LEU
2	b	196	VAL
2	c	331	LEU
2	d	312	LEU
2	d	366	LEU
2	e	312	LEU
2	g	194	LEU
2	g	312	LEU
2	g	324	THR
2	g	355	VAL
2	g	366	LEU
2	h	177	LEU
2	j	222	VAL
2	m	363	ASP
2	m	366	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	o	101	GLU
1	o	185	VAL
1	o	202	VAL
1	p	186	VAL
1	q	39	LEU
1	r	23	LEU
1	r	123	VAL
1	r	186	VAL
1	t	95	VAL
1	u	124	LEU
1	y	27	LEU
1	y	60	VAL
1	AK	22	ASP
4	0	81	THR
4	0	147	LEU
4	1	152	LEU
4	1	165	LEU
4	2	211	LEU
4	3	32	ILE
4	4	43	LEU
4	4	59	LEU
4	4	167	LEU
5	5	68	VAL
5	5	70	MET
5	5	242	LEU
6	7	72	LEU
6	9	18	LEU
7	AO	67	LEU
7	AO	87	LEU
7	AQ	56	GLU
7	AR	87	LEU
8	AS	28	THR
8	AS	56	LEU
8	AS	64	THR
8	AT	28	THR
8	AT	29	GLU
8	AT	64	THR
8	AT	76	ILE
8	AU	28	THR
8	AU	56	LEU
8	AU	64	THR
8	AV	31	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	AV	34	LEU
8	AV	76	ILE
8	AW	28	THR
8	AW	51	LEU
8	AW	56	LEU
8	AW	64	THR
8	AW	76	ILE
8	AY	56	LEU
3	A	80	LEU
3	A	111	VAL
3	A	294	VAL
3	A	304	VAL
3	A	311	VAL
3	A	335	LEU
3	A	442	THR
3	A	461	VAL
3	B	215	LEU
3	B	293	LEU
3	B	373	LEU
3	B	442	THR
3	B	454	LEU
3	B	480	THR
3	B	490	LEU
3	B	541	SER
3	C	254	LEU
3	C	294	VAL
3	C	318	LEU
3	C	372	VAL
3	C	373	LEU
3	C	405	THR
3	C	447	LEU
3	C	453	THR
3	C	480	THR
3	C	490	LEU
3	C	541	SER
3	D	40	ASP
3	D	114	LEU
3	D	294	VAL
3	D	372	VAL
3	D	373	LEU
3	D	442	THR
3	D	449	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	480	THR
3	D	490	LEU
3	D	508	VAL
3	F	111	VAL
3	F	114	LEU
3	F	226	VAL
3	F	254	LEU
3	F	372	VAL
3	F	373	LEU
3	F	412	VAL
3	F	440	THR
3	F	449	GLU
3	F	490	LEU
3	G	215	LEU
3	G	304	VAL
3	G	318	LEU
3	G	372	VAL
3	G	373	LEU
3	G	442	THR
3	G	461	VAL
3	G	490	LEU
3	H	36	VAL
3	H	58	ILE
3	H	114	LEU
3	H	185	LEU
3	H	209	THR
3	H	294	VAL
3	H	304	VAL
3	H	372	VAL
3	H	442	THR
3	H	449	GLU
3	H	461	VAL
3	H	480	THR
3	H	541	SER
3	I	294	VAL
3	I	372	VAL
3	I	440	THR
3	I	461	VAL
3	I	490	LEU
3	I	541	SER
3	J	40	ASP
3	J	51	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	192	ASP
3	J	269	ILE
3	J	294	VAL
3	J	310	ILE
3	J	312	ASP
3	J	356	VAL
3	J	373	LEU
3	J	453	THR
3	J	454	LEU
3	J	461	VAL
3	J	469	VAL
3	J	490	LEU
3	J	541	SER
3	K	138	LEU
3	K	311	VAL
3	K	318	LEU
3	K	372	VAL
3	K	453	THR
3	K	454	LEU
3	K	461	VAL
3	K	490	LEU
3	K	508	VAL
3	L	58	ILE
3	L	203	VAL
3	L	214	LEU
3	L	294	VAL
3	L	304	VAL
3	L	311	VAL
3	L	372	VAL
3	L	442	THR
3	L	454	LEU
3	L	480	THR
3	L	490	LEU
3	L	508	VAL
3	M	114	LEU
3	M	294	VAL
3	M	375	THR
3	M	412	VAL
3	M	442	THR
3	M	480	THR
3	M	490	LEU
3	N	40	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	N	111	VAL
3	N	114	LEU
3	N	207	ILE
3	N	226	VAL
3	N	254	LEU
3	N	311	VAL
3	N	318	LEU
3	N	372	VAL
3	N	394	ILE
3	N	429	GLU
3	N	453	THR
3	N	454	LEU
3	N	461	VAL
3	N	478	THR
3	N	480	THR
3	N	541	SER
3	N	545	LYS
3	O	138	LEU
3	O	294	VAL
3	O	311	VAL
3	O	329	ILE
3	O	372	VAL
3	O	440	THR
3	O	490	LEU
3	P	40	ASP
3	P	111	VAL
3	P	304	VAL
3	P	329	ILE
3	P	337	VAL
3	P	372	VAL
3	P	426	LEU
3	P	440	THR
3	P	454	LEU
3	P	461	VAL
3	P	508	VAL
3	P	541	SER
8	BD	56	LEU
8	BM	31	LEU
8	BM	51	LEU
8	BH	31	LEU
8	BH	51	LEU
8	BN	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	BI	20	VAL
8	BI	39	SER
8	BI	51	LEU
8	BO	51	LEU
8	BP	11	ASP
8	BP	23	LEU
8	BP	51	LEU
8	BT	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (352) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	33	ASN
1	AA	162	HIS
1	AB	29	GLN
1	AB	31	GLN
1	AB	40	GLN
1	AB	43	ASN
1	AB	129	HIS
1	AB	139	ASN
1	AB	162	HIS
1	AC	29	GLN
1	AC	33	ASN
1	AC	43	ASN
1	AC	162	HIS
1	AD	31	GLN
1	AE	40	GLN
1	AF	31	GLN
1	AF	33	ASN
1	AF	129	HIS
1	AF	139	ASN
1	AG	40	GLN
1	AG	47	ASN
1	AH	163	GLN
1	AI	43	ASN
1	AI	118	GLN
1	AI	129	HIS
1	AI	162	HIS
2	E	199	GLN
3	Q	97	GLN
3	Q	109	ASN
3	Q	169	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	209	GLN
2	R	229	ASN
2	S	219	ASN
2	S	318	ASN
2	S	319	HIS
2	T	209	GLN
2	T	229	ASN
2	T	309	GLN
2	T	341	GLN
2	U	229	ASN
2	U	263	GLN
2	U	318	ASN
2	U	356	GLN
2	V	219	ASN
2	V	229	ASN
2	V	310	GLN
2	V	318	ASN
2	V	319	HIS
2	W	209	GLN
2	W	372	GLN
2	X	229	ASN
2	X	318	ASN
2	Y	229	ASN
2	Y	318	ASN
2	Z	209	GLN
2	Z	265	ASN
2	Z	356	GLN
1	AL	33	ASN
1	AL	162	HIS
2	a	290	ASN
2	a	310	GLN
2	a	318	ASN
2	a	356	GLN
2	b	219	ASN
2	b	341	GLN
2	c	219	ASN
2	c	290	ASN
2	c	318	ASN
2	d	209	GLN
2	d	356	GLN
2	e	209	GLN
2	e	310	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	e	318	ASN
2	e	319	HIS
2	f	263	GLN
2	g	226	ASN
2	g	290	ASN
2	g	356	GLN
2	h	224	ASN
2	h	310	GLN
2	h	318	ASN
2	i	249	HIS
2	j	209	GLN
2	j	263	GLN
2	j	318	ASN
2	j	328	GLN
2	k	219	ASN
2	k	310	GLN
2	k	318	ASN
2	l	229	ASN
2	l	328	GLN
2	l	356	GLN
2	l	385	HIS
2	m	209	GLN
2	m	219	ASN
2	m	310	GLN
2	m	318	ASN
2	m	319	HIS
2	n	224	ASN
1	o	29	GLN
1	o	31	GLN
1	o	33	ASN
1	o	43	ASN
1	o	129	HIS
1	p	33	ASN
1	p	43	ASN
1	p	139	ASN
1	q	33	ASN
1	q	40	GLN
1	q	47	ASN
1	r	162	HIS
1	r	163	GLN
1	s	33	ASN
1	s	43	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	s	111	GLN
1	s	163	GLN
1	t	33	ASN
1	t	40	GLN
1	t	163	GLN
1	t	173	ASN
1	u	29	GLN
1	u	40	GLN
1	u	43	ASN
1	u	76	GLN
1	u	173	ASN
1	v	29	GLN
1	v	33	ASN
1	v	139	ASN
1	v	162	HIS
1	w	129	HIS
1	x	40	GLN
1	x	76	GLN
1	x	162	HIS
1	y	162	HIS
1	z	43	ASN
1	z	47	ASN
1	z	162	HIS
1	z	163	GLN
1	AJ	43	ASN
1	AJ	115	GLN
1	AJ	139	ASN
1	AJ	147	HIS
1	AJ	162	HIS
1	AK	40	GLN
1	AK	47	ASN
1	AK	147	HIS
1	AK	182	ASN
4	1	3	ASN
4	2	44	GLN
4	2	83	ASN
4	3	69	HIS
4	3	113	GLN
4	3	117	ASN
4	4	44	GLN
4	4	53	ASN
4	4	117	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	5	44	ASN
5	5	76	GLN
5	5	104	ASN
5	5	105	GLN
5	5	127	ASN
5	5	139	GLN
5	5	161	ASN
5	5	210	ASN
5	5	245	GLN
6	7	37	GLN
6	7	45	GLN
6	8	9	ASN
6	8	37	GLN
6	8	41	GLN
6	8	43	GLN
6	9	9	ASN
6	9	37	GLN
6	9	43	GLN
7	AM	71	GLN
7	AO	53	ASN
7	AO	59	ASN
7	AO	71	GLN
7	AO	78	ASN
7	AP	49	GLN
7	AP	53	ASN
7	AP	59	ASN
7	AP	71	GLN
7	AQ	59	ASN
7	AQ	71	GLN
7	AR	35	GLN
7	AR	53	ASN
8	AS	24	GLN
8	AT	61	GLN
8	AT	77	GLN
8	AV	26	GLN
8	AV	61	GLN
8	AW	24	GLN
8	AX	61	GLN
8	AX	78	ASN
8	AY	61	GLN
3	A	71	ASN
3	A	87	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	97	GLN
3	A	109	ASN
3	A	216	GLN
3	A	224	ASN
3	A	303	HIS
3	A	376	GLN
3	A	421	GLN
3	B	87	GLN
3	B	170	ASN
3	B	220	GLN
3	B	276	ASN
3	B	357	ASN
3	B	376	GLN
3	B	421	GLN
3	B	547	GLN
3	C	71	ASN
3	C	123	ASN
3	C	178	GLN
3	C	421	GLN
3	C	477	ASN
3	C	547	GLN
3	D	120	ASN
3	D	216	GLN
3	D	220	GLN
3	D	276	ASN
3	D	376	GLN
3	D	421	GLN
3	F	71	ASN
3	F	200	GLN
3	F	220	GLN
3	F	276	ASN
3	F	376	GLN
3	G	97	GLN
3	G	120	ASN
3	G	124	ASN
3	G	170	ASN
3	G	220	GLN
3	G	286	GLN
3	G	357	ASN
3	G	376	GLN
3	G	421	GLN
3	G	547	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	178	GLN
3	H	220	GLN
3	H	276	ASN
3	H	286	GLN
3	H	376	GLN
3	H	378	ASN
3	H	421	GLN
3	H	477	ASN
3	I	169	GLN
3	I	170	ASN
3	I	276	ASN
3	I	340	ASN
3	I	376	GLN
3	I	421	GLN
3	J	97	GLN
3	J	124	ASN
3	J	142	ASN
3	J	200	GLN
3	J	376	GLN
3	J	378	ASN
3	J	421	GLN
3	J	506	ASN
3	J	536	GLN
3	K	97	GLN
3	K	169	GLN
3	K	276	ASN
3	K	376	GLN
3	K	421	GLN
3	K	477	ASN
3	K	547	GLN
3	L	71	ASN
3	L	87	GLN
3	L	97	GLN
3	L	123	ASN
3	L	178	GLN
3	L	196	ASN
3	L	216	GLN
3	L	376	GLN
3	L	421	GLN
3	M	97	GLN
3	M	142	ASN
3	M	161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	261	ASN
3	M	276	ASN
3	M	314	ASN
3	M	378	ASN
3	M	421	GLN
3	M	432	ASN
3	M	547	GLN
3	N	71	ASN
3	N	75	HIS
3	N	169	GLN
3	N	170	ASN
3	N	216	GLN
3	N	376	GLN
3	N	403	HIS
3	N	421	GLN
3	N	463	HIS
3	N	536	GLN
3	O	87	GLN
3	O	169	GLN
3	O	178	GLN
3	O	200	GLN
3	O	220	GLN
3	O	276	ASN
3	O	340	ASN
3	O	378	ASN
3	O	421	GLN
3	O	477	ASN
3	P	71	ASN
3	P	87	GLN
3	P	178	GLN
3	P	196	ASN
3	P	220	GLN
3	P	261	ASN
3	P	276	ASN
3	P	421	GLN
3	P	463	HIS
3	P	547	GLN
8	AZ	59	ASN
8	BB	59	ASN
8	BB	78	ASN
8	BD	26	GLN
8	BD	61	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	BD	63	ASN
8	BE	59	ASN
8	BJ	26	GLN
8	BJ	59	ASN
8	BJ	78	ASN
8	BK	59	ASN
8	BF	59	ASN
8	BF	61	GLN
8	BL	59	ASN
8	BL	61	GLN
8	BL	77	GLN
8	BG	59	ASN
8	BM	63	ASN
8	BH	55	ASN
8	BN	26	GLN
8	BN	63	ASN
8	BN	77	GLN
8	BI	26	GLN
8	BI	59	ASN
8	BP	59	ASN
8	BQ	59	ASN
8	BQ	61	GLN
8	BC	26	GLN
8	BA	26	GLN
8	BA	59	ASN
8	BU	26	GLN
8	BT	63	ASN
8	BR	78	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

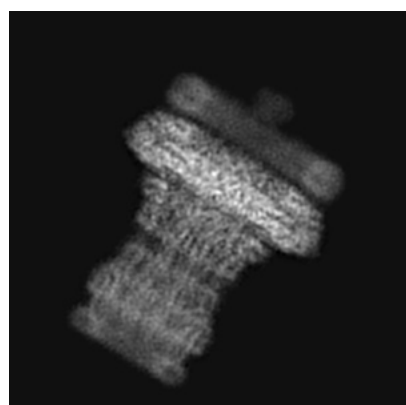
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20312. These allow visual inspection of the internal detail of the map and identification of artifacts.

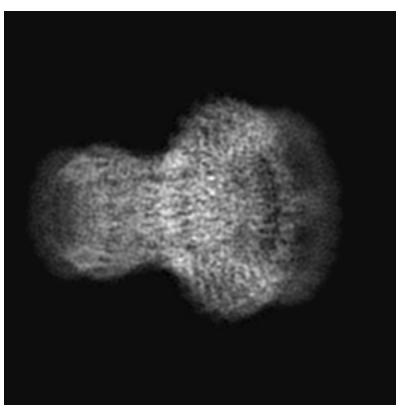
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

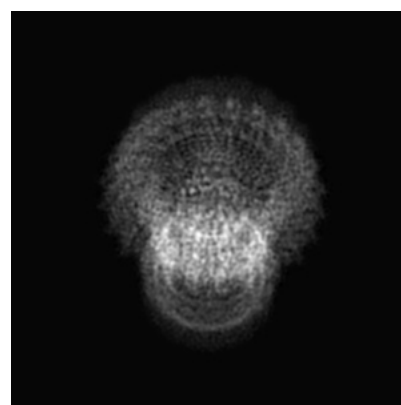
6.1.1 Primary map



X



Y

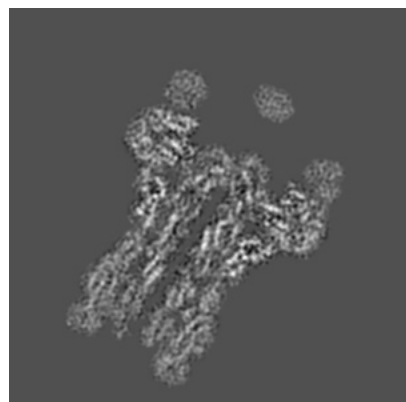


Z

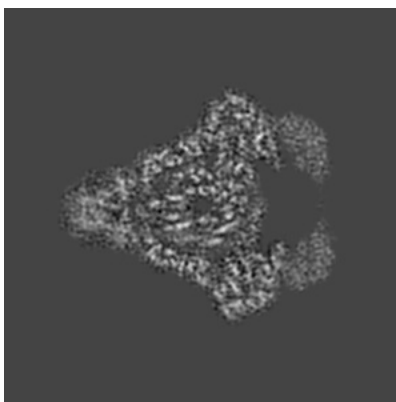
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

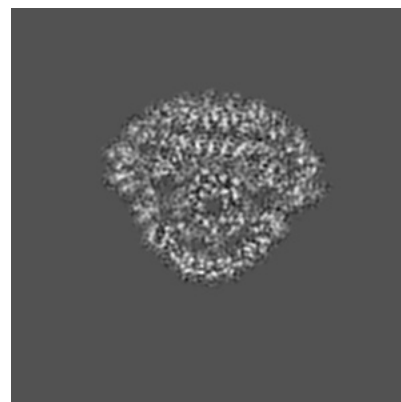
6.2.1 Primary map



X Index: 125



Y Index: 125

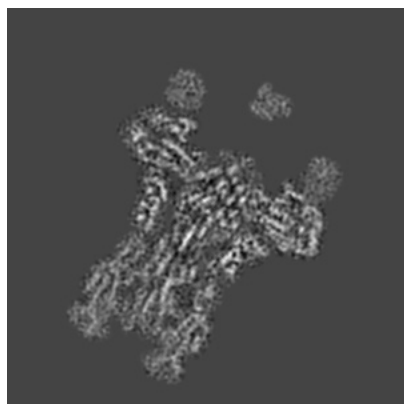


Z Index: 125

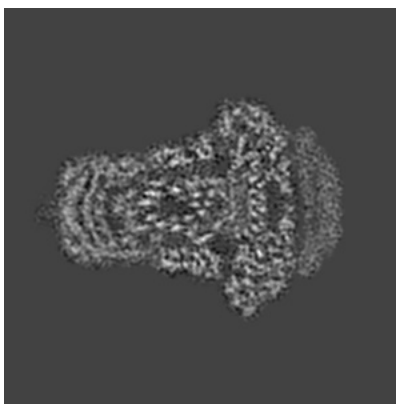
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

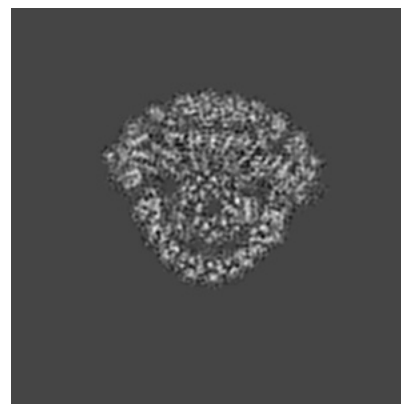
6.3.1 Primary map



X Index: 136



Y Index: 113

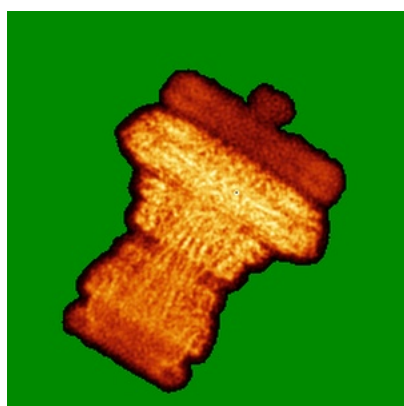


Z Index: 123

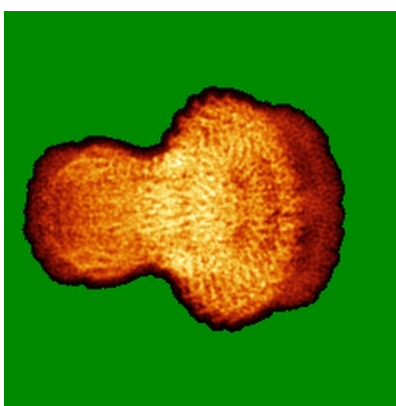
The images above show the largest variance slices of the map in three orthogonal directions.

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

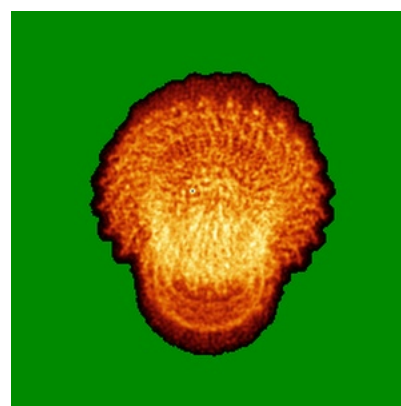
6.4.1 Primary map



X



Y

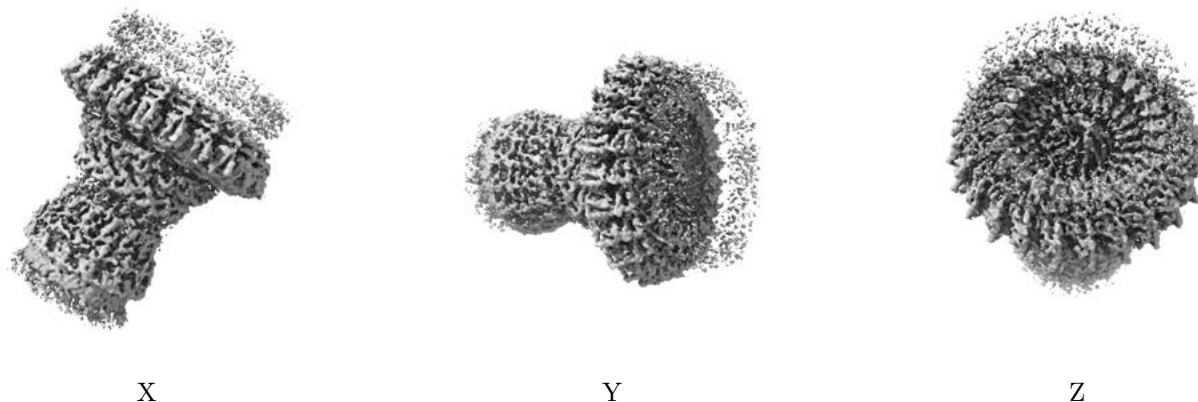


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

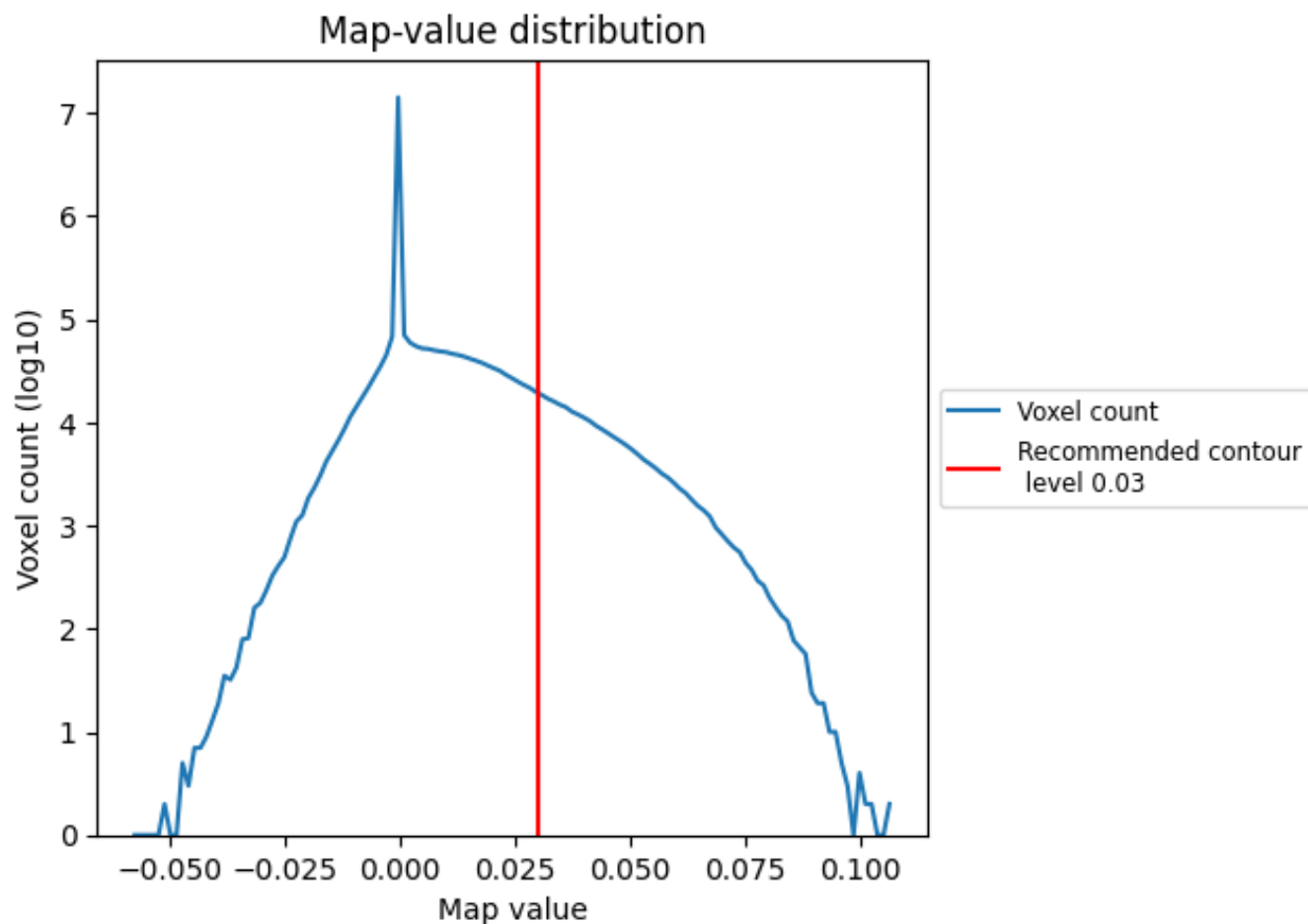
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

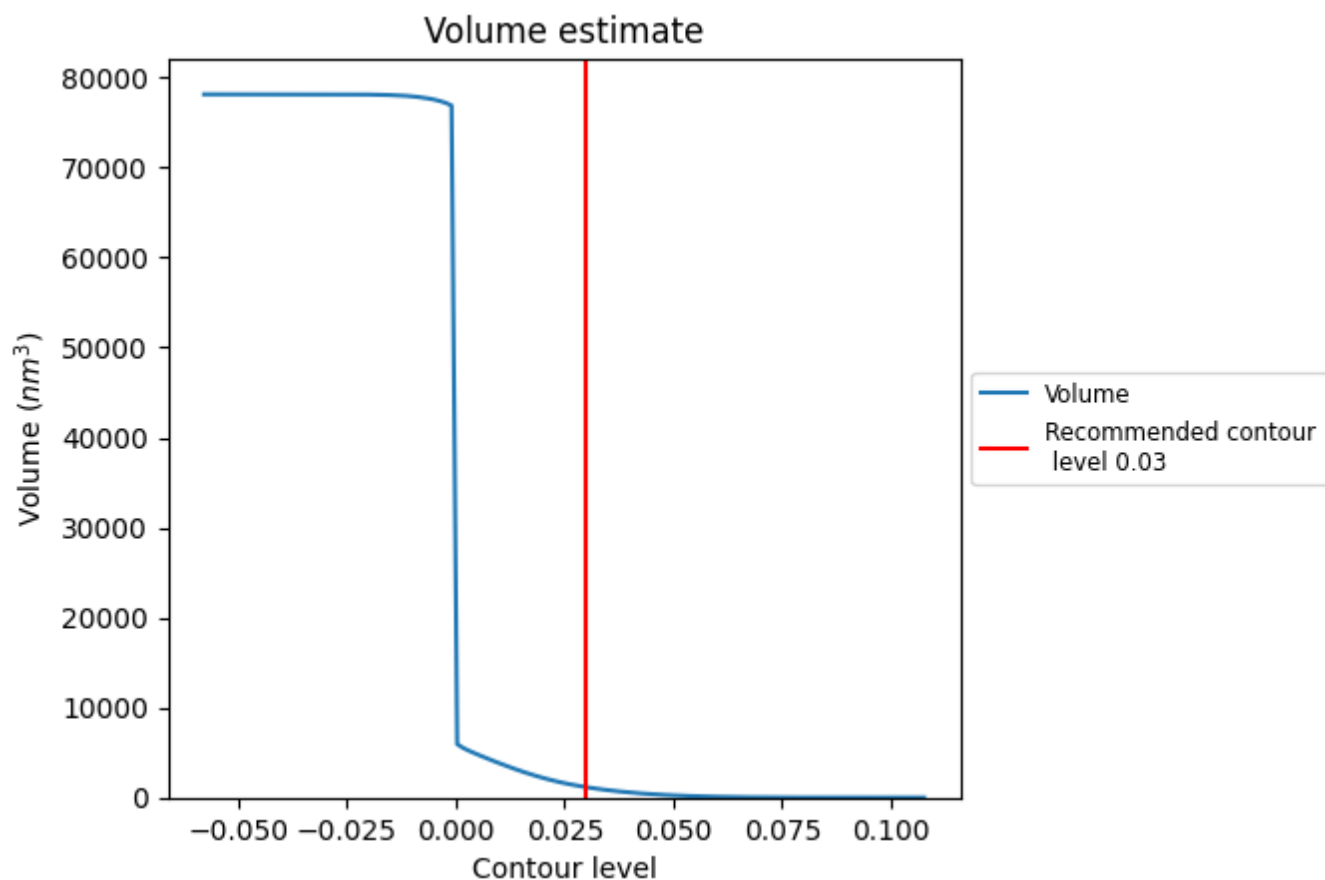
This section contains the results of statistical analysis of the map.

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.

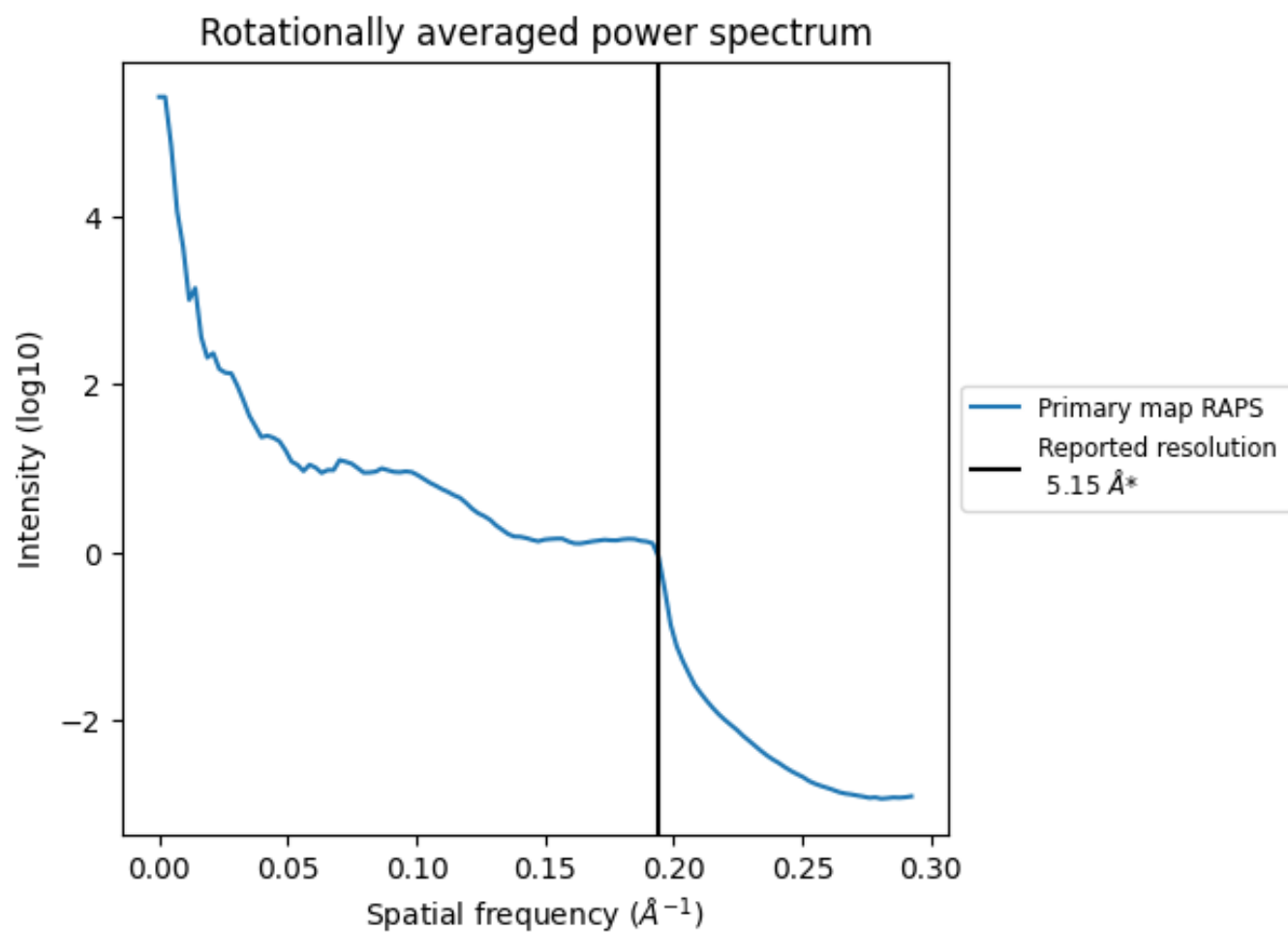
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1154 nm³; this corresponds to an approximate mass of 1042 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 0.194 Å⁻¹

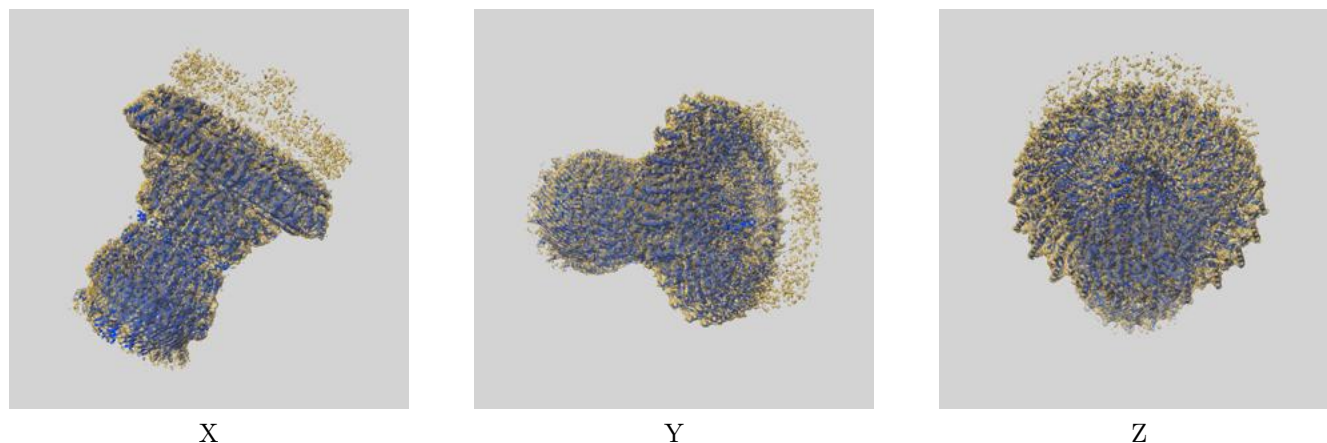
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

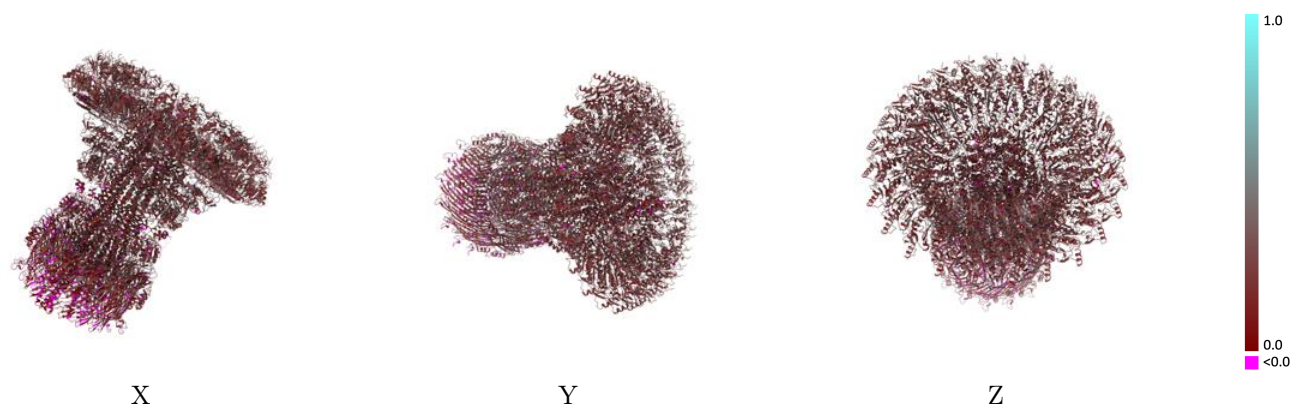
This section contains information regarding the fit between EMDB map EMD-20312 and PDB model 6Q15. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



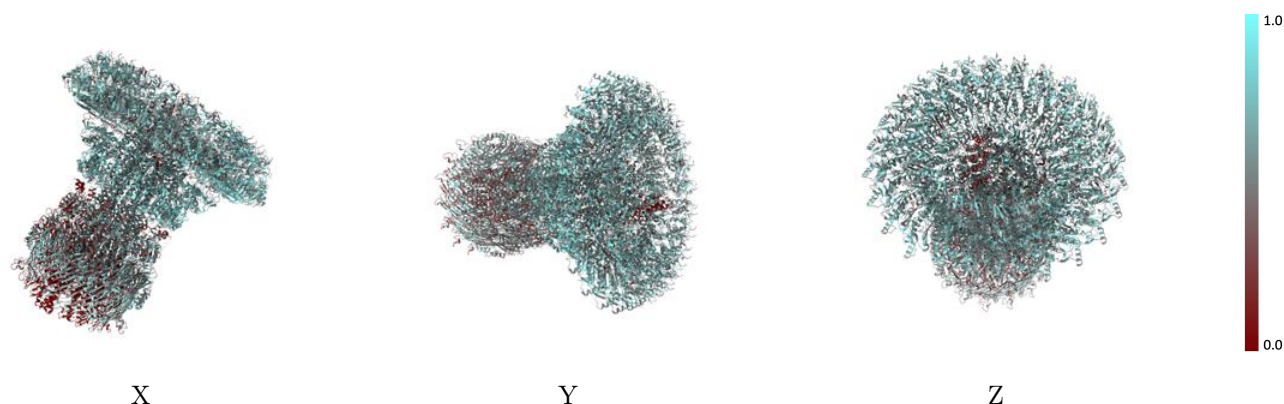
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



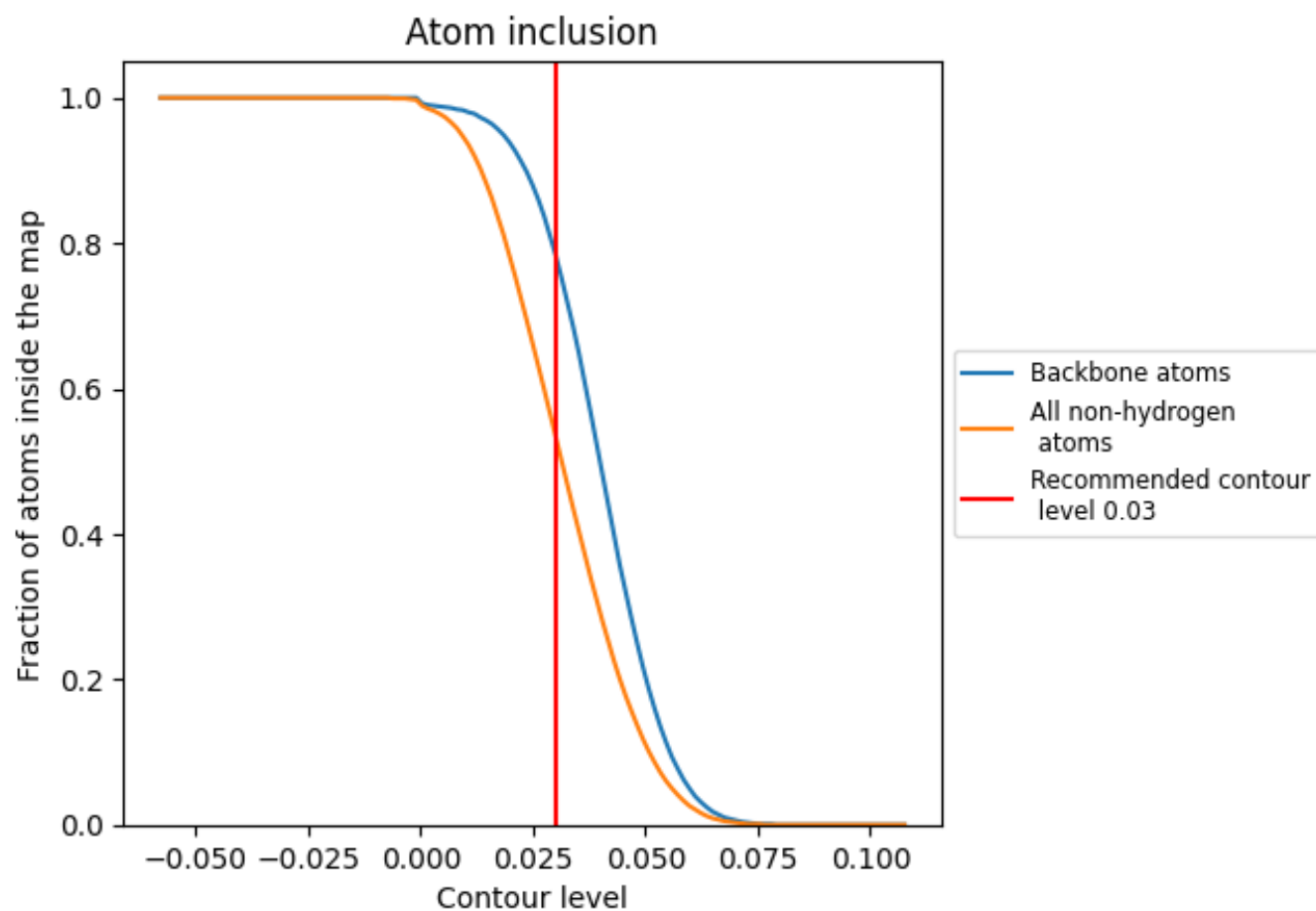
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5350	 0.2430
0	 0.5190	 0.2350
1	 0.5260	 0.2250
2	 0.5280	 0.2250
3	 0.5390	 0.2310
4	 0.5180	 0.2320
5	 0.5740	 0.2550
6	 0.1410	 0.2290
7	 0.2730	 0.2060
8	 0.4770	 0.2210
9	 0.5560	 0.2320
A	 0.4540	 0.2070
AA	 0.5920	 0.2810
AB	 0.5870	 0.2980
AC	 0.6040	 0.2980
AD	 0.5980	 0.2920
AE	 0.6110	 0.2980
AF	 0.6020	 0.3000
AG	 0.6080	 0.2910
AH	 0.5970	 0.2860
AI	 0.6140	 0.2870
AJ	 0.5870	 0.3010
AK	 0.5990	 0.2890
AL	 0.5970	 0.3010
AM	 0.5550	 0.2100
AN	 0.5640	 0.2250
AO	 0.5560	 0.2230
AP	 0.5700	 0.2400
AQ	 0.5560	 0.2440
AR	 0.5360	 0.2320
AS	 0.5690	 0.2260
AT	 0.5580	 0.2000
AU	 0.5400	 0.2020
AV	 0.5510	 0.2130
AW	 0.5990	 0.2350



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AX	 0.5030	 0.2080
AY	 0.5260	 0.2020
AZ	 0.5410	 0.2230
B	 0.4620	 0.1990
BA	 0.5220	 0.2010
BB	 0.5220	 0.2090
BC	 0.4960	 0.2100
BD	 0.4610	 0.1980
BE	 0.4730	 0.2220
BF	 0.4510	 0.2120
BG	 0.4360	 0.2090
BH	 0.4200	 0.1870
BI	 0.3710	 0.1950
BJ	 0.3330	 0.1930
BK	 0.2870	 0.1790
BL	 0.2720	 0.1920
BM	 0.2650	 0.1780
BN	 0.2260	 0.1630
BO	 0.1760	 0.1350
BP	 0.1760	 0.1330
BQ	 0.1440	 0.1280
BR	 0.0950	 0.0810
BS	 0.0630	 0.0670
BT	 0.0530	 0.0820
BU	 0.0420	 0.0490
BV	 0.0200	 0.0380
C	 0.4940	 0.2160
D	 0.5070	 0.2250
E	 0.5960	 0.2700
F	 0.5130	 0.2290
G	 0.5250	 0.2240
H	 0.5470	 0.2390
I	 0.5330	 0.2290
J	 0.5260	 0.2330
K	 0.5200	 0.2280
L	 0.5010	 0.2170
M	 0.4840	 0.2130
N	 0.4630	 0.1990
O	 0.4610	 0.1970
P	 0.4550	 0.1950
Q	 0.6730	 0.2720
R	 0.6230	 0.2710

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S	 0.6160	 0.2680
T	 0.5950	 0.2680
U	 0.6340	 0.2710
V	 0.6140	 0.2710
W	 0.5660	 0.2610
X	 0.6350	 0.2800
Y	 0.6150	 0.2690
Z	 0.5910	 0.2690
a	 0.6440	 0.2790
b	 0.6320	 0.2680
c	 0.5970	 0.2610
d	 0.6280	 0.2750
e	 0.6580	 0.2730
f	 0.6080	 0.2750
g	 0.6430	 0.2740
h	 0.6490	 0.2720
i	 0.6090	 0.2750
j	 0.6680	 0.2830
k	 0.6460	 0.2780
l	 0.5920	 0.2770
m	 0.6460	 0.2740
n	 0.6360	 0.2790
o	 0.5750	 0.2860
p	 0.5850	 0.2840
q	 0.5570	 0.2880
r	 0.5850	 0.2900
s	 0.5590	 0.2860
t	 0.5770	 0.2900
u	 0.5710	 0.2830
v	 0.5650	 0.2860
w	 0.5620	 0.2800
x	 0.5820	 0.2880
y	 0.5930	 0.2970
z	 0.5940	 0.2920