



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:43 AM UTC

PDB ID : 6V8I / pdb_00006v8i
EMDB ID : EMD-20872
Title : Composite atomic model of the Staphylococcus aureus phage 80alpha base-plate
Authors : Kizziah, J.L.; Dokland, T.
Deposited on : 2019-12-11
Resolution : 3.70 Å(reported)
Based on initial model : 5EFV

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

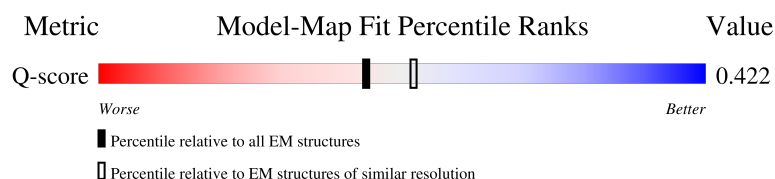
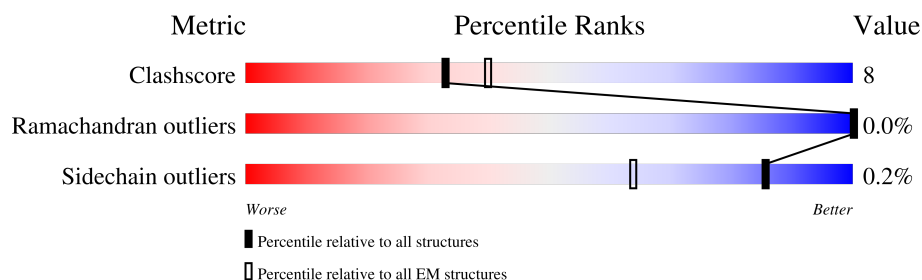
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



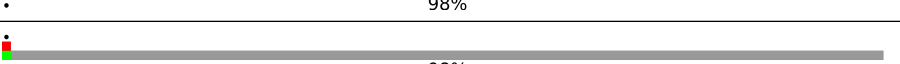
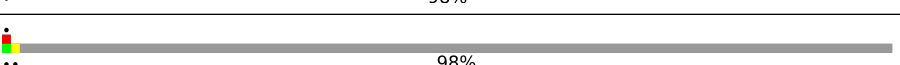
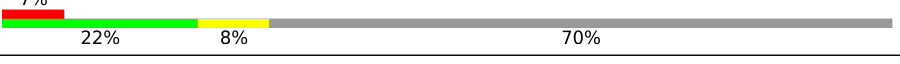
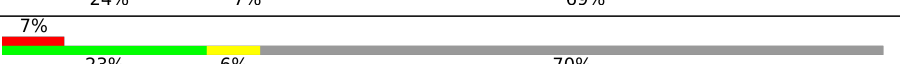
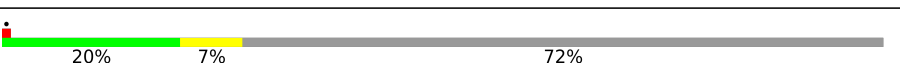
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11284 (3.19 - 4.18)

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	AC	315	 6% 81% 18%
1	AD	315	 5% 79% 20%
1	BC	315	 6% 81% 18%
1	BD	315	 1% 80% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CC	315	
1	CD	315	
2	AE	633	
2	BE	633	
2	CE	633	
3	AF	1154	
3	BF	1154	
3	CF	1154	
4	AJ	607	
4	AK	607	
4	AL	607	
4	BJ	607	
4	BK	607	
4	BL	607	
4	CJ	607	
4	CK	607	
4	CL	607	
4	DJ	607	
4	DK	607	
4	DL	607	
4	EJ	607	
4	EK	607	
4	EL	607	
4	FJ	607	
4	FK	607	

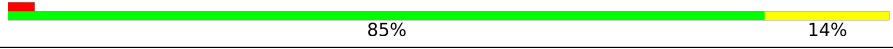
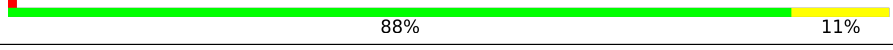
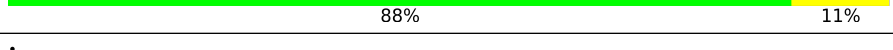
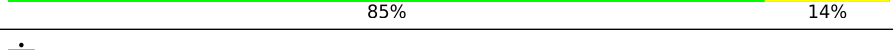
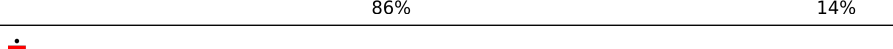
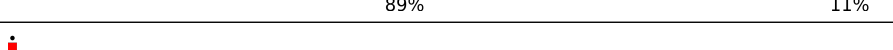
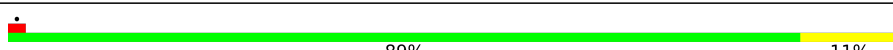
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	FL	607	
5	AM	390	
5	AN	390	
5	BM	390	
5	BN	390	
5	CM	390	
5	CN	390	
5	DM	390	
5	DN	390	
5	EM	390	
5	EN	390	
5	FM	390	
5	FN	390	
6	AA	193	
6	AB	193	
6	BA	193	
6	BB	193	
6	CA	193	
6	CB	193	
6	DA	193	
6	DB	193	
6	EA	193	
6	EB	193	
6	FA	193	
6	FB	193	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	AG	636	 89%10%
7	AH	636	 86%14%
7	AI	636	 85%14%
7	BG	636	 88%11%
7	BH	636	 85%15%
7	BI	636	 87%12%
7	CG	636	 88%11%
7	CH	636	 85%14%
7	CI	636	 86%14%
7	DG	636	 89%11%
7	DH	636	 86%13%
7	DI	636	 87%13%
7	EG	636	 89%11%
7	EH	636	 86%13%
7	EI	636	 86%14%
7	FG	636	 89%11%
7	FH	636	 86%14%
7	FI	636	 88%12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 171102 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 Distal Tail Protein, gp58.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AC	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	AD	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	CC	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	CD	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	BC	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	BD	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		

- Molecule 2 is a protein called Tail-Associated Lysin, gp59.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AE	387	Total	C	N	O	S	0	0
			3068	1944	518	598	8		
2	CE	387	Total	C	N	O	S	0	0
			3068	1944	518	598	8		
2	BE	387	Total	C	N	O	S	0	0
			3068	1944	518	598	8		

- Molecule 3 is a protein called Tape Measure Protein, gp57.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	CF	20	Total	C	N	O	0	0
			160	98	30	32		
3	BF	20	Total	C	N	O	0	0
			160	98	30	32		
3	AF	20	Total	C	N	O	0	0
			160	98	30	32		

- Molecule 4 is a protein called Fiber Lower, gp62.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	BK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	BL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	DJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	DK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	DL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	AJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	AK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	AL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	FJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	FK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	FL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	CJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	CK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	CL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	EJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	EK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	EL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		

- Molecule 5 is a protein called Fiber Upper, gp68.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	BM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	DM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		
5	AN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	AM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		
5	FN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	FM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		
5	CN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	CM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		
5	EN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	EM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		

- Molecule 6 is a protein called Major Tail Protein, gp53.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	EB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	EA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	BB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	BA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	DB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	DA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	AB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	AA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	FB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	FA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	CB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	CA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		

- Molecule 7 is a protein called Receptor Binding Protein, gp61.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	BG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	BI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	DH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	DG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	DI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	AH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	AG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	AI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	FH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	FG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	FI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	CH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	CG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	CI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	EH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	EG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	EI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		

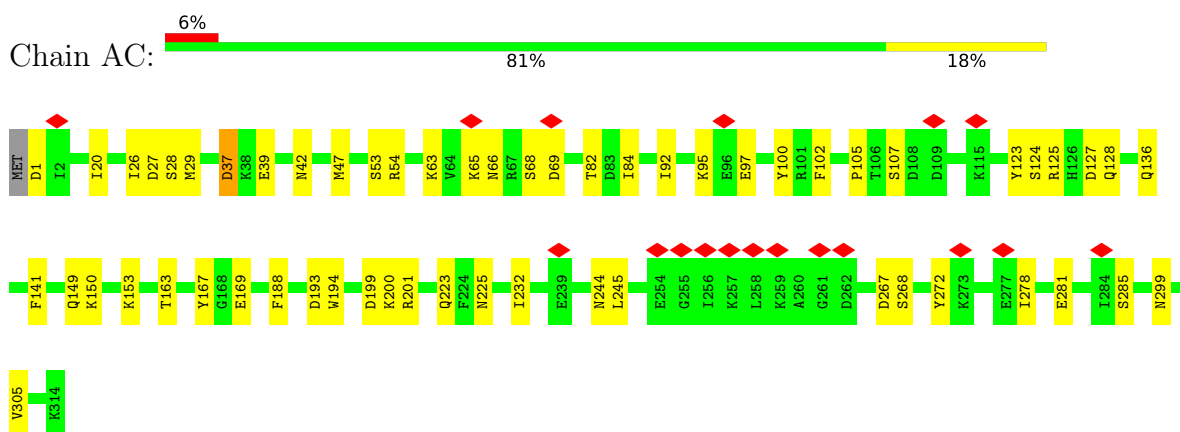
- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
8	BH	1	Total	Fe	0
			1	1	
8	DH	1	Total	Fe	0
			1	1	
8	AH	1	Total	Fe	0
			1	1	
8	FH	1	Total	Fe	0
			1	1	
8	CH	1	Total	Fe	0
			1	1	
8	EH	1	Total	Fe	0
			1	1	

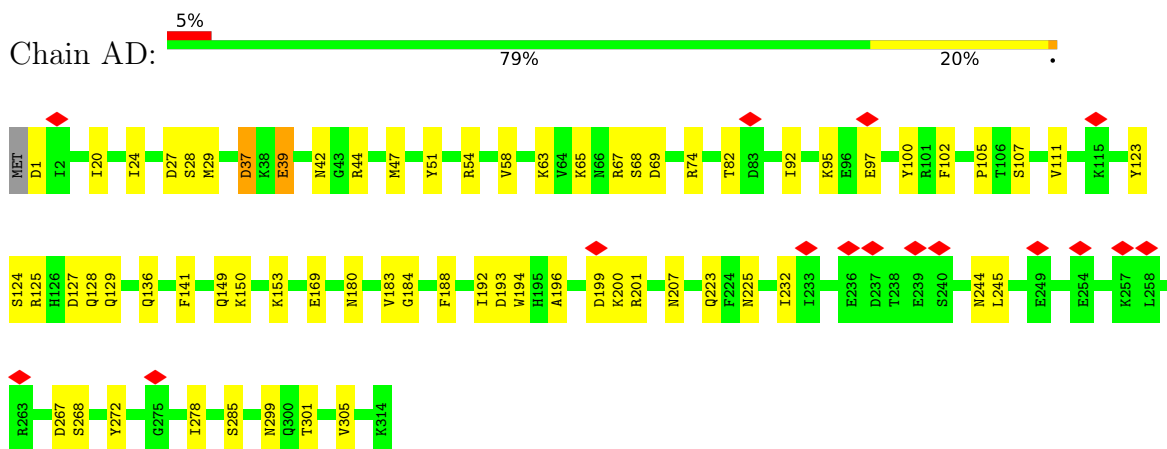
3 Residue-property plots

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.

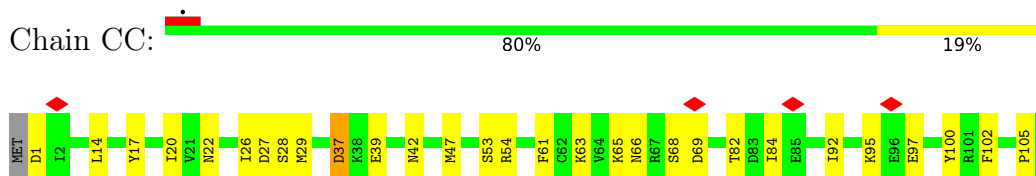
- Molecule 1: Distal Tail Protein, gp58

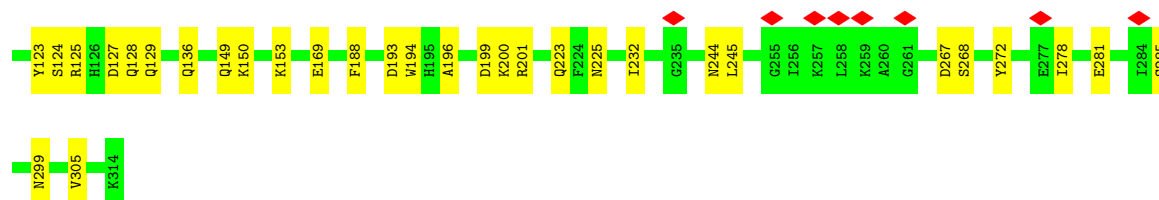


- Molecule 1: Distal Tail Protein, gp58

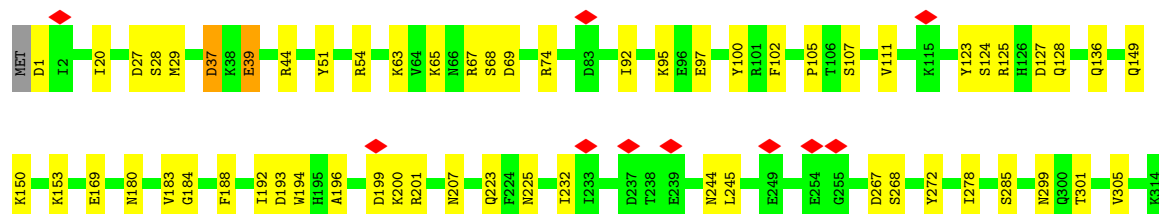
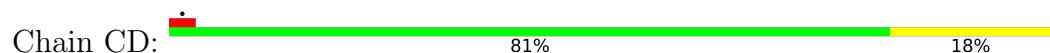


- Molecule 1: Distal Tail Protein, gp58

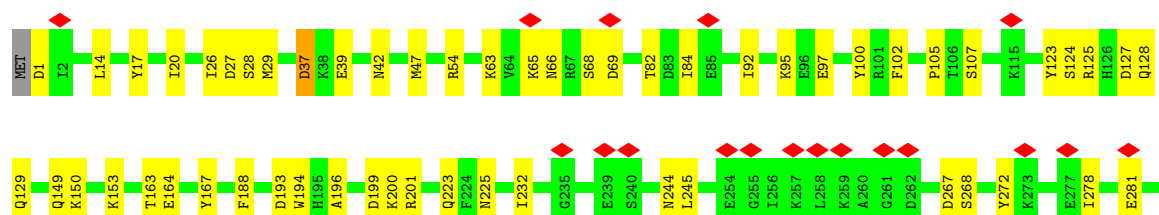
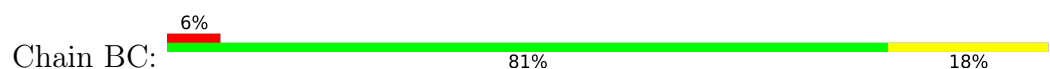




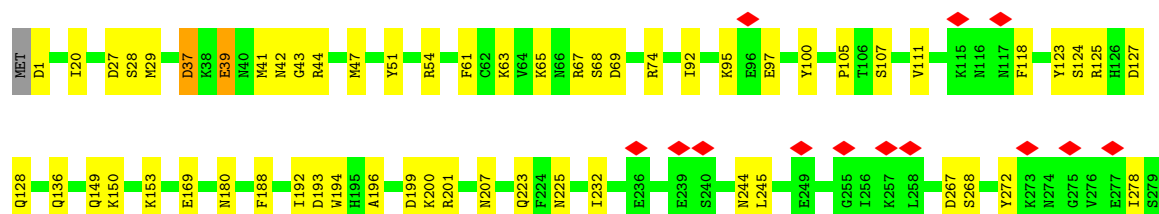
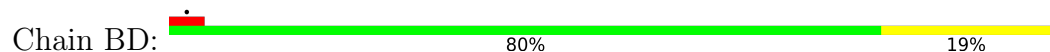
- Molecule 1: Distal Tail Protein, gp58



- Molecule 1: Distal Tail Protein, gp58

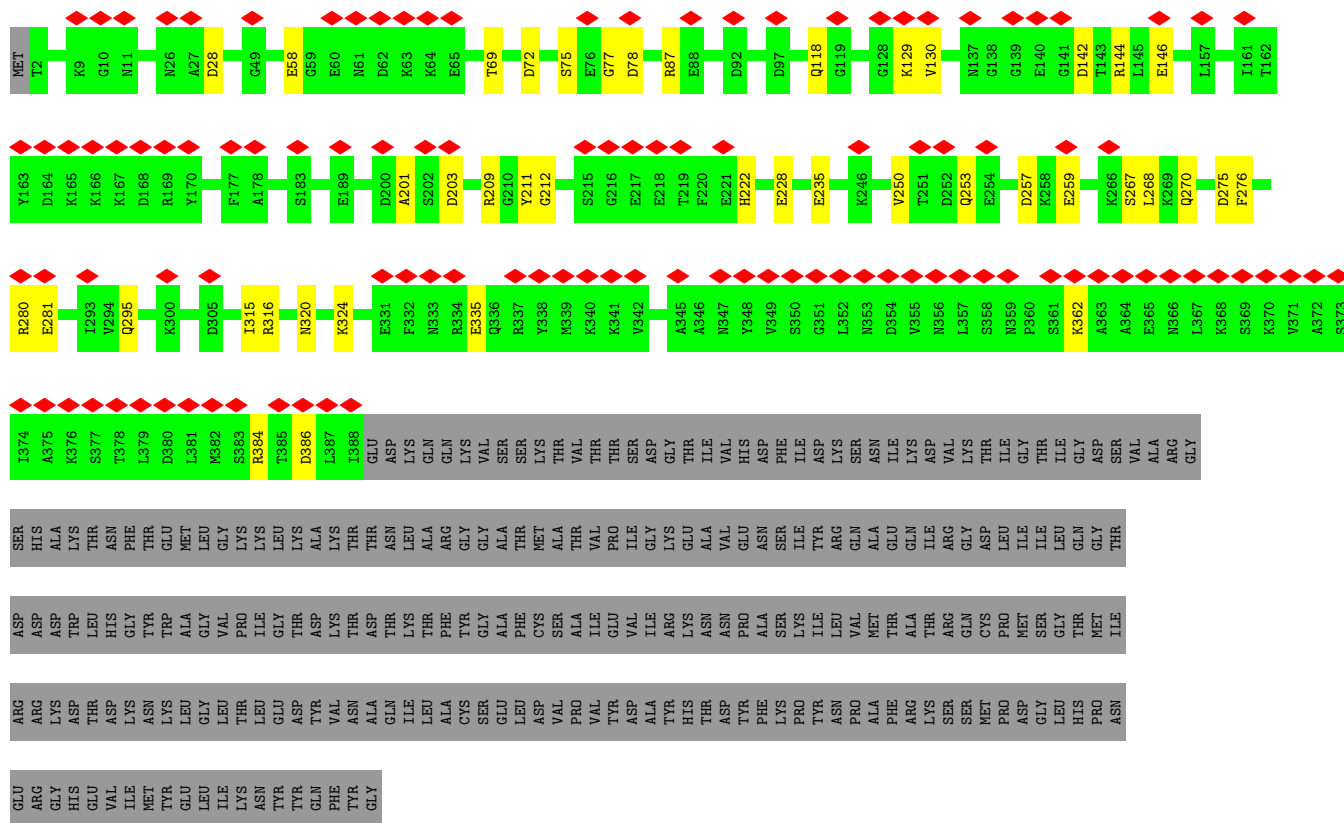


- Molecule 1: Distal Tail Protein, gp58

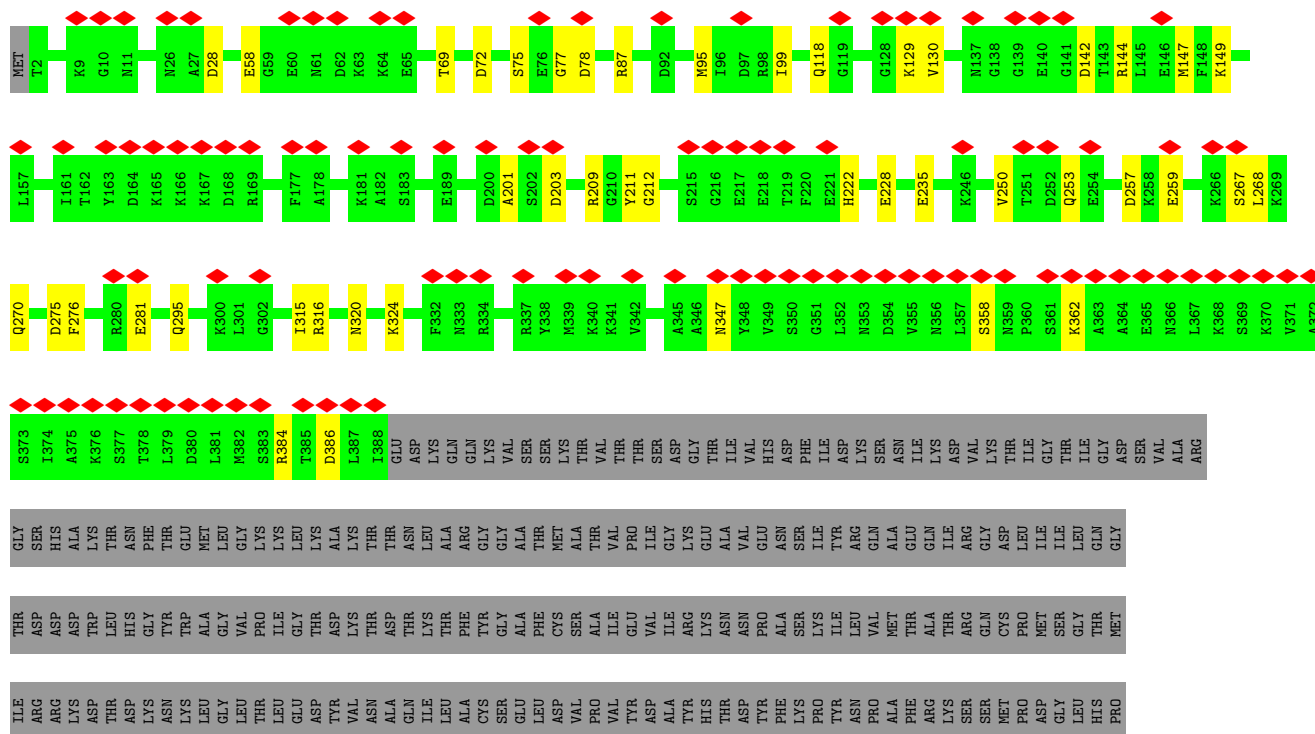


- Molecule 2: Tail-Associated Lysin, gp59



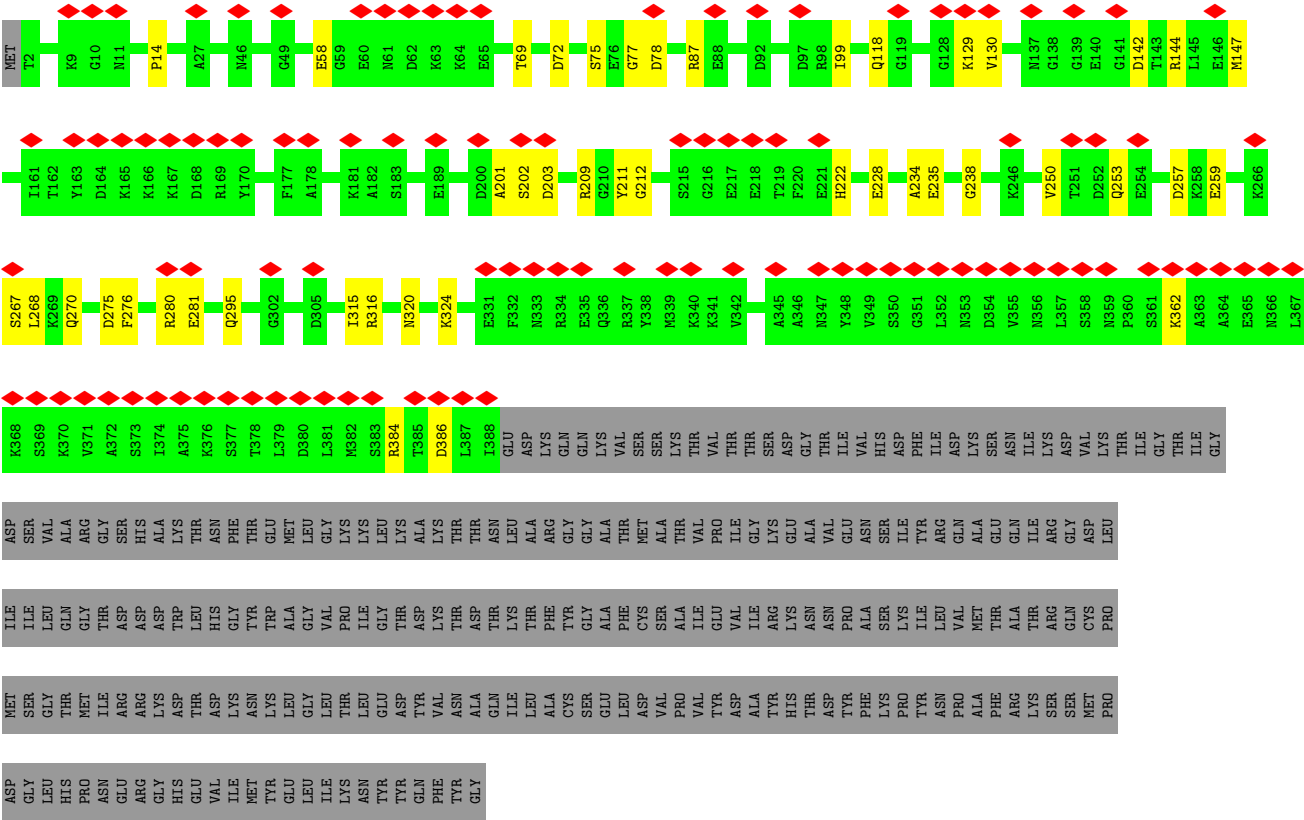


• Molecule 2: Tail-Associated Lysin, gp59

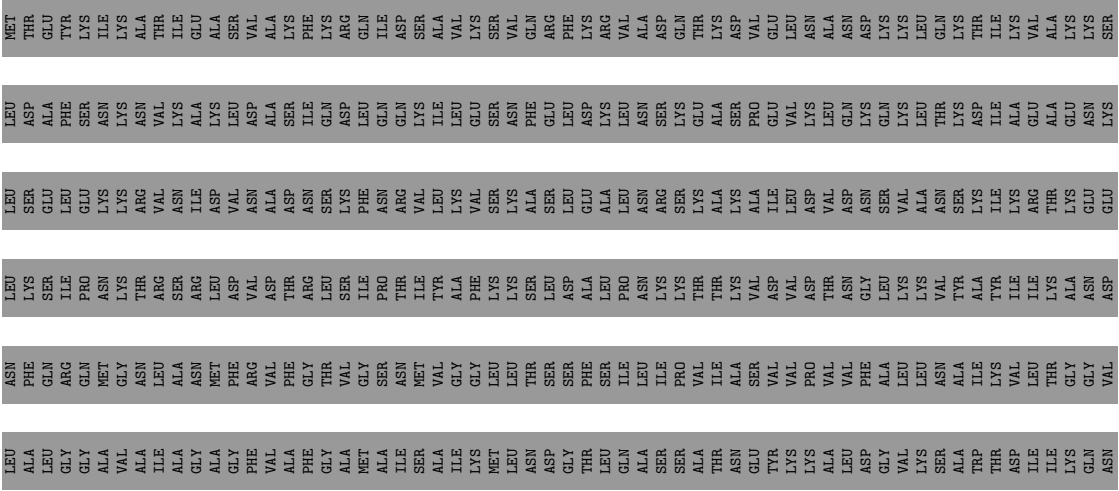


ASN
GLU
ARG
GLY
HIS
GLU
VAL
ILE
MET
TYR
GLU
LEU
ILE
LYS
ASN
TYR
GLN
PHE
TYR
GLY

● Molecule 2: Tail-Associated Lysin, gp59



● Molecule 3: Tape Measure Protein, gp57



V1141	N1142	G1143	R1144	N1145	A1146	K1147	S1150	E1151	Y1152	Y1153	L1154
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

Chain BF: 98%



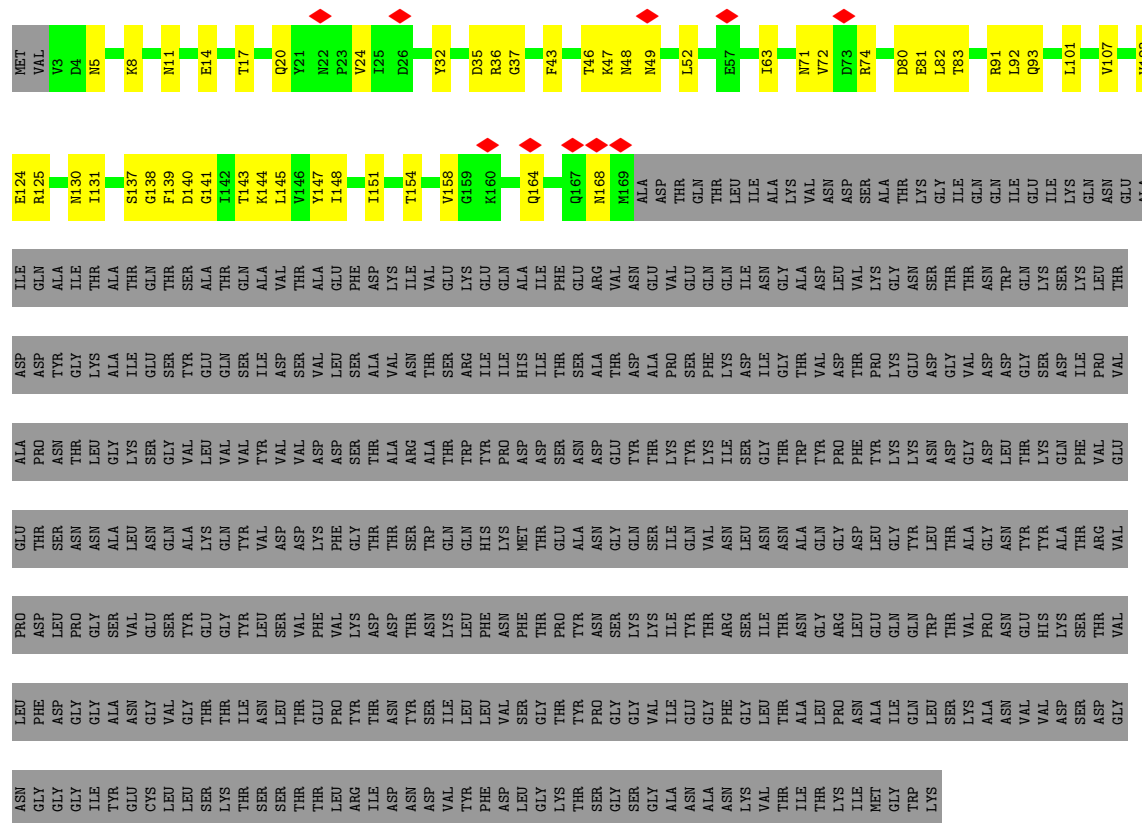
V1141	N1142	G1143	R1144	N1145	A1146	K1147	S1150	E1151	Y1152	Y1153	L1154
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

Chain AF: 98%

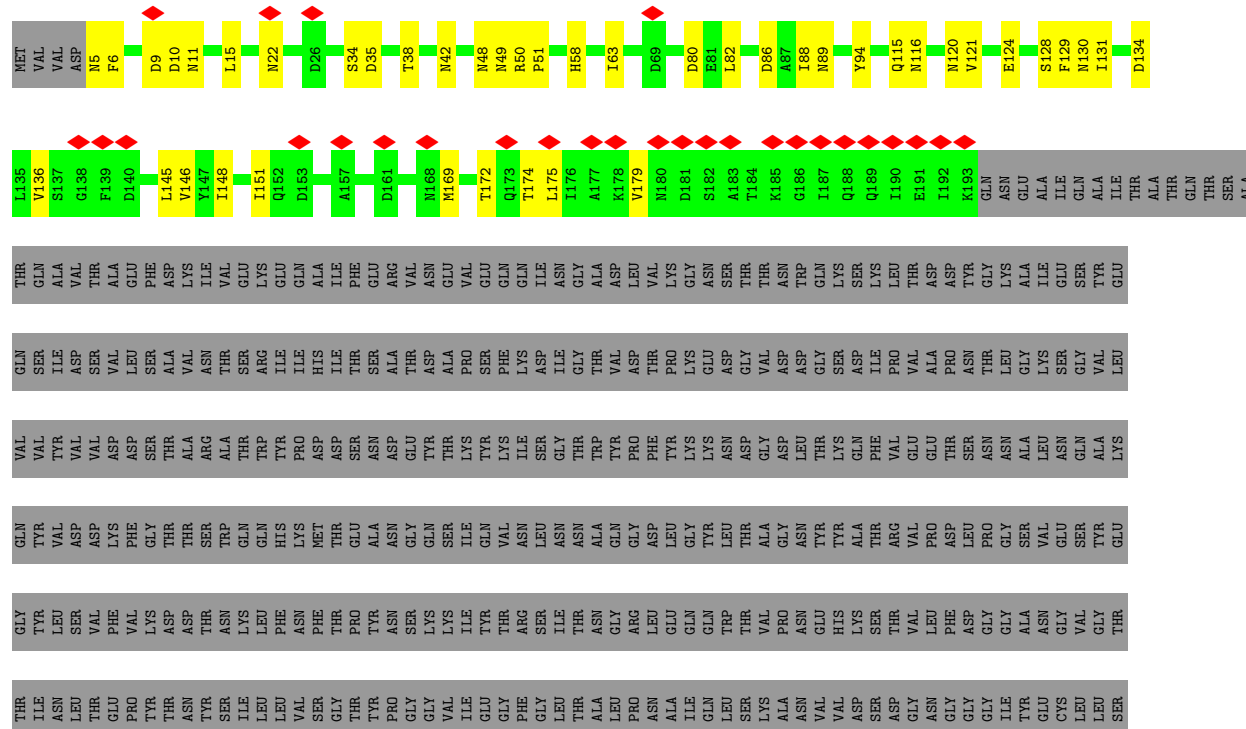
[illegible]

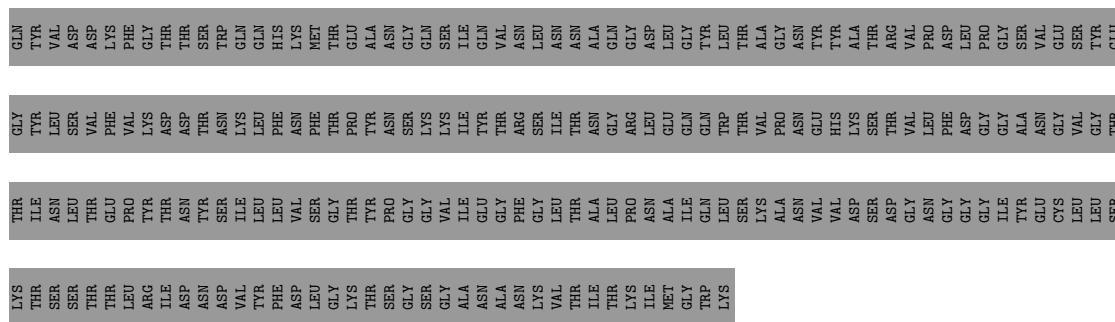
Diagram illustrating a 16-bit bus structure. The bus is divided into two 8-bit segments. The left segment contains 8 data lines (V1141 to K1147) and 8 address lines (N1142 to L1154). The right segment contains 8 data lines (S1150 to L1154) and 8 address lines (N1142 to L1154).

- 

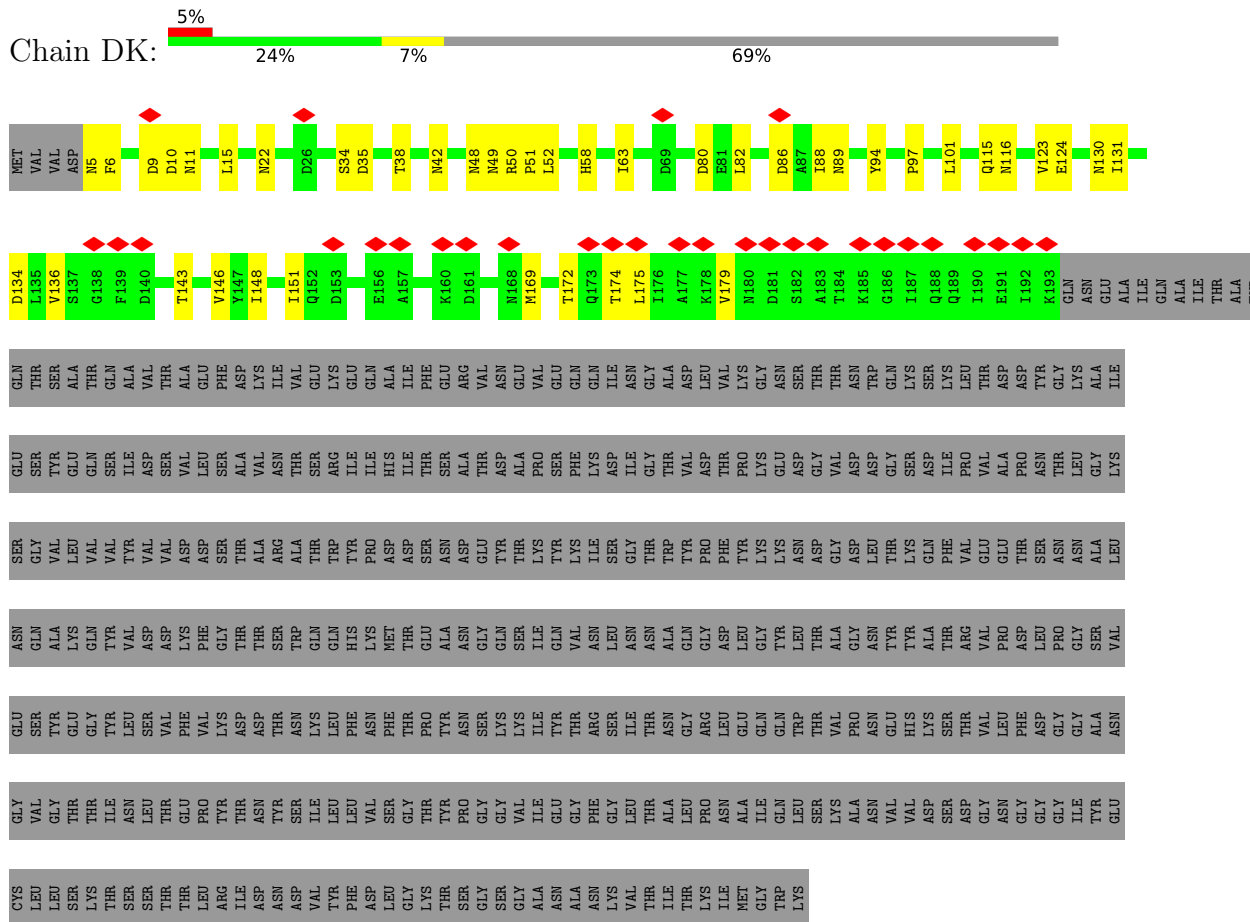


• Molecule 4: Fiber Lower, gp62

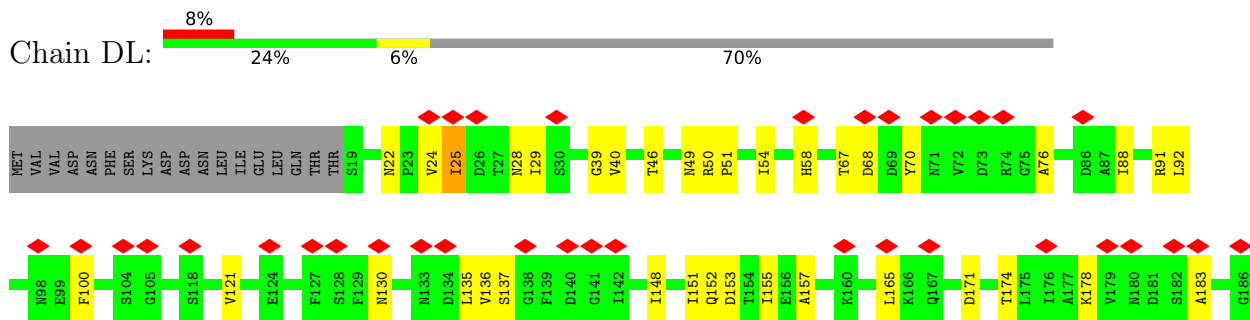




- Molecule 4: Fiber Lower, gp62



- Molecule 4: Fiber Lower, gp62

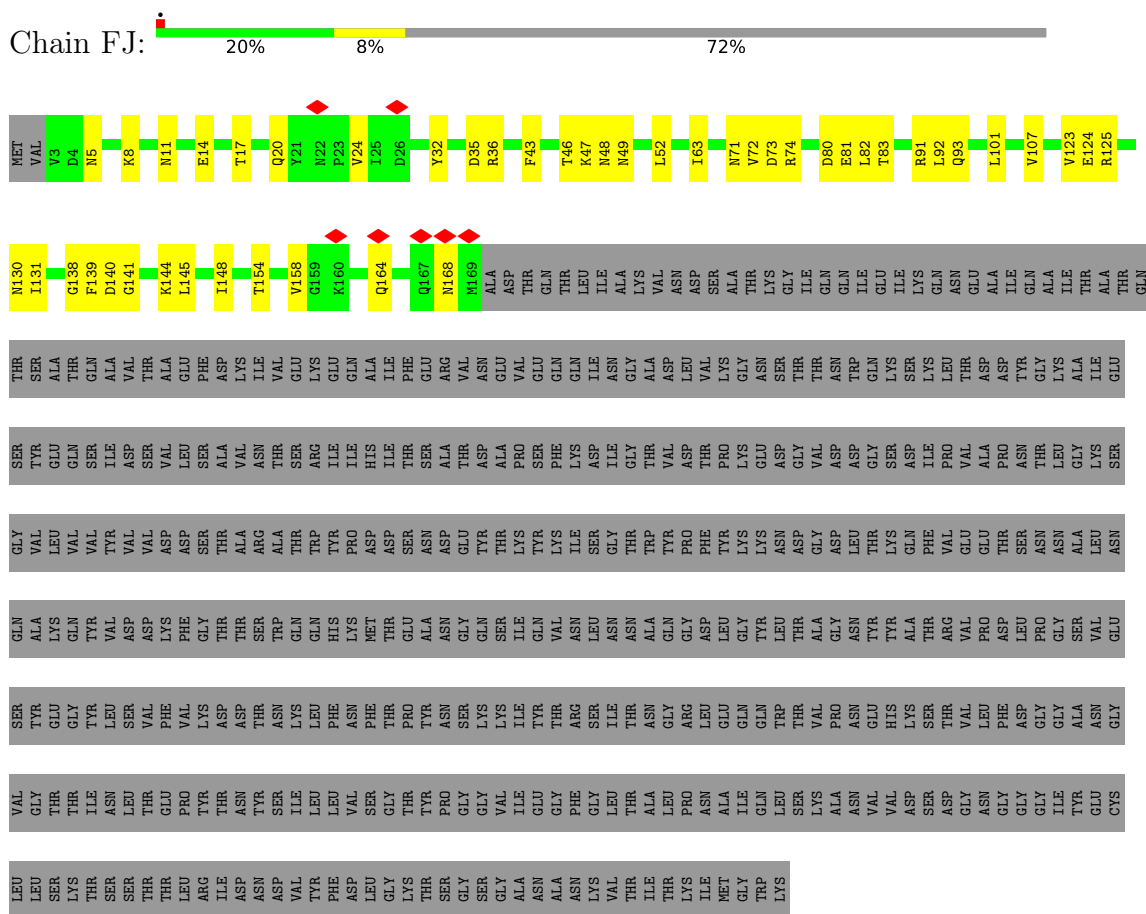


- Molecule 4: Fiber Lower, gp62

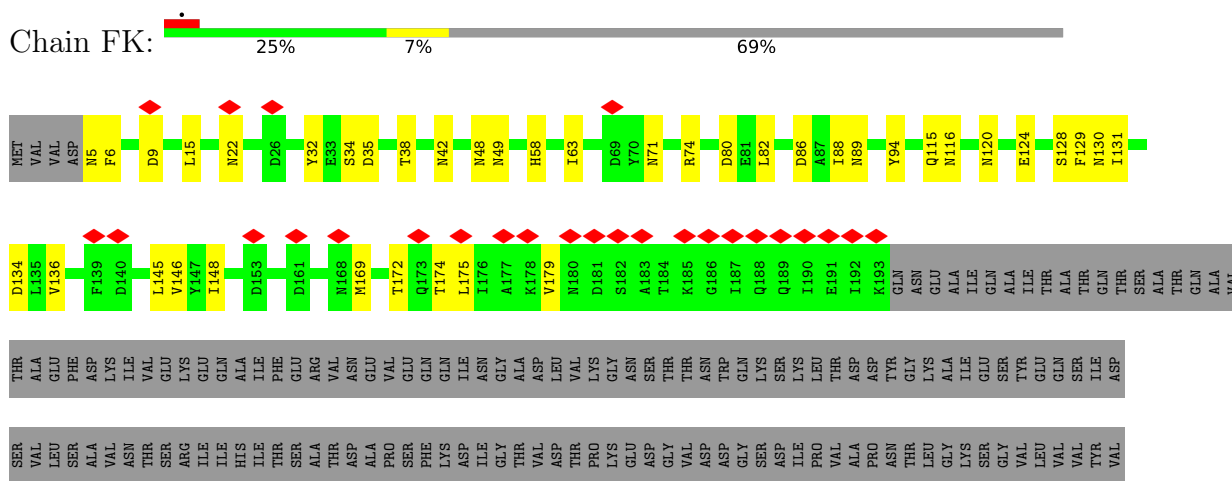
- Molecule 4: Fiber Lower, gp62



- Molecule 4: Fiber Lower, gp62

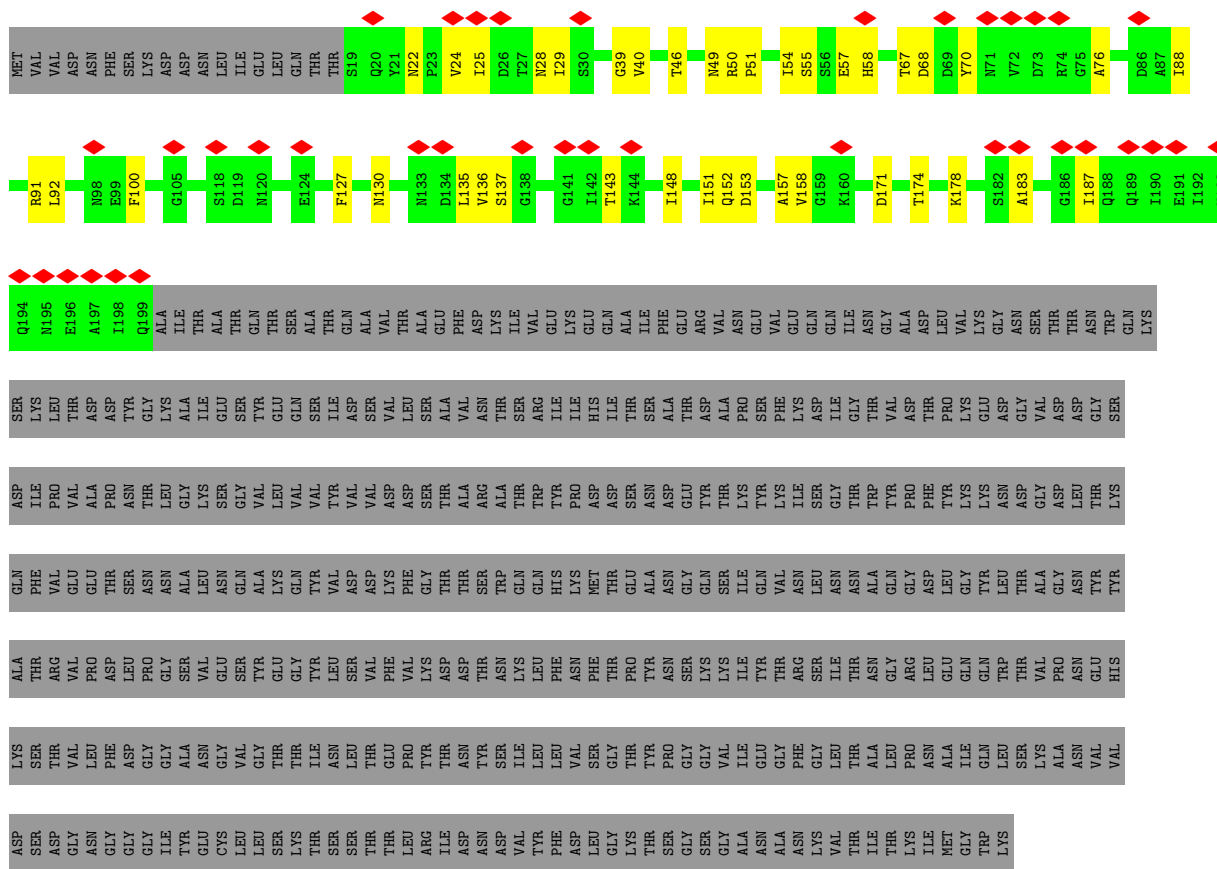


- Molecule 4: Fiber Lower, gp62

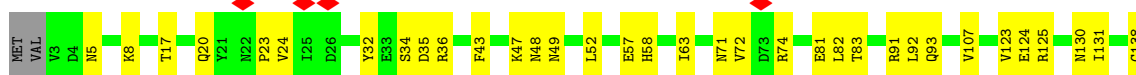


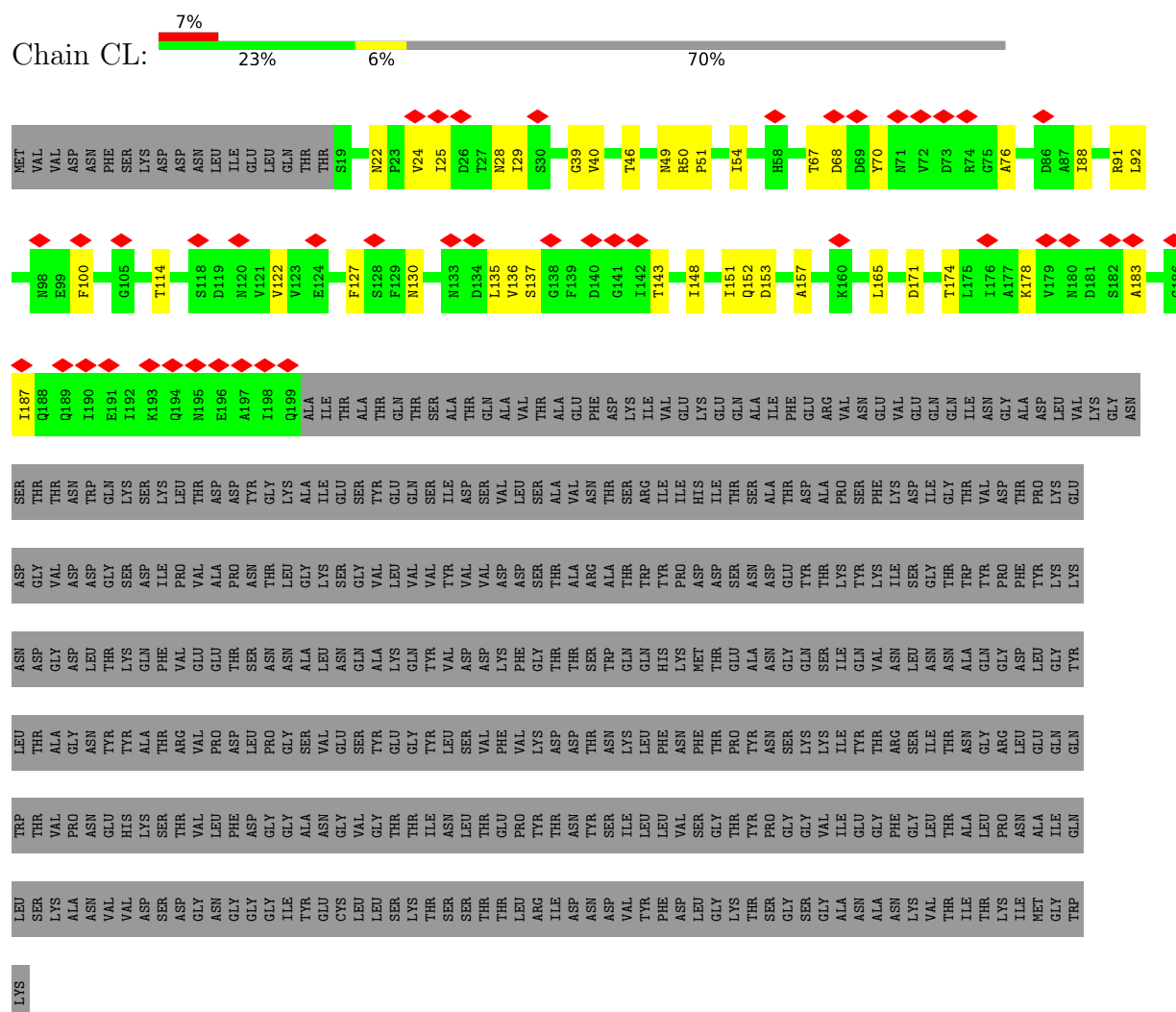
[illegible]

- Molecule 4: Fiber Lower, gp62

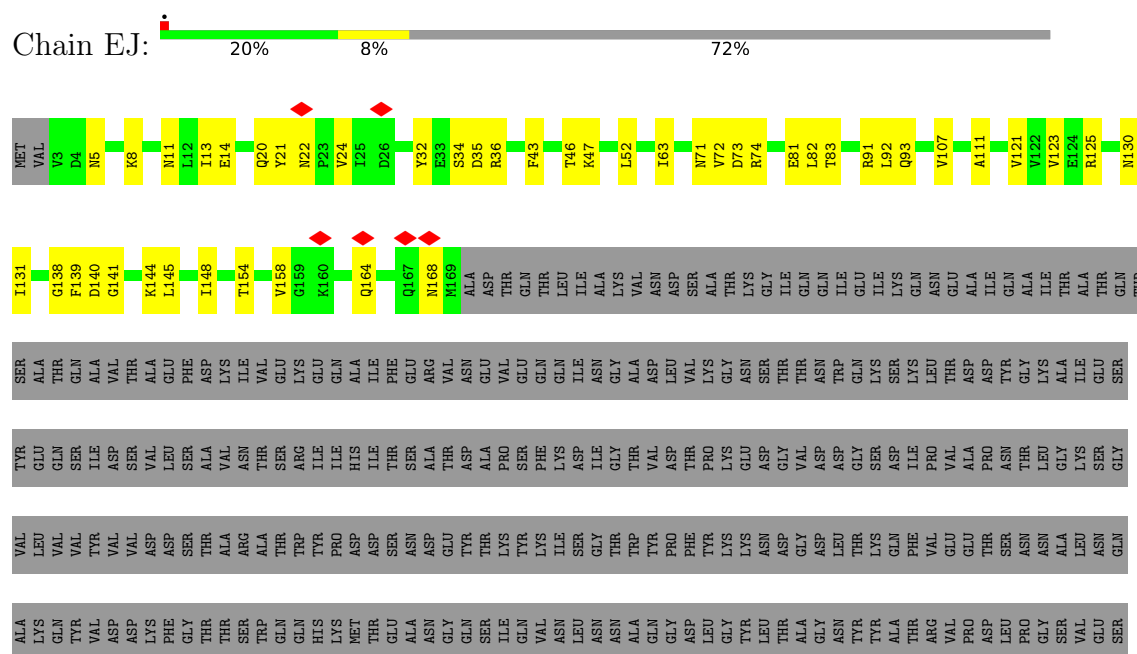


- Molecule 4: Fiber Lower, gp62

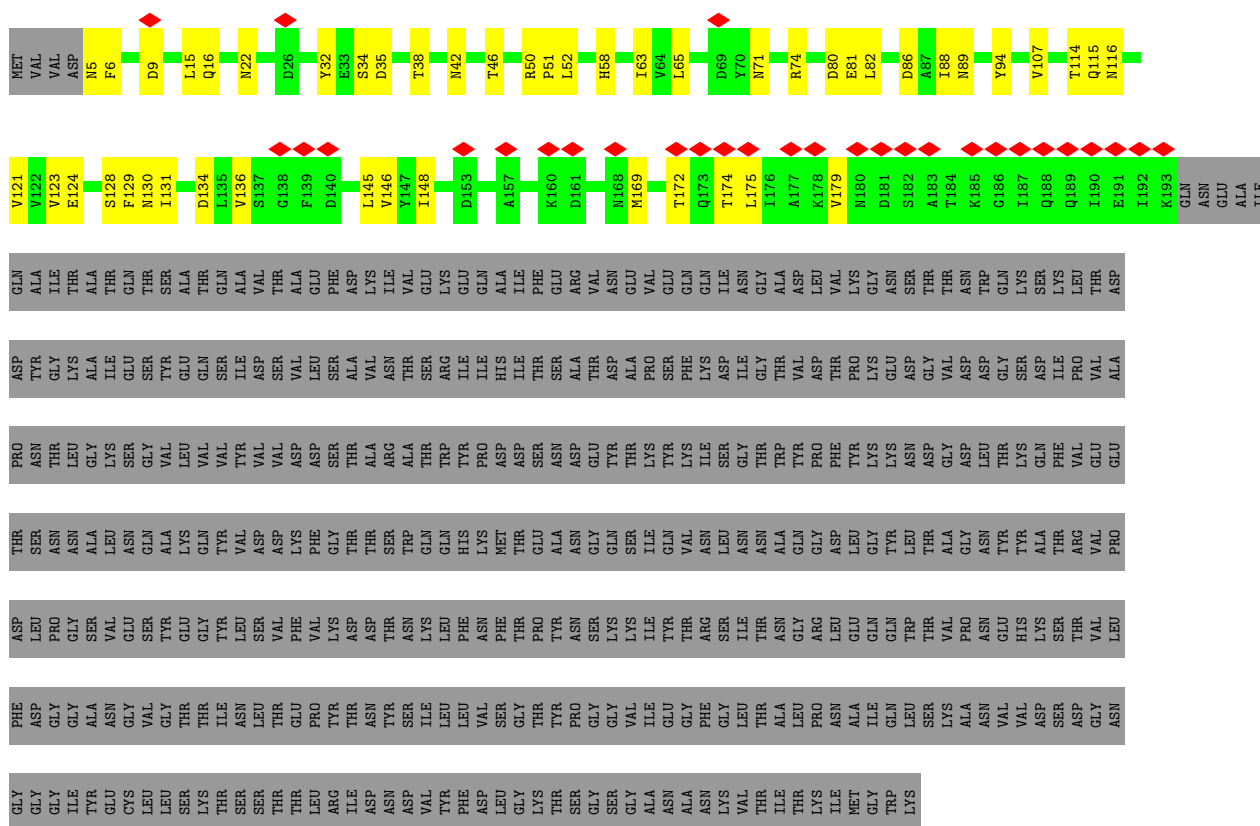




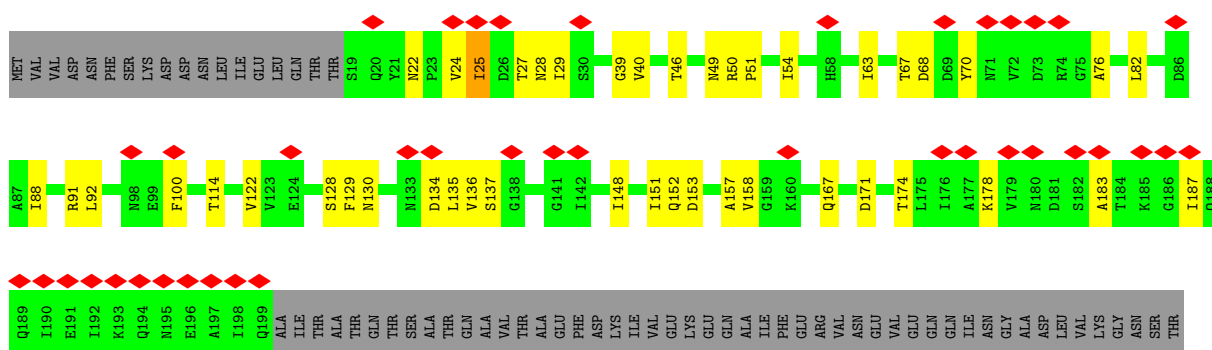
● Molecule 4: Fiber Lower, gp62

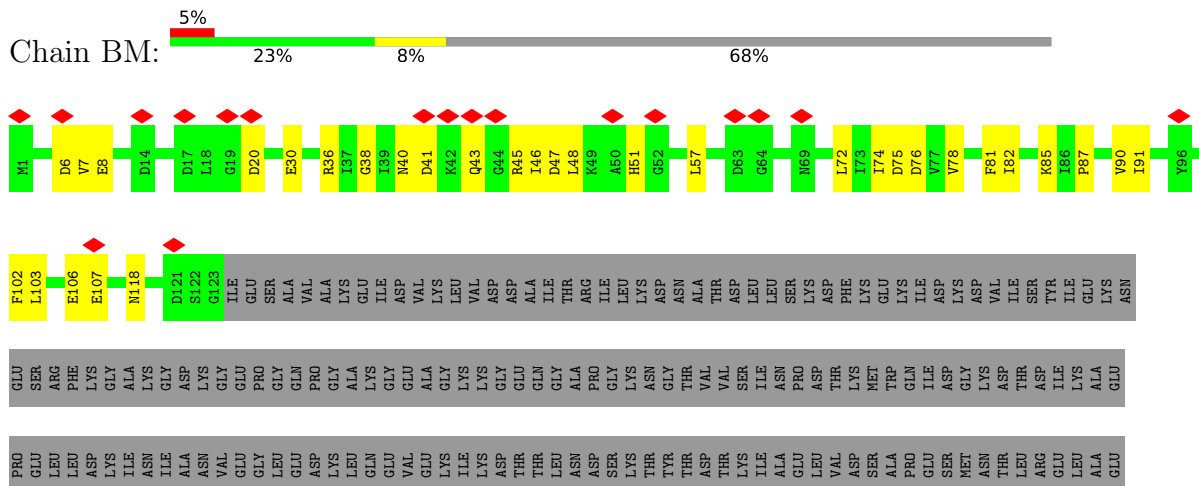


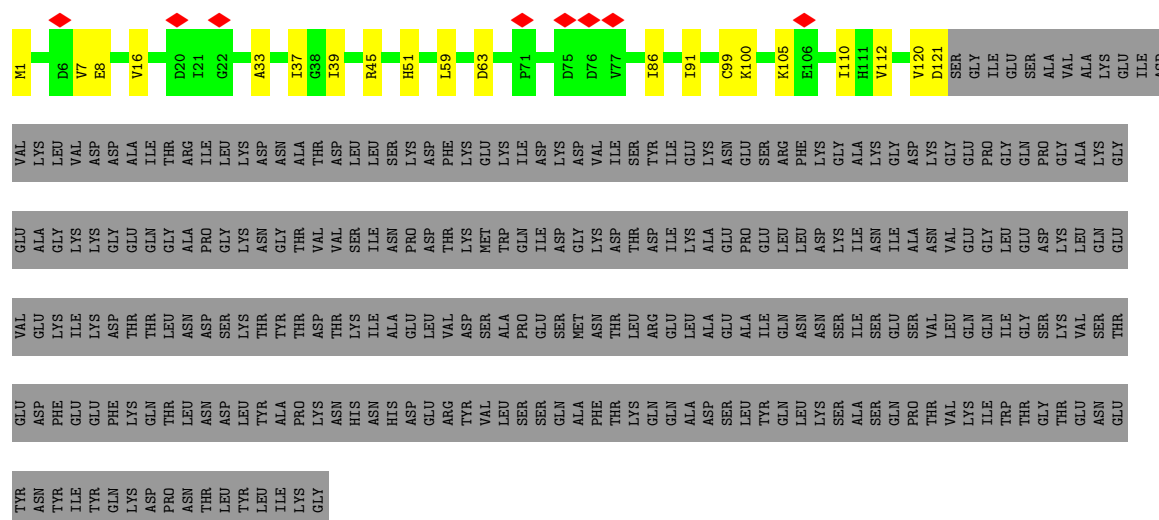
- Molecule 4: Fiber Lower, gp62



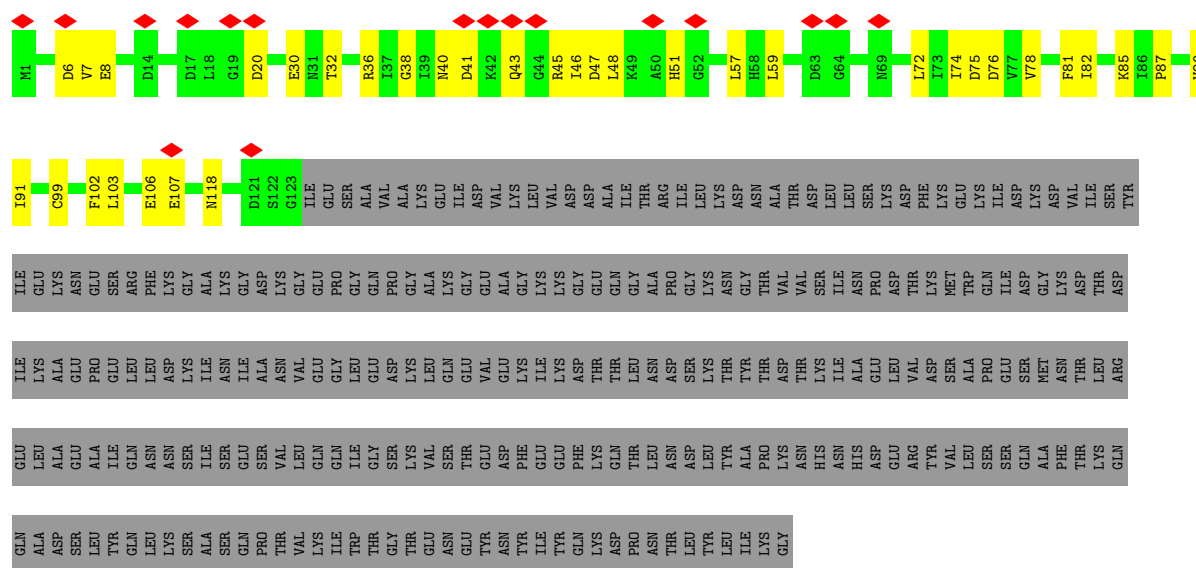
- Molecule 4: Fiber Lower, gp62



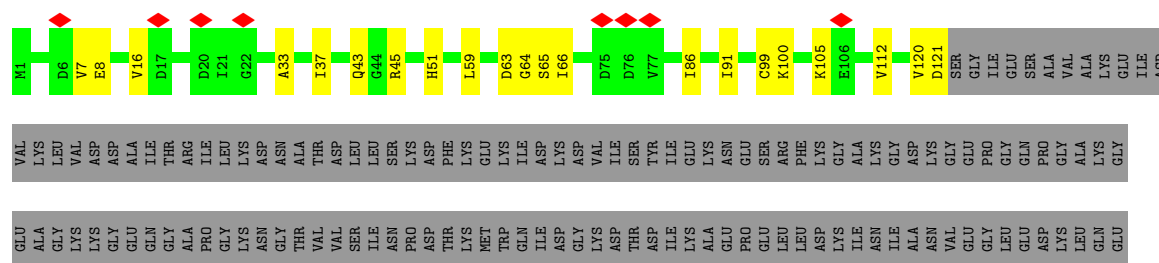




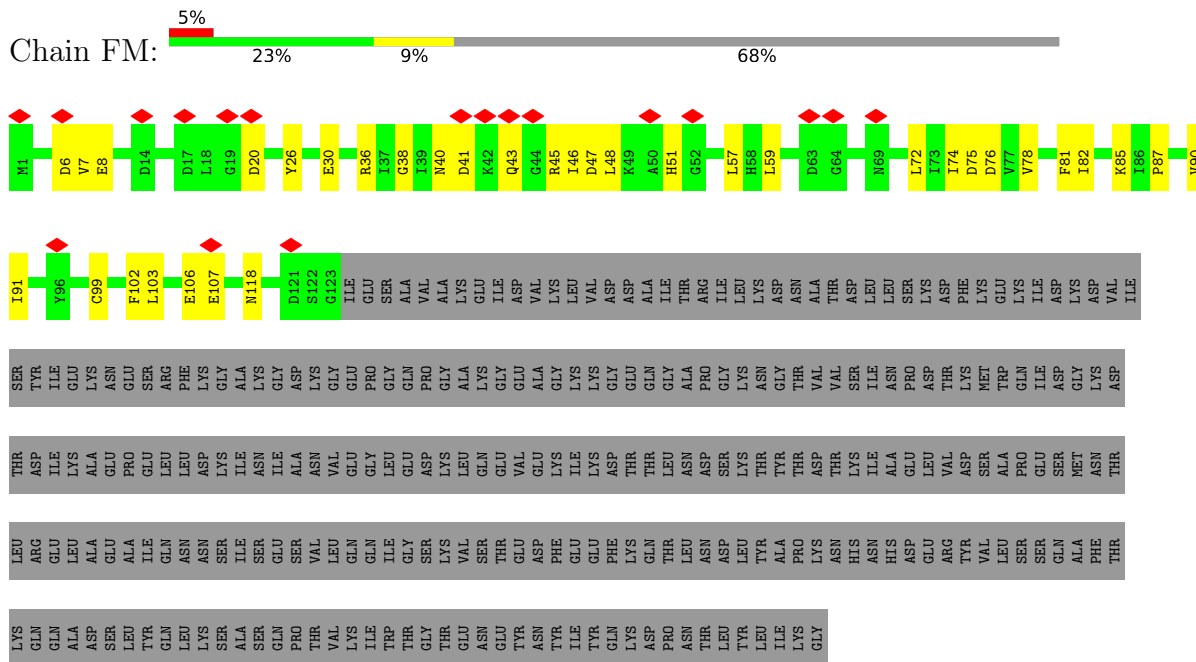
• Molecule 5: Fiber Upper, gp68



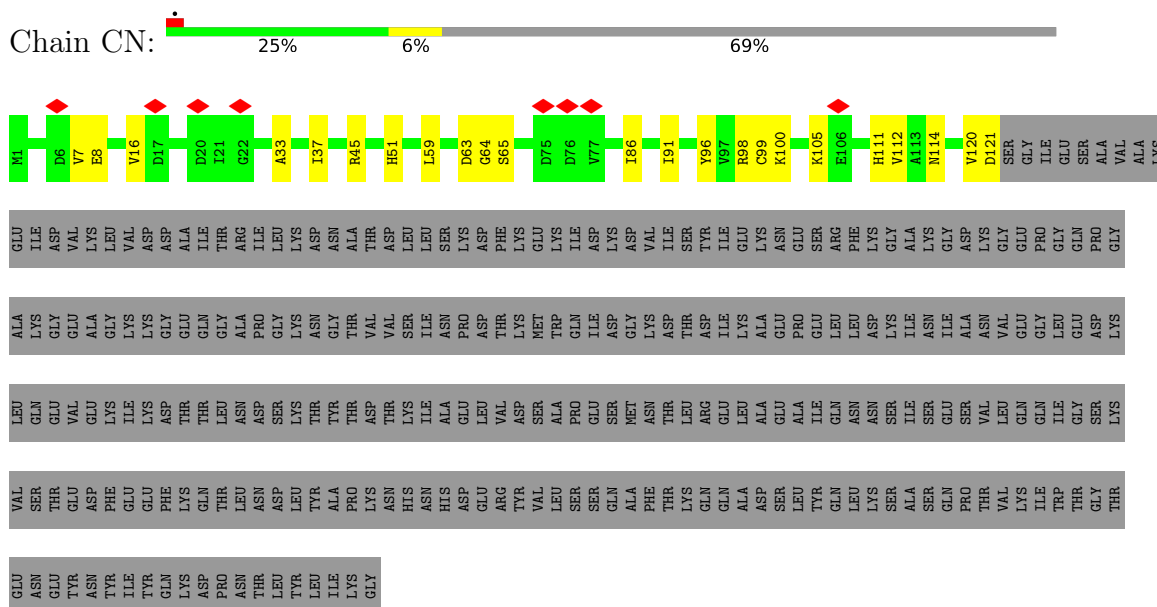
• Molecule 5: Fiber Upper, gp68



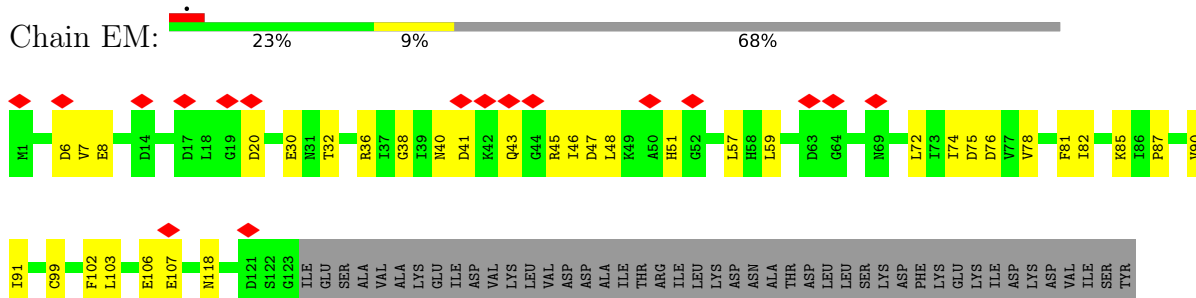
- Molecule 5: Fiber Upper, gp68



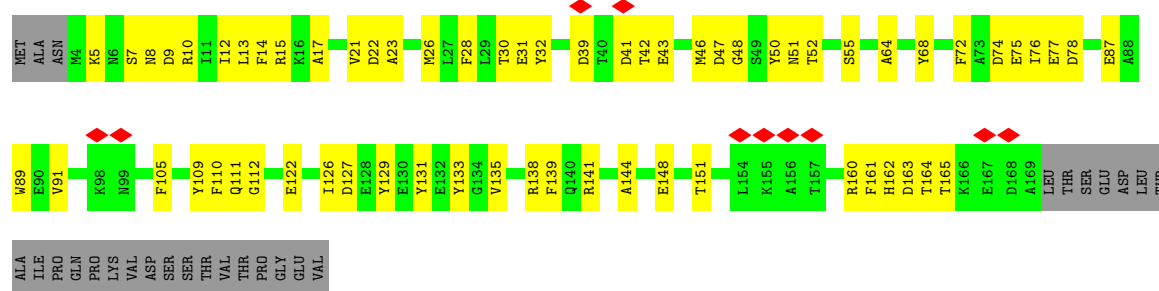
- Molecule 5: Fiber Upper, gp68



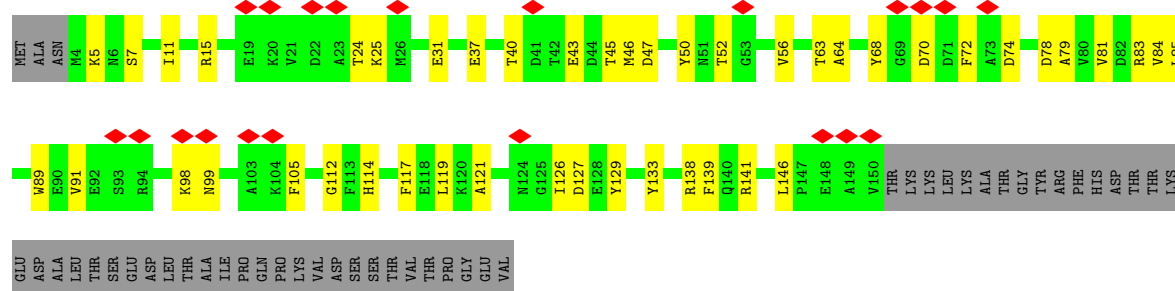
- Molecule 5: Fiber Upper, gp68



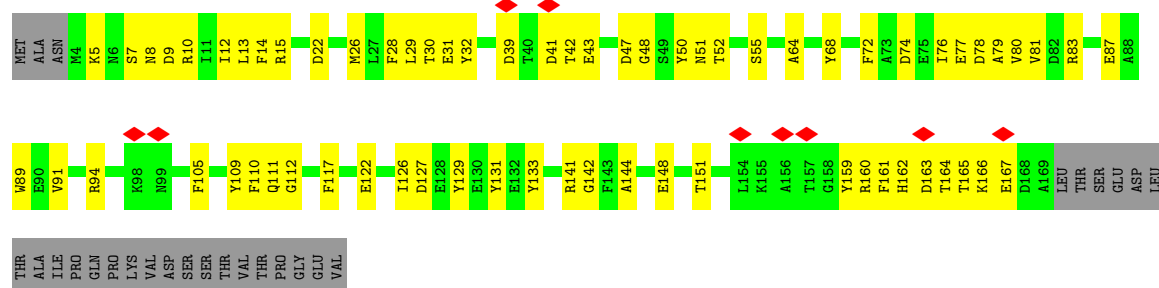
- Molecule 6: Major Tail Protein, gp53



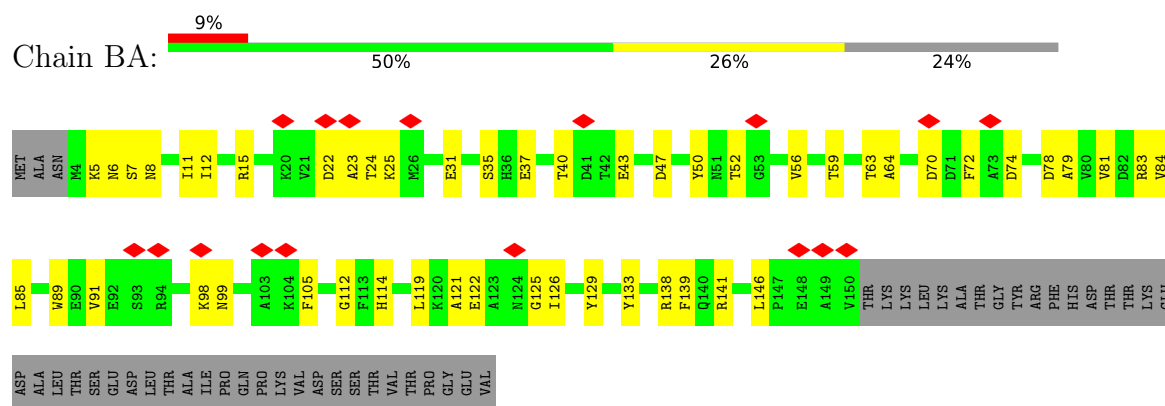
- Molecule 6: Major Tail Protein, gp53



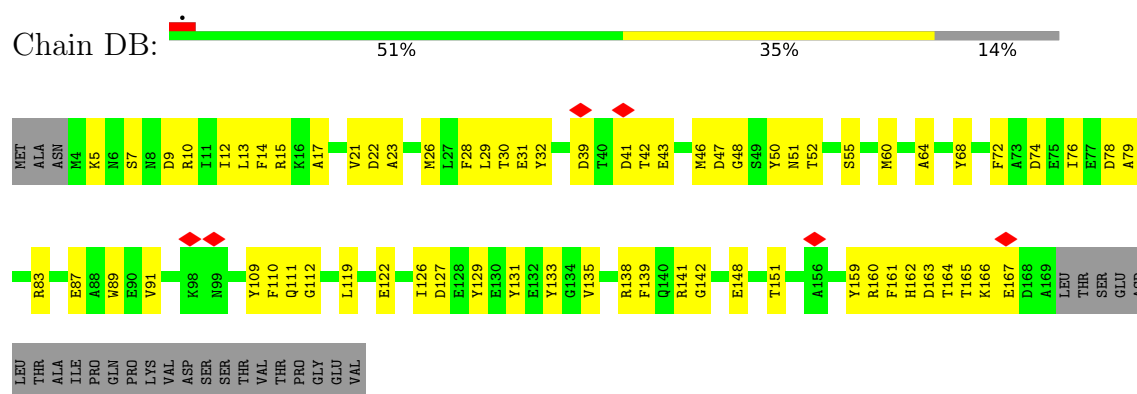
- Molecule 6: Major Tail Protein, gp53



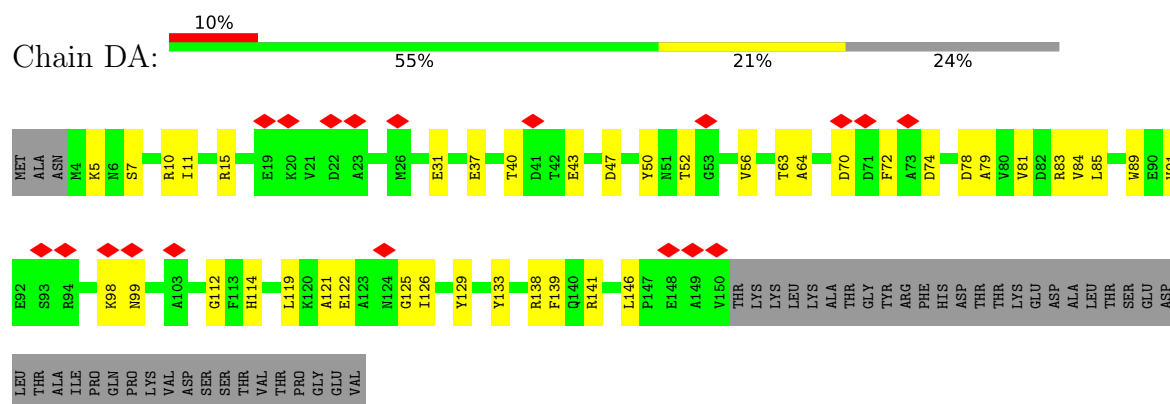
- Molecule 6: Major Tail Protein, gp53



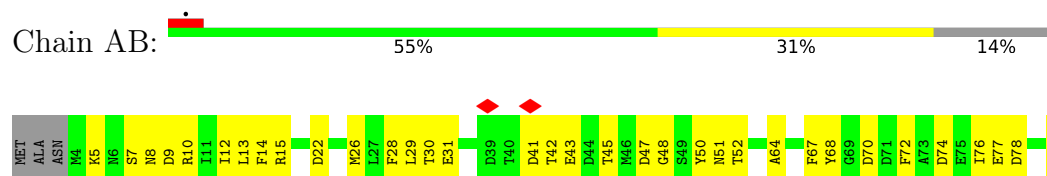
- Molecule 6: Major Tail Protein, gp53

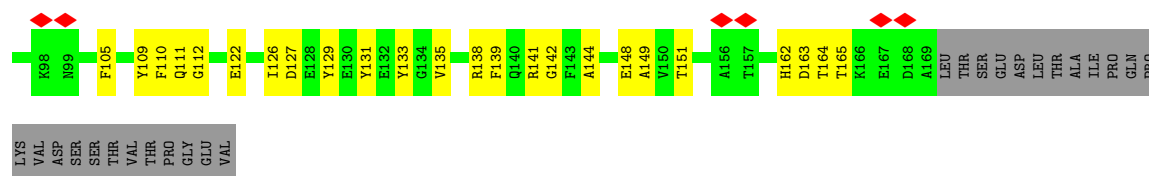


- Molecule 6: Major Tail Protein, gp53

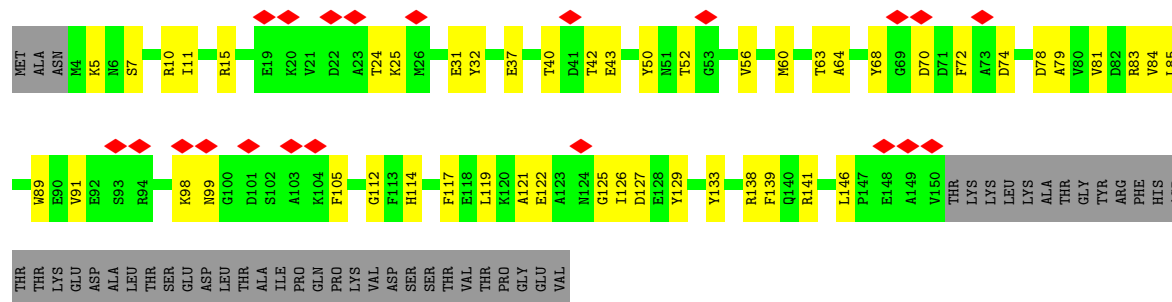


- Molecule 6: Major Tail Protein, gp53

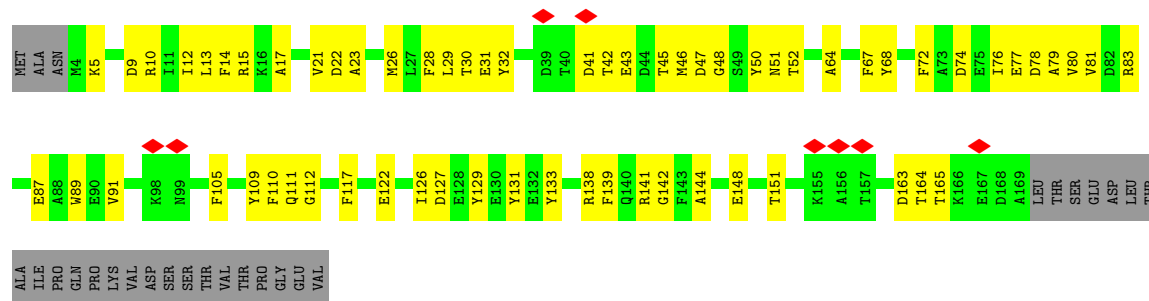




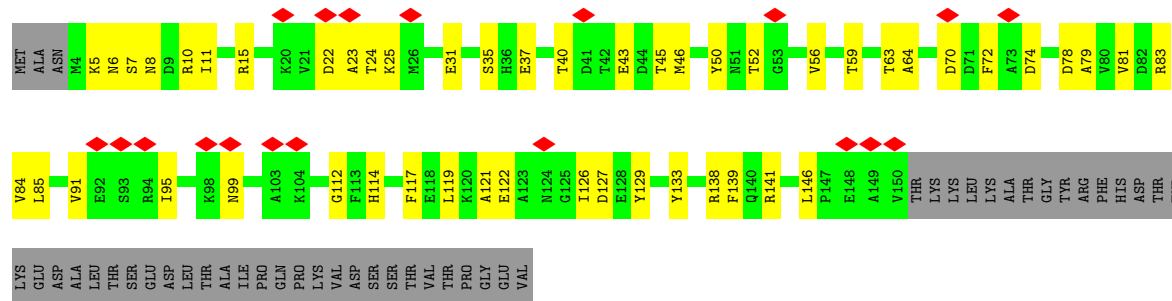
- Molecule 6: Major Tail Protein, gp53



- Molecule 6: Major Tail Protein, gp53

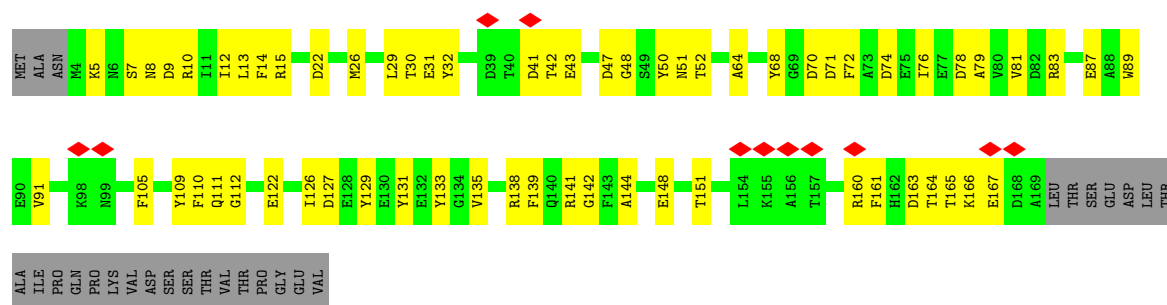


- Molecule 6: Major Tail Protein, gp53

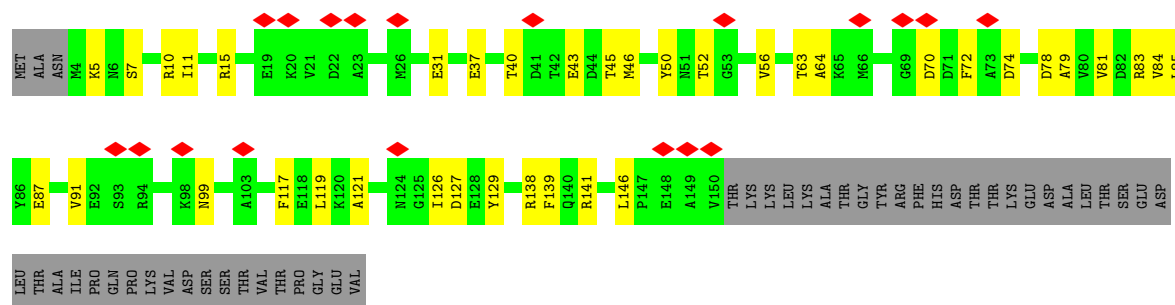


- Molecule 6: Major Tail Protein, gp53

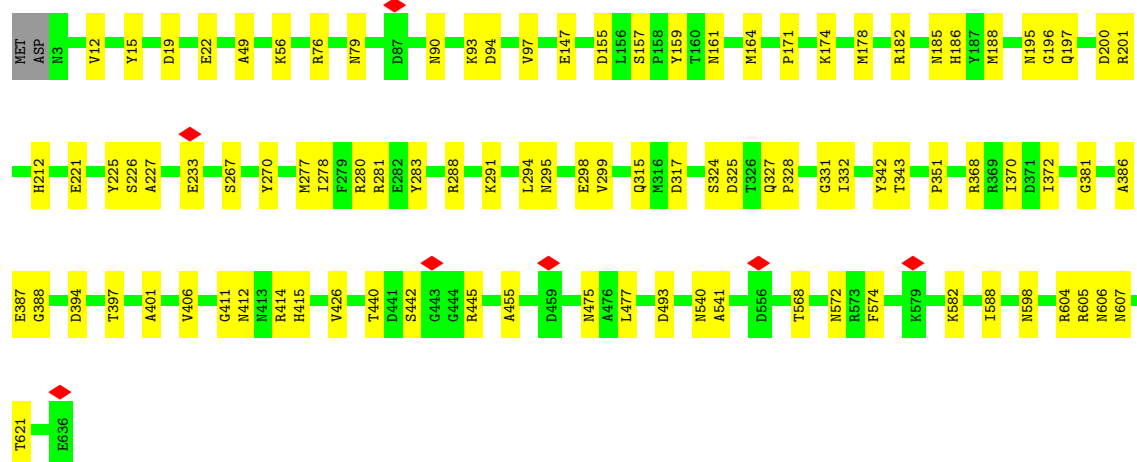




• Molecule 6: Major Tail Protein, gp53

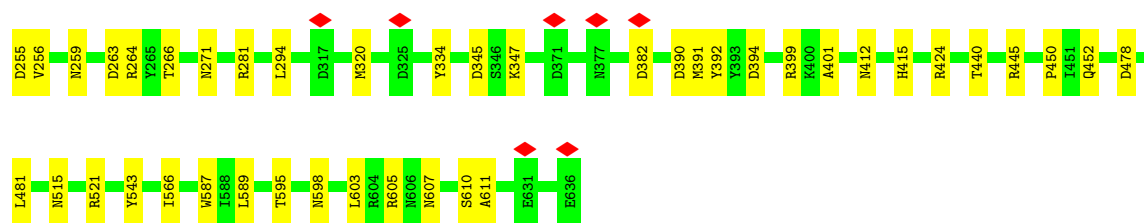


• Molecule 7: Receptor Binding Protein, gp61

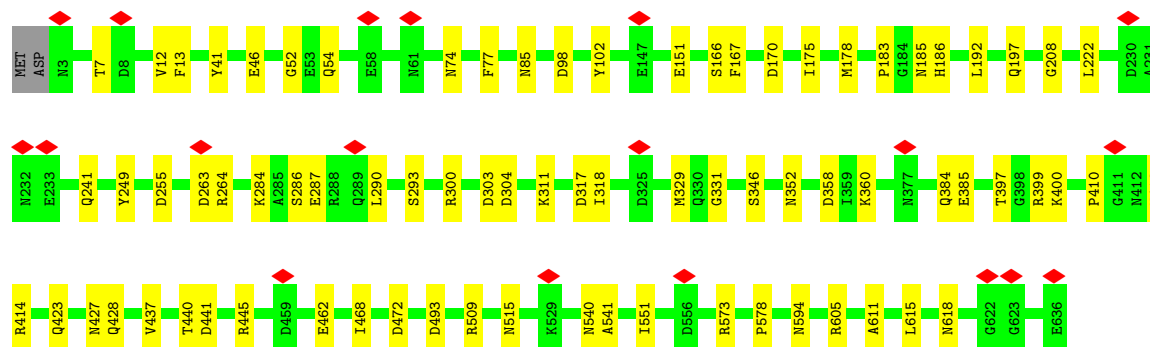
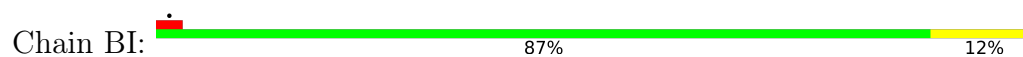


• Molecule 7: Receptor Binding Protein, gp61

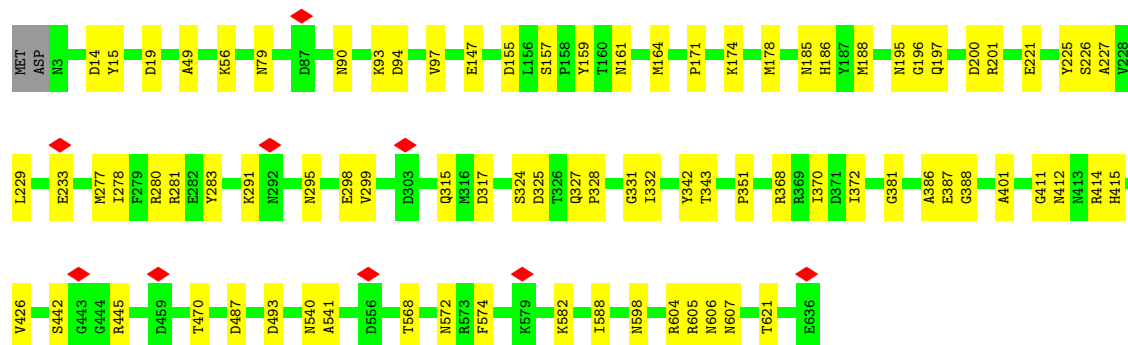
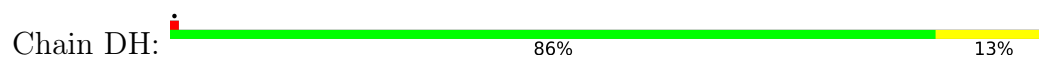




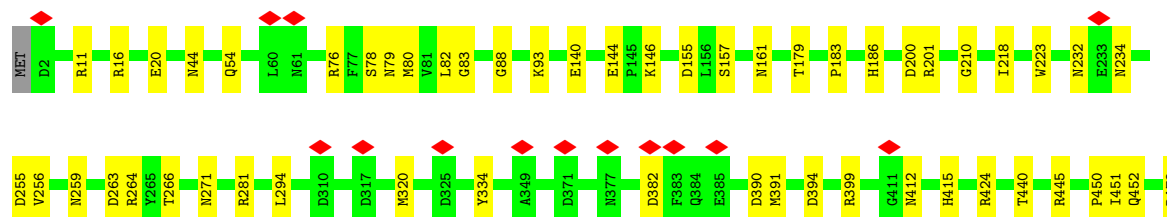
• Molecule 7: Receptor Binding Protein, gp61



• Molecule 7: Receptor Binding Protein, gp61

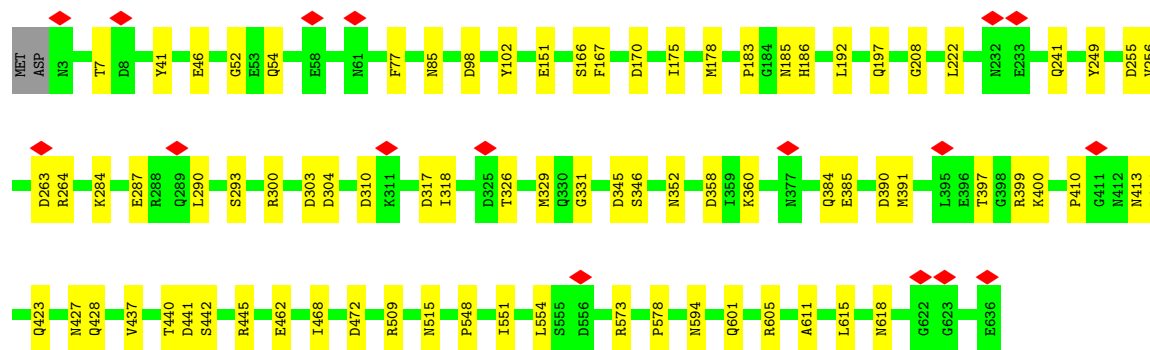


• Molecule 7: Receptor Binding Protein, gp61

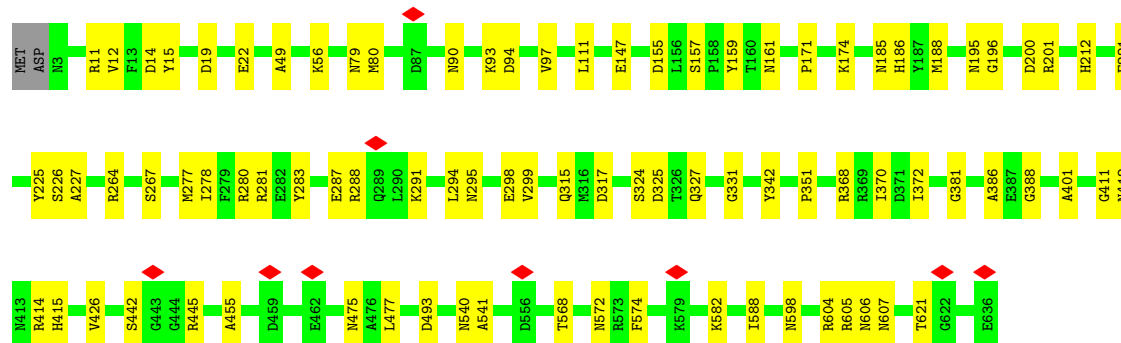
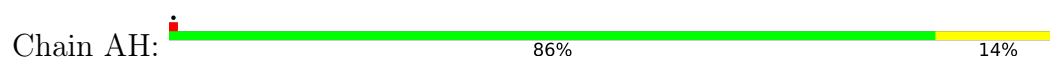




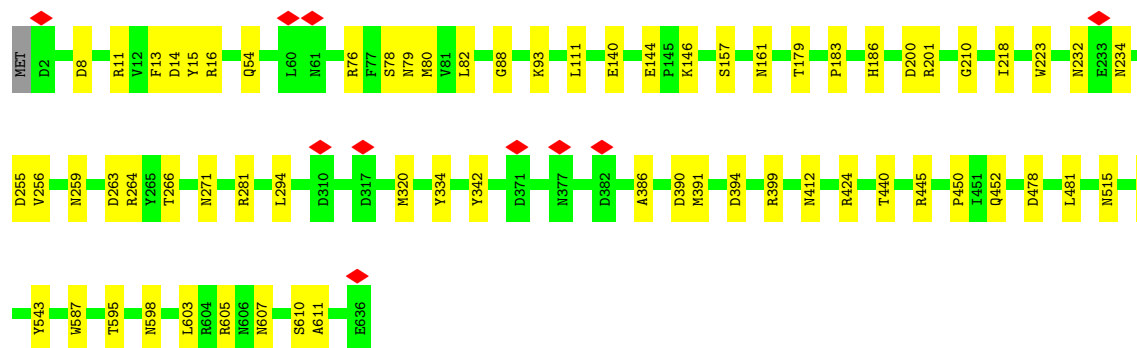
• Molecule 7: Receptor Binding Protein, gp61



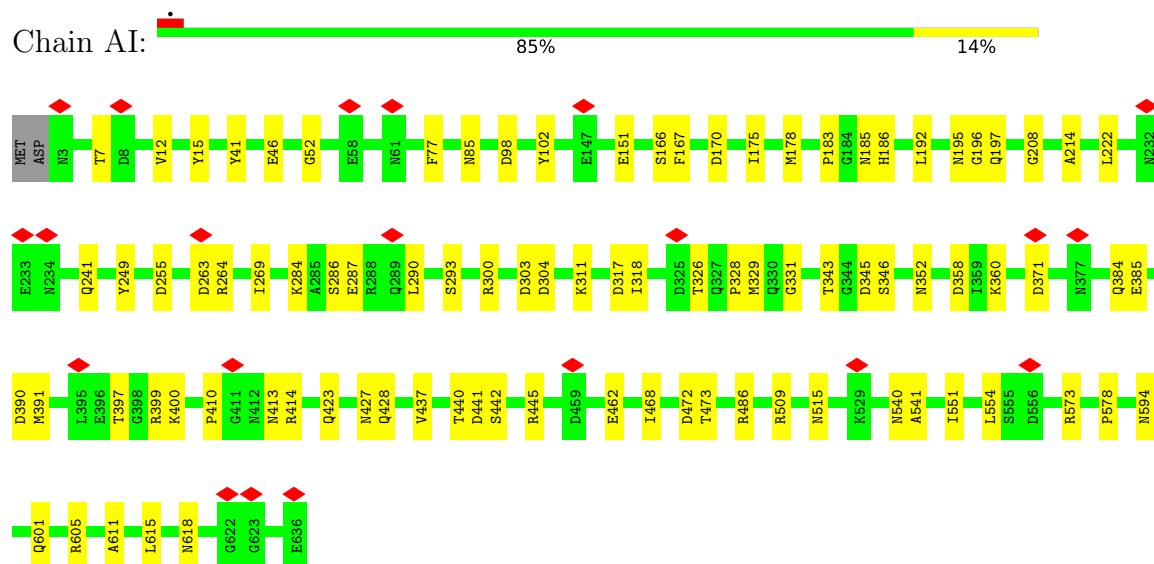
• Molecule 7: Receptor Binding Protein, gp61



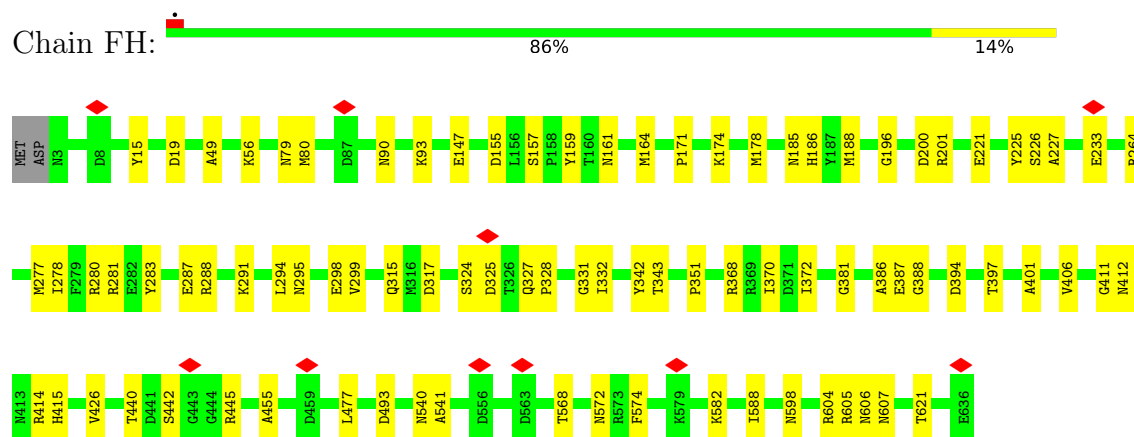
• Molecule 7: Receptor Binding Protein, gp61



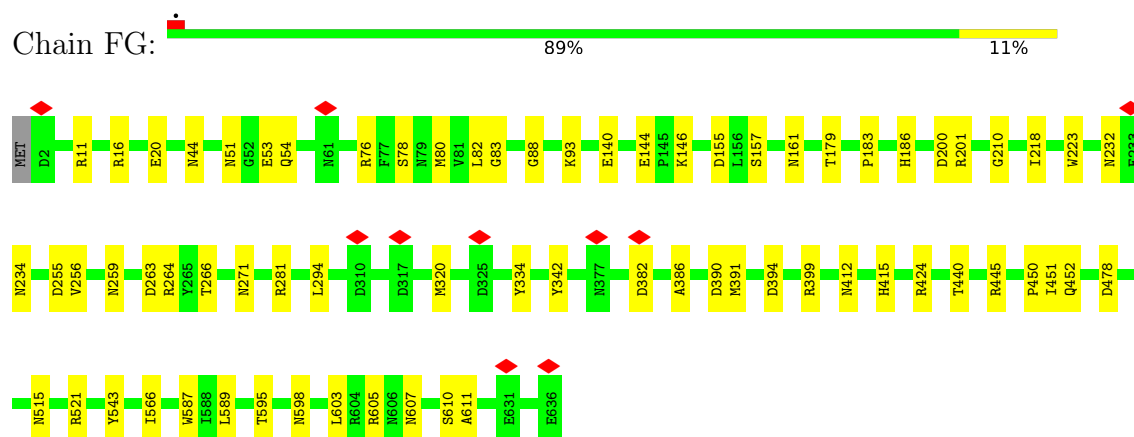
• Molecule 7: Receptor Binding Protein, gp61



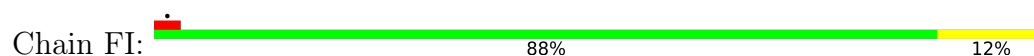
• Molecule 7: Receptor Binding Protein, gp61

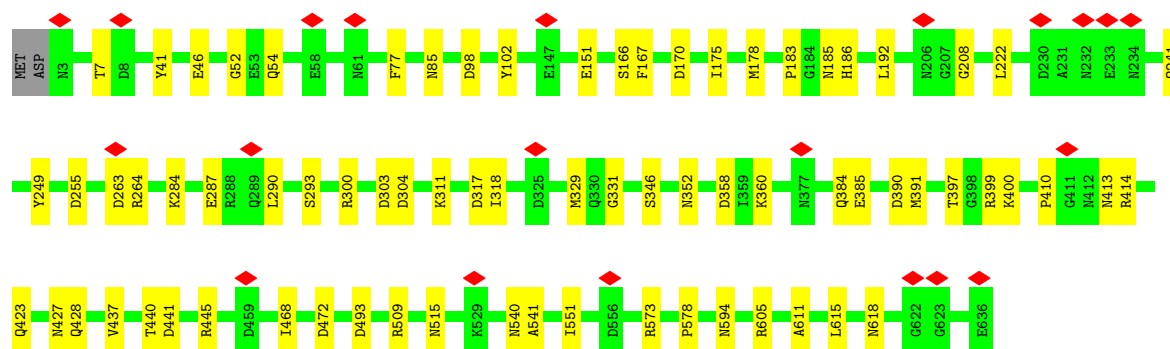


• Molecule 7: Receptor Binding Protein, gp61

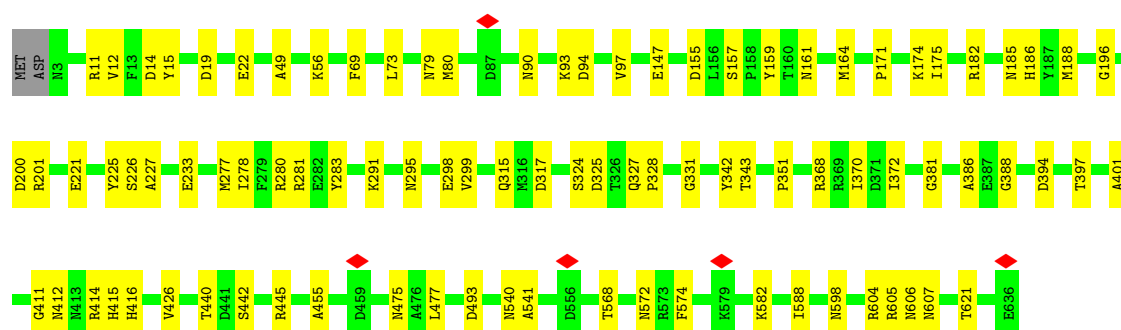


• Molecule 7: Receptor Binding Protein, gp61

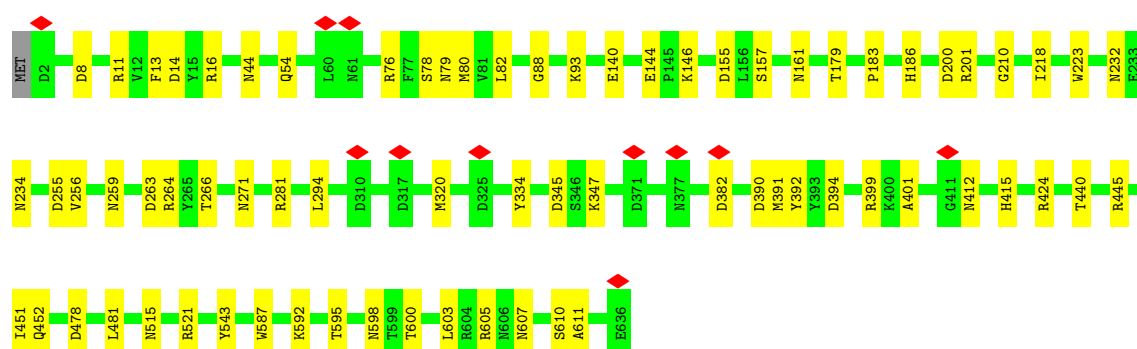




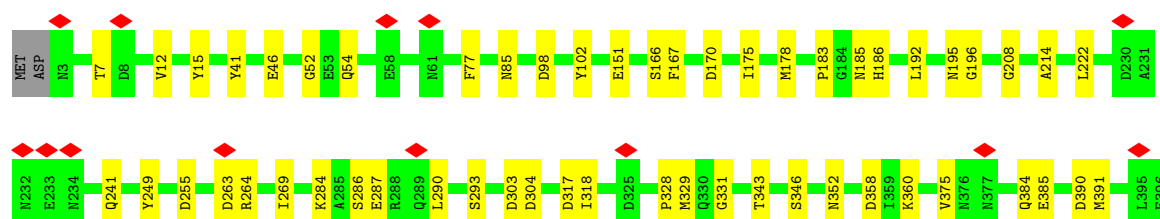
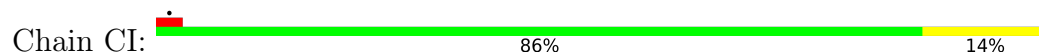
• Molecule 7: Receptor Binding Protein, gp61

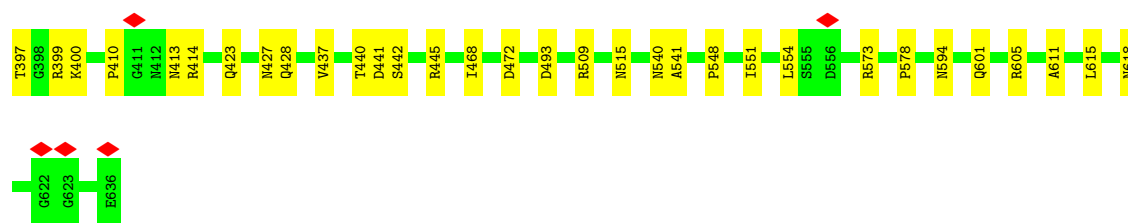


• Molecule 7: Receptor Binding Protein, gp61

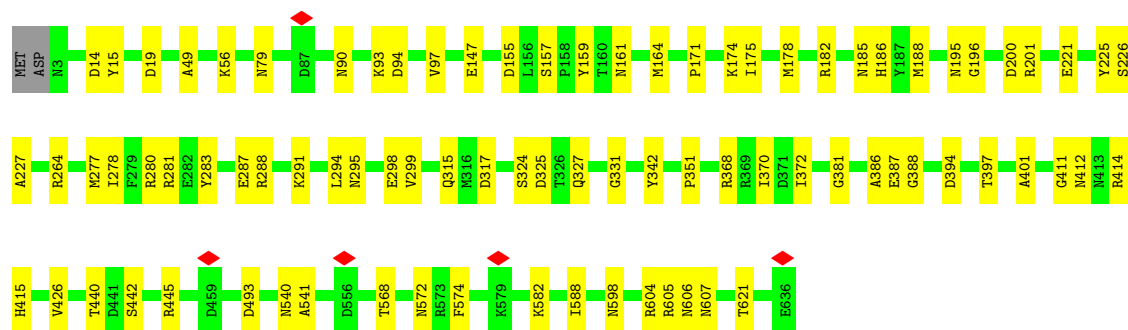


• Molecule 7: Receptor Binding Protein, gp61

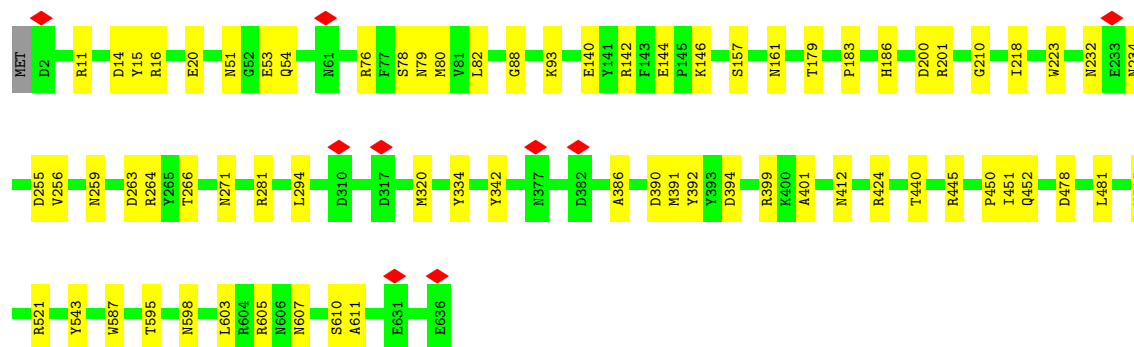




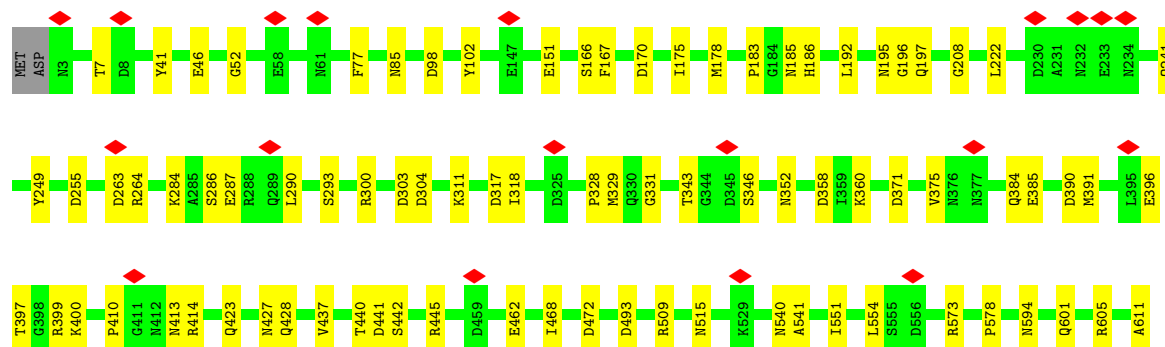
• Molecule 7: Receptor Binding Protein, gp61

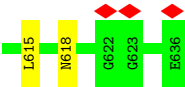


• Molecule 7: Receptor Binding Protein, gp61



• Molecule 7: Receptor Binding Protein, gp61





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	43601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	104.33	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	29000	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	28.554	Depositor
Minimum map value	-18.784	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.956	Depositor
Recommended contour level	4.5	Depositor
Map size ($\text{\AA}$)	619.52, 619.52, 619.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.21, 1.21, 1.21	Depositor

5 Model quality

5.1 Standard geometry

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

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	AC	0.46	0/2658	0.56	0/3579
1	AD	0.46	0/2658	0.56	0/3579
1	BC	0.46	0/2658	0.56	0/3579
1	BD	0.46	0/2658	0.56	0/3579
1	CC	0.46	0/2658	0.56	0/3579
1	CD	0.46	0/2658	0.56	0/3579
2	AE	0.41	0/3116	0.54	0/4198
2	BE	0.41	0/3116	0.54	0/4198
2	CE	0.41	0/3116	0.54	0/4198
3	AF	0.39	0/161	0.54	0/216
3	BF	0.38	0/161	0.54	0/216
3	CF	0.39	0/161	0.53	0/216
4	AJ	0.17	0/1353	0.31	0/1833
4	AK	0.17	0/1518	0.30	0/2055
4	AL	0.13	0/1451	0.30	0/1964
4	BJ	0.17	0/1353	0.31	0/1833
4	BK	0.16	0/1518	0.30	0/2055
4	BL	0.12	0/1451	0.28	0/1964
4	CJ	0.16	0/1353	0.30	0/1833
4	CK	0.16	0/1518	0.30	0/2055
4	CL	0.12	0/1451	0.31	1/1964 (0.1%)
4	DJ	0.16	0/1353	0.30	0/1833
4	DK	0.16	0/1518	0.30	0/2055
4	DL	0.12	0/1451	0.33	1/1964 (0.1%)
4	EJ	0.17	0/1353	0.31	0/1833
4	EK	0.17	0/1518	0.30	0/2055
4	EL	0.12	0/1451	0.32	1/1964 (0.1%)
4	FJ	0.17	0/1353	0.32	0/1833
4	FK	0.17	0/1518	0.30	0/2055
4	FL	0.13	0/1451	0.31	1/1964 (0.1%)
5	AM	0.13	0/1008	0.34	0/1351
5	AN	0.13	0/998	0.32	0/1338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	BM	0.13	0/1008	0.34	0/1351
5	BN	0.14	0/998	0.33	0/1338
5	CM	0.14	0/1008	0.35	0/1351
5	CN	0.14	0/998	0.33	0/1338
5	DM	0.14	0/1008	0.36	0/1351
5	DN	0.13	0/998	0.32	0/1338
5	EM	0.13	0/1008	0.34	0/1351
5	EN	0.13	0/998	0.32	0/1338
5	FM	0.14	0/1008	0.34	0/1351
5	FN	0.13	0/998	0.33	0/1338
6	AA	0.35	0/1188	0.39	0/1596
6	AB	0.54	0/1346	0.47	0/1807
6	BA	0.35	0/1188	0.40	0/1596
6	BB	0.53	0/1346	0.47	0/1807
6	CA	0.35	0/1188	0.39	0/1596
6	CB	0.53	0/1346	0.47	0/1807
6	DA	0.35	0/1188	0.39	0/1596
6	DB	0.53	0/1346	0.47	0/1807
6	EA	0.35	0/1188	0.39	0/1596
6	EB	0.53	0/1346	0.48	0/1807
6	FA	0.36	0/1188	0.40	0/1596
6	FB	0.54	0/1346	0.46	0/1807
7	AG	0.34	0/5332	0.46	0/7216
7	AH	0.37	0/5324	0.47	0/7205
7	AI	0.37	0/5324	0.45	0/7205
7	BG	0.36	0/5332	0.47	0/7216
7	BH	0.37	0/5324	0.47	0/7205
7	BI	0.37	0/5324	0.46	0/7205
7	CG	0.34	0/5332	0.46	0/7216
7	CH	0.37	0/5324	0.47	0/7205
7	CI	0.37	0/5324	0.46	0/7205
7	DG	0.35	0/5332	0.46	0/7216
7	DH	0.37	0/5324	0.48	0/7205
7	DI	0.37	0/5324	0.46	0/7205
7	EG	0.34	0/5332	0.46	0/7216
7	EH	0.37	0/5324	0.47	0/7205
7	EI	0.37	0/5324	0.46	0/7205
7	FG	0.35	0/5332	0.46	0/7216
7	FH	0.37	0/5324	0.47	0/7205
7	FI	0.36	0/5324	0.46	0/7205
All	All	0.35	0/174831	0.45	4/236136 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	EL	25	ILE	N-CA-C	-6.02	107.99	113.71
4	CL	25	ILE	N-CA-C	-5.89	108.11	113.71
4	FL	25	ILE	N-CA-C	-5.83	108.17	113.71
4	DL	25	ILE	N-CA-C	-5.83	108.18	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AC	2601	0	2549	90	0
1	AD	2601	0	2550	123	0
1	BC	2601	0	2549	98	0
1	BD	2601	0	2550	121	0
1	CC	2601	0	2549	94	0
1	CD	2601	0	2550	122	0
2	AE	3068	0	3098	31	0
2	BE	3068	0	3098	32	0
2	CE	3068	0	3098	32	0
3	AF	160	0	156	3	0
3	BF	160	0	156	6	0
3	CF	160	0	156	8	0
4	AJ	1331	0	1292	32	0
4	AK	1496	0	1470	36	0
4	AL	1430	0	1406	58	0
4	BJ	1331	0	1292	41	0
4	BK	1496	0	1470	34	0
4	BL	1430	0	1406	69	0
4	CJ	1331	0	1292	33	0
4	CK	1496	0	1470	33	0
4	CL	1430	0	1406	62	0
4	DJ	1331	0	1292	39	0
4	DK	1496	0	1470	31	0
4	DL	1430	0	1406	63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EJ	1331	0	1292	35	0
4	EK	1496	0	1470	39	0
4	EL	1430	0	1406	63	0
4	FJ	1331	0	1292	35	0
4	FK	1496	0	1470	33	0
4	FL	1430	0	1406	61	0
5	AM	991	0	1010	41	0
5	AN	981	0	1002	15	0
5	BM	991	0	1010	43	0
5	BN	981	0	1002	24	0
5	CM	991	0	1010	49	0
5	CN	981	0	1002	16	0
5	DM	991	0	1010	45	0
5	DN	981	0	1002	17	0
5	EM	991	0	1010	45	0
5	EN	981	0	1002	17	0
5	FM	991	0	1010	46	0
5	FN	981	0	1002	17	0
6	AA	1165	0	1085	44	0
6	AB	1320	0	1241	92	0
6	BA	1165	0	1085	46	0
6	BB	1320	0	1241	95	0
6	CA	1165	0	1085	33	0
6	CB	1320	0	1241	91	0
6	DA	1165	0	1085	41	0
6	DB	1320	0	1241	107	0
6	EA	1165	0	1085	41	0
6	EB	1320	0	1241	111	0
6	FA	1165	0	1085	41	0
6	FB	1320	0	1241	110	0
7	AG	5201	0	5001	52	0
7	AH	5193	0	4997	85	0
7	AI	5193	0	4997	61	0
7	BG	5201	0	5001	52	0
7	BH	5193	0	4997	88	0
7	BI	5193	0	4997	52	0
7	CG	5201	0	5001	53	0
7	CH	5193	0	4997	88	0
7	CI	5193	0	4997	57	0
7	DG	5201	0	5001	51	0
7	DH	5193	0	4997	65	0
7	DI	5193	0	4997	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	EG	5201	0	5001	51	0
7	EH	5193	0	4997	64	0
7	EI	5193	0	4997	59	0
7	FG	5201	0	5001	50	0
7	FH	5193	0	4997	66	0
7	FI	5193	0	4997	49	0
8	AH	1	0	0	0	0
8	BH	1	0	0	0	0
8	CH	1	0	0	0	0
8	DH	1	0	0	0	0
8	EH	1	0	0	0	0
8	FH	1	0	0	0	0
All	All	171102	0	166065	2824	0

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

All (2824) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:58:HIS:CE1	5:BN:43:GLN:HG2	1.29	1.66
4:BL:58:HIS:ND1	5:BN:43:GLN:HG2	1.41	1.35
4:FL:174:THR:OG1	7:FH:90:ASN:ND2	1.63	1.31
1:CD:149:GLN:NE2	6:AB:41:ASP:OD1	1.64	1.28
1:AD:149:GLN:NE2	6:BB:41:ASP:OD1	1.63	1.28
4:AL:174:THR:OG1	7:AH:90:ASN:ND2	1.67	1.27
1:CC:20:ILE:HD11	6:FB:50:TYR:CE2	1.69	1.27
4:BL:174:THR:OG1	7:BH:90:ASN:ND2	1.65	1.26
1:BC:69:ASP:OD2	7:BH:15:TYR:CE1	1.87	1.26
1:BD:105:PRO:HA	6:EB:15:ARG:NH2	1.49	1.25
4:CL:174:THR:OG1	7:CH:90:ASN:ND2	1.67	1.25
1:AC:69:ASP:OD2	7:AH:15:TYR:CE1	1.89	1.24
4:DL:174:THR:OG1	7:DH:90:ASN:ND2	1.68	1.24
1:AC:20:ILE:HD11	6:DB:50:TYR:CE2	1.73	1.24
4:EL:174:THR:OG1	7:EH:90:ASN:ND2	1.68	1.23
1:CC:69:ASP:OD2	7:CH:15:TYR:CE1	1.89	1.23
1:BD:107:SER:HA	6:EB:21:VAL:C	1.64	1.23
1:BD:149:GLN:NE2	6:CB:41:ASP:OD1	1.72	1.20
4:BL:58:HIS:CE1	5:BN:43:GLN:CG	2.24	1.20
4:FL:178:LYS:NZ	7:FH:93:LYS:HD3	1.54	1.18
4:BL:58:HIS:ND1	5:BN:43:GLN:CG	2.05	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:178:LYS:NZ	7:BH:93:LYS:HD3	1.56	1.18
4:EL:178:LYS:NZ	7:EH:93:LYS:HD3	1.57	1.17
4:AL:178:LYS:NZ	7:AH:93:LYS:HD3	1.56	1.17
1:AD:100:TYR:OH	6:DB:110:PHE:HA	1.47	1.15
1:CD:100:TYR:OH	6:FB:110:PHE:HA	1.46	1.13
1:BC:20:ILE:HD11	6:EB:50:TYR:CE2	1.82	1.13
1:BD:67:ARG:NH1	6:FB:47:ASP:HA	1.64	1.13
1:AD:207:ASN:HB3	7:AH:455:ALA:CB	1.77	1.12
4:CL:178:LYS:NZ	7:CH:93:LYS:HD3	1.63	1.13
1:CD:65:LYS:NZ	7:FH:19:ASP:OD1	1.82	1.12
1:AC:188:PHE:HE2	7:FG:11:ARG:HB3	1.14	1.11
1:AD:65:LYS:NZ	7:DH:19:ASP:OD1	1.84	1.11
1:BD:100:TYR:OH	6:EB:110:PHE:HA	1.49	1.09
1:CC:188:PHE:HE2	7:EG:11:ARG:HB3	1.16	1.08
1:BC:153:LYS:NZ	6:EB:43:GLU:OE2	1.86	1.08
1:BD:65:LYS:NZ	7:EH:19:ASP:OD1	1.87	1.08
4:DL:178:LYS:NZ	7:DH:93:LYS:HD3	1.67	1.08
1:AD:207:ASN:HB3	7:AH:455:ALA:HB2	1.25	1.08
1:BC:188:PHE:HE2	7:DG:11:ARG:HB3	1.13	1.07
1:AD:301:THR:HG21	7:AH:475:ASN:HA	1.38	1.06
1:AD:20:ILE:HD11	6:BB:50:TYR:CE2	1.91	1.04
1:CC:20:ILE:CD1	6:FB:50:TYR:CE2	2.40	1.03
1:AD:69:ASP:OD2	7:DH:15:TYR:CE1	2.12	1.02
1:CD:207:ASN:HB3	7:CH:455:ALA:HB2	1.39	1.02
1:BD:188:PHE:HE2	7:BG:11:ARG:HB3	1.17	1.02
4:BL:58:HIS:ND1	5:BN:43:GLN:CD	2.18	1.01
1:CD:207:ASN:HB3	7:CH:455:ALA:CB	1.89	1.01
1:CC:128:GLN:O	7:EG:16:ARG:NH2	1.94	1.01
1:CD:107:SER:HA	6:FB:21:VAL:C	1.85	1.00
1:AD:107:SER:HA	6:DB:21:VAL:C	1.87	1.00
1:AC:20:ILE:CD1	6:DB:50:TYR:CE2	2.44	1.00
1:CD:153:LYS:HB2	6:AB:52:THR:CG2	1.91	1.00
1:CC:69:ASP:OD2	7:CH:15:TYR:HE1	1.42	0.99
1:BC:128:GLN:O	7:DG:16:ARG:NH2	1.92	0.99
1:AD:153:LYS:NZ	6:BB:43:GLU:OE2	1.96	0.99
1:CD:69:ASP:OD2	7:FH:15:TYR:CE1	2.15	0.99
1:BD:188:PHE:CE2	7:BG:11:ARG:HB3	1.97	0.99
1:BD:105:PRO:HB2	6:EB:23:ALA:HB2	1.44	0.99
1:BD:111:VAL:HG21	6:EB:17:ALA:HB1	1.46	0.97
1:BC:100:TYR:CE2	6:BB:109:TYR:CE2	2.51	0.97
1:CD:68:SER:OG	7:FG:11:ARG:HG3	1.64	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:105:PRO:HA	6:EB:15:ARG:HH22	1.22	0.97
1:BD:97:GLU:OE1	6:CB:48:GLY:N	1.98	0.97
1:AC:188:PHE:CE2	7:FG:11:ARG:HB3	2.00	0.96
1:CD:301:THR:HG21	7:CH:475:ASN:HA	1.46	0.96
4:BL:58:HIS:HE1	5:BN:43:GLN:HG2	1.17	0.96
1:BD:67:ARG:HB3	6:FB:47:ASP:OD2	1.66	0.96
1:BC:100:TYR:HE2	6:BB:109:TYR:CD2	1.83	0.95
1:AC:100:TYR:OH	6:AB:110:PHE:HA	1.67	0.95
1:CD:153:LYS:HG3	6:AB:52:THR:HG21	1.46	0.95
1:BC:188:PHE:CE2	7:DG:11:ARG:HB3	2.00	0.95
1:CC:188:PHE:CE2	7:EG:11:ARG:HB3	2.03	0.94
1:BC:100:TYR:CD2	6:BB:109:TYR:HE2	1.85	0.94
4:FL:178:LYS:HZ1	7:FH:93:LYS:HD3	1.27	0.94
1:CC:100:TYR:HE2	6:CB:109:TYR:CD2	1.86	0.94
1:CD:153:LYS:HB2	6:AB:52:THR:HG21	1.49	0.93
1:CD:105:PRO:HA	6:FB:15:ARG:NH2	1.82	0.93
1:CD:153:LYS:NZ	6:AB:43:GLU:OE2	1.98	0.93
1:CD:20:ILE:HD11	6:AB:50:TYR:CE2	2.03	0.93
1:AC:69:ASP:OD2	7:AH:15:TYR:HE1	1.47	0.93
1:CC:100:TYR:CE2	6:CB:109:TYR:CE2	2.56	0.93
1:BC:20:ILE:CD1	6:EB:50:TYR:CE2	2.52	0.92
1:BC:69:ASP:OD2	7:BH:15:TYR:HE1	1.46	0.92
1:CC:100:TYR:OH	6:CB:110:PHE:HA	1.69	0.92
1:BC:100:TYR:OH	6:BB:110:PHE:HA	1.68	0.92
1:AC:100:TYR:HE2	6:AB:109:TYR:CD2	1.88	0.92
1:AC:100:TYR:CE2	6:AB:109:TYR:CE2	2.58	0.92
1:CD:105:PRO:HB2	6:FB:23:ALA:HB2	1.51	0.91
1:CC:100:TYR:CD2	6:CB:109:TYR:HE2	1.87	0.91
4:EL:178:LYS:HZ1	7:EH:93:LYS:HD3	1.26	0.91
1:AD:301:THR:HB	7:AH:475:ASN:OD1	1.69	0.91
1:BD:20:ILE:HD11	6:CB:50:TYR:CE2	2.06	0.91
1:BD:153:LYS:NZ	6:CB:43:GLU:OE2	2.03	0.91
1:AC:153:LYS:NZ	6:DB:43:GLU:OE2	2.03	0.91
4:AL:178:LYS:HZ1	7:AH:93:LYS:HD3	1.27	0.91
1:AD:68:SER:OG	7:DG:11:ARG:HG3	1.69	0.91
1:AD:207:ASN:CB	7:AH:455:ALA:HB2	2.02	0.89
1:BD:107:SER:CA	6:EB:21:VAL:C	2.45	0.89
1:AD:105:PRO:HA	6:DB:15:ARG:NH2	1.88	0.89
1:AC:128:GLN:O	7:FG:16:ARG:NH2	2.05	0.88
1:AD:67:ARG:NH1	6:EB:47:ASP:HA	1.86	0.88
1:CD:100:TYR:CD2	6:FB:109:TYR:HE2	1.90	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EL:50:ARG:HA	5:EM:81:PHE:CE2	2.08	0.88
1:CD:153:LYS:CB	6:AB:52:THR:HG21	2.03	0.88
1:AC:100:TYR:CD2	6:AB:109:TYR:HE2	1.90	0.88
1:AD:20:ILE:CD1	6:BB:50:TYR:CE2	2.57	0.88
1:CD:67:ARG:NH1	6:DB:47:ASP:HA	1.89	0.88
1:AC:153:LYS:HG3	6:DB:52:THR:HG21	1.56	0.87
1:AD:69:ASP:OD2	7:DH:15:TYR:CD1	2.27	0.87
4:BL:178:LYS:HZ1	7:BH:93:LYS:HD3	1.34	0.87
1:AD:100:TYR:CD2	6:DB:109:TYR:HE2	1.93	0.86
1:CD:153:LYS:CG	6:AB:52:THR:HG21	2.04	0.86
3:BF:1151:GLU:OE1	2:BE:87:ARG:NE	2.07	0.86
1:CC:153:LYS:NZ	6:FB:43:GLU:OE2	2.09	0.86
1:CD:69:ASP:OD2	7:FH:15:TYR:CD1	2.28	0.86
1:CC:20:ILE:CD1	6:FB:50:TYR:CZ	2.59	0.86
1:BD:107:SER:H	6:EB:22:ASP:HA	1.38	0.86
4:EK:63:ILE:HG23	4:EK:82:LEU:HD21	1.57	0.86
1:BC:153:LYS:HG3	6:EB:52:THR:HG21	1.55	0.86
1:BD:207:ASN:HB3	7:BH:455:ALA:CB	2.05	0.86
4:BK:63:ILE:HG23	4:BK:82:LEU:HD21	1.58	0.86
4:FK:63:ILE:HG23	4:FK:82:LEU:HD21	1.57	0.86
1:AD:105:PRO:HB2	6:DB:23:ALA:HB2	1.58	0.86
1:BC:100:TYR:CE2	6:BB:109:TYR:CD2	2.64	0.86
1:CD:107:SER:H	6:FB:22:ASP:HA	1.40	0.86
4:FL:50:ARG:HA	5:FM:81:PHE:CE2	2.10	0.86
1:BD:97:GLU:CD	6:CB:48:GLY:HA2	2.00	0.85
6:FB:112:GLY:N	6:FB:133:TYR:OH	2.10	0.85
1:CC:153:LYS:HG3	6:FB:52:THR:HG21	1.58	0.85
4:AK:63:ILE:HG23	4:AK:82:LEU:HD21	1.58	0.85
1:AD:188:PHE:HE2	7:AG:11:ARG:HB3	1.38	0.84
1:CD:188:PHE:HE2	7:CG:11:ARG:HB3	1.42	0.84
1:BD:100:TYR:CE2	6:EB:109:TYR:CE2	2.66	0.84
4:CL:50:ARG:HG3	5:CM:81:PHE:CE2	2.13	0.84
1:AD:301:THR:HG21	7:AH:475:ASN:CA	2.07	0.84
4:FL:178:LYS:HZ1	7:FH:93:LYS:CD	1.91	0.84
1:AD:301:THR:CB	7:AH:475:ASN:OD1	2.25	0.83
1:BC:68:SER:OG	7:BG:11:ARG:HG3	1.77	0.83
1:AC:69:ASP:OD2	7:AH:15:TYR:CD1	2.31	0.83
1:AC:68:SER:OG	7:AG:11:ARG:HG3	1.78	0.83
1:CD:301:THR:HB	7:CH:475:ASN:OD1	1.78	0.83
1:BD:67:ARG:NH1	6:FB:46:MET:O	2.10	0.83
6:BB:112:GLY:N	6:BB:133:TYR:OH	2.10	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:68:SER:OG	7:CG:11:ARG:HG3	1.78	0.83
1:BD:97:GLU:OE2	6:CB:48:GLY:HA2	1.79	0.83
1:AD:301:THR:CG2	7:AH:475:ASN:HA	2.09	0.83
1:CD:100:TYR:HH	6:FB:110:PHE:HA	1.38	0.83
1:BC:69:ASP:OD2	7:BH:15:TYR:CD1	2.32	0.83
1:BC:69:ASP:OD1	7:BG:11:ARG:NH2	2.12	0.82
1:BD:67:ARG:HH12	6:FB:47:ASP:HA	1.42	0.82
1:BD:100:TYR:CD2	6:EB:109:TYR:HE2	1.98	0.82
4:BL:178:LYS:NZ	7:BH:93:LYS:CD	2.43	0.82
1:CC:26:ILE:HD11	1:BD:74:ARG:CZ	2.09	0.82
1:BD:188:PHE:HE2	7:BG:11:ARG:CB	1.92	0.82
6:CA:138:ARG:NH2	6:CA:139:PHE:O	2.12	0.82
1:AD:128:GLN:O	7:AG:16:ARG:NH2	2.12	0.81
1:CD:100:TYR:CE2	6:FB:109:TYR:CE2	2.68	0.81
1:AD:97:GLU:OE1	6:BB:48:GLY:N	2.14	0.81
2:AE:69:THR:OG1	2:BE:201:ALA:O	1.97	0.81
1:CD:97:GLU:OE1	6:AB:48:GLY:N	2.13	0.81
1:BD:63:LYS:NZ	6:CB:52:THR:O	2.13	0.81
1:CC:100:TYR:CE2	6:CB:109:TYR:CD2	2.67	0.81
4:CK:63:ILE:HG23	4:CK:82:LEU:HD21	1.62	0.81
6:DA:138:ARG:NH2	6:DA:139:PHE:O	2.13	0.81
6:AA:138:ARG:NH2	6:AA:139:PHE:O	2.14	0.81
4:AL:178:LYS:HZ1	7:AH:93:LYS:CD	1.94	0.81
1:AC:20:ILE:CD1	6:DB:50:TYR:CZ	2.64	0.81
1:BC:153:LYS:HB2	6:EB:52:THR:HB	1.62	0.81
6:FA:138:ARG:NH2	6:FA:139:PHE:O	2.14	0.81
1:AC:100:TYR:CE2	6:AB:109:TYR:CD2	2.69	0.81
1:CC:153:LYS:HB2	6:FB:52:THR:HB	1.61	0.80
1:AD:100:TYR:HH	6:DB:110:PHE:HA	1.44	0.80
4:BL:50:ARG:HA	5:BM:81:PHE:CE2	2.15	0.80
4:DL:50:ARG:HG3	5:DM:81:PHE:CE2	2.16	0.80
1:CC:69:ASP:OD2	7:CH:15:TYR:CD1	2.33	0.80
1:BD:67:ARG:CB	6:FB:47:ASP:OD2	2.28	0.80
1:AC:69:ASP:OD1	7:AG:11:ARG:NH2	2.15	0.80
1:CC:20:ILE:HD12	6:FB:50:TYR:CZ	2.17	0.80
1:AD:100:TYR:CE2	6:DB:109:TYR:CE2	2.69	0.80
1:BD:67:ARG:HH11	6:FB:47:ASP:HA	1.46	0.80
6:EA:138:ARG:NH2	6:EA:139:PHE:O	2.14	0.80
6:BA:138:ARG:NH2	6:BA:139:PHE:O	2.15	0.80
7:AI:551:ILE:O	7:AI:573:ARG:NH1	2.15	0.80
7:EI:410:PRO:O	7:EI:414:ARG:NH2	2.15	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AE:201:ALA:O	2:CE:69:THR:OG1	1.98	0.80
4:CL:50:ARG:HA	5:CM:81:PHE:CE2	2.16	0.80
1:AC:153:LYS:HB2	6:DB:52:THR:HB	1.62	0.80
1:CC:69:ASP:OD1	7:CG:11:ARG:NH2	2.15	0.79
4:FL:178:LYS:NZ	7:FH:93:LYS:CD	2.41	0.79
7:DI:551:ILE:O	7:DI:573:ARG:NH1	2.15	0.79
7:FI:551:ILE:O	7:FI:573:ARG:NH1	2.15	0.79
2:CE:201:ALA:O	2:BE:69:THR:OG1	2.00	0.79
7:BI:551:ILE:O	7:BI:573:ARG:NH1	2.15	0.79
7:CI:410:PRO:O	7:CI:414:ARG:NH2	2.16	0.79
7:CI:551:ILE:O	7:CI:573:ARG:NH1	2.15	0.79
1:CD:100:TYR:CG	6:FB:111:GLN:NE2	2.51	0.79
4:DK:63:ILE:HG23	4:DK:82:LEU:HD21	1.63	0.79
4:EK:35:ASP:OD1	4:EK:38:THR:OG1	2.01	0.79
4:EK:169:MET:O	4:EK:172:THR:OG1	2.01	0.79
1:CD:105:PRO:HA	6:FB:15:ARG:HH22	1.43	0.79
5:FN:8:GLU:OE1	5:FN:45:ARG:NH1	2.16	0.79
7:AI:410:PRO:O	7:AI:414:ARG:NH2	2.15	0.79
4:AK:35:ASP:OD1	4:AK:38:THR:OG1	2.01	0.79
4:AL:178:LYS:NZ	7:AH:93:LYS:CD	2.44	0.79
4:CK:80:ASP:OD2	4:CK:94:TYR:OH	1.99	0.79
5:EN:8:GLU:OE1	5:EN:45:ARG:NH1	2.16	0.79
1:BD:111:VAL:CG2	6:EB:17:ALA:HB1	2.13	0.79
7:BI:410:PRO:O	7:BI:414:ARG:NH2	2.16	0.79
7:FI:410:PRO:O	7:FI:414:ARG:NH2	2.16	0.79
7:EI:551:ILE:O	7:EI:573:ARG:NH1	2.15	0.78
1:BC:20:ILE:CD1	6:EB:50:TYR:CZ	2.66	0.78
1:BD:97:GLU:OE1	6:CB:48:GLY:CA	2.31	0.78
1:AC:188:PHE:HE2	7:FG:11:ARG:CB	1.96	0.78
4:DJ:83:THR:OG1	4:DJ:93:GLN:O	2.00	0.78
6:FA:141:ARG:NH2	6:CA:78:ASP:OD1	2.16	0.78
5:BN:8:GLU:OE1	5:BN:45:ARG:NH1	2.16	0.78
5:DM:72:LEU:HD11	5:DM:82:ILE:HD12	1.66	0.78
7:BH:157:SER:OG	7:BH:196:GLY:O	2.02	0.78
4:BL:178:LYS:HZ1	7:BH:93:LYS:CD	1.96	0.78
4:EJ:83:THR:OG1	4:EJ:93:GLN:O	2.02	0.78
5:AM:72:LEU:HD11	5:AM:82:ILE:HD12	1.66	0.78
6:DA:141:ARG:NH2	6:AA:78:ASP:OD1	2.17	0.78
7:CH:157:SER:OG	7:CH:196:GLY:O	2.02	0.78
4:AK:169:MET:O	4:AK:172:THR:OG1	2.01	0.78
4:CL:178:LYS:HZ1	7:CH:93:LYS:HD3	1.45	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:188:PHE:HE2	7:DG:11:ARG:CB	1.97	0.77
4:CL:50:ARG:CG	5:CM:81:PHE:CE2	2.67	0.77
5:AN:8:GLU:OE1	5:AN:45:ARG:NH1	2.16	0.77
5:CN:8:GLU:OE1	5:CN:45:ARG:NH1	2.18	0.77
6:BA:141:ARG:NH2	6:DA:78:ASP:OD1	2.18	0.77
7:DI:410:PRO:O	7:DI:414:ARG:NH2	2.16	0.77
6:EA:78:ASP:OD1	6:CA:141:ARG:NH2	2.17	0.77
7:EH:79:ASN:ND2	7:EG:93:LYS:O	2.17	0.77
1:AD:107:SER:H	6:DB:22:ASP:HA	1.47	0.77
4:AL:50:ARG:HA	5:AM:81:PHE:CE2	2.19	0.77
5:EM:72:LEU:HD11	5:EM:82:ILE:HD12	1.66	0.77
7:FH:157:SER:OG	7:FH:196:GLY:O	2.02	0.77
4:FJ:36:ARG:NH2	4:FL:152:GLN:OE1	2.18	0.77
4:FK:35:ASP:OD1	4:FK:38:THR:OG1	2.01	0.77
5:CM:72:LEU:HD11	5:CM:82:ILE:HD12	1.66	0.77
4:AJ:83:THR:OG1	4:AJ:93:GLN:O	2.02	0.77
1:AD:188:PHE:CE2	7:AG:11:ARG:HB3	2.19	0.77
1:AD:188:PHE:HB2	7:AH:14:ASP:HA	1.64	0.77
7:EH:157:SER:OG	7:EH:196:GLY:O	2.03	0.77
4:BK:35:ASP:OD1	4:BK:38:THR:OG1	2.01	0.77
4:FJ:83:THR:OG1	4:FJ:93:GLN:O	2.03	0.77
2:AE:386:ASP:OD1	2:BE:384:ARG:NH1	2.18	0.77
4:EJ:36:ARG:NH2	4:EL:152:GLN:OE1	2.18	0.77
4:BJ:36:ARG:NH2	4:BL:152:GLN:OE1	2.17	0.76
4:EL:50:ARG:CA	5:EM:81:PHE:HE2	1.99	0.76
5:FM:72:LEU:HD11	5:FM:82:ILE:HD12	1.68	0.76
7:FH:159:TYR:O	7:FH:201:ARG:NH2	2.18	0.76
1:AC:97:GLU:OE1	6:DB:48:GLY:N	2.19	0.76
1:AD:100:TYR:CD2	6:DB:109:TYR:CE2	2.73	0.76
4:DK:80:ASP:OD2	4:DK:94:TYR:OH	2.00	0.76
7:AH:157:SER:OG	7:AH:196:GLY:O	2.02	0.76
1:AC:20:ILE:HD12	6:DB:50:TYR:CZ	2.21	0.76
1:BD:153:LYS:CE	6:CB:43:GLU:OE2	2.34	0.76
1:BD:207:ASN:HB3	7:BH:455:ALA:HB2	1.66	0.76
7:FH:79:ASN:ND2	7:FG:93:LYS:O	2.18	0.76
1:BD:125:ARG:N	7:EI:290:LEU:HD11	1.99	0.76
7:AH:79:ASN:ND2	7:AG:93:LYS:O	2.18	0.76
7:CH:79:ASN:ND2	7:CG:93:LYS:O	2.18	0.76
7:CH:159:TYR:O	7:CH:201:ARG:NH2	2.19	0.76
7:EH:159:TYR:O	7:EH:201:ARG:NH2	2.19	0.76
1:CD:301:THR:CB	7:CH:475:ASN:OD1	2.34	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:79:ASN:ND2	7:BG:93:LYS:O	2.19	0.76
7:DH:157:SER:OG	7:DH:196:GLY:O	2.03	0.76
1:BC:102:PHE:CE1	6:BB:142:GLY:HA3	2.20	0.76
1:AD:105:PRO:HA	6:DB:15:ARG:HH22	1.47	0.76
1:CD:20:ILE:CD1	6:AB:50:TYR:CE2	2.69	0.76
5:DN:8:GLU:OE1	5:DN:45:ARG:NH1	2.17	0.76
6:FB:5:LYS:O	6:CB:126:ILE:HD12	1.86	0.76
5:BM:72:LEU:HD11	5:BM:82:ILE:HD12	1.67	0.75
2:AE:77:GLY:N	1:BD:39:GLU:OE2	2.19	0.75
7:BH:159:TYR:O	7:BH:201:ARG:NH2	2.18	0.75
1:AC:153:LYS:HG3	6:DB:52:THR:CG2	2.17	0.75
4:DJ:36:ARG:NH2	4:DL:152:GLN:OE1	2.19	0.75
7:AH:159:TYR:O	7:AH:201:ARG:NH2	2.19	0.75
4:DL:50:ARG:CG	5:DM:81:PHE:CE2	2.70	0.75
1:AD:207:ASN:CB	7:AH:455:ALA:CB	2.60	0.75
1:CC:100:TYR:CD2	6:CB:109:TYR:CE2	2.72	0.75
4:BJ:83:THR:OG1	4:BJ:93:GLN:O	2.03	0.75
6:DB:112:GLY:N	6:DB:133:TYR:OH	2.20	0.75
1:CD:100:TYR:HE2	6:FB:109:TYR:CD2	2.05	0.75
4:EL:178:LYS:HZ1	7:EH:93:LYS:CD	1.98	0.75
1:AC:66:ASN:ND2	7:AH:22:GLU:OE2	2.19	0.75
4:AJ:36:ARG:NH2	4:AL:152:GLN:OE1	2.20	0.75
7:DH:159:TYR:O	7:DH:201:ARG:NH2	2.19	0.75
1:AC:95:LYS:NZ	7:FG:20:GLU:OE2	2.20	0.75
1:AD:67:ARG:HH12	6:EB:47:ASP:HA	1.50	0.75
4:FL:50:ARG:CB	5:FM:81:PHE:HE2	1.99	0.75
6:BB:5:LYS:O	6:DB:126:ILE:HD12	1.86	0.75
1:CC:66:ASN:ND2	7:CH:22:GLU:OE2	2.20	0.74
1:CC:97:GLU:OE1	6:FB:48:GLY:N	2.19	0.74
1:AD:100:TYR:HE2	6:DB:109:TYR:CD2	2.05	0.74
4:CJ:83:THR:OG1	4:CJ:93:GLN:O	2.03	0.74
7:DH:79:ASN:ND2	7:DG:93:LYS:O	2.19	0.74
1:AC:100:TYR:CD2	6:AB:109:TYR:CE2	2.76	0.74
4:DK:35:ASP:OD1	4:DK:38:THR:OG1	2.04	0.74
1:BC:153:LYS:HG3	6:EB:52:THR:CG2	2.17	0.74
1:BC:153:LYS:CE	6:EB:43:GLU:CD	2.60	0.74
1:CD:100:TYR:CD2	6:FB:109:TYR:CE2	2.75	0.74
1:BC:66:ASN:ND2	7:BH:22:GLU:OE2	2.19	0.74
4:FL:50:ARG:CA	5:FM:81:PHE:HE2	2.00	0.74
1:AC:97:GLU:OE2	6:DB:48:GLY:HA2	1.88	0.74
1:BC:100:TYR:HE2	6:BB:109:TYR:HD2	1.33	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EL:50:ARG:CB	5:EM:81:PHE:HE2	2.00	0.74
4:DL:178:LYS:HZ1	7:DH:93:LYS:HD3	1.49	0.74
1:CD:188:PHE:CE2	7:CG:11:ARG:HB3	2.23	0.74
4:BJ:8:LYS:NZ	4:BJ:35:ASP:OD2	2.21	0.74
1:CC:153:LYS:HG3	6:FB:52:THR:CG2	2.17	0.73
4:FJ:144:LYS:NZ	4:FL:148:ILE:O	2.20	0.73
6:AB:112:GLY:N	6:AB:133:TYR:OH	2.21	0.73
4:CK:35:ASP:OD1	4:CK:38:THR:OG1	2.05	0.73
1:AC:100:TYR:HE2	6:AB:109:TYR:HD2	1.37	0.73
4:EJ:5:ASN:ND2	7:EG:80:MET:O	2.17	0.73
1:BD:107:SER:HA	6:EB:21:VAL:CA	2.17	0.73
1:BD:107:SER:N	6:EB:22:ASP:HA	2.03	0.73
4:CJ:36:ARG:NH2	4:CL:152:GLN:OE1	2.20	0.73
1:BC:20:ILE:HD12	6:EB:50:TYR:CZ	2.23	0.73
6:EB:141:ARG:NH2	6:BB:74:ASP:OD1	2.22	0.73
6:BB:122:GLU:N	6:BB:122:GLU:OE2	2.21	0.73
6:AB:141:ARG:NH2	6:FB:74:ASP:OD1	2.22	0.73
6:CB:112:GLY:N	6:CB:133:TYR:OH	2.21	0.73
4:FJ:8:LYS:NZ	4:FJ:35:ASP:OD2	2.22	0.73
6:AB:5:LYS:O	6:FB:126:ILE:HD12	1.89	0.73
6:CB:122:GLU:OE2	6:CB:122:GLU:N	2.22	0.73
7:CI:151:GLU:OE1	7:CI:427:ASN:ND2	2.22	0.73
4:FL:50:ARG:HG3	5:FM:81:PHE:CE2	2.24	0.73
4:BL:50:ARG:CB	5:BM:81:PHE:HE2	2.02	0.72
7:FG:271:ASN:ND2	7:FG:334:TYR:O	2.22	0.72
4:BJ:144:LYS:NZ	4:BL:148:ILE:O	2.22	0.72
4:AL:51:PRO:O	5:AM:36:ARG:NH1	2.22	0.72
4:EL:51:PRO:O	5:EM:36:ARG:NH1	2.22	0.72
6:DB:167:GLU:OE1	6:DB:167:GLU:N	2.22	0.72
6:DB:141:ARG:NH2	6:AB:74:ASP:OD1	2.22	0.72
2:CE:384:ARG:NH1	2:BE:386:ASP:OD1	2.21	0.72
4:CL:178:LYS:NZ	7:CH:93:LYS:CD	2.49	0.72
1:CD:67:ARG:HH12	6:DB:47:ASP:HA	1.55	0.72
4:CL:50:ARG:CB	5:CM:81:PHE:HE2	2.02	0.72
7:BI:300:ARG:NH1	7:BI:311:LYS:O	2.23	0.72
4:FL:50:ARG:HA	5:FM:81:PHE:CD2	2.23	0.72
6:FB:122:GLU:N	6:FB:122:GLU:OE2	2.23	0.72
6:CB:167:GLU:OE1	6:CB:167:GLU:N	2.21	0.72
7:DI:151:GLU:OE1	7:DI:427:ASN:ND2	2.22	0.72
6:EB:5:LYS:O	6:BB:126:ILE:HD12	1.89	0.72
1:BD:223:GLN:OE1	1:BD:225:ASN:ND2	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FI:151:GLU:OE1	7:FI:427:ASN:ND2	2.22	0.72
1:BC:97:GLU:OE1	6:EB:48:GLY:N	2.22	0.71
1:BD:301:THR:HG21	7:BH:475:ASN:HA	1.71	0.71
5:DM:30:GLU:HA	5:DM:91:ILE:HD11	1.72	0.71
1:CC:97:GLU:OE2	6:FB:48:GLY:HA2	1.89	0.71
1:CD:100:TYR:CD2	6:FB:111:GLN:NE2	2.58	0.71
1:CD:128:GLN:O	7:CG:16:ARG:NH2	2.22	0.71
1:BC:97:GLU:OE2	6:EB:48:GLY:HA2	1.90	0.71
4:FL:88:ILE:HD12	5:FM:85:LYS:NZ	2.06	0.71
6:EB:112:GLY:N	6:EB:133:TYR:OH	2.23	0.71
1:AC:100:TYR:HH	6:AB:110:PHE:HA	1.53	0.71
7:AI:249:TYR:OH	7:AI:255:ASP:OD2	2.08	0.71
4:BK:80:ASP:OD2	4:BK:94:TYR:OH	2.07	0.71
4:EL:50:ARG:HA	5:EM:81:PHE:CD2	2.25	0.71
5:CM:30:GLU:HA	5:CM:91:ILE:HD11	1.72	0.71
7:BG:271:ASN:ND2	7:BG:334:TYR:O	2.23	0.71
2:AE:87:ARG:NE	3:AF:1151:GLU:OE1	2.22	0.71
1:BD:100:TYR:HE2	6:EB:109:TYR:CE2	2.08	0.71
7:CG:271:ASN:ND2	7:CG:334:TYR:O	2.24	0.71
1:BC:100:TYR:CD2	6:BB:109:TYR:CE2	2.71	0.71
7:AG:271:ASN:ND2	7:AG:334:TYR:O	2.24	0.71
4:BL:58:HIS:ND1	5:BN:43:GLN:NE2	2.37	0.71
7:FI:249:TYR:OH	7:FI:255:ASP:OD2	2.08	0.71
1:BC:223:GLN:OE1	1:BC:225:ASN:ND2	2.23	0.71
4:CL:88:ILE:CD1	5:CM:85:LYS:CE	2.68	0.71
6:EB:74:ASP:OD1	6:CB:141:ARG:NH2	2.23	0.71
7:DG:271:ASN:ND2	7:DG:334:TYR:O	2.23	0.71
7:EI:300:ARG:NH1	7:EI:311:LYS:O	2.24	0.71
1:AC:223:GLN:OE1	1:AC:225:ASN:ND2	2.23	0.71
1:CD:107:SER:N	6:FB:22:ASP:HA	2.06	0.71
6:BB:167:GLU:N	6:BB:167:GLU:OE1	2.24	0.71
6:AB:122:GLU:N	6:AB:122:GLU:OE2	2.24	0.71
4:EL:88:ILE:CD1	5:EM:85:LYS:CE	2.68	0.71
5:FM:57:LEU:HD23	5:FM:72:LEU:HD13	1.73	0.71
2:AE:209:ARG:NH2	2:AE:211:TYR:OH	2.24	0.70
1:CC:223:GLN:OE1	1:CC:225:ASN:ND2	2.23	0.70
5:FM:30:GLU:HA	5:FM:91:ILE:HD11	1.73	0.70
3:CF:1153:TYR:OH	2:CE:95:MET:SD	2.45	0.70
7:FI:300:ARG:NH1	7:FI:311:LYS:O	2.23	0.70
1:BD:20:ILE:CD1	6:CB:50:TYR:CE2	2.73	0.70
6:EA:141:ARG:NH2	6:BA:78:ASP:OD1	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:141:ARG:NH2	6:FA:78:ASP:OD1	2.25	0.70
5:BM:30:GLU:HA	5:BM:91:ILE:HD11	1.73	0.70
5:BM:57:LEU:HD23	5:BM:72:LEU:HD13	1.73	0.70
7:BI:249:TYR:OH	7:BI:255:ASP:OD2	2.08	0.70
7:AI:300:ARG:NH1	7:AI:311:LYS:O	2.23	0.70
2:CE:209:ARG:NH2	2:CE:211:TYR:OH	2.24	0.70
5:DM:57:LEU:HD23	5:DM:72:LEU:HD13	1.74	0.70
6:EB:122:GLU:N	6:EB:122:GLU:OE2	2.25	0.70
4:BL:50:ARG:HG3	5:BM:81:PHE:CE2	2.26	0.70
4:AL:50:ARG:CB	5:AM:81:PHE:HE2	2.04	0.70
4:AL:50:ARG:HG3	5:AM:81:PHE:CE2	2.26	0.70
1:AC:102:PHE:CZ	6:AB:142:GLY:O	2.45	0.70
4:BL:50:ARG:HA	5:BM:81:PHE:CD2	2.27	0.70
4:EL:50:ARG:HG3	5:EM:81:PHE:CE2	2.27	0.70
5:EM:30:GLU:HA	5:EM:91:ILE:HD11	1.74	0.70
1:AD:223:GLN:OE1	1:AD:225:ASN:ND2	2.23	0.70
1:AD:301:THR:CG2	7:AH:475:ASN:OD1	2.40	0.70
2:AE:384:ARG:NH1	2:CE:386:ASP:OD1	2.24	0.70
1:CD:223:GLN:OE1	1:CD:225:ASN:ND2	2.23	0.70
1:BC:102:PHE:CE1	6:BB:142:GLY:CA	2.75	0.70
4:DL:50:ARG:HA	5:DM:81:PHE:CE2	2.26	0.70
4:EK:134:ASP:OD1	4:EK:136:VAL:N	2.25	0.70
5:CM:57:LEU:HD23	5:CM:72:LEU:HD13	1.74	0.70
7:CI:249:TYR:OH	7:CI:255:ASP:OD2	2.09	0.70
5:BN:86:ILE:HD12	5:BN:91:ILE:HB	1.74	0.69
5:DN:86:ILE:HD12	5:DN:91:ILE:HB	1.74	0.69
1:BC:65:LYS:NZ	7:BH:19:ASP:OD1	2.25	0.69
1:BD:100:TYR:HH	6:EB:110:PHE:HA	1.55	0.69
6:EB:126:ILE:HD12	6:CB:5:LYS:O	1.90	0.69
1:AD:207:ASN:HB3	7:AH:455:ALA:HB1	1.74	0.69
1:CC:65:LYS:NZ	7:CH:19:ASP:OD1	2.24	0.69
5:AM:30:GLU:HA	5:AM:91:ILE:HD11	1.74	0.69
6:DB:122:GLU:N	6:DB:122:GLU:OE2	2.25	0.69
4:AK:134:ASP:OD1	4:AK:136:VAL:N	2.25	0.69
6:AB:15:ARG:NE	6:AB:87:GLU:OE2	2.25	0.69
6:CB:15:ARG:NE	6:CB:87:GLU:OE2	2.24	0.69
1:CC:100:TYR:HE2	6:CB:109:TYR:HD2	1.37	0.69
1:CD:301:THR:HG21	7:CH:475:ASN:CA	2.20	0.69
2:BE:209:ARG:NH2	2:BE:211:TYR:OH	2.24	0.69
4:BL:50:ARG:NH1	5:BM:6:ASP:OD2	2.25	0.69
4:BL:51:PRO:O	5:BM:36:ARG:NH1	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AH:574:PHE:O	7:AH:582:LYS:NZ	2.25	0.69
4:FK:134:ASP:OD1	4:FK:136:VAL:N	2.26	0.69
7:EH:574:PHE:O	7:EH:582:LYS:NZ	2.26	0.69
5:CN:86:ILE:HD12	5:CN:91:ILE:HB	1.74	0.69
7:FH:574:PHE:O	7:FH:582:LYS:NZ	2.25	0.69
7:EG:271:ASN:ND2	7:EG:334:TYR:O	2.24	0.69
7:EI:249:TYR:OH	7:EI:255:ASP:OD2	2.09	0.69
5:AN:86:ILE:HD12	5:AN:91:ILE:HB	1.75	0.69
5:EN:86:ILE:HD12	5:EN:91:ILE:HB	1.75	0.69
4:CL:50:ARG:HA	5:CM:81:PHE:CD2	2.27	0.69
1:AD:97:GLU:OE2	6:BB:48:GLY:HA2	1.93	0.69
1:CD:97:GLU:OE2	6:AB:48:GLY:HA2	1.93	0.69
1:BD:100:TYR:CD2	6:EB:109:TYR:CE2	2.81	0.69
1:BD:107:SER:HA	6:EB:21:VAL:O	1.92	0.69
5:DN:51:HIS:O	5:DN:105:LYS:NZ	2.26	0.69
7:BH:574:PHE:O	7:BH:582:LYS:NZ	2.25	0.69
7:FH:605:ARG:NE	7:FH:607:ASN:OD1	2.26	0.69
1:AD:100:TYR:HD2	6:DB:109:TYR:HE2	1.37	0.68
1:CC:63:LYS:NZ	6:FB:52:THR:O	2.22	0.68
4:BL:50:ARG:CA	5:BM:81:PHE:HE2	2.05	0.68
4:CL:46:THR:HG22	5:CM:78:VAL:HG22	1.75	0.68
5:FN:86:ILE:HD12	5:FN:91:ILE:HB	1.74	0.68
1:CD:301:THR:CG2	7:CH:475:ASN:HA	2.21	0.68
4:EJ:5:ASN:OD1	7:EG:78:SER:O	2.12	0.68
7:AH:605:ARG:NE	7:AH:607:ASN:OD1	2.26	0.68
1:CC:153:LYS:HG3	6:FB:52:THR:CB	2.23	0.68
4:EL:178:LYS:NZ	7:EH:93:LYS:CD	2.45	0.68
6:BB:141:ARG:NH2	6:DB:74:ASP:OD1	2.26	0.68
6:DB:15:ARG:NE	6:DB:87:GLU:OE2	2.26	0.68
1:AD:153:LYS:CE	6:BB:43:GLU:CD	2.66	0.68
1:CD:97:GLU:CD	6:AB:48:GLY:HA2	2.18	0.68
4:CL:51:PRO:HG3	5:CM:75:ASP:OD2	1.93	0.68
1:AC:63:LYS:NZ	6:DB:52:THR:O	2.26	0.68
1:CC:188:PHE:HE2	7:EG:11:ARG:CB	1.99	0.68
4:BL:88:ILE:HD12	5:BM:85:LYS:CE	2.23	0.68
6:DB:5:LYS:O	6:AB:126:ILE:HD12	1.93	0.68
7:EH:401:ALA:HB2	7:EH:426:VAL:HG21	1.76	0.68
2:AE:212:GLY:O	2:AE:250:VAL:N	2.26	0.68
4:CL:50:ARG:CA	5:CM:81:PHE:HE2	2.06	0.68
7:CH:605:ARG:NE	7:CH:607:ASN:OD1	2.27	0.68
1:BD:100:TYR:HE2	6:EB:109:TYR:CD2	2.11	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:50:ARG:CG	5:BM:81:PHE:CE2	2.77	0.68
6:FB:10:ARG:NH2	6:CB:127:ASP:OD2	2.27	0.68
6:CA:64:ALA:HB3	6:CA:129:TYR:CE1	2.29	0.68
1:CC:95:LYS:NZ	7:EG:20:GLU:OE2	2.27	0.68
1:BC:167:TYR:OH	1:BD:42:ASN:ND2	2.27	0.68
5:CN:51:HIS:O	5:CN:105:LYS:NZ	2.26	0.68
1:BC:105:PRO:HA	6:BB:15:ARG:HH22	1.59	0.68
4:BK:134:ASP:OD1	4:BK:136:VAL:N	2.27	0.68
4:CK:134:ASP:OD1	4:CK:136:VAL:N	2.27	0.68
5:EN:51:HIS:O	5:EN:105:LYS:NZ	2.27	0.68
4:FL:50:ARG:CG	5:FM:81:PHE:CE2	2.76	0.67
4:CL:50:ARG:CB	5:CM:81:PHE:CE2	2.78	0.67
6:AB:10:ARG:NH2	6:FB:127:ASP:OD2	2.27	0.67
7:CH:574:PHE:O	7:CH:582:LYS:NZ	2.26	0.67
1:CD:100:TYR:OH	6:FB:110:PHE:CA	2.35	0.67
4:EL:134:ASP:OD1	4:EL:135:LEU:N	2.28	0.67
5:BN:51:HIS:O	5:BN:105:LYS:NZ	2.28	0.67
2:CE:212:GLY:O	2:CE:250:VAL:N	2.26	0.67
4:DL:50:ARG:CB	5:DM:81:PHE:HE2	2.07	0.67
4:AL:134:ASP:OD1	4:AL:135:LEU:N	2.27	0.67
7:FH:280:ARG:NH1	7:FH:295:ASN:OD1	2.28	0.67
1:CD:153:LYS:CE	6:AB:43:GLU:CD	2.67	0.67
1:CD:188:PHE:HB2	7:CH:14:ASP:HA	1.75	0.67
2:BE:212:GLY:O	2:BE:250:VAL:N	2.26	0.67
5:FN:51:HIS:O	5:FN:105:LYS:NZ	2.28	0.67
5:EM:57:LEU:HD23	5:EM:72:LEU:HD13	1.76	0.67
6:DA:64:ALA:HB3	6:DA:129:TYR:CE1	2.30	0.67
7:DH:605:ARG:NE	7:DH:607:ASN:OD1	2.27	0.67
1:AD:97:GLU:CD	6:BB:48:GLY:HA2	2.20	0.67
4:CJ:144:LYS:NZ	4:CL:148:ILE:O	2.27	0.67
1:CD:301:THR:CG2	7:CH:475:ASN:OD1	2.43	0.67
1:BC:95:LYS:NZ	7:DG:20:GLU:OE2	2.27	0.67
4:CL:178:LYS:HZ1	7:CH:93:LYS:CD	2.08	0.67
5:CM:8:GLU:OE2	5:CM:45:ARG:NH2	2.28	0.67
6:DB:10:ARG:NH2	6:AB:127:ASP:OD2	2.27	0.67
7:DH:574:PHE:O	7:DH:582:LYS:NZ	2.27	0.67
6:EB:15:ARG:NE	6:EB:87:GLU:OE2	2.24	0.67
7:DI:249:TYR:OH	7:DI:255:ASP:OD2	2.09	0.67
1:AC:65:LYS:NZ	7:AH:19:ASP:OD1	2.26	0.67
5:DM:8:GLU:OE2	5:DM:45:ARG:NH2	2.28	0.67
5:FM:20:ASP:OD2	5:FM:118:ASN:ND2	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:EB:10:ARG:NH2	6:BB:127:ASP:OD2	2.28	0.67
1:AC:97:GLU:CD	6:DB:48:GLY:HA2	2.19	0.67
1:AD:107:SER:N	6:DB:22:ASP:HA	2.10	0.67
1:CD:100:TYR:HD2	6:FB:109:TYR:HE2	1.42	0.67
4:FK:80:ASP:OD2	4:FK:94:TYR:OH	2.07	0.67
5:AN:51:HIS:O	5:AN:105:LYS:NZ	2.27	0.67
6:BB:10:ARG:NH2	6:DB:127:ASP:OD2	2.27	0.67
7:EI:151:GLU:OE1	7:EI:427:ASN:ND2	2.28	0.67
6:AA:64:ALA:HB3	6:AA:129:TYR:CE1	2.29	0.66
7:BH:212:HIS:O	7:BH:267:SER:OG	2.13	0.66
5:AM:57:LEU:HD23	5:AM:72:LEU:HD13	1.76	0.66
4:CL:178:LYS:HZ2	7:CH:93:LYS:HD3	1.59	0.66
1:AD:111:VAL:HG21	6:DB:17:ALA:HB1	1.76	0.66
1:BC:153:LYS:HZ1	6:EB:43:GLU:CD	1.97	0.66
7:BH:605:ARG:NE	7:BH:607:ASN:OD1	2.27	0.66
1:CD:125:ARG:HA	7:FI:290:LEU:HD11	1.78	0.66
6:BB:163:ASP:OD1	6:BB:164:THR:N	2.29	0.66
1:AC:102:PHE:CZ	6:AB:142:GLY:C	2.74	0.66
1:CD:207:ASN:CB	7:CH:455:ALA:HB2	2.21	0.66
4:FL:46:THR:HG22	5:FM:78:VAL:HG22	1.78	0.66
4:EK:80:ASP:OD2	4:EK:94:TYR:OH	2.09	0.66
5:BM:20:ASP:OD2	5:BM:118:ASN:ND2	2.28	0.66
6:BA:64:ALA:HB3	6:BA:129:TYR:CE1	2.30	0.66
7:CG:140:GLU:OE2	7:CG:399:ARG:NH2	2.29	0.66
1:AD:153:LYS:CE	6:BB:43:GLU:OE2	2.43	0.66
7:AG:144:GLU:OE1	7:AG:146:LYS:NZ	2.29	0.66
4:AL:50:ARG:HA	5:AM:81:PHE:CD2	2.30	0.66
1:CD:111:VAL:HG21	6:FB:17:ALA:HB1	1.77	0.66
4:AL:28:ASN:OD1	4:AL:29:ILE:N	2.29	0.66
7:DG:140:GLU:OE2	7:DG:399:ARG:NH2	2.29	0.66
7:DI:400:LYS:N	7:DI:423:GLN:OE1	2.29	0.66
7:AI:151:GLU:OE1	7:AI:427:ASN:ND2	2.28	0.66
4:DL:178:LYS:NZ	7:DH:93:LYS:CD	2.53	0.66
6:EA:64:ALA:HB3	6:EA:129:TYR:CE1	2.30	0.66
1:CC:97:GLU:CD	6:FB:48:GLY:HA2	2.21	0.65
4:DL:88:ILE:CD1	5:DM:85:LYS:CE	2.75	0.65
4:EL:50:ARG:CB	5:EM:81:PHE:CE2	2.78	0.65
6:FA:64:ALA:HB3	6:FA:129:TYR:CE1	2.30	0.65
1:BD:97:GLU:OE1	6:CB:48:GLY:HA2	1.93	0.65
4:FL:51:PRO:HG3	5:FM:75:ASP:OD2	1.97	0.65
4:CL:51:PRO:O	5:CM:36:ARG:NH1	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FB:15:ARG:NE	6:FB:87:GLU:OE2	2.29	0.65
7:DH:401:ALA:HB2	7:DH:426:VAL:HG21	1.79	0.65
7:AI:293:SER:OG	7:AI:317:ASP:OD1	2.13	0.65
4:DL:51:PRO:O	5:DM:36:ARG:NH1	2.29	0.65
4:EJ:144:LYS:NZ	4:EL:148:ILE:O	2.28	0.65
4:EL:28:ASN:OD1	4:EL:29:ILE:N	2.29	0.65
6:EB:127:ASP:OD2	6:CB:10:ARG:NH2	2.28	0.65
7:BH:280:ARG:NH1	7:BH:295:ASN:OD1	2.30	0.65
7:DG:144:GLU:OE1	7:DG:146:LYS:NZ	2.29	0.65
7:AH:401:ALA:HB2	7:AH:426:VAL:HG21	1.78	0.65
7:EG:144:GLU:OE1	7:EG:146:LYS:NZ	2.29	0.65
4:DJ:144:LYS:NZ	4:DL:148:ILE:O	2.28	0.65
4:DK:134:ASP:OD1	4:DK:136:VAL:N	2.28	0.65
7:CI:400:LYS:N	7:CI:423:GLN:OE1	2.28	0.65
7:EH:605:ARG:NE	7:EH:607:ASN:OD1	2.26	0.65
4:FL:50:ARG:CB	5:FM:81:PHE:CE2	2.79	0.65
4:EL:50:ARG:CG	5:EM:81:PHE:CE2	2.80	0.65
5:FM:8:GLU:OE2	5:FM:45:ARG:NH2	2.30	0.65
7:EG:399:ARG:NH1	7:EG:424:ARG:O	2.29	0.65
4:AJ:144:LYS:NZ	4:AL:148:ILE:O	2.29	0.65
7:AH:221:GLU:OE1	7:AH:221:GLU:N	2.29	0.65
4:EJ:81:GLU:N	4:EJ:81:GLU:OE1	2.30	0.65
7:EI:400:LYS:N	7:EI:423:GLN:OE1	2.30	0.65
5:EM:8:GLU:OE2	5:EM:45:ARG:NH2	2.30	0.65
7:BH:221:GLU:N	7:BH:221:GLU:OE1	2.30	0.65
7:CH:401:ALA:HB2	7:CH:426:VAL:HG21	1.78	0.65
1:AC:153:LYS:HG3	6:DB:52:THR:CB	2.26	0.65
1:CC:102:PHE:CE1	6:CB:142:GLY:HA3	2.32	0.65
4:BL:28:ASN:OD1	4:BL:29:ILE:N	2.30	0.65
4:DL:28:ASN:OD1	4:DL:29:ILE:N	2.30	0.65
4:AL:50:ARG:CA	5:AM:81:PHE:HE2	2.10	0.65
4:FL:178:LYS:HZ2	7:FH:93:LYS:HD3	1.61	0.65
7:AI:400:LYS:N	7:AI:423:GLN:OE1	2.30	0.65
1:CC:102:PHE:CZ	6:CB:142:GLY:C	2.75	0.65
1:BC:63:LYS:NZ	6:EB:52:THR:O	2.27	0.65
1:BC:97:GLU:CD	6:EB:48:GLY:HA2	2.22	0.65
1:BC:153:LYS:HG3	6:EB:52:THR:CB	2.27	0.65
1:BC:163:THR:O	1:BD:44:ARG:NH1	2.29	0.65
1:BD:124:SER:C	7:EI:290:LEU:HD11	2.22	0.65
4:AJ:5:ASN:OD1	7:AG:78:SER:O	2.14	0.65
4:AL:50:ARG:CG	5:AM:81:PHE:CE2	2.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CI:293:SER:OG	7:CI:317:ASP:OD1	2.15	0.65
4:DL:50:ARG:HA	5:DM:81:PHE:CD2	2.32	0.64
4:DL:178:LYS:HZ2	7:DH:93:LYS:HD3	1.61	0.64
5:BM:8:GLU:OE2	5:BM:45:ARG:NH2	2.30	0.64
7:FH:221:GLU:OE1	7:FH:221:GLU:N	2.30	0.64
1:AD:107:SER:HA	6:DB:21:VAL:O	1.96	0.64
1:CC:102:PHE:CZ	6:CB:142:GLY:O	2.50	0.64
4:FK:130:ASN:OD1	4:FK:131:ILE:N	2.30	0.64
4:CJ:71:ASN:N	4:CJ:74:ARG:O	2.31	0.64
4:CL:28:ASN:OD1	4:CL:29:ILE:N	2.30	0.64
1:AD:193:ASP:HA	7:AH:11:ARG:O	1.97	0.64
6:DB:9:ASP:OD1	6:AB:68:TYR:OH	2.14	0.64
7:DH:221:GLU:OE1	7:DH:221:GLU:N	2.31	0.64
7:CG:155:ASP:OD2	7:CG:415:HIS:NE2	2.30	0.64
4:AJ:81:GLU:OE1	4:AJ:81:GLU:N	2.29	0.64
7:BI:400:LYS:N	7:BI:423:GLN:OE1	2.31	0.64
7:EH:221:GLU:OE1	7:EH:221:GLU:N	2.31	0.64
1:BD:100:TYR:HD2	6:EB:109:TYR:HE2	1.46	0.64
4:BL:88:ILE:CD1	5:BM:85:LYS:CE	2.76	0.64
4:DL:153:ASP:O	4:DL:157:ALA:N	2.30	0.64
4:EL:50:ARG:CA	5:EM:81:PHE:CE2	2.77	0.64
6:AB:51:ASN:OD1	6:AB:52:THR:N	2.31	0.64
6:FB:141:ARG:NH2	6:CB:74:ASP:OD1	2.31	0.64
7:FI:400:LYS:N	7:FI:423:GLN:OE1	2.31	0.64
1:AD:192:ILE:O	7:AH:12:VAL:C	2.40	0.64
7:DG:155:ASP:OD2	7:DG:415:HIS:NE2	2.31	0.64
7:CG:144:GLU:OE1	7:CG:146:LYS:NZ	2.30	0.64
4:BK:130:ASN:OD1	4:BK:131:ILE:N	2.30	0.64
7:FG:144:GLU:OE1	7:FG:146:LYS:NZ	2.30	0.64
1:AD:107:SER:HB3	6:DB:22:ASP:HB3	1.80	0.64
1:BD:128:GLN:O	7:BG:16:ARG:NH2	2.25	0.64
4:FJ:81:GLU:OE1	4:FJ:81:GLU:N	2.31	0.64
4:FL:28:ASN:OD1	4:FL:29:ILE:N	2.31	0.64
5:AM:8:GLU:OE2	5:AM:45:ARG:NH2	2.31	0.64
6:EA:141:ARG:NH2	6:BA:74:ASP:OD1	2.31	0.64
6:DB:163:ASP:OD1	6:DB:164:THR:N	2.28	0.64
7:FG:399:ARG:NH1	7:FG:424:ARG:O	2.30	0.64
1:BC:105:PRO:HG3	6:BB:89:TRP:NE1	1.78	0.64
2:BE:228:GLU:OE1	2:BE:228:GLU:N	2.31	0.64
6:AA:141:ARG:NH2	6:FA:74:ASP:OD1	2.31	0.64
7:DH:280:ARG:NH1	7:DH:295:ASN:OD1	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:88:ILE:CD1	5:BM:85:LYS:NZ	2.61	0.64
6:CB:26:MET:HE1	6:CB:131:TYR:CE1	2.33	0.64
1:AC:107:SER:HB3	6:AB:22:ASP:HB3	1.81	0.63
7:FG:342:TYR:OH	7:FG:386:ALA:HB1	1.98	0.63
2:CE:228:GLU:OE1	2:CE:228:GLU:N	2.31	0.63
4:FL:50:ARG:NH1	5:FM:6:ASP:OD2	2.31	0.63
1:AD:102:PHE:CZ	6:DB:142:GLY:O	2.51	0.63
2:AE:228:GLU:N	2:AE:228:GLU:OE1	2.31	0.63
2:AE:315:ILE:HD11	2:AE:324:LYS:HG2	1.80	0.63
4:BL:153:ASP:O	4:BL:157:ALA:N	2.31	0.63
6:EB:26:MET:HE1	6:EB:131:TYR:CE1	2.34	0.63
7:AG:399:ARG:NH1	7:AG:424:ARG:O	2.31	0.63
7:CH:221:GLU:OE1	7:CH:221:GLU:N	2.30	0.63
1:CD:193:ASP:HA	7:CH:11:ARG:O	1.99	0.63
4:BL:50:ARG:CB	5:BM:81:PHE:CE2	2.80	0.63
4:EK:58:HIS:O	4:EK:116:ASN:ND2	2.31	0.63
4:EL:88:ILE:HD13	5:EM:85:LYS:NZ	2.14	0.63
6:CB:163:ASP:OD1	6:CB:164:THR:N	2.29	0.63
7:FI:352:ASN:ND2	7:FI:384:GLN:OE1	2.32	0.63
1:AC:29:MET:SD	1:AC:29:MET:N	2.72	0.63
1:BC:102:PHE:CZ	6:BB:142:GLY:C	2.77	0.63
4:BK:48:ASN:OD1	4:BK:49:ASN:N	2.32	0.63
4:AL:153:ASP:O	4:AL:157:ALA:N	2.30	0.63
6:EB:141:ARG:NH1	6:BB:78:ASP:OD1	2.32	0.63
7:BG:515:ASN:ND2	7:BG:543:TYR:O	2.31	0.63
7:DG:399:ARG:NH1	7:DG:424:ARG:O	2.31	0.63
7:FI:293:SER:OG	7:FI:317:ASP:OD1	2.16	0.63
1:AD:301:THR:HG21	7:AH:475:ASN:OD1	1.99	0.63
6:DB:26:MET:HE1	6:DB:131:TYR:CE1	2.34	0.63
7:BI:293:SER:OG	7:BI:317:ASP:OD1	2.15	0.63
7:DG:515:ASN:ND2	7:DG:543:TYR:O	2.31	0.63
7:EH:568:THR:O	7:EH:572:ASN:ND2	2.32	0.63
7:EG:140:GLU:OE2	7:EG:399:ARG:NH2	2.32	0.63
1:AC:68:SER:OG	7:AG:11:ARG:CG	2.47	0.63
2:CE:315:ILE:HD11	2:CE:324:LYS:HG2	1.80	0.63
1:BC:68:SER:OG	7:BG:11:ARG:CG	2.46	0.63
4:DL:46:THR:HG22	5:DM:78:VAL:HG22	1.79	0.63
7:AH:568:THR:O	7:AH:572:ASN:ND2	2.32	0.63
1:AD:29:MET:N	1:AD:29:MET:SD	2.72	0.63
1:CD:29:MET:SD	1:CD:29:MET:N	2.72	0.63
1:CD:301:THR:HG21	7:CH:475:ASN:OD1	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:29:MET:N	1:BD:29:MET:SD	2.72	0.63
6:EB:42:THR:OG1	6:EB:50:TYR:O	2.13	0.63
7:DI:293:SER:OG	7:DI:317:ASP:OD1	2.15	0.63
1:BC:29:MET:N	1:BC:29:MET:SD	2.72	0.63
4:AL:50:ARG:CB	5:AM:81:PHE:CE2	2.82	0.63
4:FL:153:ASP:O	4:FL:157:ALA:N	2.30	0.63
7:AI:352:ASN:ND2	7:AI:384:GLN:OE1	2.32	0.63
7:EI:293:SER:OG	7:EI:317:ASP:OD1	2.15	0.63
4:DK:130:ASN:OD1	4:DK:131:ILE:N	2.31	0.62
7:BI:440:THR:OG1	7:BI:445:ARG:O	2.17	0.62
4:BJ:81:GLU:OE1	4:BJ:81:GLU:N	2.32	0.62
4:EL:153:ASP:O	4:EL:157:ALA:N	2.31	0.62
7:BH:401:ALA:HB2	7:BH:426:VAL:HG21	1.81	0.62
7:AG:140:GLU:OE2	7:AG:399:ARG:NH2	2.32	0.62
7:EG:515:ASN:ND2	7:EG:543:TYR:O	2.31	0.62
1:AD:192:ILE:N	7:AH:12:VAL:O	2.32	0.62
1:CD:153:LYS:CE	6:AB:43:GLU:OE2	2.47	0.62
4:DJ:81:GLU:OE1	4:DJ:81:GLU:N	2.33	0.62
6:AB:9:ASP:OD2	6:FB:68:TYR:OH	2.18	0.62
7:BG:144:GLU:OE1	7:BG:146:LYS:NZ	2.33	0.62
7:CG:515:ASN:ND2	7:CG:543:TYR:O	2.32	0.62
7:BG:399:ARG:NH1	7:BG:424:ARG:O	2.32	0.62
1:AD:63:LYS:NZ	6:BB:52:THR:O	2.28	0.62
1:BD:125:ARG:CA	7:EI:290:LEU:HD11	2.28	0.62
7:AG:183:PRO:O	7:AG:186:HIS:NE2	2.33	0.62
7:CG:399:ARG:NH1	7:CG:424:ARG:O	2.32	0.62
4:FL:88:ILE:HD12	5:FM:85:LYS:CE	2.29	0.62
4:CK:115:GLN:NE2	7:CG:82:LEU:O	2.31	0.62
6:EB:9:ASP:OD2	6:BB:68:TYR:OH	2.17	0.62
7:BI:352:ASN:ND2	7:BI:384:GLN:OE1	2.33	0.62
1:CC:29:MET:N	1:CC:29:MET:SD	2.72	0.62
6:BA:6:ASN:ND2	6:BA:8:ASN:OD1	2.32	0.62
7:FG:515:ASN:ND2	7:FG:543:TYR:O	2.31	0.62
7:EI:352:ASN:ND2	7:EI:384:GLN:OE1	2.33	0.62
1:CD:97:GLU:OE1	6:AB:48:GLY:CA	2.47	0.62
2:BE:315:ILE:HD11	2:BE:324:LYS:HG2	1.80	0.62
4:BL:50:ARG:CA	5:BM:81:PHE:CE2	2.82	0.62
4:AL:178:LYS:HZ2	7:AH:93:LYS:HD3	1.63	0.62
5:DN:99:CYS:SG	5:DN:100:LYS:N	2.73	0.62
5:EN:99:CYS:SG	5:EN:100:LYS:N	2.73	0.62
7:EI:98:ASP:OD1	7:EI:102:TYR:N	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CE:235:GLU:OE1	2:CE:235:GLU:N	2.33	0.61
4:BJ:72:VAL:O	4:BL:22:ASN:ND2	2.33	0.61
4:FJ:71:ASN:N	4:FJ:74:ARG:O	2.33	0.61
4:CK:130:ASN:OD1	4:CK:131:ILE:N	2.32	0.61
6:BB:15:ARG:NE	6:BB:87:GLU:OE2	2.27	0.61
6:FA:6:ASN:ND2	6:FA:8:ASN:OD1	2.32	0.61
6:CB:109:TYR:OH	6:CB:111:GLN:NE2	2.30	0.61
7:AH:212:HIS:O	7:AH:267:SER:OG	2.17	0.61
1:AC:125:ARG:HD3	7:AI:286:SER:HB3	1.81	0.61
4:DJ:140:ASP:OD1	4:DJ:141:GLY:N	2.34	0.61
4:CL:153:ASP:O	4:CL:157:ALA:N	2.33	0.61
4:EJ:140:ASP:OD1	4:EJ:141:GLY:N	2.32	0.61
4:EL:46:THR:HG22	5:EM:78:VAL:HG22	1.82	0.61
1:AD:1:ASP:N	1:AD:92:ILE:O	2.34	0.61
1:BC:27:ASP:OD1	1:BC:28:SER:N	2.33	0.61
4:DK:115:GLN:NE2	7:DG:82:LEU:O	2.32	0.61
4:EK:130:ASN:OD1	4:EK:131:ILE:N	2.34	0.61
5:AN:99:CYS:SG	5:AN:100:LYS:N	2.73	0.61
6:FB:89:TRP:HB3	6:FB:109:TYR:HA	1.82	0.61
1:CC:42:ASN:OD1	1:BD:223:GLN:NE2	2.34	0.61
1:CC:68:SER:OG	7:CG:11:ARG:CG	2.48	0.61
6:EB:68:TYR:OH	6:CB:9:ASP:OD2	2.17	0.61
7:FH:401:ALA:HB2	7:FH:426:VAL:HG21	1.81	0.61
1:BD:1:ASP:N	1:BD:92:ILE:O	2.34	0.61
4:AK:115:GLN:NE2	7:AG:82:LEU:O	2.32	0.61
6:BB:26:MET:HE1	6:BB:131:TYR:CE1	2.36	0.61
7:DI:440:THR:OG1	7:DI:445:ARG:O	2.18	0.61
7:CI:440:THR:OG1	7:CI:445:ARG:O	2.18	0.61
1:AC:1:ASP:N	1:AC:92:ILE:O	2.34	0.61
1:AC:27:ASP:OD1	1:AC:28:SER:N	2.34	0.61
1:AD:27:ASP:OD1	1:AD:28:SER:N	2.34	0.61
1:CC:102:PHE:CE1	6:CB:142:GLY:CA	2.83	0.61
4:DK:86:ASP:OD2	4:DK:89:ASN:ND2	2.34	0.61
4:FL:174:THR:CB	7:FH:90:ASN:HD21	2.12	0.61
5:BN:99:CYS:SG	5:BN:100:LYS:N	2.74	0.61
6:DB:109:TYR:OH	6:DB:111:GLN:NE2	2.32	0.61
7:BH:155:ASP:OD2	7:BH:415:HIS:NE2	2.34	0.61
2:AE:235:GLU:OE1	2:AE:235:GLU:N	2.33	0.61
4:BJ:5:ASN:OD1	7:BG:78:SER:O	2.18	0.61
4:BL:178:LYS:HZ3	7:BH:93:LYS:HD3	1.62	0.61
7:BG:183:PRO:O	7:BG:186:HIS:NE2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CD:1:ASP:N	1:CD:92:ILE:O	2.34	0.61
1:CD:27:ASP:OD1	1:CD:28:SER:N	2.34	0.61
1:BD:27:ASP:OD1	1:BD:28:SER:N	2.33	0.61
4:BJ:71:ASN:N	4:BJ:74:ARG:O	2.33	0.61
4:BL:51:PRO:HG3	5:BM:75:ASP:OD2	2.01	0.61
4:AK:58:HIS:O	4:AK:116:ASN:ND2	2.34	0.61
4:FL:51:PRO:O	5:FM:36:ARG:NH1	2.33	0.61
4:DK:48:ASN:OD1	4:DK:49:ASN:N	2.33	0.61
6:BB:89:TRP:HB3	6:BB:109:TYR:HA	1.81	0.61
6:AB:26:MET:HE1	6:AB:131:TYR:CE1	2.35	0.61
2:BE:235:GLU:OE1	2:BE:235:GLU:N	2.33	0.60
4:BL:174:THR:CB	7:BH:90:ASN:HD21	2.13	0.60
4:AJ:140:ASP:OD1	4:AJ:141:GLY:N	2.33	0.60
5:CN:99:CYS:SG	5:CN:100:LYS:N	2.73	0.60
7:DH:164:MET:HE2	7:DH:387:GLU:OE1	2.01	0.60
7:FG:183:PRO:O	7:FG:186:HIS:NE2	2.34	0.60
7:CG:183:PRO:O	7:CG:186:HIS:NE2	2.34	0.60
1:CC:1:ASP:N	1:CC:92:ILE:O	2.34	0.60
1:BD:97:GLU:CD	6:CB:48:GLY:CA	2.71	0.60
4:FJ:72:VAL:O	4:FL:22:ASN:ND2	2.33	0.60
4:FK:48:ASN:OD1	4:FK:49:ASN:N	2.33	0.60
1:BC:1:ASP:N	1:BC:92:ILE:O	2.34	0.60
4:AJ:24:VAL:O	4:AJ:125:ARG:NH1	2.34	0.60
7:EG:183:PRO:O	7:EG:186:HIS:NE2	2.33	0.60
4:DL:50:ARG:CB	5:DM:81:PHE:CE2	2.83	0.60
4:AL:88:ILE:CD1	5:AM:85:LYS:CE	2.79	0.60
4:CL:50:ARG:CA	5:CM:81:PHE:CE2	2.82	0.60
6:AB:141:ARG:NH1	6:FB:78:ASP:OD1	2.33	0.60
7:EH:155:ASP:OD2	7:EH:415:HIS:NE2	2.35	0.60
1:CC:27:ASP:OD1	1:CC:28:SER:N	2.33	0.60
1:BC:82:THR:O	1:BD:51:TYR:OH	2.18	0.60
1:BD:125:ARG:HA	7:EI:290:LEU:HD11	1.82	0.60
4:DJ:71:ASN:N	4:DJ:74:ARG:O	2.34	0.60
4:FL:50:ARG:CA	5:FM:81:PHE:CE2	2.78	0.60
6:EB:160:ARG:NH2	6:EB:161:PHE:O	2.34	0.60
6:CB:42:THR:OG1	6:CB:50:TYR:O	2.18	0.60
7:DG:183:PRO:O	7:DG:186:HIS:NE2	2.34	0.60
7:CI:352:ASN:ND2	7:CI:384:GLN:OE1	2.34	0.60
1:AD:20:ILE:HD12	6:BB:50:TYR:CZ	2.36	0.60
1:CC:153:LYS:CB	6:FB:52:THR:HB	2.30	0.60
1:BD:97:GLU:OE2	6:CB:48:GLY:CA	2.50	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CJ:81:GLU:OE1	4:CJ:81:GLU:N	2.35	0.60
4:CK:86:ASP:OD2	4:CK:89:ASN:ND2	2.34	0.60
4:CL:88:ILE:HD13	5:CM:85:LYS:NZ	2.17	0.60
7:DI:352:ASN:ND2	7:DI:384:GLN:OE1	2.35	0.60
1:CD:107:SER:HB3	6:FB:22:ASP:HB3	1.83	0.60
1:BD:153:LYS:CE	6:CB:43:GLU:CD	2.75	0.60
4:AK:130:ASN:OD1	4:AK:131:ILE:N	2.34	0.60
4:FK:175:LEU:HD13	4:FL:183:ALA:CB	2.32	0.60
6:DB:42:THR:OG1	6:DB:50:TYR:O	2.15	0.60
7:EH:164:MET:HE2	7:EH:387:GLU:OE1	2.01	0.60
4:BL:88:ILE:HD12	5:BM:85:LYS:NZ	2.17	0.60
4:AJ:71:ASN:N	4:AJ:74:ARG:O	2.34	0.60
6:FB:9:ASP:OD2	6:CB:68:TYR:OH	2.20	0.60
7:AG:515:ASN:ND2	7:AG:543:TYR:O	2.34	0.60
1:AC:82:THR:O	1:AD:51:TYR:OH	2.20	0.60
1:AC:102:PHE:CE1	6:AB:142:GLY:HA3	2.37	0.60
1:BD:125:ARG:HD3	7:EI:286:SER:HB3	1.84	0.60
4:FK:58:HIS:NE2	7:FH:80:MET:O	2.28	0.60
4:CJ:140:ASP:OD1	4:CJ:141:GLY:N	2.34	0.60
4:EJ:24:VAL:O	4:EJ:125:ARG:NH1	2.35	0.60
4:EK:175:LEU:HD13	4:EL:183:ALA:CB	2.32	0.60
6:FB:26:MET:HE1	6:FB:131:TYR:CE1	2.36	0.60
7:DH:155:ASP:OD2	7:DH:415:HIS:NE2	2.34	0.60
7:CH:280:ARG:NH1	7:CH:295:ASN:OD1	2.34	0.60
7:EI:397:THR:O	7:EI:399:ARG:N	2.35	0.60
1:AC:153:LYS:CE	6:DB:43:GLU:CD	2.75	0.60
4:BK:175:LEU:HD13	4:BL:183:ALA:CB	2.32	0.60
4:BL:91:ARG:C	4:BL:92:LEU:HD12	2.27	0.60
4:CJ:72:VAL:O	4:CL:22:ASN:ND2	2.34	0.60
7:BG:140:GLU:OE2	7:BG:399:ARG:NH2	2.34	0.60
7:FH:155:ASP:OD2	7:FH:415:HIS:NE2	2.33	0.60
1:AD:39:GLU:OE2	2:CE:77:GLY:N	2.31	0.59
1:AD:97:GLU:OE1	6:BB:48:GLY:CA	2.49	0.59
4:BJ:140:ASP:OD1	4:BJ:141:GLY:N	2.35	0.59
4:BL:46:THR:HG22	5:BM:78:VAL:HG22	1.83	0.59
4:CK:175:LEU:HD13	4:CL:183:ALA:CB	2.32	0.59
6:AB:163:ASP:OD1	6:AB:164:THR:N	2.34	0.59
7:BG:605:ARG:NE	7:BG:607:ASN:OD1	2.35	0.59
7:FI:440:THR:OG1	7:FI:445:ARG:O	2.20	0.59
7:CI:397:THR:O	7:CI:399:ARG:N	2.35	0.59
4:AK:175:LEU:HD13	4:AL:183:ALA:CB	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:EM:20:ASP:OD1	5:EM:118:ASN:ND2	2.35	0.59
6:CB:72:PHE:HE2	6:CB:76:ILE:HD11	1.67	0.59
6:CB:89:TRP:HB3	6:CB:109:TYR:HA	1.83	0.59
4:AL:46:THR:HG22	5:AM:78:VAL:HG22	1.83	0.59
4:EJ:71:ASN:N	4:EJ:74:ARG:O	2.34	0.59
4:FJ:140:ASP:OD1	4:FJ:141:GLY:N	2.34	0.59
4:CJ:5:ASN:OD1	7:CG:78:SER:O	2.21	0.59
6:BB:9:ASP:OD2	6:DB:68:TYR:OH	2.20	0.59
7:FH:568:THR:O	7:FH:572:ASN:ND2	2.35	0.59
7:CG:605:ARG:NE	7:CG:607:ASN:OD1	2.36	0.59
1:BC:105:PRO:HG3	6:BB:89:TRP:HE1	1.66	0.59
4:AJ:20:GLN:CD	6:DA:99:ASN:OD1	2.45	0.59
5:AM:20:ASP:OD1	5:AM:118:ASN:ND2	2.35	0.59
6:EB:163:ASP:OD1	6:EB:164:THR:N	2.34	0.59
7:AH:280:ARG:NH1	7:AH:295:ASN:OD1	2.36	0.59
1:AD:125:ARG:HA	7:DI:290:LEU:HD11	1.83	0.59
1:BD:61:PHE:CD1	6:CB:43:GLU:OE1	2.56	0.59
4:DK:175:LEU:HD13	4:DL:183:ALA:CB	2.32	0.59
5:FN:99:CYS:SG	5:FN:100:LYS:N	2.74	0.59
7:BI:151:GLU:OE1	7:BI:427:ASN:ND2	2.35	0.59
7:DI:98:ASP:OD1	7:DI:102:TYR:N	2.36	0.59
7:AI:98:ASP:OD1	7:AI:102:TYR:N	2.35	0.59
7:FI:397:THR:O	7:FI:399:ARG:N	2.35	0.59
1:AD:188:PHE:HB2	7:AH:14:ASP:CA	2.31	0.59
1:BD:207:ASN:HB3	7:BH:455:ALA:HB1	1.82	0.59
1:BD:301:THR:CG2	7:BH:475:ASN:HA	2.33	0.59
4:FK:58:HIS:O	4:FK:116:ASN:ND2	2.36	0.59
4:FL:49:ASN:O	5:FM:81:PHE:CE2	2.56	0.59
4:CJ:43:PHE:HE2	4:CJ:63:ILE:HD12	1.68	0.59
4:CL:174:THR:CB	7:CH:90:ASN:HD21	2.15	0.59
4:EJ:20:GLN:CD	6:CA:99:ASN:OD1	2.46	0.59
4:EK:86:ASP:OD2	4:EK:89:ASN:ND2	2.36	0.59
6:AB:30:THR:OG1	6:AB:31:GLU:N	2.36	0.59
7:BI:397:THR:O	7:BI:399:ARG:N	2.35	0.59
7:DH:568:THR:O	7:DH:572:ASN:ND2	2.35	0.59
7:EH:394:ASP:OD2	7:EH:397:THR:OG1	2.15	0.59
4:DL:178:LYS:HZ1	7:DH:93:LYS:CD	2.15	0.59
7:FG:140:GLU:OE2	7:FG:399:ARG:NH2	2.35	0.59
1:AC:102:PHE:CE1	6:AB:142:GLY:CA	2.86	0.59
1:BD:301:THR:HB	7:BH:475:ASN:OD1	2.03	0.59
4:BK:169:MET:O	4:BK:172:THR:OG1	2.20	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BB:141:ARG:NH1	6:DB:78:ASP:OD1	2.36	0.59
7:CH:568:THR:O	7:CH:572:ASN:ND2	2.36	0.59
1:CD:207:ASN:CB	7:CH:455:ALA:CB	2.75	0.59
4:FK:169:MET:O	4:FK:172:THR:OG1	2.19	0.59
4:FL:88:ILE:HD12	5:FM:85:LYS:HZ1	1.65	0.59
4:FL:88:ILE:CD1	5:FM:85:LYS:NZ	2.65	0.59
4:FL:91:ARG:C	4:FL:92:LEU:HD12	2.28	0.59
4:CK:48:ASN:OD1	4:CK:49:ASN:N	2.33	0.59
4:EL:51:PRO:HG3	5:EM:75:ASP:OD2	2.03	0.59
6:DB:72:PHE:HE2	6:DB:76:ILE:HD11	1.67	0.59
7:DG:605:ARG:NE	7:DG:607:ASN:OD1	2.35	0.59
6:BB:30:THR:OG1	6:BB:31:GLU:N	2.36	0.58
1:AD:20:ILE:CD1	6:BB:50:TYR:CZ	2.86	0.58
6:FB:72:PHE:HE2	6:FB:76:ILE:HD11	1.67	0.58
6:FB:163:ASP:OD1	6:FB:164:THR:N	2.34	0.58
7:BH:171:PRO:O	7:BH:174:LYS:NZ	2.31	0.58
1:CD:107:SER:HA	6:FB:21:VAL:O	2.02	0.58
4:FJ:5:ASN:OD1	7:FG:78:SER:O	2.21	0.58
4:FL:51:PRO:HD2	5:FM:81:PHE:CD2	2.38	0.58
4:DJ:24:VAL:O	4:DJ:125:ARG:NH1	2.35	0.58
4:EL:178:LYS:HZ2	7:EH:93:LYS:HD3	1.62	0.58
7:AI:397:THR:O	7:AI:399:ARG:N	2.35	0.58
7:FI:185:ASN:O	7:FI:208:GLY:N	2.37	0.58
7:CI:98:ASP:OD1	7:CI:102:TYR:N	2.36	0.58
7:EG:14:ASP:OD1	7:EG:15:TYR:N	2.36	0.58
4:DL:130:ASN:O	4:DL:137:SER:OG	2.22	0.58
7:BI:98:ASP:OD1	7:BI:102:TYR:N	2.36	0.58
7:DI:397:THR:O	7:DI:399:ARG:N	2.35	0.58
7:FI:98:ASP:OD1	7:FI:102:TYR:N	2.36	0.58
4:DL:174:THR:CB	7:DH:90:ASN:HD21	2.16	0.58
4:AK:86:ASP:OD2	4:AK:89:ASN:ND2	2.36	0.58
4:EL:49:ASN:O	5:EM:81:PHE:CE2	2.57	0.58
5:FM:41:ASP:OD2	5:FM:43:GLN:NE2	2.37	0.58
6:BB:72:PHE:HE2	6:BB:76:ILE:HD11	1.68	0.58
6:AB:42:THR:OG1	6:AB:50:TYR:O	2.19	0.58
7:BH:568:THR:O	7:BH:572:ASN:ND2	2.37	0.58
7:EI:185:ASN:O	7:EI:208:GLY:N	2.36	0.58
1:CC:107:SER:HB3	6:CB:22:ASP:HB3	1.85	0.58
7:EI:440:THR:OG1	7:EI:445:ARG:O	2.21	0.58
1:AD:67:ARG:HB3	6:EB:47:ASP:OD2	2.03	0.58
4:BK:58:HIS:O	4:BK:116:ASN:ND2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DJ:5:ASN:OD1	7:DG:78:SER:O	2.22	0.58
4:CL:88:ILE:HD13	5:CM:85:LYS:HZ1	1.68	0.58
7:EH:280:ARG:NH1	7:EH:295:ASN:OD1	2.36	0.58
4:FL:50:ARG:HA	5:FM:81:PHE:HE2	1.56	0.58
5:BN:59:LEU:HD23	5:BN:59:LEU:H	1.69	0.58
7:AH:171:PRO:O	7:AH:174:LYS:NZ	2.29	0.58
1:CD:102:PHE:CZ	6:FB:142:GLY:O	2.57	0.58
1:AC:97:GLU:OE1	6:DB:48:GLY:CA	2.52	0.57
6:AB:72:PHE:HE2	6:AB:76:ILE:HD11	1.69	0.57
6:FB:30:THR:OG1	6:FB:31:GLU:N	2.37	0.57
4:FJ:24:VAL:O	4:FJ:125:ARG:NH1	2.37	0.57
7:EH:540:ASN:OD1	7:EH:541:ALA:N	2.37	0.57
1:AD:180:ASN:HB2	7:AI:12:VAL:CG2	2.35	0.57
1:AD:193:ASP:HA	7:AH:12:VAL:HA	1.85	0.57
4:DJ:20:GLN:OE1	6:BA:98:LYS:O	2.23	0.57
6:EB:30:THR:OG1	6:EB:31:GLU:N	2.37	0.57
6:AB:89:TRP:HB3	6:AB:109:TYR:HA	1.87	0.57
5:DN:59:LEU:HD23	5:DN:59:LEU:H	1.70	0.57
7:AH:493:ASP:N	7:AH:493:ASP:OD1	2.36	0.57
4:BL:130:ASN:O	4:BL:137:SER:OG	2.23	0.57
4:CJ:8:LYS:NZ	4:CJ:35:ASP:OD2	2.37	0.57
4:DK:58:HIS:O	4:DK:116:ASN:ND2	2.37	0.57
4:CJ:24:VAL:O	4:CJ:125:ARG:NH1	2.37	0.57
7:DH:540:ASN:OD1	7:DH:541:ALA:N	2.37	0.57
7:AI:440:THR:OG1	7:AI:445:ARG:O	2.21	0.57
7:EG:605:ARG:NE	7:EG:607:ASN:OD1	2.37	0.57
1:CC:47:MET:O	2:BE:78:ASP:N	2.37	0.57
4:BJ:17:THR:HG22	4:BJ:124:GLU:OE1	2.05	0.57
4:BL:29:ILE:O	4:BL:29:ILE:HG23	2.05	0.57
4:DL:50:ARG:CA	5:DM:81:PHE:HE2	2.17	0.57
4:CL:49:ASN:O	5:CM:81:PHE:CE2	2.58	0.57
7:AG:605:ARG:NE	7:AG:607:ASN:OD1	2.38	0.57
7:FH:540:ASN:OD1	7:FH:541:ALA:N	2.37	0.57
7:FI:183:PRO:O	7:FI:186:HIS:NE2	2.38	0.57
1:CD:68:SER:OG	7:FG:11:ARG:CG	2.49	0.57
1:CD:100:TYR:CE2	6:FB:109:TYR:CD2	2.88	0.57
6:CB:30:THR:OG1	6:CB:31:GLU:N	2.38	0.57
7:CH:540:ASN:OD1	7:CH:541:ALA:N	2.37	0.57
4:BK:86:ASP:OD2	4:BK:89:ASN:ND2	2.35	0.57
4:FL:29:ILE:HG23	4:FL:29:ILE:O	2.05	0.57
4:FL:178:LYS:HZ3	7:FH:93:LYS:HD3	1.62	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EL:50:ARG:HA	5:EM:81:PHE:HE2	1.52	0.57
5:BM:41:ASP:OD2	5:BM:43:GLN:NE2	2.37	0.57
6:EB:72:PHE:HE2	6:EB:76:ILE:HD11	1.69	0.57
6:DB:72:PHE:CE2	6:DB:76:ILE:HD11	2.40	0.57
1:CC:125:ARG:HD3	7:CI:286:SER:HB3	1.87	0.57
4:AJ:130:ASN:OD1	4:AJ:131:ILE:N	2.38	0.57
4:DL:29:ILE:HG23	4:DL:29:ILE:O	2.05	0.56
4:AL:174:THR:CB	7:AH:90:ASN:HD21	2.18	0.56
4:FK:86:ASP:OD2	4:FK:89:ASN:ND2	2.38	0.56
4:CL:91:ARG:C	4:CL:92:LEU:HD12	2.30	0.56
7:CG:345:ASP:O	7:CG:347:LYS:N	2.38	0.56
1:AD:111:VAL:CG2	6:DB:17:ALA:HB1	2.35	0.56
1:BD:107:SER:N	6:EB:22:ASP:CA	2.68	0.56
4:CJ:5:ASN:ND2	7:CG:80:MET:O	2.31	0.56
6:AB:109:TYR:OH	6:AB:111:GLN:NE2	2.36	0.56
7:BH:185:ASN:OD1	7:BH:186:HIS:N	2.38	0.56
1:CC:124:SER:OG	1:CC:127:ASP:OD1	2.24	0.56
1:BD:193:ASP:O	1:BD:201:ARG:NH1	2.39	0.56
4:AL:50:ARG:CA	5:AM:81:PHE:CE2	2.86	0.56
4:CJ:74:ARG:HB3	4:CL:24:VAL:HG22	1.87	0.56
5:AN:59:LEU:HD23	5:AN:59:LEU:H	1.70	0.56
5:EN:59:LEU:HD23	5:EN:59:LEU:H	1.70	0.56
6:DB:91:VAL:O	6:DB:91:VAL:HG13	2.05	0.56
6:CB:72:PHE:CE2	6:CB:76:ILE:HD11	2.41	0.56
7:BH:394:ASP:OD2	7:BH:397:THR:OG1	2.13	0.56
7:BH:540:ASN:OD1	7:BH:541:ALA:N	2.38	0.56
7:AG:587:TRP:NE1	7:AG:603:LEU:HD21	2.21	0.56
7:AI:185:ASN:O	7:AI:208:GLY:N	2.39	0.56
7:FG:605:ARG:NE	7:FG:607:ASN:OD1	2.38	0.56
7:CH:445:ARG:NH2	7:CI:414:ARG:O	2.39	0.56
4:DL:91:ARG:C	4:DL:92:LEU:HD12	2.30	0.56
4:CL:130:ASN:O	4:CL:137:SER:OG	2.22	0.56
4:EL:91:ARG:C	4:EL:92:LEU:HD12	2.31	0.56
6:EB:89:TRP:HB3	6:EB:109:TYR:HA	1.86	0.56
7:DH:171:PRO:O	7:DH:174:LYS:NZ	2.32	0.56
7:EI:183:PRO:O	7:EI:186:HIS:NE2	2.38	0.56
1:BC:124:SER:OG	1:BC:127:ASP:OD1	2.24	0.56
4:BK:115:GLN:NE2	7:BG:82:LEU:O	2.38	0.56
4:CK:58:HIS:O	4:CK:116:ASN:ND2	2.39	0.56
4:EJ:43:PHE:HE2	4:EJ:63:ILE:HD12	1.71	0.56
5:DM:20:ASP:OD1	5:DM:118:ASN:ND2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CM:20:ASP:OD1	5:CM:118:ASN:ND2	2.38	0.56
6:EB:91:VAL:HG13	6:EB:91:VAL:O	2.04	0.56
6:BB:42:THR:OG1	6:BB:50:TYR:O	2.18	0.56
7:DG:587:TRP:NE1	7:DG:603:LEU:HD21	2.21	0.56
1:BD:124:SER:OG	1:BD:127:ASP:OD1	2.24	0.56
4:DJ:91:ARG:C	4:DJ:92:LEU:HD12	2.30	0.56
4:AK:63:ILE:HD11	4:AK:94:TYR:CE2	2.40	0.56
4:AL:29:ILE:HG23	4:AL:29:ILE:O	2.06	0.56
4:FL:55:SER:OG	4:FL:58:HIS:ND1	2.33	0.56
6:DB:30:THR:OG1	6:DB:31:GLU:N	2.38	0.56
7:DH:445:ARG:NH2	7:DI:414:ARG:O	2.38	0.56
7:AH:540:ASN:OD1	7:AH:541:ALA:N	2.37	0.56
1:AC:153:LYS:CB	6:DB:52:THR:HB	2.33	0.56
1:CC:97:GLU:OE1	6:FB:48:GLY:CA	2.54	0.56
4:BL:178:LYS:HZ2	7:BH:93:LYS:HD3	1.60	0.56
4:AJ:72:VAL:O	4:AL:22:ASN:ND2	2.39	0.56
4:EJ:130:ASN:OD1	4:EJ:131:ILE:N	2.39	0.56
4:EL:88:ILE:CD1	5:EM:85:LYS:NZ	2.69	0.56
5:CM:48:LEU:HD12	5:CM:74:ILE:HD11	1.88	0.56
6:DB:89:TRP:HB3	6:DB:109:TYR:HA	1.87	0.56
6:FB:141:ARG:NH1	6:CB:78:ASP:OD1	2.37	0.56
1:AC:124:SER:OG	1:AC:127:ASP:OD1	2.24	0.56
1:CC:20:ILE:HD11	6:FB:50:TYR:CD2	2.37	0.56
1:BC:153:LYS:CB	6:EB:52:THR:HB	2.33	0.56
4:AL:91:ARG:C	4:AL:92:LEU:HD12	2.31	0.56
7:BI:185:ASN:O	7:BI:208:GLY:N	2.38	0.56
7:FH:185:ASN:OD1	7:FH:186:HIS:N	2.39	0.56
7:FH:493:ASP:OD1	7:FH:493:ASP:N	2.36	0.56
1:BC:193:ASP:O	1:BC:201:ARG:NH1	2.39	0.56
4:BJ:20:GLN:CD	6:EA:99:ASN:OD1	2.48	0.56
4:AL:130:ASN:O	4:AL:137:SER:OG	2.23	0.56
4:CK:52:LEU:HD12	7:CG:79:ASN:O	2.06	0.56
4:CL:88:ILE:CD1	5:CM:85:LYS:NZ	2.69	0.56
4:EL:174:THR:CB	7:EH:90:ASN:HD21	2.17	0.56
6:FB:72:PHE:CE2	6:FB:76:ILE:HD11	2.40	0.56
1:AC:193:ASP:O	1:AC:201:ARG:NH1	2.39	0.56
1:CD:63:LYS:NZ	6:AB:52:THR:O	2.34	0.56
1:BD:97:GLU:OE1	6:CB:47:ASP:C	2.48	0.56
4:AL:50:ARG:HA	5:AM:81:PHE:HE2	1.64	0.56
4:AL:178:LYS:HZ3	7:AH:93:LYS:HD3	1.65	0.56
4:FJ:20:GLN:CD	6:AA:99:ASN:OD1	2.49	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:FJ:74:ARG:HB3	4:FL:24:VAL:HG22	1.87	0.56
4:CJ:48:ASN:OD1	4:CJ:49:ASN:N	2.36	0.56
6:BB:148:GLU:O	6:BB:151:THR:OG1	2.18	0.56
7:CH:171:PRO:O	7:CH:174:LYS:NZ	2.34	0.56
7:EG:587:TRP:NE1	7:EG:603:LEU:HD21	2.21	0.56
1:CC:82:THR:O	1:CD:51:TYR:OH	2.22	0.55
4:BK:34:SER:N	4:BK:134:ASP:OD2	2.37	0.55
4:BK:148:ILE:HG23	4:BL:151:ILE:HD11	1.87	0.55
5:FN:59:LEU:HD23	5:FN:59:LEU:H	1.69	0.55
6:DB:141:ARG:NH1	6:AB:78:ASP:OD1	2.37	0.55
7:FH:49:ALA:N	7:FG:54:GLN:O	2.39	0.55
1:AD:153:LYS:HE3	6:BB:43:GLU:CD	2.31	0.55
4:EK:34:SER:N	4:EK:134:ASP:OD2	2.37	0.55
4:EL:29:ILE:HG23	4:EL:29:ILE:O	2.06	0.55
6:BB:72:PHE:CE2	6:BB:76:ILE:HD11	2.41	0.55
6:BB:160:ARG:NH2	6:BB:161:PHE:O	2.39	0.55
6:FB:42:THR:OG1	6:FB:50:TYR:O	2.20	0.55
6:FB:91:VAL:O	6:FB:91:VAL:HG13	2.07	0.55
6:CB:148:GLU:O	6:CB:151:THR:OG1	2.21	0.55
1:CD:180:ASN:HB2	7:CI:12:VAL:CG2	2.36	0.55
1:CD:199:ASP:OD1	1:CD:200:LYS:N	2.40	0.55
4:FJ:20:GLN:NE2	6:AA:99:ASN:OD1	2.40	0.55
5:CM:41:ASP:OD2	5:CM:43:GLN:NE2	2.40	0.55
1:AC:149:GLN:OE1	6:DB:41:ASP:HB3	2.07	0.55
1:AD:184:GLY:HA2	7:AG:13:PHE:O	2.07	0.55
4:BL:174:THR:CG2	7:BH:90:ASN:HD21	2.19	0.55
4:AK:88:ILE:O	7:AG:76:ARG:NH1	2.39	0.55
4:CJ:43:PHE:CE2	4:CJ:63:ILE:HD12	2.41	0.55
5:DM:48:LEU:HD12	5:DM:74:ILE:HD11	1.88	0.55
6:EB:78:ASP:OD1	6:CB:141:ARG:NH1	2.38	0.55
7:BH:493:ASP:N	7:BH:493:ASP:OD1	2.37	0.55
7:FI:264:ARG:NH1	7:FI:287:GLU:OE1	2.40	0.55
1:AD:107:SER:CA	6:DB:21:VAL:C	2.73	0.55
4:BL:54:ILE:HD13	4:BL:92:LEU:HD11	1.88	0.55
4:AJ:5:ASN:ND2	7:AG:80:MET:O	2.25	0.55
6:FB:12:ILE:O	6:FB:13:LEU:HD12	2.06	0.55
7:AI:183:PRO:O	7:AI:186:HIS:NE2	2.39	0.55
7:CI:264:ARG:NH1	7:CI:287:GLU:OE1	2.40	0.55
1:AD:199:ASP:OD1	1:AD:200:LYS:N	2.40	0.55
7:BG:587:TRP:NE1	7:BG:603:LEU:HD21	2.22	0.55
7:CH:185:ASN:OD1	7:CH:186:HIS:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:100:TYR:CE2	6:DB:109:TYR:CD2	2.88	0.55
1:CC:149:GLN:OE1	6:FB:41:ASP:HB3	2.06	0.55
1:CD:124:SER:OG	1:CD:127:ASP:OD1	2.24	0.55
1:BC:107:SER:HB3	6:BB:22:ASP:HB3	1.89	0.55
4:BK:88:ILE:O	7:BG:76:ARG:NH1	2.39	0.55
4:DL:88:ILE:HD13	5:DM:85:LYS:NZ	2.22	0.55
4:EK:63:ILE:HD11	4:EK:94:TYR:CE2	2.42	0.55
5:CN:59:LEU:HD23	5:CN:59:LEU:H	1.70	0.55
6:DB:148:GLU:O	6:DB:151:THR:OG1	2.21	0.55
7:AH:155:ASP:OD2	7:AH:415:HIS:NE2	2.39	0.55
7:CH:342:TYR:CE2	7:CH:386:ALA:HB1	2.42	0.55
1:AD:37:ASP:OD2	1:AD:37:ASP:N	2.40	0.55
1:AD:188:PHE:HE2	7:AG:11:ARG:CB	2.15	0.55
1:CC:153:LYS:CE	6:FB:43:GLU:CD	2.80	0.55
4:CL:88:ILE:HD12	5:CM:85:LYS:HE2	1.87	0.55
6:BB:91:VAL:HG13	6:BB:91:VAL:O	2.06	0.55
6:CB:12:ILE:C	6:CB:13:LEU:HD12	2.32	0.55
1:CC:199:ASP:OD1	1:CC:200:LYS:N	2.40	0.55
1:BD:207:ASN:CB	7:BH:455:ALA:HB2	2.36	0.55
4:BL:51:PRO:HD2	5:BM:81:PHE:CD2	2.41	0.55
4:DK:146:VAL:HG23	4:DK:146:VAL:O	2.07	0.55
4:FL:130:ASN:O	4:FL:137:SER:OG	2.23	0.55
4:CL:29:ILE:HG23	4:CL:29:ILE:O	2.06	0.55
6:BB:163:ASP:O	6:BA:15:ARG:NH1	2.40	0.55
7:BI:346:SER:O	7:BI:346:SER:OG	2.24	0.55
7:FH:164:MET:HE2	7:FH:387:GLU:OE1	2.07	0.55
7:EG:595:THR:OG1	7:EG:598:ASN:OD1	2.23	0.55
1:CD:39:GLU:OE2	2:BE:77:GLY:N	2.38	0.55
1:CD:100:TYR:CE1	6:FB:111:GLN:HG2	2.41	0.55
1:BD:68:SER:OG	7:EG:11:ARG:HG3	2.06	0.55
4:DJ:72:VAL:O	4:DL:22:ASN:ND2	2.40	0.55
4:CL:51:PRO:HD2	5:CM:81:PHE:CD2	2.42	0.55
6:AB:91:VAL:O	6:AB:91:VAL:HG13	2.07	0.55
6:CB:91:VAL:O	6:CB:91:VAL:HG13	2.06	0.55
1:AC:97:GLU:OE1	6:DB:48:GLY:HA2	2.06	0.54
1:AD:124:SER:OG	1:AD:127:ASP:OD1	2.24	0.54
1:CD:244:ASN:OD1	1:CD:245:LEU:N	2.39	0.54
1:BD:199:ASP:OD1	1:BD:200:LYS:N	2.40	0.54
4:BJ:20:GLN:NE2	6:EA:99:ASN:OD1	2.39	0.54
4:AL:51:PRO:HG3	5:AM:75:ASP:OD2	2.07	0.54
7:AH:185:ASN:OD1	7:AH:186:HIS:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:EI:346:SER:O	7:EI:346:SER:OG	2.25	0.54
1:AD:193:ASP:O	1:AD:201:ARG:NH1	2.39	0.54
1:CC:188:PHE:HB2	7:EH:14:ASP:HA	1.88	0.54
1:BC:37:ASP:OD2	1:BC:37:ASP:N	2.40	0.54
1:BC:97:GLU:OE1	6:EB:48:GLY:CA	2.55	0.54
1:BC:244:ASN:OD1	1:BC:245:LEU:N	2.39	0.54
5:AM:76:ASP:OD1	5:AM:78:VAL:HG23	2.07	0.54
6:DB:41:ASP:O	6:DB:52:THR:OG1	2.21	0.54
7:AG:595:THR:OG1	7:AG:598:ASN:OD1	2.23	0.54
1:CD:97:GLU:OE1	6:AB:48:GLY:HA2	2.08	0.54
4:BJ:74:ARG:HB3	4:BL:24:VAL:HG22	1.89	0.54
6:DB:12:ILE:C	6:DB:13:LEU:HD12	2.33	0.54
7:BH:164:MET:HE2	7:BH:387:GLU:OE1	2.07	0.54
7:FG:587:TRP:NE1	7:FG:603:LEU:HD21	2.22	0.54
7:CH:56:LYS:O	7:CI:52:GLY:N	2.41	0.54
1:CD:153:LYS:HE3	6:AB:43:GLU:CD	2.32	0.54
4:CJ:130:ASN:OD1	4:CJ:131:ILE:N	2.40	0.54
7:DH:493:ASP:N	7:DH:493:ASP:OD1	2.40	0.54
1:BD:244:ASN:OD1	1:BD:245:LEU:N	2.39	0.54
4:AJ:91:ARG:C	4:AJ:92:LEU:HD12	2.33	0.54
6:BB:12:ILE:O	6:BB:13:LEU:HD12	2.07	0.54
6:DB:160:ARG:NH2	6:DB:161:PHE:O	2.40	0.54
1:AC:199:ASP:OD1	1:AC:200:LYS:N	2.40	0.54
2:AE:268:LEU:O	2:AE:270:GLN:NE2	2.41	0.54
1:CC:37:ASP:N	1:CC:37:ASP:OD2	2.40	0.54
1:CD:188:PHE:HB2	7:CH:14:ASP:CA	2.38	0.54
2:CE:142:ASP:OD2	2:BE:362:LYS:NZ	2.40	0.54
4:BJ:24:VAL:O	4:BJ:125:ARG:NH1	2.41	0.54
5:BM:40:ASN:OD1	5:BM:41:ASP:N	2.41	0.54
5:FM:40:ASN:OD1	5:FM:41:ASP:N	2.41	0.54
7:DI:346:SER:O	7:DI:346:SER:OG	2.26	0.54
7:EG:610:SER:OG	7:EG:611:ALA:N	2.41	0.54
1:BD:37:ASP:N	1:BD:37:ASP:OD2	2.40	0.54
4:DJ:5:ASN:ND2	7:DG:80:MET:O	2.26	0.54
4:AJ:43:PHE:HE2	4:AJ:63:ILE:HD12	1.72	0.54
4:CK:88:ILE:O	7:CG:76:ARG:NH1	2.41	0.54
5:DM:41:ASP:OD2	5:DM:43:GLN:NE2	2.40	0.54
7:BH:49:ALA:N	7:BG:54:GLN:O	2.40	0.54
1:AD:244:ASN:OD1	1:AD:245:LEU:N	2.39	0.54
2:CE:259:GLU:N	2:CE:259:GLU:OE1	2.41	0.54
4:DJ:155:ILE:CD1	4:DL:165:LEU:HD13	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:FK:146:VAL:O	4:FK:146:VAL:HG23	2.06	0.54
1:AD:153:LYS:HG3	6:BB:52:THR:HG21	1.89	0.54
1:CC:244:ASN:OD1	1:CC:245:LEU:N	2.39	0.54
1:BC:199:ASP:OD1	1:BC:200:LYS:N	2.40	0.54
4:DL:50:ARG:CA	5:DM:81:PHE:CE2	2.91	0.54
4:EJ:72:VAL:O	4:EL:22:ASN:ND2	2.40	0.54
7:DH:185:ASN:OD1	7:DH:186:HIS:N	2.41	0.54
7:DH:411:GLY:O	7:DH:414:ARG:NH1	2.41	0.54
1:CC:193:ASP:O	1:CC:201:ARG:NH1	2.39	0.54
1:CD:193:ASP:O	1:CD:201:ARG:NH1	2.39	0.54
2:BE:268:LEU:O	2:BE:270:GLN:NE2	2.41	0.54
4:DJ:74:ARG:HB3	4:DL:24:VAL:HG22	1.90	0.54
5:EM:41:ASP:OD2	5:EM:43:GLN:NE2	2.41	0.54
7:CI:183:PRO:O	7:CI:186:HIS:NE2	2.41	0.54
7:EH:185:ASN:OD1	7:EH:186:HIS:N	2.41	0.54
1:AD:67:ARG:NH1	6:EB:46:MET:O	2.40	0.53
1:CD:67:ARG:HB3	6:DB:47:ASP:OD2	2.08	0.53
1:CD:111:VAL:CG2	6:FB:17:ALA:HB1	2.37	0.53
1:BC:149:GLN:OE1	6:EB:41:ASP:HB3	2.08	0.53
4:AJ:154:THR:O	4:AJ:158:VAL:HG22	2.08	0.53
4:CK:146:VAL:O	4:CK:146:VAL:HG23	2.07	0.53
7:BG:595:THR:OG1	7:BG:598:ASN:OD1	2.23	0.53
7:BI:264:ARG:NH1	7:BI:287:GLU:OE1	2.41	0.53
7:AI:264:ARG:NH1	7:AI:287:GLU:OE1	2.41	0.53
7:CH:155:ASP:OD2	7:CH:415:HIS:NE2	2.38	0.53
1:CD:37:ASP:OD2	1:CD:37:ASP:N	2.40	0.53
2:CE:268:LEU:O	2:CE:270:GLN:NE2	2.41	0.53
4:EL:174:THR:CG2	7:EH:90:ASN:HD21	2.21	0.53
5:AM:41:ASP:OD2	5:AM:43:GLN:NE2	2.41	0.53
6:AB:148:GLU:O	6:AB:151:THR:OG1	2.21	0.53
7:DI:185:ASN:O	7:DI:208:GLY:N	2.42	0.53
7:CH:233:GLU:N	7:CH:233:GLU:OE2	2.41	0.53
7:CI:329:MET:SD	7:CI:331:GLY:N	2.82	0.53
7:CI:540:ASN:OD1	7:CI:541:ALA:N	2.41	0.53
1:CC:97:GLU:OE1	6:FB:48:GLY:HA2	2.09	0.53
1:CC:128:GLN:C	7:EG:16:ARG:HH22	2.07	0.53
4:CL:174:THR:CG2	7:CH:90:ASN:HD21	2.21	0.53
7:BI:293:SER:OG	7:BI:318:ILE:O	2.27	0.53
1:AC:125:ARG:HA	7:AI:290:LEU:HD11	1.90	0.53
2:AE:259:GLU:OE1	2:AE:259:GLU:N	2.41	0.53
1:CD:184:GLY:HA2	7:CG:13:PHE:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:102:PHE:CZ	6:BB:142:GLY:O	2.62	0.53
1:BD:192:ILE:N	7:BH:12:VAL:O	2.42	0.53
2:BE:259:GLU:OE1	2:BE:259:GLU:N	2.41	0.53
4:BK:146:VAL:HG23	4:BK:146:VAL:O	2.07	0.53
4:DK:88:ILE:O	7:DG:76:ARG:NH1	2.41	0.53
4:AJ:74:ARG:HB3	4:AL:24:VAL:HG22	1.90	0.53
7:DG:394:ASP:N	7:DG:399:ARG:O	2.41	0.53
7:AI:329:MET:SD	7:AI:331:GLY:N	2.82	0.53
7:FH:233:GLU:N	7:FH:233:GLU:OE2	2.41	0.53
7:FI:329:MET:SD	7:FI:331:GLY:N	2.82	0.53
7:CG:587:TRP:NE1	7:CG:603:LEU:HD21	2.23	0.53
7:CG:595:THR:OG1	7:CG:598:ASN:OD1	2.24	0.53
7:EH:56:LYS:O	7:EI:52:GLY:N	2.42	0.53
4:DJ:8:LYS:NZ	4:DJ:35:ASP:OD2	2.41	0.53
4:DL:174:THR:CG2	7:DH:90:ASN:HD21	2.21	0.53
5:FM:76:ASP:OD1	5:FM:78:VAL:HG23	2.07	0.53
5:EM:76:ASP:OD1	5:EM:78:VAL:HG23	2.09	0.53
4:EL:130:ASN:O	4:EL:137:SER:OG	2.24	0.53
6:BB:41:ASP:O	6:BB:52:THR:OG1	2.22	0.53
7:DI:329:MET:SD	7:DI:331:GLY:N	2.82	0.53
7:CI:185:ASN:O	7:CI:208:GLY:N	2.41	0.53
1:AC:37:ASP:OD2	1:AC:37:ASP:N	2.40	0.53
1:CC:20:ILE:CD1	6:FB:50:TYR:CD2	2.91	0.53
1:CD:67:ARG:NH1	6:DB:46:MET:O	2.42	0.53
6:CB:160:ARG:NH2	6:CB:161:PHE:O	2.41	0.53
7:BH:598:ASN:OD1	7:BH:621:THR:N	2.41	0.53
7:BI:183:PRO:O	7:BI:186:HIS:NE2	2.41	0.53
1:BC:125:ARG:HD3	7:BI:286:SER:HB3	1.90	0.53
4:EJ:154:THR:O	4:EJ:158:VAL:HG22	2.08	0.53
7:DG:610:SER:OG	7:DG:611:ALA:N	2.42	0.53
7:EH:598:ASN:OD1	7:EH:621:THR:N	2.42	0.53
1:AC:244:ASN:OD1	1:AC:245:LEU:N	2.39	0.53
1:BD:100:TYR:OH	6:EB:110:PHE:CA	2.39	0.53
4:AK:15:LEU:HD13	4:AK:124:GLU:OE1	2.09	0.53
7:BI:329:MET:SD	7:BI:331:GLY:N	2.82	0.53
1:BD:107:SER:CA	6:EB:22:ASP:N	2.73	0.52
4:DK:169:MET:O	4:DK:172:THR:OG1	2.24	0.52
4:DL:54:ILE:HD13	4:DL:92:LEU:HD11	1.90	0.52
4:CL:50:ARG:HA	5:CM:81:PHE:HE2	1.63	0.52
4:EJ:164:GLN:O	4:EJ:168:ASN:ND2	2.43	0.52
4:EK:52:LEU:HD12	7:EG:79:ASN:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EK:115:GLN:NE2	7:EG:82:LEU:O	2.41	0.52
6:CB:12:ILE:O	6:CB:13:LEU:HD12	2.09	0.52
7:DI:264:ARG:NH1	7:DI:287:GLU:OE1	2.40	0.52
7:FI:293:SER:OG	7:FI:318:ILE:O	2.27	0.52
7:CH:49:ALA:N	7:CG:54:GLN:O	2.41	0.52
1:CD:192:ILE:O	7:CH:12:VAL:C	2.52	0.52
4:BK:63:ILE:HD11	4:BK:94:TYR:CE2	2.45	0.52
4:FK:63:ILE:HD11	4:FK:94:TYR:CE2	2.44	0.52
5:BM:48:LEU:HD12	5:BM:74:ILE:HD11	1.92	0.52
6:BA:141:ARG:NH2	6:DA:74:ASP:OD1	2.42	0.52
6:DA:79:ALA:O	6:DA:83:ARG:N	2.41	0.52
7:BH:233:GLU:N	7:BH:233:GLU:OE2	2.41	0.52
1:AD:192:ILE:O	7:AH:12:VAL:O	2.26	0.52
1:AD:223:GLN:NE2	1:BC:42:ASN:OD1	2.41	0.52
1:CC:153:LYS:HG3	6:FB:52:THR:HB	1.90	0.52
1:BD:63:LYS:CE	6:CB:52:THR:O	2.57	0.52
1:BD:207:ASN:CB	7:BH:455:ALA:CB	2.85	0.52
4:BL:49:ASN:O	5:BM:81:PHE:CE2	2.62	0.52
4:FK:179:VAL:HG22	4:FL:187:ILE:HG13	1.91	0.52
5:AM:40:ASN:OD1	5:AM:41:ASP:N	2.43	0.52
5:AM:48:LEU:HD12	5:AM:74:ILE:HD11	1.91	0.52
6:BB:12:ILE:C	6:BB:13:LEU:HD12	2.35	0.52
7:DH:56:LYS:O	7:DI:52:GLY:N	2.42	0.52
7:CG:394:ASP:N	7:CG:399:ARG:O	2.41	0.52
1:AC:100:TYR:CE2	6:AB:109:TYR:HE2	2.07	0.52
4:CK:169:MET:O	4:CK:172:THR:OG1	2.24	0.52
6:EA:79:ALA:O	6:EA:83:ARG:N	2.40	0.52
1:CC:105:PRO:HA	6:CB:15:ARG:HH22	1.74	0.52
4:EK:88:ILE:O	7:EG:76:ARG:NH1	2.42	0.52
5:EM:48:LEU:HD12	5:EM:74:ILE:HD11	1.92	0.52
6:DA:141:ARG:NH2	6:AA:74:ASP:OD1	2.42	0.52
7:AG:394:ASP:N	7:AG:399:ARG:O	2.43	0.52
7:FH:56:LYS:O	7:FI:52:GLY:N	2.42	0.52
7:CH:598:ASN:OD1	7:CH:621:THR:N	2.43	0.52
7:EI:540:ASN:OD1	7:EI:541:ALA:N	2.43	0.52
1:BD:107:SER:HB2	6:EB:21:VAL:HA	1.92	0.52
4:CL:54:ILE:HD13	4:CL:92:LEU:HD11	1.90	0.52
4:EJ:74:ARG:HB3	4:EL:24:VAL:HG22	1.92	0.52
4:EL:51:PRO:HD2	5:EM:81:PHE:CD2	2.44	0.52
5:FM:48:LEU:HD12	5:FM:74:ILE:HD11	1.92	0.52
6:EA:74:ASP:OD1	6:CA:141:ARG:NH2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FH:411:GLY:O	7:FH:414:ARG:NH1	2.43	0.52
7:FI:540:ASN:OD1	7:FI:541:ALA:N	2.43	0.52
7:CH:411:GLY:O	7:CH:414:ARG:NH1	2.43	0.52
1:CD:180:ASN:O	7:CI:12:VAL:HG23	2.09	0.52
1:BC:97:GLU:OE1	6:EB:47:ASP:C	2.53	0.52
4:AJ:20:GLN:NE2	6:DA:98:LYS:O	2.43	0.52
4:EK:15:LEU:HD13	4:EK:124:GLU:OE1	2.10	0.52
4:EK:179:VAL:HG22	4:EL:187:ILE:HG13	1.92	0.52
5:CM:40:ASN:OD1	5:CM:41:ASP:N	2.43	0.52
5:EM:40:ASN:OD1	5:EM:41:ASP:N	2.43	0.52
7:BI:540:ASN:OD1	7:BI:541:ALA:N	2.43	0.52
7:DH:233:GLU:N	7:DH:233:GLU:OE2	2.43	0.52
7:AH:56:LYS:O	7:AI:52:GLY:N	2.42	0.52
7:EI:329:MET:SD	7:EI:331:GLY:N	2.82	0.52
1:CD:100:TYR:CZ	6:FB:111:GLN:HG2	2.45	0.52
1:BD:301:THR:CG2	7:BH:475:ASN:OD1	2.58	0.52
4:DJ:130:ASN:OD1	4:DJ:131:ILE:N	2.42	0.52
4:EK:148:ILE:HG23	4:EL:151:ILE:HD11	1.92	0.52
4:EL:88:ILE:HD12	5:EM:85:LYS:HE2	1.91	0.52
6:BB:105:PHE:N	6:BB:144:ALA:O	2.38	0.52
6:AB:72:PHE:CE2	6:AB:76:ILE:HD11	2.44	0.52
6:FA:138:ARG:HD2	6:CA:81:VAL:HG11	1.92	0.52
7:BH:342:TYR:CE2	7:BH:386:ALA:HB1	2.45	0.52
6:AA:79:ALA:O	6:AA:83:ARG:N	2.40	0.52
7:BH:56:LYS:O	7:BI:52:GLY:N	2.42	0.52
1:BC:97:GLU:OE1	6:EB:48:GLY:HA2	2.09	0.52
4:DJ:20:GLN:NE2	6:BA:99:ASN:OD1	2.43	0.52
4:FL:174:THR:CG2	7:FH:90:ASN:HD21	2.23	0.52
5:DM:40:ASN:OD1	5:DM:41:ASP:N	2.43	0.52
6:AB:12:ILE:C	6:AB:13:LEU:HD12	2.35	0.52
6:FB:148:GLU:O	6:FB:151:THR:OG1	2.20	0.52
7:DI:183:PRO:O	7:DI:186:HIS:NE2	2.42	0.52
4:EL:54:ILE:HD13	4:EL:92:LEU:HD11	1.92	0.51
7:DH:161:ASN:ND2	7:DH:412:ASN:O	2.44	0.51
7:AI:540:ASN:OD1	7:AI:541:ALA:N	2.43	0.51
7:FH:598:ASN:OD1	7:FH:621:THR:N	2.42	0.51
7:EI:264:ARG:NH1	7:EI:287:GLU:OE1	2.43	0.51
4:BJ:154:THR:O	4:BJ:158:VAL:HG22	2.09	0.51
4:AK:146:VAL:HG23	4:AK:146:VAL:O	2.10	0.51
4:FJ:154:THR:O	4:FJ:158:VAL:HG22	2.09	0.51
4:EJ:43:PHE:CE2	4:EJ:63:ILE:HD12	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FB:12:ILE:C	6:FB:13:LEU:HD12	2.35	0.51
7:BH:372:ILE:HG22	7:BH:406:VAL:HG11	1.92	0.51
7:AI:166:SER:OG	7:AI:167:PHE:N	2.43	0.51
7:CH:493:ASP:OD1	7:CH:493:ASP:N	2.40	0.51
1:BD:301:THR:HG21	7:BH:475:ASN:CA	2.39	0.51
4:BK:5:ASN:OD1	4:BK:6:PHE:N	2.43	0.51
6:BA:79:ALA:O	6:BA:83:ARG:N	2.41	0.51
7:DH:598:ASN:OD1	7:DH:621:THR:N	2.43	0.51
7:AI:303:ASP:OD1	7:AI:304:ASP:N	2.43	0.51
7:FI:346:SER:O	7:FI:346:SER:OG	2.25	0.51
7:EI:441:ASP:OD1	7:EI:442:SER:N	2.43	0.51
4:BK:179:VAL:HG22	4:BL:187:ILE:HG13	1.91	0.51
4:DK:179:VAL:HG22	4:DL:187:ILE:HG13	1.92	0.51
4:DL:88:ILE:CD1	5:DM:85:LYS:NZ	2.74	0.51
4:AJ:8:LYS:NZ	4:AJ:35:ASP:OD2	2.44	0.51
4:AJ:164:GLN:O	4:AJ:168:ASN:ND2	2.42	0.51
7:FG:394:ASP:N	7:FG:399:ARG:O	2.44	0.51
7:FI:170:ASP:OD1	7:FI:175:ILE:N	2.42	0.51
7:EI:170:ASP:OD1	7:EI:175:ILE:N	2.40	0.51
1:AC:42:ASN:OD1	1:CD:223:GLN:NE2	2.43	0.51
4:DK:5:ASN:OD1	4:DK:6:PHE:N	2.44	0.51
6:FA:141:ARG:NH2	6:CA:74:ASP:OD1	2.44	0.51
7:AH:200:ASP:N	7:AH:200:ASP:OD1	2.43	0.51
7:AI:346:SER:O	7:AI:346:SER:OG	2.27	0.51
7:EI:166:SER:OG	7:EI:167:PHE:N	2.43	0.51
4:DL:49:ASN:O	5:DM:81:PHE:CE2	2.64	0.51
4:FK:88:ILE:O	7:FG:76:ARG:NH1	2.44	0.51
7:BH:411:GLY:O	7:BH:414:ARG:NH1	2.44	0.51
7:FH:342:TYR:CE2	7:FH:386:ALA:HB1	2.45	0.51
7:EH:493:ASP:OD1	7:EH:493:ASP:N	2.41	0.51
7:EG:394:ASP:N	7:EG:399:ARG:O	2.42	0.51
1:AC:20:ILE:HD11	6:DB:50:TYR:CD2	2.39	0.51
1:AC:97:GLU:OE1	6:DB:47:ASP:C	2.54	0.51
1:AD:97:GLU:OE1	6:BB:48:GLY:HA2	2.10	0.51
4:DJ:154:THR:O	4:DJ:158:VAL:HG22	2.11	0.51
4:AK:5:ASN:OD1	4:AK:6:PHE:N	2.44	0.51
6:EA:81:VAL:HG11	6:CA:138:ARG:HD2	1.93	0.51
7:AI:441:ASP:OD1	7:AI:442:SER:N	2.43	0.51
7:FH:440:THR:OG1	7:FH:445:ARG:O	2.23	0.51
7:CI:41:TYR:O	7:CI:46:GLU:N	2.43	0.51
4:FK:148:ILE:HG23	4:FL:151:ILE:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CM:76:ASP:OD1	5:CM:78:VAL:HG23	2.11	0.51
6:EB:72:PHE:CE2	6:EB:76:ILE:HD11	2.45	0.51
6:DB:163:ASP:O	6:DA:15:ARG:NH1	2.44	0.51
7:BG:610:SER:OG	7:BG:611:ALA:N	2.44	0.51
7:DI:346:SER:N	7:DI:385:GLU:OE1	2.44	0.51
7:AG:610:SER:OG	7:AG:611:ALA:N	2.41	0.51
1:CC:97:GLU:OE1	6:FB:47:ASP:C	2.53	0.51
4:DL:50:ARG:HA	5:DM:81:PHE:HE2	1.74	0.51
7:DG:595:THR:OG1	7:DG:598:ASN:OD1	2.23	0.51
7:AH:370:ILE:HB	7:AH:372:ILE:HD11	1.93	0.51
7:FH:381:GLY:N	7:FG:450:PRO:O	2.44	0.51
1:AC:267:ASP:OD1	1:AC:268:SER:N	2.43	0.51
1:AD:100:TYR:OH	6:DB:110:PHE:CA	2.39	0.51
1:CD:20:ILE:HD12	6:AB:50:TYR:CZ	2.46	0.51
4:AL:50:ARG:NH1	5:AM:6:ASP:OD2	2.44	0.51
6:EA:138:ARG:HD2	6:BA:81:VAL:HG11	1.93	0.51
6:BA:138:ARG:HD2	6:DA:81:VAL:HG11	1.93	0.51
7:DG:179:THR:HG21	7:DG:210:GLY:O	2.11	0.51
7:FH:372:ILE:HG22	7:FH:406:VAL:HG11	1.92	0.51
7:FG:610:SER:OG	7:FG:611:ALA:N	2.43	0.51
7:EG:51:ASN:ND2	7:EG:53:GLU:OE1	2.44	0.51
1:AD:180:ASN:O	7:AI:12:VAL:HG23	2.11	0.50
4:FJ:130:ASN:OD1	4:FJ:131:ILE:N	2.44	0.50
4:CJ:20:GLN:NE2	6:FA:99:ASN:OD1	2.43	0.50
6:EB:148:GLU:O	6:EB:151:THR:OG1	2.20	0.50
7:DH:188:MET:HE1	7:DH:201:ARG:CZ	2.41	0.50
7:DH:328:PRO:O	7:DH:343:THR:OG1	2.14	0.50
7:CI:263:ASP:O	7:CI:284:LYS:NZ	2.44	0.50
7:EH:411:GLY:O	7:EH:414:ARG:NH1	2.44	0.50
2:AE:335:GLU:OE1	3:CF:1142:ASN:HB3	2.12	0.50
1:BD:105:PRO:CA	6:EB:15:ARG:NH2	2.45	0.50
4:DK:52:LEU:HD12	7:DG:79:ASN:O	2.11	0.50
4:AK:179:VAL:HG22	4:AL:187:ILE:HG13	1.94	0.50
4:FK:5:ASN:OD1	4:FK:6:PHE:N	2.44	0.50
4:CK:179:VAL:HG22	4:CL:187:ILE:HG13	1.92	0.50
6:DA:138:ARG:HD2	6:AA:81:VAL:HG11	1.93	0.50
7:AH:381:GLY:N	7:AG:450:PRO:O	2.44	0.50
7:CI:166:SER:OG	7:CI:167:PHE:N	2.44	0.50
7:CI:170:ASP:OD1	7:CI:175:ILE:N	2.41	0.50
1:AC:102:PHE:HZ	6:AB:142:GLY:O	1.91	0.50
4:BK:50:ARG:HB2	4:BK:51:PRO:HD2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:40:VAL:HG23	4:BL:40:VAL:O	2.11	0.50
4:CK:58:HIS:NE2	7:CH:80:MET:O	2.27	0.50
4:CL:40:VAL:HG23	4:CL:40:VAL:O	2.12	0.50
5:AN:120:VAL:HG12	5:AN:121:ASP:H	1.77	0.50
6:AA:138:ARG:HD2	6:FA:81:VAL:HG11	1.93	0.50
6:FB:138:ARG:HG3	6:CB:81:VAL:HG11	1.93	0.50
7:BG:14:ASP:OD2	7:BG:15:TYR:N	2.43	0.50
7:BI:346:SER:N	7:BI:385:GLU:OE1	2.45	0.50
7:DI:41:TYR:O	7:DI:46:GLU:N	2.44	0.50
7:AH:188:MET:HE1	7:AH:201:ARG:CZ	2.41	0.50
7:FH:225:TYR:CE2	7:FH:277:MET:HE1	2.46	0.50
1:CD:125:ARG:CA	7:FI:290:LEU:HD11	2.41	0.50
1:CD:188:PHE:HE2	7:CG:11:ARG:CB	2.19	0.50
1:BC:100:TYR:CE2	6:BB:109:TYR:HE2	2.00	0.50
4:AL:68:ASP:O	4:AL:70:TYR:N	2.43	0.50
4:FL:40:VAL:HG23	4:FL:40:VAL:O	2.11	0.50
6:EB:109:TYR:OH	6:EB:111:GLN:NE2	2.35	0.50
7:EH:445:ARG:NH2	7:EI:414:ARG:O	2.44	0.50
4:BL:58:HIS:HE1	5:BN:43:GLN:CG	1.98	0.50
4:BL:58:HIS:HA	5:BN:43:GLN:NE2	2.26	0.50
4:CK:145:LEU:HD23	4:CK:145:LEU:H	1.76	0.50
7:DH:49:ALA:N	7:DG:54:GLN:O	2.44	0.50
7:DH:200:ASP:N	7:DH:200:ASP:OD1	2.43	0.50
7:AH:161:ASN:ND2	7:AH:412:ASN:O	2.45	0.50
7:AI:346:SER:N	7:AI:385:GLU:OE1	2.45	0.50
7:EH:188:MET:HE1	7:EH:201:ARG:CZ	2.41	0.50
1:BD:272:TYR:CD1	1:BD:278:ILE:HG22	2.47	0.50
4:DK:148:ILE:HG23	4:DL:151:ILE:HD11	1.94	0.50
4:FJ:43:PHE:CE2	4:FJ:63:ILE:HD12	2.46	0.50
4:CJ:154:THR:O	4:CJ:158:VAL:HG22	2.11	0.50
4:EL:50:ARG:HB2	5:EM:81:PHE:HE2	1.77	0.50
6:BB:79:ALA:O	6:BB:83:ARG:N	2.43	0.50
6:DB:12:ILE:O	6:DB:13:LEU:HD12	2.11	0.50
6:CB:79:ALA:O	6:CB:83:ARG:N	2.45	0.50
6:CA:79:ALA:O	6:CA:83:ARG:N	2.44	0.50
7:DI:166:SER:OG	7:DI:167:PHE:N	2.44	0.50
2:AE:281:GLU:OE1	2:AE:281:GLU:N	2.45	0.50
1:CC:272:TYR:CD1	1:CC:278:ILE:HG22	2.47	0.50
1:CD:20:ILE:CD1	6:AB:50:TYR:CZ	2.95	0.50
1:CD:193:ASP:HA	7:CH:12:VAL:HA	1.94	0.50
2:CE:281:GLU:OE1	2:CE:281:GLU:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BJ:43:PHE:CE2	4:BJ:63:ILE:HD12	2.47	0.50
4:DL:50:ARG:HG3	5:DM:81:PHE:CD2	2.46	0.50
7:BG:394:ASP:N	7:BG:399:ARG:O	2.43	0.50
7:DH:164:MET:HE3	7:DH:178:MET:HE3	1.93	0.50
7:DI:303:ASP:OD1	7:DI:304:ASP:N	2.44	0.50
7:CG:179:THR:HG21	7:CG:210:GLY:O	2.11	0.50
7:EI:346:SER:N	7:EI:385:GLU:OE1	2.44	0.50
1:AC:66:ASN:ND2	7:AG:8:ASP:OD1	2.45	0.50
3:CF:1152:TYR:OH	2:CE:347:ASN:ND2	2.42	0.50
1:CD:107:SER:CA	6:FB:21:VAL:C	2.73	0.50
1:CD:301:THR:OG1	7:CH:477:LEU:HD11	2.12	0.50
4:AK:50:ARG:HB2	4:AK:51:PRO:HD2	1.93	0.50
5:AN:33:ALA:HB3	5:AN:86:ILE:HD11	1.94	0.50
6:DB:12:ILE:HD11	6:DB:32:TYR:CE2	2.46	0.50
7:BI:303:ASP:OD1	7:BI:304:ASP:N	2.45	0.50
7:AH:411:GLY:O	7:AH:414:ARG:NH1	2.45	0.50
7:AI:326:THR:OG1	7:AI:345:ASP:OD2	2.18	0.50
7:FG:255:ASP:OD1	7:FG:256:VAL:N	2.45	0.50
7:CH:188:MET:HE1	7:CH:201:ARG:CZ	2.41	0.50
7:CI:346:SER:N	7:CI:385:GLU:OE1	2.44	0.50
1:AC:105:PRO:HA	6:AB:15:ARG:HH22	1.77	0.50
1:CD:267:ASP:OD1	1:CD:268:SER:N	2.43	0.50
2:CE:203:ASP:O	2:CE:267:SER:OG	2.29	0.50
3:AF:1135:ASP:OD1	3:AF:1135:ASP:N	2.45	0.50
4:DJ:32:TYR:OH	4:DK:22:ASN:O	2.29	0.50
4:AL:54:ILE:HD13	4:AL:92:LEU:HD11	1.93	0.50
4:FL:57:GLU:C	5:FN:43:GLN:HE22	2.20	0.50
7:BI:166:SER:OG	7:BI:167:PHE:N	2.45	0.50
7:DH:283:TYR:OH	7:DH:291:LYS:NZ	2.45	0.50
7:EH:161:ASN:ND2	7:EH:412:ASN:O	2.44	0.50
1:BC:272:TYR:CD1	1:BC:278:ILE:HG22	2.47	0.49
4:AK:148:ILE:HG23	4:AL:151:ILE:HD11	1.93	0.49
7:BH:381:GLY:N	7:BG:450:PRO:O	2.45	0.49
7:DI:170:ASP:OD1	7:DI:175:ILE:N	2.40	0.49
7:FH:200:ASP:N	7:FH:200:ASP:OD1	2.44	0.49
7:FH:445:ARG:NH2	7:FI:414:ARG:O	2.44	0.49
7:FI:303:ASP:OD1	7:FI:304:ASP:N	2.45	0.49
7:CI:303:ASP:OD1	7:CI:304:ASP:N	2.45	0.49
7:EI:303:ASP:OD1	7:EI:304:ASP:N	2.45	0.49
1:AC:47:MET:O	2:CE:78:ASP:N	2.45	0.49
1:BC:123:TYR:N	1:BC:127:ASP:OD2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BE:203:ASP:O	2:BE:267:SER:OG	2.29	0.49
4:AK:34:SER:N	4:AK:134:ASP:OD2	2.38	0.49
4:AL:174:THR:CG2	7:AH:90:ASN:HD21	2.25	0.49
4:FL:54:ILE:HD13	4:FL:92:LEU:HD11	1.94	0.49
4:CL:50:ARG:HD3	5:CM:81:PHE:CZ	2.47	0.49
4:EK:114:THR:HG22	4:EK:121:VAL:HG12	1.95	0.49
7:DH:381:GLY:N	7:DG:450:PRO:O	2.45	0.49
7:AH:342:TYR:CE2	7:AH:386:ALA:HB1	2.47	0.49
7:CH:200:ASP:OD1	7:CH:200:ASP:N	2.43	0.49
7:EH:381:GLY:N	7:EG:450:PRO:O	2.44	0.49
1:AD:299:ASN:N	1:AD:299:ASN:OD1	2.45	0.49
1:CD:123:TYR:N	1:CD:127:ASP:OD2	2.45	0.49
1:CD:192:ILE:N	7:CH:12:VAL:O	2.45	0.49
1:CD:272:TYR:CD1	1:CD:278:ILE:HG22	2.47	0.49
1:BD:107:SER:HB3	6:EB:22:ASP:N	2.26	0.49
4:DL:88:ILE:HD12	5:DM:85:LYS:HE2	1.94	0.49
4:CL:88:ILE:HD12	5:CM:85:LYS:CE	2.41	0.49
4:EL:50:ARG:NH1	5:EM:6:ASP:OD2	2.44	0.49
4:EL:68:ASP:O	4:EL:70:TYR:N	2.43	0.49
6:EB:51:ASN:OD1	6:EB:52:THR:N	2.46	0.49
7:BH:200:ASP:OD1	7:BH:200:ASP:N	2.43	0.49
1:AC:20:ILE:CD1	6:DB:50:TYR:CD2	2.94	0.49
1:AC:123:TYR:N	1:AC:127:ASP:OD2	2.45	0.49
1:AC:272:TYR:CD1	1:AC:278:ILE:HG22	2.47	0.49
1:BD:123:TYR:N	1:BD:127:ASP:OD2	2.45	0.49
1:BD:301:THR:HG21	7:BH:475:ASN:OD1	2.12	0.49
4:EK:146:VAL:HG23	4:EK:146:VAL:O	2.10	0.49
5:EN:120:VAL:HG12	5:EN:121:ASP:H	1.77	0.49
7:BG:179:THR:HG21	7:BG:210:GLY:O	2.12	0.49
7:DH:470:THR:OG1	7:DH:487:ASP:O	2.22	0.49
7:AI:41:TYR:O	7:AI:46:GLU:N	2.45	0.49
7:EH:225:TYR:CE2	7:EH:277:MET:HE1	2.48	0.49
1:AD:123:TYR:N	1:AD:127:ASP:OD2	2.45	0.49
4:BJ:82:LEU:O	4:BJ:83:THR:OG1	2.29	0.49
4:AL:88:ILE:HD13	5:AM:85:LYS:NZ	2.27	0.49
7:BI:170:ASP:OD1	7:BI:175:ILE:N	2.42	0.49
7:DH:225:TYR:CE2	7:DH:277:MET:HE1	2.47	0.49
7:DG:157:SER:OG	7:DG:157:SER:O	2.30	0.49
7:FG:51:ASN:ND2	7:FG:53:GLU:OE1	2.45	0.49
7:FI:346:SER:N	7:FI:385:GLU:OE1	2.45	0.49
7:EH:200:ASP:OD1	7:EH:200:ASP:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:EI:293:SER:OG	7:EI:318:ILE:O	2.30	0.49
7:EI:468:ILE:HD11	7:EI:472:ASP:HB3	1.94	0.49
1:BC:125:ARG:HA	7:BI:290:LEU:HD11	1.93	0.49
4:DJ:82:LEU:O	4:DJ:83:THR:OG1	2.30	0.49
4:DL:40:VAL:HG23	4:DL:40:VAL:O	2.12	0.49
6:BA:31:GLU:HG2	6:BA:63:THR:HG22	1.95	0.49
7:BH:161:ASN:ND2	7:BH:412:ASN:O	2.44	0.49
7:AH:111:LEU:HD21	7:AG:111:LEU:HD21	1.94	0.49
7:AH:225:TYR:CE2	7:AH:277:MET:HE1	2.47	0.49
7:FI:166:SER:OG	7:FI:167:PHE:N	2.45	0.49
7:CH:394:ASP:OD2	7:CH:397:THR:OG1	2.15	0.49
7:CG:157:SER:O	7:CG:157:SER:OG	2.30	0.49
7:EH:342:TYR:CE2	7:EH:386:ALA:HB1	2.48	0.49
1:AC:153:LYS:HG3	6:DB:52:THR:HB	1.94	0.49
1:BD:201:ARG:NH2	7:BI:13:PHE:HD2	2.10	0.49
4:AK:145:LEU:HD23	4:AK:145:LEU:H	1.78	0.49
4:FK:34:SER:N	4:FK:134:ASP:OD2	2.38	0.49
4:CK:50:ARG:HB2	4:CK:51:PRO:HD2	1.95	0.49
6:EB:122:GLU:O	6:CB:7:SER:OG	2.26	0.49
6:FA:40:THR:HG22	6:FA:52:THR:O	2.13	0.49
7:DH:331:GLY:HA3	7:DH:388:GLY:HA2	1.95	0.49
4:FL:88:ILE:CD1	5:FM:85:LYS:CE	2.91	0.49
5:BM:76:ASP:OD1	5:BM:78:VAL:HG23	2.13	0.49
5:DN:120:VAL:HG12	5:DN:121:ASP:H	1.78	0.49
6:EB:12:ILE:C	6:EB:13:LEU:HD12	2.37	0.49
6:EA:31:GLU:HG2	6:EA:63:THR:HG22	1.94	0.49
6:DB:79:ALA:O	6:DB:83:ARG:N	2.44	0.49
7:BH:188:MET:HE1	7:BH:201:ARG:CZ	2.42	0.49
7:BG:255:ASP:OD1	7:BG:256:VAL:N	2.45	0.49
7:EI:41:TYR:O	7:EI:46:GLU:N	2.45	0.49
6:EB:64:ALA:HB3	6:EB:129:TYR:CZ	2.48	0.49
7:FG:595:THR:OG1	7:FG:598:ASN:OD1	2.24	0.49
7:EI:328:PRO:O	7:EI:343:THR:OG1	2.29	0.49
1:AC:153:LYS:HZ1	6:DB:43:GLU:CD	2.10	0.49
1:AD:272:TYR:CD1	1:AD:278:ILE:HG22	2.47	0.49
2:AE:142:ASP:OD2	2:CE:362:LYS:NZ	2.45	0.49
5:DM:38:GLY:HA3	5:DM:81:PHE:CE1	2.48	0.49
7:BH:331:GLY:HA3	7:BH:388:GLY:HA2	1.95	0.49
7:FH:188:MET:HE1	7:FH:201:ARG:CZ	2.43	0.49
7:FH:394:ASP:OD2	7:FH:397:THR:OG1	2.13	0.49
7:CI:178:MET:SD	7:CI:192:LEU:HD11	2.53	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:193:ASP:CG	7:AH:11:ARG:O	2.56	0.48
1:CC:123:TYR:N	1:CC:127:ASP:OD2	2.45	0.48
1:BC:299:ASN:N	1:BC:299:ASN:OD1	2.45	0.48
4:CK:5:ASN:OD1	4:CK:6:PHE:N	2.46	0.48
4:CL:178:LYS:HZ3	7:CH:93:LYS:HD3	1.68	0.48
5:CN:120:VAL:HG12	5:CN:121:ASP:N	2.28	0.48
6:EB:110:PHE:HB2	6:EB:135:VAL:HG13	1.95	0.48
6:BA:43:GLU:HB2	6:BA:50:TYR:OH	2.13	0.48
6:CB:12:ILE:HD11	6:CB:32:TYR:CE2	2.48	0.48
7:DG:88:GLY:N	7:DI:85:ASN:OD1	2.46	0.48
1:AD:267:ASP:OD1	1:AD:268:SER:N	2.43	0.48
2:AE:146:GLU:OE2	2:CE:358:SER:OG	2.27	0.48
1:BC:223:GLN:HA	1:BD:41:MET:CE	2.44	0.48
4:AJ:107:VAL:O	4:AJ:107:VAL:HG13	2.13	0.48
4:EK:145:LEU:HD23	4:EK:145:LEU:H	1.77	0.48
4:EL:25:ILE:HG23	4:EL:27:THR:H	1.78	0.48
4:EL:158:VAL:O	4:EL:158:VAL:HG12	2.13	0.48
5:EN:16:VAL:HG13	5:EN:16:VAL:O	2.13	0.48
6:FB:41:ASP:O	6:FB:52:THR:OG1	2.22	0.48
7:BH:225:TYR:CE2	7:BH:277:MET:HE1	2.48	0.48
7:BH:445:ARG:NH2	7:BI:414:ARG:O	2.46	0.48
7:CH:225:TYR:CE2	7:CH:277:MET:HE1	2.47	0.48
7:CH:381:GLY:N	7:CG:450:PRO:O	2.46	0.48
1:BD:299:ASN:OD1	1:BD:299:ASN:N	2.45	0.48
4:BL:158:VAL:O	4:BL:158:VAL:HG12	2.13	0.48
4:AJ:43:PHE:CE2	4:AJ:63:ILE:HD12	2.47	0.48
4:FL:158:VAL:O	4:FL:158:VAL:HG12	2.14	0.48
4:EJ:34:SER:HB3	4:EK:123:VAL:HG21	1.95	0.48
4:EK:5:ASN:OD1	4:EK:6:PHE:N	2.46	0.48
5:DN:33:ALA:HB3	5:DN:86:ILE:HD11	1.94	0.48
5:EN:120:VAL:HG12	5:EN:121:ASP:N	2.29	0.48
6:FA:79:ALA:O	6:FA:83:ARG:N	2.41	0.48
7:AH:445:ARG:NH2	7:AI:414:ARG:O	2.45	0.48
7:FG:440:THR:OG1	7:FG:445:ARG:O	2.31	0.48
7:CH:161:ASN:ND2	7:CH:412:ASN:O	2.45	0.48
5:CN:120:VAL:HG12	5:CN:121:ASP:H	1.78	0.48
6:DA:84:VAL:HG22	6:DA:85:LEU:N	2.28	0.48
7:DI:222:LEU:O	7:DI:241:GLN:NE2	2.46	0.48
7:AG:161:ASN:ND2	7:AG:412:ASN:O	2.43	0.48
1:CC:102:PHE:HZ	6:CB:142:GLY:O	1.96	0.48
1:CC:267:ASP:OD1	1:CC:268:SER:N	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BE:281:GLU:OE1	2:BE:281:GLU:N	2.45	0.48
4:BK:128:SER:OG	4:BK:129:PHE:N	2.46	0.48
4:AL:49:ASN:O	5:AM:81:PHE:CE2	2.67	0.48
5:BN:120:VAL:HG12	5:BN:121:ASP:N	2.28	0.48
5:FN:120:VAL:HG12	5:FN:121:ASP:N	2.28	0.48
6:EB:164:THR:HG23	6:EB:165:THR:HG22	1.96	0.48
6:BB:77:GLU:CD	6:BB:77:GLU:C	2.81	0.48
7:FH:161:ASN:ND2	7:FH:412:ASN:O	2.44	0.48
7:FH:171:PRO:O	7:FH:174:LYS:NZ	2.32	0.48
7:EH:331:GLY:HA3	7:EH:388:GLY:HA2	1.96	0.48
7:EH:440:THR:OG1	7:EH:445:ARG:O	2.26	0.48
7:EG:179:THR:HG21	7:EG:210:GLY:O	2.13	0.48
7:EI:222:LEU:O	7:EI:241:GLN:NE2	2.47	0.48
3:BF:1135:ASP:N	3:BF:1135:ASP:OD1	2.45	0.48
4:BL:25:ILE:HG23	4:BL:27:THR:H	1.78	0.48
4:AJ:21:TYR:O	4:AJ:22:ASN:ND2	2.47	0.48
4:AK:128:SER:OG	4:AK:129:PHE:N	2.46	0.48
4:CK:15:LEU:HD13	4:CK:124:GLU:OE1	2.14	0.48
4:EJ:21:TYR:O	4:EJ:22:ASN:ND2	2.46	0.48
6:EA:112:GLY:N	6:EA:133:TYR:OH	2.44	0.48
6:AA:84:VAL:HG22	6:AA:85:LEU:N	2.29	0.48
6:FA:84:VAL:HG22	6:FA:85:LEU:N	2.29	0.48
7:CG:263:ASP:OD1	7:CG:264:ARG:N	2.46	0.48
1:BD:192:ILE:O	7:BH:12:VAL:O	2.32	0.48
4:AL:25:ILE:HG23	4:AL:27:THR:H	1.78	0.48
4:FJ:17:THR:HG22	4:FJ:124:GLU:OE1	2.13	0.48
6:EB:138:ARG:HG3	6:BB:81:VAL:HG11	1.96	0.48
6:AB:64:ALA:HB3	6:AB:129:TYR:CZ	2.49	0.48
7:DH:342:TYR:CE2	7:DH:386:ALA:HB1	2.49	0.48
7:AG:179:THR:HG21	7:AG:210:GLY:O	2.12	0.48
7:CG:440:THR:OG1	7:CG:445:ARG:O	2.32	0.48
4:BJ:130:ASN:OD1	4:BJ:131:ILE:N	2.46	0.48
4:FJ:82:LEU:O	4:FJ:83:THR:OG1	2.29	0.48
4:EK:169:MET:C	4:EK:172:THR:HG1	2.20	0.48
4:EL:88:ILE:HD13	5:EM:85:LYS:HZ1	1.77	0.48
4:EL:128:SER:OG	4:EL:129:PHE:N	2.47	0.48
5:DN:16:VAL:HG13	5:DN:16:VAL:O	2.13	0.48
5:AN:16:VAL:O	5:AN:16:VAL:HG13	2.13	0.48
5:EN:33:ALA:HB3	5:EN:86:ILE:HD11	1.94	0.48
6:EA:84:VAL:HG22	6:EA:85:LEU:N	2.29	0.48
7:AH:598:ASN:OD1	7:AH:621:THR:N	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FI:41:TYR:O	7:FI:46:GLU:N	2.45	0.48
1:CC:105:PRO:HG3	6:CB:89:TRP:NE1	1.89	0.48
6:BB:51:ASN:OD1	6:BB:52:THR:N	2.47	0.48
6:BB:164:THR:O	6:BB:165:THR:HG22	2.13	0.48
7:DH:281:ARG:NH2	7:DH:298:GLU:OE2	2.46	0.48
7:FH:331:GLY:HA3	7:FH:388:GLY:HA2	1.95	0.48
7:FG:161:ASN:ND2	7:FG:412:ASN:O	2.45	0.48
7:EH:370:ILE:HB	7:EH:372:ILE:HD11	1.96	0.48
1:BD:267:ASP:OD1	1:BD:268:SER:N	2.43	0.48
4:EJ:91:ARG:C	4:EJ:92:LEU:HD12	2.39	0.48
5:FM:46:ILE:HD11	5:FM:51:HIS:HE1	1.79	0.48
5:CN:96:TYR:OH	5:CN:98:ARG:NH2	2.46	0.48
6:EB:77:GLU:CD	6:EB:77:GLU:C	2.82	0.48
6:DA:31:GLU:HG2	6:DA:63:THR:HG22	1.95	0.48
6:AB:12:ILE:O	6:AB:13:LEU:HD12	2.13	0.48
6:FB:51:ASN:OD1	6:FB:52:THR:N	2.47	0.48
6:FB:64:ALA:HB3	6:FB:129:TYR:CZ	2.49	0.48
6:CA:84:VAL:HG22	6:CA:85:LEU:N	2.28	0.48
7:FG:179:THR:HG21	7:FG:210:GLY:O	2.12	0.48
4:FK:128:SER:OG	4:FK:129:PHE:N	2.47	0.47
5:AN:120:VAL:HG12	5:AN:121:ASP:N	2.29	0.47
5:CN:33:ALA:HB3	5:CN:86:ILE:HD11	1.94	0.47
6:AA:31:GLU:HG2	6:AA:63:THR:HG22	1.94	0.47
6:FB:77:GLU:C	6:FB:77:GLU:CD	2.81	0.47
7:AI:170:ASP:OD1	7:AI:175:ILE:N	2.39	0.47
7:FH:288:ARG:HD2	7:FH:294:LEU:HD23	1.95	0.47
7:EI:263:ASP:O	7:EI:284:LYS:NZ	2.46	0.47
1:BD:107:SER:CB	6:EB:22:ASP:N	2.77	0.47
4:CJ:145:LEU:HA	4:CJ:148:ILE:HG22	1.96	0.47
4:EJ:145:LEU:HA	4:EJ:148:ILE:HG22	1.97	0.47
5:CN:16:VAL:O	5:CN:16:VAL:HG13	2.13	0.47
6:AA:32:TYR:OH	6:AA:60:MET:SD	2.69	0.47
6:FA:31:GLU:HG2	6:FA:63:THR:HG22	1.95	0.47
7:CH:283:TYR:OH	7:CH:291:LYS:NZ	2.46	0.47
3:CF:1135:ASP:N	3:CF:1135:ASP:OD1	2.45	0.47
3:CF:1151:GLU:OE1	2:CE:87:ARG:NE	2.48	0.47
4:BJ:43:PHE:HE2	4:BJ:63:ILE:HD12	1.80	0.47
4:DJ:155:ILE:HD11	4:DL:165:LEU:HD13	1.95	0.47
4:EK:9:ASP:OD1	4:EK:42:ASN:ND2	2.38	0.47
5:DM:76:ASP:OD1	5:DM:78:VAL:HG23	2.13	0.47
6:CA:31:GLU:HG2	6:CA:63:THR:HG22	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:41:TYR:O	7:BI:46:GLU:N	2.45	0.47
7:CI:441:ASP:OD1	7:CI:442:SER:N	2.47	0.47
4:FJ:43:PHE:HE2	4:FJ:63:ILE:HD12	1.80	0.47
4:CL:50:ARG:HG3	5:CM:81:PHE:CD2	2.47	0.47
5:DN:120:VAL:HG12	5:DN:121:ASP:N	2.28	0.47
6:BB:64:ALA:HB3	6:BB:129:TYR:CZ	2.49	0.47
6:AB:164:THR:HG23	6:AB:165:THR:HG22	1.96	0.47
6:CB:70:ASP:OD1	6:CB:72:PHE:N	2.48	0.47
7:BI:263:ASP:O	7:BI:284:LYS:NZ	2.47	0.47
7:DG:263:ASP:OD1	7:DG:264:ARG:N	2.46	0.47
7:DI:441:ASP:OD1	7:DI:442:SER:N	2.47	0.47
1:AD:67:ARG:HH11	6:EB:47:ASP:HA	1.74	0.47
1:CC:69:ASP:CG	7:CH:15:TYR:HE1	2.19	0.47
1:CD:299:ASN:N	1:CD:299:ASN:OD1	2.45	0.47
1:BC:153:LYS:HG3	6:EB:52:THR:HB	1.96	0.47
1:BC:267:ASP:OD1	1:BC:268:SER:N	2.43	0.47
4:BL:68:ASP:O	4:BL:70:TYR:N	2.43	0.47
4:DK:175:LEU:HD13	4:DL:183:ALA:HB3	1.96	0.47
4:AL:128:SER:OG	4:AL:129:PHE:N	2.47	0.47
4:EJ:107:VAL:HG13	4:EJ:107:VAL:O	2.14	0.47
5:AM:38:GLY:HA3	5:AM:81:PHE:CE1	2.48	0.47
6:BA:112:GLY:O	6:BA:133:TYR:OH	2.29	0.47
7:DI:293:SER:OG	7:DI:318:ILE:O	2.31	0.47
7:CH:328:PRO:O	7:CH:343:THR:OG1	2.19	0.47
7:CG:610:SER:OG	7:CG:611:ALA:N	2.45	0.47
1:AC:124:SER:C	7:AI:290:LEU:HD11	2.40	0.47
1:CD:183:VAL:HG12	7:CG:14:ASP:HA	1.95	0.47
4:FL:50:ARG:HB2	5:FM:81:PHE:HE2	1.78	0.47
5:BN:16:VAL:HG13	5:BN:16:VAL:O	2.15	0.47
6:BA:84:VAL:HG22	6:BA:85:LEU:N	2.29	0.47
6:DB:112:GLY:C	6:DB:133:TYR:HE1	2.22	0.47
6:CA:40:THR:HG22	6:CA:52:THR:O	2.15	0.47
7:BI:358:ASP:OD1	7:BI:360:LYS:N	2.47	0.47
7:AG:88:GLY:N	7:AI:85:ASN:OD1	2.47	0.47
7:AI:554:LEU:O	7:AI:601:GLN:NE2	2.43	0.47
7:FH:442:SER:O	7:FI:437:VAL:HG22	2.14	0.47
1:AC:299:ASN:N	1:AC:299:ASN:OD1	2.45	0.47
1:AD:125:ARG:CA	7:DI:290:LEU:HD11	2.45	0.47
1:BC:105:PRO:HA	6:BB:15:ARG:NH2	2.27	0.47
4:DK:50:ARG:HB2	4:DK:51:PRO:HD2	1.95	0.47
4:CK:175:LEU:HD13	4:CL:183:ALA:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EJ:82:LEU:O	4:EJ:83:THR:OG1	2.28	0.47
4:EK:71:ASN:N	4:EK:74:ARG:O	2.47	0.47
6:EB:105:PHE:N	6:EB:144:ALA:O	2.42	0.47
6:BB:14:PHE:HD2	6:BB:72:PHE:CZ	2.33	0.47
6:BB:164:THR:O	6:BB:167:GLU:OE1	2.32	0.47
6:AB:77:GLU:C	6:AB:77:GLU:CD	2.82	0.47
6:AB:138:ARG:HG3	6:FB:81:VAL:HG11	1.96	0.47
6:FB:164:THR:HG23	6:FB:165:THR:HG22	1.96	0.47
6:CB:41:ASP:O	6:CB:52:THR:OG1	2.25	0.47
7:BG:294:LEU:HD21	7:BG:320:MET:SD	2.54	0.47
7:BI:440:THR:OG1	7:BI:441:ASP:N	2.47	0.47
7:AI:263:ASP:O	7:AI:284:LYS:NZ	2.46	0.47
7:FI:358:ASP:OD1	7:FI:360:LYS:N	2.48	0.47
7:CI:358:ASP:OD1	7:CI:360:LYS:N	2.47	0.47
7:EH:606:ASN:ND2	7:EI:594:ASN:OD1	2.48	0.47
7:EG:88:GLY:N	7:EI:85:ASN:OD1	2.47	0.47
7:EI:554:LEU:O	7:EI:601:GLN:NE2	2.43	0.47
1:CD:207:ASN:HB3	7:CH:455:ALA:HB1	1.89	0.47
4:BJ:48:ASN:OD1	4:BJ:49:ASN:N	2.45	0.47
4:FJ:138:GLY:O	4:FJ:139:PHE:CD1	2.68	0.47
6:EB:112:GLY:C	6:EB:133:TYR:HE1	2.23	0.47
6:AB:112:GLY:C	6:AB:133:TYR:HE1	2.23	0.47
7:BG:440:THR:OG1	7:BG:445:ARG:O	2.31	0.47
7:DH:370:ILE:HB	7:DH:372:ILE:HD11	1.97	0.47
7:DI:358:ASP:OD1	7:DI:360:LYS:N	2.48	0.47
7:EI:358:ASP:OD1	7:EI:360:LYS:N	2.47	0.47
1:AD:124:SER:N	1:AD:127:ASP:OD2	2.47	0.47
4:BJ:138:GLY:O	4:BJ:139:PHE:CD1	2.68	0.47
4:DK:34:SER:N	4:DK:134:ASP:OD2	2.40	0.47
4:AK:52:LEU:HD12	7:AG:79:ASN:O	2.15	0.47
4:EL:88:ILE:HD12	5:EM:85:LYS:CE	2.45	0.47
5:CN:16:VAL:H	5:CM:26:TYR:HH	1.62	0.47
5:CN:63:ASP:OD1	5:CN:63:ASP:N	2.48	0.47
7:BH:281:ARG:NH2	7:BH:298:GLU:OE2	2.46	0.47
7:DG:80:MET:HE1	7:DI:77:PHE:CE1	2.50	0.47
7:DG:294:LEU:HD21	7:DG:320:MET:SD	2.55	0.47
7:DI:178:MET:SD	7:DI:192:LEU:HD11	2.54	0.47
7:AG:14:ASP:OD1	7:AG:15:TYR:N	2.48	0.47
2:CE:58:GLU:N	2:CE:320:ASN:OD1	2.48	0.47
4:BJ:145:LEU:HA	4:BJ:148:ILE:HG22	1.97	0.47
4:DL:51:PRO:HD2	5:DM:81:PHE:CD2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DL:178:LYS:HZ3	7:DH:93:LYS:HD3	1.72	0.47
4:AL:51:PRO:HD2	5:AM:81:PHE:CD2	2.50	0.47
4:CJ:82:LEU:O	4:CJ:83:THR:OG1	2.29	0.47
7:BI:178:MET:SD	7:BI:192:LEU:HD11	2.54	0.47
7:EH:442:SER:O	7:EI:437:VAL:HG22	2.15	0.47
4:BL:88:ILE:HD12	5:BM:85:LYS:HZ1	1.79	0.46
4:DL:50:ARG:HD3	5:DM:81:PHE:CZ	2.50	0.46
4:FK:71:ASN:N	4:FK:74:ARG:O	2.46	0.46
6:EB:163:ASP:O	6:EA:15:ARG:NH1	2.48	0.46
6:BA:40:THR:HG22	6:BA:52:THR:O	2.14	0.46
6:CB:112:GLY:C	6:CB:133:TYR:HE1	2.22	0.46
7:BH:442:SER:O	7:BI:437:VAL:HG22	2.15	0.46
7:BI:413:ASN:N	7:BI:413:ASN:OD1	2.47	0.46
7:AG:263:ASP:OD1	7:AG:264:ARG:N	2.47	0.46
7:FH:327:GLN:NE2	7:FH:351:PRO:O	2.48	0.46
7:FI:468:ILE:HD11	7:FI:472:ASP:HB3	1.98	0.46
7:CG:294:LEU:HD21	7:CG:320:MET:SD	2.55	0.46
2:AE:362:LYS:NZ	2:BE:142:ASP:OD2	2.47	0.46
1:BD:69:ASP:OD2	7:EH:15:TYR:CE1	2.68	0.46
1:BD:153:LYS:HE3	6:CB:43:GLU:CD	2.40	0.46
2:BE:58:GLU:N	2:BE:320:ASN:OD1	2.48	0.46
4:DL:68:ASP:O	4:DL:70:TYR:N	2.43	0.46
4:AJ:145:LEU:HA	4:AJ:148:ILE:HG22	1.97	0.46
4:CL:114:THR:HG23	4:CL:122:VAL:HG22	1.96	0.46
6:DB:51:ASN:OD1	6:DB:52:THR:N	2.48	0.46
7:AH:327:GLN:NE2	7:AH:351:PRO:O	2.47	0.46
7:AG:294:LEU:HD21	7:AG:320:MET:SD	2.55	0.46
7:FG:263:ASP:OD1	7:FG:264:ARG:N	2.47	0.46
7:FI:263:ASP:O	7:FI:284:LYS:NZ	2.47	0.46
7:EG:80:MET:HE1	7:EI:77:PHE:CE1	2.49	0.46
3:CF:1154:LEU:HD23	2:CE:149:LYS:CG	2.46	0.46
1:CC:125:ARG:HA	7:CI:290:LEU:HD11	1.97	0.46
1:BC:66:ASN:ND2	7:BG:8:ASP:OD1	2.49	0.46
1:BC:129:GLN:O	7:DG:16:ARG:NH1	2.46	0.46
1:BD:301:THR:CB	7:BH:475:ASN:OD1	2.62	0.46
4:DJ:43:PHE:HE2	4:DJ:63:ILE:HD12	1.80	0.46
4:DJ:145:LEU:HA	4:DJ:148:ILE:HG22	1.96	0.46
4:DL:58:HIS:CE1	5:DN:43:GLN:HG2	2.51	0.46
4:AJ:138:GLY:O	4:AJ:139:PHE:CD1	2.69	0.46
4:FJ:145:LEU:HA	4:FJ:148:ILE:HG22	1.96	0.46
5:BN:120:VAL:HG12	5:BN:121:ASP:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BM:47:ASP:OD1	5:BM:47:ASP:N	2.48	0.46
5:FN:16:VAL:O	5:FN:16:VAL:HG13	2.15	0.46
7:DI:263:ASP:O	7:DI:284:LYS:NZ	2.46	0.46
7:FG:294:LEU:HD21	7:FG:320:MET:SD	2.55	0.46
7:CG:161:ASN:ND2	7:CG:412:ASN:O	2.45	0.46
7:EG:390:ASP:OD1	7:EG:391:MET:N	2.49	0.46
1:CD:63:LYS:HE2	6:AB:52:THR:HG23	1.98	0.46
4:BJ:20:GLN:OE1	6:EA:98:LYS:O	2.34	0.46
4:BJ:107:VAL:HG13	4:BJ:107:VAL:O	2.15	0.46
4:FK:115:GLN:NE2	7:FG:82:LEU:O	2.42	0.46
4:FL:51:PRO:CD	5:FM:81:PHE:HD2	2.29	0.46
4:CJ:47:LYS:HB2	4:CJ:52:LEU:HD21	1.97	0.46
4:EK:175:LEU:HD13	4:EL:183:ALA:HB3	1.97	0.46
5:DN:63:ASP:N	5:DN:63:ASP:OD1	2.48	0.46
6:EB:126:ILE:CD1	6:CB:5:LYS:H	2.29	0.46
6:DA:40:THR:HG22	6:DA:52:THR:O	2.15	0.46
6:AB:105:PHE:N	6:AB:144:ALA:O	2.40	0.46
6:FB:79:ALA:O	6:FB:83:ARG:N	2.44	0.46
7:AH:331:GLY:HA3	7:AH:388:GLY:HA2	1.97	0.46
7:AH:606:ASN:ND2	7:AI:594:ASN:OD1	2.49	0.46
7:EH:327:GLN:NE2	7:EH:351:PRO:O	2.47	0.46
2:AE:58:GLU:N	2:AE:320:ASN:OD1	2.48	0.46
2:AE:203:ASP:O	2:AE:267:SER:OG	2.29	0.46
1:CD:124:SER:N	1:CD:127:ASP:OD2	2.47	0.46
4:BJ:151:ILE:HG21	4:BK:151:ILE:HD11	1.98	0.46
4:DK:15:LEU:HD13	4:DK:124:GLU:OE1	2.15	0.46
4:AJ:34:SER:HB3	4:AK:123:VAL:HG21	1.97	0.46
4:EJ:13:ILE:HD12	4:EJ:43:PHE:CE1	2.51	0.46
4:EL:40:VAL:O	4:EL:40:VAL:HG23	2.16	0.46
5:EM:38:GLY:HA3	5:EM:81:PHE:CE1	2.51	0.46
6:DB:139:PHE:CD1	6:DB:139:PHE:C	2.94	0.46
6:DA:31:GLU:HB3	6:AA:122:GLU:OE2	2.16	0.46
7:BI:468:ILE:HD11	7:BI:472:ASP:HB3	1.97	0.46
7:AH:315:GLN:NE2	7:AH:317:ASP:OD1	2.46	0.46
7:FI:222:LEU:O	7:FI:241:GLN:NE2	2.48	0.46
7:CH:278:ILE:HG22	7:CH:299:VAL:HG22	1.97	0.46
7:EG:294:LEU:HD21	7:EG:320:MET:SD	2.55	0.46
1:CC:53:SER:OG	1:CD:44:ARG:NH2	2.46	0.46
4:DJ:43:PHE:CE2	4:DJ:63:ILE:HD12	2.50	0.46
5:DN:96:TYR:OH	5:DN:98:ARG:NH2	2.46	0.46
5:CM:46:ILE:HD11	5:CM:51:HIS:HE1	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FB:14:PHE:HD2	6:FB:72:PHE:CZ	2.33	0.46
7:DH:315:GLN:NE2	7:DH:317:ASP:OD1	2.46	0.46
7:DG:161:ASN:ND2	7:DG:412:ASN:O	2.44	0.46
7:AH:442:SER:O	7:AI:437:VAL:HG22	2.15	0.46
7:AH:588:ILE:HG21	7:AH:604:ARG:NH1	2.31	0.46
7:FI:605:ARG:NH1	7:FI:611:ALA:O	2.47	0.46
7:CH:164:MET:HE2	7:CH:416:HIS:HA	1.98	0.46
7:CI:293:SER:OG	7:CI:318:ILE:O	2.32	0.46
1:CC:299:ASN:OD1	1:CC:299:ASN:N	2.45	0.46
4:BL:88:ILE:CD1	5:BM:85:LYS:HE3	2.46	0.46
4:AL:50:ARG:HB2	5:AM:81:PHE:HE2	1.77	0.46
5:BN:66:ILE:HG23	5:BN:66:ILE:O	2.16	0.46
5:FN:63:ASP:N	5:FN:63:ASP:OD1	2.49	0.46
5:FN:120:VAL:HG12	5:FN:121:ASP:H	1.79	0.46
5:EM:47:ASP:OD1	5:EM:47:ASP:N	2.48	0.46
6:EB:12:ILE:HD11	6:EB:32:TYR:CE2	2.51	0.46
6:FB:163:ASP:O	6:FA:15:ARG:NH1	2.49	0.46
7:DH:442:SER:O	7:DI:437:VAL:HG22	2.16	0.46
7:AG:255:ASP:OD1	7:AG:256:VAL:N	2.49	0.46
7:EH:588:ILE:HG21	7:EH:604:ARG:NH1	2.31	0.46
4:BK:15:LEU:HD13	4:BK:124:GLU:OE1	2.16	0.46
4:FJ:73:ASP:OD1	4:FJ:74:ARG:N	2.49	0.46
4:FJ:107:VAL:O	4:FJ:107:VAL:HG13	2.15	0.46
4:FK:9:ASP:OD1	4:FK:42:ASN:ND2	2.36	0.46
4:CJ:91:ARG:C	4:CJ:92:LEU:HD12	2.40	0.46
6:AB:110:PHE:HB2	6:AB:135:VAL:HG13	1.98	0.46
7:DH:278:ILE:HG22	7:DH:299:VAL:HG22	1.97	0.46
7:AI:328:PRO:O	7:AI:343:THR:OG1	2.28	0.46
7:FH:164:MET:HE3	7:FH:178:MET:HE3	1.98	0.46
7:EG:255:ASP:OD1	7:EG:256:VAL:N	2.49	0.46
1:AC:149:GLN:CD	6:DB:41:ASP:HB3	2.41	0.46
4:BJ:47:LYS:HB2	4:BJ:52:LEU:HD21	1.98	0.46
4:CJ:164:GLN:O	4:CJ:168:ASN:ND2	2.49	0.46
4:CK:143:THR:O	4:CK:143:THR:HG23	2.16	0.46
4:EL:76:ALA:HB1	4:EL:100:PHE:CE2	2.51	0.46
7:DH:226:SER:OG	7:DH:227:ALA:N	2.49	0.46
1:AD:107:SER:HB3	6:DB:22:ASP:CB	2.46	0.46
4:AJ:140:ASP:OD2	4:AJ:143:THR:OG1	2.25	0.46
4:AK:48:ASN:OD1	4:AK:49:ASN:N	2.44	0.46
5:AM:46:ILE:HD11	5:AM:51:HIS:HE1	1.81	0.46
6:AB:14:PHE:HD2	6:AB:72:PHE:CZ	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AB:163:ASP:O	6:AA:15:ARG:NH1	2.48	0.46
6:FA:24:THR:OG1	6:FA:25:LYS:N	2.49	0.46
7:DH:324:SER:OG	7:DH:325:ASP:N	2.49	0.46
7:DG:440:THR:OG1	7:DG:445:ARG:O	2.32	0.46
7:AG:390:ASP:OD1	7:AG:391:MET:N	2.49	0.46
7:AI:413:ASN:OD1	7:AI:413:ASN:N	2.49	0.46
7:CG:80:MET:HE1	7:CI:77:PHE:CE1	2.50	0.46
7:EI:413:ASN:N	7:EI:413:ASN:OD1	2.49	0.46
3:CF:1144:ARG:HG2	3:BF:1138:THR:HG21	1.98	0.45
1:CC:124:SER:N	1:CC:127:ASP:OD2	2.47	0.45
5:FN:66:ILE:O	5:FN:66:ILE:HG23	2.16	0.45
5:CM:38:GLY:HA3	5:CM:81:PHE:CE1	2.51	0.45
6:AA:37:GLU:O	6:AA:56:VAL:HG13	2.16	0.45
7:BH:188:MET:HE1	7:BH:201:ARG:NE	2.31	0.45
7:BG:263:ASP:OD1	7:BG:264:ARG:N	2.47	0.45
7:AG:440:THR:OG1	7:AG:445:ARG:O	2.31	0.45
7:AI:605:ARG:NH1	7:AI:611:ALA:O	2.46	0.45
7:EH:324:SER:OG	7:EH:325:ASP:N	2.49	0.45
1:BD:124:SER:N	1:BD:127:ASP:OD2	2.47	0.45
2:BE:275:ASP:OD1	2:BE:276:PHE:N	2.50	0.45
4:DJ:20:GLN:CD	6:BA:98:LYS:O	2.59	0.45
4:DJ:138:GLY:O	4:DJ:139:PHE:CD1	2.70	0.45
4:DL:135:LEU:HD12	4:DL:136:VAL:O	2.17	0.45
4:AJ:14:GLU:OE2	4:AJ:46:THR:HG21	2.15	0.45
5:FN:7:VAL:HB	5:FN:37:ILE:HG22	1.98	0.45
6:AA:7:SER:OG	6:FA:122:GLU:O	2.32	0.45
7:CG:88:GLY:N	7:CI:85:ASN:OD1	2.49	0.45
7:CI:413:ASN:OD1	7:CI:413:ASN:N	2.48	0.45
7:EI:178:MET:SD	7:EI:192:LEU:HD11	2.57	0.45
1:CD:97:GLU:OE2	6:AB:48:GLY:CA	2.64	0.45
1:CD:107:SER:N	6:FB:22:ASP:CA	2.77	0.45
1:BD:67:ARG:NH1	6:FB:47:ASP:CA	2.57	0.45
1:BD:105:PRO:CA	6:EB:15:ARG:HH22	2.11	0.45
4:DK:9:ASP:OD1	4:DK:42:ASN:ND2	2.38	0.45
4:FJ:5:ASN:ND2	7:FG:80:MET:O	2.33	0.45
4:FJ:32:TYR:OH	4:FK:22:ASN:O	2.34	0.45
4:FL:51:PRO:HD2	5:FM:81:PHE:HD2	1.81	0.45
4:EJ:138:GLY:O	4:EJ:139:PHE:CD1	2.69	0.45
5:DM:46:ILE:HD11	5:DM:51:HIS:HE1	1.80	0.45
5:FN:33:ALA:HB3	5:FN:86:ILE:HD11	1.98	0.45
5:FM:38:GLY:HA3	5:FM:81:PHE:CE1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:327:GLN:NE2	7:BH:351:PRO:O	2.48	0.45
7:DG:390:ASP:OD1	7:DG:391:MET:N	2.50	0.45
7:FI:178:MET:SD	7:FI:192:LEU:HD11	2.55	0.45
7:CG:390:ASP:OD1	7:CG:391:MET:N	2.49	0.45
1:CC:66:ASN:ND2	7:CG:8:ASP:OD1	2.49	0.45
4:AK:169:MET:C	4:AK:172:THR:HG1	2.20	0.45
5:BM:46:ILE:HD11	5:BM:51:HIS:HE1	1.79	0.45
7:AH:324:SER:OG	7:AH:325:ASP:N	2.49	0.45
7:FH:188:MET:HE1	7:FH:201:ARG:NE	2.32	0.45
7:EI:605:ARG:NH1	7:EI:611:ALA:O	2.46	0.45
1:AC:53:SER:OG	1:AD:44:ARG:NH2	2.47	0.45
2:AE:78:ASP:N	1:BC:47:MET:O	2.45	0.45
2:AE:275:ASP:OD1	2:AE:276:PHE:N	2.50	0.45
1:BD:47:MET:O	2:BE:280:ARG:NH2	2.49	0.45
4:BL:135:LEU:HD12	4:BL:136:VAL:O	2.17	0.45
4:DK:174:THR:O	4:DK:174:THR:HG22	2.17	0.45
4:CL:49:ASN:O	5:CM:78:VAL:CG1	2.65	0.45
5:BM:38:GLY:HA3	5:BM:81:PHE:CE1	2.50	0.45
6:EB:14:PHE:HD2	6:EB:72:PHE:CZ	2.34	0.45
6:EA:37:GLU:O	6:EA:56:VAL:HG13	2.16	0.45
6:AA:40:THR:HG22	6:AA:52:THR:O	2.17	0.45
7:DH:606:ASN:OD1	7:DI:618:ASN:ND2	2.49	0.45
7:AG:80:MET:HE1	7:AI:77:PHE:CE1	2.51	0.45
1:AD:183:VAL:HG12	7:AG:14:ASP:HA	1.98	0.45
4:DJ:73:ASP:OD1	4:DJ:74:ARG:N	2.50	0.45
4:AL:40:VAL:HG23	4:AL:40:VAL:O	2.16	0.45
4:CJ:32:TYR:OH	4:CK:22:ASN:O	2.34	0.45
4:CL:135:LEU:HD12	4:CL:136:VAL:O	2.17	0.45
4:EJ:8:LYS:NZ	4:EJ:35:ASP:OD2	2.50	0.45
5:FM:57:LEU:CD2	5:FM:72:LEU:HD13	2.45	0.45
6:CB:139:PHE:CD1	6:CB:139:PHE:C	2.94	0.45
7:FH:606:ASN:OD1	7:FI:618:ASN:ND2	2.50	0.45
1:CD:107:SER:HB3	6:FB:22:ASP:CB	2.47	0.45
2:CE:275:ASP:OD1	2:CE:276:PHE:N	2.50	0.45
1:BD:180:ASN:HB2	7:BI:12:VAL:CG2	2.47	0.45
4:BL:76:ALA:HB1	4:BL:100:PHE:CE2	2.52	0.45
4:CJ:138:GLY:O	4:CJ:139:PHE:CD1	2.69	0.45
4:CL:76:ALA:HB1	4:CL:100:PHE:CE2	2.52	0.45
4:EK:63:ILE:HD11	4:EK:94:TYR:CD2	2.52	0.45
5:FN:16:VAL:H	5:FM:26:TYR:HH	1.64	0.45
5:EM:46:ILE:HD11	5:EM:51:HIS:HE1	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CA:15:ARG:NE	6:CA:87:GLU:OE2	2.50	0.45
7:AH:278:ILE:HG22	7:AH:299:VAL:HG22	1.99	0.45
7:FG:88:GLY:N	7:FI:85:ASN:OD1	2.49	0.45
7:FI:578:PRO:HG3	7:FI:615:LEU:HD22	1.99	0.45
7:EG:200:ASP:OD1	7:EG:201:ARG:N	2.49	0.45
1:AC:149:GLN:OE1	6:DB:41:ASP:CB	2.64	0.45
1:AD:128:GLN:C	7:AG:16:ARG:HH22	2.17	0.45
1:BD:68:SER:HG	7:EG:11:ARG:HG3	1.81	0.45
2:BE:129:LYS:NZ	2:BE:130:VAL:O	2.46	0.45
4:AJ:13:ILE:HD12	4:AJ:43:PHE:CE1	2.52	0.45
4:AL:135:LEU:HD12	4:AL:136:VAL:O	2.17	0.45
5:BN:63:ASP:OD1	5:BN:63:ASP:N	2.49	0.45
6:DB:5:LYS:H	6:AB:126:ILE:CD1	2.29	0.45
1:CC:153:LYS:CG	6:FB:52:THR:HB	2.47	0.45
4:BJ:14:GLU:OE2	4:BJ:46:THR:HG21	2.17	0.45
4:DJ:20:GLN:CD	6:BA:99:ASN:OD1	2.60	0.45
4:AK:58:HIS:NE2	7:AH:80:MET:O	2.33	0.45
4:CJ:57:GLU:OE1	4:CJ:58:HIS:ND1	2.49	0.45
4:CL:50:ARG:CD	5:CM:81:PHE:CZ	2.99	0.45
4:EL:135:LEU:HD12	4:EL:136:VAL:O	2.17	0.45
6:BA:112:GLY:N	6:BA:133:TYR:OH	2.47	0.45
7:BH:588:ILE:HG21	7:BH:604:ARG:NH1	2.31	0.45
7:DI:326:THR:OG1	7:DI:345:ASP:OD2	2.20	0.45
7:CH:442:SER:O	7:CI:437:VAL:HG22	2.17	0.45
7:CH:606:ASN:OD1	7:CI:618:ASN:ND2	2.50	0.45
7:CI:509:ARG:NH2	7:CI:515:ASN:O	2.47	0.45
7:EG:440:THR:OG1	7:EG:445:ARG:O	2.31	0.45
1:CC:281:GLU:O	2:CE:295:GLN:NE2	2.50	0.45
1:BC:281:GLU:O	2:BE:295:GLN:NE2	2.49	0.45
4:BK:174:THR:O	4:BK:174:THR:HG22	2.17	0.45
4:AK:6:PHE:O	4:AK:6:PHE:CG	2.70	0.45
4:FJ:20:GLN:OE1	6:AA:98:LYS:O	2.35	0.45
4:EJ:14:GLU:OE2	4:EJ:46:THR:HG21	2.17	0.45
5:BN:7:VAL:HB	5:BN:37:ILE:HG22	1.98	0.45
7:BI:578:PRO:HG3	7:BI:615:LEU:HD22	1.98	0.45
7:FH:588:ILE:HG21	7:FH:604:ARG:NH1	2.31	0.45
7:EH:49:ALA:N	7:EG:54:GLN:O	2.50	0.45
7:EG:478:ASP:OD1	7:EG:521:ARG:NH2	2.49	0.45
1:CC:149:GLN:CD	6:FB:41:ASP:HB3	2.42	0.44
1:BC:128:GLN:C	7:DG:16:ARG:HH22	2.06	0.44
4:AL:76:ALA:HB1	4:AL:100:PHE:CE2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DN:7:VAL:HB	5:DN:37:ILE:HG22	1.98	0.44
6:BB:5:LYS:H	6:DB:126:ILE:CD1	2.29	0.44
6:CB:51:ASN:OD1	6:CB:52:THR:N	2.50	0.44
6:CB:70:ASP:OD1	6:CB:71:ASP:N	2.50	0.44
6:CB:105:PHE:N	6:CB:144:ALA:O	2.41	0.44
7:BH:226:SER:OG	7:BH:227:ALA:N	2.50	0.44
7:BG:88:GLY:N	7:BI:85:ASN:OD1	2.51	0.44
7:BG:390:ASP:OD1	7:BG:391:MET:N	2.50	0.44
7:FH:147:GLU:O	7:FH:368:ARG:NH2	2.50	0.44
7:FH:226:SER:OG	7:FH:227:ALA:N	2.51	0.44
7:CH:315:GLN:NE2	7:CH:317:ASP:OD1	2.46	0.44
1:CC:149:GLN:OE1	6:FB:41:ASP:CB	2.65	0.44
1:BC:153:LYS:HE3	6:EB:43:GLU:CD	2.38	0.44
4:EK:6:PHE:O	4:EK:6:PHE:CG	2.71	0.44
6:EA:11:ILE:HB	6:EA:91:VAL:HG13	1.99	0.44
6:EA:40:THR:HG22	6:EA:52:THR:O	2.17	0.44
6:BA:24:THR:OG1	6:BA:25:LYS:N	2.49	0.44
6:DB:129:TYR:CD1	6:DB:129:TYR:C	2.95	0.44
7:BH:147:GLU:O	7:BH:368:ARG:NH2	2.50	0.44
7:DI:578:PRO:HG3	7:DI:615:LEU:HD22	1.99	0.44
7:AI:509:ARG:NH2	7:AI:515:ASN:O	2.50	0.44
7:FH:324:SER:OG	7:FH:325:ASP:N	2.48	0.44
7:FH:606:ASN:ND2	7:FI:594:ASN:OD1	2.51	0.44
7:FI:440:THR:OG1	7:FI:441:ASP:N	2.49	0.44
7:CH:440:THR:OG1	7:CH:445:ARG:O	2.24	0.44
7:CH:588:ILE:HG21	7:CH:604:ARG:NH1	2.32	0.44
1:CD:67:ARG:HH11	6:DB:47:ASP:HA	1.74	0.44
4:BL:50:ARG:HB2	5:BM:81:PHE:HE2	1.77	0.44
4:DJ:164:GLN:O	4:DJ:168:ASN:ND2	2.50	0.44
4:CK:148:ILE:HG23	4:CL:151:ILE:HD11	1.98	0.44
5:BN:33:ALA:HB3	5:BN:86:ILE:HD11	1.98	0.44
5:DM:102:PHE:C	5:DM:103:LEU:HD12	2.43	0.44
5:CM:102:PHE:C	5:CM:103:LEU:HD12	2.43	0.44
6:DB:14:PHE:HD2	6:DB:72:PHE:CZ	2.35	0.44
6:DB:138:ARG:HG2	6:DB:139:PHE:O	2.16	0.44
6:AA:112:GLY:N	6:AA:133:TYR:OH	2.44	0.44
7:DH:588:ILE:HG21	7:DH:604:ARG:NH1	2.32	0.44
7:DG:255:ASP:OD1	7:DG:256:VAL:N	2.51	0.44
7:AH:281:ARG:NH2	7:AH:298:GLU:OE2	2.49	0.44
7:FG:44:ASN:O	7:FI:54:GLN:NE2	2.50	0.44
7:CH:281:ARG:NH2	7:CH:298:GLU:OE2	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:EH:164:MET:HE3	7:EH:178:MET:HE3	1.98	0.44
7:EH:606:ASN:OD1	7:EI:618:ASN:ND2	2.51	0.44
2:CE:129:LYS:NZ	2:CE:130:VAL:O	2.46	0.44
1:BC:124:SER:N	1:BC:127:ASP:OD2	2.47	0.44
5:FM:47:ASP:OD1	5:FM:47:ASP:N	2.48	0.44
6:DB:159:TYR:OH	6:DA:138:ARG:O	2.28	0.44
6:DA:7:SER:N	6:AA:125:GLY:O	2.38	0.44
7:BI:222:LEU:O	7:BI:241:GLN:NE2	2.51	0.44
7:AI:178:MET:SD	7:AI:192:LEU:HD11	2.57	0.44
7:FI:317:ASP:OD1	7:FI:318:ILE:N	2.49	0.44
7:FI:413:ASN:OD1	7:FI:413:ASN:N	2.48	0.44
7:CH:606:ASN:ND2	7:CI:594:ASN:OD1	2.51	0.44
1:CD:100:TYR:CZ	6:FB:110:PHE:HA	2.44	0.44
1:BC:102:PHE:CD1	6:BB:142:GLY:HA3	2.52	0.44
1:BC:188:PHE:HB2	7:DH:14:ASP:HA	1.98	0.44
4:CK:174:THR:HG22	4:CK:174:THR:O	2.17	0.44
5:CM:47:ASP:OD1	5:CM:47:ASP:N	2.48	0.44
6:EB:139:PHE:CD1	6:EB:139:PHE:C	2.96	0.44
6:EA:37:GLU:C	6:EA:56:VAL:HG13	2.42	0.44
6:FB:5:LYS:H	6:CB:126:ILE:CD1	2.29	0.44
6:CB:14:PHE:HD2	6:CB:72:PHE:CZ	2.35	0.44
7:FH:281:ARG:NH2	7:FH:298:GLU:OE2	2.47	0.44
7:CH:147:GLU:O	7:CH:368:ARG:NH2	2.50	0.44
1:AD:301:THR:OG1	7:AH:477:LEU:HD11	2.18	0.44
3:BF:1141:VAL:HG21	3:AF:1141:VAL:HG11	1.98	0.44
4:DK:6:PHE:O	4:DK:6:PHE:CG	2.70	0.44
4:FK:6:PHE:CG	4:FK:6:PHE:O	2.70	0.44
4:EL:174:THR:HG21	7:EH:90:ASN:HD21	1.83	0.44
6:AB:139:PHE:HE2	6:FB:77:GLU:OE2	2.01	0.44
7:BH:324:SER:OG	7:BH:325:ASP:N	2.48	0.44
7:BG:155:ASP:OD2	7:BG:415:HIS:NE2	2.49	0.44
7:DI:509:ARG:NH2	7:DI:515:ASN:O	2.49	0.44
7:CH:370:ILE:HB	7:CH:372:ILE:HD11	2.00	0.44
7:CI:578:PRO:HG3	7:CI:615:LEU:HD22	2.00	0.44
1:BC:149:GLN:CD	6:EB:41:ASP:HB3	2.43	0.44
4:BL:67:THR:HB	4:BL:76:ALA:HB3	2.00	0.44
4:DJ:11:ASN:OD1	4:DJ:11:ASN:N	2.51	0.44
4:DK:10:ASP:OD1	4:DK:11:ASN:N	2.51	0.44
4:FL:135:LEU:HD12	4:FL:136:VAL:O	2.17	0.44
4:CK:6:PHE:O	4:CK:6:PHE:CG	2.70	0.44
4:CK:97:PRO:O	4:CK:101:LEU:HD23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EJ:73:ASP:OD1	4:EJ:74:ARG:N	2.51	0.44
4:EL:67:THR:HB	4:EL:76:ALA:HB3	2.00	0.44
5:BM:87:PRO:HG2	5:BM:90:VAL:HG23	2.00	0.44
5:DN:111:HIS:NE2	5:DN:114:ASN:OD1	2.44	0.44
5:AN:7:VAL:HB	5:AN:37:ILE:HG22	2.00	0.44
5:FM:46:ILE:HD11	5:FM:51:HIS:CE1	2.53	0.44
5:CN:7:VAL:HB	5:CN:37:ILE:HG22	1.98	0.44
6:EB:5:LYS:H	6:BB:126:ILE:CD1	2.30	0.44
6:CB:110:PHE:HB2	6:CB:135:VAL:HG13	2.00	0.44
7:BH:164:MET:HE3	7:BH:178:MET:HE3	1.99	0.44
7:BH:328:PRO:O	7:BH:343:THR:OG1	2.17	0.44
7:EG:218:ILE:HD12	7:EG:223:TRP:CD1	2.53	0.44
1:AD:97:GLU:OE2	6:BB:48:GLY:CA	2.64	0.44
1:CC:129:GLN:O	7:EG:16:ARG:NH1	2.51	0.44
1:BC:149:GLN:OE1	6:EB:41:ASP:CB	2.66	0.44
4:AK:63:ILE:HD11	4:AK:94:TYR:CD2	2.53	0.44
4:AL:88:ILE:HD12	5:AM:85:LYS:HE2	2.00	0.44
4:AL:158:VAL:HG12	4:AL:158:VAL:O	2.18	0.44
4:CK:34:SER:N	4:CK:134:ASP:OD2	2.41	0.44
5:BM:46:ILE:HD11	5:BM:51:HIS:CE1	2.53	0.44
5:DM:46:ILE:HD11	5:DM:51:HIS:CE1	2.53	0.44
6:DA:112:GLY:O	6:DA:133:TYR:OH	2.32	0.44
6:AA:7:SER:HB2	6:FA:121:ALA:HB1	2.00	0.44
6:FB:29:LEU:HD23	6:FB:29:LEU:H	1.82	0.44
6:CA:11:ILE:HB	6:CA:91:VAL:HG13	2.00	0.44
7:FG:478:ASP:OD1	7:FG:521:ARG:NH2	2.48	0.44
7:FI:427:ASN:OD1	7:FI:428:GLN:N	2.51	0.44
7:CG:255:ASP:OD1	7:CG:256:VAL:N	2.51	0.44
7:CI:468:ILE:HD11	7:CI:472:ASP:HB3	2.00	0.44
7:EI:509:ARG:NH2	7:EI:515:ASN:O	2.51	0.44
1:AD:74:ARG:CZ	1:BC:26:ILE:HD11	2.47	0.44
1:BD:95:LYS:NZ	7:BG:20:GLU:OE2	2.51	0.44
4:DL:171:ASP:O	4:DL:174:THR:HG22	2.18	0.44
4:FK:15:LEU:HD13	4:FK:124:GLU:OE1	2.17	0.44
4:EK:174:THR:O	4:EK:174:THR:HG22	2.18	0.44
5:FM:106:GLU:O	5:FM:107:GLU:HB3	2.18	0.44
5:EN:7:VAL:HB	5:EN:37:ILE:HG22	2.00	0.44
5:EN:16:VAL:HG21	5:EN:112:VAL:O	2.18	0.44
6:BA:47:ASP:OD2	6:DB:28:PHE:N	2.44	0.44
6:AB:29:LEU:HD23	6:AB:29:LEU:H	1.83	0.44
6:AA:37:GLU:C	6:AA:56:VAL:HG13	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FA:22:ASP:OD1	6:FA:23:ALA:N	2.51	0.44
6:FA:43:GLU:HB3	6:FA:50:TYR:OH	2.17	0.44
6:CB:129:TYR:CD1	6:CB:129:TYR:C	2.95	0.44
6:CB:138:ARG:HG2	6:CB:139:PHE:O	2.18	0.44
7:BH:606:ASN:ND2	7:BI:594:ASN:OD1	2.51	0.44
7:BH:606:ASN:OD1	7:BI:618:ASN:ND2	2.51	0.44
7:DH:147:GLU:O	7:DH:368:ARG:NH2	2.51	0.44
7:AH:606:ASN:OD1	7:AI:618:ASN:ND2	2.50	0.44
7:AG:200:ASP:OD1	7:AG:201:ARG:N	2.49	0.44
7:AI:468:ILE:HD11	7:AI:472:ASP:HB3	2.00	0.44
7:EH:188:MET:HE1	7:EH:201:ARG:NE	2.33	0.44
1:CC:26:ILE:HD11	1:BD:74:ARG:NE	2.32	0.43
1:BC:164:GLU:O	1:BD:44:ARG:N	2.46	0.43
4:DK:143:THR:HG23	4:DK:143:THR:O	2.17	0.43
4:AJ:111:ALA:O	4:AJ:123:VAL:HG23	2.18	0.43
4:FL:76:ALA:HB1	4:FL:100:PHE:CE2	2.53	0.43
4:EL:88:ILE:CD1	5:EM:85:LYS:HE2	2.44	0.43
5:BM:46:ILE:HD13	5:EN:1:MET:HE2	2.00	0.43
5:DM:7:VAL:HG22	5:DM:8:GLU:N	2.33	0.43
5:CN:16:VAL:HG21	5:CN:112:VAL:O	2.17	0.43
5:CM:7:VAL:HG22	5:CM:8:GLU:N	2.33	0.43
6:AB:5:LYS:H	6:FB:126:ILE:CD1	2.30	0.43
6:FA:141:ARG:HH22	6:CA:78:ASP:CG	2.25	0.43
7:BH:76:ARG:NH1	7:BI:74:ASN:OD1	2.46	0.43
7:BI:427:ASN:OD1	7:BI:428:GLN:N	2.50	0.43
7:DH:188:MET:HE1	7:DH:201:ARG:NE	2.33	0.43
7:AH:49:ALA:N	7:AG:54:GLN:O	2.49	0.43
7:AG:478:ASP:OD1	7:AG:521:ARG:NH2	2.50	0.43
7:FH:278:ILE:HG22	7:FH:299:VAL:HG22	2.00	0.43
7:EH:283:TYR:OH	7:EH:291:LYS:NZ	2.51	0.43
1:AD:180:ASN:HB2	7:AI:12:VAL:HG22	2.00	0.43
1:CC:232:ILE:HG22	1:CC:305:VAL:HG23	2.01	0.43
4:BK:6:PHE:O	4:BK:6:PHE:CG	2.71	0.43
4:AK:174:THR:O	4:AK:174:THR:HG22	2.17	0.43
4:AK:175:LEU:HD13	4:AL:183:ALA:HB3	2.00	0.43
4:FK:174:THR:HG22	4:FK:174:THR:O	2.17	0.43
5:AN:1:MET:HE2	5:FM:46:ILE:HD13	2.00	0.43
5:EN:63:ASP:OD1	5:EN:63:ASP:N	2.49	0.43
6:EA:43:GLU:HB3	6:EA:50:TYR:OH	2.18	0.43
6:DB:60:MET:SD	6:DB:133:TYR:HB3	2.58	0.43
6:DA:47:ASP:OD2	6:AB:28:PHE:N	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FA:7:SER:HB2	6:CA:121:ALA:HB1	2.00	0.43
6:FA:37:GLU:O	6:FA:56:VAL:HG13	2.18	0.43
7:BG:80:MET:HE1	7:BI:77:PHE:CE1	2.53	0.43
7:BG:478:ASP:OD1	7:BG:521:ARG:NH2	2.49	0.43
7:BI:605:ARG:NH1	7:BI:611:ALA:O	2.47	0.43
7:AI:293:SER:OG	7:AI:318:ILE:O	2.34	0.43
7:CH:331:GLY:HA3	7:CH:388:GLY:HA2	1.99	0.43
7:EH:171:PRO:O	7:EH:174:LYS:NZ	2.30	0.43
1:CC:100:TYR:HH	6:CB:110:PHE:HA	1.81	0.43
1:BC:153:LYS:NZ	6:EB:43:GLU:CD	2.61	0.43
1:BD:20:ILE:HD11	6:CB:50:TYR:CD2	2.51	0.43
4:DJ:34:SER:HB3	4:DK:123:VAL:HG21	2.01	0.43
4:DL:174:THR:HG21	7:DH:90:ASN:HD21	1.83	0.43
5:AM:46:ILE:HD11	5:AM:51:HIS:CE1	2.53	0.43
6:EA:7:SER:OG	6:BA:122:GLU:O	2.32	0.43
6:CA:37:GLU:O	6:CA:56:VAL:HG13	2.18	0.43
7:BG:218:ILE:HD12	7:BG:223:TRP:CD1	2.53	0.43
7:BG:266:THR:HG23	7:BG:281:ARG:CG	2.49	0.43
7:DH:327:GLN:NE2	7:DH:351:PRO:O	2.49	0.43
7:DI:317:ASP:OD1	7:DI:318:ILE:N	2.49	0.43
7:AI:317:ASP:OD1	7:AI:318:ILE:N	2.50	0.43
7:FG:155:ASP:OD1	7:FG:415:HIS:NE2	2.52	0.43
7:CH:188:MET:HE1	7:CH:201:ARG:NE	2.33	0.43
7:CH:226:SER:OG	7:CH:227:ALA:N	2.50	0.43
7:CG:218:ILE:HD12	7:CG:223:TRP:CD1	2.54	0.43
7:EH:278:ILE:HG22	7:EH:299:VAL:HG22	2.00	0.43
1:AC:232:ILE:HG22	1:AC:305:VAL:HG23	2.01	0.43
1:CD:232:ILE:HG22	1:CD:305:VAL:HG23	2.01	0.43
1:BC:20:ILE:CD1	6:EB:50:TYR:CD2	3.01	0.43
4:BJ:5:ASN:ND2	7:BG:80:MET:O	2.34	0.43
4:EK:16:GLN:OE1	4:EK:46:THR:OG1	2.19	0.43
5:BM:106:GLU:O	5:BM:107:GLU:HB3	2.18	0.43
5:EM:87:PRO:HG2	5:EM:90:VAL:HG23	2.01	0.43
6:BB:9:ASP:OD1	6:BB:94:ARG:NH2	2.51	0.43
6:DB:29:LEU:HD23	6:DB:29:LEU:H	1.84	0.43
6:DA:7:SER:OG	6:AA:122:GLU:O	2.28	0.43
6:AA:43:GLU:HB3	6:AA:50:TYR:OH	2.18	0.43
6:FA:112:GLY:O	6:FA:133:TYR:OH	2.29	0.43
7:BG:44:ASN:O	7:BI:54:GLN:NE2	2.51	0.43
7:BG:161:ASN:ND2	7:BG:412:ASN:O	2.44	0.43
7:DG:200:ASP:OD1	7:DG:201:ARG:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AH:264:ARG:NH1	7:AH:287:GLU:OE2	2.51	0.43
7:AG:218:ILE:HD12	7:AG:223:TRP:CD1	2.53	0.43
7:EG:142:ARG:NH1	7:EI:396:GLU:OE2	2.51	0.43
1:AD:136:GLN:NE2	1:AD:169:GLU:OE1	2.50	0.43
1:AD:232:ILE:HG22	1:AD:305:VAL:HG23	2.01	0.43
1:CC:136:GLN:NE2	1:CC:169:GLU:OE1	2.50	0.43
1:BD:280:THR:HG23	2:BE:14:PRO:HD3	2.00	0.43
4:BJ:137:SER:O	4:BL:120:ASN:ND2	2.51	0.43
4:FJ:36:ARG:H	4:FJ:101:LEU:HD12	1.83	0.43
5:BN:16:VAL:HG21	5:BN:112:VAL:O	2.18	0.43
5:FN:16:VAL:HG21	5:FN:112:VAL:O	2.18	0.43
6:EB:15:ARG:NH1	6:EB:87:GLU:OE2	2.52	0.43
6:EA:7:SER:HB2	6:BA:121:ALA:HB1	2.00	0.43
6:DA:43:GLU:HB3	6:DA:50:TYR:OH	2.19	0.43
7:BH:315:GLN:NE2	7:BH:317:ASP:OD1	2.50	0.43
7:DI:468:ILE:HD11	7:DI:472:ASP:HB3	2.00	0.43
7:DI:548:PRO:O	7:DI:573:ARG:NH1	2.52	0.43
7:EI:578:PRO:HG3	7:EI:615:LEU:HD22	2.00	0.43
1:BC:232:ILE:HG22	1:BC:305:VAL:HG23	2.01	0.43
4:BL:88:ILE:HD12	5:BM:85:LYS:HE2	1.97	0.43
4:DK:97:PRO:O	4:DK:101:LEU:HD23	2.18	0.43
4:AK:32:TYR:HB2	4:FJ:123:VAL:CG1	2.49	0.43
4:FK:175:LEU:HD13	4:FL:183:ALA:HB3	2.00	0.43
5:AN:16:VAL:HG21	5:AN:112:VAL:O	2.18	0.43
5:CM:46:ILE:HD11	5:CM:51:HIS:CE1	2.53	0.43
5:CM:87:PRO:HG2	5:CM:90:VAL:HG23	2.00	0.43
6:EB:12:ILE:O	6:EB:13:LEU:HD12	2.19	0.43
6:BB:162:HIS:O	6:BA:89:TRP:HH2	2.02	0.43
6:AA:11:ILE:HB	6:AA:91:VAL:HG13	2.00	0.43
7:BH:288:ARG:HD2	7:BH:294:LEU:HD22	2.00	0.43
7:DH:606:ASN:ND2	7:DI:594:ASN:OD1	2.51	0.43
7:AI:222:LEU:O	7:AI:241:GLN:NE2	2.51	0.43
7:CH:327:GLN:NE2	7:CH:351:PRO:O	2.47	0.43
7:CI:554:LEU:O	7:CI:601:GLN:NE2	2.43	0.43
1:AD:97:GLU:OE1	6:BB:47:ASP:C	2.60	0.43
1:BD:125:ARG:N	7:EI:290:LEU:CD1	2.76	0.43
4:BK:175:LEU:HD13	4:BL:183:ALA:HB3	2.00	0.43
4:AJ:73:ASP:OD1	4:AJ:74:ARG:N	2.52	0.43
4:FJ:91:ARG:C	4:FJ:92:LEU:HD12	2.44	0.43
4:EJ:35:ASP:O	4:EK:121:VAL:HG22	2.18	0.43
5:DN:16:VAL:HG21	5:DN:112:VAL:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DB:110:PHE:HB2	6:DB:135:VAL:HG13	1.99	0.43
6:DA:70:ASP:OD1	6:DA:72:PHE:N	2.52	0.43
6:AB:139:PHE:CD1	6:AB:139:PHE:C	2.97	0.43
6:AA:24:THR:OG1	6:AA:25:LYS:N	2.52	0.43
7:BG:157:SER:O	7:BG:157:SER:OG	2.33	0.43
7:BG:200:ASP:OD1	7:BG:201:ARG:N	2.51	0.43
7:DG:218:ILE:HD12	7:DG:223:TRP:CD1	2.53	0.43
7:FH:411:GLY:N	7:FG:452:GLN:OE1	2.52	0.43
7:FG:382:ASP:N	7:FG:382:ASP:OD2	2.52	0.43
7:CI:493:ASP:OD1	7:CI:493:ASP:N	2.50	0.43
7:EH:411:GLY:N	7:EG:452:GLN:OE1	2.52	0.43
7:EG:161:ASN:ND2	7:EG:412:ASN:O	2.45	0.43
1:AD:68:SER:OG	7:DG:11:ARG:CG	2.54	0.43
1:AD:194:TRP:HB3	7:AI:15:TYR:HA	1.99	0.43
1:CC:61:PHE:CD1	6:FB:43:GLU:OE1	2.72	0.43
4:BL:174:THR:HG21	7:BH:90:ASN:HD21	1.83	0.43
4:DL:76:ALA:HB1	4:DL:100:PHE:CE2	2.54	0.43
4:CJ:34:SER:HB3	4:CK:123:VAL:HG21	2.00	0.43
5:DM:57:LEU:CD2	5:DM:72:LEU:HD13	2.46	0.43
5:AM:87:PRO:HG2	5:AM:90:VAL:HG23	2.01	0.43
6:EA:24:THR:OG1	6:EA:25:LYS:N	2.52	0.43
6:EA:146:LEU:N	6:EA:146:LEU:HD12	2.34	0.43
6:AA:70:ASP:OD1	6:AA:72:PHE:N	2.52	0.43
6:FA:11:ILE:HB	6:FA:91:VAL:HG13	2.00	0.43
7:DI:440:THR:OG1	7:DI:441:ASP:N	2.51	0.43
7:DI:605:ARG:NH1	7:DI:611:ALA:O	2.47	0.43
7:AH:411:GLY:N	7:AG:452:GLN:OE1	2.51	0.43
7:CG:392:TYR:N	7:CG:401:ALA:O	2.50	0.43
7:CI:7:THR:HG22	7:CI:7:THR:O	2.18	0.43
7:CI:328:PRO:O	7:CI:343:THR:OG1	2.31	0.43
1:AD:95:LYS:HD3	7:AG:8:ASP:O	2.19	0.43
4:BK:10:ASP:OD1	4:BK:11:ASN:N	2.52	0.43
4:AL:67:THR:HB	4:AL:76:ALA:HB3	2.01	0.43
4:FL:68:ASP:O	4:FL:70:TYR:N	2.43	0.43
4:CL:174:THR:HG21	7:CH:90:ASN:HD21	1.84	0.43
4:EL:114:THR:HG23	4:EL:122:VAL:HG22	2.01	0.43
5:EM:102:PHE:C	5:EM:103:LEU:HD12	2.44	0.43
6:BA:22:ASP:OD1	6:BA:23:ALA:N	2.51	0.43
6:BA:37:GLU:O	6:BA:56:VAL:HG13	2.18	0.43
6:DA:119:LEU:HA	6:DA:129:TYR:HA	2.01	0.43
7:BH:278:ILE:HG22	7:BH:299:VAL:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:DH:94:ASP:O	7:DH:97:VAL:HG12	2.19	0.43
7:DG:382:ASP:OD1	7:DG:382:ASP:N	2.52	0.43
7:DI:7:THR:O	7:DI:7:THR:HG22	2.19	0.43
7:AH:188:MET:HE1	7:AH:201:ARG:NE	2.33	0.43
7:AH:283:TYR:OH	7:AH:291:LYS:NZ	2.51	0.43
7:AI:358:ASP:OD1	7:AI:360:LYS:N	2.51	0.43
7:EI:195:ASN:OD1	7:EI:196:GLY:N	2.52	0.43
1:CD:97:GLU:CD	6:AB:48:GLY:CA	2.88	0.43
3:BF:1151:GLU:HG3	2:BE:87:ARG:HB3	2.01	0.43
1:BC:29:MET:SD	1:BC:54:ARG:NE	2.92	0.43
4:CL:68:ASP:O	4:CL:70:TYR:N	2.44	0.43
5:FM:87:PRO:HG2	5:FM:90:VAL:HG23	2.00	0.43
6:EB:139:PHE:HE2	6:BB:77:GLU:OE2	2.02	0.43
6:DA:83:ARG:NH1	6:DA:114:HIS:O	2.52	0.43
7:AI:7:THR:O	7:AI:7:THR:HG22	2.19	0.43
7:EG:259:ASN:OD1	7:EG:259:ASN:N	2.52	0.43
2:AE:129:LYS:NZ	2:AE:130:VAL:O	2.46	0.42
1:CD:136:GLN:NE2	1:CD:169:GLU:OE1	2.50	0.42
1:CD:194:TRP:HB3	7:CI:15:TYR:HA	2.01	0.42
4:DK:151:ILE:HD13	4:DL:155:ILE:HG12	2.01	0.42
4:FJ:164:GLN:O	4:FJ:168:ASN:ND2	2.52	0.42
4:FK:32:TYR:HB2	4:CJ:123:VAL:CG1	2.49	0.42
4:FK:63:ILE:HD11	4:FK:94:TYR:CD2	2.54	0.42
4:EL:51:PRO:CD	5:EM:81:PHE:HD2	2.32	0.42
5:AM:106:GLU:O	5:AM:107:GLU:HB3	2.19	0.42
5:EM:46:ILE:HD11	5:EM:51:HIS:CE1	2.53	0.42
6:BB:29:LEU:HD23	6:BB:29:LEU:H	1.84	0.42
6:BB:165:THR:HG23	6:BB:165:THR:O	2.19	0.42
6:BA:7:SER:HB2	6:DA:121:ALA:HB1	2.00	0.42
6:DA:5:LYS:O	6:AA:126:ILE:HA	2.19	0.42
7:FG:259:ASN:OD1	7:FG:259:ASN:N	2.52	0.42
7:CH:324:SER:OG	7:CH:325:ASP:N	2.50	0.42
7:CG:44:ASN:O	7:CI:54:GLN:NE2	2.52	0.42
1:AD:111:VAL:HG11	6:DB:111:GLN:HE22	1.84	0.42
1:BD:193:ASP:OD1	1:BD:194:TRP:N	2.52	0.42
1:BD:232:ILE:HG22	1:BD:305:VAL:HG23	2.01	0.42
2:BE:222:HIS:O	2:BE:222:HIS:ND1	2.50	0.42
4:BK:63:ILE:HD11	4:BK:94:TYR:CD2	2.54	0.42
4:BL:171:ASP:O	4:BL:174:THR:HG22	2.19	0.42
4:DJ:107:VAL:O	4:DJ:107:VAL:HG13	2.18	0.42
4:DJ:111:ALA:O	4:DJ:123:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AL:88:ILE:CD1	5:AM:85:LYS:NZ	2.83	0.42
4:CJ:107:VAL:O	4:CJ:107:VAL:HG13	2.18	0.42
5:DM:106:GLU:O	5:DM:107:GLU:HB3	2.19	0.42
5:EM:7:VAL:HG22	5:EM:8:GLU:N	2.33	0.42
6:EB:7:SER:OG	6:BB:122:GLU:O	2.34	0.42
6:EA:105:PHE:CD1	6:EA:105:PHE:N	2.86	0.42
6:BA:11:ILE:HB	6:BA:91:VAL:HG13	2.00	0.42
6:BA:35:SER:OG	6:BA:59:THR:O	2.36	0.42
6:AB:15:ARG:NH1	6:AB:87:GLU:OE2	2.50	0.42
6:AA:119:LEU:HA	6:AA:129:TYR:HA	2.01	0.42
6:FB:112:GLY:C	6:FB:133:TYR:HE1	2.27	0.42
6:CA:43:GLU:HB3	6:CA:50:TYR:OH	2.19	0.42
7:AG:157:SER:O	7:AG:157:SER:OG	2.35	0.42
7:AG:259:ASN:OD1	7:AG:259:ASN:N	2.52	0.42
7:FH:283:TYR:OH	7:FH:291:LYS:NZ	2.52	0.42
7:EG:157:SER:O	7:EG:157:SER:OG	2.35	0.42
1:BC:100:TYR:CG	6:BB:111:GLN:NE2	2.87	0.42
1:BD:194:TRP:O	1:BD:196:ALA:N	2.52	0.42
4:BJ:80:ASP:OD1	4:BJ:80:ASP:N	2.52	0.42
4:FL:67:THR:HB	4:FL:76:ALA:HB3	2.00	0.42
4:CL:88:ILE:CD1	5:CM:85:LYS:HE3	2.49	0.42
6:BA:83:ARG:NH1	6:BA:114:HIS:O	2.52	0.42
6:DA:11:ILE:HB	6:DA:91:VAL:HG13	2.00	0.42
6:AB:7:SER:O	6:AB:8:ASN:C	2.63	0.42
7:FG:390:ASP:OD1	7:FG:391:MET:N	2.52	0.42
7:CI:440:THR:OG1	7:CI:441:ASP:N	2.51	0.42
7:EH:147:GLU:O	7:EH:368:ARG:NH2	2.51	0.42
7:EH:226:SER:OG	7:EH:227:ALA:N	2.53	0.42
7:EH:264:ARG:NH1	7:EH:287:GLU:OE2	2.52	0.42
7:EG:263:ASP:OD1	7:EG:264:ARG:N	2.47	0.42
1:AC:26:ILE:HD11	1:CD:74:ARG:CZ	2.49	0.42
1:AC:281:GLU:O	2:AE:295:GLN:NE2	2.50	0.42
1:AD:20:ILE:HD11	6:BB:50:TYR:CD2	2.47	0.42
1:AD:129:GLN:O	7:AG:16:ARG:NH1	2.52	0.42
1:BC:223:GLN:HA	1:BD:41:MET:HE1	2.01	0.42
4:DL:88:ILE:HD12	5:DM:85:LYS:CE	2.47	0.42
4:CL:67:THR:HB	4:CL:76:ALA:HB3	2.00	0.42
4:EJ:111:ALA:O	4:EJ:123:VAL:HG23	2.19	0.42
4:EK:80:ASP:N	4:EK:80:ASP:OD1	2.51	0.42
5:AM:7:VAL:HG22	5:AM:8:GLU:N	2.33	0.42
5:AM:102:PHE:C	5:AM:103:LEU:HD12	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CM:106:GLU:O	5:CM:107:GLU:HB3	2.19	0.42
6:EA:7:SER:N	6:BA:125:GLY:O	2.37	0.42
6:BB:166:LYS:HG2	6:BB:166:LYS:O	2.19	0.42
6:BA:7:SER:OG	6:DA:122:GLU:O	2.34	0.42
6:BA:40:THR:HG21	6:DA:83:ARG:NH2	2.34	0.42
6:FA:40:THR:HG21	6:CA:83:ARG:NH2	2.34	0.42
7:AH:226:SER:OG	7:AH:227:ALA:N	2.52	0.42
7:FH:370:ILE:HB	7:FH:372:ILE:HD11	2.01	0.42
7:FG:266:THR:HG23	7:FG:281:ARG:CG	2.49	0.42
7:CH:94:ASP:O	7:CH:97:VAL:HG12	2.19	0.42
7:CG:259:ASN:OD1	7:CG:259:ASN:N	2.53	0.42
1:AC:102:PHE:CE1	6:AB:142:GLY:O	2.72	0.42
1:AC:136:GLN:NE2	1:AC:169:GLU:OE1	2.50	0.42
1:AC:163:THR:O	1:AD:44:ARG:NH1	2.52	0.42
1:AD:69:ASP:CG	7:DH:15:TYR:CE1	2.95	0.42
1:AD:193:ASP:OD1	1:AD:194:TRP:N	2.53	0.42
1:CD:97:GLU:OE1	6:AB:47:ASP:C	2.61	0.42
1:BD:29:MET:SD	1:BD:54:ARG:NE	2.92	0.42
4:BJ:164:GLN:O	4:BJ:168:ASN:ND2	2.53	0.42
4:BL:49:ASN:O	5:BM:78:VAL:CG1	2.68	0.42
4:AK:81:GLU:C	4:AK:82:LEU:HD22	2.44	0.42
4:FL:91:ARG:HH22	5:FM:76:ASP:N	2.17	0.42
4:CL:114:THR:CG2	4:CL:122:VAL:HG22	2.50	0.42
5:BM:7:VAL:HG22	5:BM:8:GLU:N	2.34	0.42
5:FM:7:VAL:HG22	5:FM:8:GLU:N	2.34	0.42
5:CN:111:HIS:NE2	5:CN:114:ASN:OD1	2.44	0.42
6:EA:119:LEU:HA	6:EA:129:TYR:HA	2.01	0.42
6:DB:119:LEU:C	6:DB:119:LEU:HD12	2.44	0.42
6:DB:162:HIS:O	6:DA:89:TRP:HH2	2.03	0.42
6:DA:37:GLU:O	6:DA:56:VAL:HG13	2.18	0.42
6:CA:119:LEU:HA	6:CA:129:TYR:HA	2.01	0.42
7:DH:411:GLY:N	7:DG:452:GLN:OE1	2.52	0.42
7:DI:554:LEU:O	7:DI:601:GLN:NE2	2.44	0.42
7:CG:200:ASP:OD1	7:CG:201:ARG:N	2.50	0.42
7:CG:592:LYS:HB2	7:CG:600:THR:HG23	2.01	0.42
7:CI:427:ASN:OD1	7:CI:428:GLN:N	2.53	0.42
7:EH:94:ASP:O	7:EH:97:VAL:HG12	2.20	0.42
7:EH:315:GLN:NE2	7:EH:317:ASP:OD1	2.46	0.42
7:EI:7:THR:O	7:EI:7:THR:HG22	2.19	0.42
7:EI:427:ASN:OD1	7:EI:428:GLN:N	2.53	0.42
1:CD:29:MET:SD	1:CD:54:ARG:NE	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:39:GLY:H	4:BL:136:VAL:HG12	1.85	0.42
4:DL:25:ILE:HG12	4:DL:121:VAL:HG21	2.01	0.42
4:DL:151:ILE:O	4:DL:151:ILE:HG12	2.20	0.42
4:FJ:48:ASN:OD1	4:FJ:49:ASN:N	2.46	0.42
4:CJ:17:THR:O	4:CJ:17:THR:OG1	2.37	0.42
6:EB:72:PHE:O	6:EB:75:GLU:N	2.52	0.42
6:FB:12:ILE:HD11	6:FB:32:TYR:CE2	2.55	0.42
7:BG:382:ASP:N	7:BG:382:ASP:OD1	2.52	0.42
7:BI:7:THR:O	7:BI:7:THR:HG22	2.18	0.42
7:AH:147:GLU:O	7:AH:368:ARG:NH2	2.53	0.42
7:CH:455:ALA:O	7:CH:477:LEU:N	2.52	0.42
7:CI:222:LEU:O	7:CI:241:GLN:NE2	2.52	0.42
7:CI:317:ASP:OD1	7:CI:318:ILE:N	2.50	0.42
2:AE:118:GLN:O	2:AE:144:ARG:NH2	2.53	0.42
2:AE:253:GLN:NE2	2:AE:257:ASP:OD2	2.53	0.42
1:CD:95:LYS:HD3	7:CG:8:ASP:O	2.19	0.42
1:CD:107:SER:CA	6:FB:22:ASP:N	2.83	0.42
4:BJ:32:TYR:OH	4:BK:22:ASN:O	2.37	0.42
4:BJ:35:ASP:O	4:BK:121:VAL:HG22	2.19	0.42
4:BL:151:ILE:HG12	4:BL:151:ILE:O	2.20	0.42
4:DL:88:ILE:CD1	5:DM:85:LYS:HE2	2.50	0.42
4:AJ:32:TYR:OH	4:AK:22:ASN:O	2.37	0.42
4:FK:148:ILE:CG2	4:FL:151:ILE:HD11	2.49	0.42
4:EJ:11:ASN:OD1	4:EJ:11:ASN:N	2.53	0.42
4:EL:171:ASP:O	4:EL:174:THR:HG22	2.20	0.42
6:BB:7:SER:OG	6:DB:122:GLU:O	2.24	0.42
6:AA:146:LEU:HD12	6:AA:146:LEU:N	2.35	0.42
6:FA:112:GLY:N	6:FA:133:TYR:OH	2.47	0.42
7:AH:94:ASP:O	7:AH:97:VAL:HG12	2.20	0.42
7:FG:232:ASN:O	7:FG:234:ASN:N	2.53	0.42
7:EI:197:GLN:NE2	7:EI:462:GLU:OE1	2.53	0.42
7:EI:390:ASP:OD1	7:EI:391:MET:N	2.53	0.42
2:AE:222:HIS:O	2:AE:222:HIS:ND1	2.50	0.42
4:DL:49:ASN:O	5:DM:78:VAL:CG1	2.68	0.42
4:CK:128:SER:OG	4:CK:129:PHE:N	2.52	0.42
5:AM:47:ASP:OD1	5:AM:47:ASP:N	2.48	0.42
6:EA:5:LYS:O	6:BA:126:ILE:HA	2.20	0.42
6:AB:148:GLU:HG2	6:AB:149:ALA:N	2.35	0.42
6:CA:146:LEU:HD12	6:CA:146:LEU:N	2.34	0.42
7:DH:195:ASN:ND2	7:DH:197:GLN:OE1	2.50	0.42
7:CI:548:PRO:O	7:CI:573:ARG:NH1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:193:ASP:OD1	1:AC:194:TRP:N	2.53	0.42
3:CF:1140:ILE:HD11	3:BF:1135:ASP:N	2.34	0.42
1:CC:22:ASN:HA	6:FB:45:THR:HG22	2.01	0.42
1:CD:193:ASP:CG	7:CH:11:ARG:O	2.63	0.42
4:DL:51:PRO:HG3	5:DM:75:ASP:OD2	2.20	0.42
4:FL:171:ASP:O	4:FL:174:THR:HG22	2.19	0.42
6:DB:64:ALA:HB3	6:DB:129:TYR:CZ	2.54	0.42
6:FB:28:PHE:CD2	6:FB:67:PHE:CD1	3.08	0.42
6:CA:37:GLU:C	6:CA:56:VAL:HG13	2.45	0.42
7:BG:345:ASP:O	7:BG:347:LYS:N	2.52	0.42
7:BI:317:ASP:OD1	7:BI:318:ILE:N	2.50	0.42
7:DI:197:GLN:NE2	7:DI:462:GLU:OE1	2.53	0.42
7:AI:427:ASN:OD1	7:AI:428:GLN:N	2.52	0.42
7:AI:473:THR:O	7:AI:486:ARG:NH2	2.53	0.42
7:CH:401:ALA:CB	7:CH:426:VAL:HG21	2.49	0.42
2:CE:222:HIS:O	2:CE:222:HIS:ND1	2.50	0.42
1:BC:153:LYS:HE2	6:EB:43:GLU:CD	2.43	0.42
4:FJ:11:ASN:OD1	4:FJ:11:ASN:N	2.53	0.42
4:CL:39:GLY:H	4:CL:136:VAL:HG12	1.85	0.42
4:CL:171:ASP:O	4:CL:174:THR:HG22	2.19	0.42
6:EB:41:ASP:O	6:EB:52:THR:OG1	2.24	0.42
6:BB:12:ILE:HD11	6:BB:32:TYR:CE2	2.55	0.42
6:FA:5:LYS:O	6:CA:126:ILE:HA	2.19	0.42
7:BH:411:GLY:N	7:BG:452:GLN:OE1	2.53	0.42
7:BH:440:THR:OG1	7:BH:445:ARG:O	2.23	0.42
7:DI:427:ASN:OD1	7:DI:428:GLN:N	2.52	0.42
7:AI:195:ASN:OD1	7:AI:196:GLY:N	2.52	0.42
7:FI:509:ARG:NH2	7:FI:515:ASN:O	2.52	0.42
7:CG:232:ASN:O	7:CG:234:ASN:N	2.53	0.42
7:CG:382:ASP:N	7:CG:382:ASP:OD1	2.51	0.42
1:BC:14:LEU:O	1:BC:17:TYR:N	2.48	0.41
1:BC:194:TRP:O	1:BC:196:ALA:N	2.52	0.41
1:BD:192:ILE:O	7:BH:12:VAL:C	2.63	0.41
4:FL:39:GLY:H	4:FL:136:VAL:HG12	1.85	0.41
4:CK:10:ASP:OD1	4:CK:11:ASN:N	2.53	0.41
4:EK:50:ARG:HB2	4:EK:51:PRO:HD2	2.02	0.41
5:BM:57:LEU:CD2	5:BM:72:LEU:HD13	2.45	0.41
5:DM:87:PRO:HG2	5:DM:90:VAL:HG23	2.01	0.41
5:AM:57:LEU:CD2	5:AM:72:LEU:HD13	2.47	0.41
5:AM:59:LEU:HA	5:AM:99:CYS:HA	2.02	0.41
5:EM:106:GLU:O	5:EM:107:GLU:HB3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:EA:47:ASP:OD2	6:BB:28:PHE:N	2.47	0.41
6:BA:5:LYS:O	6:DA:126:ILE:HA	2.19	0.41
6:BA:119:LEU:HA	6:BA:129:TYR:HA	2.01	0.41
6:AA:42:THR:OG1	6:AA:50:TYR:O	2.35	0.41
7:FH:264:ARG:NH1	7:FH:287:GLU:OE2	2.53	0.41
7:FG:218:ILE:HD12	7:FG:223:TRP:CD1	2.55	0.41
7:CI:605:ARG:NH1	7:CI:611:ALA:O	2.47	0.41
1:CC:153:LYS:CE	6:FB:43:GLU:OE2	2.68	0.41
1:CD:180:ASN:HB2	7:CI:12:VAL:HG22	2.01	0.41
1:BC:193:ASP:OD1	1:BC:194:TRP:N	2.53	0.41
2:BE:118:GLN:O	2:BE:144:ARG:NH2	2.53	0.41
4:BJ:36:ARG:H	4:BJ:101:LEU:HD12	1.85	0.41
4:BJ:123:VAL:CG1	4:EK:32:TYR:HB2	2.50	0.41
5:DM:47:ASP:OD1	5:DM:47:ASP:N	2.48	0.41
5:DM:103:LEU:HD12	5:DM:103:LEU:N	2.35	0.41
6:BA:70:ASP:OD1	6:BA:72:PHE:N	2.53	0.41
6:AB:139:PHE:CE2	6:FB:77:GLU:OE2	2.74	0.41
6:FB:80:VAL:HG21	6:FB:117:PHE:HB2	2.02	0.41
6:FA:146:LEU:HD12	6:FA:146:LEU:N	2.35	0.41
7:BG:392:TYR:N	7:BG:401:ALA:O	2.50	0.41
7:DG:478:ASP:OD1	7:DG:521:ARG:NH2	2.53	0.41
7:DI:413:ASN:N	7:DI:413:ASN:OD1	2.50	0.41
7:FG:157:SER:O	7:FG:157:SER:OG	2.33	0.41
7:FG:200:ASP:OD1	7:FG:201:ARG:N	2.49	0.41
7:CG:266:THR:HG23	7:CG:281:ARG:CG	2.50	0.41
7:EH:182:ARG:NE	7:EH:188:MET:SD	2.93	0.41
7:EG:392:TYR:N	7:EG:401:ALA:O	2.50	0.41
1:AC:124:SER:N	1:AC:127:ASP:OD2	2.47	0.41
1:AD:153:LYS:HB2	6:BB:52:THR:HB	2.01	0.41
1:CD:193:ASP:OD1	1:CD:194:TRP:N	2.53	0.41
4:AL:114:THR:HG23	4:AL:122:VAL:HG22	2.01	0.41
4:AL:190:ILE:O	4:AL:194:GLN:HG2	2.20	0.41
4:CL:50:ARG:HB2	5:CM:81:PHE:HE2	1.80	0.41
4:CL:88:ILE:CD1	5:CM:85:LYS:HE2	2.44	0.41
6:EA:121:ALA:HB1	6:CA:7:SER:HB2	2.01	0.41
6:EA:127:ASP:OD2	6:CA:10:ARG:NH2	2.53	0.41
6:BB:7:SER:O	6:BB:8:ASN:C	2.63	0.41
6:BB:112:GLY:C	6:BB:133:TYR:HE1	2.28	0.41
6:DA:37:GLU:C	6:DA:56:VAL:HG13	2.45	0.41
6:DA:146:LEU:HD12	6:DA:146:LEU:N	2.34	0.41
6:AA:10:ARG:NH2	6:FA:127:ASP:OD2	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FA:10:ARG:NH2	6:CA:127:ASP:OD2	2.54	0.41
6:FA:119:LEU:HA	6:FA:129:TYR:HA	2.01	0.41
6:CB:166:LYS:O	6:CB:166:LYS:HG2	2.20	0.41
7:BG:259:ASN:OD1	7:BG:259:ASN:N	2.52	0.41
7:AI:390:ASP:OD1	7:AI:391:MET:N	2.53	0.41
7:FH:278:ILE:HD12	7:FH:332:ILE:HD11	2.03	0.41
7:EH:281:ARG:NH2	7:EH:298:GLU:OE2	2.48	0.41
2:CE:118:GLN:O	2:CE:144:ARG:NH2	2.53	0.41
4:AL:39:GLY:H	4:AL:136:VAL:HG12	1.86	0.41
4:FK:58:HIS:HB3	7:FG:83:GLY:N	2.36	0.41
4:FK:145:LEU:H	4:FK:145:LEU:HD23	1.86	0.41
4:EK:128:SER:OG	4:EK:129:PHE:N	2.53	0.41
5:BN:97:VAL:O	5:BN:97:VAL:HG23	2.20	0.41
5:CM:103:LEU:HD12	5:CM:103:LEU:N	2.35	0.41
6:EA:70:ASP:OD1	6:EA:72:PHE:N	2.53	0.41
6:DA:112:GLY:N	6:DA:133:TYR:OH	2.48	0.41
6:AA:105:PHE:CD1	6:AA:105:PHE:N	2.86	0.41
7:BH:278:ILE:HD12	7:BH:332:ILE:HD11	2.03	0.41
7:BH:283:TYR:OH	7:BH:291:LYS:NZ	2.54	0.41
7:AI:214:ALA:HB2	7:AI:269:ILE:HA	2.02	0.41
7:CH:69:PHE:O	7:CH:73:LEU:HD23	2.20	0.41
1:CC:193:ASP:OD1	1:CC:194:TRP:N	2.53	0.41
1:BC:223:GLN:HE22	1:BD:43:GLY:HA3	1.85	0.41
2:BE:253:GLN:NE2	2:BE:257:ASP:OD2	2.53	0.41
4:BK:145:LEU:HD23	4:BK:145:LEU:H	1.84	0.41
4:AK:65:LEU:HD11	4:AK:107:VAL:HG11	2.03	0.41
5:AN:110:ILE:CG1	5:AM:32:THR:HG21	2.51	0.41
6:EB:162:HIS:O	6:EA:89:TRP:HH2	2.03	0.41
6:EA:126:ILE:HA	6:CA:5:LYS:O	2.19	0.41
6:BB:159:TYR:OH	6:BA:138:ARG:O	2.29	0.41
6:FB:105:PHE:N	6:FB:144:ALA:O	2.44	0.41
6:FA:83:ARG:NH1	6:FA:114:HIS:O	2.53	0.41
7:BH:182:ARG:NE	7:BH:188:MET:SD	2.93	0.41
7:DG:232:ASN:O	7:DG:234:ASN:N	2.53	0.41
7:DG:451:ILE:HG22	7:DG:452:GLN:N	2.36	0.41
7:AH:288:ARG:HD2	7:AH:294:LEU:HD22	2.01	0.41
7:AI:197:GLN:NE2	7:AI:462:GLU:OE1	2.53	0.41
7:AI:440:THR:OG1	7:AI:441:ASP:N	2.53	0.41
7:EI:371:ASP:OD2	7:EI:371:ASP:N	2.50	0.41
1:CC:14:LEU:O	1:CC:17:TYR:N	2.48	0.41
2:CE:99:ILE:HD11	2:CE:147:MET:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CE:253:GLN:NE2	2:CE:257:ASP:OD2	2.53	0.41
1:BC:124:SER:C	7:BI:290:LEU:HD11	2.45	0.41
4:BK:50:ARG:NE	7:BG:79:ASN:OD1	2.53	0.41
4:DL:50:ARG:CD	5:DM:81:PHE:CZ	3.03	0.41
4:AJ:17:THR:HG22	4:AJ:124:GLU:OE2	2.20	0.41
4:AK:143:THR:HG23	4:AK:143:THR:O	2.21	0.41
4:AL:91:ARG:O	4:AL:92:LEU:HD12	2.21	0.41
4:CJ:17:THR:HG22	4:CJ:124:GLU:OE2	2.20	0.41
4:CJ:143:THR:HG22	4:CJ:147:TYR:HD2	1.85	0.41
5:BM:102:PHE:C	5:BM:103:LEU:HD12	2.46	0.41
5:AN:63:ASP:OD1	5:AN:63:ASP:N	2.49	0.41
6:EB:7:SER:O	6:EB:8:ASN:C	2.63	0.41
6:DB:7:SER:OG	6:AB:122:GLU:O	2.27	0.41
6:DA:7:SER:HB2	6:AA:121:ALA:HB1	2.01	0.41
6:DA:10:ARG:NH2	6:AA:127:ASP:OD2	2.53	0.41
7:BG:232:ASN:O	7:BG:234:ASN:N	2.53	0.41
7:DI:390:ASP:OD1	7:DI:391:MET:N	2.53	0.41
7:FG:80:MET:HE1	7:FI:77:PHE:CE1	2.55	0.41
1:AC:167:TYR:OH	1:AD:42:ASN:ND2	2.53	0.41
2:CE:58:GLU:OE1	2:CE:316:ARG:NH2	2.54	0.41
4:DJ:119:ASP:OD1	4:DJ:119:ASP:N	2.54	0.41
4:DJ:139:PHE:CD2	4:DJ:139:PHE:C	2.99	0.41
4:DJ:143:THR:HG22	4:DJ:147:TYR:HD2	1.85	0.41
4:EK:148:ILE:CG2	4:EL:151:ILE:HD11	2.50	0.41
4:EL:39:GLY:H	4:EL:136:VAL:HG12	1.85	0.41
6:BB:39:ASP:HB3	6:BB:55:SER:OG	2.20	0.41
6:DB:164:THR:OG1	6:DB:165:THR:N	2.54	0.41
6:DB:166:LYS:O	6:DB:166:LYS:HG2	2.19	0.41
6:AA:5:LYS:O	6:FA:126:ILE:HA	2.20	0.41
7:FI:263:ASP:OD2	7:FI:263:ASP:N	2.52	0.41
7:CG:451:ILE:HG22	7:CG:452:GLN:N	2.36	0.41
7:EH:288:ARG:HD2	7:EH:294:LEU:HD22	2.02	0.41
7:EI:493:ASP:OD1	7:EI:493:ASP:N	2.50	0.41
1:CC:194:TRP:O	1:CC:196:ALA:N	2.52	0.41
1:BC:69:ASP:CG	7:BH:15:TYR:HE1	2.22	0.41
2:BE:234:ALA:O	2:BE:238:GLY:N	2.49	0.41
4:BJ:141:GLY:O	4:BL:114:THR:CG2	2.69	0.41
4:FL:58:HIS:CE1	5:FN:43:GLN:HG2	2.56	0.41
4:CK:9:ASP:OD1	4:CK:42:ASN:ND2	2.39	0.41
4:CL:127:PHE:HB3	4:CL:143:THR:HG23	2.03	0.41
4:EK:65:LEU:HD11	4:EK:107:VAL:HG11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BM:103:LEU:HD12	5:BM:103:LEU:N	2.36	0.41
5:EM:103:LEU:HD12	5:EM:103:LEU:N	2.36	0.41
6:BA:146:LEU:N	6:BA:146:LEU:HD12	2.36	0.41
6:DA:141:ARG:HH22	6:AA:78:ASP:CG	2.29	0.41
6:AA:83:ARG:NH1	6:AA:114:HIS:O	2.53	0.41
6:CB:164:THR:OG1	6:CB:165:THR:N	2.53	0.41
6:CA:117:PHE:C	6:CA:117:PHE:CD1	2.99	0.41
7:BH:94:ASP:O	7:BH:97:VAL:HG12	2.21	0.41
7:BH:195:ASN:ND2	7:BH:197:GLN:OE1	2.47	0.41
7:FH:315:GLN:NE2	7:FH:317:ASP:OD1	2.51	0.41
7:CH:175:ILE:HD11	7:CI:375:VAL:CG1	2.51	0.41
1:AC:102:PHE:CE1	6:AB:142:GLY:C	2.99	0.41
1:AD:47:MET:O	2:AE:280:ARG:NH2	2.54	0.41
2:AE:58:GLU:OE1	2:AE:316:ARG:NH2	2.54	0.41
2:AE:87:ARG:NH2	2:BE:202:SER:OG	2.54	0.41
1:BD:97:GLU:OE2	6:CB:48:GLY:C	2.64	0.41
4:BJ:35:ASP:O	4:BJ:37:GLY:N	2.54	0.41
4:BK:9:ASP:OD1	4:BK:42:ASN:ND2	2.38	0.41
4:BL:127:PHE:HB3	4:BL:143:THR:HG23	2.03	0.41
4:DK:58:HIS:HB3	7:DG:83:GLY:N	2.35	0.41
4:DL:121:VAL:O	4:DL:121:VAL:HG13	2.20	0.41
4:AL:63:ILE:HG13	4:AL:82:LEU:HD21	2.03	0.41
4:FJ:47:LYS:HB2	4:FJ:52:LEU:HD21	2.02	0.41
4:EJ:32:TYR:OH	4:EK:22:ASN:O	2.39	0.41
4:EK:81:GLU:C	4:EK:82:LEU:HD22	2.46	0.41
4:EL:63:ILE:HG13	4:EL:82:LEU:HD21	2.03	0.41
4:EL:91:ARG:O	4:EL:92:LEU:HD12	2.21	0.41
4:EL:167:GLN:NE2	4:EL:171:ASP:OD1	2.54	0.41
5:DM:59:LEU:HA	5:DM:99:CYS:HA	2.03	0.41
5:FM:102:PHE:C	5:FM:103:LEU:HD12	2.46	0.41
5:EN:64:GLY:O	5:EN:65:SER:C	2.64	0.41
5:EM:75:ASP:HB2	5:EM:81:PHE:O	2.21	0.41
6:EB:39:ASP:HB3	6:EB:55:SER:OG	2.20	0.41
6:EA:83:ARG:NH1	6:EA:114:HIS:O	2.53	0.41
6:EA:117:PHE:CD1	6:EA:117:PHE:C	2.99	0.41
6:BB:80:VAL:HG21	6:BB:117:PHE:HB2	2.03	0.41
6:DB:15:ARG:NH1	6:DB:87:GLU:OE2	2.53	0.41
6:FA:70:ASP:OD1	6:FA:72:PHE:N	2.53	0.41
6:CB:7:SER:O	6:CB:8:ASN:C	2.63	0.41
6:CB:15:ARG:NH1	6:CB:87:GLU:OE2	2.54	0.41
7:BG:566:ILE:HD11	7:BG:589:LEU:HD23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:493:ASP:OD1	7:BI:493:ASP:N	2.53	0.41
7:BI:509:ARG:NH2	7:BI:515:ASN:O	2.53	0.41
7:DH:229:LEU:HD23	7:DH:229:LEU:H	1.86	0.41
7:DG:259:ASN:OD1	7:DG:259:ASN:N	2.53	0.41
7:AI:371:ASP:OD2	7:AI:371:ASP:N	2.50	0.41
7:FH:328:PRO:O	7:FH:343:THR:OG1	2.18	0.41
7:FH:455:ALA:O	7:FH:477:LEU:N	2.54	0.41
7:FG:566:ILE:HD11	7:FG:589:LEU:HD23	2.02	0.41
7:FI:7:THR:HG22	7:FI:7:THR:O	2.19	0.41
7:CG:478:ASP:OD1	7:CG:521:ARG:NH2	2.54	0.41
7:CI:390:ASP:OD1	7:CI:391:MET:N	2.54	0.41
7:EH:401:ALA:CB	7:EH:426:VAL:HG21	2.48	0.41
7:EG:232:ASN:O	7:EG:234:ASN:N	2.53	0.41
7:EG:266:THR:HG23	7:EG:281:ARG:CG	2.51	0.41
7:EI:440:THR:OG1	7:EI:441:ASP:N	2.53	0.41
1:AC:125:ARG:N	7:AI:290:LEU:HD11	2.36	0.41
1:AD:125:ARG:N	7:DI:290:LEU:HD11	2.36	0.41
1:CC:29:MET:SD	1:CC:54:ARG:NE	2.92	0.41
2:BE:99:ILE:HD11	2:BE:147:MET:HG3	2.03	0.41
4:DL:50:ARG:HB2	5:DM:81:PHE:HE2	1.81	0.41
4:FL:127:PHE:HB3	4:FL:143:THR:HG23	2.03	0.41
4:EJ:47:LYS:HB2	4:EJ:52:LEU:HD21	2.02	0.41
5:FM:75:ASP:HB2	5:FM:81:PHE:O	2.21	0.41
5:EN:60:PHE:N	5:EN:60:PHE:CD1	2.89	0.41
6:DA:5:LYS:HE3	6:AA:68:TYR:HA	2.03	0.41
6:AB:162:HIS:O	6:AA:89:TRP:HH2	2.04	0.41
6:CB:64:ALA:HB3	6:CB:129:TYR:CZ	2.56	0.41
6:CB:165:THR:O	6:CB:167:GLU:OE1	2.39	0.41
7:AH:195:ASN:OD1	7:AH:196:GLY:N	2.54	0.41
7:FI:390:ASP:OD1	7:FI:391:MET:N	2.54	0.41
7:CI:195:ASN:OD1	7:CI:196:GLY:N	2.54	0.41
7:EI:317:ASP:OD1	7:EI:318:ILE:N	2.50	0.41
1:AC:84:ILE:HG23	1:AD:51:TYR:CE1	2.56	0.40
1:AD:20:ILE:CD1	6:BB:50:TYR:CD2	3.01	0.40
1:AD:29:MET:SD	1:AD:54:ARG:NE	2.92	0.40
1:BC:84:ILE:HG23	1:BD:51:TYR:CE1	2.56	0.40
4:BJ:11:ASN:OD1	4:BJ:11:ASN:N	2.54	0.40
4:BJ:143:THR:HG22	4:BJ:147:TYR:HD2	1.86	0.40
4:BK:120:ASN:OD1	4:BK:120:ASN:N	2.54	0.40
4:DL:67:THR:HB	4:DL:76:ALA:HB3	2.03	0.40
4:AK:103:HIS:CE1	4:AK:145:LEU:HD22	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CJ:155:ILE:HD11	4:CL:165:LEU:HD13	2.03	0.40
5:CM:17:ASP:OD1	5:CM:17:ASP:N	2.54	0.40
5:CM:75:ASP:HB2	5:CM:81:PHE:O	2.21	0.40
5:EM:59:LEU:HA	5:EM:99:CYS:HA	2.02	0.40
6:EB:28:PHE:O	6:EB:64:ALA:HA	2.21	0.40
6:EA:141:ARG:CZ	6:BA:74:ASP:OD1	2.69	0.40
6:BA:7:SER:N	6:DA:125:GLY:O	2.36	0.40
6:BA:105:PHE:N	6:BA:105:PHE:CD1	2.88	0.40
6:AA:117:PHE:CD1	6:AA:117:PHE:C	2.99	0.40
6:FA:117:PHE:CD1	6:FA:117:PHE:C	2.99	0.40
7:DG:44:ASN:O	7:DI:54:GLN:NE2	2.54	0.40
7:EG:342:TYR:CE2	7:EG:386:ALA:HB1	2.57	0.40
7:EG:451:ILE:HG22	7:EG:452:GLN:N	2.37	0.40
2:AE:28:ASP:OD1	2:AE:28:ASP:N	2.54	0.40
1:CC:84:ILE:HG23	1:CD:51:TYR:CE1	2.56	0.40
1:BD:118:PHE:HE1	6:CB:51:ASN:O	2.05	0.40
1:BD:136:GLN:NE2	1:BD:169:GLU:OE1	2.50	0.40
2:BE:58:GLU:OE1	2:BE:316:ARG:NH2	2.54	0.40
4:BJ:140:ASP:OD2	4:BJ:143:THR:OG1	2.27	0.40
4:BK:80:ASP:OD1	4:BK:80:ASP:N	2.54	0.40
4:DJ:35:ASP:O	4:DJ:37:GLY:N	2.54	0.40
4:FJ:14:GLU:OE2	4:FJ:46:THR:HG21	2.21	0.40
4:FK:120:ASN:OD1	4:FK:120:ASN:N	2.54	0.40
5:DN:4:ILE:HA	5:DN:34:SER:O	2.21	0.40
6:EB:139:PHE:CE2	6:BB:77:GLU:OE2	2.73	0.40
6:EA:45:THR:HG22	6:EA:46:MET:N	2.36	0.40
6:AA:141:ARG:CZ	6:FA:74:ASP:OD1	2.69	0.40
6:FB:138:ARG:HG2	6:FB:139:PHE:O	2.21	0.40
6:FA:95:ILE:O	6:FA:95:ILE:HG22	2.21	0.40
7:DH:278:ILE:HD12	7:DH:332:ILE:HD11	2.03	0.40
7:DG:266:THR:HG23	7:DG:281:ARG:CG	2.51	0.40
7:DG:566:ILE:HD11	7:DG:589:LEU:HD23	2.03	0.40
7:DI:256:VAL:O	7:DI:256:VAL:HG23	2.22	0.40
7:FI:493:ASP:OD1	7:FI:493:ASP:N	2.53	0.40
7:CH:182:ARG:NE	7:CH:188:MET:SD	2.93	0.40
1:AC:29:MET:SD	1:AC:54:ARG:NE	2.92	0.40
1:BD:301:THR:OG1	7:BH:477:LEU:HD11	2.22	0.40
4:BJ:91:ARG:C	4:BJ:92:LEU:HD12	2.47	0.40
4:DL:39:GLY:H	4:DL:136:VAL:HG12	1.85	0.40
4:FL:174:THR:HG21	7:FH:90:ASN:HD21	1.87	0.40
4:CK:38:THR:OG1	4:EJ:121:VAL:O	2.40	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EJ:63:ILE:HB	4:EJ:82:LEU:HD21	2.04	0.40
5:BN:27:THR:OG1	5:BN:28:GLU:OE1	2.39	0.40
5:DN:27:THR:OG1	5:DN:28:GLU:OE1	2.40	0.40
5:FN:64:GLY:O	5:FN:65:SER:C	2.64	0.40
5:CM:112:VAL:HG13	5:CM:113:ALA:N	2.37	0.40
6:EA:68:TYR:HA	6:CA:5:LYS:HE3	2.03	0.40
6:EA:78:ASP:CG	6:CA:141:ARG:HH22	2.29	0.40
6:BA:11:ILE:C	6:BA:12:ILE:HD12	2.47	0.40
6:BA:37:GLU:C	6:BA:56:VAL:HG13	2.46	0.40
6:DB:39:ASP:HB3	6:DB:55:SER:OG	2.21	0.40
6:AB:138:ARG:HG2	6:AB:139:PHE:O	2.21	0.40
6:FA:37:GLU:C	6:FA:56:VAL:HG13	2.46	0.40
6:CB:26:MET:HE2	6:CB:64:ALA:HB2	2.03	0.40
6:CB:29:LEU:HD23	6:CB:29:LEU:H	1.84	0.40
7:BI:197:GLN:NE2	7:BI:462:GLU:OE1	2.54	0.40
7:AG:266:THR:HG23	7:AG:281:ARG:CG	2.51	0.40
7:CI:214:ALA:HB2	7:CI:269:ILE:HA	2.03	0.40
1:AC:153:LYS:CG	6:DB:52:THR:HB	2.51	0.40
1:AD:24:ILE:HG22	1:AD:58:VAL:HG22	2.03	0.40
1:AD:82:THR:HG22	1:AD:141:PHE:CE2	2.57	0.40
1:AD:194:TRP:O	1:AD:196:ALA:N	2.52	0.40
1:CD:107:SER:CB	6:FB:22:ASP:N	2.84	0.40
1:CD:194:TRP:O	1:CD:196:ALA:N	2.52	0.40
4:DJ:17:THR:HG22	4:DJ:124:GLU:CD	2.47	0.40
4:AK:13:ILE:HD13	4:AK:27:THR:HG22	2.03	0.40
4:AL:125:ARG:HE	4:AL:143:THR:HG21	1.86	0.40
4:FJ:80:ASP:OD1	4:FJ:80:ASP:N	2.52	0.40
5:AN:39:ILE:O	5:AN:45:ARG:HA	2.21	0.40
5:AM:75:ASP:HB2	5:AM:81:PHE:O	2.21	0.40
5:EN:66:ILE:HG23	5:EN:66:ILE:O	2.22	0.40
5:EN:110:ILE:CG1	5:EM:32:THR:HG21	2.51	0.40
6:EB:138:ARG:HG2	6:EB:139:PHE:O	2.22	0.40
6:AB:45:THR:OG1	6:AB:48:GLY:N	2.55	0.40
6:CA:45:THR:HG22	6:CA:46:MET:N	2.37	0.40
7:BH:270:TYR:HB2	7:BH:277:MET:HE2	2.02	0.40
7:BH:370:ILE:HB	7:BH:372:ILE:HD11	2.03	0.40
7:DI:300:ARG:NH1	7:DI:310:ASP:OD1	2.54	0.40
7:AG:232:ASN:O	7:AG:234:ASN:N	2.53	0.40
7:AG:342:TYR:CE2	7:AG:386:ALA:HB1	2.57	0.40
7:AI:578:PRO:HG3	7:AI:615:LEU:HD22	2.02	0.40
7:EH:195:ASN:OD1	7:EH:196:GLY:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:82:THR:HG22	1:AC:141:PHE:CE2	2.57	0.40
1:AD:188:PHE:CD1	7:AH:15:TYR:N	2.90	0.40
1:CC:102:PHE:CE1	6:CB:142:GLY:C	3.00	0.40
1:CC:105:PRO:HG3	6:CB:89:TRP:HE1	1.82	0.40
2:CE:28:ASP:N	2:CE:28:ASP:OD1	2.54	0.40
4:DJ:63:ILE:HB	4:DJ:82:LEU:HD21	2.04	0.40
5:FM:59:LEU:HA	5:FM:99:CYS:HA	2.03	0.40
5:CN:64:GLY:O	5:CN:65:SER:C	2.64	0.40
6:AB:67:PHE:CZ	6:AB:70:ASP:HB2	2.57	0.40
6:FA:35:SER:OG	6:FA:59:THR:O	2.36	0.40
6:FA:45:THR:HG22	6:FA:46:MET:N	2.36	0.40
6:CA:70:ASP:OD1	6:CA:72:PHE:N	2.54	0.40
7:AH:401:ALA:CB	7:AH:426:VAL:HG21	2.50	0.40
7:FG:451:ILE:HG22	7:FG:452:GLN:N	2.36	0.40
7:EH:175:ILE:HD11	7:EI:375:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	AD	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	BC	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	BD	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	CC	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	CD	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
2	AE	385/633 (61%)	339 (88%)	46 (12%)	0	100	100
2	BE	385/633 (61%)	339 (88%)	46 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CE	385/633 (61%)	339 (88%)	46 (12%)	0	100	100
3	AF	18/1154 (2%)	17 (94%)	1 (6%)	0	100	100
3	BF	18/1154 (2%)	17 (94%)	1 (6%)	0	100	100
3	CF	18/1154 (2%)	17 (94%)	1 (6%)	0	100	100
4	AJ	165/607 (27%)	137 (83%)	28 (17%)	0	100	100
4	AK	187/607 (31%)	169 (90%)	18 (10%)	0	100	100
4	AL	179/607 (30%)	158 (88%)	21 (12%)	0	100	100
4	BJ	165/607 (27%)	133 (81%)	32 (19%)	0	100	100
4	BK	187/607 (31%)	166 (89%)	21 (11%)	0	100	100
4	BL	179/607 (30%)	157 (88%)	22 (12%)	0	100	100
4	CJ	165/607 (27%)	136 (82%)	28 (17%)	1 (1%)	21	52
4	CK	187/607 (31%)	169 (90%)	18 (10%)	0	100	100
4	CL	179/607 (30%)	159 (89%)	20 (11%)	0	100	100
4	DJ	165/607 (27%)	136 (82%)	29 (18%)	0	100	100
4	DK	187/607 (31%)	168 (90%)	19 (10%)	0	100	100
4	DL	179/607 (30%)	160 (89%)	19 (11%)	0	100	100
4	EJ	165/607 (27%)	137 (83%)	28 (17%)	0	100	100
4	EK	187/607 (31%)	166 (89%)	21 (11%)	0	100	100
4	EL	179/607 (30%)	158 (88%)	21 (12%)	0	100	100
4	FJ	165/607 (27%)	133 (81%)	32 (19%)	0	100	100
4	FK	187/607 (31%)	166 (89%)	21 (11%)	0	100	100
4	FL	179/607 (30%)	158 (88%)	21 (12%)	0	100	100
5	AM	121/390 (31%)	102 (84%)	19 (16%)	0	100	100
5	AN	119/390 (30%)	103 (87%)	16 (13%)	0	100	100
5	BM	121/390 (31%)	101 (84%)	20 (16%)	0	100	100
5	BN	119/390 (30%)	106 (89%)	13 (11%)	0	100	100
5	CM	121/390 (31%)	101 (84%)	20 (16%)	0	100	100
5	CN	119/390 (30%)	104 (87%)	15 (13%)	0	100	100
5	DM	121/390 (31%)	100 (83%)	21 (17%)	0	100	100
5	DN	119/390 (30%)	104 (87%)	15 (13%)	0	100	100
5	EM	121/390 (31%)	102 (84%)	19 (16%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	EN	119/390 (30%)	103 (87%)	16 (13%)	0	100	100
5	FM	121/390 (31%)	102 (84%)	19 (16%)	0	100	100
5	FN	119/390 (30%)	106 (89%)	13 (11%)	0	100	100
6	AA	145/193 (75%)	139 (96%)	6 (4%)	0	100	100
6	AB	164/193 (85%)	152 (93%)	12 (7%)	0	100	100
6	BA	145/193 (75%)	140 (97%)	5 (3%)	0	100	100
6	BB	164/193 (85%)	147 (90%)	17 (10%)	0	100	100
6	CA	145/193 (75%)	142 (98%)	3 (2%)	0	100	100
6	CB	164/193 (85%)	146 (89%)	18 (11%)	0	100	100
6	DA	145/193 (75%)	142 (98%)	3 (2%)	0	100	100
6	DB	164/193 (85%)	149 (91%)	15 (9%)	0	100	100
6	EA	145/193 (75%)	139 (96%)	6 (4%)	0	100	100
6	EB	164/193 (85%)	150 (92%)	14 (8%)	0	100	100
6	FA	145/193 (75%)	141 (97%)	4 (3%)	0	100	100
6	FB	164/193 (85%)	148 (90%)	16 (10%)	0	100	100
7	AG	633/636 (100%)	567 (90%)	65 (10%)	1 (0%)	43	72
7	AH	632/636 (99%)	576 (91%)	56 (9%)	0	100	100
7	AI	632/636 (99%)	579 (92%)	53 (8%)	0	100	100
7	BG	633/636 (100%)	570 (90%)	62 (10%)	1 (0%)	43	72
7	BH	632/636 (99%)	576 (91%)	56 (9%)	0	100	100
7	BI	632/636 (99%)	581 (92%)	51 (8%)	0	100	100
7	CG	633/636 (100%)	567 (90%)	65 (10%)	1 (0%)	43	72
7	CH	632/636 (99%)	577 (91%)	55 (9%)	0	100	100
7	CI	632/636 (99%)	582 (92%)	50 (8%)	0	100	100
7	DG	633/636 (100%)	567 (90%)	65 (10%)	1 (0%)	43	72
7	DH	632/636 (99%)	576 (91%)	56 (9%)	0	100	100
7	DI	632/636 (99%)	582 (92%)	50 (8%)	0	100	100
7	EG	633/636 (100%)	570 (90%)	62 (10%)	1 (0%)	43	72
7	EH	632/636 (99%)	576 (91%)	56 (9%)	0	100	100
7	EI	632/636 (99%)	580 (92%)	52 (8%)	0	100	100
7	FG	633/636 (100%)	569 (90%)	63 (10%)	1 (0%)	43	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	FH	632/636 (99%)	571 (90%)	61 (10%)	0	100	100
7	FI	632/636 (99%)	578 (92%)	54 (8%)	0	100	100
All	All	20943/36621 (57%)	18815 (90%)	2121 (10%)	7 (0%)	100	100

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	DG	481	LEU
7	CG	481	LEU
7	BG	481	LEU
7	AG	481	LEU
7	FG	481	LEU
7	EG	481	LEU
4	CJ	23	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	AC	288/290 (99%)	284 (99%)	4 (1%)	59	70
1	AD	288/290 (99%)	284 (99%)	4 (1%)	59	70
1	BC	288/290 (99%)	284 (99%)	4 (1%)	59	70
1	BD	288/290 (99%)	284 (99%)	4 (1%)	59	70
1	CC	288/290 (99%)	284 (99%)	4 (1%)	59	70
1	CD	288/290 (99%)	284 (99%)	4 (1%)	59	70
2	AE	339/549 (62%)	337 (99%)	2 (1%)	78	79
2	BE	339/549 (62%)	337 (99%)	2 (1%)	78	79
2	CE	339/549 (62%)	337 (99%)	2 (1%)	78	79
3	AF	17/965 (2%)	17 (100%)	0	100	100
3	BF	17/965 (2%)	17 (100%)	0	100	100
3	CF	17/965 (2%)	17 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AJ	152/526 (29%)	152 (100%)	0	100	100
4	AK	170/526 (32%)	170 (100%)	0	100	100
4	AL	161/526 (31%)	161 (100%)	0	100	100
4	BJ	152/526 (29%)	152 (100%)	0	100	100
4	BK	170/526 (32%)	170 (100%)	0	100	100
4	BL	161/526 (31%)	161 (100%)	0	100	100
4	CJ	152/526 (29%)	152 (100%)	0	100	100
4	CK	170/526 (32%)	170 (100%)	0	100	100
4	CL	161/526 (31%)	161 (100%)	0	100	100
4	DJ	152/526 (29%)	152 (100%)	0	100	100
4	DK	170/526 (32%)	170 (100%)	0	100	100
4	DL	161/526 (31%)	161 (100%)	0	100	100
4	EJ	152/526 (29%)	152 (100%)	0	100	100
4	EK	170/526 (32%)	170 (100%)	0	100	100
4	EL	161/526 (31%)	161 (100%)	0	100	100
4	FJ	152/526 (29%)	152 (100%)	0	100	100
4	FK	170/526 (32%)	170 (100%)	0	100	100
4	FL	161/526 (31%)	161 (100%)	0	100	100
5	AM	109/342 (32%)	109 (100%)	0	100	100
5	AN	108/342 (32%)	108 (100%)	0	100	100
5	BM	109/342 (32%)	109 (100%)	0	100	100
5	BN	108/342 (32%)	108 (100%)	0	100	100
5	CM	109/342 (32%)	109 (100%)	0	100	100
5	CN	108/342 (32%)	108 (100%)	0	100	100
5	DM	109/342 (32%)	109 (100%)	0	100	100
5	DN	108/342 (32%)	108 (100%)	0	100	100
5	EM	109/342 (32%)	109 (100%)	0	100	100
5	EN	108/342 (32%)	108 (100%)	0	100	100
5	FM	109/342 (32%)	109 (100%)	0	100	100
5	FN	108/342 (32%)	108 (100%)	0	100	100
6	AA	120/160 (75%)	120 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AB	136/160 (85%)	136 (100%)	0	100	100
6	BA	120/160 (75%)	120 (100%)	0	100	100
6	BB	136/160 (85%)	136 (100%)	0	100	100
6	CA	120/160 (75%)	120 (100%)	0	100	100
6	CB	136/160 (85%)	136 (100%)	0	100	100
6	DA	120/160 (75%)	120 (100%)	0	100	100
6	DB	136/160 (85%)	136 (100%)	0	100	100
6	EA	120/160 (75%)	120 (100%)	0	100	100
6	EB	136/160 (85%)	136 (100%)	0	100	100
6	FA	120/160 (75%)	120 (100%)	0	100	100
6	FB	136/160 (85%)	136 (100%)	0	100	100
7	AG	561/562 (100%)	561 (100%)	0	100	100
7	AH	560/562 (100%)	560 (100%)	0	100	100
7	AI	560/562 (100%)	560 (100%)	0	100	100
7	BG	561/562 (100%)	561 (100%)	0	100	100
7	BH	560/562 (100%)	560 (100%)	0	100	100
7	BI	560/562 (100%)	560 (100%)	0	100	100
7	CG	561/562 (100%)	561 (100%)	0	100	100
7	CH	560/562 (100%)	560 (100%)	0	100	100
7	CI	560/562 (100%)	560 (100%)	0	100	100
7	DG	561/562 (100%)	561 (100%)	0	100	100
7	DH	560/562 (100%)	560 (100%)	0	100	100
7	DI	560/562 (100%)	560 (100%)	0	100	100
7	EG	561/562 (100%)	561 (100%)	0	100	100
7	EH	560/562 (100%)	560 (100%)	0	100	100
7	EI	560/562 (100%)	560 (100%)	0	100	100
7	FG	561/562 (100%)	561 (100%)	0	100	100
7	FH	560/562 (100%)	560 (100%)	0	100	100
7	FI	560/562 (100%)	560 (100%)	0	100	100
All	All	18618/31890 (58%)	18588 (100%)	30 (0%)	85	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AC	37	ASP
1	AC	39	GLU
1	AC	150	LYS
1	AC	285	SER
1	AD	37	ASP
1	AD	39	GLU
1	AD	150	LYS
1	AD	285	SER
2	AE	72	ASP
2	AE	75	SER
1	CC	37	ASP
1	CC	39	GLU
1	CC	150	LYS
1	CC	285	SER
1	CD	37	ASP
1	CD	39	GLU
1	CD	150	LYS
1	CD	285	SER
2	CE	72	ASP
2	CE	75	SER
1	BC	37	ASP
1	BC	39	GLU
1	BC	150	LYS
1	BC	285	SER
1	BD	37	ASP
1	BD	39	GLU
1	BD	150	LYS
1	BD	285	SER
2	BE	72	ASP
2	BE	75	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	AC	50	ASN
1	AC	207	ASN
1	AD	40	ASN
1	AD	207	ASN
2	AE	154	HIS
2	AE	343	ASN
2	AE	347	ASN
2	AE	359	ASN
3	CF	1145	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	CF	1149	ASN
1	CC	50	ASN
1	CC	207	ASN
1	CD	40	ASN
1	CD	207	ASN
2	CE	347	ASN
3	BF	1149	ASN
1	BC	207	ASN
1	BC	223	GLN
1	BC	225	ASN
1	BD	42	ASN
1	BD	66	ASN
1	BD	207	ASN
2	BE	343	ASN
2	BE	347	ASN
3	AF	1149	ASN
4	BJ	5	ASN
4	BJ	22	ASN
4	BJ	126	GLN
4	BJ	168	ASN
4	BK	173	GLN
4	DJ	5	ASN
4	DJ	22	ASN
4	DJ	126	GLN
4	DJ	168	ASN
4	DK	173	GLN
4	AJ	5	ASN
4	AJ	20	GLN
4	AJ	22	ASN
4	AJ	126	GLN
4	AJ	168	ASN
4	AK	173	GLN
4	FJ	5	ASN
4	FJ	22	ASN
4	FJ	126	GLN
4	FJ	168	ASN
4	FK	173	GLN
4	CJ	5	ASN
4	CJ	22	ASN
4	CJ	126	GLN
4	CJ	168	ASN
4	CK	173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	EJ	5	ASN
4	EJ	22	ASN
4	EJ	126	GLN
4	EJ	168	ASN
4	EL	89	ASN
5	BN	118	ASN
5	DN	118	ASN
5	DM	118	ASN
5	AN	118	ASN
5	FN	43	GLN
5	FN	118	ASN
5	FM	118	ASN
5	CN	43	GLN
5	CN	118	ASN
5	EN	43	GLN
5	EN	118	ASN
6	BB	111	GLN
6	BB	162	HIS
6	BA	111	GLN
6	DB	111	GLN
6	DA	111	GLN
6	FB	162	HIS
6	FA	111	GLN
6	CB	162	HIS
6	CA	111	GLN
7	BH	3	ASN
7	BH	90	ASN
7	BH	350	ASN
7	BH	510	ASN
7	BH	613	GLN
7	BH	618	ASN
7	BG	90	ASN
7	BG	500	ASN
7	BI	165	GLN
7	BI	377	ASN
7	BI	613	GLN
7	DH	90	ASN
7	DH	235	ASN
7	DH	327	GLN
7	DH	350	ASN
7	DH	613	GLN
7	DH	618	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	DG	90	ASN
7	DG	352	ASN
7	DG	500	ASN
7	AH	90	ASN
7	AH	148	GLN
7	AH	235	ASN
7	AH	327	GLN
7	AH	350	ASN
7	AH	613	GLN
7	AH	618	ASN
7	AG	61	ASN
7	AG	90	ASN
7	AG	352	ASN
7	AG	500	ASN
7	AI	613	GLN
7	FH	90	ASN
7	FH	350	ASN
7	FH	510	ASN
7	FH	613	GLN
7	FH	618	ASN
7	FG	90	ASN
7	FG	500	ASN
7	FI	613	GLN
7	CH	90	ASN
7	CH	235	ASN
7	CH	350	ASN
7	CH	613	GLN
7	CH	618	ASN
7	CG	3	ASN
7	CG	61	ASN
7	CG	90	ASN
7	CG	352	ASN
7	CG	500	ASN
7	CG	510	ASN
7	CI	539	GLN
7	EH	90	ASN
7	EH	235	ASN
7	EH	350	ASN
7	EH	613	GLN
7	EH	618	ASN
7	EG	61	ASN
7	EG	90	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	EG	500	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 ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

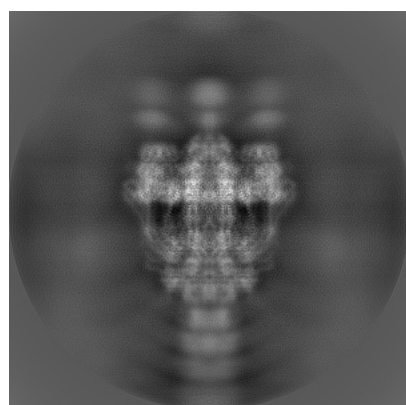
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20872. These allow visual inspection of the internal detail of the map and identification of artifacts.

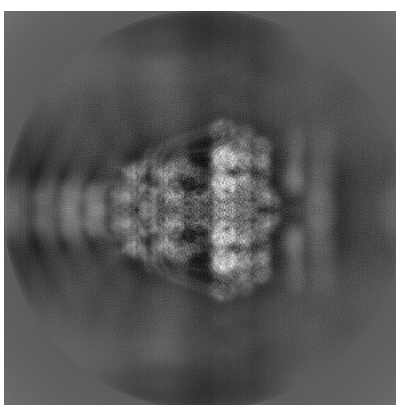
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

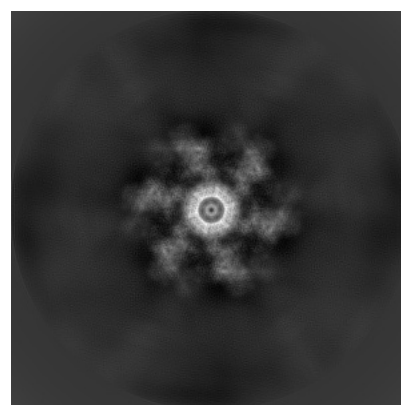
6.1.1 Primary map



X



Y

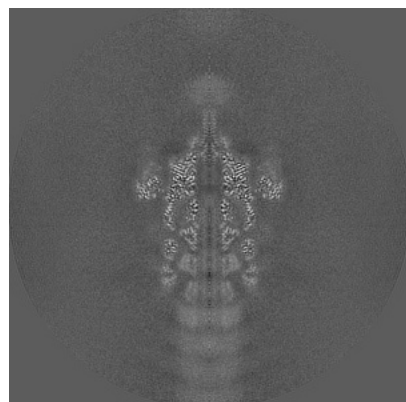


Z

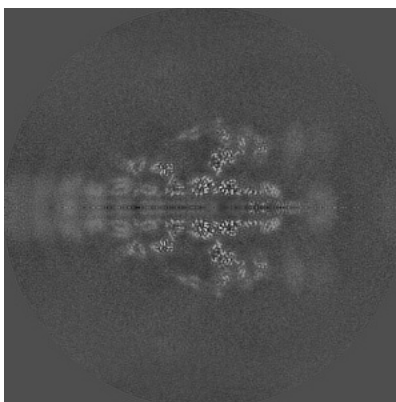
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

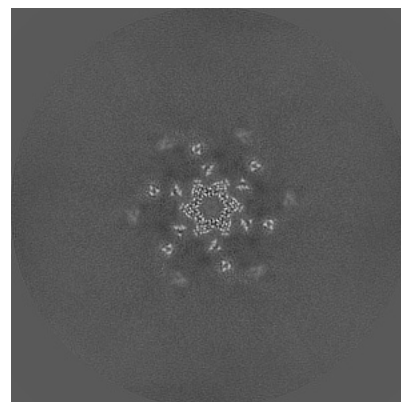
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

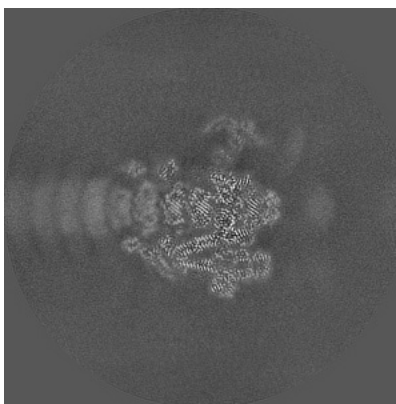
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

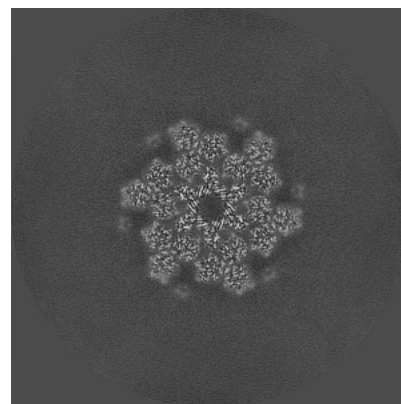
6.3.1 Primary map



X Index: 238



Y Index: 274

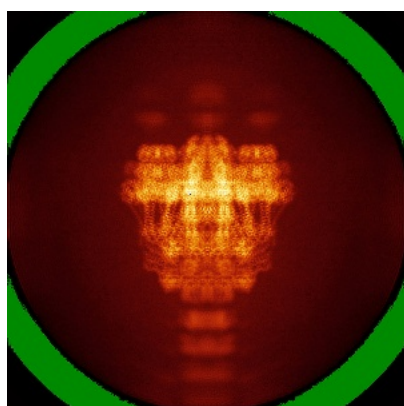


Z Index: 278

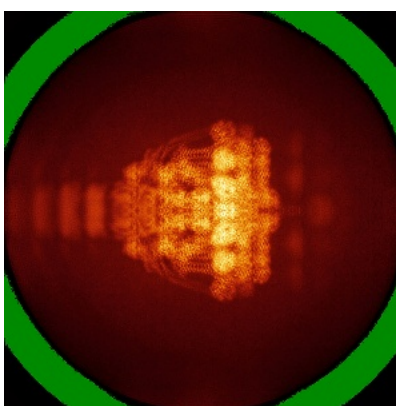
The images above show the largest variance slices of the map in three orthogonal directions.

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

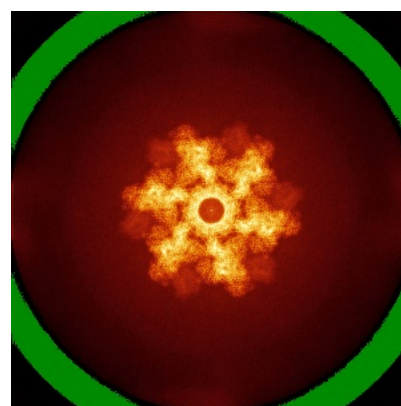
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

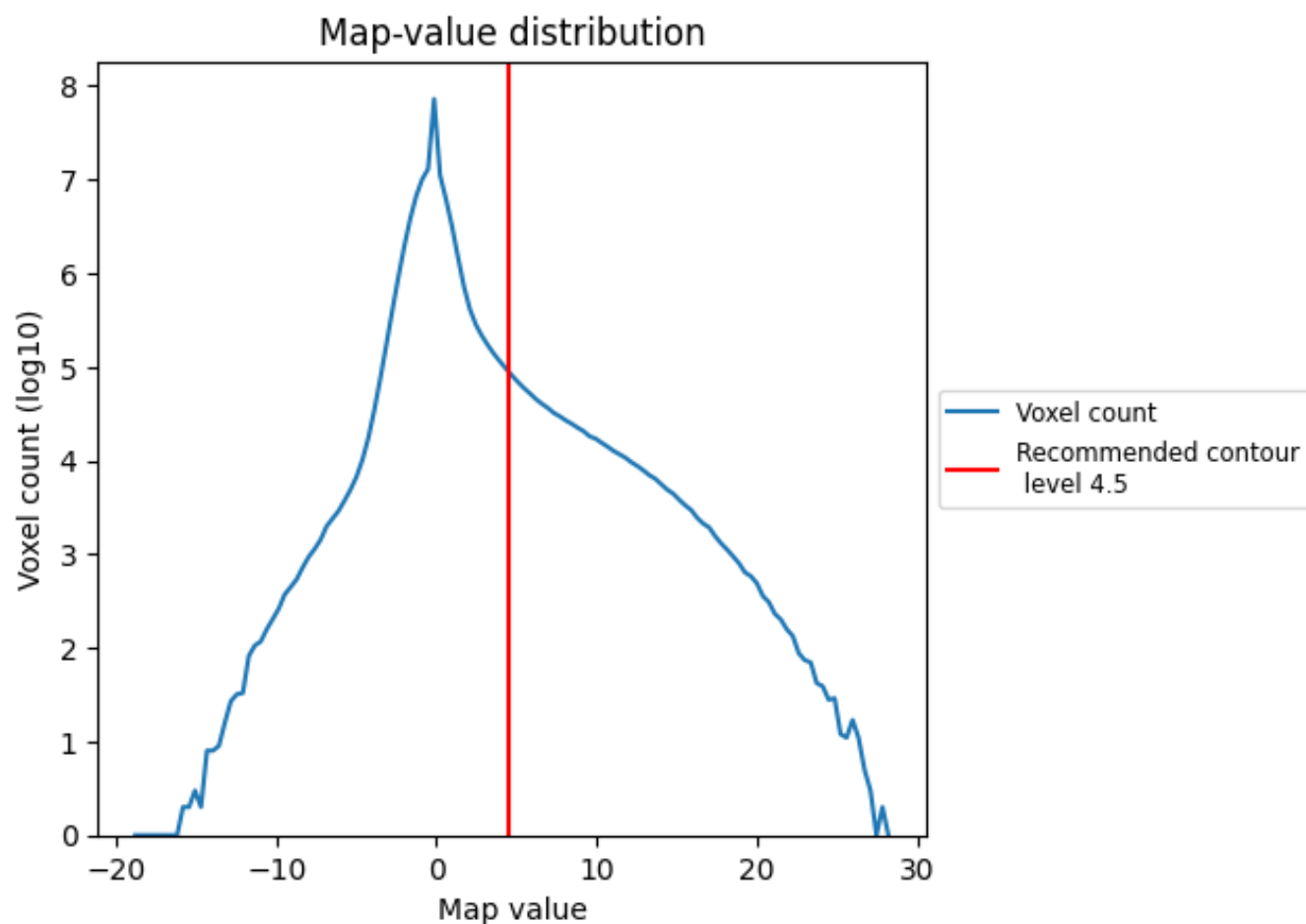
6.6 Mask visualisation

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

7 Map analysis [i](#)

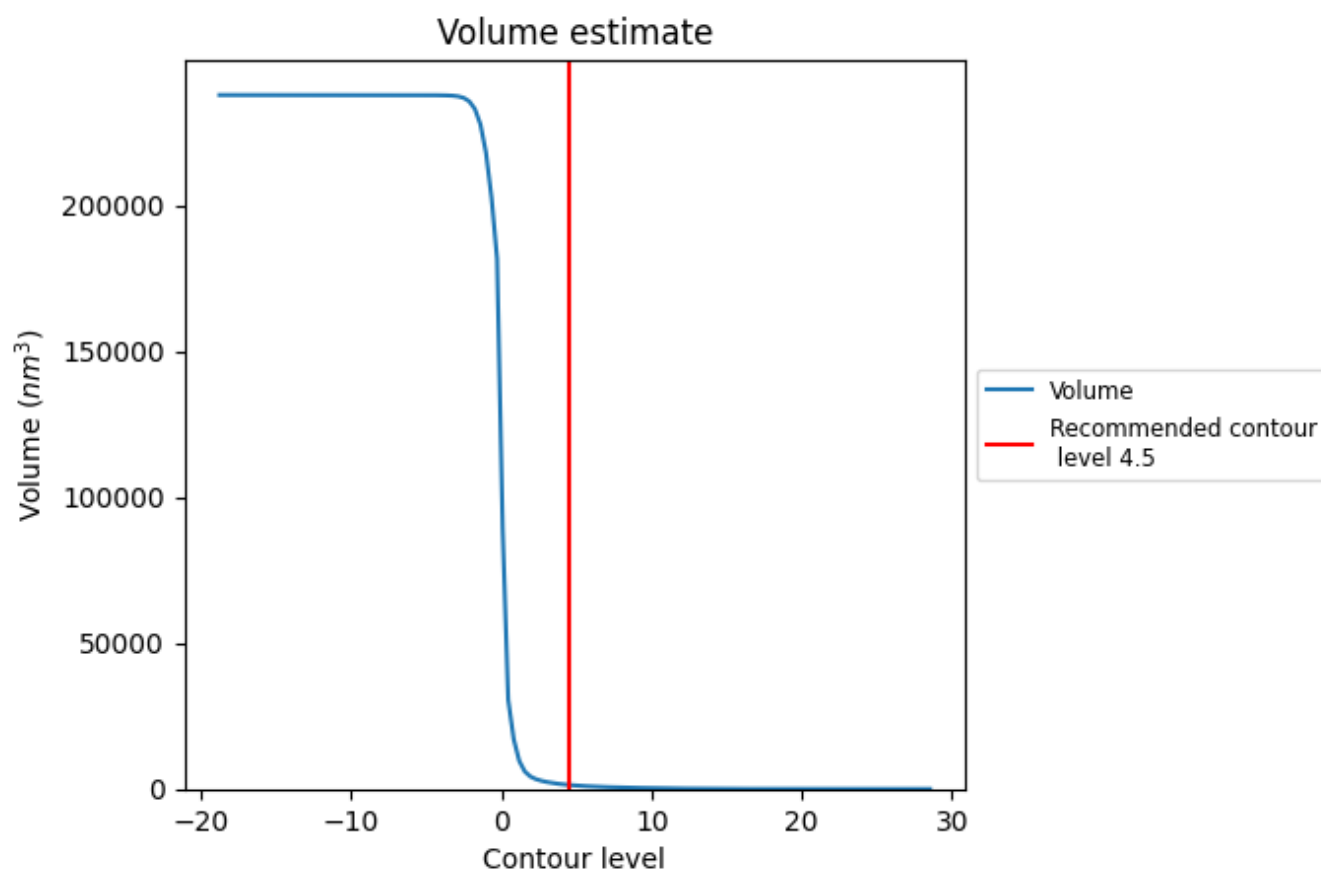
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

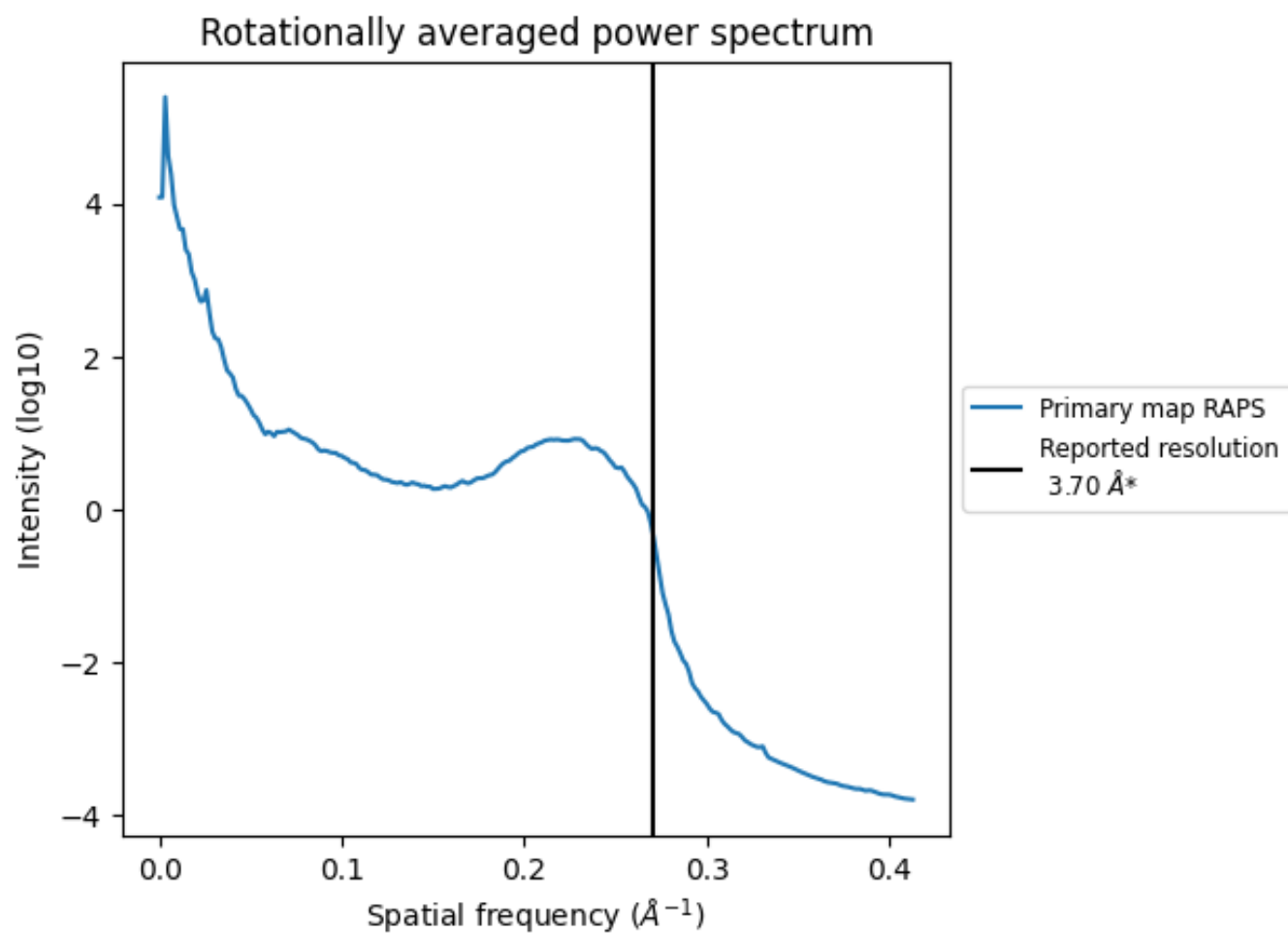
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1367 nm^3 ; this corresponds to an approximate mass of 1235 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 ⓘ

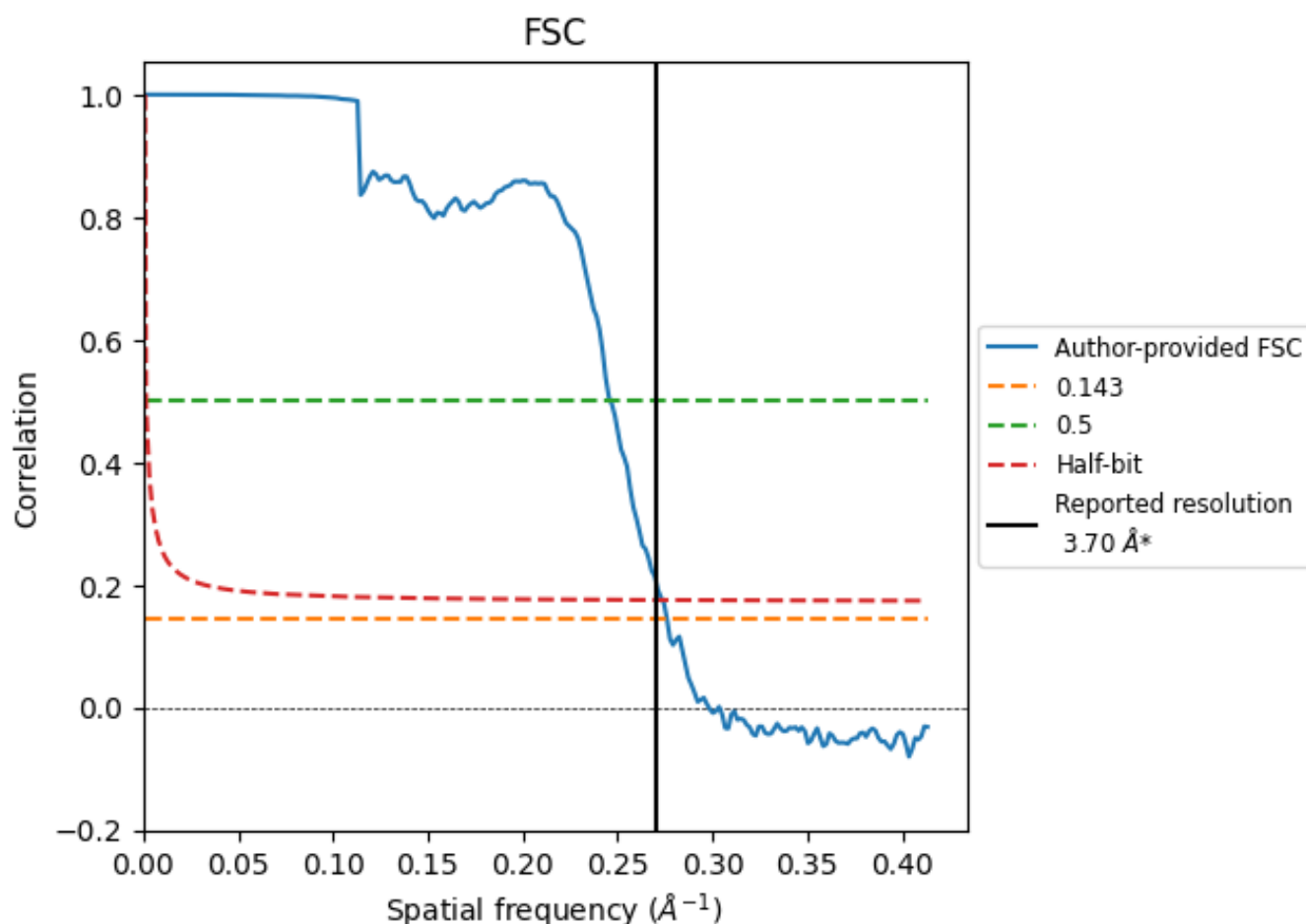


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

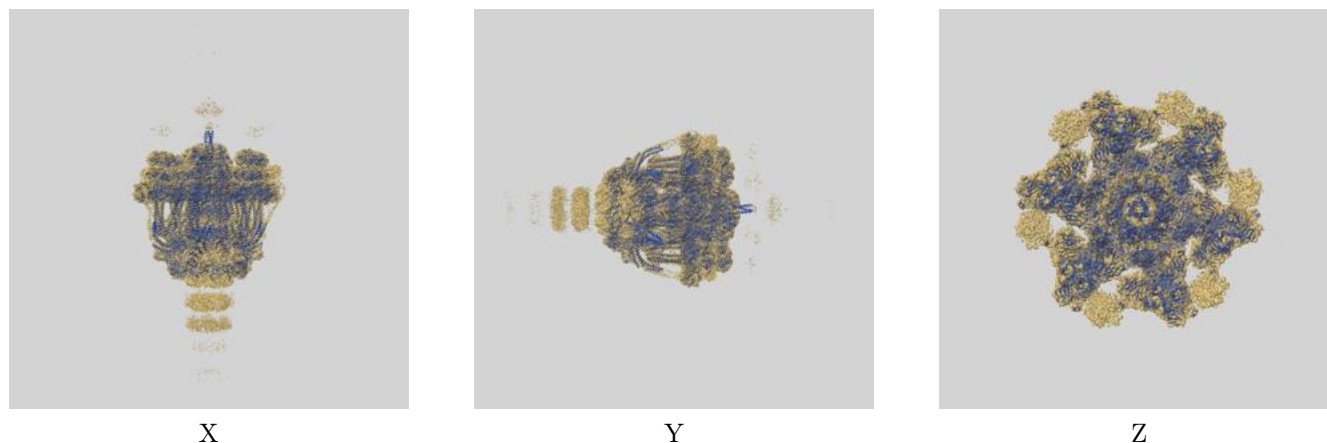
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.62	4.06	3.66
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

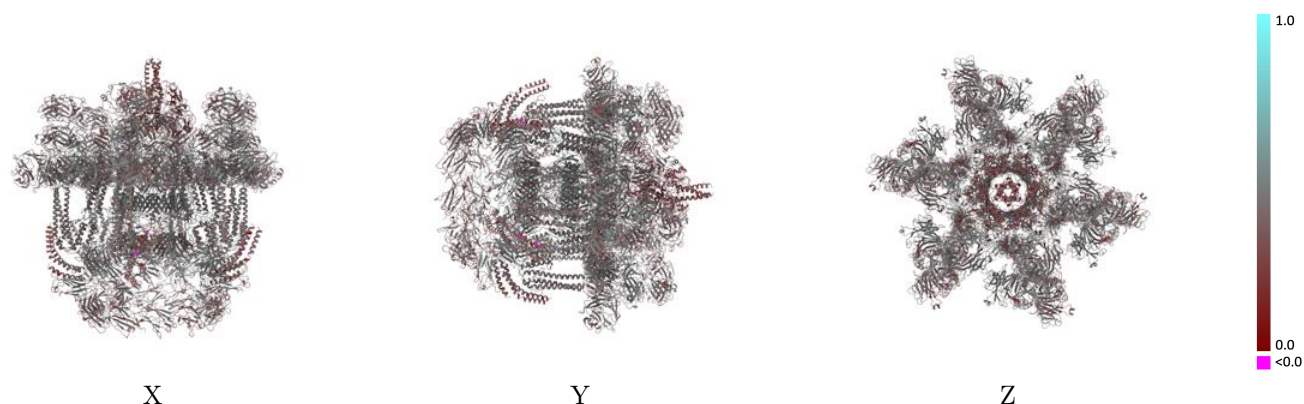
This section contains information regarding the fit between EMDB map EMD-20872 and PDB model 6V8I. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 4.5 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](#)

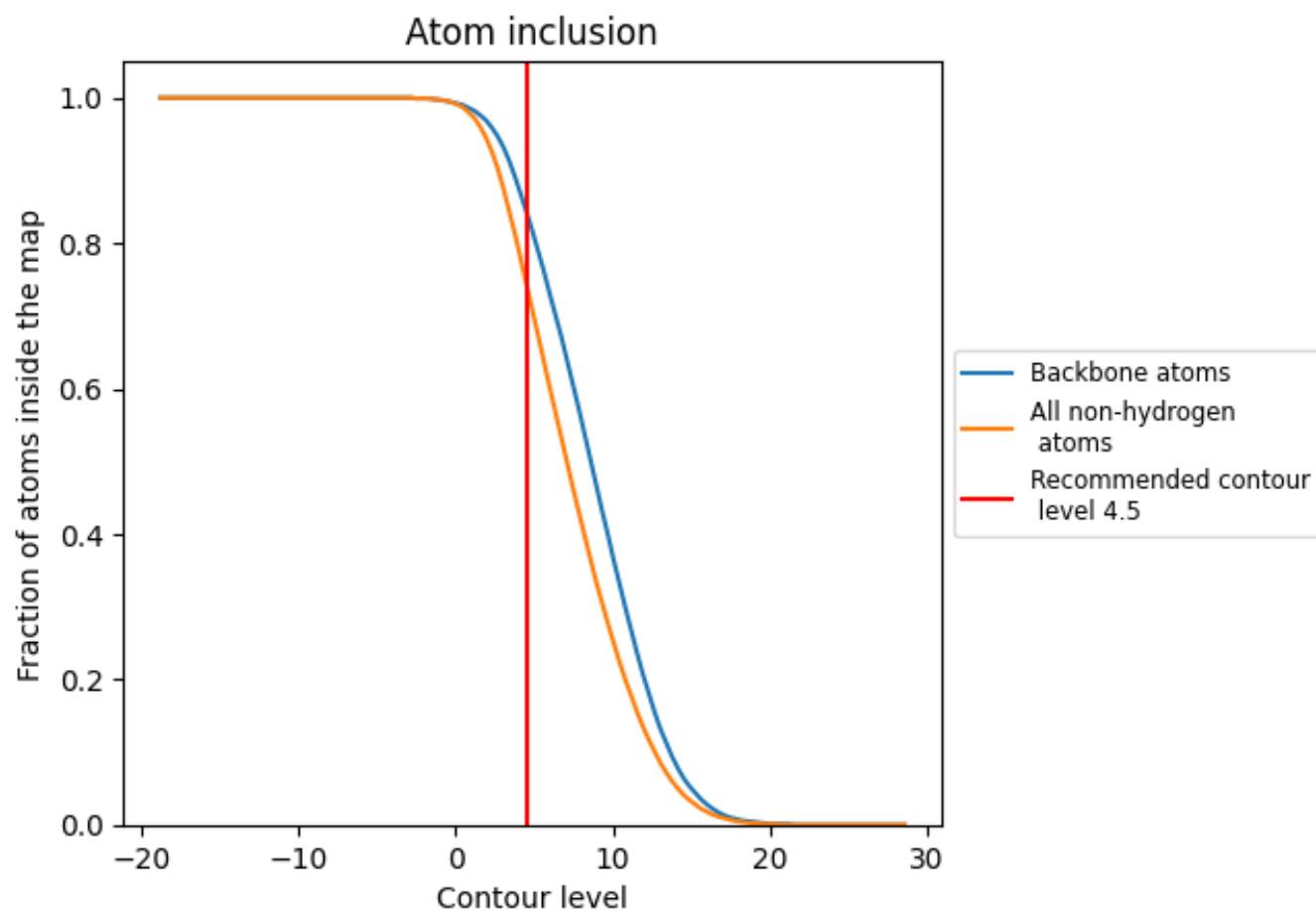


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7440	 0.4220
AA	 0.6780	 0.4270
AB	 0.7670	 0.4670
AC	 0.7490	 0.4050
AD	 0.7530	 0.4100
AE	 0.5700	 0.3290
AF	 0.2010	 0.2290
AG	 0.8100	 0.4310
AH	 0.7810	 0.4390
AI	 0.7740	 0.4370
AJ	 0.7400	 0.4380
AK	 0.6760	 0.4360
AL	 0.5620	 0.3830
AM	 0.7020	 0.3750
AN	 0.6860	 0.3900
BA	 0.6870	 0.4270
BB	 0.7810	 0.4660
BC	 0.7560	 0.4040
BD	 0.7630	 0.4200
BE	 0.5750	 0.3290
BF	 0.2010	 0.2370
BG	 0.8190	 0.4310
BH	 0.7860	 0.4400
BI	 0.7700	 0.4370
BJ	 0.7200	 0.4390
BK	 0.6970	 0.4420
BL	 0.5750	 0.3790
BM	 0.6930	 0.3720
BN	 0.6880	 0.3880
CA	 0.6910	 0.4300
CB	 0.7840	 0.4680
CC	 0.7610	 0.4070
CD	 0.7590	 0.4070
CE	 0.5770	 0.3270
CF	 0.1560	 0.1870



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
CG	 0.8240	 0.4300
CH	 0.7910	 0.4400
CI	 0.7710	 0.4390
CJ	 0.7280	 0.4390
CK	 0.6990	 0.4350
CL	 0.5700	 0.3850
CM	 0.7010	 0.3760
CN	 0.6930	 0.3880
DA	 0.6990	 0.4300
DB	 0.7890	 0.4650
DG	 0.8140	 0.4300
DH	 0.7770	 0.4400
DI	 0.7830	 0.4370
DJ	 0.7350	 0.4360
DK	 0.6970	 0.4370
DL	 0.5560	 0.3830
DM	 0.6990	 0.3740
DN	 0.6940	 0.3900
EA	 0.6870	 0.4290
EB	 0.7530	 0.4670
EG	 0.8210	 0.4320
EH	 0.7870	 0.4390
EI	 0.7710	 0.4360
EJ	 0.7380	 0.4420
EK	 0.6820	 0.4370
EL	 0.5690	 0.3850
EM	 0.7020	 0.3740
EN	 0.6860	 0.3880
FA	 0.6900	 0.4310
FB	 0.7810	 0.4680
FG	 0.8140	 0.4320
FH	 0.7780	 0.4390
FI	 0.7750	 0.4360
FJ	 0.7290	 0.4380
FK	 0.6970	 0.4390
FL	 0.5790	 0.3820
FM	 0.6950	 0.3750
FN	 0.6890	 0.3910