



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:22 AM UTC

PDB ID : 7QOI / pdb_00007qoi
EMDB ID : EMD-14091
Title : Unique vertex of the phicrAss001 virion
Authors : Bayfield, O.W.; Shkoporov, A.N.; Yutin, N.; Khokhlova, E.V.; Smith, J.L.R.;
Hawkins, D.E.D.P.; Koonin, E.V.; Hill, C.; Antson, A.A.
Deposited on : 2021-12-24
Resolution : 3.62 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

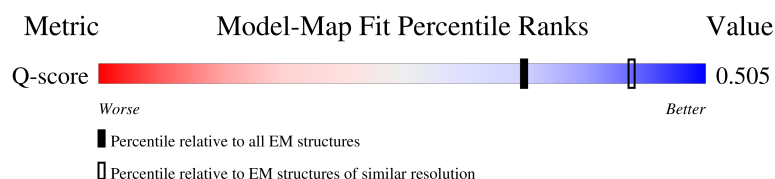
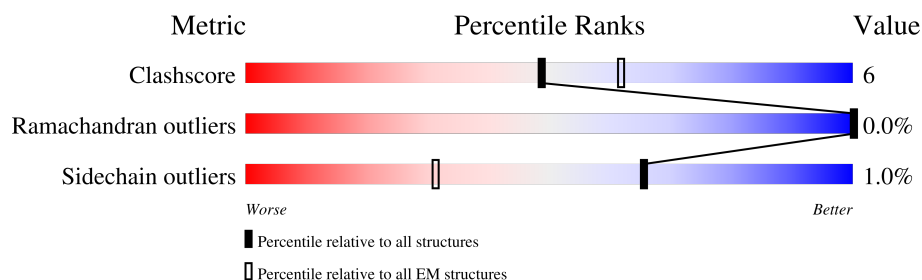
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.62 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	11773 (3.12 - 4.12)

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

Mol	Chain	Length	Quality of chain
1	AA	504	
1	AB	504	
1	AC	504	
1	AD	504	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AE	504	
1	AF	504	
1	BA	504	
1	BB	504	
1	BC	504	
1	BD	504	
1	BE	504	
1	BF	504	
1	CA	504	
1	CB	504	
1	CC	504	
1	CD	504	
1	CE	504	
1	CF	504	
1	DA	504	
1	DB	504	
1	DC	504	
1	DD	504	
1	DE	504	
1	DF	504	
1	EA	504	
1	EB	504	
1	EC	504	
1	ED	504	
1	EE	504	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	EF	504	
2	Aa	333	
2	Ab	333	
2	Ad	333	
2	Ae	333	
2	Af	333	
2	Ba	333	
2	Bb	333	
2	Bd	333	
2	Be	333	
2	Bf	333	
2	Ca	333	
2	Cb	333	
2	Cd	333	
2	Ce	333	
2	Cf	333	
2	Da	333	
2	Db	333	
2	Dd	333	
2	De	333	
2	Df	333	
2	Ea	333	
2	Eb	333	
2	Ed	333	
2	Ee	333	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Ef	333	
3	Ag	104	
3	Ah	104	
3	Bg	104	
3	Bh	104	
3	Cg	104	
3	Ch	104	
3	Dg	104	
3	Dh	104	
3	Eg	104	
3	Eh	104	
4	Ai	97	
4	Aj	97	
4	Ak	97	
4	Bi	97	
4	Bj	97	
4	Bk	97	
4	Ci	97	
4	Cj	97	
4	Ck	97	
4	Di	97	
4	Dj	97	
4	Dk	97	
4	Ei	97	
4	Ej	97	

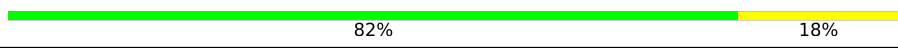
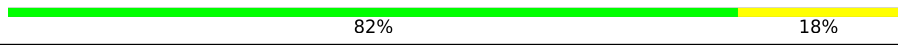
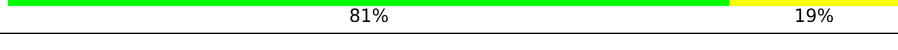
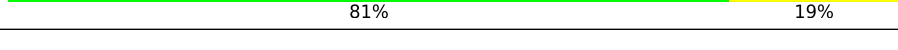
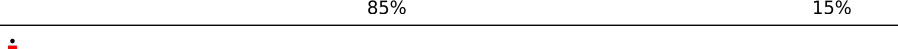
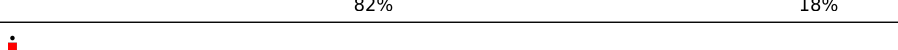
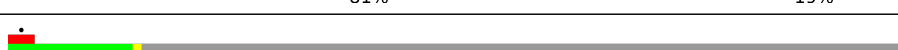
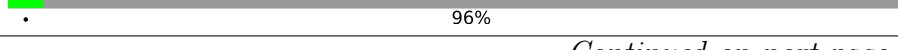
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Ek	97	
5	FA	806	
5	FB	806	
5	FC	806	
5	FD	806	
5	FE	806	
5	FF	806	
5	FG	806	
5	FH	806	
5	FI	806	
5	FJ	806	
5	FK	806	
5	FL	806	
6	FM	236	
6	FN	236	
6	FO	236	
6	FP	236	
6	FQ	236	
6	FR	236	
6	FS	236	
6	FT	236	
6	FU	236	
6	FV	236	
6	FW	236	
6	FX	236	

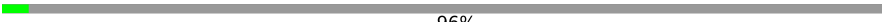
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	FY	225	 88%12%
7	FZ	225	 81%19%
7	GA	225	 82%18%
7	GB	225	 82%18%
7	GC	225	 83%17%
7	GD	225	 87%13%
7	GE	225	 81%19%
7	GF	225	 81%19%
7	GG	225	 85%15%
7	GH	225	 82%18%
7	GI	225	 89%11%
7	GJ	225	 81%19%
8	GK	842	 14%85%
8	GL	842	 13%85%
8	GM	842	 13%85%
8	GN	842	 14%85%
8	GO	842	 13%85%
8	GP	842	 13%85%
8	GQ	842	 13%85%
8	GR	842	 13%85%
8	GS	842	 12%85%
8	GT	842	 12%85%
8	GU	842	 13%85%
8	GV	842	 12%85%
8	IK	842	 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	IL	842	 96%
8	IM	842	 96%
8	IN	842	 96%
8	IO	842	 96%
8	IP	842	 96%
8	IQ	842	 96%
8	IR	842	 96%
8	IS	842	 96%
8	IT	842	 96%
8	IU	842	 96%
8	IV	842	 96%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 310209 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 Major capsid protein gp32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	484	Total	C	N	O	S	0	0
			3861	2451	668	723	19		
1	AB	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	AC	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	AD	456	Total	C	N	O	S	0	0
			3649	2329	631	671	18		
1	AE	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	AF	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	BA	485	Total	C	N	O	S	0	0
			3868	2455	669	725	19		
1	BB	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	BC	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	BD	456	Total	C	N	O	S	0	0
			3649	2329	631	671	18		
1	BE	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	BF	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	CA	483	Total	C	N	O	S	0	0
			3855	2448	667	721	19		
1	CB	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	CC	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	CD	451	Total	C	N	O	S	0	0
			3612	2307	623	664	18		
1	CE	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CF	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	DA	485	Total	C	N	O	S	0	0
			3868	2455	669	725	19		
1	DB	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	DC	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	DD	456	Total	C	N	O	S	0	0
			3649	2329	631	671	18		
1	DE	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	DF	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	EA	485	Total	C	N	O	S	0	0
			3868	2455	669	725	19		
1	EB	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	EC	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	ED	456	Total	C	N	O	S	0	0
			3649	2329	631	671	18		
1	EE	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	EF	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		

- Molecule 2 is a protein called Auxiliary capsid protein gp36.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Aa	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Ab	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Ad	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Ae	267	Total	C	N	O	S	0	0
			2077	1335	332	401	9		
2	Af	185	Total	C	N	O	S	0	0
			1434	919	226	283	6		
2	Ba	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bb	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Bd	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Be	266	Total	C	N	O	S	0	0
			2070	1330	331	400	9		
2	Bf	185	Total	C	N	O	S	0	0
			1434	919	226	283	6		
2	Ca	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Cb	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Cd	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Ce	267	Total	C	N	O	S	0	0
			2077	1335	332	401	9		
2	Cf	185	Total	C	N	O	S	0	0
			1434	919	226	283	6		
2	Da	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Db	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Dd	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	De	267	Total	C	N	O	S	0	0
			2077	1335	332	401	9		
2	Df	185	Total	C	N	O	S	0	0
			1434	919	226	283	6		
2	Ea	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Eb	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Ed	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Ee	267	Total	C	N	O	S	0	0
			2077	1335	332	401	9		
2	Ef	185	Total	C	N	O	S	0	0
			1434	919	226	283	6		

- Molecule 3 is a protein called Portal vertex capsid protein gp57.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ag	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Ah	73	Total	C	N	O	S	0	0
			563	359	91	105	8		
3	Bg	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Bh	73	Total	C	N	O	S	0	0
			563	359	91	105	8		
3	Cg	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Ch	73	Total	C	N	O	S	0	0
			563	359	91	105	8		
3	Dg	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Dh	73	Total	C	N	O	S	0	0
			563	359	91	105	8		
3	Eg	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Eh	73	Total	C	N	O	S	0	0
			563	359	91	105	8		

- Molecule 4 is a protein called Head fiber trimer protein gp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ai	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Aj	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ak	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Bi	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Bj	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Bk	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ci	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Cj	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ck	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Di	38	Total	C	N	O	S	0	0
			310	201	51	56	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Dj	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Dk	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ei	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ej	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ek	38	Total	C	N	O	S	0	0
			310	201	51	56	2		

- Molecule 5 is a protein called Portal protein gp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	FA	688	Total	C	N	O	S	0	0
			5617	3558	957	1077	25		
5	FB	678	Total	C	N	O	S	0	0
			5545	3519	941	1062	23		
5	FC	684	Total	C	N	O	S	0	0
			5597	3550	951	1072	24		
5	FD	705	Total	C	N	O	S	0	0
			5759	3657	976	1102	24		
5	FE	660	Total	C	N	O	S	0	0
			5400	3426	920	1031	23		
5	FF	684	Total	C	N	O	S	0	0
			5593	3543	952	1074	24		
5	FG	680	Total	C	N	O	S	0	0
			5569	3531	948	1066	24		
5	FH	689	Total	C	N	O	S	0	0
			5618	3558	958	1078	24		
5	FI	694	Total	C	N	O	S	0	0
			5671	3601	961	1085	24		
5	FJ	698	Total	C	N	O	S	0	0
			5699	3613	967	1094	25		
5	FK	669	Total	C	N	O	S	0	0
			5478	3483	929	1043	23		
5	FL	681	Total	C	N	O	S	0	0
			5563	3529	945	1066	23		

- Molecule 6 is a protein called Ring protein 1 gp43.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	FM	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FN	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FO	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FP	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FQ	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FR	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FS	229	Total	C	N	O	S	0	0
			1868	1204	314	341	9		
6	FT	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FU	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FV	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FW	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FX	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		

- Molecule 7 is a protein called Ring protein 2 gp40.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	FY	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	FZ	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GA	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GB	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GC	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GD	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GE	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GF	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	GG	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GH	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GI	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GJ	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		

- Molecule 8 is a protein called Cargo protein 1 gp45.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	GK	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GL	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GM	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GN	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GO	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GP	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GQ	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GR	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GS	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GT	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GU	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GV	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	IK	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IL	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IM	32	Total	C	N	O	S	0	0
			251	157	44	49	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	IN	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IO	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IP	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IQ	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IR	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IS	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IT	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IU	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IV	32	Total	C	N	O	S	0	0
			251	157	44	49	1		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	AB	1	Total	Mg	0
			1	1	
9	AC	1	Total	Mg	0
			1	1	
9	AD	1	Total	Mg	0
			1	1	
9	AE	1	Total	Mg	0
			1	1	
9	BB	1	Total	Mg	0
			1	1	
9	BD	1	Total	Mg	0
			1	1	
9	CB	1	Total	Mg	0
			1	1	
9	CD	1	Total	Mg	0
			1	1	
9	CE	1	Total	Mg	0
			1	1	
9	CF	1	Total	Mg	0
			1	1	

Continued on next page...

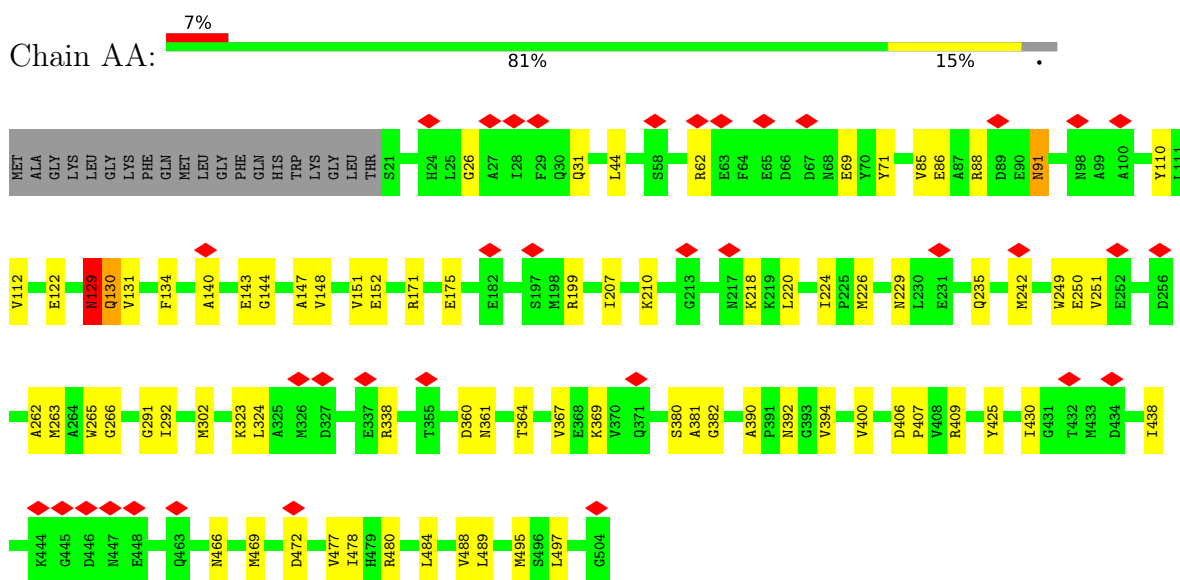
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
9	DB	1	Total 1	Mg 1	0
9	DE	1	Total 1	Mg 1	0
9	DF	1	Total 1	Mg 1	0
9	EB	1	Total 1	Mg 1	0
9	ED	1	Total 1	Mg 1	0
9	FA	1	Total 1	Mg 1	0
9	FB	1	Total 1	Mg 1	0
9	FC	1	Total 1	Mg 1	0
9	FD	1	Total 1	Mg 1	0
9	FE	1	Total 1	Mg 1	0
9	FF	1	Total 1	Mg 1	0
9	FG	1	Total 1	Mg 1	0
9	FH	1	Total 1	Mg 1	0
9	FI	1	Total 1	Mg 1	0
9	FJ	1	Total 1	Mg 1	0
9	FK	1	Total 1	Mg 1	0
9	FL	1	Total 1	Mg 1	0

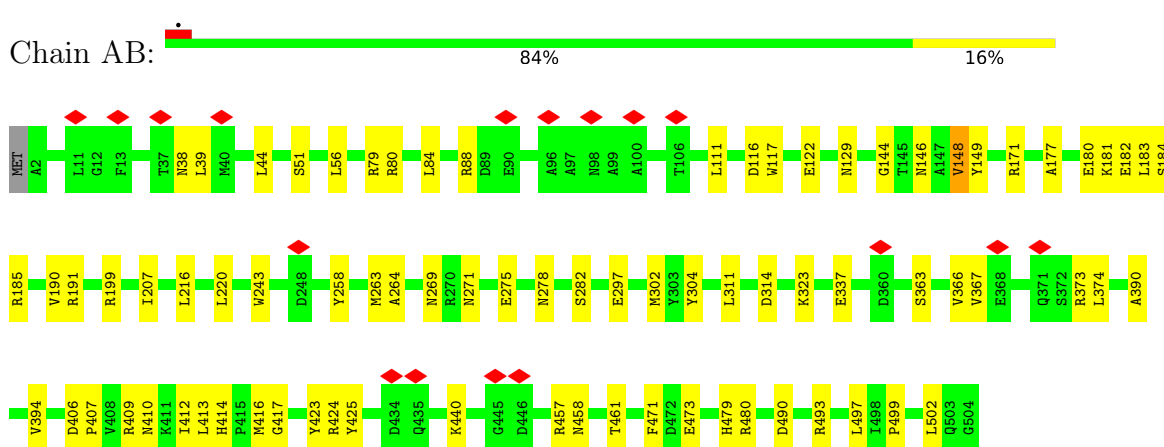
3 Residue-property plots

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.

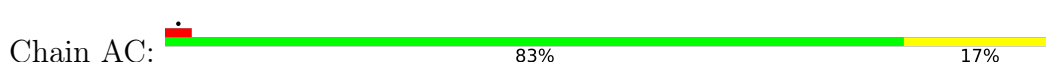
- Molecule 1: Major capsid protein gp32

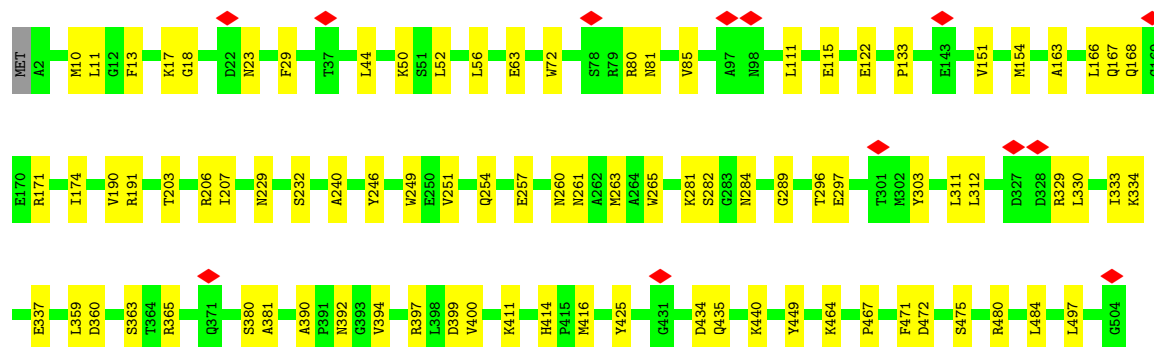


- Molecule 1: Major capsid protein gp32



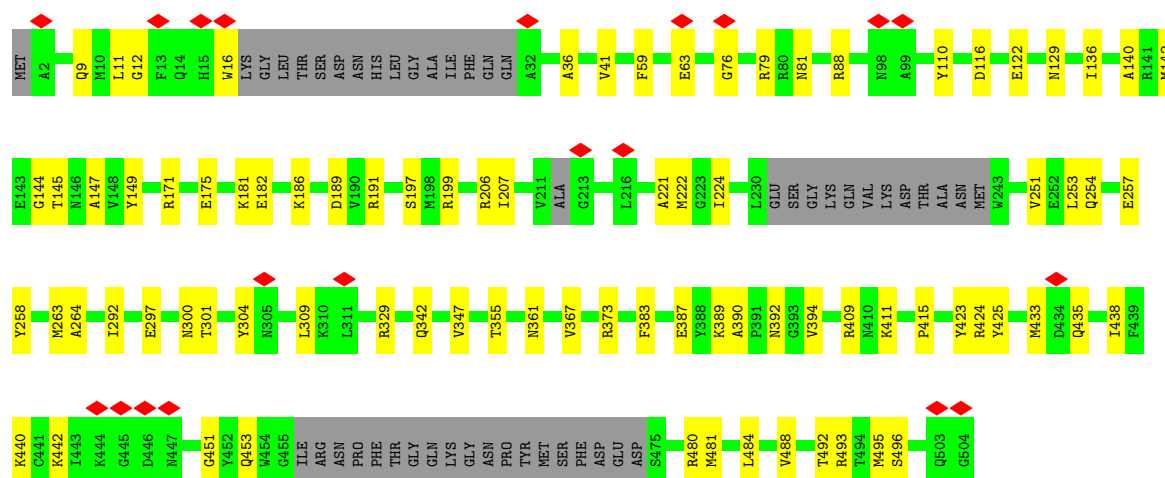
- Molecule 1: Major capsid protein gp32





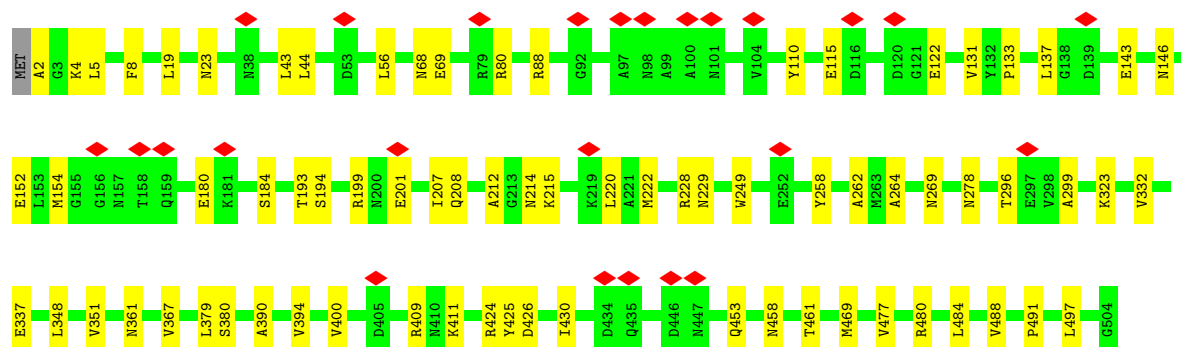
- Molecule 1: Major capsid protein gp32

Chain AD: 74% 17% 10%



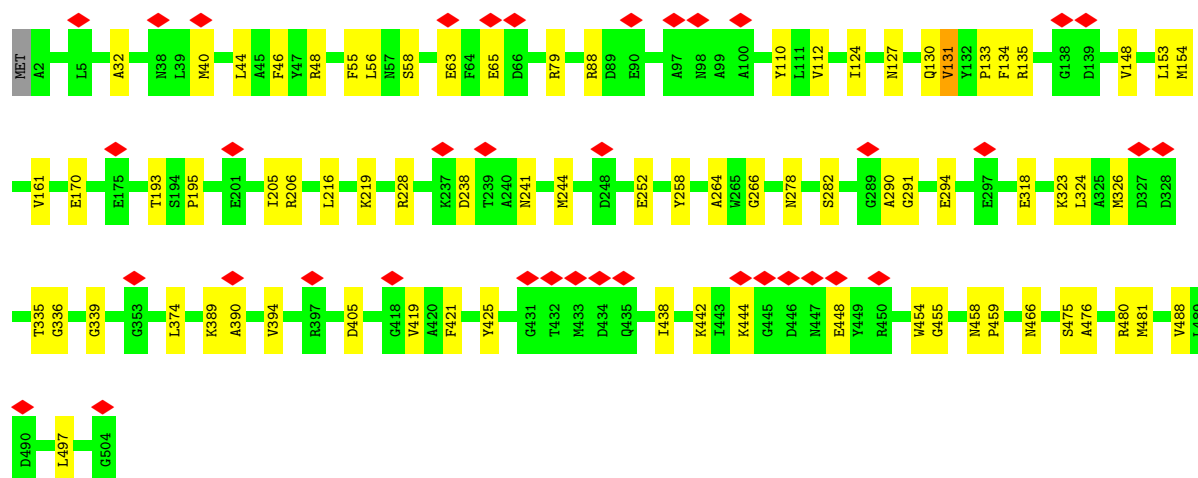
- Molecule 1: Major capsid protein gp32

Chain AE: 5% 85% 15%

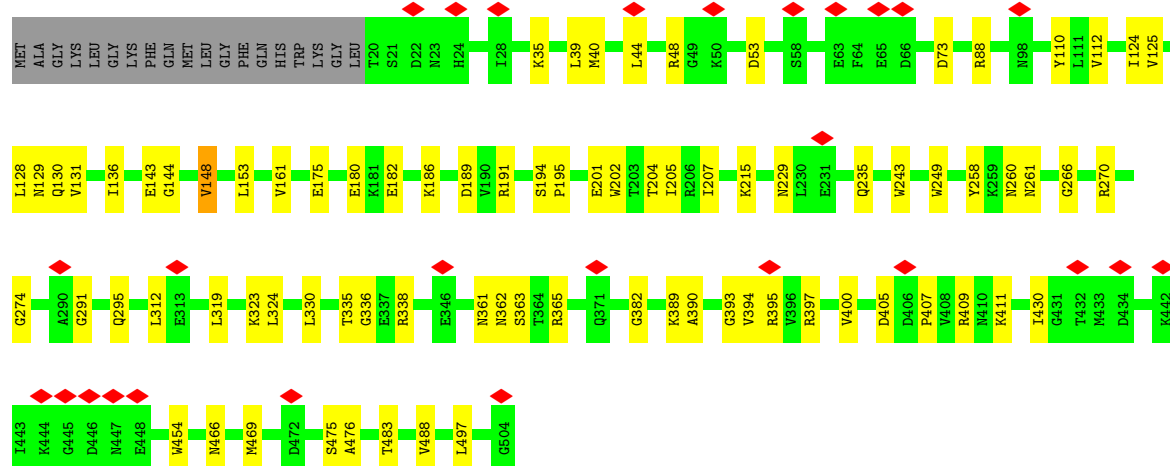
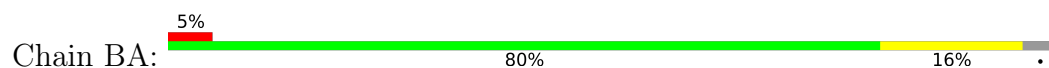


- Molecule 1: Major capsid protein gp32

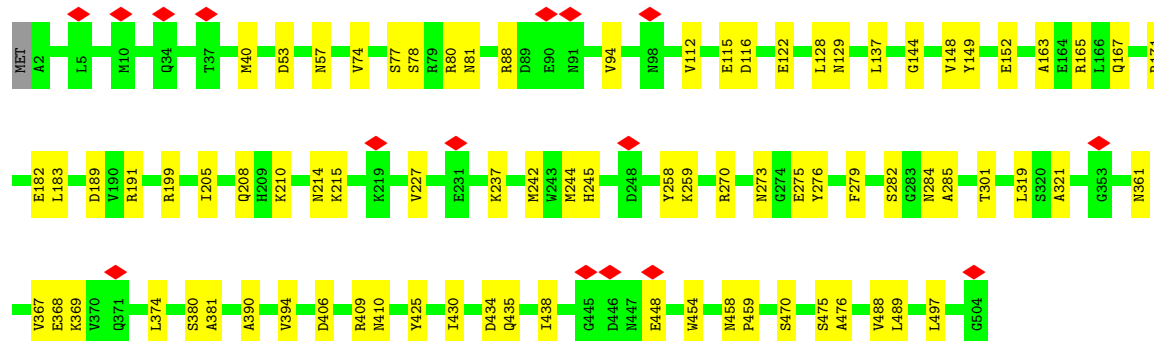
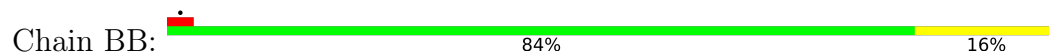
Chain AF: 8% 85% 15%



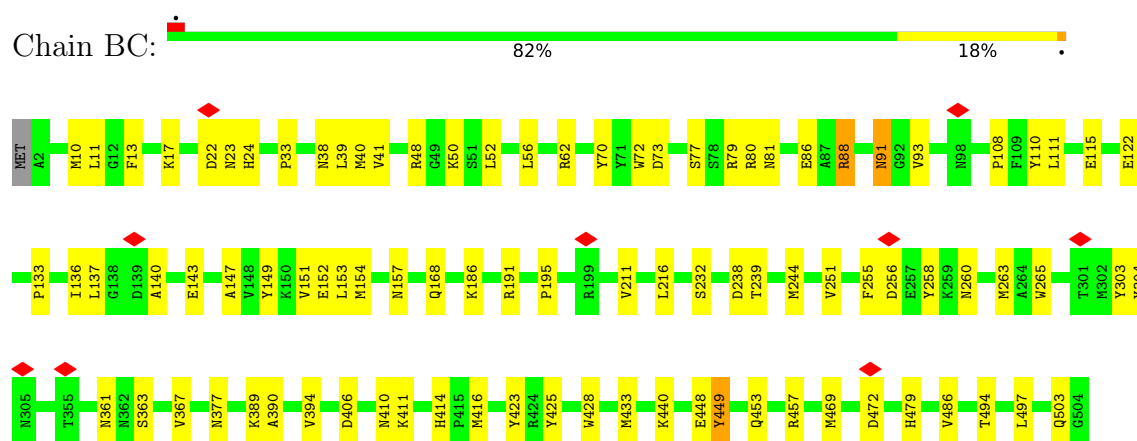
- Molecule 1: Major capsid protein gp32



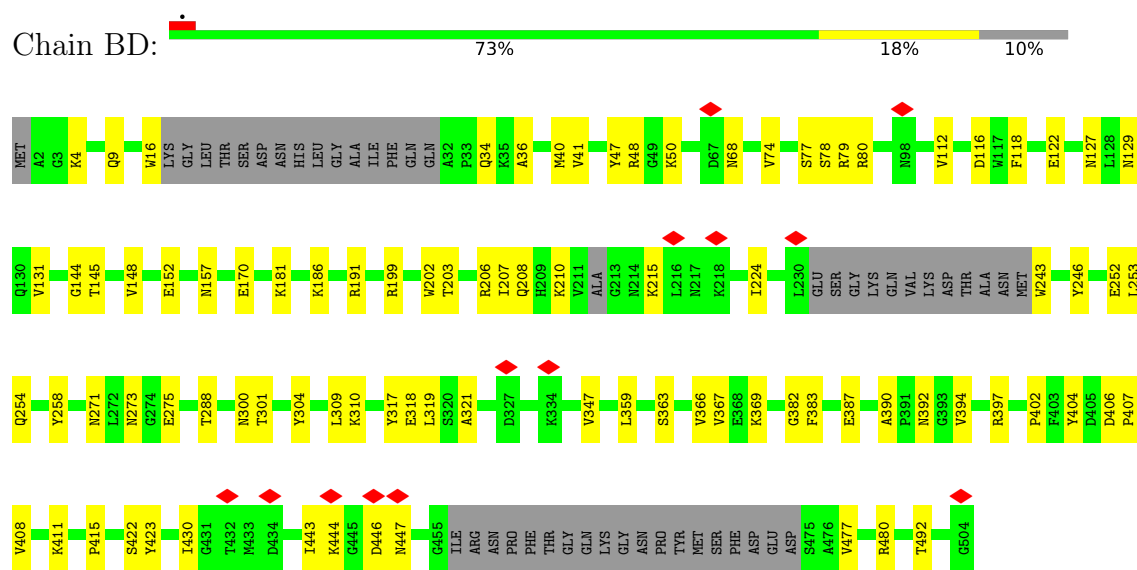
- Molecule 1: Major capsid protein gp32



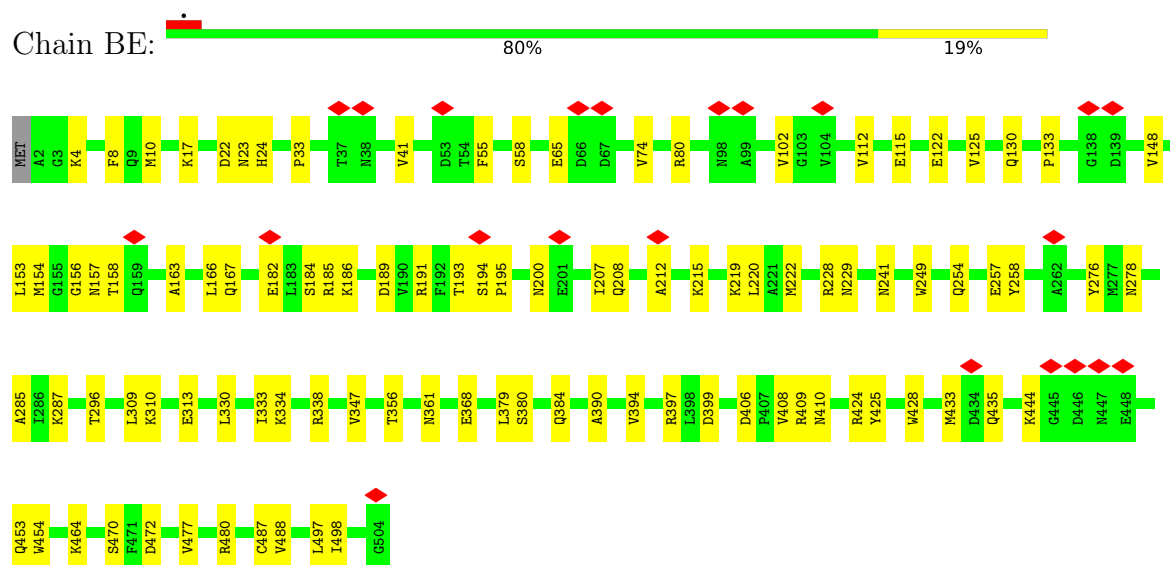
- Molecule 1: Major capsid protein gp32



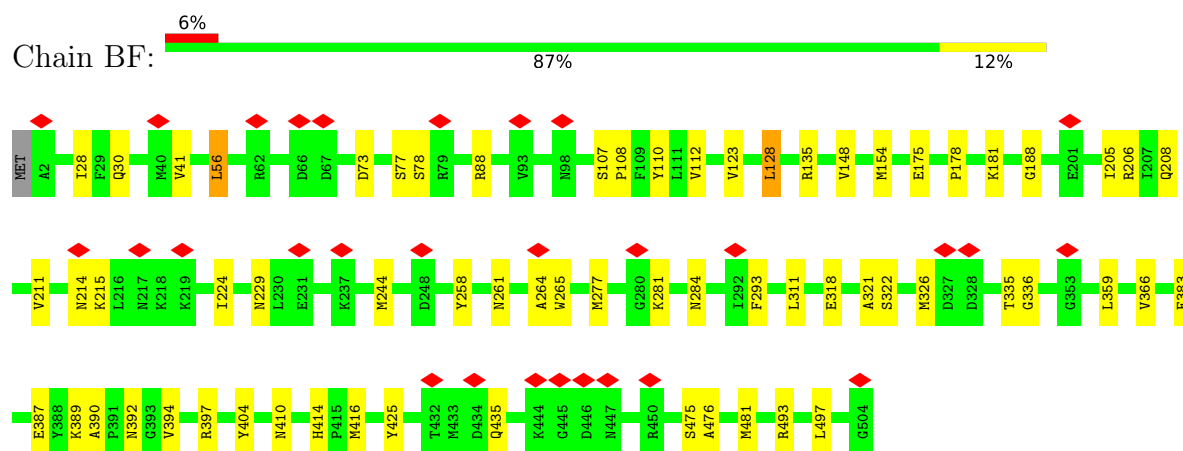
• Molecule 1: Major capsid protein gp32



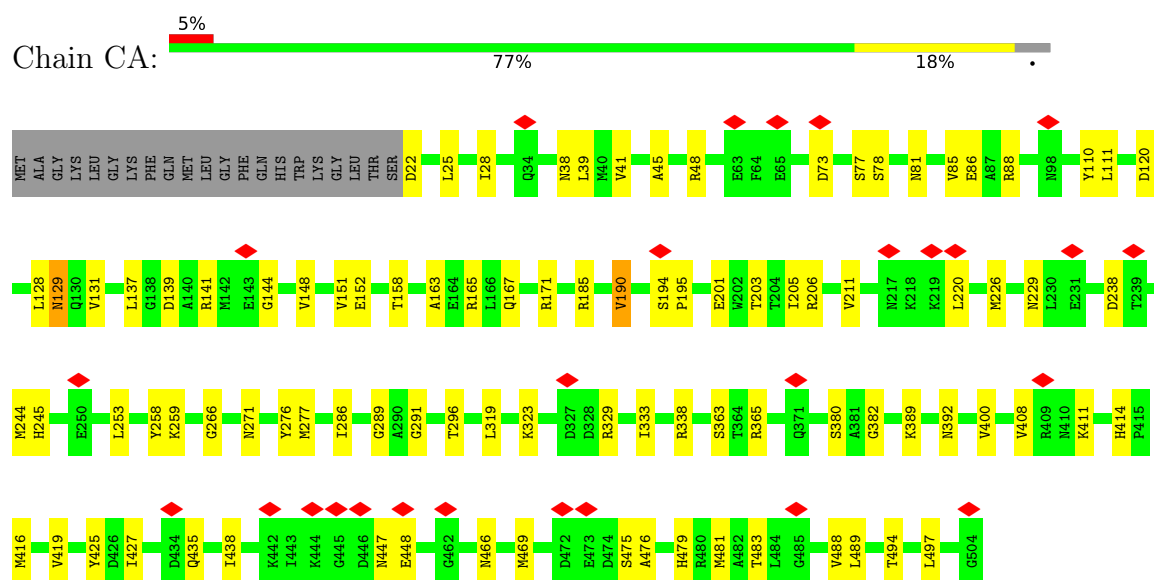
• Molecule 1: Major capsid protein gp32



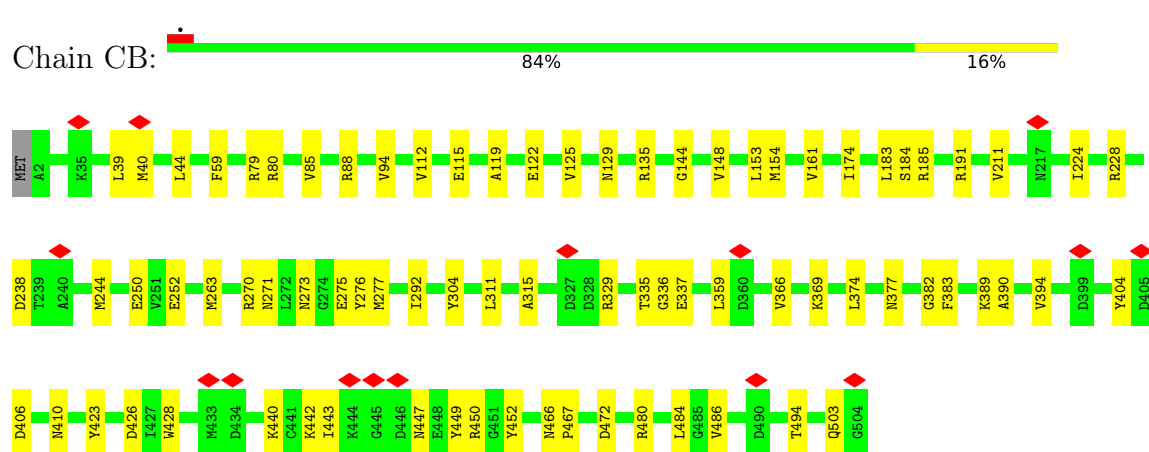
- Molecule 1: Major capsid protein gp32



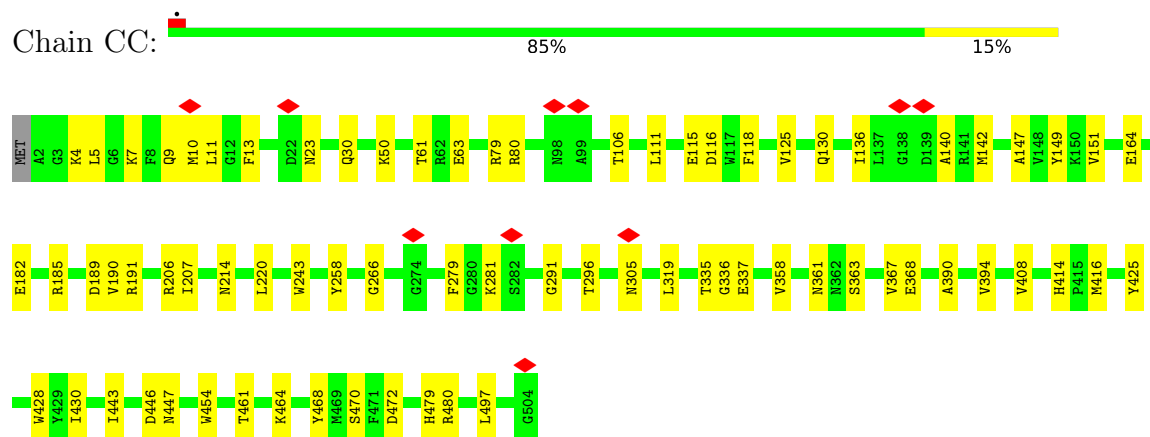
- Molecule 1: Major capsid protein gp32



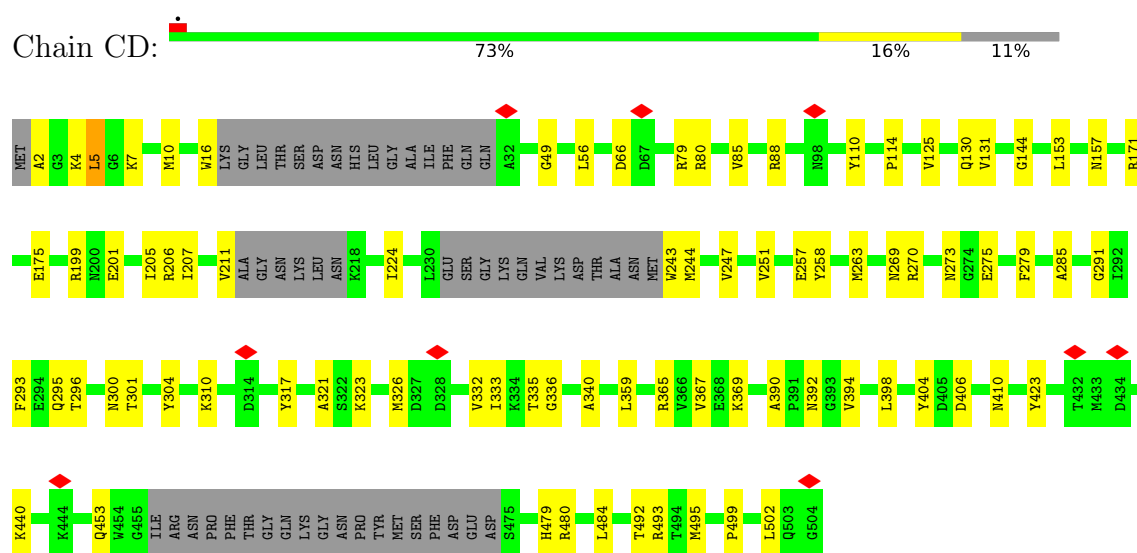
- Molecule 1: Major capsid protein gp32



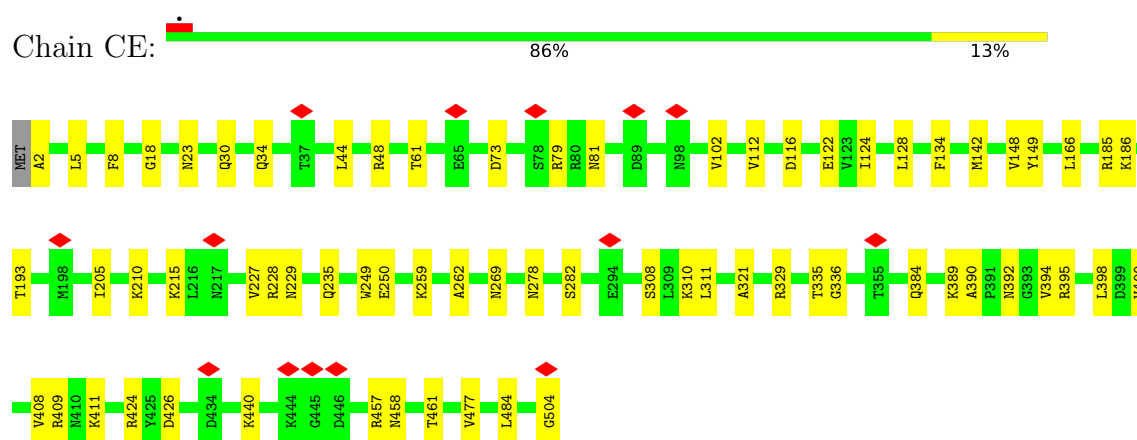
- Molecule 1: Major capsid protein gp32



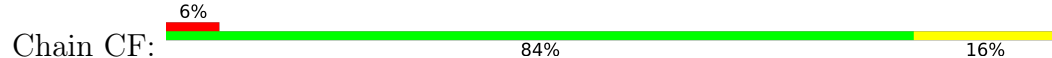
• Molecule 1: Major capsid protein gp32

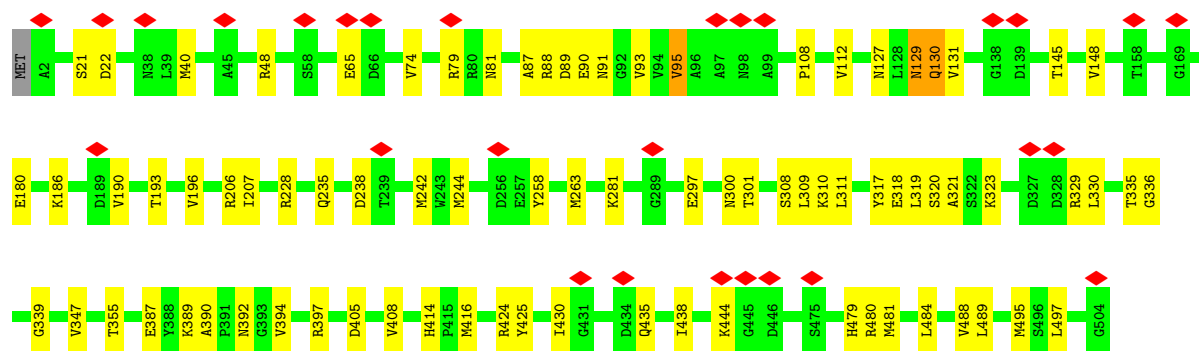


• Molecule 1: Major capsid protein gp32

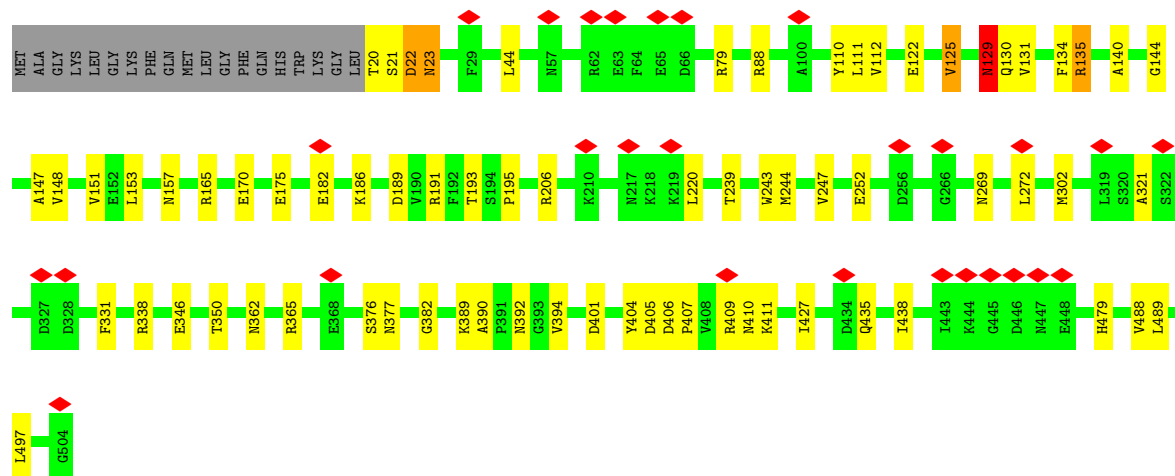
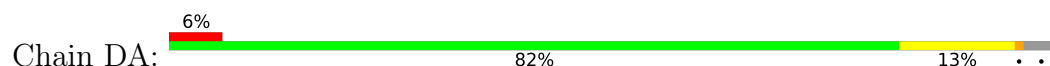


• Molecule 1: Major capsid protein gp32

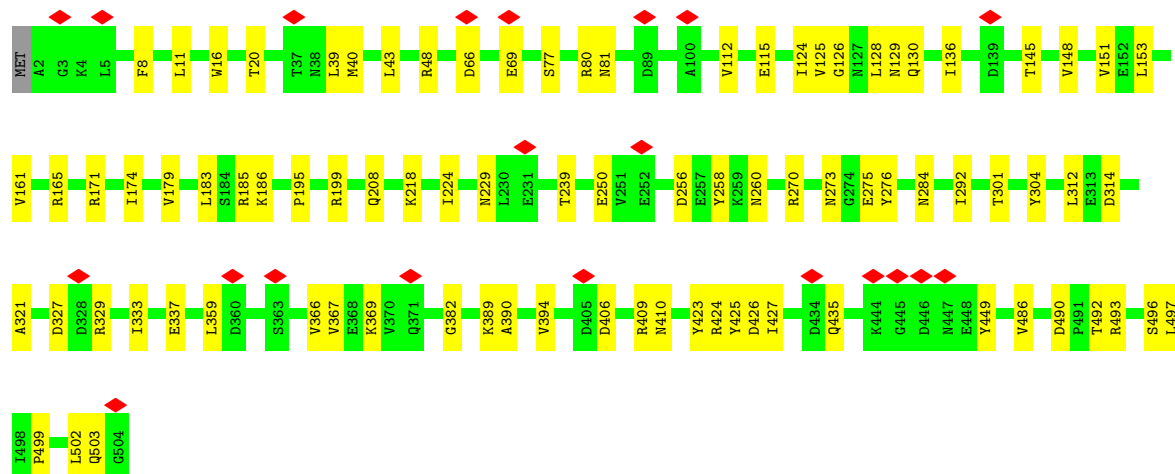
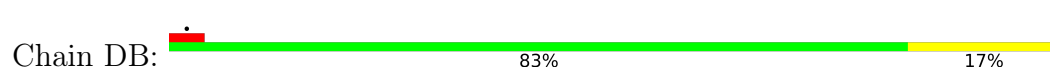




• Molecule 1: Major capsid protein gp32

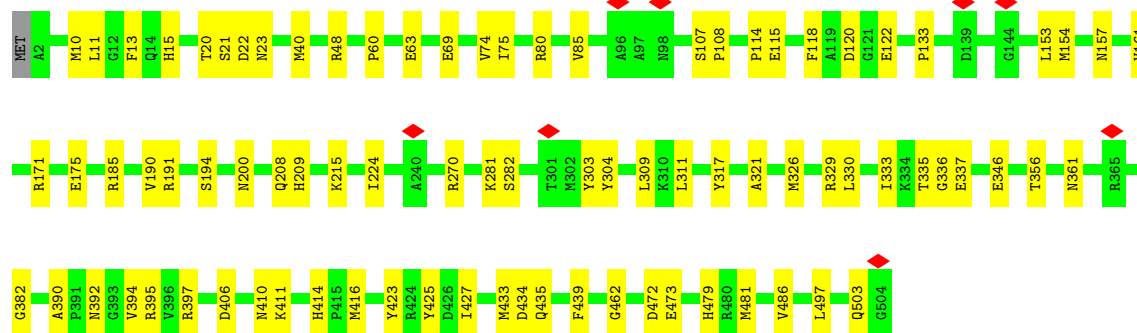


• Molecule 1: Major capsid protein gp32



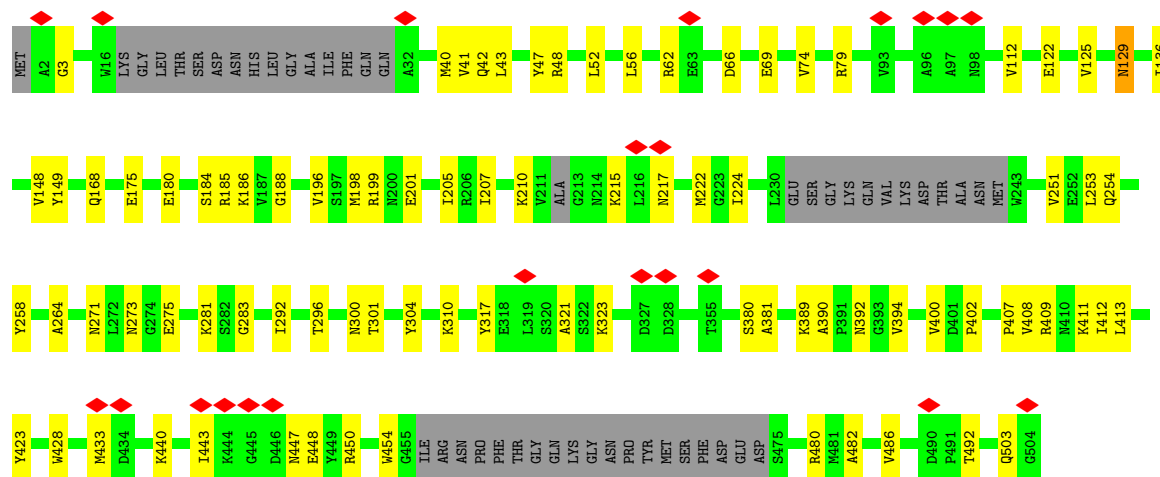
• Molecule 1: Major capsid protein gp32

Chain DC:  83% 17%



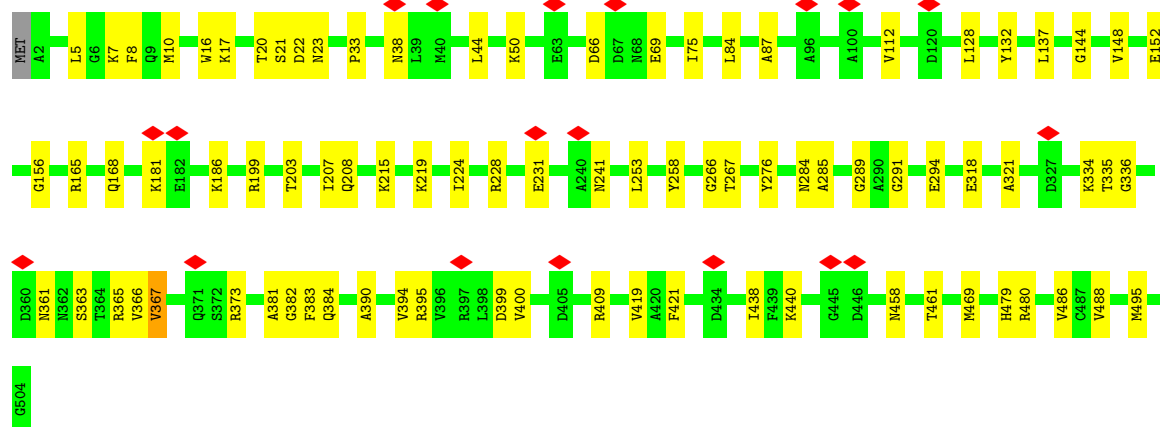
- Molecule 1: Major capsid protein gp32

Chain DD:  73% 17% 10%

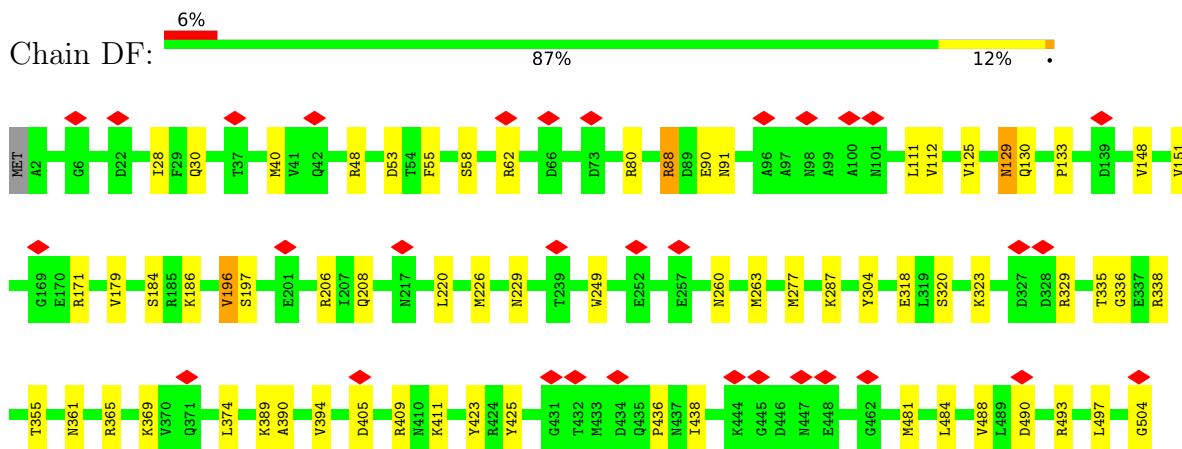


- Molecule 1: Major capsid protein gp32

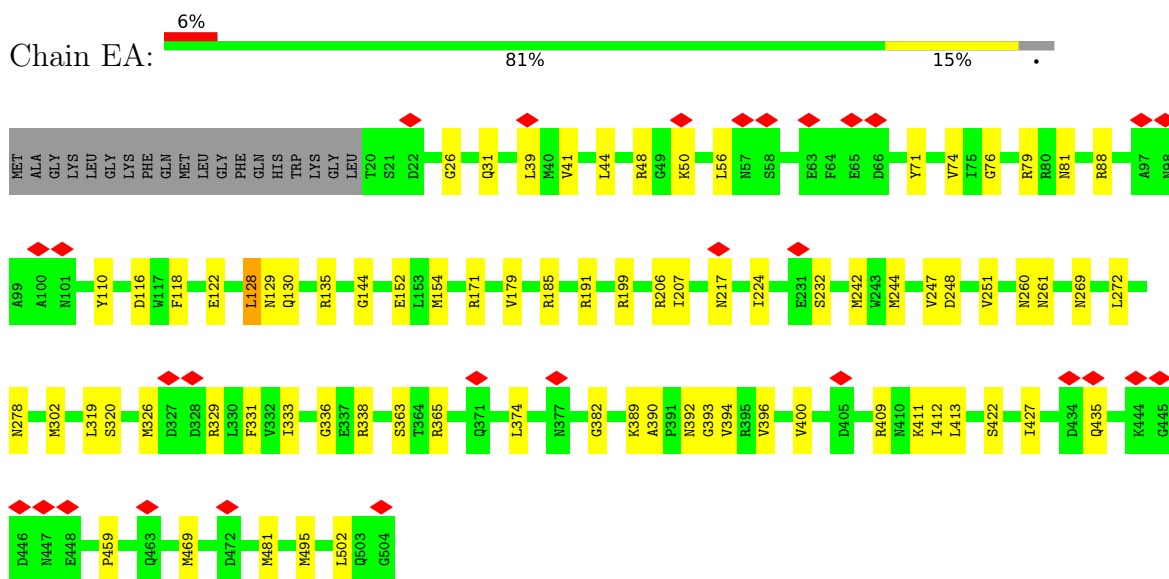
Chain DE:  83% 16%



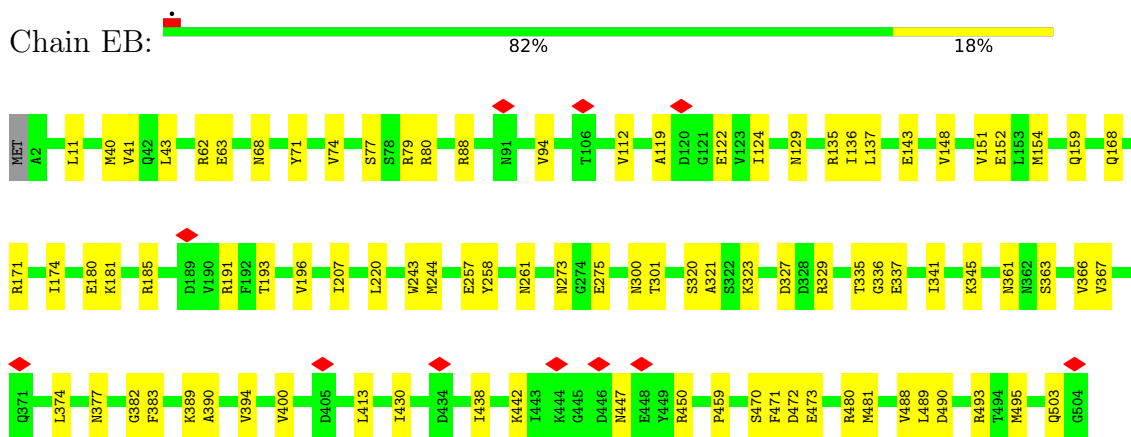
- Molecule 1: Major capsid protein gp32



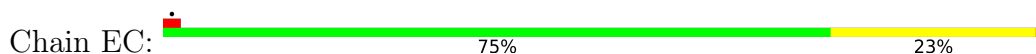
• Molecule 1: Major capsid protein gp32

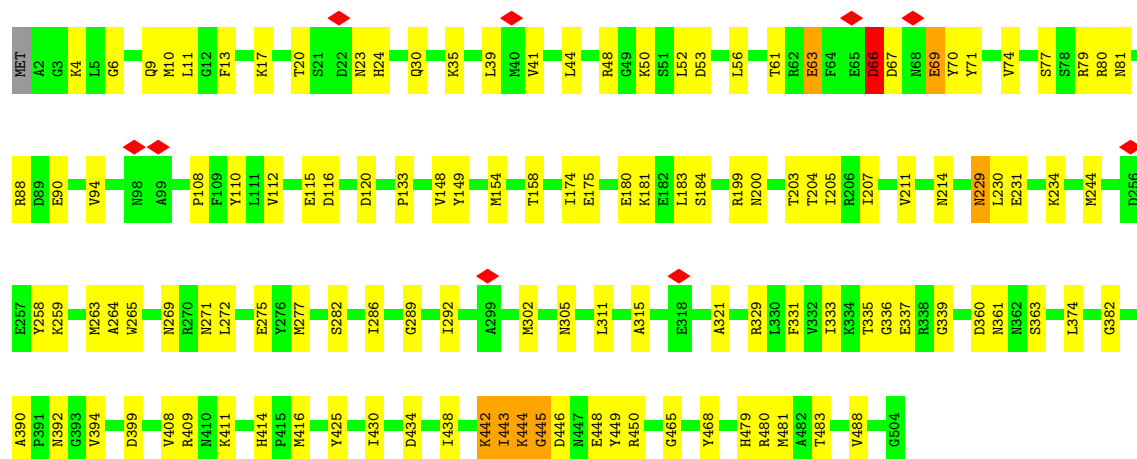


• Molecule 1: Major capsid protein gp32

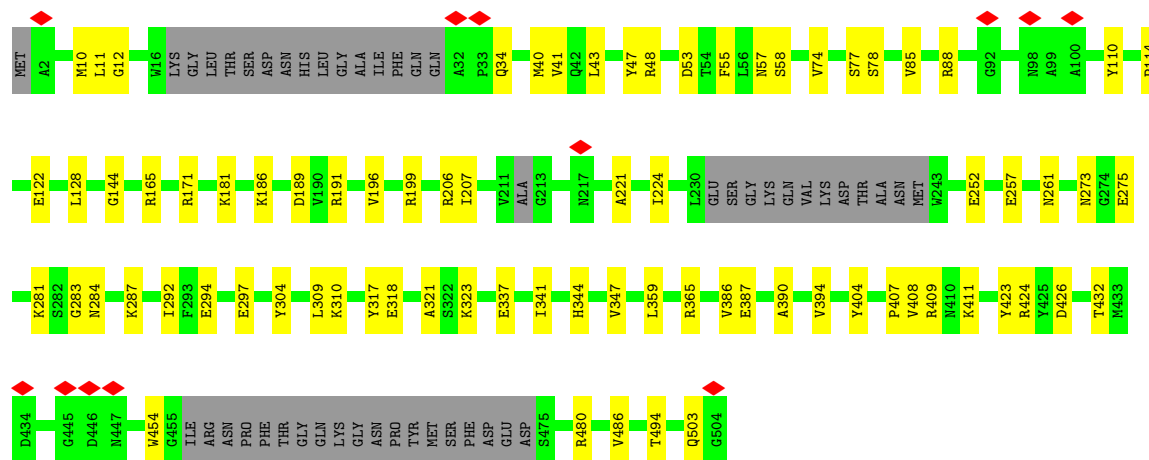
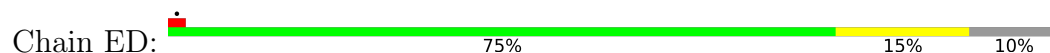


• Molecule 1: Major capsid protein gp32

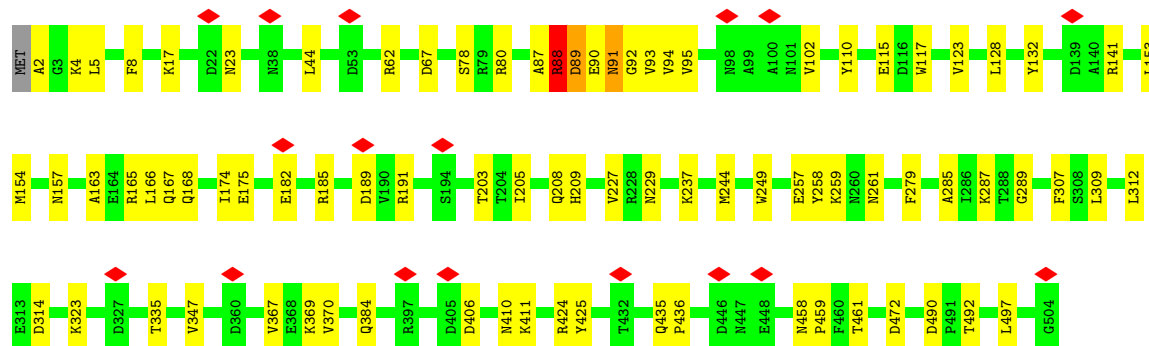
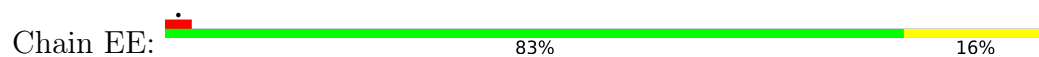




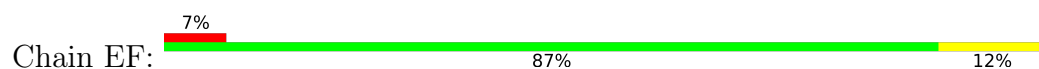
• Molecule 1: Major capsid protein gp32

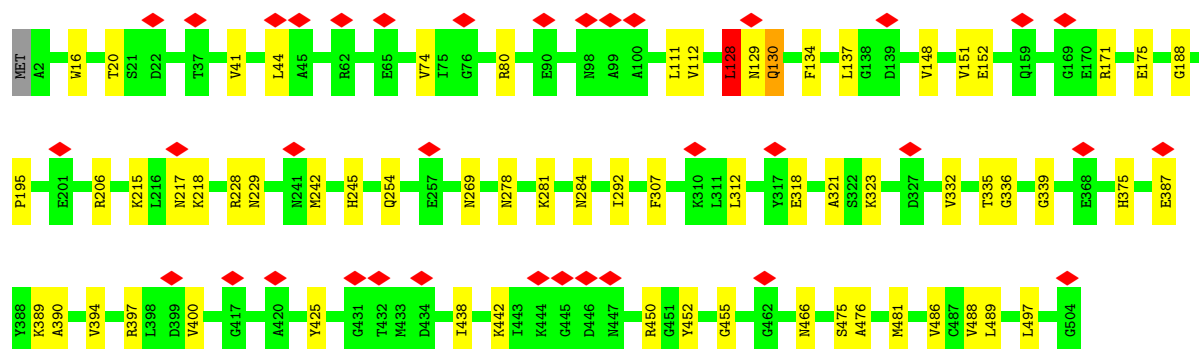


• Molecule 1: Major capsid protein gp32

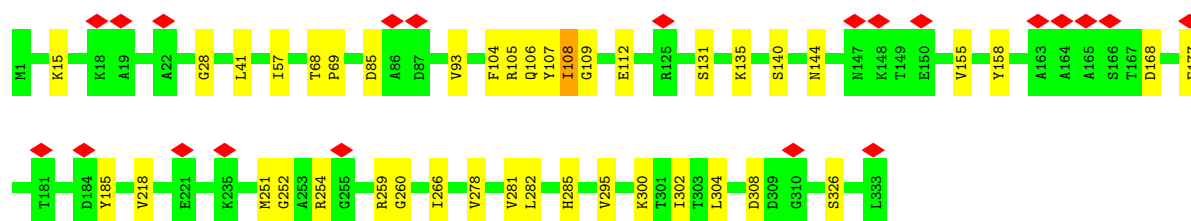


• Molecule 1: Major capsid protein gp32

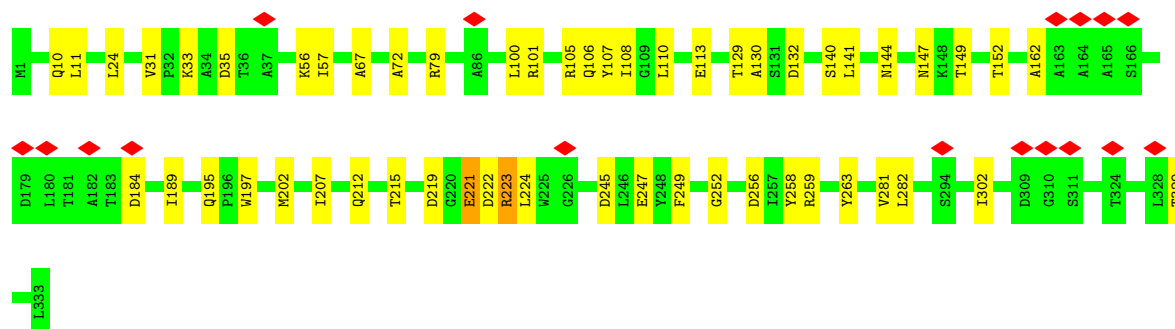
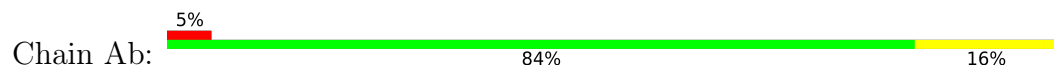




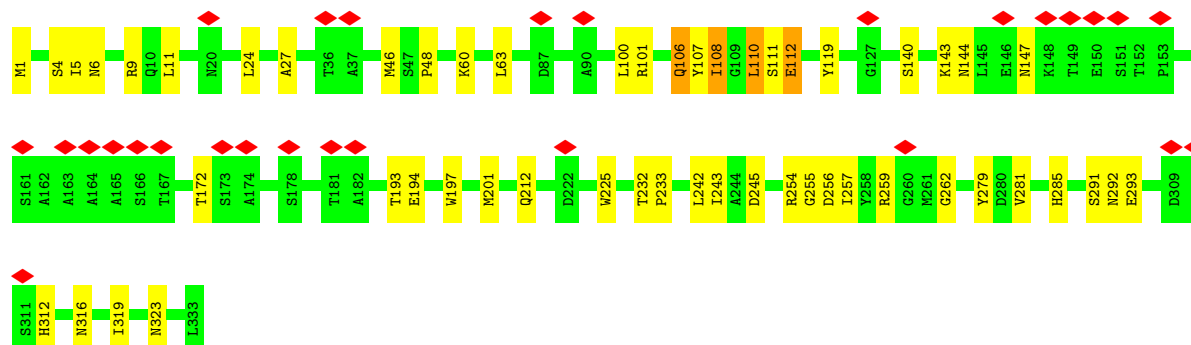
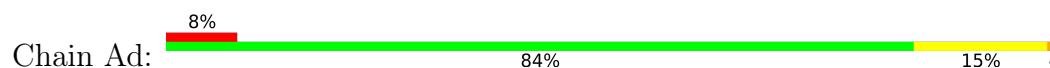
• Molecule 2: Auxiliary capsid protein gp36



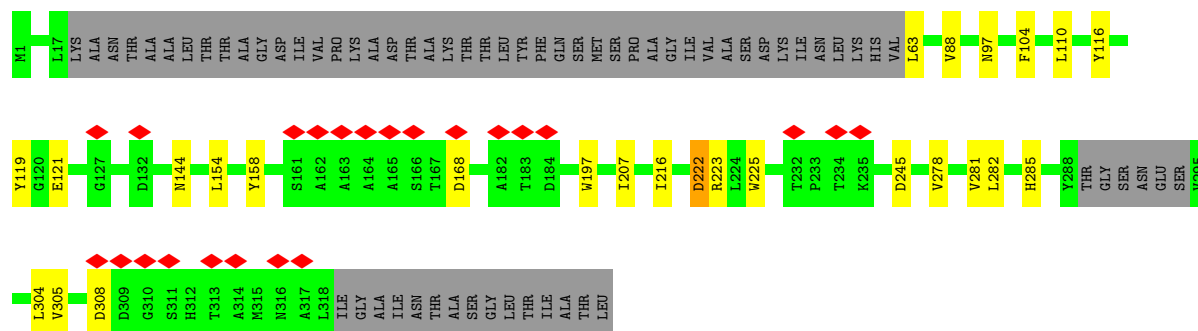
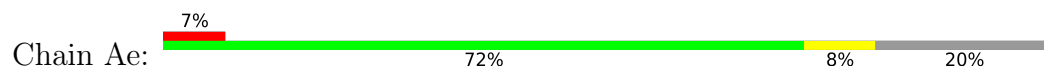
• Molecule 2: Auxiliary capsid protein gp36



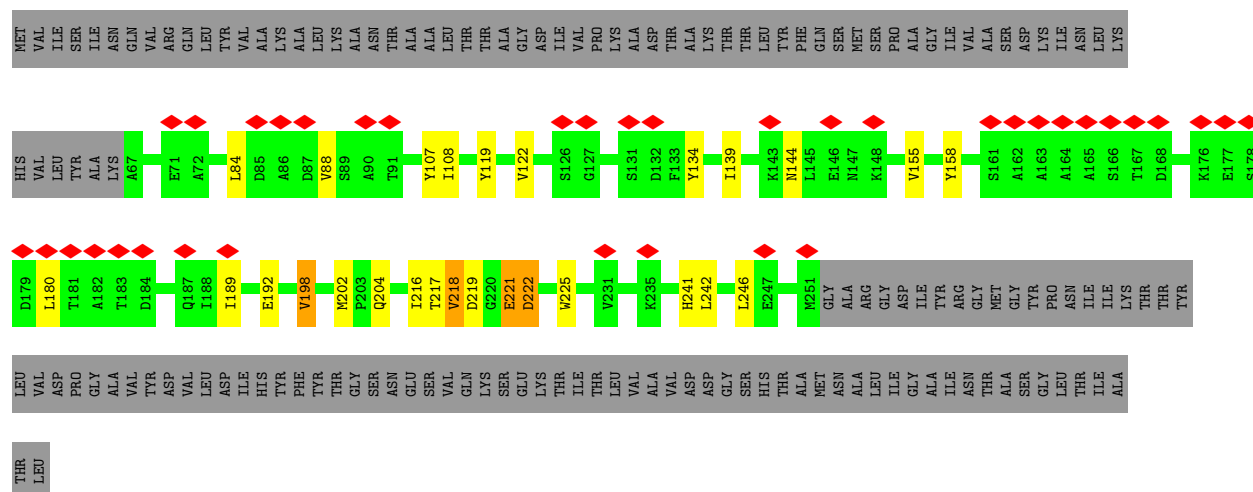
• Molecule 2: Auxiliary capsid protein gp36



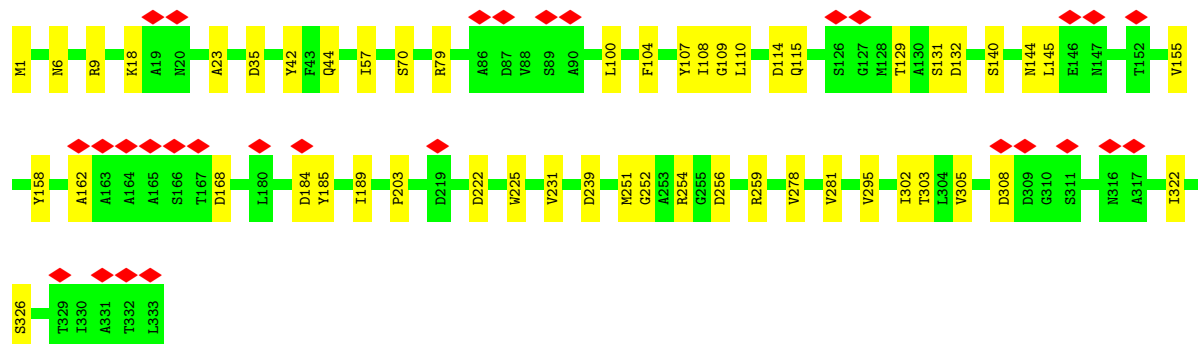
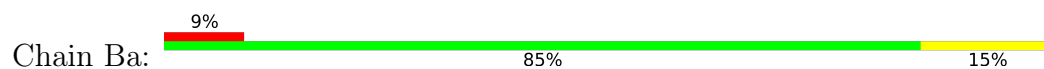
- Molecule 2: Auxiliary capsid protein gp36



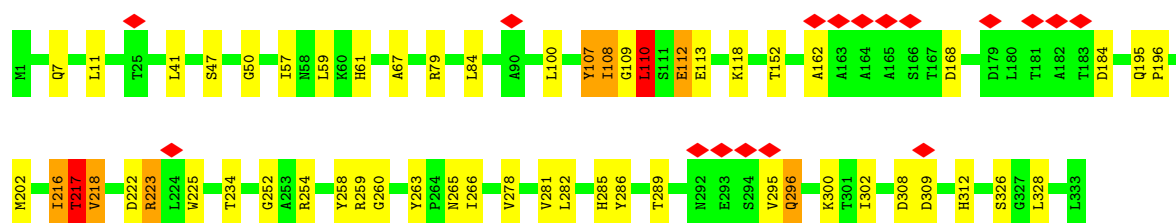
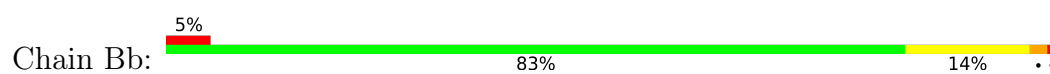
- Molecule 2: Auxiliary capsid protein gp36



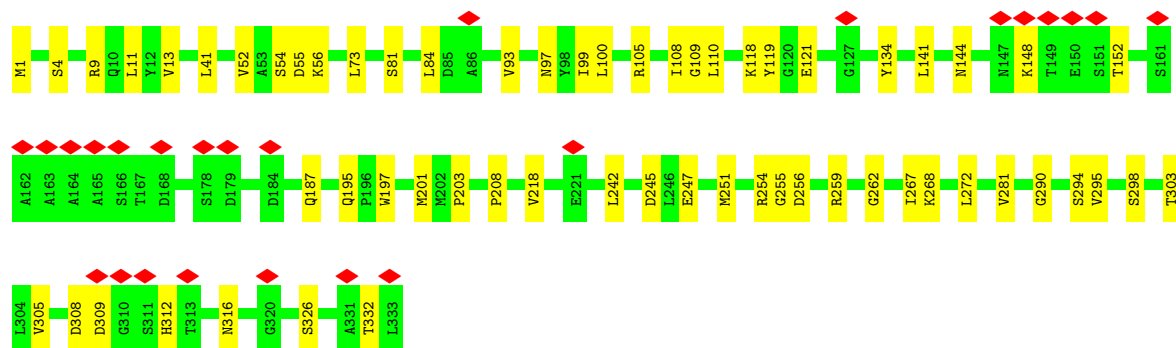
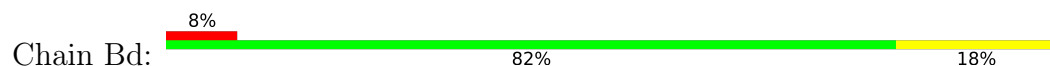
- Molecule 2: Auxiliary capsid protein gp36



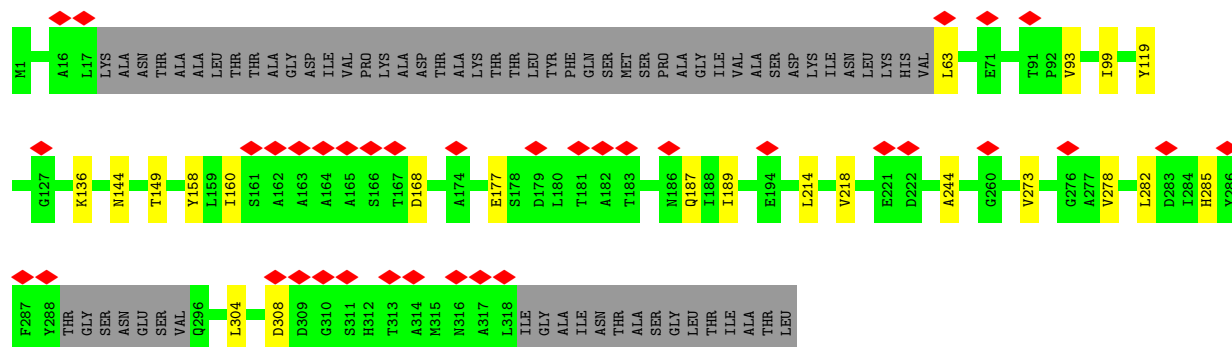
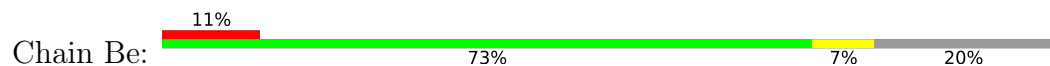
- Molecule 2: Auxiliary capsid protein gp36



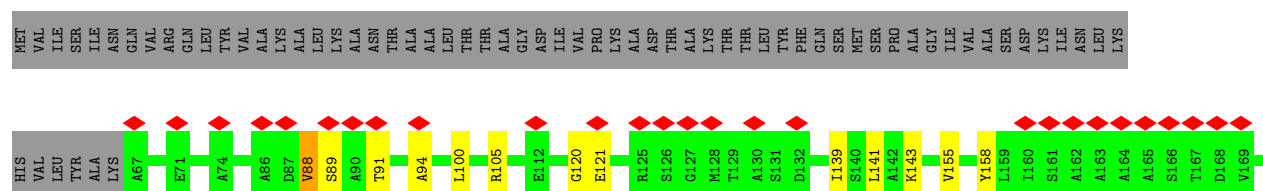
• Molecule 2: Auxiliary capsid protein gp36

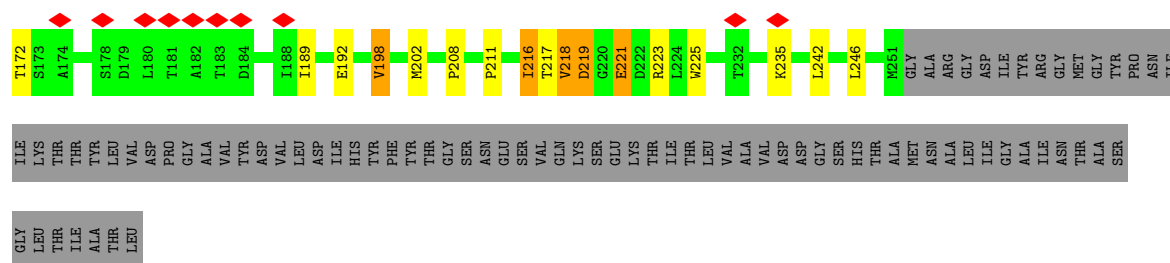


• Molecule 2: Auxiliary capsid protein gp36

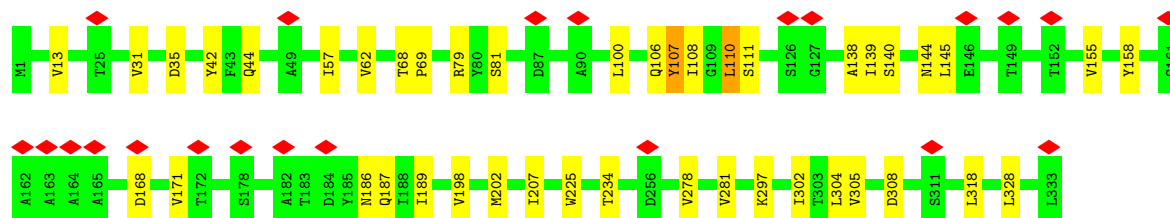
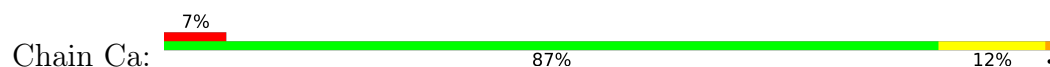


• Molecule 2: Auxiliary capsid protein gp36

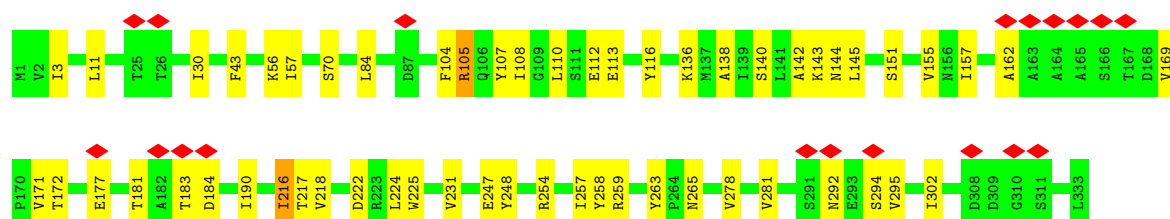
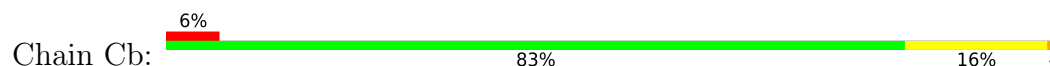




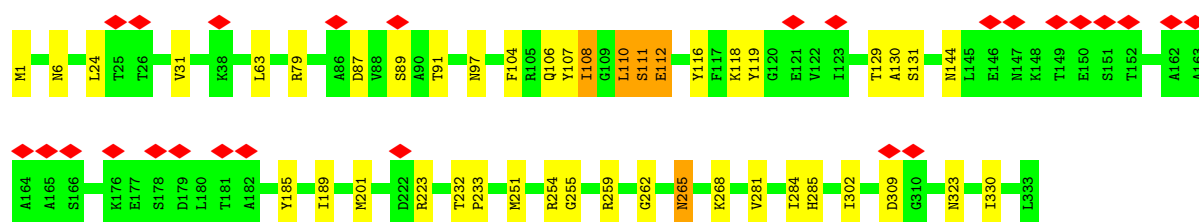
• Molecule 2: Auxiliary capsid protein gp36



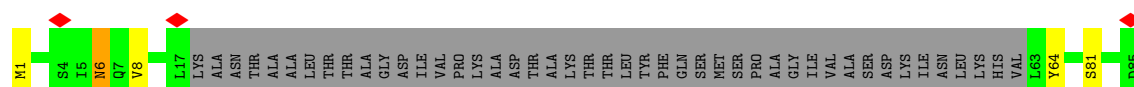
• Molecule 2: Auxiliary capsid protein gp36

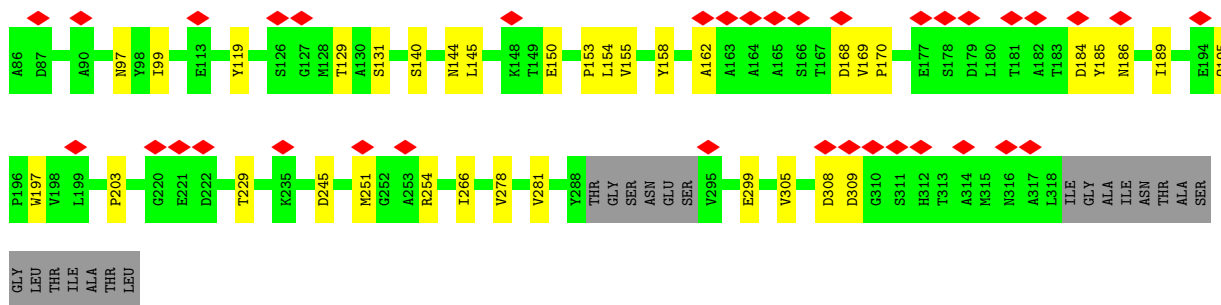


• Molecule 2: Auxiliary capsid protein gp36

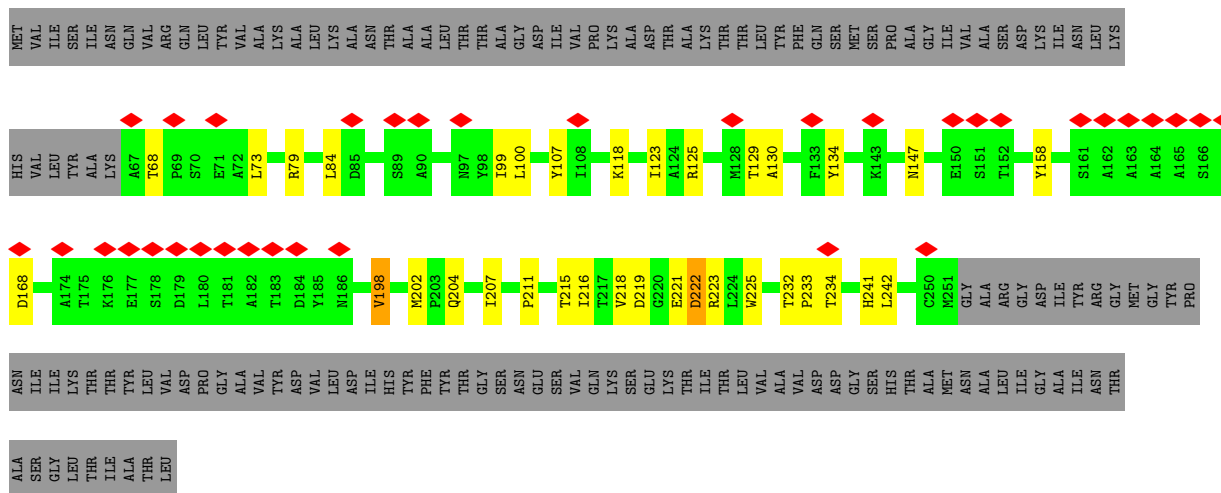


• Molecule 2: Auxiliary capsid protein gp36

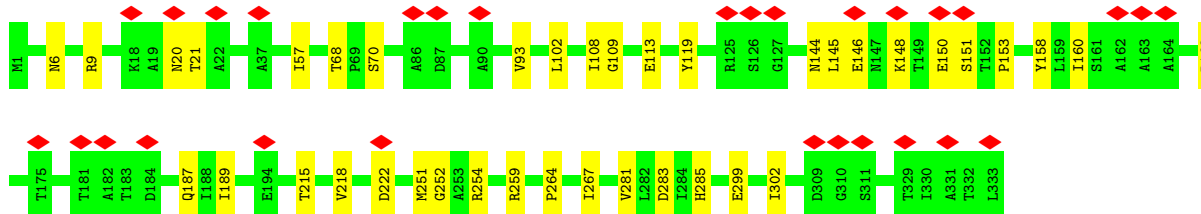
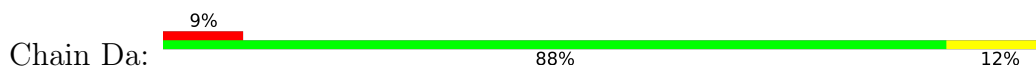




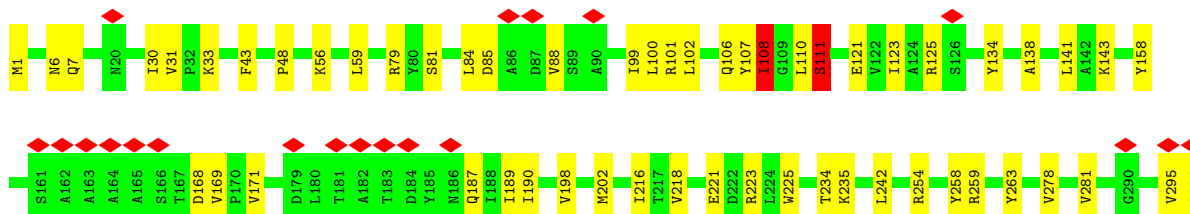
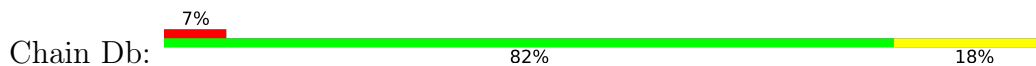
• Molecule 2: Auxiliary capsid protein gp36



• Molecule 2: Auxiliary capsid protein gp36



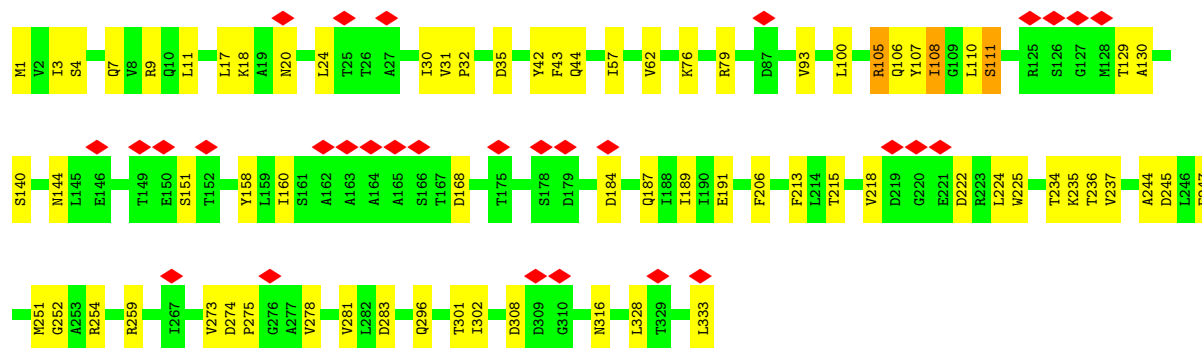
• Molecule 2: Auxiliary capsid protein gp36



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

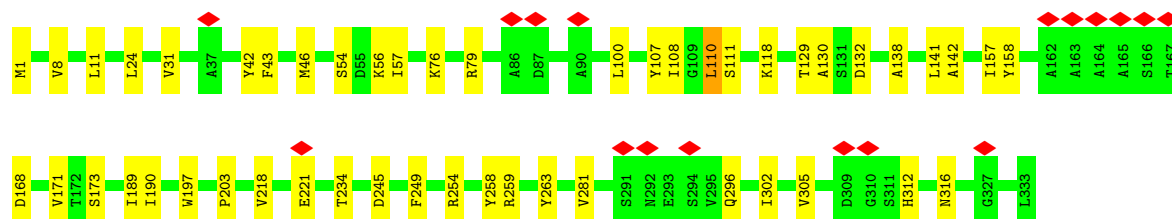
• Molecule 2: Auxiliary capsid protein gp36

Chain Ea: 9% 78% 21%



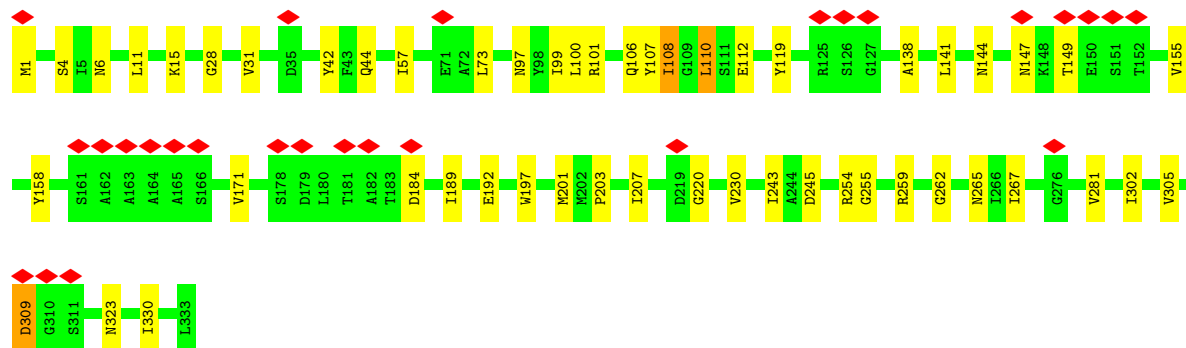
• Molecule 2: Auxiliary capsid protein gp36

Chain Eb: 5% 85% 14%



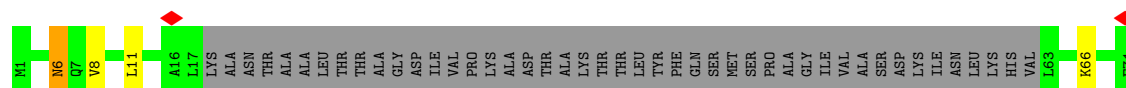
• Molecule 2: Auxiliary capsid protein gp36

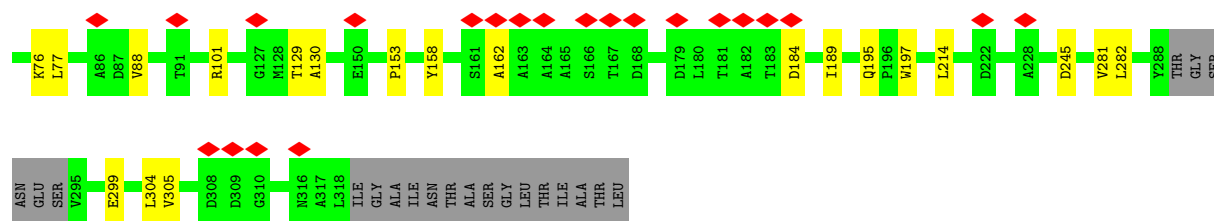
Chain Ed: 8% 84% 15%



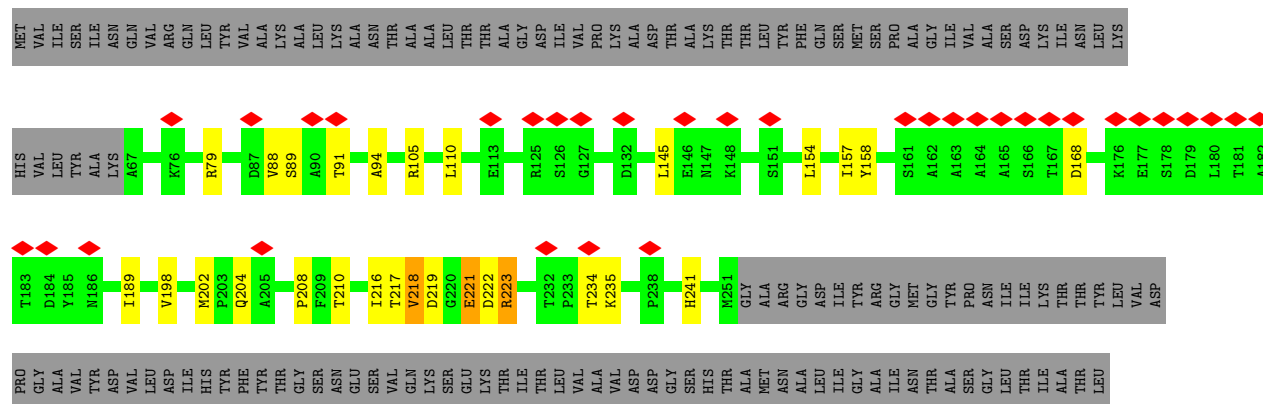
• Molecule 2: Auxiliary capsid protein gp36

Chain Ee: 7% 73% 20%

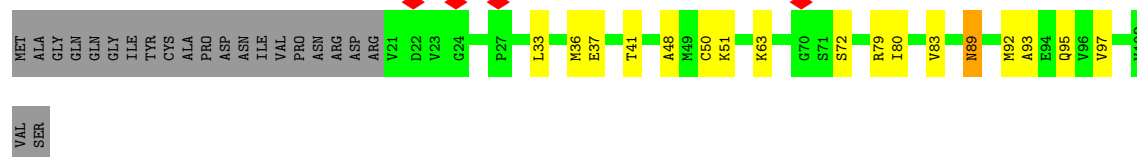




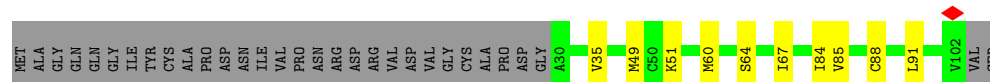
• Molecule 2: Auxiliary capsid protein gp36



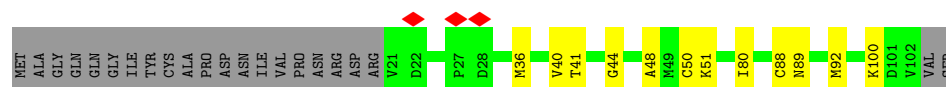
• Molecule 3: Portal vertex capsid protein gp57



• Molecule 3: Portal vertex capsid protein gp57

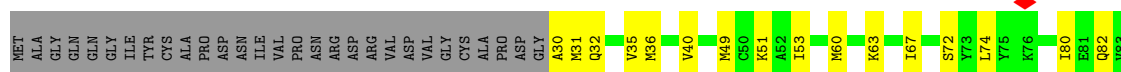


• Molecule 3: Portal vertex capsid protein gp57



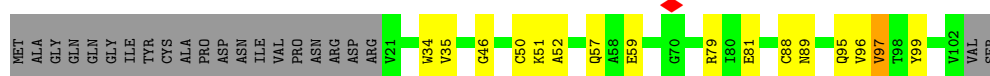
• Molecule 3: Portal vertex capsid protein gp57

Chain Bh:  52% 18% 30%



- Molecule 3: Portal vertex capsid protein gp57

Chain Cg:  63% 14% 21%



- Molecule 3: Portal vertex capsid protein gp57

Chain Ch:  5% 56% 14% 30%



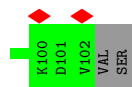
- Molecule 3: Portal vertex capsid protein gp57

Chain Dg:  64% 14% 21%



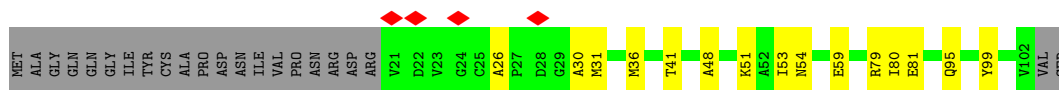
- Molecule 3: Portal vertex capsid protein gp57

Chain Dh:  55% 15% 30%

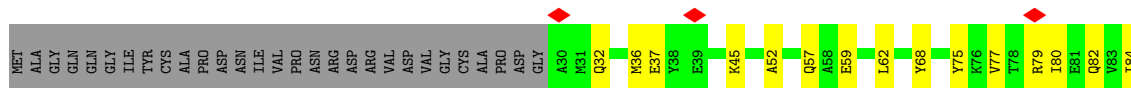


- Molecule 3: Portal vertex capsid protein gp57

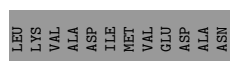
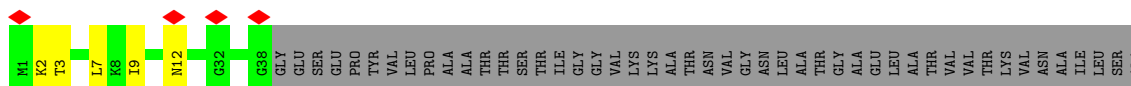
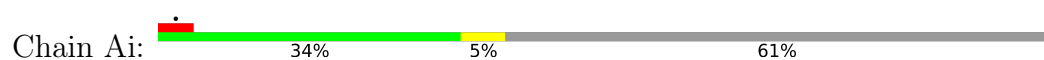
Chain Eg:  64% 14% 21%



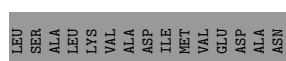
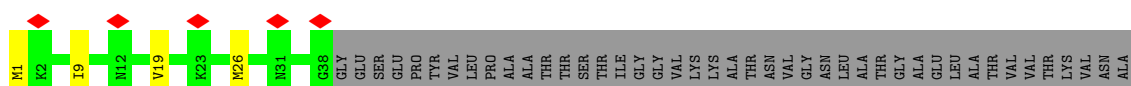
- Molecule 3: Portal vertex capsid protein gp57



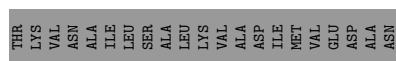
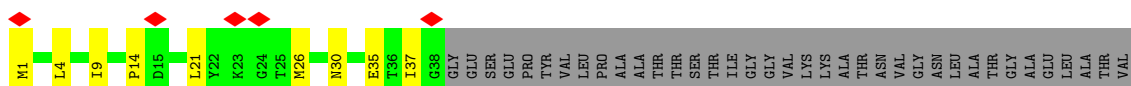
- Molecule 4: Head fiber trimer protein gp21



- Molecule 4: Head fiber trimer protein gp21

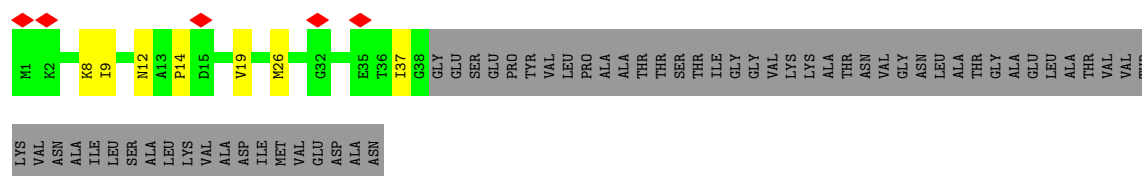


- Molecule 4: Head fiber trimer protein gp21

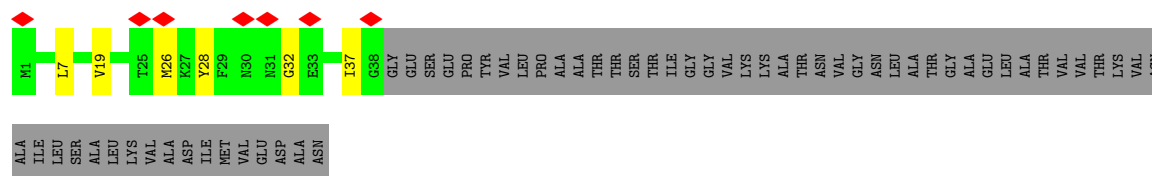


- Molecule 4: Head fiber trimer protein gp21

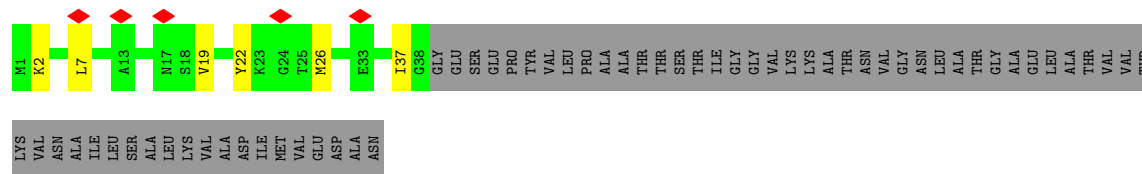
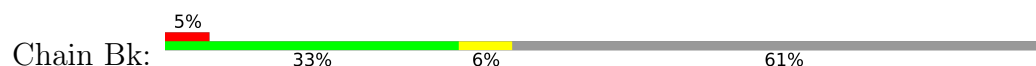




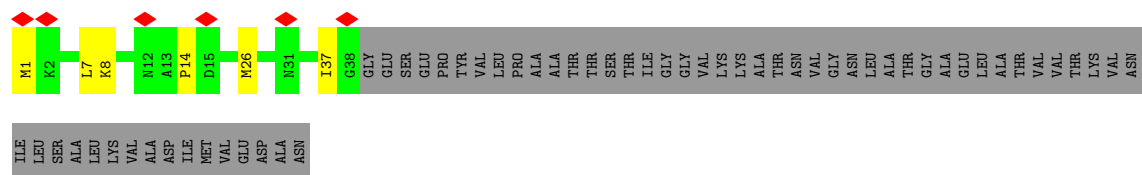
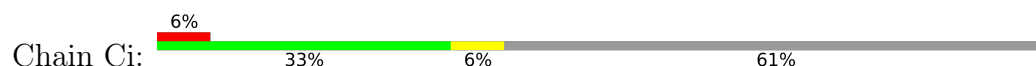
• Molecule 4: Head fiber trimer protein gp21



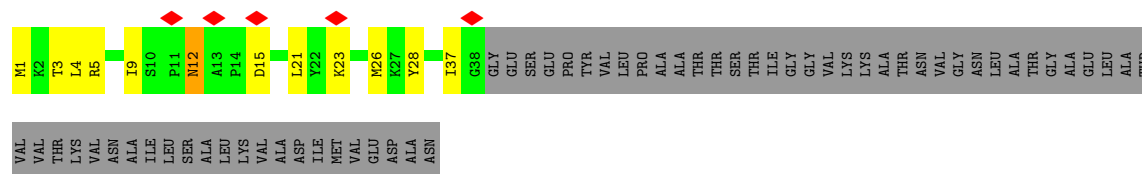
• Molecule 4: Head fiber trimer protein gp21



• Molecule 4: Head fiber trimer protein gp21

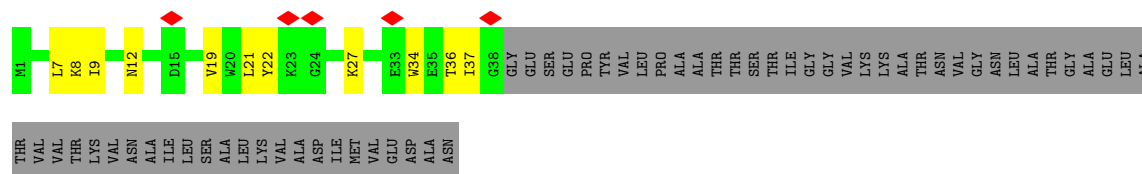


• Molecule 4: Head fiber trimer protein gp21

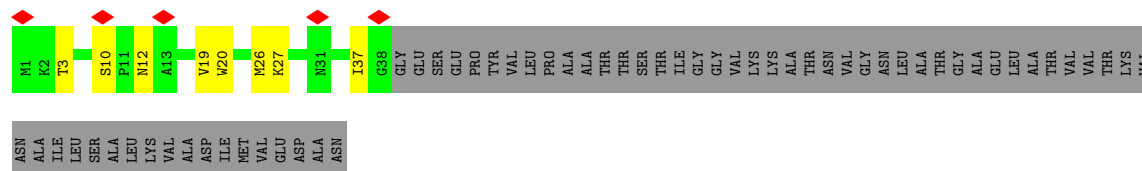


• Molecule 4: Head fiber trimer protein gp21

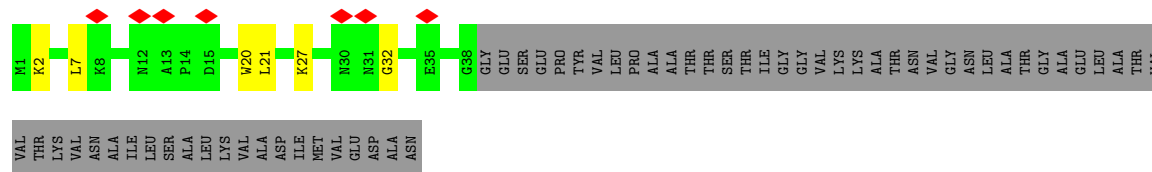
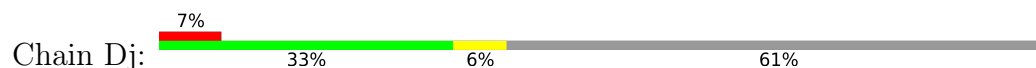




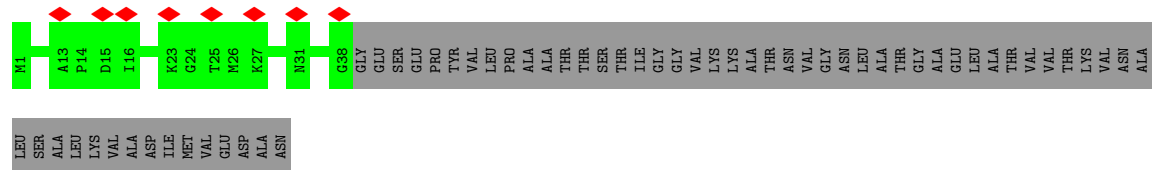
• Molecule 4: Head fiber trimer protein gp21



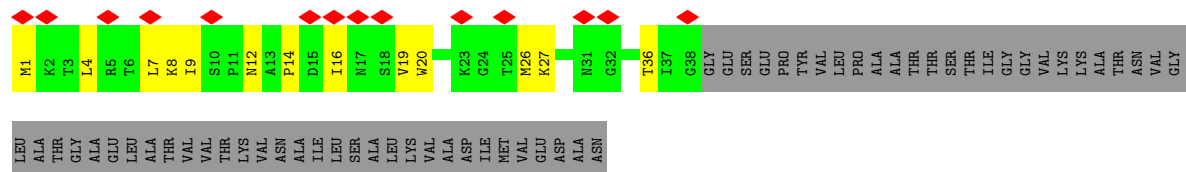
• Molecule 4: Head fiber trimer protein gp21



• Molecule 4: Head fiber trimer protein gp21

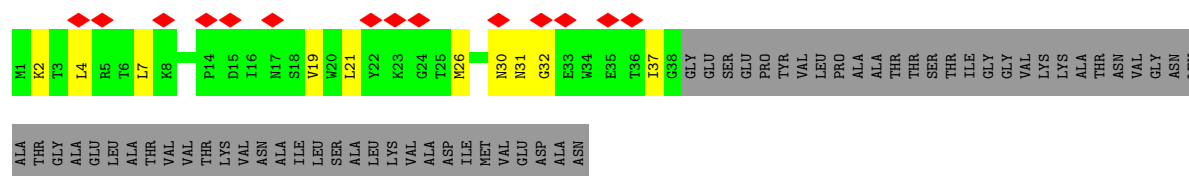


• Molecule 4: Head fiber trimer protein gp21

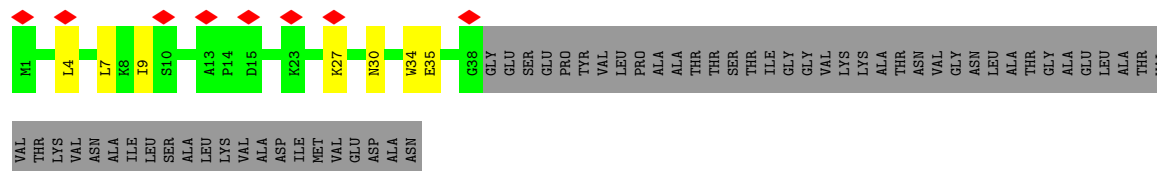
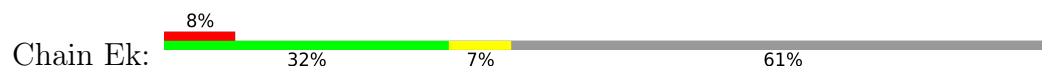


• Molecule 4: Head fiber trimer protein gp21

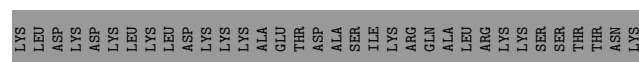
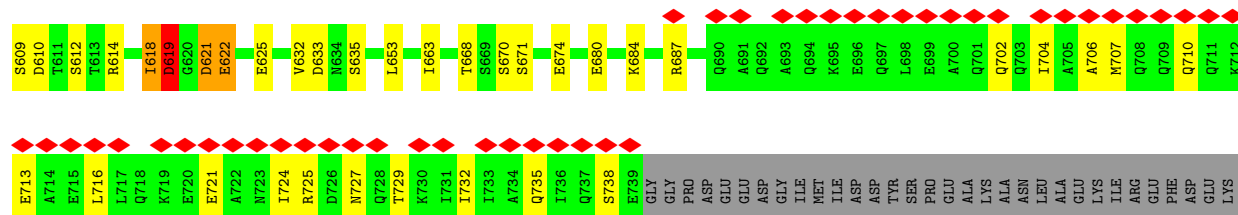
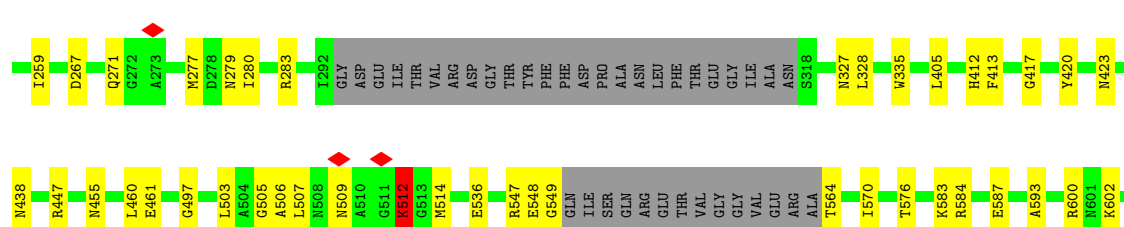
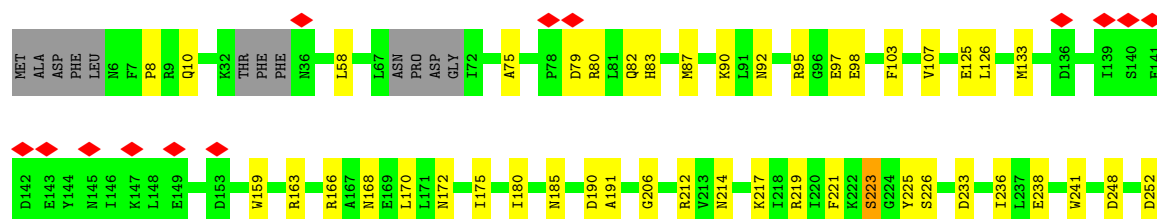
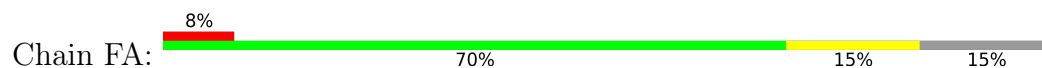




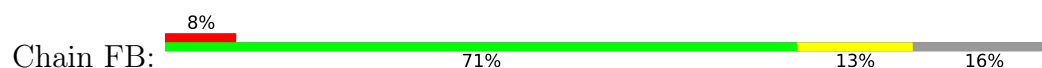
• Molecule 4: Head fiber trimer protein gp21

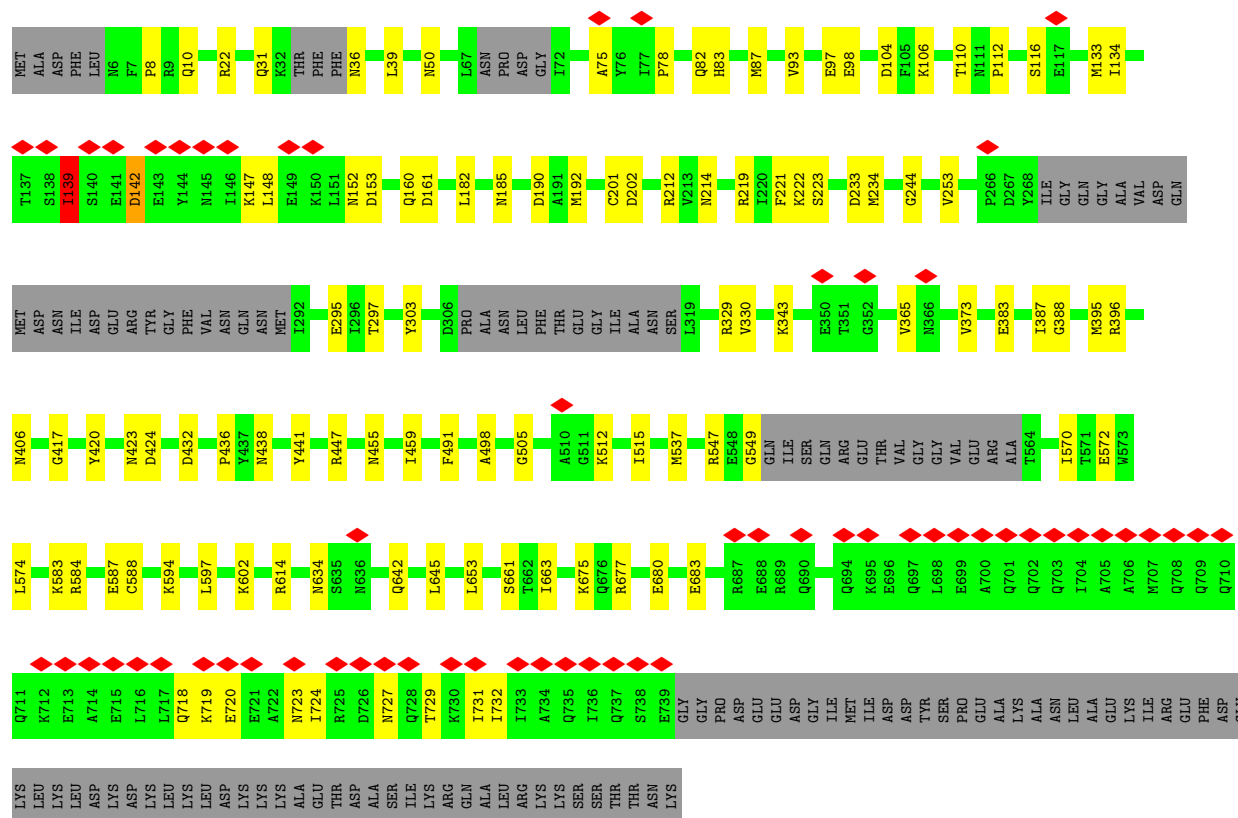


• Molecule 5: Portal protein gp20

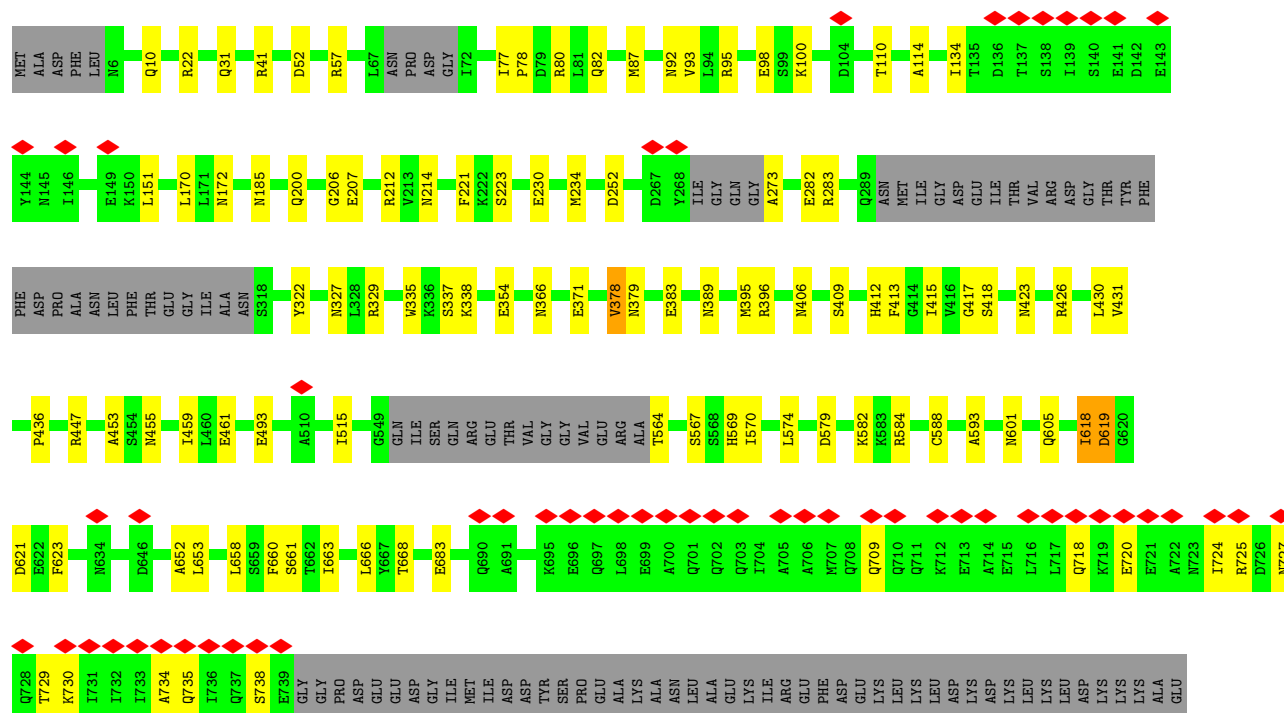
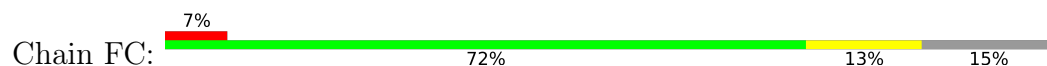


• Molecule 5: Portal protein gp20

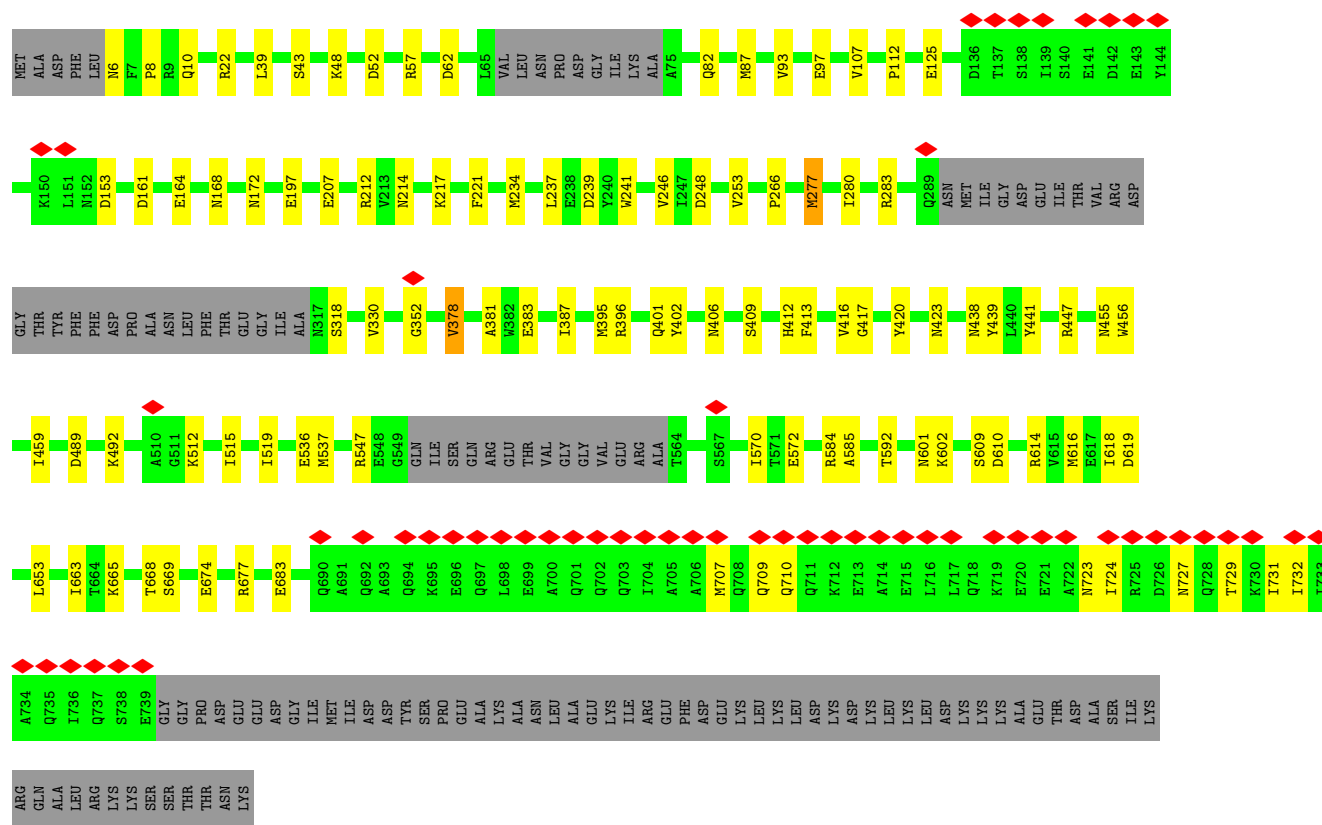
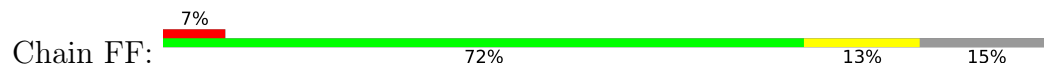




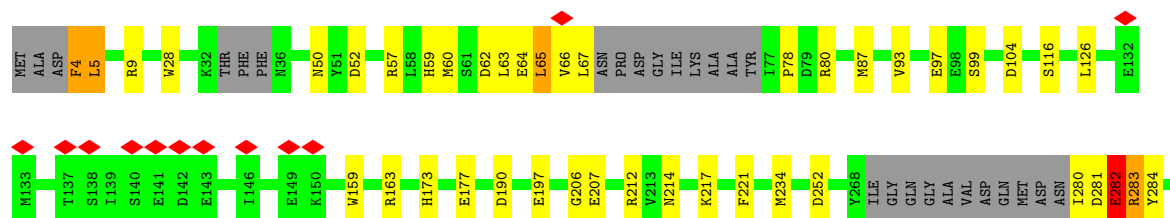
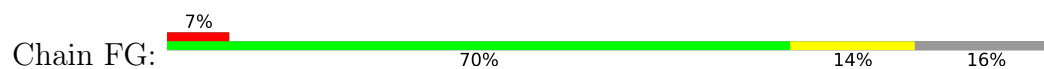
• Molecule 5: Portal protein gp20

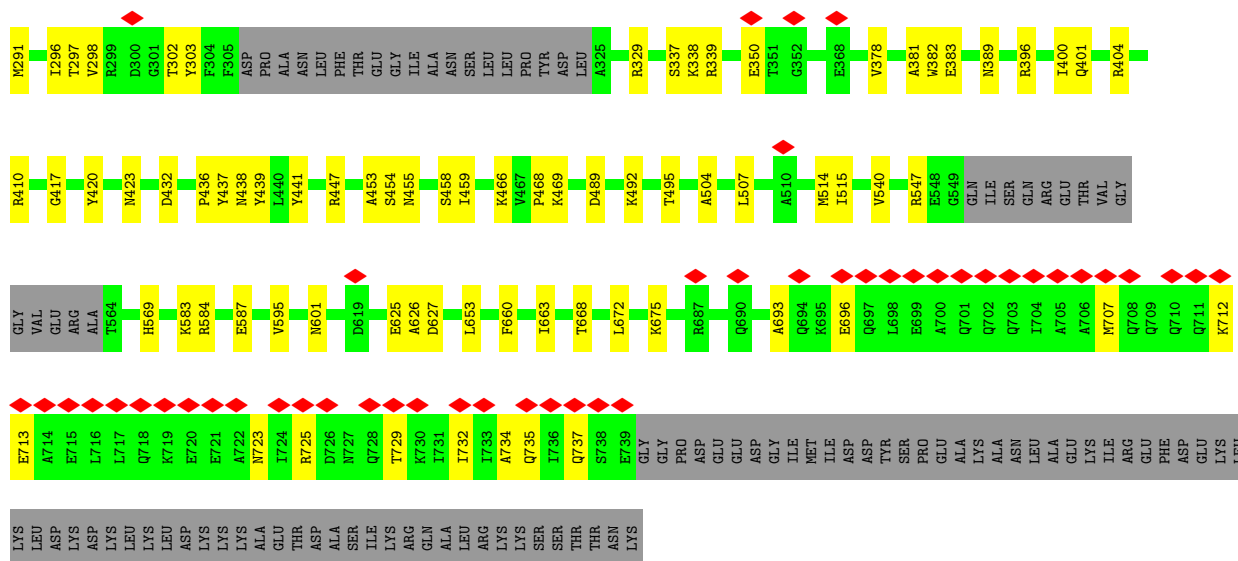


- Molecule 5: Portal protein gp20

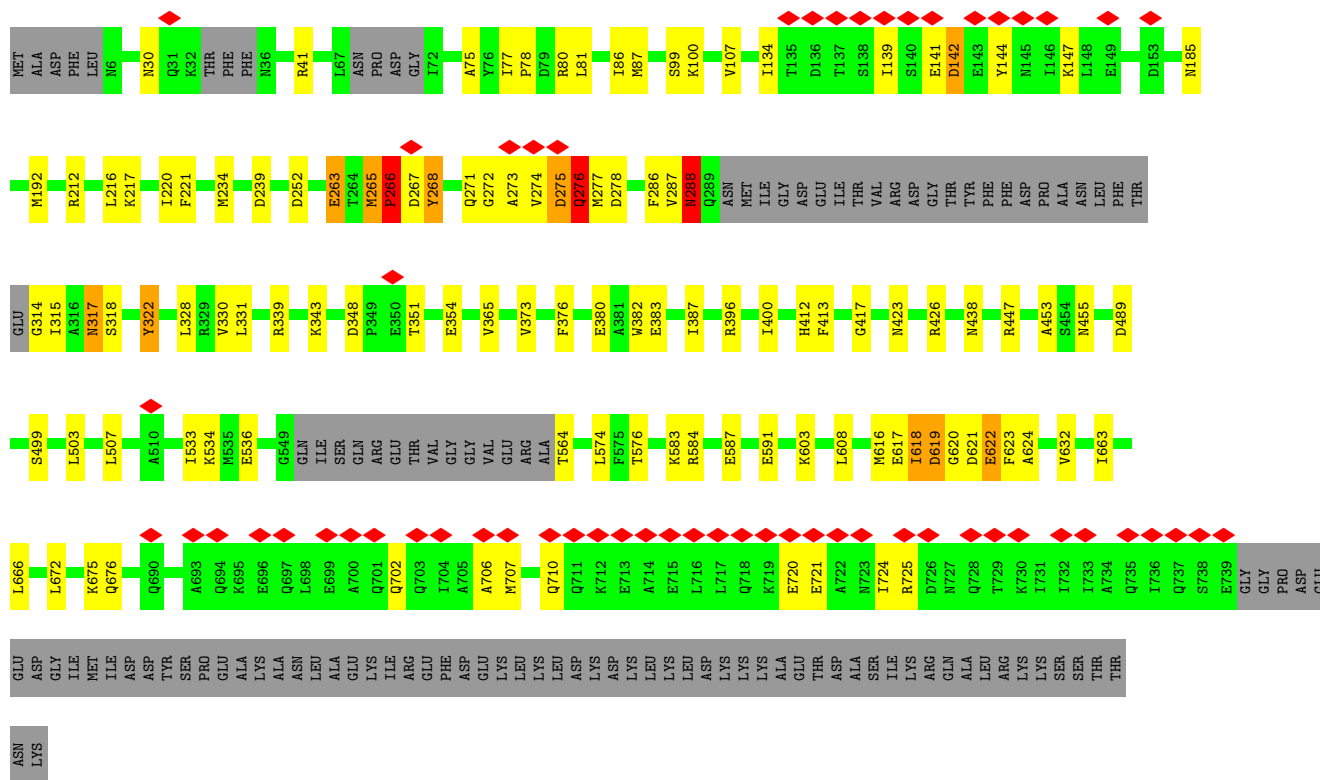


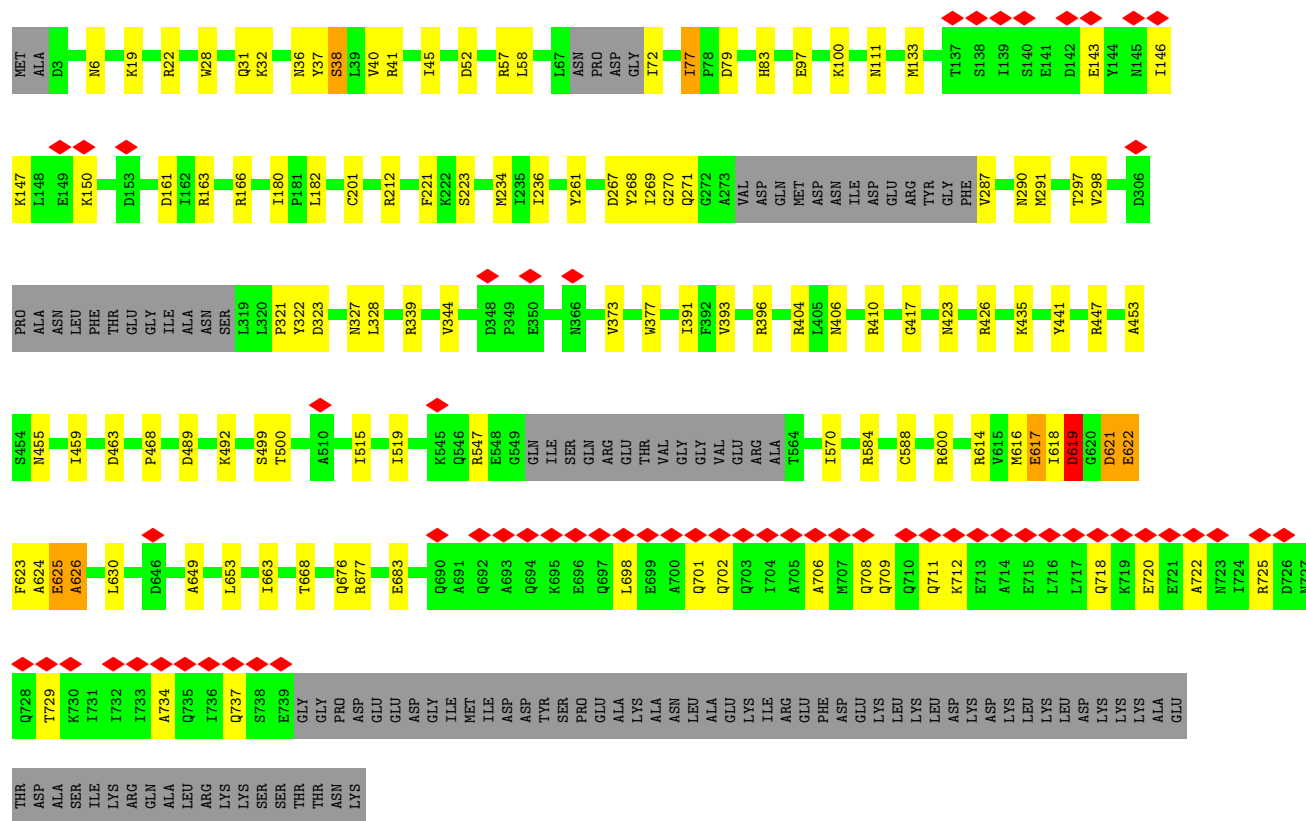
- Molecule 5: Portal protein gp20



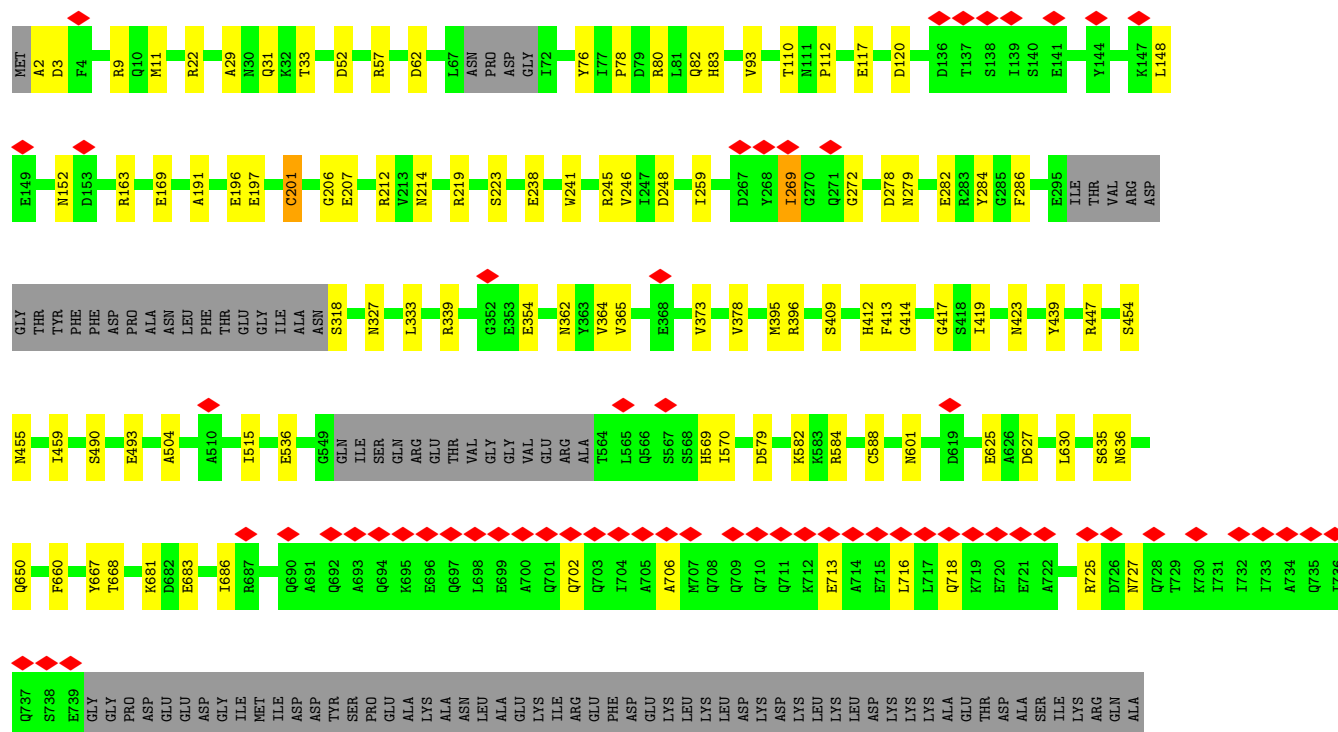
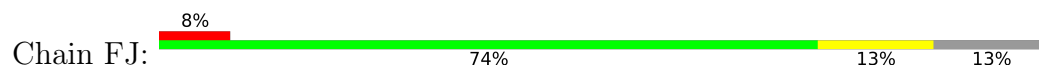


• Molecule 5: Portal protein gp20





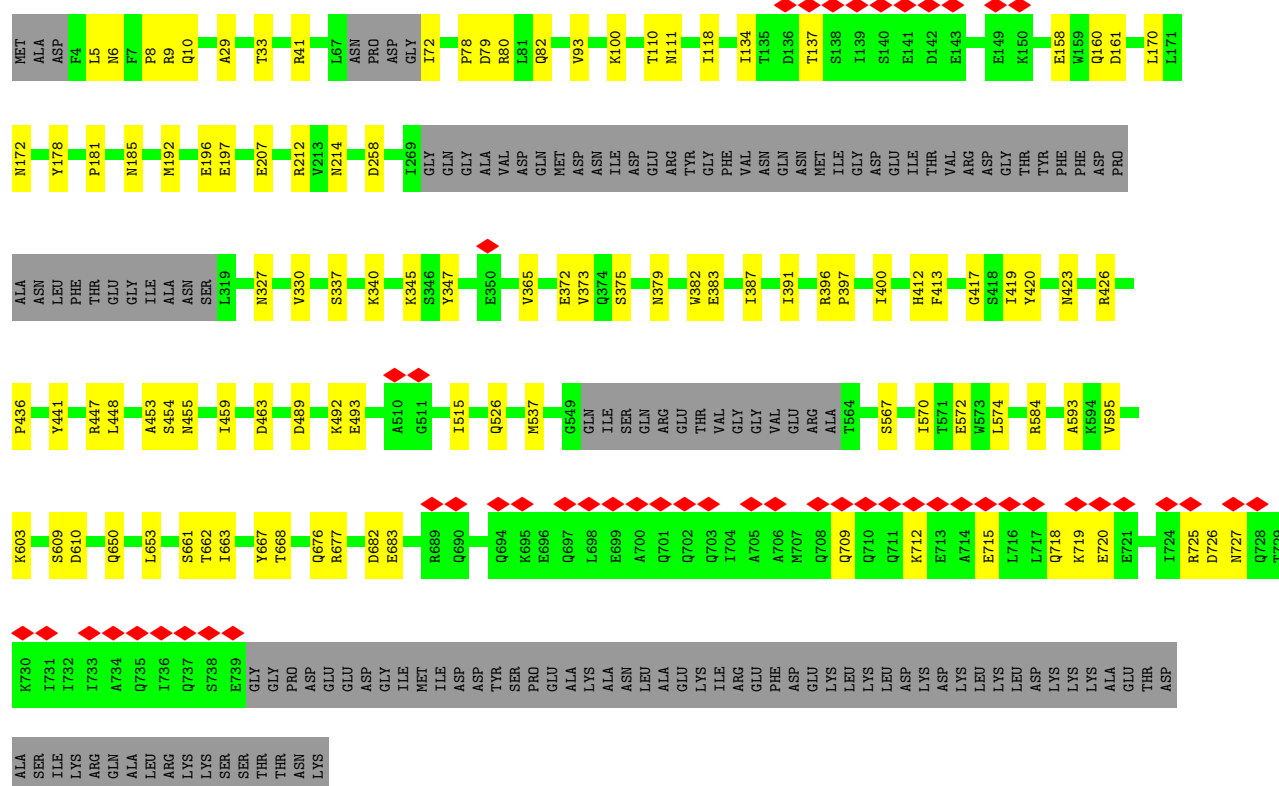
• Molecule 5: Portal protein gp20



LEU
ARG
LYS
LYS
SER
SER
THR
THR
ASN
LYS

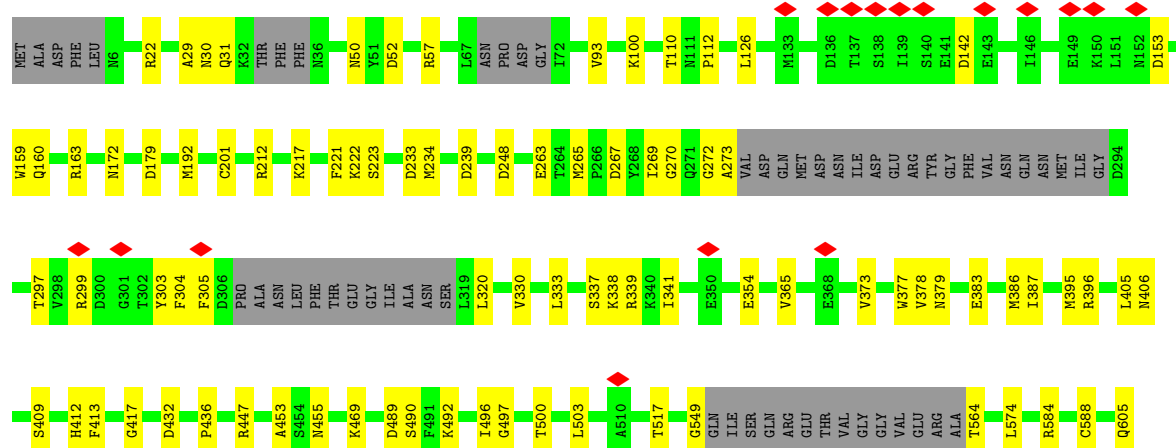
• Molecule 5: Portal protein gp20

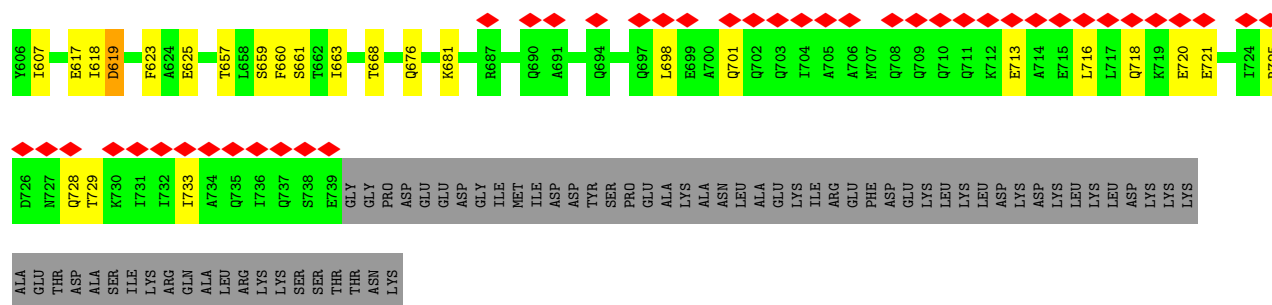
Chain FK: 



• Molecule 5: Portal protein gp20

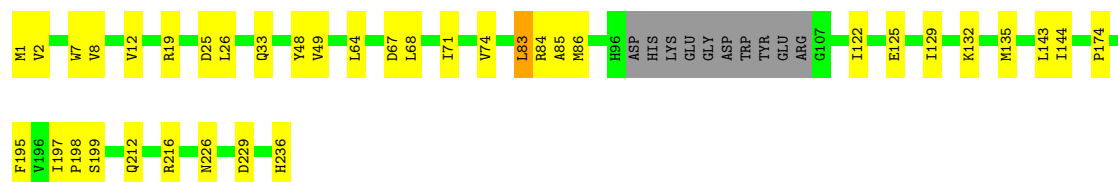
Chain FL: 





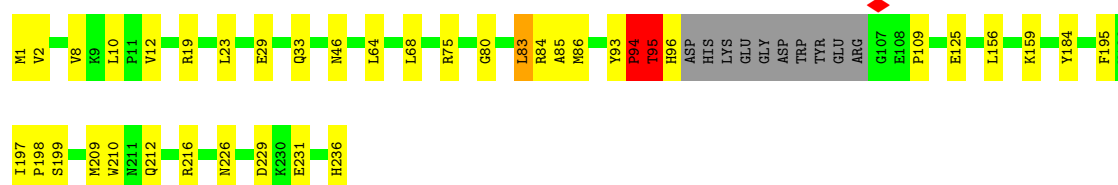
- Molecule 6: Ring protein 1 gp43

Chain FM: 80% 15% .



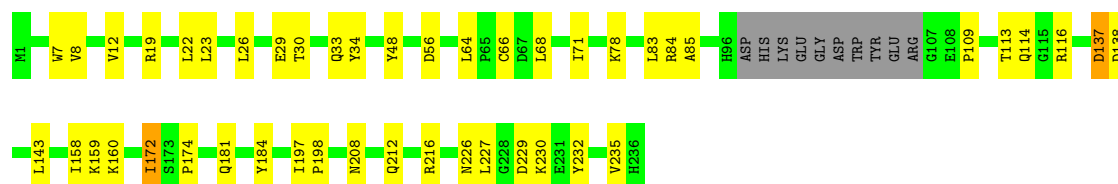
- Molecule 6: Ring protein 1 gp43

Chain FN: 79% 15% . .



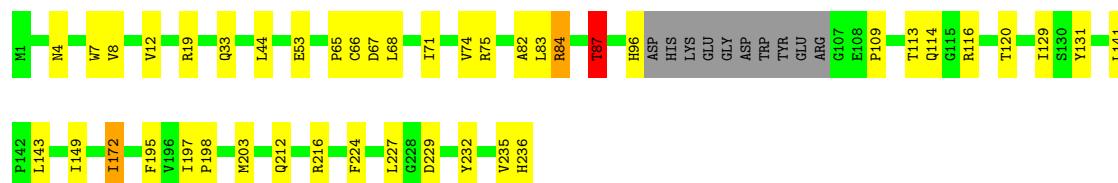
- Molecule 6: Ring protein 1 gp43

Chain FO: 76% 19% . .

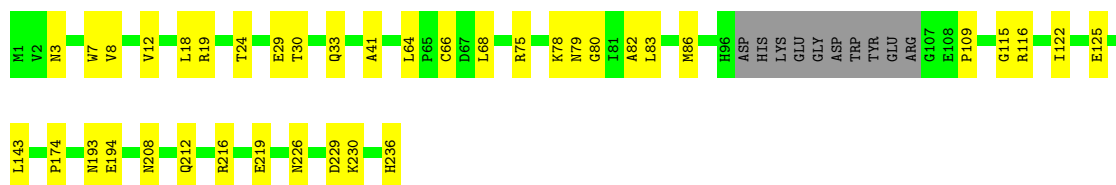


- Molecule 6: Ring protein 1 gp43

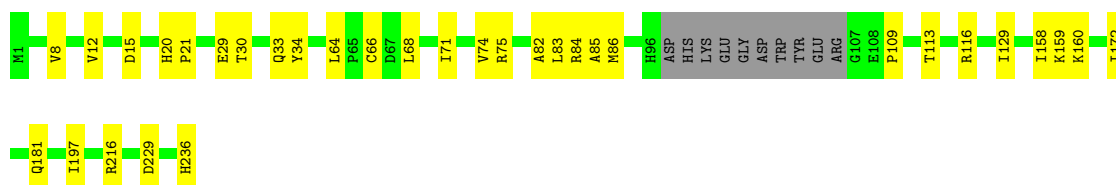
Chain FP: 78% 17% . .



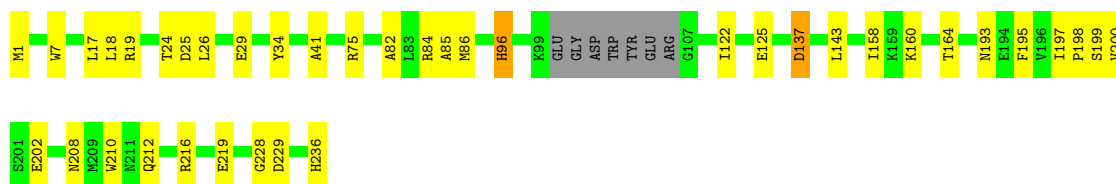
• Molecule 6: Ring protein 1 gp43

Chain FQ:  80% 16% .

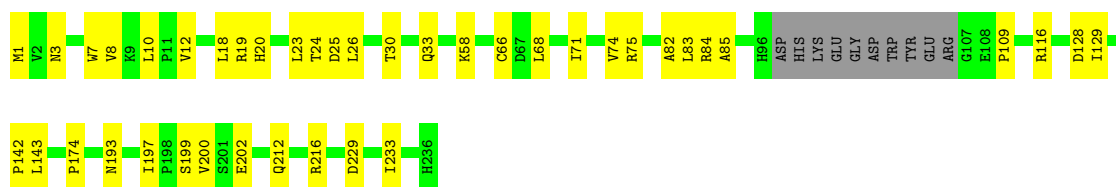
• Molecule 6: Ring protein 1 gp43

Chain FR:  82% 14% .

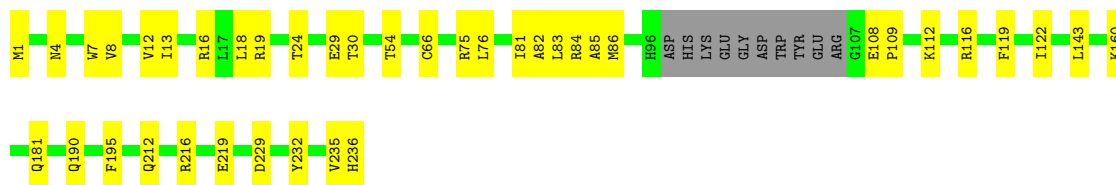
• Molecule 6: Ring protein 1 gp43

Chain FS:  81% 16% ..

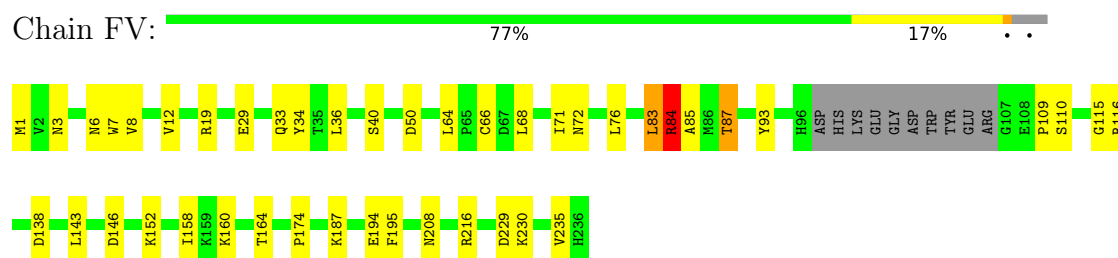
• Molecule 6: Ring protein 1 gp43

Chain FT:  78% 17% .

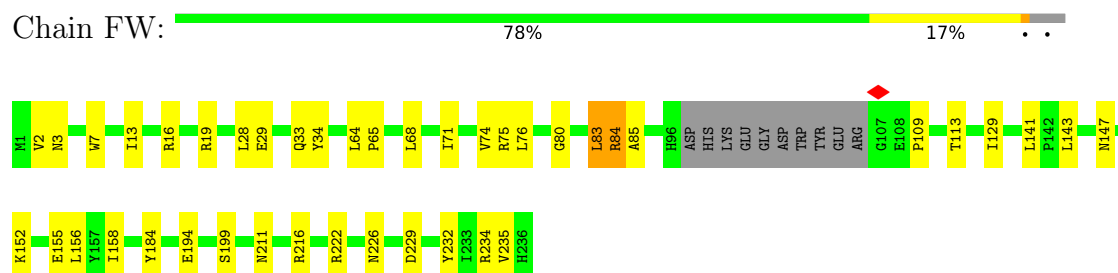
• Molecule 6: Ring protein 1 gp43

Chain FU:  79% 17% .

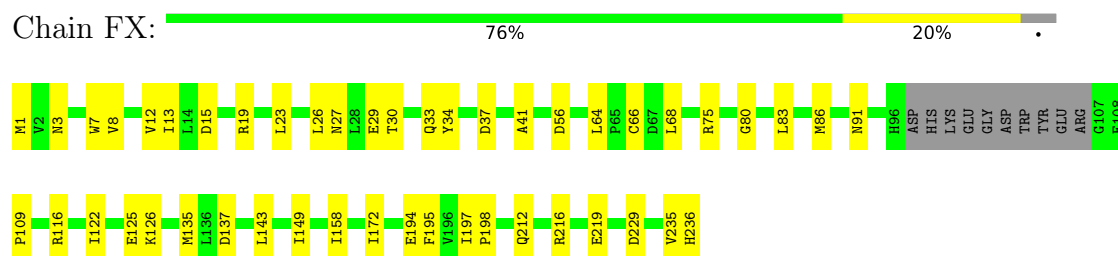
- Molecule 6: Ring protein 1 gp43



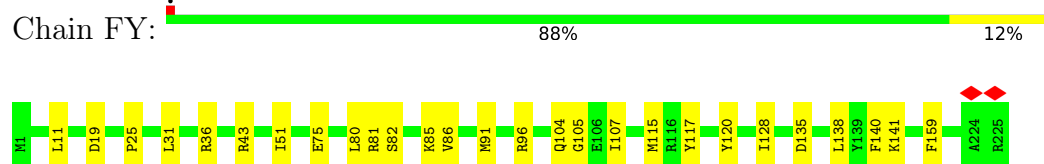
- Molecule 6: Ring protein 1 gp43



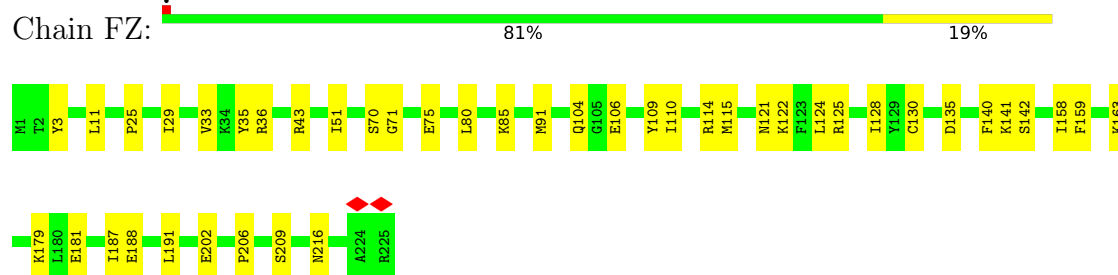
- Molecule 6: Ring protein 1 gp43



- Molecule 7: Ring protein 2 gp40

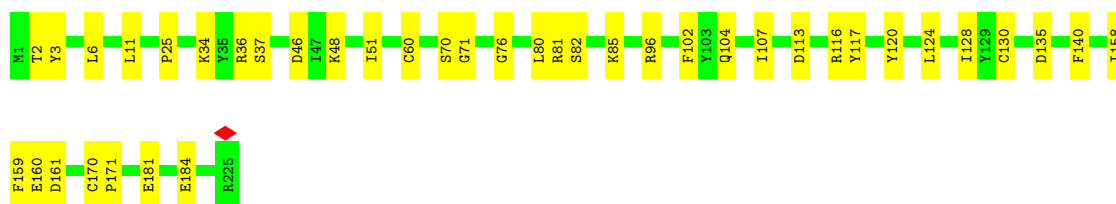


- Molecule 7: Ring protein 2 gp40



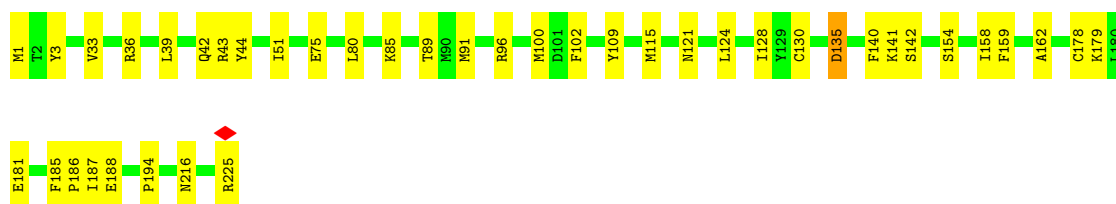
- Molecule 7: Ring protein 2 gp40

Chain GA:  82% 18%



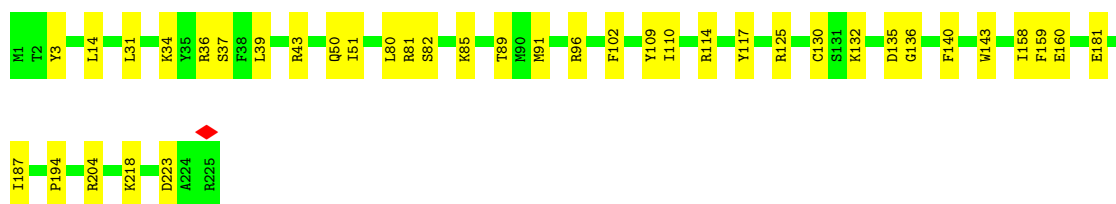
- Molecule 7: Ring protein 2 gp40

Chain GB:  82% 18%



- Molecule 7: Ring protein 2 gp40

Chain GC:  83% 17%



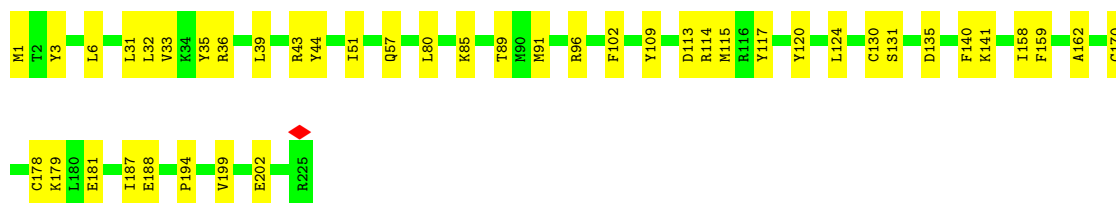
- Molecule 7: Ring protein 2 gp40

Chain GD:  87% 13%



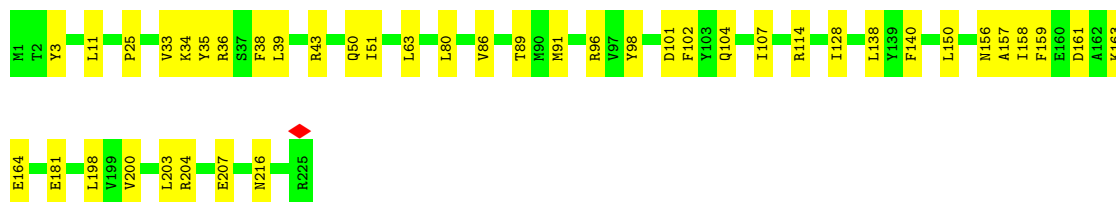
- Molecule 7: Ring protein 2 gp40

Chain GE:  81% 19%



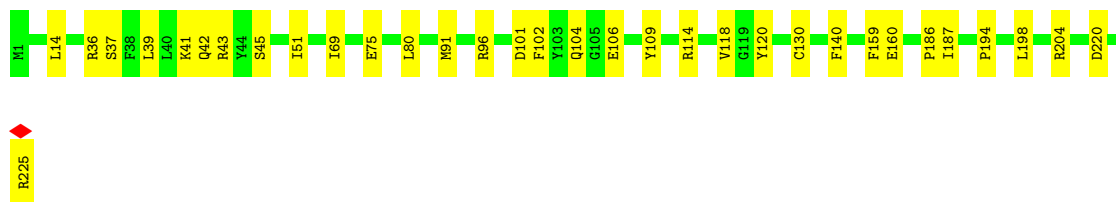
- Molecule 7: Ring protein 2 gp40

Chain GF:  81% 19%



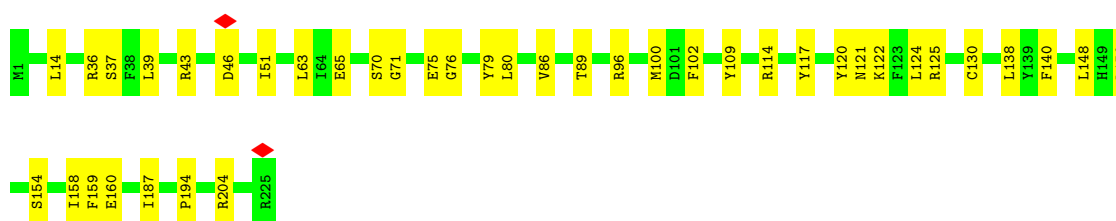
- Molecule 7: Ring protein 2 gp40

Chain GG:  85% 15%



- Molecule 7: Ring protein 2 gp40

Chain GH:  82% 18%



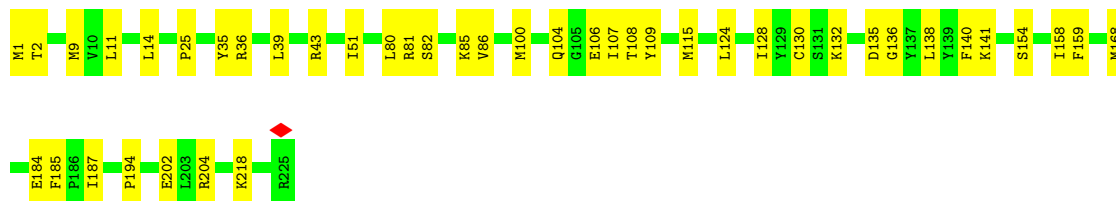
- Molecule 7: Ring protein 2 gp40

Chain GI:  89% 11%

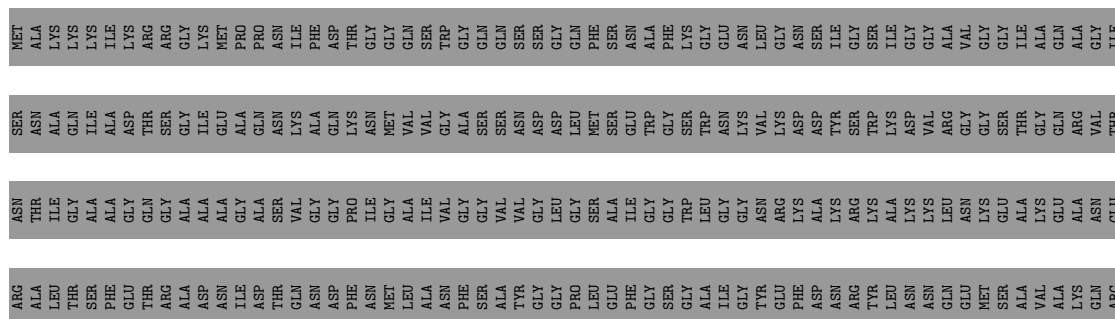
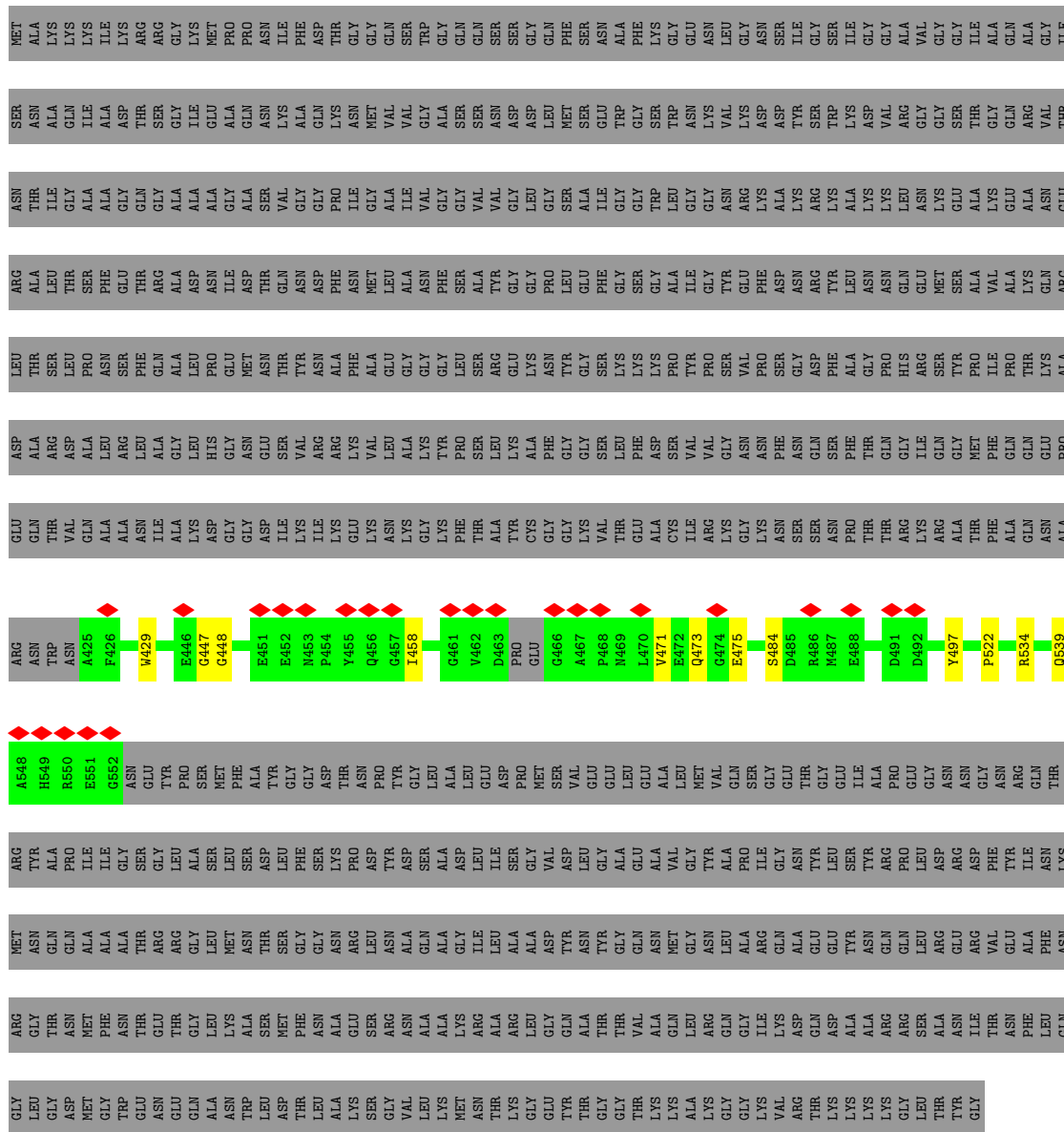


- Molecule 7: Ring protein 2 gp40

Chain GJ:  81% 19%



- Molecule 8: Cargo protein 1 gp45



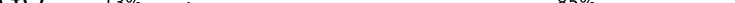


[illegible]

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

[illegible]

- Molecule 8: Cargo protein 1 gp45

Chain GQ:  13% 85%

[illegible]

[illegible]

- Molecule 8: Cargo protein 1 gp45

Chain IK: 96%

[illegible]

- Molecule 8: Cargo protein 1 gp45

96%

- Molecule 8: Cargo protein 1 gp45

96%

[illegible]

[illegible]

- Molecule 8: Cargo protein 1 gp45

Chain IO: 96%

[illegible]

Chain IQ:



[illegible]

- Molecule 8: Cargo protein 1 gp45

Chain IS: 96%

Tyr	Phe	Lys	Val	Tyr	Arg	Asn	Ser	Met
Lys	Thr	Ile	Arg	Asn	Ala	Thr	Asn	Met
Leu	Asn	Lys	Arg	Ala	Leu	Ile	Ala	Lys
Arg	Gly	Glu	Lys	Phe	Thr	Gly	Gln	Lys
Gly	Val	Lys	Val	Ala	Ser	Ala	Ile	Lys
Lys	Thr	Asn	Leu	Glu	Phe	Ala	Ala	Ile
Thr	Phe	Lys	Ala	Gly	Glu	Gly	Asp	Lys
Phe	Ile	Gly	Lys	Gly	Thr	Thr	Thr	Arg
Asn	Asn	Phe	Tyr	Leu	Arg	Gly	Ser	Gly
Lys	Glu	Phe	Pro	Gly	Ala	Ala	Gly	Lys
Ala	Gly	Thr	Leu	Ser	Asp	Ala	Ile	Lys
Ala	Gly	Ala	Leu	Arg	Asn	Ala	Glu	Met
Lys	Ser	Tyr	Lys	Glu	Ile	Gly	Ala	Pro
Ser	His	Lys	Ala	Lys	Asp	Ala	Gln	Pro
Ala	Glu	Gly	Phe	Asn	Thr	Ser	Asn	Asn
Gln	Glu	Gly	Gly	Tyr	Gln	Val	Lys	Ile
Arg	Asn	Lys	Gly	Gly	Asn	Gly	Ala	Phe
Glu	Pro	Val	Ser	Ser	Asp	Gly	Gln	Asp
Ser	Tyr	Thr	Leu	Lys	Phe	Pro	Lys	Thr
Glu	Gln	Glu	Phe	Lys	Asn	Ile	Asn	Gly
Glu	Gly	Ala	Asp	Lys	Met	Gly	Met	Gly
Arg	Ile	Cys	Ser	Pro	Leu	Ala	Val	Gln
Pro	Gln	Ile	Val	Tyr	Ala	Ile	Val	Ser
Asn	Tle	Arg	Val	Pro	Asn	Val	Gly	Trp
Asp	Gly	Lys	Gly	Ser	Phe	Gly	Ala	Gly
Pro	Val	Gly	Asn	Pro	Ser	Gly	Ser	Gln
Pro	Asp	Lys	Asn	Ala	Lys	Val	Ser	Asn
Leu	Asp	Lys	Phe	Ser	Tyr	Val	Asn	Ser
Ser	Pro	Asn	Asn	Gly	Gly	Gly	Asp	Ser
Thr	Glu	Ser	Gln	Asp	Gly	Leu	Asp	Gly
Lys	Gly	Ser	Gln	Asn	Pro	Gly	Leu	Gln
Gly	Ala	Asn	Ser	Phe	Leu	Ser	Met	Phe
Leu	Pro	Pro	Phe	Ala	Leu	Ser	Ser	Ser
Gln	Asn	Thr	Thr	Gly	Glu	Ile	Glu	Asn
Ala	Leu	Thr	Gln	Pro	F214	Ile	Trp	Ala
Ala	Val	Arg	Gly	His	Y221	Gly	Gly	Phe
Met	Glu	Lys	Ile	Arg	E222	Trp	Gly	Lys
Glu	Gln	Arg	Gln	Ser		Trp	Ser	Leu
Arg	Gly	Ala	Gly	Thr	N225	Gly	Asn	Gly
Ile	Glu	Thr	Met	Pro	R226	Asn	Lys	Asn
Ala	Val	Phe	Phe	Ile		Gln	Val	Leu
Val	Ala	Ala	Gln	Pro	N229	Asn	Val	Lys
Thr	Val	Ala	Gln	Thr		Arg	Lys	Gly
Ala	Tyr	Gln	Gln	Pro		Arg	Asp	Asn
Gln	Asp	Asn	Glu	Lys	Q239	Lys	Asp	Ser
Leu	Asp	Ala	Pro	Ala		Ala	Asn	Ala
Glu	Tyr	Arg	Glu	Asp		Glu	Tyr	Ile
Ala	Val	Asn	Gln	Ala	T242	Arg	Ser	Gly
Arg	Phe	Trp	Thr	Arg	S243	Lys	Trp	Ser
Gln	Ser	Asn	Val	Asp	L244	Ala	Lys	Ile
Arg	Asp	Ala	Gln	Ala	P245	Lys	Asp	Gly
Lys	Met	Phe	Ala	Leu	Asn	Val	Val	Gly
Glu	Arg	Gly	Ala	Ser	Ser	Leu	Arg	Ala
His	Tle	Trp	Ile	Leu	Phe	Gln	Gly	Gly
Arg	Pro	Leu	Ala	Gly	Ala	Asn	Ser	Gly
Glu	Asp	Lys	Lys	Leu	Ala	Thr	Gly	Ile
Gly	Thr	Asn	Asp	Leu	Leu	Ala	Thr	Lys
Asn	Ile	Gly	Gly	His	Pro	Lys	Gln	Ala
Glu	Arg	Gln	Gly	Asn	Glu	Gly	Arg	Ala
Pro	Cys	Asp	Tle	Ser	Thr	Asn	Val	Lys
	Glu	Ser	Asp	Glu	Thr	Glu	Val	Gly

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	-0.478	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	398.71204, 398.71204, 398.71204	wwPDB
Map dimensions	286, 286, 286	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.394098, 1.394098, 1.394098	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.22	0/3950	0.50	3/5346 (0.1%)
1	AB	0.22	0/4106	0.46	0/5553
1	AC	0.25	0/4106	0.47	0/5553
1	AD	0.24	0/3732	0.48	0/5044
1	AE	0.22	0/4106	0.45	2/5553 (0.0%)
1	AF	0.26	0/4106	0.49	0/5553
1	BA	0.25	0/3957	0.50	2/5356 (0.0%)
1	BB	0.22	0/4106	0.44	0/5553
1	BC	0.27	0/4106	0.54	1/5553 (0.0%)
1	BD	0.24	0/3732	0.48	0/5044
1	BE	0.21	0/4106	0.44	0/5553
1	BF	0.21	0/4106	0.46	0/5553
1	CA	0.22	0/3944	0.47	1/5338 (0.0%)
1	CB	0.23	0/4106	0.46	0/5553
1	CC	0.26	0/4106	0.50	0/5553
1	CD	0.25	0/3695	0.49	1/4995 (0.0%)
1	CE	0.21	0/4106	0.42	0/5553
1	CF	0.27	0/4106	0.55	2/5553 (0.0%)
1	DA	0.27	0/3957	0.52	4/5356 (0.1%)
1	DB	0.22	0/4106	0.45	0/5553
1	DC	0.25	0/4106	0.46	0/5553
1	DD	0.24	0/3732	0.48	4/5044 (0.1%)
1	DE	0.21	0/4106	0.43	0/5553
1	DF	0.23	0/4106	0.48	0/5553
1	EA	0.23	0/3957	0.47	2/5356 (0.0%)
1	EB	0.22	0/4106	0.43	0/5553
1	EC	0.33	0/4106	0.72	9/5553 (0.2%)
1	ED	0.24	0/3732	0.46	0/5044
1	EE	0.25	0/4106	0.50	1/5553 (0.0%)
1	EF	0.23	0/4106	0.48	2/5553 (0.0%)
2	Aa	0.24	0/2591	0.50	0/3533
2	Ab	0.29	0/2591	0.58	3/3533 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Ad	0.27	0/2591	0.53	3/3533 (0.1%)
2	Ae	0.19	0/2119	0.46	0/2887
2	Af	0.24	0/1465	0.53	0/2001
2	Ba	0.24	0/2591	0.55	3/3533 (0.1%)
2	Bb	0.35	0/2591	0.64	5/3533 (0.1%)
2	Bd	0.27	0/2591	0.51	1/3533 (0.0%)
2	Be	0.20	0/2112	0.46	0/2877
2	Bf	0.25	0/1465	0.56	1/2001 (0.0%)
2	Ca	0.24	0/2591	0.55	3/3533 (0.1%)
2	Cb	0.31	0/2591	0.60	3/3533 (0.1%)
2	Cd	0.26	0/2591	0.50	1/3533 (0.0%)
2	Ce	0.18	0/2119	0.45	2/2887 (0.1%)
2	Cf	0.28	0/1465	0.61	1/2001 (0.0%)
2	Da	0.23	0/2591	0.52	3/3533 (0.1%)
2	Db	0.32	1/2591 (0.0%)	0.56	1/3533 (0.0%)
2	Dd	0.26	0/2591	0.57	5/3533 (0.1%)
2	De	0.19	0/2119	0.45	0/2887
2	Df	0.26	0/1465	0.52	0/2001
2	Ea	0.25	0/2591	0.51	0/3533
2	Eb	0.29	0/2591	0.59	2/3533 (0.1%)
2	Ed	0.26	0/2591	0.52	1/3533 (0.0%)
2	Ee	0.19	0/2119	0.43	2/2887 (0.1%)
2	Ef	0.27	0/1465	0.60	3/2001 (0.1%)
3	Ag	0.26	0/629	0.45	0/852
3	Ah	0.27	0/572	0.55	0/773
3	Bg	0.24	0/629	0.45	0/852
3	Bh	0.27	0/572	0.56	0/773
3	Cg	0.24	0/629	0.43	0/852
3	Ch	0.27	0/572	0.59	1/773 (0.1%)
3	Dg	0.24	0/629	0.43	0/852
3	Dh	0.28	0/572	0.58	0/773
3	Eg	0.25	0/629	0.43	0/852
3	Eh	0.29	0/572	0.59	0/773
4	Ai	0.20	0/318	0.43	0/430
4	Aj	0.19	0/318	0.44	0/430
4	Ak	0.19	0/318	0.45	0/430
4	Bi	0.18	0/318	0.39	0/430
4	Bj	0.17	0/318	0.42	0/430
4	Bk	0.18	0/318	0.45	0/430
4	Ci	0.20	0/318	0.50	0/430
4	Cj	0.18	0/318	0.49	0/430
4	Ck	0.24	0/318	0.60	0/430
4	Di	0.22	0/318	0.51	0/430

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	Dj	0.16	0/318	0.43	0/430
4	Dk	0.18	0/318	0.51	0/430
4	Ei	0.19	0/318	0.39	0/430
4	Ej	0.19	0/318	0.44	0/430
4	Ek	0.23	0/318	0.49	0/430
5	FA	0.38	0/5718	0.64	8/7713 (0.1%)
5	FB	0.33	0/5646	0.54	3/7616 (0.0%)
5	FC	0.36	0/5700	0.57	3/7690 (0.0%)
5	FD	0.42	2/5868 (0.0%)	0.71	19/7920 (0.2%)
5	FE	0.38	2/5500 (0.0%)	0.63	10/7419 (0.1%)
5	FF	0.34	0/5697	0.56	1/7687 (0.0%)
5	FG	0.35	0/5670	0.59	4/7645 (0.1%)
5	FH	0.41	0/5719	0.71	9/7715 (0.1%)
5	FI	0.44	5/5776 (0.1%)	0.71	16/7793 (0.2%)
5	FJ	0.33	0/5804	0.54	1/7831 (0.0%)
5	FK	0.33	0/5581	0.52	0/7531
5	FL	0.38	0/5664	0.61	7/7640 (0.1%)
6	FM	0.45	1/1881 (0.1%)	0.61	1/2548 (0.0%)
6	FN	0.41	1/1881 (0.1%)	0.69	4/2548 (0.2%)
6	FO	0.38	0/1881	0.55	0/2548
6	FP	0.47	1/1881 (0.1%)	0.65	2/2548 (0.1%)
6	FQ	0.37	0/1881	0.57	0/2548
6	FR	0.38	0/1881	0.53	0/2548
6	FS	0.37	0/1909	0.56	0/2585
6	FT	0.37	0/1881	0.58	0/2548
6	FU	0.38	0/1881	0.55	0/2548
6	FV	0.49	1/1881 (0.1%)	0.66	4/2548 (0.2%)
6	FW	0.46	1/1881 (0.1%)	0.62	1/2548 (0.0%)
6	FX	0.37	0/1881	0.53	1/2548 (0.0%)
7	FY	0.36	0/1886	0.52	0/2552
7	FZ	0.36	0/1886	0.52	0/2552
7	GA	0.35	0/1886	0.49	0/2552
7	GB	0.35	0/1886	0.50	0/2552
7	GC	0.35	0/1886	0.49	0/2552
7	GD	0.36	0/1886	0.49	0/2552
7	GE	0.36	0/1886	0.51	0/2552
7	GF	0.36	0/1886	0.52	0/2552
7	GG	0.38	0/1886	0.51	0/2552
7	GH	0.36	0/1886	0.51	0/2552
7	GI	0.37	0/1886	0.48	0/2552
7	GJ	0.36	0/1886	0.51	0/2552
8	GK	0.30	0/1003	0.63	0/1347
8	GL	0.25	0/1003	0.58	0/1347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	GM	0.26	0/1003	0.60	0/1347
8	GN	0.25	0/1003	0.58	0/1347
8	GO	0.29	0/1003	0.62	0/1347
8	GP	0.34	0/1003	0.66	1/1347 (0.1%)
8	GQ	0.33	0/1003	0.68	1/1347 (0.1%)
8	GR	0.25	0/1003	0.58	0/1347
8	GS	0.26	0/1003	0.58	0/1347
8	GT	0.25	0/1003	0.56	0/1347
8	GU	0.25	0/1003	0.56	0/1347
8	GV	0.33	0/1003	0.71	2/1347 (0.1%)
8	IK	0.27	0/255	0.56	0/342
8	IL	0.26	0/255	0.47	0/342
8	IM	0.25	0/255	0.51	0/342
8	IN	0.25	0/255	0.47	0/342
8	IO	0.25	0/255	0.51	0/342
8	IP	0.23	0/255	0.53	0/342
8	IQ	0.27	0/255	0.61	1/342 (0.3%)
8	IR	0.22	0/255	0.48	0/342
8	IS	0.55	0/255	0.97	3/342 (0.9%)
8	IT	0.23	0/255	0.50	0/342
8	IU	0.23	0/255	0.48	0/342
8	IV	0.23	0/255	0.48	0/342
All	All	0.30	15/316732 (0.0%)	0.54	180/428688 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BF	0	1
2	Ab	0	1
2	Ad	0	2
2	Bb	0	2
2	Bd	0	1
2	Cb	0	1
2	Cd	0	2
2	Db	0	1
2	Dd	0	1
2	Eb	0	1
2	Ed	0	2
3	Ah	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	Eh	0	1
6	FS	0	1
All	All	0	18

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	FE	256	PRO	C-O	-7.76	1.14	1.24
5	FI	626	ALA	C-O	-6.36	1.16	1.24
5	FD	321	PRO	C-O	-6.32	1.16	1.23
5	FE	260	LYS	C-O	-6.30	1.16	1.24
5	FI	323	ASP	C-O	-6.07	1.17	1.23
5	FI	270	GLY	CA-C	-6.00	1.47	1.52
6	FM	85	ALA	CA-CB	-5.88	1.43	1.53
5	FI	625	GLU	C-O	-5.68	1.17	1.24
6	FN	10	LEU	C-N	5.65	1.39	1.34
5	FD	255	SER	CA-CB	-5.40	1.45	1.53
5	FI	626	ALA	CA-CB	-5.39	1.44	1.53
6	FV	84	ARG	C-O	-5.35	1.17	1.23
6	FP	84	ARG	C-O	-5.34	1.16	1.23
6	FW	84	ARG	C-O	-5.11	1.17	1.23
2	Db	111	SER	CA-CB	-5.03	1.45	1.53

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EC	66	ASP	CB-CA-C	-25.40	87.17	116.63
6	FN	95	THR	CB-CA-C	-18.15	80.82	111.31
5	FE	266	PRO	N-CA-C	17.28	138.19	113.47
5	FD	34	PHE	N-CA-C	-13.05	91.98	112.99
5	FG	284	TYR	N-CA-C	-12.74	97.44	113.23
5	FD	37	TYR	CB-CA-C	12.00	131.86	111.22
5	FI	269	ILE	N-CA-C	-11.06	93.70	109.63
5	FG	282	GLU	CB-CA-C	-10.75	92.73	111.22
5	FD	35	PHE	CB-CA-C	10.69	127.66	110.88
1	EC	67	ASP	CB-CA-C	10.23	130.77	110.42
5	FD	321	PRO	CB-CA-C	-10.02	99.33	111.46
5	FA	621	ASP	CB-CA-C	-9.92	92.16	110.01
2	Ba	107	TYR	CB-CA-C	9.82	127.84	116.54
5	FH	621	ASP	N-CA-C	-9.80	101.48	113.15
1	EC	445	GLY	N-CA-C	-9.71	99.17	112.18
5	FH	266	PRO	CA-N-CD	-9.65	98.48	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	FA	619	ASP	CB-CA-C	-9.60	93.79	109.72
1	BA	131	VAL	N-CA-C	-9.48	101.14	110.72
5	FH	619	ASP	N-CA-C	9.39	121.96	110.41
5	FA	223	SER	N-CA-C	-9.29	97.13	110.59
2	Dd	107	TYR	N-CA-C	9.16	120.88	111.07
1	CF	129	ASN	CB-CA-C	-9.11	97.04	110.16
5	FI	323	ASP	CB-CA-C	-9.08	96.16	110.14
5	FH	288	ASN	CB-CA-C	-9.02	106.17	116.63
5	FI	269	ILE	CA-C-N	-8.99	115.77	122.33
5	FI	269	ILE	C-N-CA	-8.99	115.77	122.33
5	FC	619	ASP	N-CA-C	8.91	122.29	110.53
2	Ad	112	GLU	CB-CA-C	8.91	127.03	110.11
5	FD	36	ASN	CB-CA-C	8.72	125.28	111.51
5	FE	267	ASP	CB-CA-C	-8.71	100.18	111.86
2	Ca	110	LEU	CA-C-N	-8.34	107.85	123.27
2	Ca	110	LEU	C-N-CA	-8.34	107.85	123.27
2	Eb	107	TYR	N-CA-C	8.13	119.77	111.07
2	Dd	108	ILE	N-CA-C	-8.09	106.03	113.71
8	GV	454	PRO	CB-CA-C	-8.08	98.23	111.56
1	EC	445	GLY	CA-C-O	-7.84	115.76	121.88
5	FA	225	TYR	N-CA-C	-7.79	104.21	112.93
1	AA	131	VAL	N-CA-C	-7.78	104.17	111.48
1	AA	129	ASN	CB-CA-C	-7.77	96.82	109.72
1	EC	444	LYS	CB-CA-C	7.76	123.82	111.48
5	FB	139	ILE	N-CA-C	-7.73	98.94	109.37
2	Ad	108	ILE	N-CA-C	-7.65	98.27	108.06
8	IS	245	PRO	CB-CA-C	-7.63	95.60	110.10
6	FN	94	PRO	N-CA-CB	-7.56	95.31	103.25
2	Cb	217	THR	CB-CA-C	-7.45	99.90	111.83
5	FL	179	ASP	CA-C-N	7.33	124.86	120.24
5	FL	179	ASP	C-N-CA	7.33	124.86	120.24
5	FI	271	GLN	N-CA-C	7.21	120.26	108.08
1	DA	135	ARG	CB-CA-C	-7.18	98.55	110.19
5	FG	283	ARG	CB-CA-C	7.18	122.08	111.89
1	CA	129	ASN	N-CA-C	7.10	118.71	110.97
5	FI	623	PHE	CA-CB-CG	7.03	120.83	113.80
5	FA	621	ASP	N-CA-C	-7.02	104.45	113.16
2	Bb	110	LEU	N-CA-C	7.01	118.92	111.28
8	IS	245	PRO	N-CA-CB	-6.92	95.39	103.00
5	FL	270	GLY	CA-C-O	-6.89	117.34	122.37
5	FE	256	PRO	CB-CA-C	-6.86	101.51	112.21
6	FV	87	THR	CB-CA-C	6.83	120.85	109.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	FD	33	THR	N-CA-C	6.83	118.98	109.15
1	EF	128	LEU	N-CA-C	-6.81	99.95	110.10
1	EF	130	GLN	N-CA-C	-6.74	103.24	113.89
2	Ab	107	TYR	CB-CA-C	6.73	121.32	110.29
5	FI	40	VAL	CA-C-O	-6.68	112.81	120.42
5	FC	623	PHE	CB-CA-C	6.60	120.93	109.65
5	FD	323	ASP	CB-CA-C	6.56	119.81	110.24
2	Eb	110	LEU	N-CA-C	-6.55	105.86	114.31
6	FW	85	ALA	N-CA-CB	-6.55	100.34	110.29
8	IQ	219	ILE	N-CA-C	-6.55	106.41	112.96
1	CD	4	LYS	CB-CA-C	-6.53	99.48	110.19
1	BA	128	LEU	N-CA-C	-6.49	99.44	109.76
5	FD	324	LEU	CA-C-O	-6.47	113.80	121.11
5	FI	327	ASN	CA-C-O	-6.45	113.80	121.60
6	FP	87	THR	CB-CA-C	6.42	120.81	109.65
5	FD	251	TYR	N-CA-C	-6.37	104.38	111.71
5	FD	519	ILE	N-CA-C	-6.35	106.32	112.29
5	FD	311	PHE	CA-C-N	6.34	133.65	121.54
5	FD	311	PHE	C-N-CA	6.34	133.65	121.54
2	Bb	217	THR	CB-CA-C	-6.33	99.76	109.89
2	Dd	105	ARG	CA-C-N	-6.31	114.57	123.03
2	Dd	105	ARG	C-N-CA	-6.31	114.57	123.03
6	FN	93	TYR	CB-CA-C	6.29	118.45	109.08
1	CF	131	VAL	N-CA-C	-6.27	104.39	110.72
5	FI	624	ALA	CA-C-O	-6.25	114.31	121.19
1	EC	67	ASP	CA-C-N	-6.22	112.59	122.29
1	EC	67	ASP	C-N-CA	-6.22	112.59	122.29
1	EE	88	ARG	CB-CA-C	6.19	120.71	109.62
5	FE	267	ASP	N-CA-C	-6.19	102.85	111.52
2	Bb	112	GLU	CB-CA-C	6.15	121.75	110.36
5	FH	623	PHE	CA-CB-CG	6.14	119.94	113.80
2	Cd	110	LEU	N-CA-C	-6.12	105.46	113.17
5	FL	623	PHE	CB-CA-C	6.10	120.76	109.54
6	FN	95	THR	CA-C-O	-6.09	114.26	120.84
5	FI	626	ALA	CA-C-O	-6.09	114.05	120.63
5	FH	266	PRO	N-CA-CB	-6.08	96.86	103.25
5	FH	322	TYR	CB-CA-C	6.06	121.25	110.16
5	FD	35	PHE	CA-CB-CG	6.05	119.85	113.80
5	FH	266	PRO	CB-CA-C	6.05	121.54	111.56
5	FF	614	ARG	CB-CA-C	6.03	119.20	109.07
2	Cb	295	VAL	N-CA-C	-6.01	106.64	112.29
8	GV	462	VAL	N-CA-C	-6.00	106.47	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	FD	327	ASN	CB-CA-C	5.98	118.81	109.84
1	BC	251	VAL	N-CA-C	-5.96	106.94	113.43
2	Ca	107	TYR	N-CA-C	5.93	117.61	111.03
2	Dd	107	TYR	CA-C-O	-5.92	114.61	120.82
5	FE	260	LYS	N-CA-CB	5.89	118.78	110.12
5	FE	266	PRO	CB-CA-C	-5.88	103.71	113.06
6	FP	87	THR	N-CA-C	-5.87	106.17	113.38
5	FI	519	ILE	N-CA-C	-5.84	106.80	112.29
6	FV	83	LEU	N-CA-CB	-5.82	101.49	110.04
2	Ef	217	THR	CB-CA-C	-5.78	101.47	111.30
5	FD	318	SER	CA-C-O	-5.77	114.80	121.26
5	FL	619	ASP	CB-CA-C	-5.76	100.42	109.70
1	EC	66	ASP	CA-CB-CG	5.76	118.36	112.60
2	Ef	219	ASP	N-CA-C	-5.76	106.20	113.23
1	AA	129	ASN	CA-C-O	-5.74	114.88	121.19
5	FC	621	ASP	N-CA-C	-5.70	106.17	113.01
5	FE	260	LYS	CA-C-O	-5.69	114.52	120.55
5	FJ	269	ILE	N-CA-C	-5.68	107.75	113.20
5	FE	262	ILE	N-CA-C	-5.67	105.63	113.00
8	GQ	457	GLY	CA-C-O	-5.62	118.35	122.23
2	Bb	222	ASP	CB-CA-C	5.62	120.54	112.12
5	FG	282	GLU	CA-C-O	-5.57	114.35	120.70
5	FA	619	ASP	N-CA-C	5.55	118.28	110.23
8	IS	242	THR	CB-CA-C	5.52	121.08	109.65
2	Bb	109	GLY	CA-C-O	-5.50	116.78	121.57
5	FD	38	SER	N-CA-C	-5.48	100.09	109.24
1	DA	125	VAL	N-CA-CB	-5.47	104.87	112.52
1	DA	129	ASN	N-CA-C	5.44	116.89	111.07
5	FL	31	GLN	CA-C-N	5.43	131.47	121.70
5	FL	31	GLN	C-N-CA	5.43	131.47	121.70
2	Cf	222	ASP	CB-CA-C	-5.42	101.40	110.29
5	FH	624	ALA	CA-C-O	-5.41	115.20	121.15
2	Ef	221	GLU	CB-CA-C	5.41	121.18	110.42
2	Ab	105	ARG	CA-C-N	-5.40	115.09	122.87
2	Ab	105	ARG	C-N-CA	-5.40	115.09	122.87
6	FV	84	ARG	CB-CA-C	-5.40	100.00	109.71
2	Ad	108	ILE	N-CA-CB	5.39	118.47	111.19
5	FE	266	PRO	CA-C-O	-5.38	112.23	120.03
2	Db	108	ILE	CB-CA-C	5.38	120.11	111.29
2	Bf	216	ILE	CA-C-O	-5.38	116.56	121.72
3	Ch	85	VAL	N-CA-C	5.37	120.48	108.88
2	Bd	109	GLY	CA-C-O	-5.36	115.52	121.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DA	125	VAL	CA-C-O	-5.36	116.21	121.67
6	FV	85	ALA	N-CA-C	5.32	117.59	110.35
1	EC	443	ILE	N-CA-C	5.32	116.41	108.54
2	Ed	110	LEU	N-CA-C	-5.30	106.49	113.17
2	Cb	216	ILE	N-CA-C	-5.28	100.71	108.11
5	FI	622	GLU	N-CA-C	-5.26	105.58	113.89
1	DD	129	ASN	CA-C-N	5.24	131.55	121.54
1	DD	129	ASN	C-N-CA	5.24	131.55	121.54
5	FA	506	ALA	N-CA-C	-5.23	107.27	113.97
5	FA	512	LYS	N-CA-CB	-5.21	101.72	109.69
2	Ba	6	ASN	CA-C-N	5.20	131.48	121.54
2	Ba	6	ASN	C-N-CA	5.20	131.48	121.54
2	Ce	6	ASN	CA-C-N	5.20	131.47	121.54
2	Ce	6	ASN	C-N-CA	5.20	131.47	121.54
5	FD	321	PRO	CA-C-O	-5.20	115.10	121.03
5	FI	618	ILE	N-CA-C	-5.20	102.35	109.37
2	Da	109	GLY	CA-C-O	-5.18	116.17	121.61
5	FB	142	ASP	CA-C-N	-5.15	114.57	122.60
5	FB	142	ASP	C-N-CA	-5.15	114.57	122.60
2	Ee	6	ASN	CA-C-N	5.12	131.31	121.54
2	Ee	6	ASN	C-N-CA	5.12	131.31	121.54
5	FI	619	ASP	N-CA-C	5.12	117.65	110.23
2	Da	6	ASN	CA-C-N	5.11	131.29	121.54
2	Da	6	ASN	C-N-CA	5.11	131.29	121.54
5	FD	326	GLY	N-CA-C	-5.11	107.69	115.66
6	FM	85	ALA	N-CA-CB	-5.10	102.47	109.97
5	FD	321	PRO	N-CA-CB	-5.10	98.88	103.36
1	DD	433	MET	CA-C-N	5.09	131.26	121.54
1	DD	433	MET	C-N-CA	5.09	131.26	121.54
8	GP	460	ILE	N-CA-C	-5.07	108.56	113.53
5	FE	259	ILE	N-CA-C	-5.04	105.48	110.62
1	AE	131	VAL	N-CA-C	-5.04	107.92	112.96
1	AE	201	GLU	CA-CB-CG	5.03	124.16	114.10
1	EA	128	LEU	N-CA-C	-5.02	99.59	108.23
6	FX	91	ASN	N-CA-C	5.02	116.44	110.97
1	EA	129	ASN	N-CA-C	5.02	116.44	111.07
5	FI	327	ASN	CA-CB-CG	5.01	117.61	112.60
5	FI	621	ASP	CB-CA-C	-5.01	104.82	111.88

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Ab	263	TYR	Peptide
2	Ad	262	GLY	Peptide
2	Ad	6	ASN	Peptide
3	Ah	85	VAL	Peptide
1	BF	128	LEU	Peptide
2	Bb	263	TYR	Peptide
2	Bb	296	GLN	Peptide
2	Bd	262	GLY	Peptide
2	Cb	263	TYR	Peptide
2	Cd	262	GLY	Peptide
2	Cd	6	ASN	Peptide
2	Db	263	TYR	Peptide
2	Dd	262	GLY	Peptide
2	Eb	263	TYR	Peptide
2	Ed	262	GLY	Peptide
2	Ed	6	ASN	Peptide
3	Eh	85	VAL	Peptide
6	FS	96	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	3861	0	3765	56	0
1	AB	4012	0	3920	61	0
1	AC	4012	0	3921	67	0
1	AD	3649	0	3574	66	0
1	AE	4012	0	3920	54	0
1	AF	4012	0	3921	51	0
1	BA	3868	0	3772	55	0
1	BB	4012	0	3921	59	0
1	BC	4012	0	3921	73	0
1	BD	3649	0	3574	73	0
1	BE	4012	0	3921	67	0
1	BF	4012	0	3921	47	0
1	CA	3855	0	3760	64	0
1	CB	4012	0	3921	61	0
1	CC	4012	0	3921	62	0
1	CD	3612	0	3535	59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CE	4012	0	3920	53	0
1	CF	4012	0	3920	59	0
1	DA	3868	0	3772	52	0
1	DB	4012	0	3921	70	0
1	DC	4012	0	3921	70	0
1	DD	3649	0	3574	71	0
1	DE	4012	0	3920	65	0
1	DF	4012	0	3921	46	0
1	EA	3868	0	3772	58	0
1	EB	4012	0	3921	70	0
1	EC	4012	0	3921	96	0
1	ED	3649	0	3574	60	0
1	EE	4012	0	3921	60	0
1	EF	4012	0	3921	48	0
2	Aa	2542	0	2558	26	0
2	Ab	2542	0	2558	37	0
2	Ad	2542	0	2558	34	0
2	Ae	2077	0	2075	14	0
2	Af	1434	0	1419	14	0
2	Ba	2542	0	2558	29	0
2	Bb	2542	0	2558	41	0
2	Bd	2542	0	2558	42	0
2	Be	2070	0	2066	13	0
2	Bf	1434	0	1419	17	0
2	Ca	2542	0	2558	24	0
2	Cb	2542	0	2558	35	0
2	Cd	2542	0	2558	34	0
2	Ce	2077	0	2075	22	0
2	Cf	1434	0	1419	20	0
2	Da	2542	0	2558	23	0
2	Db	2542	0	2558	44	0
2	Dd	2542	0	2558	37	0
2	De	2077	0	2075	24	0
2	Df	1434	0	1419	10	0
2	Ea	2542	0	2558	44	0
2	Eb	2542	0	2558	36	0
2	Ed	2542	0	2558	38	0
2	Ee	2077	0	2075	14	0
2	Ef	1434	0	1419	19	0
3	Ag	619	0	619	14	0
3	Ah	563	0	570	7	0
3	Bg	619	0	619	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Bh	563	0	570	15	0
3	Cg	619	0	619	14	0
3	Ch	563	0	570	10	0
3	Dg	619	0	619	15	0
3	Dh	563	0	570	11	0
3	Eg	619	0	619	13	0
3	Eh	563	0	570	11	0
4	Ai	310	0	313	5	0
4	Aj	310	0	313	3	0
4	Ak	310	0	313	9	0
4	Bi	310	0	313	6	0
4	Bj	310	0	313	6	0
4	Bk	310	0	313	5	0
4	Ci	310	0	313	7	0
4	Cj	310	0	313	11	0
4	Ck	310	0	313	11	0
4	Di	310	0	313	5	0
4	Dj	310	0	313	5	0
4	Dk	310	0	313	0	0
4	Ei	310	0	313	10	0
4	Ej	310	0	313	9	0
4	Ek	310	0	313	7	0
5	FA	5617	0	5565	83	0
5	FB	5545	0	5492	79	0
5	FC	5597	0	5537	84	0
5	FD	5759	0	5692	106	0
5	FE	5400	0	5357	73	0
5	FF	5593	0	5522	74	0
5	FG	5569	0	5507	89	0
5	FH	5618	0	5564	78	0
5	FI	5671	0	5610	80	0
5	FJ	5699	0	5631	78	0
5	FK	5478	0	5443	79	0
5	FL	5563	0	5508	73	0
6	FM	1841	0	1864	24	0
6	FN	1841	0	1864	25	0
6	FO	1841	0	1864	34	0
6	FP	1841	0	1864	34	0
6	FQ	1841	0	1864	29	0
6	FR	1841	0	1864	23	0
6	FS	1868	0	1888	30	0
6	FT	1841	0	1864	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	FU	1841	0	1864	30	0
6	FV	1841	0	1864	33	0
6	FW	1841	0	1864	36	0
6	FX	1841	0	1864	33	0
7	FY	1841	0	1801	16	0
7	FZ	1841	0	1801	28	0
7	GA	1841	0	1801	23	0
7	GB	1841	0	1801	25	0
7	GC	1841	0	1801	22	0
7	GD	1841	0	1801	21	0
7	GE	1841	0	1801	27	0
7	GF	1841	0	1801	25	0
7	GG	1841	0	1801	26	0
7	GH	1841	0	1801	26	0
7	GI	1841	0	1801	16	0
7	GJ	1841	0	1801	27	0
8	GK	987	0	930	7	0
8	GL	987	0	930	10	0
8	GM	987	0	930	13	0
8	GN	987	0	930	6	0
8	GO	987	0	930	11	0
8	GP	987	0	930	8	0
8	GQ	987	0	930	8	0
8	GR	987	0	930	10	0
8	GS	987	0	930	12	0
8	GT	987	0	930	12	0
8	GU	987	0	930	10	0
8	GV	987	0	930	20	0
8	IK	251	0	239	2	0
8	IL	251	0	239	3	0
8	IM	251	0	239	5	0
8	IN	251	0	239	6	0
8	IO	251	0	239	2	0
8	IP	251	0	239	4	0
8	IQ	251	0	239	4	0
8	IR	251	0	239	4	0
8	IS	251	0	239	13	0
8	IT	251	0	239	6	0
8	IU	251	0	239	4	0
8	IV	251	0	239	6	0
9	AB	1	0	0	0	0
9	AC	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AD	1	0	0	0	0
9	AE	1	0	0	0	0
9	BB	1	0	0	0	0
9	BD	1	0	0	0	0
9	CB	1	0	0	0	0
9	CD	1	0	0	0	0
9	CE	1	0	0	0	0
9	CF	1	0	0	0	0
9	DB	1	0	0	0	0
9	DE	1	0	0	0	0
9	DF	1	0	0	0	0
9	EB	1	0	0	0	0
9	ED	1	0	0	1	0
9	FA	1	0	0	0	0
9	FB	1	0	0	0	0
9	FC	1	0	0	0	0
9	FD	1	0	0	0	0
9	FE	1	0	0	0	0
9	FF	1	0	0	0	0
9	FG	1	0	0	0	0
9	FH	1	0	0	0	0
9	FI	1	0	0	0	0
9	FJ	1	0	0	0	0
9	FK	1	0	0	0	0
9	FL	1	0	0	0	0
All	All	310209	0	306018	3568	0

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

All (3568) 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)
5:FG:280:ILE:HG21	5:FG:302:THR:CG2	1.59	1.30
5:FD:269:ILE:CG1	5:FD:325:ALA:H	1.49	1.23
5:FD:269:ILE:HG12	5:FD:325:ALA:CA	1.70	1.22
5:FD:269:ILE:HG12	5:FD:325:ALA:N	1.56	1.18
5:FG:280:ILE:CG2	5:FG:302:THR:HG21	1.73	1.17
5:FD:269:ILE:CD1	5:FD:325:ALA:H	1.58	1.17
5:FG:280:ILE:HG21	5:FG:302:THR:HG21	1.21	1.13
5:FD:269:ILE:HG12	5:FD:325:ALA:HA	1.37	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FG:280:ILE:HG21	5:FG:302:THR:HG22	1.40	1.04
1:CD:5:LEU:HD11	3:Cg:35:VAL:HG21	1.44	1.00
5:FD:269:ILE:CG1	5:FD:325:ALA:N	2.20	0.98
8:IS:243:SER:O	8:IS:243:SER:OG	1.83	0.89
8:GV:447:GLY:HA3	8:GV:458:ILE:HD11	1.54	0.89
8:IR:245:PRO:HA	8:IS:243:SER:HB2	1.56	0.87
5:FG:280:ILE:CG2	5:FG:302:THR:CG2	2.40	0.87
5:FD:269:ILE:HD11	5:FD:325:ALA:H	1.41	0.85
5:FH:141:GLU:O	5:FH:141:GLU:HG2	1.77	0.84
5:FH:141:GLU:HA	5:FH:144:TYR:HB2	1.58	0.84
8:GV:444:ILE:HD13	8:GV:460:ILE:HG21	1.58	0.83
5:FD:269:ILE:CD1	5:FD:325:ALA:N	2.41	0.82
5:FD:269:ILE:CG1	5:FD:325:ALA:CA	2.59	0.81
2:Cd:108:ILE:H	2:Cd:108:ILE:HD13	1.47	0.80
2:Cd:108:ILE:HD13	2:Cd:108:ILE:N	1.97	0.80
5:FG:280:ILE:HG22	5:FG:302:THR:HG21	1.63	0.79
5:FD:269:ILE:CG1	5:FD:325:ALA:HA	2.13	0.78
2:Cf:216:ILE:HG12	2:Cf:225:TRP:HB3	1.67	0.76
8:GV:459:GLN:NE2	8:GV:459:GLN:O	2.19	0.75
5:FB:139:ILE:HD12	5:FB:139:ILE:H	1.51	0.75
2:Bb:217:THR:O	2:Bb:217:THR:OG1	1.99	0.75
2:Db:108:ILE:HD13	2:Db:108:ILE:H	1.51	0.75
6:FW:83:LEU:N	6:FW:83:LEU:HD23	2.02	0.75
8:GO:444:ILE:HD13	8:GO:460:ILE:HG21	1.67	0.75
5:FC:618:ILE:HD13	5:FC:618:ILE:N	2.02	0.74
2:Db:108:ILE:HD13	2:Db:108:ILE:N	2.01	0.73
5:FA:619:ASP:OD1	5:FA:619:ASP:N	2.19	0.73
2:Ed:112:GLU:N	2:Ed:112:GLU:OE1	2.21	0.72
1:CA:253:LEU:HD21	1:CF:79:ARG:HH22	1.54	0.72
1:BD:80:ARG:HD3	2:Bd:110:LEU:HG	1.71	0.72
2:Aa:108:ILE:HG23	2:Aa:108:ILE:O	1.88	0.71
5:FB:139:ILE:HD12	5:FB:139:ILE:N	2.05	0.71
6:FW:76:LEU:HG	6:FW:83:LEU:HD21	1.72	0.71
1:AB:413:LEU:HD11	2:Aa:105:ARG:HH22	1.56	0.71
8:IS:244:LEU:HD12	8:IS:245:PRO:HD2	1.71	0.70
1:BB:361:ASN:HD21	1:BB:367:VAL:H	1.39	0.70
2:Dd:112:GLU:OE1	2:Dd:112:GLU:N	2.25	0.70
2:Df:222:ASP:N	2:Df:222:ASP:OD1	2.23	0.70
1:BB:137:LEU:HD11	1:BB:152:GLU:HG3	1.74	0.69
5:FC:724:ILE:HG23	5:FD:725:ARG:HH11	1.55	0.69
2:Da:108:ILE:HG13	2:Da:108:ILE:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ed:108:ILE:HG23	2:Ed:108:ILE:O	1.92	0.68
1:AA:130:GLN:HG3	1:AA:130:GLN:O	1.94	0.68
5:FE:267:ASP:O	5:FE:267:ASP:CG	2.34	0.68
8:GV:444:ILE:CD1	8:GV:460:ILE:HG21	2.23	0.68
1:AC:191:ARG:H	1:AD:254:GLN:HE22	1.42	0.68
1:CF:263:MET:HG3	1:CF:484:LEU:HD12	1.75	0.68
2:Db:216:ILE:O	2:Db:216:ILE:HG13	1.93	0.68
5:FA:622:GLU:HG3	8:GK:522:PRO:HG3	1.75	0.67
1:EE:91:ASN:OD1	1:EE:91:ASN:N	2.26	0.67
8:IR:245:PRO:HA	8:IS:243:SER:CB	2.24	0.67
5:FJ:716:LEU:HD11	5:FK:718:GLN:HG2	1.75	0.67
1:AD:361:ASN:HD21	1:AD:367:VAL:H	1.39	0.67
1:DD:79:ARG:O	2:Dd:111:SER:HB2	1.93	0.67
5:FK:727:ASN:HB3	5:FL:729:THR:HG21	1.77	0.67
1:DA:390:ALA:HB3	1:DA:394:VAL:HB	1.77	0.67
2:Dd:110:LEU:HD22	1:EC:13:PHE:HB3	1.76	0.67
1:EC:77:SER:H	1:ED:10:MET:HE1	1.60	0.66
1:AC:263:MET:HG3	1:AC:484:LEU:HD12	1.76	0.66
1:BF:206:ARG:HG3	1:BF:481:MET:HB3	1.75	0.66
1:AC:10:MET:N	1:AC:10:MET:SD	2.69	0.66
1:ED:292:ILE:HG12	1:ED:486:VAL:HG21	1.77	0.66
8:GL:494:ARG:HH22	8:GL:502:LYS:HA	1.61	0.66
2:Eb:221:GLU:HG2	2:Eb:221:GLU:O	1.95	0.66
5:FE:727:ASN:HB3	5:FF:729:THR:HG21	1.78	0.66
1:CC:10:MET:N	1:CC:10:MET:SD	2.69	0.66
5:FI:722:ALA:HA	5:FI:725:ARG:HE	1.60	0.66
1:CF:87:ALA:O	1:CF:95:VAL:HB	1.96	0.65
1:EC:434:ASP:HB3	5:FC:31:GLN:HG3	1.77	0.65
2:Bf:221:GLU:OE1	2:Bf:221:GLU:HA	1.94	0.65
1:DE:318:GLU:HG3	1:DF:338:ARG:HH22	1.60	0.65
5:FE:653:LEU:HD13	5:FE:663:ILE:HG13	1.78	0.65
8:GO:448:GLY:H	8:GO:473:GLN:HB3	1.59	0.65
5:FJ:31:GLN:NE2	5:FJ:284:TYR:OH	2.29	0.65
2:Ae:88:VAL:HG22	2:Ae:223:ARG:HE	1.62	0.65
5:FA:460:LEU:HD11	5:FA:512:LYS:HB3	1.77	0.65
1:DD:292:ILE:HG12	1:DD:486:VAL:HG11	1.79	0.65
5:FG:4:PHE:N	5:FG:4:PHE:CD1	2.65	0.65
1:BD:246:TYR:HH	5:FJ:318:SER:N	1.94	0.64
5:FH:141:GLU:HA	5:FH:144:TYR:CB	2.26	0.64
2:Ce:278:VAL:HG23	2:Ce:308:ASP:HB3	1.80	0.64
1:EA:382:GLY:HA3	1:EF:389:LYS:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FA:455:ASN:O	5:FL:447:ARG:NH1	2.31	0.64
7:GG:80:LEU:HB2	7:GG:140:PHE:HB2	1.79	0.64
7:GD:80:LEU:HB2	7:GD:140:PHE:HB2	1.77	0.64
1:BC:133:PRO:HB2	1:BC:154:MET:HB3	1.79	0.64
6:FO:160:LYS:HE3	6:FO:181:GLN:HG2	1.79	0.64
2:Bb:278:VAL:HG23	2:Bb:308:ASP:HB3	1.80	0.64
1:CF:130:GLN:HE21	1:CF:130:GLN:C	2.05	0.64
2:Ef:88:VAL:HG13	2:Ef:218:VAL:HG11	1.80	0.64
5:FF:731:ILE:HD11	5:FG:729:THR:HB	1.79	0.64
5:FG:404:ARG:HG3	5:FG:410:ARG:HD3	1.79	0.64
2:Eb:138:ALA:HB1	2:Eb:171:VAL:HG11	1.79	0.64
5:FA:729:THR:HA	5:FA:732:ILE:HD12	1.80	0.64
5:FG:5:LEU:HB3	5:FG:28:TRP:HE1	1.63	0.64
4:Ei:7:LEU:HB2	4:Ek:4:LEU:HB2	1.80	0.64
5:FD:240:TYR:OH	5:FD:321:PRO:O	2.09	0.64
1:DC:390:ALA:HB3	1:DC:394:VAL:HB	1.80	0.64
5:FD:253:VAL:O	5:FD:253:VAL:HG22	1.97	0.64
5:FH:288:ASN:ND2	5:FH:317:ASN:OD1	2.31	0.63
6:FT:216:ARG:NH2	6:FT:229:ASP:O	2.30	0.63
2:Aa:252:GLY:HA3	2:Aa:259:ARG:HH21	1.62	0.63
2:Bb:295:VAL:HG23	2:Bb:296:GLN:HG2	1.79	0.63
1:DA:409:ARG:NH1	1:DA:410:ASN:OD1	2.31	0.63
1:EB:413:LEU:HD11	2:Ea:105:ARG:HH22	1.63	0.63
1:EF:206:ARG:HG3	1:EF:481:MET:HB3	1.80	0.63
5:FH:620:GLY:C	5:FH:622:GLU:H	2.05	0.63
7:FY:86:VAL:HG21	7:FY:138:LEU:HB2	1.80	0.63
1:DA:88:ARG:HB2	1:DA:110:TYR:HB2	1.80	0.63
5:FD:269:ILE:HD11	5:FD:325:ALA:N	2.08	0.63
5:FD:447:ARG:NH1	5:FE:455:ASN:O	2.32	0.63
6:FP:19:ARG:NH1	6:FQ:33:GLN:OE1	2.32	0.63
2:Bd:290:GLY:HA3	2:Bd:294:SER:HB2	1.80	0.63
1:CC:461:THR:O	5:FI:32:LYS:NZ	2.31	0.63
5:FC:570:ILE:HG12	5:FD:93:VAL:HG22	1.80	0.63
1:AF:112:VAL:HG22	1:AF:148:VAL:HG22	1.80	0.63
1:EC:10:MET:SD	1:EC:10:MET:N	2.71	0.63
7:GG:36:ARG:NH2	7:GG:159:PHE:O	2.31	0.63
1:AC:449:TYR:HB2	5:FB:303:TYR:HD2	1.64	0.63
1:DB:77:SER:OG	2:Db:111:SER:OG	2.08	0.63
1:DF:206:ARG:HG3	1:DF:481:MET:HB3	1.79	0.63
5:FB:221:PHE:HB2	5:FB:234:MET:HB3	1.81	0.63
1:EC:80:ARG:NH2	1:EC:115:GLU:OE1	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ef:158:TYR:HB2	2:Ef:189:ILE:HB	1.80	0.63
5:FB:720:GLU:HA	5:FC:725:ARG:HH22	1.64	0.63
7:GI:80:LEU:HB2	7:GI:140:PHE:HB2	1.79	0.63
2:Aa:105:ARG:HG3	2:Aa:106:GLN:HG3	1.80	0.63
1:BC:93:VAL:O	1:BC:93:VAL:HG23	1.98	0.63
1:CC:447:ASN:HB2	5:FI:321:PRO:HG2	1.81	0.63
6:FR:216:ARG:NH2	6:FR:229:ASP:O	2.32	0.63
1:AE:4:LYS:HG2	2:Bb:202:MET:HE1	1.81	0.62
2:Ce:150:GLU:HG2	2:Ce:154:LEU:HD11	1.82	0.62
2:Ea:278:VAL:HG13	2:Ea:308:ASP:HB3	1.80	0.62
6:FV:1:MET:HG3	6:FV:195:PHE:HA	1.80	0.62
1:AA:69:GLU:HG3	1:AA:199:ARG:HH21	1.63	0.62
1:CC:61:THR:HB	5:FI:268:TYR:HD1	1.62	0.62
1:DC:191:ARG:H	1:DD:254:GLN:HE22	1.47	0.62
5:FG:723:ASN:HB3	5:FH:725:ARG:HH21	1.64	0.62
5:FI:709:GLN:HA	5:FI:712:LYS:HE3	1.81	0.62
6:FQ:83:LEU:HD22	6:FQ:109:PRO:HB2	1.81	0.62
1:AA:129:ASN:H	1:AA:129:ASN:ND2	1.95	0.62
1:AE:425:TYR:HB2	1:AE:497:LEU:HB2	1.81	0.62
7:GC:36:ARG:HG3	7:GC:187:ILE:HD12	1.80	0.62
2:Da:146:GLU:HG3	2:Da:153:PRO:HG3	1.81	0.62
1:EB:321:ALA:O	1:EC:48:ARG:NH2	2.32	0.62
6:FV:216:ARG:NH2	6:FV:229:ASP:O	2.32	0.62
1:AE:214:ASN:HD21	1:BA:182:GLU:HG2	1.65	0.62
1:BB:435:GLN:NE2	1:BC:40:MET:O	2.33	0.62
1:CE:79:ARG:HB3	1:CF:408:VAL:HG11	1.81	0.62
1:BA:201:GLU:OE2	1:BA:270:ARG:NH1	2.33	0.62
1:BD:127:ASN:HB2	1:BD:170:GLU:HG3	1.82	0.62
1:BE:65:GLU:HA	1:BE:444:LYS:HE2	1.79	0.62
2:Dd:24:LEU:HD23	2:Dd:29:ASP:HB3	1.82	0.62
5:FB:723:ASN:HB3	5:FC:725:ARG:HH21	1.63	0.62
5:FJ:52:ASP:HB3	5:FJ:57:ARG:HB2	1.81	0.62
1:BA:330:LEU:HD21	1:BA:397:ARG:HE	1.64	0.62
1:BB:390:ALA:HB3	1:BB:394:VAL:HB	1.82	0.62
1:BC:91:ASN:HD22	1:BC:91:ASN:H	1.47	0.62
1:EE:203:THR:HB	1:EE:289:GLY:H	1.63	0.62
1:EF:16:TRP:HE1	1:EF:20:THR:HG22	1.63	0.62
5:FI:163:ARG:NH1	5:FI:625:GLU:OE1	2.33	0.62
5:FK:447:ARG:NH1	5:FL:455:ASN:O	2.32	0.62
6:FX:27:ASN:HD22	7:GJ:108:THR:HG23	1.64	0.62
7:GJ:80:LEU:HB2	7:GJ:140:PHE:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:390:ALA:HB3	1:BA:394:VAL:HB	1.82	0.62
1:BC:91:ASN:H	1:BC:91:ASN:ND2	1.98	0.62
6:FO:19:ARG:NH1	6:FP:33:GLN:OE1	2.32	0.62
1:AE:154:MET:SD	1:AF:278:ASN:ND2	2.73	0.62
3:Dh:35:VAL:HG11	3:Dh:92:MET:HB3	1.82	0.62
1:BC:191:ARG:H	1:BD:254:GLN:HE22	1.47	0.61
5:FG:447:ARG:NH1	5:FH:455:ASN:O	2.33	0.61
6:FT:7:TRP:HB3	6:FT:143:LEU:HG	1.82	0.61
6:FV:19:ARG:NH1	6:FW:33:GLN:OE1	2.33	0.61
7:FZ:110:ILE:HD12	7:FZ:114:ARG:HG2	1.82	0.61
8:GO:444:ILE:CD1	8:GO:460:ILE:HG21	2.30	0.61
2:Bf:216:ILE:HD13	2:Bf:225:TRP:HB3	1.82	0.61
1:CA:323:LYS:HB3	1:CB:44:LEU:HD22	1.82	0.61
1:CC:125:VAL:HG21	1:CC:130:GLN:H	1.64	0.61
1:CF:242:MET:HE2	1:CF:244:MET:HB2	1.81	0.61
1:EC:133:PRO:HB2	1:EC:154:MET:HB3	1.82	0.61
2:Ea:108:ILE:HG22	2:Ea:108:ILE:O	2.01	0.61
5:FB:570:ILE:HG12	5:FC:93:VAL:HG22	1.83	0.61
5:FI:38:SER:O	5:FI:426:ARG:NH1	2.33	0.61
6:FU:19:ARG:NH1	6:FV:33:GLN:OE1	2.33	0.61
7:GD:36:ARG:NH2	7:GD:159:PHE:O	2.33	0.61
1:BB:425:TYR:HB2	1:BB:497:LEU:HB2	1.82	0.61
5:FG:381:ALA:H	5:FG:401:GLN:HE22	1.46	0.61
6:FW:216:ARG:NH2	6:FW:229:ASP:O	2.34	0.61
7:GJ:36:ARG:NH2	7:GJ:159:PHE:O	2.33	0.61
1:AB:181:LYS:HG3	1:AB:182:GLU:HG3	1.82	0.61
4:Ak:9:ILE:HG22	4:Ak:21:LEU:HB2	1.80	0.61
5:FJ:504:ALA:HA	8:IS:245:PRO:HG3	1.80	0.61
2:Ef:88:VAL:HG11	2:Ef:216:ILE:HD11	1.82	0.61
1:CD:263:MET:HG3	1:CD:484:LEU:HD13	1.83	0.61
1:EE:153:LEU:HD22	1:EE:157:ASN:HD22	1.65	0.61
5:FF:97:GLU:OE2	5:FF:547:ARG:NH1	2.33	0.61
5:FF:164:GLU:OE2	5:FF:168:ASN:ND2	2.33	0.61
5:FJ:78:PRO:HG2	6:FW:232:TYR:HA	1.82	0.61
8:GT:497:TYR:O	8:GT:534:ARG:NH1	2.33	0.61
3:Eh:45:LYS:HD3	3:Eh:95:GLN:HG2	1.83	0.61
5:FC:329:ARG:NH2	5:FC:389:ASN:OD1	2.34	0.61
1:AA:88:ARG:HB2	1:AA:110:TYR:HB2	1.83	0.61
1:AE:390:ALA:HB3	1:AE:394:VAL:HB	1.82	0.61
1:AF:390:ALA:HB3	1:AF:394:VAL:HB	1.82	0.61
1:BB:189:ASP:O	1:BB:191:ARG:NH1	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bd:119:TYR:O	2:Bd:144:ASN:ND2	2.33	0.61
1:DE:366:VAL:HG13	1:DE:383:PHE:HB3	1.83	0.61
1:EA:88:ARG:HB2	1:EA:110:TYR:HB2	1.83	0.61
1:EA:261:ASN:HD22	1:EF:175:GLU:HA	1.65	0.61
8:GV:497:TYR:O	8:GV:534:ARG:NH1	2.34	0.61
3:Ag:37:GLU:OE2	3:Ag:95:GLN:NE2	2.34	0.61
1:DB:128:LEU:HD23	1:DB:165:ARG:HD2	1.83	0.61
5:FA:417:GLY:O	5:FA:584:ARG:NH2	2.32	0.61
5:FJ:423:ASN:OD1	5:FK:212:ARG:NH2	2.34	0.61
7:GF:36:ARG:NH2	7:GF:159:PHE:O	2.34	0.61
1:AC:52:LEU:HD22	1:AC:260:ASN:HB3	1.82	0.60
1:EC:66:ASP:HA	1:EC:443:ILE:HG23	1.82	0.60
5:FI:52:ASP:HB3	5:FI:57:ARG:HB2	1.82	0.60
6:FO:66:CYS:SG	6:FO:116:ARG:NH2	2.72	0.60
8:IP:229:ASN:OD1	8:IQ:226:ARG:NH2	2.34	0.60
1:BC:52:LEU:HD11	1:BC:265:TRP:HE1	1.66	0.60
1:AB:220:LEU:HD21	1:AB:243:TRP:HB2	1.83	0.60
2:Aa:108:ILE:O	2:Aa:108:ILE:CG2	2.48	0.60
1:CA:271:ASN:HD21	1:CA:277:MET:HE3	1.66	0.60
5:FH:622:GLU:HG3	8:GR:522:PRO:HG3	1.82	0.60
7:GE:36:ARG:NH2	7:GE:159:PHE:O	2.34	0.60
2:Db:221:GLU:O	2:Db:221:GLU:HG3	2.01	0.60
1:EA:44:LEU:HG	1:EF:323:LYS:HB3	1.83	0.60
6:FU:66:CYS:SG	6:FU:116:ARG:NH1	2.74	0.60
4:Ai:7:LEU:HB2	4:Ak:4:LEU:HB2	1.84	0.60
2:Ee:11:LEU:HD11	2:Ee:305:VAL:HG13	1.82	0.60
5:FG:63:LEU:HD23	5:FG:63:LEU:H	1.65	0.60
6:FS:216:ARG:NH2	6:FS:229:ASP:O	2.34	0.60
2:Cb:138:ALA:HB1	2:Cb:171:VAL:HG21	1.83	0.60
1:EB:168:GLN:HE22	2:Eb:76:LYS:HB2	1.67	0.60
5:FG:417:GLY:O	5:FG:584:ARG:NH2	2.34	0.60
7:GB:51:ILE:HG21	7:GB:158:ILE:HD11	1.84	0.60
8:GK:497:TYR:O	8:GK:534:ARG:NH1	2.34	0.60
2:Cb:11:LEU:HD22	2:Cb:247:GLU:HG3	1.84	0.60
1:EC:450:ARG:HB3	5:FD:287:VAL:HG12	1.83	0.60
5:FG:339:ARG:NH1	8:GQ:521:ASP:OD2	2.34	0.60
8:GT:446:GLU:H	8:GT:473:GLN:HE21	1.50	0.60
4:Bi:26:MET:HE2	4:Bi:37:ILE:HG13	1.84	0.60
6:FM:19:ARG:NH1	6:FN:33:GLN:OE1	2.34	0.60
6:FS:29:GLU:OE2	7:GE:114:ARG:NH2	2.35	0.60
7:GB:43:ARG:NH1	8:IN:221:TYR:OH	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:390:ALA:HB3	1:BF:394:VAL:HB	1.83	0.60
1:DB:129:ASN:OD1	1:DC:411:LYS:NZ	2.34	0.60
1:EA:435:GLN:NE2	1:EB:40:MET:O	2.35	0.60
5:FD:723:ASN:HB3	5:FE:725:ARG:HH21	1.67	0.60
5:FH:30:ASN:HD22	5:FH:331:LEU:HD22	1.67	0.60
1:BC:88:ARG:HG3	1:BC:110:TYR:HB2	1.84	0.60
5:FA:653:LEU:HD13	5:FA:663:ILE:HG13	1.84	0.60
5:FC:447:ARG:NH1	5:FD:455:ASN:O	2.35	0.60
6:FR:66:CYS:SG	6:FR:116:ARG:NH1	2.73	0.60
6:FW:3:ASN:ND2	6:FW:194:GLU:OE2	2.35	0.60
7:FY:36:ARG:NH2	7:FY:159:PHE:O	2.35	0.60
7:FZ:36:ARG:NH2	7:FZ:159:PHE:O	2.35	0.60
8:GT:453:ASN:ND2	8:GT:457:GLY:O	2.35	0.60
1:AC:133:PRO:HB2	1:AC:154:MET:HB3	1.84	0.59
2:Ad:119:TYR:O	2:Ad:144:ASN:ND2	2.35	0.59
2:Ca:278:VAL:HG13	2:Ca:308:ASP:HB3	1.84	0.59
7:GB:115:MET:HE3	7:GB:141:LYS:HB3	1.82	0.59
7:GE:80:LEU:HB2	7:GE:140:PHE:HB2	1.84	0.59
7:GG:220:ASP:HB3	7:GG:225:ARG:HD2	1.83	0.59
8:IO:229:ASN:OD1	8:IP:226:ARG:NH2	2.35	0.59
2:Ae:282:LEU:HD23	2:Ae:304:LEU:HD12	1.82	0.59
5:FE:200:GLN:HG3	5:FE:415:ILE:HG13	1.84	0.59
5:FK:192:MET:HG2	5:FK:574:LEU:HD21	1.84	0.59
7:GH:80:LEU:HB2	7:GH:140:PHE:HB2	1.84	0.59
1:BA:39:LEU:HA	1:BF:435:GLN:HE22	1.66	0.59
1:CC:454:TRP:NE1	5:FI:290:ASN:OD1	2.35	0.59
1:EC:305:ASN:ND2	3:Eg:59:GLU:OE1	2.35	0.59
5:FB:139:ILE:H	5:FB:139:ILE:CD1	2.15	0.59
7:GB:80:LEU:HB2	7:GB:140:PHE:HB2	1.84	0.59
1:CE:2:ALA:N	2:Db:106:GLN:O	2.35	0.59
2:Cb:248:TYR:O	2:Cb:259:ARG:NH1	2.35	0.59
1:EF:438:ILE:HG12	1:EF:488:VAL:HG22	1.85	0.59
5:FA:133:MET:SD	5:FA:614:ARG:NH1	2.75	0.59
5:FB:329:ARG:NH2	5:FB:388:GLY:O	2.36	0.59
7:FZ:43:ARG:NH1	8:IL:221:TYR:OH	2.35	0.59
7:GB:36:ARG:NH2	7:GB:159:PHE:O	2.35	0.59
7:GE:51:ILE:HG21	7:GE:158:ILE:HD11	1.85	0.59
5:FE:200:GLN:HE22	5:FE:332:ARG:HH12	1.51	0.59
5:FE:694:GLN:HA	5:FE:697:GLN:HE21	1.68	0.59
6:FO:216:ARG:NH2	6:FO:229:ASP:O	2.36	0.59
2:Ba:278:VAL:HG23	2:Ba:308:ASP:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:190:VAL:HG21	1:CD:251:VAL:HG22	1.85	0.59
5:FD:722:ALA:HA	5:FD:725:ARG:HE	1.66	0.59
5:FG:338:LYS:NZ	5:FH:263:GLU:HB3	2.18	0.59
6:FS:7:TRP:HB3	6:FS:143:LEU:HG	1.85	0.59
7:FY:75:GLU:O	7:GJ:104:GLN:NE2	2.35	0.59
8:IS:229:ASN:OD1	8:IT:226:ARG:NH2	2.35	0.59
2:Cd:268:LYS:HE2	2:Db:198:VAL:HG13	1.84	0.59
1:DA:389:LYS:HB2	1:DB:382:GLY:HA3	1.84	0.59
5:FC:273:ALA:N	5:FC:322:TYR:HH	2.01	0.59
5:FC:447:ARG:NH2	6:FQ:212:GLN:O	2.35	0.59
5:FC:653:LEU:HD13	5:FC:663:ILE:HG13	1.84	0.59
5:FF:423:ASN:OD1	5:FG:212:ARG:NH2	2.35	0.59
5:FG:338:LYS:HZ3	5:FH:263:GLU:HB3	1.68	0.59
5:FH:507:LEU:HD11	5:FI:499:SER:HB2	1.84	0.59
5:FH:724:ILE:HG23	5:FI:725:ARG:HH11	1.68	0.59
6:FX:66:CYS:SG	6:FX:116:ARG:NH1	2.75	0.59
1:AA:144:GLY:HA2	2:Aa:281:VAL:HG11	1.85	0.59
1:EA:435:GLN:HE22	1:EB:40:MET:H	1.50	0.59
1:ED:181:LYS:HD2	1:EE:287:LYS:HD2	1.85	0.59
2:Ef:223:ARG:HG2	2:Ef:223:ARG:NH1	2.18	0.59
2:Ae:278:VAL:HG23	2:Ae:308:ASP:HB3	1.85	0.59
2:Da:160:ILE:HD12	2:Da:187:GLN:HE21	1.67	0.59
5:FB:653:LEU:HD13	5:FB:663:ILE:HG13	1.85	0.59
5:FE:447:ARG:NH1	5:FF:455:ASN:O	2.36	0.59
5:FH:142:ASP:OD1	5:FH:142:ASP:N	2.36	0.59
8:IM:229:ASN:OD1	8:IN:226:ARG:NH2	2.36	0.59
1:AD:144:GLY:HA2	2:Ad:281:VAL:HG11	1.85	0.58
2:Aa:251:MET:SD	2:Aa:254:ARG:NH2	2.75	0.58
1:DE:168:GLN:NE2	2:De:76:LYS:O	2.34	0.58
2:Ea:42:TYR:HE2	2:Ea:44:GLN:HE21	1.51	0.58
5:FA:327:ASN:ND2	5:FL:223:SER:O	2.36	0.58
5:FD:570:ILE:HG12	5:FE:93:VAL:HG22	1.84	0.58
5:FD:693:ALA:HA	5:FD:696:GLU:HG2	1.84	0.58
5:FJ:207:GLU:HG3	5:FJ:601:ASN:HD21	1.68	0.58
5:FK:709:GLN:HA	5:FK:712:LYS:HE2	1.85	0.58
8:GL:497:TYR:O	8:GL:534:ARG:NH1	2.36	0.58
1:AD:451:GLY:HA3	1:BC:469:MET:HE3	1.85	0.58
1:BC:153:LEU:HD13	1:BC:157:ASN:HB3	1.85	0.58
2:Ed:11:LEU:O	2:Ed:254:ARG:NH2	2.35	0.58
5:FB:133:MET:SD	5:FB:614:ARG:NH1	2.76	0.58
5:FE:265:MET:SD	5:FE:265:MET:C	2.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FP:7:TRP:HB3	6:FP:143:LEU:HG	1.84	0.58
6:FV:12:VAL:HG22	7:GI:120:TYR:HB3	1.85	0.58
7:FZ:121:ASN:HB3	7:FZ:124:LEU:HD12	1.85	0.58
2:Bb:59:LEU:HD22	2:Bb:328:LEU:HD21	1.85	0.58
1:CE:193:THR:OG1	1:CF:235:GLN:NE2	2.36	0.58
1:EC:50:LYS:HD3	1:EC:231:GLU:HG3	1.86	0.58
4:Ei:20:TRP:HB3	4:Ei:27:LYS:HB2	1.85	0.58
5:FL:417:GLY:O	5:FL:584:ARG:NH2	2.35	0.58
6:FV:29:GLU:HG2	7:GH:124:LEU:HD22	1.85	0.58
7:GB:85:LYS:NZ	7:GB:135:ASP:O	2.36	0.58
1:EC:63:GLU:HB3	5:FD:269:ILE:O	2.03	0.58
1:EE:88:ARG:HG2	1:EE:110:TYR:HB2	1.85	0.58
2:Ea:1:MET:HG2	2:Ea:245:ASP:HB3	1.84	0.58
5:FC:418:SER:HB2	5:FC:584:ARG:HH12	1.67	0.58
1:AB:390:ALA:HB3	1:AB:394:VAL:HB	1.86	0.58
2:Dd:290:GLY:HA3	2:Dd:294:SER:HB2	1.85	0.58
5:FE:381:ALA:H	5:FE:401:GLN:HE22	1.51	0.58
5:FK:447:ARG:NH2	6:FM:212:GLN:O	2.37	0.58
7:GI:173:GLU:OE2	7:GJ:81:ARG:NH2	2.36	0.58
8:GT:494:ARG:HH22	8:GT:502:LYS:HA	1.68	0.58
1:AC:334:LYS:NZ	1:AC:399:ASP:OD2	2.36	0.58
1:CB:390:ALA:HB3	1:CB:394:VAL:HB	1.84	0.58
1:EA:389:LYS:HB2	1:EB:382:GLY:HA3	1.86	0.58
1:EB:88:ARG:NH2	1:EB:143:GLU:OE1	2.37	0.58
5:FA:727:ASN:HB3	5:FB:729:THR:HG21	1.85	0.58
5:FJ:110:THR:O	5:FK:172:ASN:ND2	2.37	0.58
5:FJ:570:ILE:HG12	5:FK:93:VAL:HG22	1.85	0.58
2:Bd:11:LEU:HD22	2:Bd:247:GLU:HG3	1.86	0.58
2:Cd:131:SER:HB2	2:Cd:185:TYR:H	1.69	0.58
1:DC:63:GLU:HB2	5:FF:318:SER:HB3	1.85	0.58
1:ED:186:LYS:HB2	1:EE:208:GLN:HG2	1.86	0.58
5:FE:50:ASN:ND2	5:FE:432:ASP:OD1	2.34	0.58
5:FK:6:ASN:ND2	5:FL:267:ASP:OD1	2.36	0.58
5:FL:30:ASN:ND2	5:FL:386:MET:SD	2.76	0.58
6:FM:2:VAL:HA	6:FM:199:SER:HB3	1.84	0.58
6:FR:29:GLU:OE2	7:GD:114:ARG:NH2	2.33	0.58
7:GB:96:ARG:NH2	7:GB:102:PHE:O	2.36	0.58
2:Bf:94:ALA:HB3	4:Bj:32:GLY:HA3	1.86	0.58
1:CB:450:ARG:NH1	1:CB:452:TYR:OH	2.37	0.58
1:DD:42:GLN:OE1	5:FF:283:ARG:NH1	2.37	0.58
1:EC:211:VAL:HG21	1:EC:244:MET:HE1	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FD:45:ILE:HG23	5:FD:317:ASN:HD22	1.69	0.58
6:FQ:19:ARG:NH1	6:FR:33:GLN:OE1	2.37	0.58
7:GC:81:ARG:NH1	7:GC:82:SER:O	2.37	0.58
7:GH:39:LEU:HD21	7:GH:194:PRO:HB2	1.85	0.58
8:IT:229:ASN:OD1	8:IU:226:ARG:NH2	2.36	0.58
1:BD:152:GLU:OE2	1:BE:278:ASN:ND2	2.37	0.58
2:Be:93:VAL:HG21	2:Be:218:VAL:HG12	1.86	0.58
1:CF:297:GLU:OE2	1:CF:424:ARG:NH2	2.37	0.58
2:Cb:30:ILE:HD11	2:Cb:43:PHE:HB3	1.85	0.58
4:Cj:9:ILE:HG22	4:Cj:21:LEU:HB2	1.86	0.58
1:DD:503:GLN:NE2	2:Dd:147:ASN:OD1	2.37	0.58
2:Db:158:TYR:OH	2:Db:235:LYS:NZ	2.35	0.58
4:Di:20:TRP:HB3	4:Di:27:LYS:HB2	1.85	0.58
5:FH:423:ASN:OD1	5:FI:212:ARG:NH2	2.34	0.58
5:FI:77:ILE:HG13	6:FV:235:VAL:HG22	1.86	0.58
6:FM:174:PRO:HG3	8:IV:239:GLN:HB3	1.85	0.58
6:FU:109:PRO:HB3	6:FU:122:ILE:HD11	1.84	0.58
7:GJ:81:ARG:NH1	7:GJ:82:SER:O	2.35	0.58
1:CB:252:GLU:OE1	1:CB:480:ARG:NH1	2.36	0.57
4:Ck:27:LYS:HB3	4:Ck:34:TRP:HB3	1.86	0.57
5:FB:724:ILE:HD13	5:FC:725:ARG:HD2	1.86	0.57
5:FE:38:SER:O	5:FE:426:ARG:NH1	2.37	0.57
5:FH:417:GLY:O	5:FH:584:ARG:NH2	2.32	0.57
5:FF:52:ASP:HB3	5:FF:57:ARG:HB2	1.86	0.57
8:IU:229:ASN:OD1	8:IV:226:ARG:NH2	2.37	0.57
1:AA:207:ILE:HG22	1:AA:480:ARG:HB2	1.87	0.57
1:AD:142:MET:SD	2:Ad:9:ARG:NH1	2.78	0.57
1:BC:414:HIS:HD2	1:BC:416:MET:H	1.52	0.57
1:EE:163:ALA:O	1:EE:167:GLN:NE2	2.37	0.57
5:FA:549:GLY:O	5:FL:564:THR:N	2.37	0.57
6:FV:29:GLU:OE2	7:GH:114:ARG:NH2	2.37	0.57
1:AB:117:TRP:O	1:AB:191:ARG:NH1	2.36	0.57
1:AF:206:ARG:HG3	1:AF:481:MET:HB3	1.87	0.57
2:Bb:218:VAL:O	2:Bb:218:VAL:HG12	2.04	0.57
1:CA:88:ARG:HB2	1:CA:110:TYR:HB2	1.84	0.57
1:CB:406:ASP:O	1:CB:410:ASN:ND2	2.37	0.57
2:Db:123:ILE:HD13	2:Db:125:ARG:HH21	1.69	0.57
2:De:160:ILE:HG13	2:De:187:GLN:HE21	1.69	0.57
5:FA:172:ASN:ND2	5:FL:110:THR:O	2.37	0.57
5:FC:221:PHE:HB2	5:FC:234:MET:HB3	1.86	0.57
6:FU:12:VAL:HG22	7:GH:120:TYR:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:GI:36:ARG:HG3	7:GI:187:ILE:HD12	1.86	0.57
8:GN:497:TYR:O	8:GN:534:ARG:NH1	2.36	0.57
1:AC:203:THR:HG22	1:AC:289:GLY:H	1.69	0.57
1:DA:206:ARG:NH1	1:DF:184:SER:OG	2.37	0.57
2:Db:138:ALA:HB1	2:Db:171:VAL:HG11	1.87	0.57
5:FB:343:LYS:NZ	8:GM:436:ASP:OD1	2.38	0.57
5:FK:720:GLU:HB3	5:FL:718:GLN:HE21	1.70	0.57
7:GG:109:TYR:HA	7:GG:130:CYS:HB2	1.87	0.57
1:CD:131:VAL:HG11	1:CE:504:GLY:HA3	1.86	0.57
1:CD:199:ARG:NH2	2:Db:258:TYR:OH	2.38	0.57
2:Cf:198:VAL:H	2:Cf:202:MET:HB2	1.70	0.57
1:DB:186:LYS:HD2	1:DC:208:GLN:HG3	1.87	0.57
1:DE:219:LYS:HG2	1:DE:241:ASN:HD22	1.70	0.57
1:EC:438:ILE:HG12	1:EC:488:VAL:HG22	1.86	0.57
1:ED:11:LEU:HD12	1:ED:224:ILE:HD12	1.86	0.57
1:ED:365:ARG:HB2	1:EE:369:LYS:HE3	1.87	0.57
5:FB:192:MET:HG2	5:FB:574:LEU:HD21	1.87	0.57
5:FC:354:GLU:O	5:FD:600:ARG:NH1	2.33	0.57
5:FC:366:ASN:HB3	5:FC:371:GLU:HG3	1.86	0.57
5:FG:329:ARG:NH2	5:FG:389:ASN:OD1	2.36	0.57
5:FK:80:ARG:HD2	6:FX:235:VAL:HG11	1.86	0.57
5:FL:447:ARG:NH2	6:FN:212:GLN:O	2.35	0.57
6:FW:16:ARG:NH2	6:FX:37:ASP:OD2	2.36	0.57
8:IR:229:ASN:OD1	8:IS:226:ARG:NH2	2.37	0.57
1:DC:80:ARG:NH2	1:DC:115:GLU:OE1	2.38	0.57
1:DD:199:ARG:NH2	2:Eb:258:TYR:OH	2.38	0.57
1:EC:61:THR:OG1	5:FD:269:ILE:HG22	2.05	0.57
5:FB:729:THR:HA	5:FB:732:ILE:HD12	1.86	0.57
5:FJ:163:ARG:NH1	5:FJ:625:GLU:OE1	2.37	0.57
5:FL:221:PHE:HB2	5:FL:234:MET:HB3	1.86	0.57
5:FL:713:GLU:HA	5:FL:716:LEU:HB3	1.87	0.57
1:BC:137:LEU:HD11	1:BC:152:GLU:HG2	1.85	0.57
2:Bd:54:SER:OG	2:Bd:55:ASP:N	2.37	0.57
1:CA:141:ARG:HG3	1:CA:148:VAL:HG13	1.87	0.57
1:DD:389:LYS:HB2	1:DE:382:GLY:HA3	1.85	0.57
2:De:278:VAL:HG13	2:De:308:ASP:HB3	1.87	0.57
1:EE:87:ALA:O	1:EE:95:VAL:HG12	2.05	0.57
1:EE:323:LYS:HB3	1:EF:44:LEU:HG	1.86	0.57
5:FB:459:ILE:HB	5:FB:515:ILE:HB	1.87	0.57
7:GD:43:ARG:NH1	8:IP:221:TYR:OH	2.38	0.57
7:GG:43:ARG:NH2	8:IS:225:ASN:OD1	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:479:HIS:NE2	1:EE:472:ASP:OD1	2.38	0.57
1:AE:361:ASN:HD21	1:AE:367:VAL:H	1.52	0.57
1:BA:409:ARG:NH2	1:BF:175:GLU:OE2	2.38	0.57
2:Cb:104:PHE:HB2	2:Cb:116:TYR:HB3	1.87	0.57
2:Dd:79:ARG:NH2	2:Dd:168:ASP:OD2	2.38	0.57
1:EF:111:LEU:HD12	1:EF:151:VAL:HG21	1.86	0.57
5:FI:396:ARG:NH2	8:GS:433:GLN:OE1	2.37	0.57
6:FN:216:ARG:NH2	6:FN:229:ASP:O	2.38	0.57
6:FW:83:LEU:HD23	6:FW:83:LEU:H	1.70	0.57
7:GH:36:ARG:NH2	7:GH:159:PHE:O	2.38	0.57
1:AB:314:ASP:OD2	2:Ab:101:ARG:NH1	2.37	0.57
1:AE:23:ASN:OD1	2:Bb:259:ARG:NH2	2.37	0.57
1:DF:390:ALA:HB3	1:DF:394:VAL:HB	1.87	0.57
5:FB:406:ASN:HD22	5:FC:206:GLY:HA3	1.69	0.57
5:FE:110:THR:O	5:FF:172:ASN:ND2	2.37	0.57
5:FH:447:ARG:NH1	5:FI:455:ASN:O	2.37	0.57
5:FI:720:GLU:O	5:FJ:725:ARG:NH2	2.38	0.57
7:GA:70:SER:OG	7:GA:71:GLY:N	2.38	0.57
8:GK:448:GLY:H	8:GK:473:GLN:HB2	1.70	0.57
8:GU:497:TYR:O	8:GU:534:ARG:NH1	2.37	0.57
1:AB:88:ARG:HH21	1:AB:148:VAL:HG21	1.70	0.56
2:Be:160:ILE:HG13	2:Be:187:GLN:HE21	1.68	0.56
2:Dd:13:VAL:HG11	2:Dd:272:LEU:HB2	1.86	0.56
1:EB:244:MET:HE3	1:EB:459:PRO:HB2	1.87	0.56
5:FI:653:LEU:HD13	5:FI:663:ILE:HG13	1.87	0.56
5:FK:572:GLU:HG3	5:FL:100:LYS:HE3	1.87	0.56
1:DD:69:GLU:OE1	2:Eb:258:TYR:OH	2.21	0.56
1:DE:84:LEU:HD21	1:DE:87:ALA:HB2	1.86	0.56
1:ED:386:VAL:HG23	1:ED:387:GLU:HG2	1.88	0.56
2:Ed:323:ASN:HD21	2:Ed:330:ILE:H	1.52	0.56
2:Ef:198:VAL:H	2:Ef:202:MET:HB2	1.70	0.56
5:FG:87:MET:HE2	5:FG:438:ASN:HD22	1.69	0.56
5:FG:653:LEU:HD13	5:FG:663:ILE:HG13	1.86	0.56
7:FZ:80:LEU:HB2	7:FZ:140:PHE:HB2	1.86	0.56
1:AA:220:LEU:HD13	1:AA:226:MET:HG3	1.87	0.56
1:AB:129:ASN:OD1	1:AC:411:LYS:NZ	2.38	0.56
1:AB:144:GLY:HA2	2:Ab:281:VAL:HG11	1.87	0.56
1:AB:425:TYR:HB2	1:AB:497:LEU:HB2	1.87	0.56
1:BA:389:LYS:NZ	1:BB:380:SER:OG	2.38	0.56
1:CB:273:ASN:ND2	1:CB:275:GLU:OE2	2.38	0.56
1:CD:326:MET:HE1	1:CE:400:VAL:HG11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:23:ASN:OD1	2:Db:259:ARG:NH2	2.38	0.56
1:DE:156:GLY:HA2	1:DF:277:MET:HE1	1.87	0.56
2:Ef:223:ARG:HG2	2:Ef:223:ARG:HH11	1.70	0.56
5:FB:572:GLU:HG3	5:FC:100:LYS:HE3	1.87	0.56
5:FH:266:PRO:HG3	5:FH:322:TYR:CE1	2.40	0.56
5:FI:97:GLU:OE2	5:FI:547:ARG:NH1	2.36	0.56
6:FM:216:ARG:NH2	6:FM:229:ASP:O	2.37	0.56
6:FN:12:VAL:HG22	7:GA:120:TYR:HB3	1.87	0.56
6:FO:48:TYR:O	6:FP:114:GLN:NE2	2.38	0.56
7:GJ:43:ARG:NH1	8:IV:221:TYR:OH	2.35	0.56
8:GM:472:GLU:HG3	8:GM:474:GLY:H	1.70	0.56
8:GU:448:GLY:H	8:GU:473:GLN:HB2	1.69	0.56
8:IM:242:THR:OG1	8:IN:240:ARG:NH1	2.39	0.56
1:AA:382:GLY:HA3	1:AF:389:LYS:HB2	1.88	0.56
1:AC:63:GLU:OE1	5:FA:219:ARG:NH2	2.38	0.56
2:Ab:259:ARG:NH2	1:EE:23:ASN:OD1	2.38	0.56
1:BC:433:MET:HE1	1:BD:41:VAL:HG13	1.86	0.56
1:EC:264:ALA:HA	1:EC:292:ILE:HG22	1.88	0.56
5:FE:423:ASN:OD1	5:FF:212:ARG:NH2	2.38	0.56
1:BD:9:GLN:NE2	3:Bg:89:ASN:O	2.38	0.56
1:BD:181:LYS:HD2	1:BE:287:LYS:HD2	1.88	0.56
1:CA:365:ARG:O	1:CB:377:ASN:ND2	2.39	0.56
1:CD:125:VAL:HG21	1:CD:130:GLN:H	1.71	0.56
1:DE:75:ILE:HG13	1:DF:40:MET:HE3	1.87	0.56
2:Da:158:TYR:HB3	2:Da:168:ASP:HB2	1.86	0.56
1:EC:390:ALA:HB3	1:EC:394:VAL:HB	1.88	0.56
5:FJ:80:ARG:HD2	6:FW:235:VAL:HG21	1.87	0.56
6:FN:95:THR:O	6:FN:95:THR:OG1	2.00	0.56
6:FX:216:ARG:NH2	6:FX:229:ASP:O	2.38	0.56
7:FY:104:GLN:NE2	7:FZ:75:GLU:O	2.38	0.56
1:AA:175:GLU:OE2	1:AB:409:ARG:NH1	2.39	0.56
1:AB:171:ARG:HB2	1:AC:411:LYS:HD3	1.88	0.56
1:AC:435:GLN:HE22	1:AD:41:VAL:HG22	1.71	0.56
2:Bd:9:ARG:HE	2:Bd:303:THR:HG21	1.70	0.56
3:Bg:41:THR:HA	4:Bi:12:ASN:HD21	1.69	0.56
3:Bh:36:MET:HG2	3:Bh:80:ILE:HG12	1.87	0.56
1:DA:20:THR:HG23	1:DA:20:THR:O	2.06	0.56
2:Da:158:TYR:HB2	2:Da:189:ILE:HB	1.88	0.56
3:Eg:36:MET:HG2	3:Eg:80:ILE:HG12	1.87	0.56
5:FG:163:ARG:NH1	5:FG:625:GLU:OE1	2.39	0.56
5:FH:400:ILE:HD11	5:FH:591:GLU:HG3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:2:ALA:N	2:Bb:107:TYR:O	2.38	0.56
1:AF:153:LEU:HD11	1:AF:161:VAL:HG13	1.88	0.56
1:CC:361:ASN:HD21	1:CC:367:VAL:HB	1.71	0.56
1:DD:199:ARG:HH22	1:DE:33:PRO:HB3	1.70	0.56
1:DE:334:LYS:NZ	1:DE:399:ASP:OD2	2.37	0.56
1:EC:275:GLU:OE1	6:FS:96:HIS:ND1	2.39	0.56
5:FB:447:ARG:NH2	5:FC:453:ALA:O	2.39	0.56
5:FK:161:ASP:OD2	5:FK:677:ARG:NH1	2.39	0.56
5:FK:650:GLN:NE2	5:FK:667:TYR:OH	2.37	0.56
5:FL:52:ASP:HB3	5:FL:57:ARG:HB2	1.87	0.56
6:FW:74:VAL:HG22	6:FW:129:ILE:HG12	1.88	0.56
1:CB:183:LEU:H	5:FI:297:THR:HG22	1.70	0.56
2:Dd:312:HIS:O	2:Dd:316:ASN:ND2	2.38	0.56
1:EE:89:ASP:OD1	1:EE:90:GLU:N	2.39	0.56
5:FJ:2:ALA:N	5:FJ:272:GLY:O	2.39	0.56
6:FQ:216:ARG:NH2	6:FQ:229:ASP:O	2.39	0.56
6:FS:1:MET:HG3	6:FS:195:PHE:HA	1.87	0.56
7:FZ:51:ILE:HG21	7:FZ:158:ILE:HD11	1.88	0.56
7:GE:115:MET:SD	7:GE:131:SER:OG	2.61	0.56
7:GJ:51:ILE:HG21	7:GJ:158:ILE:HD11	1.88	0.56
8:GR:497:TYR:O	8:GR:534:ARG:NH1	2.39	0.56
1:AE:269:ASN:HD22	1:AE:278:ASN:HB2	1.71	0.56
1:BA:48:ARG:HD2	1:BA:407:PRO:HD3	1.88	0.56
1:CD:243:TRP:HB2	5:FH:286:PHE:HD1	1.71	0.56
1:CF:206:ARG:HG3	1:CF:481:MET:HB3	1.86	0.56
3:Cg:51:LYS:NZ	3:Ch:84:ILE:O	2.39	0.56
1:DA:438:ILE:HG12	1:DA:488:VAL:HG13	1.88	0.56
2:Db:88:VAL:HG12	2:Db:223:ARG:HD2	1.87	0.56
5:FI:570:ILE:HG12	5:FJ:93:VAL:HG22	1.88	0.56
1:AD:438:ILE:HG23	1:AD:488:VAL:HG22	1.87	0.56
1:CF:89:ASP:C	1:CF:89:ASP:OD1	2.49	0.56
4:Ck:27:LYS:HG2	4:Ck:36:THR:HG22	1.88	0.56
1:DC:326:MET:HG2	5:FF:277:MET:HE1	1.88	0.56
5:FA:423:ASN:ND2	5:FB:214:ASN:OD1	2.37	0.56
5:FD:222:LYS:HE2	5:FE:243:PRO:HG2	1.88	0.56
7:GA:85:LYS:NZ	7:GA:135:ASP:O	2.39	0.56
1:AD:390:ALA:HB3	1:AD:394:VAL:HB	1.88	0.55
1:BB:112:VAL:HG22	1:BB:148:VAL:HG22	1.89	0.55
1:BF:425:TYR:HB2	1:BF:497:LEU:HB2	1.87	0.55
1:DB:136:ILE:HG12	1:DB:151:VAL:HG12	1.86	0.55
1:DC:171:ARG:HB2	1:DD:411:LYS:HD2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dd:119:TYR:O	2:Dd:144:ASN:ND2	2.37	0.55
5:FE:266:PRO:HB2	5:FE:268:TYR:HB2	1.87	0.55
5:FF:709:GLN:HE21	5:FG:707:MET:HE2	1.72	0.55
5:FH:447:ARG:NH2	5:FI:453:ALA:O	2.39	0.55
5:FL:618:ILE:HG22	5:FL:618:ILE:O	2.05	0.55
6:FM:8:VAL:HB	6:FM:12:VAL:HG21	1.88	0.55
7:GA:51:ILE:HG21	7:GA:158:ILE:HD11	1.88	0.55
8:GQ:497:TYR:O	8:GQ:534:ARG:NH1	2.38	0.55
1:AD:415:PRO:HA	3:Ah:67:ILE:HG22	1.87	0.55
1:AE:296:THR:HG22	1:AE:488:VAL:HG11	1.88	0.55
2:Ae:216:ILE:HG12	2:Ae:225:TRP:HB3	1.88	0.55
1:BF:88:ARG:HB2	1:BF:110:TYR:HB2	1.87	0.55
1:CC:185:ARG:NH2	2:Db:296:GLN:O	2.39	0.55
2:Cf:123:ILE:O	2:Cf:125:ARG:NH1	2.39	0.55
1:DB:406:ASP:O	1:DB:410:ASN:ND2	2.39	0.55
1:DC:321:ALA:O	1:DC:329:ARG:NH2	2.40	0.55
1:EB:361:ASN:HD21	1:EB:367:VAL:HB	1.70	0.55
3:Eg:79:ARG:NH2	3:Eg:95:GLN:OE1	2.39	0.55
5:FB:110:THR:O	5:FC:172:ASN:ND2	2.40	0.55
5:FD:38:SER:HB3	5:FD:41:ARG:HG2	1.88	0.55
5:FG:583:LYS:NZ	5:FG:587:GLU:OE2	2.39	0.55
3:Ag:79:ARG:NH2	3:Ag:95:GLN:OE1	2.39	0.55
4:Bi:8:LYS:HD2	4:Bi:14:PRO:HB3	1.89	0.55
5:FE:379:ASN:ND2	5:FF:248:ASP:OD1	2.40	0.55
5:FF:447:ARG:NH1	5:FG:455:ASN:O	2.39	0.55
6:FV:138:ASP:OD1	6:FV:138:ASP:N	2.38	0.55
7:GA:36:ARG:NH2	7:GA:159:PHE:O	2.40	0.55
2:Cd:323:ASN:HD21	2:Cd:330:ILE:H	1.54	0.55
1:EC:183:LEU:HD12	1:ED:284:ASN:HD21	1.71	0.55
1:ED:297:GLU:OE2	1:ED:424:ARG:NH2	2.39	0.55
1:ED:310:LYS:NZ	2:Ed:97:ASN:O	2.39	0.55
6:FR:83:LEU:HD22	6:FR:109:PRO:HB2	1.89	0.55
7:GE:36:ARG:HG3	7:GE:187:ILE:HD12	1.88	0.55
1:AA:224:ILE:HD12	1:AF:195:PRO:HD2	1.87	0.55
2:Ad:319:ILE:O	2:Ad:323:ASN:ND2	2.39	0.55
1:CC:111:LEU:HD12	1:CC:151:VAL:HG21	1.88	0.55
1:CE:61:THR:HG22	1:CE:440:LYS:HB2	1.87	0.55
3:Ch:31:MET:HG3	3:Ch:53:ILE:HG22	1.89	0.55
1:DC:330:LEU:HB2	1:DC:395:ARG:HH21	1.72	0.55
5:FB:383:GLU:OE2	5:FB:396:ARG:NH1	2.39	0.55
5:FG:97:GLU:OE1	5:FG:547:ARG:NH2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FI:447:ARG:NH1	5:FJ:455:ASN:O	2.39	0.55
5:FK:8:PRO:O	5:FK:10:GLN:NE2	2.40	0.55
6:FQ:18:LEU:HD22	6:FQ:24:THR:HA	1.88	0.55
6:FV:76:LEU:HG	6:FV:83:LEU:HD11	1.89	0.55
7:GD:122:LYS:HA	7:GD:125:ARG:HD2	1.89	0.55
7:GG:104:GLN:NE2	7:GH:75:GLU:O	2.40	0.55
8:GV:450:HIS:O	8:GV:456:GLN:HA	2.07	0.55
2:Aa:93:VAL:HG21	2:Aa:218:VAL:HG12	1.89	0.55
1:BA:48:ARG:NH2	1:BF:321:ALA:O	2.40	0.55
1:BE:80:ARG:NH2	1:BE:115:GLU:OE2	2.39	0.55
1:BE:130:GLN:HE22	1:BF:293:PHE:HB3	1.71	0.55
2:Be:136:LYS:NZ	2:Be:177:GLU:OE2	2.40	0.55
1:DB:435:GLN:NE2	1:DC:40:MET:O	2.39	0.55
1:DC:175:GLU:OE2	1:DD:409:ARG:NH2	2.36	0.55
3:Dg:36:MET:HG2	3:Dg:80:ILE:HG12	1.88	0.55
1:EB:129:ASN:ND2	1:EC:409:ARG:O	2.39	0.55
1:EE:62:ARG:HH21	1:EE:436:PRO:HD2	1.72	0.55
1:EE:458:ASN:ND2	1:EE:461:THR:OG1	2.40	0.55
5:FB:8:PRO:O	5:FB:10:GLN:NE2	2.37	0.55
6:FP:216:ARG:HH12	6:FP:229:ASP:HB2	1.70	0.55
6:FS:19:ARG:NH1	6:FT:33:GLN:OE1	2.39	0.55
7:GH:46:ASP:OD1	7:GH:46:ASP:N	2.38	0.55
8:IS:244:LEU:O	8:IS:245:PRO:C	2.49	0.55
1:AE:133:PRO:HB2	1:AE:154:MET:HB2	1.87	0.55
2:Ab:11:LEU:HD22	2:Ab:247:GLU:HG3	1.88	0.55
2:Bb:84:LEU:HD23	2:Bb:225:TRP:HE1	1.72	0.55
2:Be:119:TYR:O	2:Be:144:ASN:ND2	2.40	0.55
1:CA:382:GLY:HA3	1:CF:389:LYS:HB2	1.89	0.55
1:CF:112:VAL:HG22	1:CF:148:VAL:HG22	1.89	0.55
1:DA:302:MET:HE3	1:DA:497:LEU:HD13	1.89	0.55
1:DD:253:LEU:HD11	5:FF:280:ILE:HD11	1.88	0.55
2:Df:79:ARG:NH1	2:Df:234:THR:OG1	2.39	0.55
3:Dh:79:ARG:NH2	3:Dh:92:MET:O	2.39	0.55
1:EA:269:ASN:HD22	1:EA:278:ASN:HB2	1.71	0.55
5:FG:383:GLU:OE2	5:FG:396:ARG:NH1	2.37	0.55
5:FL:272:GLY:HA2	5:FL:305:PHE:HE1	1.72	0.55
6:FN:212:GLN:HG2	6:FN:231:GLU:HG3	1.87	0.55
6:FP:68:LEU:HD21	6:FP:71:ILE:HG13	1.88	0.55
7:GC:85:LYS:NZ	7:GC:135:ASP:O	2.39	0.55
8:GM:449:SER:HA	8:GM:472:GLU:HB2	1.89	0.55
8:GO:497:TYR:O	8:GO:534:ARG:NH1	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:424:ARG:NH2	1:AE:426:ASP:OD2	2.40	0.55
2:Ad:143:LYS:O	2:Ad:147:ASN:ND2	2.40	0.55
1:BC:91:ASN:ND2	1:BC:91:ASN:N	2.54	0.55
1:CB:80:ARG:NH2	1:CB:115:GLU:OE2	2.40	0.55
1:DC:133:PRO:HB2	1:DC:154:MET:HB3	1.88	0.55
1:EC:203:THR:HG22	1:EC:289:GLY:H	1.71	0.55
5:FC:567:SER:HB2	5:FD:549:GLY:HA2	1.89	0.55
5:FD:417:GLY:O	5:FD:584:ARG:NH2	2.39	0.55
5:FK:400:ILE:HB	5:FK:595:VAL:HG11	1.88	0.55
7:GB:36:ARG:NH1	7:GB:186:PRO:O	2.39	0.55
1:AA:152:GLU:OE1	1:AB:278:ASN:ND2	2.39	0.55
1:CB:59:PHE:O	1:CB:440:LYS:NZ	2.40	0.55
1:CE:112:VAL:HG22	1:CE:148:VAL:HG12	1.88	0.55
2:Cd:259:ARG:HH22	1:DC:23:ASN:HB2	1.70	0.55
1:DC:60:PRO:HG2	1:DC:439:PHE:HB3	1.88	0.55
1:DC:473:GLU:OE2	2:Db:7:GLN:NE2	2.40	0.55
1:EC:329:ARG:NH1	1:EC:392:ASN:O	2.40	0.55
5:FK:383:GLU:OE2	5:FK:396:ARG:NH1	2.39	0.55
6:FW:19:ARG:NH1	6:FX:33:GLN:OE1	2.39	0.55
1:AF:244:MET:HE3	1:AF:459:PRO:HB2	1.88	0.55
1:BC:10:MET:SD	1:BC:10:MET:N	2.80	0.55
1:BC:70:TYR:HB3	1:BD:34:GLN:HG3	1.88	0.55
1:BD:310:LYS:NZ	2:Bd:97:ASN:O	2.39	0.55
1:CB:85:VAL:HB	1:CB:112:VAL:HG23	1.89	0.55
1:CF:425:TYR:HB2	1:CF:497:LEU:HB2	1.88	0.55
2:Cd:265:ASN:O	1:DB:199:ARG:NH1	2.40	0.55
2:Db:85:ASP:HB3	2:Db:88:VAL:HG22	1.88	0.55
1:EC:74:VAL:HG12	1:ED:41:VAL:HB	1.88	0.55
2:Ea:140:SER:O	2:Ea:144:ASN:ND2	2.40	0.55
5:FC:564:THR:N	5:FD:549:GLY:O	2.40	0.55
5:FD:297:THR:HB	5:FD:304:PHE:HB2	1.88	0.55
6:FO:29:GLU:HG2	7:GA:124:LEU:HD22	1.88	0.55
6:FQ:78:LYS:NZ	6:FQ:79:ASN:OD1	2.39	0.55
8:IT:243:SER:OG	8:IT:244:LEU:N	2.34	0.55
1:BD:390:ALA:HB3	1:BD:394:VAL:HB	1.89	0.54
2:Cd:110:LEU:HD22	1:DC:13:PHE:HB3	1.89	0.54
1:DA:411:LYS:HG2	1:DF:171:ARG:HB2	1.89	0.54
1:EA:365:ARG:O	1:EB:377:ASN:ND2	2.40	0.54
5:FA:447:ARG:NH2	6:FO:212:GLN:O	2.39	0.54
5:FC:417:GLY:O	5:FC:584:ARG:NH2	2.40	0.54
5:FF:417:GLY:O	5:FF:584:ARG:NH2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FJ:339:ARG:NH2	8:GT:521:ASP:OD2	2.39	0.54
7:GF:107:ILE:HG23	7:GF:128:ILE:HB	1.89	0.54
7:GI:36:ARG:NH2	7:GI:159:PHE:O	2.40	0.54
8:GP:448:GLY:H	8:GP:473:GLN:HB2	1.72	0.54
1:AB:146:ASN:ND2	2:Ab:72:ALA:O	2.41	0.54
1:AD:12:GLY:HA2	1:AD:221:ALA:HA	1.90	0.54
2:Af:88:VAL:HG13	2:Af:218:VAL:HG11	1.87	0.54
1:BA:466:ASN:HB3	1:BA:469:MET:HG2	1.88	0.54
1:BF:56:LEU:HD11	1:BF:264:ALA:HB2	1.90	0.54
1:CB:80:ARG:HD2	2:Cb:110:LEU:HB3	1.89	0.54
1:EF:112:VAL:HG22	1:EF:148:VAL:HG22	1.88	0.54
5:FB:82:GLN:NE2	5:FB:83:HIS:O	2.41	0.54
6:FQ:122:ILE:HD12	6:FQ:125:GLU:HB2	1.89	0.54
6:FW:216:ARG:NH1	6:FW:226:ASN:O	2.40	0.54
1:CB:185:ARG:HB2	1:CC:281:LYS:HE3	1.89	0.54
1:CD:206:ARG:NH2	1:DC:472:ASP:O	2.38	0.54
1:CD:390:ALA:HB3	1:CD:394:VAL:HB	1.89	0.54
2:Cf:158:TYR:HB3	2:Cf:168:ASP:HB2	1.89	0.54
6:FV:66:CYS:SG	6:FV:116:ARG:NH1	2.80	0.54
7:GF:86:VAL:HG21	7:GF:138:LEU:HB2	1.90	0.54
1:AC:282:SER:OG	1:AC:284:ASN:ND2	2.41	0.54
1:AC:464:LYS:HD3	5:FB:31:GLN:HB3	1.90	0.54
1:BB:80:ARG:NH2	1:BB:115:GLU:OE2	2.41	0.54
2:Cd:255:GLY:HA2	1:DB:275:GLU:HA	1.89	0.54
1:DB:273:ASN:ND2	1:DB:275:GLU:OE2	2.40	0.54
1:DF:88:ARG:HH11	1:DF:88:ARG:HG3	1.72	0.54
1:EC:204:THR:HG22	1:EC:483:THR:HG23	1.89	0.54
5:FC:52:ASP:HB3	5:FC:57:ARG:HB2	1.89	0.54
6:FR:74:VAL:HG22	6:FR:129:ILE:HG12	1.90	0.54
7:FY:43:ARG:NH1	8:IK:221:TYR:OH	2.39	0.54
7:GC:96:ARG:NH2	7:GC:102:PHE:O	2.40	0.54
7:GG:104:GLN:HE22	7:GH:76:GLY:HA3	1.71	0.54
1:BD:271:ASN:HB3	1:BD:273:ASN:H	1.72	0.54
1:BD:300:ASN:ND2	1:BD:492:THR:O	2.40	0.54
1:CA:238:ASP:OD2	1:CA:245:HIS:NE2	2.41	0.54
1:CD:56:LEU:HD12	1:CD:440:LYS:HD3	1.89	0.54
2:Cd:108:ILE:N	2:Cd:108:ILE:CD1	2.70	0.54
3:Dg:51:LYS:HD2	3:Dh:88:CYS:HA	1.90	0.54
5:FB:112:PRO:HG2	5:FC:668:THR:HB	1.87	0.54
5:FD:653:LEU:HD13	5:FD:663:ILE:HG13	1.89	0.54
5:FH:252:ASP:N	5:FH:252:ASP:OD1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FY:81:ARG:NH1	7:FY:82:SER:O	2.39	0.54
7:GE:96:ARG:NH2	7:GE:102:PHE:O	2.40	0.54
7:GF:80:LEU:HB2	7:GF:140:PHE:HB2	1.88	0.54
7:GJ:86:VAL:HG21	7:GJ:138:LEU:HB2	1.90	0.54
1:AB:183:LEU:H	5:FB:297:THR:HG22	1.73	0.54
1:AD:329:ARG:NH1	1:AD:392:ASN:O	2.40	0.54
2:Ae:197:TRP:NE1	2:Ae:245:ASP:OD2	2.40	0.54
2:Bf:219:ASP:OD1	2:Bf:219:ASP:N	2.41	0.54
1:CC:189:ASP:O	1:CC:191:ARG:NH1	2.41	0.54
1:CE:308:SER:OG	2:Ce:97:ASN:ND2	2.41	0.54
1:DB:301:THR:HG23	1:DB:496:SER:HB2	1.89	0.54
1:DD:112:VAL:HG22	1:DD:148:VAL:HG22	1.89	0.54
1:EC:230:LEU:HD12	1:EC:234:LYS:HB3	1.89	0.54
1:ED:74:VAL:HB	1:ED:196:VAL:HG23	1.88	0.54
5:FI:404:ARG:HG3	5:FI:410:ARG:HD3	1.89	0.54
6:FX:1:MET:HG3	6:FX:195:PHE:HA	1.89	0.54
1:AC:163:ALA:O	1:AC:167:GLN:NE2	2.39	0.54
1:AD:438:ILE:HG12	1:AD:488:VAL:HG13	1.89	0.54
4:Ak:26:MET:HE3	4:Ak:37:ILE:HD13	1.89	0.54
2:Ba:281:VAL:HG22	2:Ba:305:VAL:HG12	1.88	0.54
4:Ck:9:ILE:HG22	4:Ck:21:LEU:HB2	1.88	0.54
1:EB:490:ASP:HB3	1:EB:493:ARG:HG3	1.89	0.54
5:FA:8:PRO:O	5:FA:10:GLN:NE2	2.32	0.54
5:FJ:447:ARG:NH1	5:FK:455:ASN:O	2.41	0.54
6:FN:2:VAL:HA	6:FN:199:SER:HB3	1.88	0.54
6:FO:138:ASP:N	6:FO:138:ASP:OD1	2.40	0.54
2:Af:216:ILE:HG13	2:Af:216:ILE:O	2.06	0.54
1:BE:390:ALA:HB3	1:BE:394:VAL:HB	1.88	0.54
1:BF:112:VAL:HG22	1:BF:148:VAL:HG22	1.89	0.54
1:CA:48:ARG:NH2	1:CF:321:ALA:O	2.40	0.54
1:CD:144:GLY:HA2	2:Cd:281:VAL:HG11	1.89	0.54
1:DB:229:ASN:ND2	1:DB:250:GLU:OE2	2.38	0.54
3:Dh:73:TYR:O	3:Dh:76:LYS:NZ	2.41	0.54
1:EA:206:ARG:HG3	1:EA:481:MET:HG3	1.89	0.54
1:EE:102:VAL:HG21	1:EE:166:LEU:HD12	1.89	0.54
1:EF:269:ASN:HD22	1:EF:278:ASN:HB2	1.71	0.54
5:FB:583:LYS:NZ	5:FB:587:GLU:OE2	2.41	0.54
5:FC:110:THR:O	5:FD:172:ASN:ND2	2.40	0.54
5:FG:104:ASP:N	5:FG:104:ASP:OD1	2.41	0.54
5:FH:268:TYR:N	5:FH:268:TYR:CD1	2.76	0.54
6:FU:216:ARG:NH2	6:FU:229:ASP:O	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:GG:37:SER:OG	7:GG:160:GLU:O	2.25	0.54
1:AB:79:ARG:NH1	2:Ab:113:GLU:OE2	2.41	0.54
1:AC:81:ASN:HB2	1:AC:171:ARG:HB3	1.90	0.54
1:AC:85:VAL:HA	1:AC:168:GLN:HG3	1.90	0.54
1:BB:122:GLU:OE2	1:BC:258:TYR:OH	2.26	0.54
1:BB:475:SER:OG	1:BB:476:ALA:N	2.41	0.54
1:BE:184:SER:OG	1:BF:206:ARG:NH1	2.39	0.54
2:Ba:239:ASP:H	2:Ba:278:VAL:HG12	1.73	0.54
2:Bb:79:ARG:NH1	2:Bb:234:THR:OG1	2.41	0.54
2:Bf:105:ARG:HB2	2:Bf:208:PRO:HG2	1.89	0.54
3:Cg:34:TRP:NE1	3:Cg:52:ALA:O	2.39	0.54
1:DF:88:ARG:HG3	1:DF:88:ARG:NH1	2.23	0.54
2:Dd:251:MET:SD	2:Dd:254:ARG:NH2	2.81	0.54
1:ED:128:LEU:HD23	1:ED:165:ARG:HD2	1.89	0.54
3:Eh:36:MET:HG2	3:Eh:80:ILE:HG12	1.90	0.54
5:FA:219:ARG:NH1	5:FA:238:GLU:OE2	2.41	0.54
5:FA:447:ARG:NH1	5:FB:455:ASN:O	2.40	0.54
5:FA:461:GLU:OE2	5:FB:512:LYS:NZ	2.37	0.54
5:FD:594:LYS:NZ	5:FD:625:GLU:OE2	2.41	0.54
5:FH:354:GLU:O	5:FI:600:ARG:NH1	2.39	0.54
8:GO:541:GLU:OE1	8:GO:544:GLN:NE2	2.41	0.54
8:GV:448:GLY:H	8:GV:473:GLN:HB2	1.73	0.54
3:Ag:51:LYS:HD2	3:Ah:88:CYS:HA	1.89	0.54
1:CA:163:ALA:O	1:CA:167:GLN:NE2	2.38	0.54
1:CB:311:LEU:O	1:CB:315:ALA:N	2.41	0.54
1:CC:390:ALA:HB3	1:CC:394:VAL:HB	1.90	0.54
1:DB:256:ASP:O	1:DB:260:ASN:ND2	2.41	0.54
1:EB:438:ILE:HG23	1:EB:488:VAL:HG22	1.90	0.54
1:EC:81:ASN:HD22	1:ED:411:LYS:HG2	1.73	0.54
5:FA:725:ARG:NH2	5:FL:720:GLU:OE1	2.40	0.54
5:FD:379:ASN:ND2	5:FE:248:ASP:OD1	2.40	0.54
6:FM:1:MET:HG3	6:FM:195:PHE:HA	1.90	0.54
6:FT:66:CYS:SG	6:FT:116:ARG:NH1	2.71	0.54
1:AB:414:HIS:HD2	1:AB:416:MET:HB2	1.73	0.53
1:BC:361:ASN:HD21	1:BC:367:VAL:HB	1.73	0.53
1:CF:319:LEU:HD21	1:CF:430:ILE:HD13	1.90	0.53
1:DE:440:LYS:HA	1:DE:486:VAL:HG23	1.88	0.53
2:De:6:ASN:ND2	2:De:299:GLU:OE1	2.40	0.53
3:Dg:79:ARG:NH1	3:Dg:81:GLU:OE1	2.41	0.53
4:Dj:20:TRP:HB3	4:Dj:27:LYS:HB2	1.90	0.53
1:EB:112:VAL:HG22	1:EB:148:VAL:HG22	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:129:ASN:OD1	1:EC:411:LYS:NZ	2.41	0.53
5:FJ:76:TYR:OH	6:FW:234:ARG:NH1	2.41	0.53
6:FP:53:GLU:HG3	6:FP:131:TYR:HE1	1.73	0.53
7:GI:85:LYS:NZ	7:GI:135:ASP:O	2.41	0.53
1:AC:207:ILE:HG22	1:AC:480:ARG:HB2	1.91	0.53
4:Ak:26:MET:HB3	4:Ak:37:ILE:HG12	1.89	0.53
1:CA:425:TYR:HB2	1:CA:497:LEU:HB3	1.90	0.53
4:Ci:1:MET:HB2	4:Cj:9:ILE:HG13	1.90	0.53
1:DA:79:ARG:NH2	2:Da:113:GLU:OE2	2.41	0.53
1:DC:10:MET:N	1:DC:10:MET:SD	2.82	0.53
1:DF:263:MET:HG3	1:DF:484:LEU:HD12	1.90	0.53
2:Ea:234:THR:HG23	2:Ea:235:LYS:HG3	1.91	0.53
4:Ei:8:LYS:HD2	4:Ei:14:PRO:HB3	1.90	0.53
5:FB:75:ALA:HB1	6:FO:235:VAL:HG22	1.90	0.53
5:FF:724:ILE:HA	5:FF:727:ASN:HD22	1.72	0.53
7:GA:34:LYS:NZ	7:GA:161:ASP:OD1	2.42	0.53
1:AA:390:ALA:HB3	1:AA:394:VAL:HB	1.91	0.53
1:AC:56:LEU:O	1:AC:440:LYS:NZ	2.40	0.53
1:BB:259:LYS:NZ	1:BB:448:GLU:OE2	2.38	0.53
2:Ba:251:MET:SD	2:Ba:254:ARG:NH2	2.81	0.53
4:Bi:9:ILE:HB	4:Bk:2:LYS:HB2	1.90	0.53
1:DD:323:LYS:HB3	1:DE:44:LEU:HG	1.90	0.53
5:FF:82:GLN:NE2	6:FS:236:HIS:OXT	2.41	0.53
5:FJ:447:ARG:NH2	6:FX:212:GLN:O	2.41	0.53
6:FQ:216:ARG:NH1	6:FQ:226:ASN:O	2.41	0.53
6:FU:29:GLU:OE2	7:GG:114:ARG:NH2	2.42	0.53
7:GE:33:VAL:HG22	7:GE:162:ALA:HB3	1.90	0.53
1:AB:366:VAL:HG23	1:AB:367:VAL:HG23	1.91	0.53
1:AC:23:ASN:HB2	2:Ed:259:ARG:HH22	1.72	0.53
1:AF:127:ASN:HB2	1:AF:170:GLU:OE2	2.09	0.53
2:Ab:147:ASN:ND2	2:Ab:149:THR:OG1	2.42	0.53
2:Ab:258:TYR:OH	1:ED:199:ARG:NH2	2.41	0.53
1:BA:144:GLY:HA2	2:Ba:281:VAL:HG11	1.90	0.53
1:BB:53:ASP:N	1:BB:53:ASP:OD1	2.38	0.53
1:BD:199:ARG:NH2	2:Cb:258:TYR:OH	2.41	0.53
2:Be:282:LEU:HD23	2:Be:304:LEU:HD12	1.91	0.53
1:CA:41:VAL:HB	1:CF:74:VAL:HG22	1.90	0.53
1:CC:443:ILE:HB	1:CC:446:ASP:HB2	1.89	0.53
1:CE:311:LEU:HD13	2:Ce:99:ILE:HD13	1.91	0.53
1:DB:124:ILE:HG22	1:DB:174:ILE:HA	1.88	0.53
1:EA:411:LYS:HG2	1:EF:171:ARG:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:363:SER:OG	1:EC:361:ASN:ND2	2.41	0.53
1:EE:189:ASP:O	1:EE:191:ARG:NH1	2.42	0.53
1:EF:128:LEU:N	1:EF:128:LEU:HD23	2.23	0.53
1:EF:228:ARG:HD3	1:EF:245:HIS:HE1	1.72	0.53
6:FU:1:MET:HG3	6:FU:195:PHE:HA	1.90	0.53
7:GB:128:ILE:HA	7:GB:142:SER:HB2	1.89	0.53
7:GH:65:GLU:HG3	7:GH:148:LEU:HD22	1.90	0.53
2:Ad:312:HIS:O	2:Ad:316:ASN:ND2	2.41	0.53
2:Ba:140:SER:O	2:Ba:144:ASN:ND2	2.42	0.53
2:Bd:281:VAL:HG22	2:Bd:305:VAL:HG12	1.90	0.53
2:Be:158:TYR:HB2	2:Be:189:ILE:HB	1.89	0.53
1:DB:8:PHE:HB3	2:Da:267:ILE:HD12	1.91	0.53
1:DB:80:ARG:NH2	1:DB:115:GLU:OE2	2.42	0.53
1:EC:449:TYR:OH	5:FD:291:MET:SD	2.66	0.53
1:ED:503:GLN:NE2	2:Ed:147:ASN:OD1	2.41	0.53
5:FB:447:ARG:NH1	5:FC:455:ASN:O	2.42	0.53
5:FD:167:ALA:HB1	5:FD:590:LEU:HD21	1.90	0.53
5:FE:609:SER:OG	5:FE:610:ASP:N	2.41	0.53
5:FI:734:ALA:O	5:FI:737:GLN:NE2	2.42	0.53
5:FK:9:ARG:HE	5:FL:263:GLU:HG2	1.72	0.53
5:FL:378:VAL:HG13	5:FL:409:SER:HA	1.90	0.53
6:FV:34:TYR:HD2	6:FV:158:ILE:HG23	1.74	0.53
8:GV:462:VAL:HA	8:GV:467:ALA:O	2.07	0.53
1:AB:80:ARG:HH11	2:Ab:110:LEU:HB3	1.73	0.53
1:AB:207:ILE:HG22	1:AB:480:ARG:HB2	1.91	0.53
1:BA:53:ASP:OD2	1:BA:260:ASN:ND2	2.41	0.53
1:BA:153:LEU:HD11	1:BA:161:VAL:HG23	1.90	0.53
2:Bb:41:LEU:HD13	2:Bb:326:SER:HB3	1.89	0.53
4:Ci:7:LEU:HD22	4:Ck:19:VAL:HG21	1.90	0.53
1:DE:8:PHE:HA	1:DE:10:MET:HE2	1.91	0.53
2:Da:252:GLY:HA3	2:Da:259:ARG:HH21	1.73	0.53
1:EA:48:ARG:NH2	1:EF:321:ALA:O	2.38	0.53
5:FA:564:THR:N	5:FB:549:GLY:O	2.41	0.53
5:FE:536:GLU:OE2	5:FF:441:TYR:OH	2.26	0.53
5:FG:489:ASP:HB3	5:FG:492:LYS:HG3	1.90	0.53
5:FH:277:MET:O	5:FH:278:ASP:HB2	2.09	0.53
7:FY:11:LEU:HD11	7:FY:25:PRO:HG3	1.90	0.53
1:BB:129:ASN:OD1	1:BC:411:LYS:NZ	2.41	0.53
1:CA:201:GLU:OE2	1:CA:276:TYR:OH	2.26	0.53
1:EA:390:ALA:HB3	1:EA:394:VAL:HB	1.91	0.53
1:EF:390:ALA:HB3	1:EF:394:VAL:HB	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FK:41:ARG:O	5:FK:426:ARG:NH1	2.38	0.53
6:FV:50:ASP:OD2	6:FV:72:ASN:ND2	2.42	0.53
7:GC:109:TYR:HA	7:GC:130:CYS:HB2	1.91	0.53
7:GG:43:ARG:NH1	8:IS:221:TYR:OH	2.42	0.53
1:AC:190:VAL:HG21	1:AD:251:VAL:HG22	1.89	0.53
1:AF:290:ALA:HB1	1:AF:294:GLU:HB3	1.91	0.53
1:BA:48:ARG:HH22	1:BF:322:SER:HA	1.74	0.53
1:BA:261:ASN:HD22	1:BF:175:GLU:HA	1.74	0.53
1:BE:186:LYS:HB2	1:BF:208:GLN:HG2	1.90	0.53
1:DC:200:ASN:ND2	1:DC:486:VAL:O	2.42	0.53
1:ED:40:MET:O	5:FC:283:ARG:NH1	2.41	0.53
1:ED:122:GLU:OE2	1:EE:258:TYR:OH	2.27	0.53
6:FV:83:LEU:N	6:FV:83:LEU:HD12	2.23	0.53
6:FW:83:LEU:N	6:FW:83:LEU:CD2	2.71	0.53
1:AA:466:ASN:HB3	1:AA:469:MET:HG2	1.90	0.53
1:AE:80:ARG:NH2	1:AE:115:GLU:OE2	2.42	0.53
1:CC:207:ILE:HG22	1:CC:480:ARG:HB2	1.90	0.53
1:CD:201:GLU:OE2	1:CD:270:ARG:NH1	2.40	0.53
2:Ca:140:SER:O	2:Ca:144:ASN:ND2	2.41	0.53
2:Ca:158:TYR:HB2	2:Ca:189:ILE:HB	1.90	0.53
2:Db:79:ARG:NH2	2:Db:168:ASP:OD2	2.39	0.53
1:EC:445:GLY:O	1:EC:446:ASP:C	2.51	0.53
1:EE:88:ARG:HG3	1:EE:92:GLY:HA2	1.91	0.53
5:FG:423:ASN:OD1	5:FH:212:ARG:NH2	2.41	0.53
5:FH:383:GLU:OE2	5:FH:396:ARG:NH1	2.42	0.53
5:FL:50:ASN:ND2	5:FL:432:ASP:OD1	2.35	0.53
7:GC:43:ARG:NH1	8:IO:221:TYR:OH	2.41	0.53
7:GC:80:LEU:HB2	7:GC:140:PHE:HB2	1.89	0.53
7:GE:43:ARG:NH1	8:IQ:221:TYR:OH	2.42	0.53
1:AC:50:LYS:HD2	1:AC:232:SER:HB3	1.89	0.53
2:Bd:259:ARG:HH22	1:CC:23:ASN:HB2	1.74	0.53
4:Bj:26:MET:HG2	4:Bj:37:ILE:HD12	1.91	0.53
1:CE:458:ASN:ND2	1:CE:461:THR:OG1	2.42	0.53
2:Cd:108:ILE:HG22	2:Cd:108:ILE:O	2.08	0.53
1:DA:405:ASP:OD1	1:DA:405:ASP:N	2.42	0.53
1:DB:112:VAL:HG22	1:DB:148:VAL:HG12	1.91	0.53
4: Ei:27:LYS:HE2	4: Ei:36:THR:HG22	1.91	0.53
5:FD:219:ARG:NH2	5:FD:238:GLU:OE2	2.42	0.53
5:FF:489:ASP:OD1	6:FQ:193:ASN:ND2	2.38	0.53
5:FG:627:ASP:HA	5:FH:603:LYS:HE3	1.91	0.53
5:FH:134:ILE:HD12	5:FH:147:LYS:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FL:365:VAL:HG11	5:FL:373:VAL:HB	1.91	0.53
7:FZ:33:VAL:HG21	7:FZ:163:LYS:HG3	1.91	0.53
1:AB:458:ASN:ND2	1:AB:461:THR:OG1	2.42	0.52
1:AD:207:ILE:HG22	1:AD:480:ARG:HB2	1.90	0.52
1:BB:128:LEU:HD13	1:BB:165:ARG:HD2	1.91	0.52
1:BD:68:ASN:O	1:BD:202:TRP:NE1	2.40	0.52
2:Bd:93:VAL:HG11	2:Bd:218:VAL:HG13	1.91	0.52
2:Bd:316:ASN:ND2	2:Bd:332:THR:OG1	2.42	0.52
3:Bg:89:ASN:OD1	3:Bh:30:ALA:N	2.41	0.52
1:CC:182:GLU:OE2	1:DC:215:LYS:NZ	2.42	0.52
1:CD:207:ILE:HG22	1:CD:480:ARG:HB2	1.91	0.52
1:CF:355:THR:O	4:Cj:5:ARG:NH2	2.39	0.52
1:DD:188:GLY:O	1:DE:208:GLN:NE2	2.42	0.52
1:EA:374:LEU:HD11	1:EF:400:VAL:HG21	1.91	0.52
5:FC:436:PRO:HG3	6:FQ:236:HIS:HB2	1.91	0.52
5:FE:90:LYS:NZ	5:FE:548:GLU:OE2	2.34	0.52
5:FF:609:SER:OG	5:FF:610:ASP:N	2.42	0.52
5:FH:221:PHE:HB2	5:FH:234:MET:HB3	1.91	0.52
6:FP:212:GLN:HE21	6:FP:216:ARG:HH21	1.55	0.52
7:GG:106:GLU:OE2	7:GH:117:TYR:OH	2.27	0.52
8:IT:237:ALA:O	8:IT:240:ARG:NH2	2.41	0.52
1:AD:300:ASN:ND2	1:AD:492:THR:O	2.42	0.52
1:AE:262:ALA:HB3	1:AE:484:LEU:HD11	1.92	0.52
2:Cb:84:LEU:HD22	2:Cb:225:TRP:HE1	1.74	0.52
3:Dg:36:MET:HB2	3:Dg:48:ALA:HB3	1.92	0.52
1:EC:269:ASN:ND2	1:EC:286:ILE:O	2.36	0.52
5:FA:248:ASP:OD1	5:FL:379:ASN:ND2	2.42	0.52
5:FE:402:TYR:OH	5:FE:592:THR:OG1	2.27	0.52
5:FE:727:ASN:HA	5:FE:730:LYS:HE2	1.91	0.52
5:FG:52:ASP:HB3	5:FG:57:ARG:HB2	1.90	0.52
6:FV:83:LEU:CD1	6:FV:83:LEU:H	2.22	0.52
8:GP:494:ARG:HH22	8:GP:502:LYS:HA	1.73	0.52
2:Ae:119:TYR:O	2:Ae:144:ASN:ND2	2.43	0.52
1:BE:330:LEU:HD11	1:BE:397:ARG:HD3	1.92	0.52
1:CA:466:ASN:HB3	1:CA:469:MET:HG2	1.91	0.52
2:Dd:294:SER:O	1:EA:185:ARG:NH2	2.43	0.52
1:EC:321:ALA:O	1:EC:329:ARG:NH2	2.41	0.52
5:FA:107:VAL:HG22	5:FA:632:VAL:HG22	1.90	0.52
5:FC:223:SER:O	5:FD:327:ASN:ND2	2.42	0.52
5:FC:383:GLU:OE2	5:FC:396:ARG:NH1	2.41	0.52
5:FD:269:ILE:H	5:FD:325:ALA:HA	1.72	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FG:280:ILE:HD13	5:FG:302:THR:HG22	1.91	0.52
6:FS:75:ARG:HA	6:FS:82:ALA:HA	1.91	0.52
6:FS:216:ARG:NH1	6:FS:219:GLU:OE2	2.41	0.52
2:Af:222:ASP:N	2:Af:222:ASP:OD1	2.42	0.52
1:BD:443:ILE:HB	1:BD:447:ASN:HB3	1.91	0.52
1:CA:128:LEU:HD12	1:CA:165:ARG:HD2	1.92	0.52
1:DD:275:GLU:OE2	2:Eb:254:ARG:NH1	2.43	0.52
1:DE:390:ALA:HB3	1:DE:394:VAL:HB	1.91	0.52
1:EA:135:ARG:HB2	1:EA:154:MET:HG2	1.90	0.52
1:EB:135:ARG:NH2	1:EB:152:GLU:OE1	2.41	0.52
1:EC:66:ASP:O	1:ED:34:GLN:NE2	2.42	0.52
5:FI:161:ASP:OD2	5:FI:677:ARG:NH1	2.42	0.52
6:FO:22:LEU:O	7:GA:48:LYS:NZ	2.38	0.52
1:AA:171:ARG:NH2	2:Aa:112:GLU:OE1	2.43	0.52
1:AC:337:GLU:HG2	1:AC:400:VAL:HG11	1.91	0.52
1:AC:472:ASP:O	1:ED:206:ARG:NH2	2.41	0.52
2:Ca:100:LEU:HB2	2:Ca:225:TRP:HZ2	1.74	0.52
2:Df:106:GLN:NE2	2:Df:112:GLU:OE2	2.43	0.52
2:Ea:160:ILE:HD12	2:Ea:187:GLN:HE21	1.74	0.52
5:FB:423:ASN:OD1	5:FC:212:ARG:NH2	2.42	0.52
5:FK:396:ARG:NH2	8:GU:432:THR:OG1	2.43	0.52
7:GH:14:LEU:HA	7:GH:204:ARG:HH12	1.74	0.52
1:AF:438:ILE:HG12	1:AF:488:VAL:HG13	1.90	0.52
1:BE:112:VAL:HG22	1:BE:148:VAL:HG12	1.92	0.52
1:CE:30:GLN:NE2	1:DC:224:ILE:O	2.43	0.52
1:CE:185:ARG:HD3	1:CF:281:LYS:HG2	1.90	0.52
4:Di:26:MET:HG2	4:Di:37:ILE:HD12	1.90	0.52
1:EB:88:ARG:HG2	1:EB:94:VAL:HA	1.91	0.52
1:EC:4:LYS:HG2	1:EC:9:GLN:HB3	1.91	0.52
1:EC:363:SER:OG	1:ED:365:ARG:NH1	2.43	0.52
1:EE:154:MET:HA	1:EF:278:ASN:HD21	1.74	0.52
2:Ea:107:TYR:O	2:Ea:108:ILE:C	2.52	0.52
5:FB:112:PRO:O	5:FB:160:GLN:NE2	2.43	0.52
5:FB:417:GLY:O	5:FB:584:ARG:NH2	2.41	0.52
5:FC:170:LEU:HD22	5:FC:593:ALA:HB1	1.92	0.52
5:FH:80:ARG:HG2	5:FH:81:LEU:H	1.74	0.52
6:FR:29:GLU:HG2	7:GD:124:LEU:HD22	1.90	0.52
6:FW:64:LEU:HG	6:FW:68:LEU:HD13	1.90	0.52
1:BA:88:ARG:HB2	1:BA:110:TYR:HB2	1.92	0.52
1:BC:168:GLN:HB3	3:Bh:60:MET:HE3	1.92	0.52
1:BE:200:ASN:ND2	1:BE:487:CYS:SG	2.82	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CF:320:SER:O	1:CF:329:ARG:NH2	2.42	0.52
1:DB:183:LEU:H	5:FG:297:THR:HG22	1.73	0.52
1:DC:69:GLU:OE2	1:DC:270:ARG:NH2	2.43	0.52
2:Db:281:VAL:HG22	2:Db:305:VAL:HG22	1.90	0.52
2:De:77:LEU:HD11	2:De:237:VAL:HG13	1.92	0.52
5:FE:546:GLN:NE2	5:FE:564:THR:OG1	2.43	0.52
5:FL:222:LYS:HB2	5:FL:233:ASP:HB2	1.91	0.52
6:FM:226:ASN:ND2	6:FM:229:ASP:OD2	2.42	0.52
6:FW:71:ILE:HD12	6:FW:113:THR:HG21	1.92	0.52
7:GI:100:MET:SD	7:GI:154:SER:OG	2.68	0.52
1:AD:116:ASP:HB3	2:Ad:4:SER:HB2	1.92	0.52
1:AD:129:ASN:HD22	1:AE:409:ARG:HE	1.56	0.52
1:AF:425:TYR:HB2	1:AF:497:LEU:HB3	1.91	0.52
1:BB:214:ASN:OD1	1:BB:215:LYS:NZ	2.43	0.52
1:BB:406:ASP:O	1:BB:410:ASN:ND2	2.43	0.52
1:BC:303:TYR:HB2	3:Bg:80:ILE:HB	1.91	0.52
2:Ba:252:GLY:HA3	2:Ba:259:ARG:HH21	1.75	0.52
2:Bb:308:ASP:OD2	2:Bb:312:HIS:ND1	2.40	0.52
1:ED:390:ALA:HB3	1:ED:394:VAL:HB	1.91	0.52
5:FJ:365:VAL:HG11	5:FJ:373:VAL:HB	1.91	0.52
5:FL:163:ARG:NH1	5:FL:625:GLU:OE2	2.43	0.52
6:FX:216:ARG:NH1	6:FX:219:GLU:OE2	2.43	0.52
7:GF:51:ILE:HG21	7:GF:158:ILE:HD11	1.92	0.52
7:GJ:2:THR:HA	7:GJ:184:GLU:HA	1.91	0.52
1:BA:189:ASP:O	1:BA:191:ARG:NH1	2.42	0.52
1:BD:16:TRP:HE1	1:BD:224:ILE:HD11	1.75	0.52
1:CB:374:LEU:HD12	1:CF:392:ASN:HD22	1.74	0.52
1:CE:390:ALA:HB3	1:CE:394:VAL:HB	1.92	0.52
1:EB:323:LYS:HB3	1:EC:44:LEU:HG	1.91	0.52
3:Eg:99:TYR:HB3	3:Eh:102:VAL:HG23	1.92	0.52
5:FD:104:ASP:OD1	5:FD:104:ASP:N	2.39	0.52
5:FE:447:ARG:NH2	6:FS:212:GLN:O	2.37	0.52
5:FE:594:LYS:NZ	5:FE:623:PHE:O	2.40	0.52
5:FK:423:ASN:OD1	5:FL:212:ARG:NH2	2.43	0.52
6:FU:7:TRP:HB3	6:FU:143:LEU:HG	1.92	0.52
6:FW:19:ARG:NH2	6:FX:29:GLU:OE2	2.42	0.52
7:GA:96:ARG:NH2	7:GA:102:PHE:O	2.43	0.52
7:GG:14:LEU:HD23	7:GG:204:ARG:HH11	1.75	0.52
7:GJ:85:LYS:NZ	7:GJ:135:ASP:O	2.43	0.52
1:AA:85:VAL:HG12	1:AA:86:GLU:HG3	1.92	0.52
1:BE:163:ALA:O	1:BE:167:GLN:NE2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:193:THR:OG1	1:DB:229:ASN:OD1	2.25	0.52
1:DD:390:ALA:HB3	1:DD:394:VAL:HB	1.91	0.52
5:FB:116:SER:OG	5:FC:605:GLN:O	2.26	0.52
5:FH:672:LEU:HA	5:FH:675:LYS:HG2	1.91	0.52
5:FJ:378:VAL:HG13	5:FJ:409:SER:HA	1.92	0.52
5:FJ:536:GLU:OE2	5:FK:441:TYR:OH	2.26	0.52
5:FJ:579:ASP:HA	5:FJ:582:LYS:HD3	1.91	0.52
1:AA:263:MET:HG3	1:AA:484:LEU:HD12	1.92	0.51
1:BF:387:GLU:OE1	1:BF:397:ARG:NH1	2.43	0.51
3:Bg:88:CYS:SG	3:Bg:89:ASN:N	2.82	0.51
4:Bj:37:ILE:HD13	4:Bk:26:MET:HB2	1.92	0.51
2:Cf:216:ILE:O	2:Cf:216:ILE:HG13	2.10	0.51
1:EC:120:ASP:OD2	1:ED:281:LYS:NZ	2.43	0.51
5:FF:112:PRO:HG2	5:FG:668:THR:HB	1.91	0.51
5:FG:173:HIS:NE2	5:FG:177:GLU:OE1	2.43	0.51
5:FJ:447:ARG:NH2	5:FK:453:ALA:O	2.43	0.51
5:FL:721:GLU:OE1	5:FL:725:ARG:NH1	2.39	0.51
6:FM:33:GLN:OE1	6:FX:19:ARG:NH1	2.43	0.51
6:FV:152:LYS:HG2	6:FV:187:LYS:HE2	1.92	0.51
8:GR:484:SER:H	8:GR:539:GLN:HE22	1.59	0.51
2:Ab:221:GLU:HB3	4:Ak:1:MET:HE3	1.91	0.51
1:CD:171:ARG:HB2	1:CE:411:LYS:HG2	1.92	0.51
4:Ci:26:MET:HG2	4:Ci:37:ILE:HD12	1.92	0.51
2:Dd:74:ALA:HB1	2:Dd:236:THR:HB	1.92	0.51
2:Dd:105:ARG:HB3	2:Dd:112:GLU:HG3	1.92	0.51
5:FD:600:ARG:HB2	8:GN:436:ASP:HB2	1.92	0.51
7:GF:96:ARG:NH2	7:GF:102:PHE:O	2.43	0.51
7:GH:70:SER:OG	7:GH:71:GLY:N	2.43	0.51
2:Aa:140:SER:O	2:Aa:144:ASN:ND2	2.43	0.51
1:BF:404:TYR:O	1:BF:410:ASN:ND2	2.41	0.51
4:Bi:26:MET:HB2	4:Bk:37:ILE:HG21	1.92	0.51
2:Ca:35:ASP:OD1	2:Ca:35:ASP:N	2.43	0.51
2:Cb:216:ILE:O	2:Cb:216:ILE:HG13	2.10	0.51
1:ED:318:GLU:OE2	2:Ed:101:ARG:NH1	2.43	0.51
2:Ee:6:ASN:ND2	2:Ee:299:GLU:OE1	2.43	0.51
5:FK:653:LEU:HD13	5:FK:663:ILE:HG13	1.90	0.51
6:FN:75:ARG:HD2	6:FN:80:GLY:HA2	1.93	0.51
7:GH:43:ARG:NH1	8:IT:221:TYR:OH	2.43	0.51
7:GH:122:LYS:HA	7:GH:125:ARG:HD2	1.92	0.51
8:IM:228:LEU:HD13	8:IN:226:ARG:HB3	1.92	0.51
1:AC:434:ASP:OD2	5:FA:283:ARG:NH2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ag:50:CYS:HB3	3:Ah:91:LEU:HD23	1.93	0.51
3:Cg:79:ARG:NH1	3:Cg:81:GLU:OE1	2.43	0.51
1:DF:438:ILE:HG23	1:DF:488:VAL:HG22	1.92	0.51
2:Ed:138:ALA:HB1	2:Ed:171:VAL:HG11	1.92	0.51
5:FC:379:ASN:ND2	5:FD:248:ASP:OD1	2.42	0.51
5:FE:383:GLU:OE1	5:FE:398:ARG:NH1	2.43	0.51
5:FJ:362:ASN:ND2	8:GT:514:GLU:OE1	2.43	0.51
5:FK:447:ARG:NH2	5:FL:453:ALA:O	2.44	0.51
6:FQ:8:VAL:HB	6:FQ:12:VAL:HG21	1.90	0.51
7:GA:3:TYR:HB2	7:GA:181:GLU:HA	1.92	0.51
1:AA:112:VAL:HG22	1:AA:148:VAL:HG12	1.92	0.51
1:BC:390:ALA:HB3	1:BC:394:VAL:HB	1.92	0.51
2:Bd:298:SER:OG	1:CA:185:ARG:NH1	2.44	0.51
1:CF:48:ARG:NH1	1:CF:405:ASP:O	2.43	0.51
2:Db:308:ASP:OD2	2:Db:312:HIS:ND1	2.44	0.51
1:EF:425:TYR:HB2	1:EF:497:LEU:HB2	1.93	0.51
5:FA:259:ILE:HD13	5:FL:377:TRP:HB2	1.93	0.51
5:FA:412:HIS:ND1	5:FA:413:PHE:O	2.44	0.51
5:FG:50:ASN:ND2	5:FG:432:ASP:OD1	2.44	0.51
5:FI:468:PRO:HB3	6:FT:197:ILE:HD13	1.93	0.51
8:GM:447:GLY:HA3	8:GM:458:ILE:HD11	1.93	0.51
1:AC:111:LEU:HD21	1:AC:166:LEU:HD22	1.92	0.51
1:AF:63:GLU:HG3	1:AF:442:LYS:HE3	1.92	0.51
2:Bd:251:MET:SD	2:Bd:254:ARG:NH2	2.84	0.51
1:CB:153:LEU:HD11	1:CB:161:VAL:HG23	1.91	0.51
1:CF:228:ARG:NE	1:CF:238:ASP:OD2	2.41	0.51
1:DC:153:LEU:HD11	1:DC:161:VAL:HG13	1.92	0.51
1:DD:122:GLU:OE2	1:DE:258:TYR:OH	2.29	0.51
1:EA:338:ARG:NH2	1:EF:318:GLU:OE1	2.42	0.51
6:FV:83:LEU:HD12	6:FV:83:LEU:H	1.75	0.51
6:FW:19:ARG:HH21	6:FX:30:THR:HA	1.75	0.51
8:GP:497:TYR:O	8:GP:534:ARG:NH1	2.44	0.51
1:AB:56:LEU:HD21	1:AB:264:ALA:HB2	1.93	0.51
1:AF:438:ILE:HG23	1:AF:488:VAL:HG22	1.92	0.51
1:BB:199:ARG:HH22	1:BC:33:PRO:HG3	1.75	0.51
1:BC:440:LYS:HA	1:BC:486:VAL:HG12	1.93	0.51
1:CD:79:ARG:HG2	1:CE:408:VAL:HG11	1.92	0.51
2:Cb:107:TYR:HB2	2:Cb:116:TYR:HB2	1.93	0.51
1:EE:123:VAL:HG23	1:EE:175:GLU:HB2	1.92	0.51
5:FB:719:LYS:HE2	5:FC:718:GLN:HE22	1.75	0.51
5:FG:404:ARG:HH12	5:FG:626:ALA:HB3	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FH:265:MET:HE3	5:FH:322:TYR:CE2	2.46	0.51
5:FI:143:GLU:HA	5:FI:146:ILE:HD12	1.93	0.51
5:FI:267:ASP:OD1	5:FI:267:ASP:N	2.44	0.51
6:FN:23:LEU:HD11	6:FN:159:LYS:HG3	1.93	0.51
6:FU:18:LEU:HD22	6:FU:24:THR:HA	1.93	0.51
7:GA:80:LEU:HB2	7:GA:140:PHE:HB2	1.92	0.51
8:GM:497:TYR:O	8:GM:534:ARG:NH1	2.43	0.51
1:BD:48:ARG:HB2	5:FJ:279:ASN:HD22	1.75	0.51
2:Bb:286:TYR:HE1	2:Bb:302:ILE:HG13	1.76	0.51
2:Bd:1:MET:HG3	2:Bd:203:PRO:HB3	1.93	0.51
3:Bh:40:VAL:HG13	3:Bh:74:LEU:HB3	1.93	0.51
1:CC:335:THR:OG1	1:CC:336:GLY:N	2.44	0.51
1:CC:414:HIS:HD2	1:CC:416:MET:H	1.59	0.51
1:DA:392:ASN:ND2	1:DB:337:GLU:O	2.44	0.51
2:De:93:VAL:HG21	2:De:218:VAL:HG12	1.92	0.51
5:FB:106:LYS:NZ	5:FB:642:GLN:OE1	2.44	0.51
5:FE:163:ARG:NH1	5:FE:625:GLU:OE2	2.44	0.51
5:FK:340:LYS:HE3	5:FK:375:SER:HB3	1.92	0.51
6:FO:7:TRP:HB3	6:FO:143:LEU:HG	1.92	0.51
1:AA:266:GLY:O	1:AA:291:GLY:N	2.43	0.51
1:AE:458:ASN:ND2	1:AE:461:THR:OG1	2.41	0.51
2:Ad:243:ILE:HG13	2:Ad:279:TYR:HB2	1.93	0.51
1:BD:116:ASP:HB3	2:Bd:4:SER:HB3	1.93	0.51
2:Bd:197:TRP:NE1	2:Bd:245:ASP:OD2	2.40	0.51
1:CA:475:SER:OG	1:CA:476:ALA:N	2.41	0.51
2:Cb:157:ILE:HG22	2:Cb:190:ILE:HG23	1.93	0.51
1:DC:304:TYR:OH	1:DC:423:TYR:O	2.27	0.51
1:DC:462:GLY:O	5:FG:389:ASN:ND2	2.39	0.51
1:DE:438:ILE:HG23	1:DE:488:VAL:HG12	1.93	0.51
1:EB:79:ARG:HB3	1:EC:408:VAL:HG11	1.92	0.51
1:EB:301:THR:O	2:Eb:118:LYS:NZ	2.44	0.51
1:EB:327:ASP:N	1:EB:327:ASP:OD1	2.41	0.51
2:Ed:197:TRP:NE1	2:Ed:245:ASP:OD2	2.37	0.51
5:FE:195:GLY:O	5:FE:420:TYR:N	2.41	0.51
5:FG:469:LYS:NZ	6:FS:41:ALA:O	2.43	0.51
5:FH:339:ARG:NH1	8:GR:521:ASP:OD2	2.38	0.51
5:FK:181:PRO:O	5:FK:185:ASN:ND2	2.44	0.51
7:GD:42:GLN:OE1	8:IP:225:ASN:ND2	2.44	0.51
1:AA:380:SER:OG	1:AA:381:ALA:N	2.44	0.51
1:BA:88:ARG:NH2	1:BA:143:GLU:OE1	2.40	0.51
2:Bf:139:ILE:HD11	2:Bf:143:LYS:HE3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:79:ARG:NH1	1:CD:257:GLU:OE2	2.44	0.51
1:DD:409:ARG:O	1:DD:411:LYS:NZ	2.39	0.51
1:EE:406:ASP:O	1:EE:410:ASN:ND2	2.43	0.51
4:Ej:4:LEU:HD11	4:Ek:9:ILE:HD11	1.92	0.51
5:FB:78:PRO:HG2	6:FO:232:TYR:HA	1.91	0.51
5:FJ:191:ALA:HB2	5:FJ:197:GLU:HB2	1.92	0.51
5:FK:110:THR:O	5:FL:172:ASN:ND2	2.43	0.51
5:FK:489:ASP:HB3	5:FK:492:LYS:HG3	1.93	0.51
1:AA:229:ASN:O	1:AA:249:TRP:NE1	2.36	0.50
1:AB:471:PHE:HD1	1:AB:473:GLU:H	1.57	0.50
3:Ag:41:THR:HA	4:Ai:12:ASN:HD21	1.76	0.50
1:BA:323:LYS:NZ	2:Ba:115:GLN:O	2.43	0.50
1:BC:363:SER:O	1:BD:369:LYS:NZ	2.41	0.50
1:BD:207:ILE:HG22	1:BD:480:ARG:HB2	1.93	0.50
1:BE:220:LEU:HB2	1:BE:222:MET:HE2	1.92	0.50
1:CB:389:LYS:NZ	1:CC:368:GLU:OE2	2.44	0.50
1:CD:175:GLU:HG2	1:CE:409:ARG:HH12	1.76	0.50
1:DF:355:THR:HG21	4:Dj:2:LYS:HD2	1.92	0.50
1:EC:292:ILE:HD11	1:EC:438:ILE:HD13	1.92	0.50
2:Ef:218:VAL:HG13	2:Ef:218:VAL:O	2.10	0.50
5:FB:447:ARG:NH2	6:FP:212:GLN:O	2.44	0.50
5:FG:466:LYS:HE2	5:FG:495:THR:HG21	1.93	0.50
6:FQ:3:ASN:ND2	6:FQ:194:GLU:OE2	2.45	0.50
7:FY:96:ARG:NH2	7:FY:105:GLY:O	2.43	0.50
7:GC:51:ILE:HG21	7:GC:158:ILE:HD11	1.93	0.50
7:GH:89:THR:HA	7:GH:159:PHE:HA	1.93	0.50
1:AC:257:GLU:O	1:AC:261:ASN:ND2	2.44	0.50
1:AE:212:ALA:HB3	1:AE:215:LYS:HZ2	1.76	0.50
1:BE:254:GLN:NE2	1:BE:257:GLU:OE1	2.44	0.50
3:Bg:51:LYS:HD2	3:Bh:88:CYS:HA	1.92	0.50
1:CA:111:LEU:HD12	1:CA:151:VAL:HG21	1.94	0.50
1:CA:195:PRO:HD2	1:CB:224:ILE:HD12	1.92	0.50
1:DB:359:LEU:HA	1:DC:361:ASN:HB2	1.93	0.50
1:DE:458:ASN:ND2	1:DE:461:THR:OG1	2.44	0.50
1:DE:469:MET:O	1:EB:470:SER:OG	2.26	0.50
2:Da:119:TYR:O	2:Da:144:ASN:ND2	2.42	0.50
1:EC:52:LEU:HD11	1:EC:265:TRP:HE1	1.77	0.50
1:EC:69:GLU:HG2	1:EC:200:ASN:O	2.10	0.50
1:EE:279:PHE:HA	1:EE:285:ALA:HA	1.92	0.50
2:Ea:251:MET:SD	2:Ea:254:ARG:NH2	2.83	0.50
5:FG:447:ARG:NH2	6:FU:212:GLN:O	2.38	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FG:507:LEU:HD11	5:FH:499:SER:HB3	1.92	0.50
6:FN:46:ASN:O	6:FO:114:GLN:NE2	2.44	0.50
8:GO:503:THR:HG22	8:GO:505:ALA:H	1.76	0.50
1:AC:174:ILE:O	1:AD:409:ARG:NH2	2.44	0.50
1:AC:425:TYR:HB2	1:AC:497:LEU:HB3	1.92	0.50
1:AD:481:MET:SD	1:BC:457:ARG:NH2	2.85	0.50
1:BB:273:ASN:ND2	1:BB:275:GLU:OE2	2.44	0.50
1:BC:216:LEU:HD12	1:BC:457:ARG:HB3	1.91	0.50
1:BC:256:ASP:O	1:BC:260:ASN:ND2	2.42	0.50
1:BC:406:ASP:O	1:BC:410:ASN:ND2	2.45	0.50
1:CA:190:VAL:HG11	1:CB:250:GLU:HB3	1.93	0.50
1:DD:224:ILE:HG21	3:Dg:87:PRO:HG2	1.92	0.50
1:EE:490:ASP:OD2	1:EE:492:THR:OG1	2.27	0.50
5:FA:82:GLN:NE2	6:FN:236:HIS:OXT	2.44	0.50
6:FP:67:ASP:OD1	6:FP:67:ASP:N	2.36	0.50
6:FV:3:ASN:ND2	6:FV:194:GLU:OE2	2.45	0.50
7:GA:60:CYS:SG	7:GA:171:PRO:HD2	2.51	0.50
7:GJ:11:LEU:HD11	7:GJ:25:PRO:HG3	1.92	0.50
1:BD:392:ASN:H	1:BE:384:GLN:HE22	1.59	0.50
1:BE:23:ASN:OD1	2:Cb:259:ARG:NH2	2.44	0.50
1:CA:435:GLN:NE2	1:CB:40:MET:O	2.44	0.50
2:Ca:107:TYR:HD1	2:Ca:207:ILE:HD13	1.75	0.50
1:DA:377:ASN:ND2	1:DF:365:ARG:O	2.44	0.50
1:DB:69:GLU:OE2	1:DB:270:ARG:NH2	2.45	0.50
5:FI:417:GLY:O	5:FI:584:ARG:NH2	2.43	0.50
5:FL:469:LYS:NZ	6:FX:41:ALA:O	2.43	0.50
6:FM:7:TRP:HB3	6:FM:143:LEU:HG	1.94	0.50
6:FQ:7:TRP:HB3	6:FQ:143:LEU:HG	1.94	0.50
6:FQ:216:ARG:NH1	6:FQ:219:GLU:OE2	2.45	0.50
6:FR:34:TYR:HD2	6:FR:158:ILE:HG23	1.76	0.50
6:FS:29:GLU:HG2	7:GE:124:LEU:HD22	1.93	0.50
7:GA:113:ASP:OD1	7:GA:116:ARG:NH1	2.42	0.50
8:GV:462:VAL:O	8:GV:462:VAL:CG1	2.59	0.50
1:AB:363:SER:OG	1:AC:365:ARG:NH1	2.44	0.50
1:AD:76:GLY:HA2	1:AE:43:LEU:HD13	1.93	0.50
2:Aa:278:VAL:HG23	2:Aa:308:ASP:HB3	1.94	0.50
1:BD:118:PHE:HA	1:BD:191:ARG:HH21	1.76	0.50
1:BE:24:HIS:NE2	2:Cb:3:ILE:O	2.44	0.50
1:BE:276:TYR:HB2	1:BE:285:ALA:HB1	1.93	0.50
2:Bb:216:ILE:O	2:Bb:216:ILE:CG1	2.59	0.50
2:Ce:1:MET:HB3	2:Ce:203:PRO:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:195:PRO:HD2	1:DB:224:ILE:HD12	1.94	0.50
1:EE:94:VAL:HG13	1:EE:94:VAL:O	2.11	0.50
2:Ea:110:LEU:O	2:Ea:110:LEU:HG	2.10	0.50
2:Eb:11:LEU:O	2:Eb:254:ARG:NH2	2.37	0.50
2:Eb:221:GLU:OE1	2:Eb:221:GLU:N	2.44	0.50
2:Eb:281:VAL:HG22	2:Eb:305:VAL:HG12	1.93	0.50
5:FA:10:GLN:OE1	5:FA:335:TRP:NE1	2.43	0.50
5:FB:98:GLU:OE1	5:FB:185:ASN:ND2	2.44	0.50
5:FB:724:ILE:HD12	5:FB:727:ASN:HB2	1.93	0.50
8:GS:447:GLY:HA3	8:GS:458:ILE:HD11	1.94	0.50
1:AA:62:ARG:HH22	1:AB:38:ASN:HB3	1.77	0.50
1:AA:400:VAL:O	1:AB:373:ARG:NH2	2.45	0.50
1:AB:297:GLU:OE2	1:AB:424:ARG:NH2	2.45	0.50
1:AB:490:ASP:HB3	1:AB:493:ARG:HG3	1.94	0.50
1:AD:453:GLN:HA	1:BC:469:MET:HB2	1.94	0.50
1:AF:219:LYS:HG3	1:AF:241:ASN:HD22	1.77	0.50
1:CD:317:TYR:OH	1:CD:392:ASN:ND2	2.39	0.50
2:Cd:119:TYR:O	2:Cd:144:ASN:ND2	2.39	0.50
1:EE:182:GLU:O	1:EF:284:ASN:ND2	2.40	0.50
1:EE:425:TYR:HB2	1:EE:497:LEU:HB2	1.94	0.50
3:Eg:79:ARG:NH1	3:Eg:81:GLU:OE1	2.44	0.50
5:FJ:29:ALA:HB2	5:FJ:333:LEU:HD22	1.93	0.50
6:FX:29:GLU:HG2	7:GJ:124:LEU:HD22	1.93	0.50
7:GC:37:SER:OG	7:GC:160:GLU:O	2.30	0.50
2:Ab:202:MET:HE1	1:EE:4:LYS:HG2	1.92	0.50
1:BC:428:TRP:HA	1:BC:494:THR:HG23	1.93	0.50
2:Ba:42:TYR:HE2	2:Ba:44:GLN:HE21	1.59	0.50
1:CA:363:SER:O	1:CB:369:LYS:NZ	2.42	0.50
1:CB:79:ARG:NH1	2:Cb:113:GLU:OE2	2.42	0.50
1:DA:22:ASP:OD1	1:DA:22:ASP:N	2.42	0.50
1:DA:134:PHE:HB3	1:DA:151:VAL:HG13	1.94	0.50
1:DD:175:GLU:HG2	1:DE:409:ARG:HH12	1.77	0.50
1:DF:125:VAL:HG12	1:DF:133:PRO:HA	1.93	0.50
2:De:197:TRP:NE1	2:De:245:ASP:OD2	2.39	0.50
1:EC:56:LEU:HD13	1:EC:263:MET:HE2	1.94	0.50
1:EE:229:ASN:O	1:EE:249:TRP:NE1	2.35	0.50
2:Eb:108:ILE:HG22	2:Eb:108:ILE:O	2.11	0.50
5:FG:447:ARG:NH2	5:FH:453:ALA:O	2.45	0.50
5:FI:22:ARG:NH2	8:GS:517:GLU:OE1	2.40	0.50
5:FK:111:ASN:ND2	5:FL:607:ILE:O	2.44	0.50
7:FY:115:MET:HE2	7:FY:141:LYS:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:79:ARG:HH21	2:Ab:189:ILE:HD12	1.77	0.50
2:Ae:281:VAL:HG22	2:Ae:305:VAL:HG12	1.92	0.50
1:CB:472:ASP:OD1	1:CB:472:ASP:N	2.45	0.50
2:Cd:309:ASP:N	2:Cd:309:ASP:OD1	2.45	0.50
1:DA:435:GLN:NE2	1:DB:40:MET:O	2.38	0.50
1:EB:171:ARG:HB2	1:EC:411:LYS:HD3	1.92	0.50
2:Ea:158:TYR:HB3	2:Ea:168:ASP:HB3	1.92	0.50
2:Ef:79:ARG:NH1	2:Ef:234:THR:OG1	2.44	0.50
5:FC:41:ARG:O	5:FC:426:ARG:NH1	2.43	0.50
5:FC:727:ASN:HA	5:FC:730:LYS:HE2	1.94	0.50
5:FI:344:VAL:HG12	5:FI:373:VAL:HG23	1.93	0.50
5:FI:720:GLU:HB3	5:FJ:718:GLN:HE21	1.76	0.50
6:FP:4:ASN:ND2	6:FQ:115:GLY:O	2.44	0.50
6:FQ:12:VAL:HG22	7:GD:120:TYR:HB3	1.94	0.50
7:GH:96:ARG:NH2	7:GH:102:PHE:O	2.45	0.50
7:GJ:100:MET:SD	7:GJ:154:SER:OG	2.69	0.50
1:AB:190:VAL:HG21	1:AC:251:VAL:HG22	1.94	0.50
1:AD:186:LYS:HB2	1:AE:208:GLN:HG2	1.94	0.50
1:AE:56:LEU:HD11	1:AE:264:ALA:HB2	1.94	0.50
2:Ba:100:LEU:HB2	2:Ba:225:TRP:HZ2	1.77	0.50
1:CA:211:VAL:HG11	1:CA:244:MET:HE1	1.94	0.50
2:Cb:105:ARG:CZ	2:Cb:105:ARG:HB2	2.42	0.50
1:DC:335:THR:OG1	1:DC:336:GLY:N	2.43	0.50
1:EB:74:VAL:HG22	1:EC:41:VAL:HB	1.93	0.50
2:Ee:162:ALA:HB3	2:Ee:184:ASP:HB2	1.94	0.50
5:FD:665:LYS:O	5:FD:669:SER:OG	2.29	0.50
5:FH:343:LYS:HE2	5:FH:376:PHE:HE2	1.77	0.50
6:FN:1:MET:HG3	6:FN:195:PHE:HA	1.94	0.50
1:AE:453:GLN:HB3	1:AE:477:VAL:HG22	1.93	0.49
1:AF:339:GLY:O	1:AF:425:TYR:OH	2.29	0.49
2:Ab:140:SER:O	2:Ab:144:ASN:ND2	2.40	0.49
1:BF:366:VAL:HG23	1:BF:383:PHE:HB3	1.94	0.49
1:CC:80:ARG:NH2	1:CC:115:GLU:OE1	2.44	0.49
2:Cd:110:LEU:HD21	1:DC:15:HIS:ND1	2.27	0.49
1:EB:366:VAL:HG23	1:EB:383:PHE:HB3	1.94	0.49
5:FA:600:ARG:NH1	5:FL:354:GLU:O	2.45	0.49
5:FD:712:LYS:HA	5:FD:715:GLU:HG2	1.92	0.49
5:FH:721:GLU:OE1	5:FH:725:ARG:NH1	2.45	0.49
5:FL:112:PRO:O	5:FL:160:GLN:NE2	2.45	0.49
6:FN:29:GLU:HG2	7:FZ:124:LEU:HD22	1.93	0.49
7:GC:39:LEU:HD21	7:GC:194:PRO:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:GD:51:ILE:HG21	7:GD:158:ILE:HD11	1.93	0.49
7:GD:106:GLU:OE2	7:GE:117:TYR:OH	2.29	0.49
1:AB:271:ASN:HD22	1:AB:275:GLU:HB2	1.77	0.49
1:AF:56:LEU:HD21	1:AF:264:ALA:HB2	1.94	0.49
1:AF:475:SER:OG	1:AF:476:ALA:N	2.46	0.49
2:Ab:10:GLN:NE2	1:ED:283:GLY:O	2.45	0.49
2:Ab:252:GLY:HA3	2:Ab:259:ARG:HH21	1.75	0.49
1:BA:205:ILE:HD12	1:BA:258:TYR:HB3	1.93	0.49
1:BD:79:ARG:HB3	1:BE:408:VAL:HG21	1.93	0.49
1:BE:310:LYS:HE2	2:Be:99:ILE:HD12	1.94	0.49
1:CB:174:ILE:HG21	1:CB:191:ARG:HH22	1.77	0.49
1:CD:79:ARG:O	2:Cd:111:SER:HB3	2.12	0.49
1:CE:205:ILE:HD11	1:CE:259:LYS:HG3	1.94	0.49
1:CF:300:ASN:HB3	1:CF:495:MET:HG3	1.95	0.49
2:Ce:309:ASP:OD1	2:Ce:309:ASP:N	2.40	0.49
3:Ch:59:GLU:HG3	3:Ch:77:VAL:HG21	1.93	0.49
1:DC:120:ASP:OD2	1:DD:281:LYS:NZ	2.40	0.49
1:DC:479:HIS:ND1	5:FG:291:MET:SD	2.85	0.49
1:DD:186:LYS:HD3	1:DE:479:HIS:HE1	1.76	0.49
1:EB:471:PHE:HD1	1:EB:473:GLU:H	1.60	0.49
1:ED:88:ARG:HB2	1:ED:110:TYR:HB2	1.95	0.49
5:FD:35:PHE:CE2	5:FD:37:TYR:HB3	2.47	0.49
5:FF:683:GLU:HG3	5:FG:660:PHE:HB2	1.94	0.49
6:FV:7:TRP:HB3	6:FV:143:LEU:HG	1.92	0.49
7:FZ:206:PRO:HA	7:FZ:209:SER:HB2	1.94	0.49
7:GG:39:LEU:HD21	7:GG:194:PRO:HB2	1.93	0.49
1:BD:317:TYR:O	1:BD:321:ALA:N	2.44	0.49
1:BD:415:PRO:HA	3:Bh:67:ILE:HG12	1.95	0.49
2:Ba:1:MET:HE2	2:Ba:203:PRO:HB3	1.94	0.49
2:Bd:99:ILE:HG12	2:Bd:121:GLU:HG3	1.94	0.49
1:DB:366:VAL:HG23	1:DB:367:VAL:HG23	1.95	0.49
1:DD:304:TYR:OH	1:DD:423:TYR:O	2.30	0.49
1:DE:181:LYS:HD2	1:DF:287:LYS:HD2	1.94	0.49
1:EA:144:GLY:HA2	2:Ea:281:VAL:HG11	1.93	0.49
6:FN:94:PRO:O	6:FN:94:PRO:HG2	2.12	0.49
6:FP:74:VAL:HG22	6:FP:129:ILE:HG12	1.94	0.49
6:FT:174:PRO:HG3	8:IQ:239:GLN:HB3	1.94	0.49
6:FU:76:LEU:HD12	6:FU:81:ILE:HB	1.95	0.49
7:FY:80:LEU:HB2	7:FY:140:PHE:HB2	1.94	0.49
8:GS:497:TYR:O	8:GS:534:ARG:NH1	2.45	0.49
1:AC:13:PHE:HB2	2:Ed:110:LEU:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:143:GLU:HG3	1:AE:146:ASN:HB2	1.95	0.49
2:Ad:197:TRP:NE1	2:Ad:245:ASP:OD2	2.40	0.49
1:DA:244:MET:HA	1:DA:247:VAL:HG22	1.94	0.49
1:DB:292:ILE:HG13	1:DB:486:VAL:HG11	1.94	0.49
1:DC:414:HIS:HD2	1:DC:416:MET:H	1.60	0.49
1:DE:112:VAL:HG22	1:DE:148:VAL:HG22	1.95	0.49
1:DE:231:GLU:HG3	1:DE:253:LEU:HD13	1.94	0.49
1:EB:335:THR:OG1	1:EB:336:GLY:N	2.45	0.49
5:FJ:62:ASP:OD2	5:FJ:439:TYR:OH	2.30	0.49
6:FO:23:LEU:HD11	6:FO:159:LYS:HG3	1.94	0.49
6:FV:6:ASN:ND2	6:FV:146:ASP:OD2	2.42	0.49
6:FW:28:LEU:HD21	6:FW:141:LEU:HD11	1.93	0.49
7:FY:117:TYR:OH	7:GJ:106:GLU:OE1	2.30	0.49
7:GB:100:MET:SD	7:GB:154:SER:OG	2.70	0.49
7:GF:43:ARG:NH1	8:IR:221:TYR:OH	2.44	0.49
8:GV:462:VAL:O	8:GV:467:ALA:HA	2.13	0.49
8:IQ:233:MET:HA	8:IQ:236:VAL:HG22	1.94	0.49
1:CA:220:LEU:HD12	1:CA:226:MET:HE3	1.93	0.49
1:CB:135:ARG:NH2	1:CC:279:PHE:O	2.45	0.49
2:De:11:LEU:O	2:De:254:ARG:NH2	2.37	0.49
1:EB:450:ARG:HG3	1:EB:480:ARG:HG2	1.93	0.49
1:ED:273:ASN:ND2	1:ED:275:GLU:OE2	2.45	0.49
2:Ea:158:TYR:HB2	2:Ea:189:ILE:HB	1.95	0.49
2:Eb:157:ILE:HG22	2:Eb:190:ILE:HG23	1.93	0.49
2:Eb:249:PHE:O	2:Eb:259:ARG:NH2	2.45	0.49
2:Ee:281:VAL:HG22	2:Ee:305:VAL:HG12	1.95	0.49
5:FA:505:GLY:O	5:FA:509:ASN:HB2	2.12	0.49
5:FC:98:GLU:OE1	5:FC:185:ASN:ND2	2.45	0.49
5:FF:161:ASP:OD2	5:FF:677:ARG:NH1	2.46	0.49
6:FM:64:LEU:HG	6:FM:68:LEU:HD13	1.93	0.49
6:FT:199:SER:OG	6:FT:200:VAL:N	2.44	0.49
7:GB:109:TYR:HA	7:GB:130:CYS:HB2	1.92	0.49
7:GJ:107:ILE:HG23	7:GJ:128:ILE:HB	1.93	0.49
1:AA:88:ARG:NH2	1:AA:143:GLU:OE1	2.46	0.49
1:AB:323:LYS:HB3	1:AC:44:LEU:HG	1.95	0.49
1:AC:254:GLN:NE2	1:AC:257:GLU:OE1	2.45	0.49
2:Ab:256:ASP:OD1	2:Ab:256:ASP:N	2.44	0.49
2:Bd:52:VAL:HG12	1:CB:277:MET:HG2	1.94	0.49
2:De:118:LYS:NZ	2:De:150:GLU:OE1	2.45	0.49
1:EF:450:ARG:NH1	1:EF:452:TYR:OH	2.46	0.49
5:FA:75:ALA:HA	5:FA:80:ARG:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FB:202:ASP:OD1	8:GL:433:GLN:NE2	2.45	0.49
5:FK:459:ILE:HB	5:FK:515:ILE:HB	1.94	0.49
6:FM:68:LEU:HD21	6:FM:71:ILE:HG13	1.93	0.49
6:FW:29:GLU:HG2	7:GI:124:LEU:HD22	1.94	0.49
8:GU:492:ASP:N	8:GU:492:ASP:OD1	2.42	0.49
2:Ad:107:TYR:CD1	2:Ad:107:TYR:O	2.66	0.49
1:BD:122:GLU:OE2	1:BE:258:TYR:OH	2.27	0.49
1:CA:85:VAL:HG12	1:CA:86:GLU:HG2	1.94	0.49
1:DD:400:VAL:O	1:DE:373:ARG:NH2	2.46	0.49
2:Dd:57:ILE:HD11	2:Dd:302:ILE:HD12	1.94	0.49
1:EE:257:GLU:O	1:EE:261:ASN:ND2	2.46	0.49
2:Ed:243:ILE:HG21	2:Ed:305:VAL:HG21	1.95	0.49
4:Ej:2:LYS:HE3	4:Ek:9:ILE:HD12	1.95	0.49
5:FB:87:MET:HE2	5:FB:438:ASN:HD22	1.78	0.49
5:FC:207:GLU:HG3	5:FC:601:ASN:HD21	1.77	0.49
6:FN:216:ARG:NH1	6:FN:226:ASN:O	2.46	0.49
6:FU:83:LEU:HD22	6:FU:109:PRO:HB2	1.94	0.49
8:GQ:518:ARG:HB2	8:GQ:521:ASP:HB2	1.95	0.49
8:GV:459:GLN:HE21	8:GV:459:GLN:C	2.20	0.49
1:AF:228:ARG:NE	1:AF:238:ASP:OD2	2.39	0.49
1:BA:48:ARG:NE	1:BA:405:ASP:OD2	2.46	0.49
1:BD:144:GLY:HA3	2:Bd:73:LEU:HD21	1.95	0.49
1:CF:301:THR:O	2:Cf:118:LYS:NZ	2.45	0.49
2:Cb:142:ALA:HB2	2:Cb:157:ILE:HD11	1.95	0.49
2:Ce:153:PRO:O	2:Ce:195:GLN:NE2	2.46	0.49
1:DE:400:VAL:HG21	1:DF:374:LEU:HD21	1.93	0.49
5:FE:734:ALA:O	5:FE:737:GLN:NE2	2.45	0.49
6:FX:135:MET:HG2	6:FX:143:LEU:HD23	1.95	0.49
3:Ag:89:ASN:N	3:Ag:89:ASN:OD1	2.46	0.49
1:BA:124:ILE:HD11	1:BA:136:ILE:HD11	1.95	0.49
1:DB:304:TYR:OH	1:DB:423:TYR:O	2.30	0.49
1:DD:454:TRP:HD1	1:EC:468:TYR:HD1	1.61	0.49
1:EB:472:ASP:OD1	1:EB:472:ASP:N	2.45	0.49
1:ED:304:TYR:OH	1:ED:423:TYR:O	2.31	0.49
5:FB:222:LYS:HB2	5:FB:233:ASP:HB2	1.95	0.49
5:FB:731:ILE:HD11	5:FC:729:THR:HB	1.95	0.49
5:FC:406:ASN:ND2	5:FD:207:GLU:OE2	2.44	0.49
5:FE:330:VAL:HG22	5:FE:387:ILE:HG23	1.95	0.49
5:FI:676:GLN:HE22	5:FJ:668:THR:HG21	1.77	0.49
5:FK:662:THR:OG1	5:FK:682:ASP:OD2	2.25	0.49
6:FQ:64:LEU:HG	6:FQ:68:LEU:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FZ:115:MET:HE3	7:FZ:141:LYS:HB3	1.94	0.49
7:GF:101:ASP:HB2	7:GG:69:ILE:HG12	1.95	0.49
1:CB:144:GLY:HA2	2:Cb:281:VAL:HG11	1.95	0.49
3:Cg:57:GLN:HG2	3:Ch:89:ASN:HD21	1.78	0.49
1:DA:338:ARG:NH2	1:DF:318:GLU:OE1	2.39	0.49
1:DC:157:ASN:OD1	2:Dd:148:LYS:NZ	2.44	0.49
1:DD:210:LYS:O	1:DD:217:ASN:ND2	2.46	0.49
1:DF:229:ASN:O	1:DF:249:TRP:NE1	2.37	0.49
2:Da:285:HIS:NE2	2:Da:299:GLU:OE1	2.45	0.49
1:EE:205:ILE:HD11	1:EE:259:LYS:HG3	1.94	0.49
5:FD:354:GLU:O	5:FE:600:ARG:NH1	2.46	0.49
5:FF:536:GLU:OE2	5:FG:441:TYR:OH	2.24	0.49
5:FG:63:LEU:HD23	5:FG:63:LEU:N	2.27	0.49
5:FG:672:LEU:HA	5:FG:675:LYS:HG2	1.93	0.49
5:FH:192:MET:HG2	5:FH:574:LEU:HD21	1.94	0.49
5:FH:620:GLY:C	5:FH:622:GLU:N	2.65	0.49
5:FH:720:GLU:O	5:FI:725:ARG:NH1	2.43	0.49
7:GF:3:TYR:HB2	7:GF:181:GLU:HA	1.94	0.49
1:AD:309:LEU:HD11	1:AD:347:VAL:HG22	1.95	0.48
2:Ad:256:ASP:HB3	1:BB:270:ARG:HH12	1.77	0.48
1:CB:503:GLN:NE2	2:Cb:143:LYS:O	2.46	0.48
1:CC:363:SER:OG	1:CD:365:ARG:NH1	2.44	0.48
1:CC:425:TYR:HB2	1:CC:497:LEU:HB3	1.95	0.48
1:CD:301:THR:O	2:Cd:118:LYS:NZ	2.42	0.48
1:DC:122:GLU:OE2	1:DD:258:TYR:OH	2.28	0.48
1:DE:224:ILE:O	1:EC:30:GLN:NE2	2.38	0.48
2:Db:6:ASN:ND2	2:Db:299:GLU:OE1	2.46	0.48
1:EA:71:TYR:HB3	1:EA:199:ARG:HG2	1.93	0.48
1:EC:479:HIS:NE2	5:FD:294:ASP:OD2	2.43	0.48
2:Ea:100:LEU:HB2	2:Ea:225:TRP:HZ2	1.77	0.48
5:FC:22:ARG:HB3	5:FC:395:MET:HB3	1.95	0.48
5:FC:252:ASP:OD1	5:FC:252:ASP:N	2.47	0.48
5:FD:424:ASP:OD2	5:FE:214:ASN:ND2	2.46	0.48
5:FJ:112:PRO:HG2	5:FK:668:THR:HB	1.95	0.48
5:FK:82:GLN:NE2	6:FX:236:HIS:OXT	2.46	0.48
6:FW:147:ASN:HD21	6:FW:194:GLU:HG2	1.77	0.48
1:BA:270:ARG:HE	1:BA:274:GLY:HA2	1.78	0.48
1:CE:210:LYS:HB2	1:CE:477:VAL:HG22	1.94	0.48
1:DA:165:ARG:NH1	1:DA:170:GLU:OE2	2.47	0.48
1:DA:479:HIS:HE1	1:DF:186:LYS:HD3	1.78	0.48
1:DD:300:ASN:ND2	1:DD:492:THR:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:80:ARG:HH11	2:Eb:110:LEU:HB3	1.78	0.48
2:Ef:145:LEU:HD22	2:Ef:154:LEU:HD23	1.94	0.48
5:FE:352:GLY:HA2	8:GP:460:ILE:O	2.13	0.48
5:FH:583:LYS:NZ	5:FH:587:GLU:OE2	2.45	0.48
5:FH:663:ILE:HA	5:FH:666:LEU:HD12	1.95	0.48
5:FH:720:GLU:HA	5:FI:725:ARG:HH22	1.77	0.48
5:FI:221:PHE:HE2	5:FI:236:ILE:HD12	1.78	0.48
5:FJ:245:ARG:HA	5:FJ:248:ASP:HB2	1.95	0.48
5:FK:29:ALA:O	5:FK:33:THR:OG1	2.28	0.48
5:FK:609:SER:OG	5:FK:610:ASP:N	2.46	0.48
6:FT:18:LEU:HD22	6:FT:24:THR:HA	1.94	0.48
7:GE:85:LYS:NZ	7:GE:135:ASP:O	2.47	0.48
7:GE:115:MET:HE3	7:GE:141:LYS:HB2	1.94	0.48
7:GF:161:ASP:HB3	7:GF:164:GLU:HB2	1.95	0.48
1:AC:122:GLU:OE2	1:AD:258:TYR:OH	2.31	0.48
1:AF:419:VAL:HG12	1:AF:421:PHE:H	1.76	0.48
1:AF:448:GLU:OE2	1:AF:480:ARG:NE	2.45	0.48
2:Ab:184:ASP:N	2:Ab:184:ASP:OD1	2.45	0.48
1:BE:433:MET:HG2	1:BE:435:GLN:HB3	1.94	0.48
1:CB:329:ARG:NH2	1:CC:337:GLU:OE2	2.38	0.48
1:CD:321:ALA:O	1:CE:48:ARG:NH2	2.42	0.48
2:Cd:87:ASP:OD2	2:Cd:223:ARG:NH2	2.44	0.48
2:Cf:79:ARG:NH1	2:Cf:234:THR:OG1	2.46	0.48
2:Dd:201:MET:HB3	1:EC:11:LEU:HD23	1.96	0.48
2:Df:146:GLU:OE1	2:Df:172:THR:OG1	2.30	0.48
5:FA:460:LEU:HB2	5:FA:514:MET:HE3	1.95	0.48
5:FD:536:GLU:OE2	5:FE:441:TYR:OH	2.28	0.48
6:FO:64:LEU:HG	6:FO:68:LEU:HD13	1.94	0.48
6:FP:224:PHE:HD1	6:FP:227:LEU:HD13	1.78	0.48
7:GJ:39:LEU:HD21	7:GJ:194:PRO:HB2	1.95	0.48
1:AC:414:HIS:HD2	1:AC:416:MET:H	1.60	0.48
1:BA:362:ASN:O	1:BA:365:ARG:NH1	2.46	0.48
2:Bb:252:GLY:HA3	2:Bb:259:ARG:HH21	1.78	0.48
2:Bd:13:VAL:HG11	2:Bd:272:LEU:HB2	1.95	0.48
1:CA:137:LEU:HD11	1:CA:152:GLU:HB3	1.94	0.48
1:CA:259:LYS:NZ	1:CA:448:GLU:OE2	2.46	0.48
1:CB:442:LYS:NZ	1:CB:443:ILE:O	2.46	0.48
1:CF:390:ALA:HB3	1:CF:394:VAL:HB	1.95	0.48
2:Cd:63:LEU:HB2	2:Cd:285:HIS:HD2	1.79	0.48
4:Ci:8:LYS:HD2	4:Ci:14:PRO:HB3	1.95	0.48
1:DB:425:TYR:HB2	1:DB:497:LEU:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:360:ASP:OD1	1:EC:360:ASP:N	2.46	0.48
1:ED:171:ARG:HB2	1:EE:411:LYS:HG2	1.95	0.48
2:Ea:79:ARG:NH1	2:Ea:191:GLU:OE1	2.46	0.48
2:Eb:1:MET:HB3	2:Eb:203:PRO:HB3	1.95	0.48
5:FC:22:ARG:NH2	8:GM:517:GLU:OE1	2.46	0.48
5:FF:383:GLU:OE2	5:FF:396:ARG:NH1	2.47	0.48
5:FI:6:ASN:O	5:FI:28:TRP:NE1	2.45	0.48
6:FW:152:LYS:NZ	6:FW:155:GLU:OE2	2.38	0.48
7:GG:42:GLN:OE1	8:IS:225:ASN:ND2	2.46	0.48
7:GH:37:SER:OG	7:GH:160:GLU:O	2.29	0.48
8:GU:463:ASP:OD1	8:GU:463:ASP:N	2.45	0.48
1:AA:302:MET:HE1	1:AA:495:MET:HE2	1.94	0.48
1:AC:296:THR:HG23	1:AC:297:GLU:HG3	1.95	0.48
2:Ad:110:LEU:HD13	2:Ad:110:LEU:N	2.28	0.48
3:Ah:35:VAL:HG12	3:Ah:49:MET:HG3	1.95	0.48
1:BA:175:GLU:OE2	1:BB:409:ARG:NH2	2.46	0.48
1:BA:229:ASN:O	1:BA:249:TRP:NE1	2.39	0.48
1:BA:295:GLN:HG2	1:BA:488:VAL:HB	1.93	0.48
1:BC:72:TRP:HB3	1:BD:36:ALA:HB3	1.95	0.48
1:BE:22:ASP:HB3	2:Cb:257:ILE:HD13	1.95	0.48
2:Bb:108:ILE:HG22	2:Bb:108:ILE:O	2.14	0.48
1:CA:25:LEU:HD12	1:CA:28:ILE:HD11	1.96	0.48
2:Cd:112:GLU:OE1	2:Cd:112:GLU:N	2.46	0.48
1:DA:438:ILE:HG23	1:DA:488:VAL:HG22	1.96	0.48
2:Ef:223:ARG:HH11	2:Ef:223:ARG:CG	2.27	0.48
5:FB:161:ASP:OD2	5:FB:677:ARG:NH1	2.39	0.48
5:FF:6:ASN:OD1	5:FF:6:ASN:N	2.45	0.48
5:FI:708:GLN:O	5:FI:711:GLN:NE2	2.46	0.48
7:GE:35:TYR:OH	7:GE:202:GLU:OE1	2.25	0.48
1:AC:467:PRO:O	1:ED:454:TRP:NE1	2.46	0.48
1:AD:140:ALA:HB1	1:AD:147:ALA:HB1	1.94	0.48
2:Bf:198:VAL:H	2:Bf:202:MET:HB2	1.79	0.48
1:CE:262:ALA:HB3	1:CE:484:LEU:HD11	1.96	0.48
1:DA:22:ASP:O	1:DA:23:ASN:C	2.55	0.48
1:DA:129:ASN:HB2	1:DB:409:ARG:NH2	2.28	0.48
1:DC:185:ARG:NH2	2:Eb:296:GLN:O	2.43	0.48
1:DD:52:LEU:HB3	1:DD:56:LEU:HD23	1.94	0.48
1:EA:79:ARG:O	2:Ea:111:SER:HB3	2.13	0.48
1:EC:88:ARG:HG3	1:EC:94:VAL:HA	1.96	0.48
1:EC:116:ASP:OD1	1:EC:149:TYR:OH	2.29	0.48
2:Ed:42:TYR:HE2	2:Ed:44:GLN:HE21	1.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FG:197:GLU:OE1	5:FG:420:TYR:OH	2.25	0.48
5:FG:734:ALA:O	5:FG:737:GLN:NE2	2.46	0.48
5:FI:31:GLN:NE2	5:FI:322:TYR:OH	2.45	0.48
5:FJ:627:ASP:HA	5:FK:603:LYS:HE3	1.96	0.48
5:FL:383:GLU:OE1	5:FL:396:ARG:NH1	2.45	0.48
6:FR:8:VAL:HB	6:FR:12:VAL:HG21	1.95	0.48
7:GH:100:MET:SD	7:GH:154:SER:OG	2.69	0.48
8:GV:475:GLU:HG2	8:GV:484:SER:HA	1.95	0.48
1:AD:81:ASN:N	1:AD:81:ASN:OD1	2.46	0.48
1:BB:227:VAL:HG12	1:BB:237:LYS:HA	1.96	0.48
1:BD:112:VAL:HG22	1:BD:148:VAL:HG22	1.95	0.48
1:CA:411:LYS:HD2	1:CF:81:ASN:HD22	1.78	0.48
1:CD:300:ASN:ND2	1:CD:492:THR:O	2.47	0.48
1:CE:457:ARG:NH1	1:DB:449:TYR:OH	2.46	0.48
2:De:101:ARG:HE	2:De:212:GLN:HE21	1.60	0.48
1:EA:56:LEU:HD12	1:EA:260:ASN:HD22	1.79	0.48
1:EC:449:TYR:HB3	1:EC:481:MET:H	1.79	0.48
5:FB:223:SER:O	5:FC:327:ASN:ND2	2.35	0.48
5:FC:396:ARG:HE	8:GM:432:THR:HG21	1.78	0.48
5:FE:712:LYS:O	5:FE:716:LEU:N	2.47	0.48
6:FR:84:ARG:HG3	6:FR:85:ALA:H	1.79	0.48
6:FT:12:VAL:HG22	7:GG:120:TYR:HB3	1.95	0.48
6:FU:54:THR:OG1	6:FV:93:TYR:OH	2.30	0.48
7:GF:50:GLN:NE2	7:GG:91:MET:SD	2.87	0.48
1:AA:251:VAL:HG11	1:AA:478:ILE:HD11	1.95	0.48
2:Ab:221:GLU:HB3	4:Ak:1:MET:CE	2.44	0.48
2:Bb:57:ILE:HD11	2:Bb:302:ILE:HD12	1.94	0.48
2:Be:158:TYR:HB3	2:Be:168:ASP:HB2	1.95	0.48
1:CA:319:LEU:O	1:CA:323:LYS:N	2.46	0.48
2:Cf:79:ARG:NH2	2:Cf:168:ASP:OD2	2.47	0.48
3:Cg:50:CYS:HB3	3:Ch:91:LEU:HD23	1.95	0.48
1:DD:62:ARG:HH22	1:DE:38:ASN:HB3	1.78	0.48
1:DD:283:GLY:HA3	2:Eb:8:VAL:HG11	1.95	0.48
1:DE:66:ASP:OD1	1:DE:66:ASP:N	2.45	0.48
1:EA:135:ARG:NH1	1:EA:152:GLU:OE2	2.46	0.48
1:ED:77:SER:OG	1:ED:78:SER:N	2.46	0.48
1:EE:78:SER:O	1:EE:78:SER:OG	2.32	0.48
5:FD:265:MET:HE1	5:FD:328:LEU:HD21	1.96	0.48
5:FF:447:ARG:NH2	5:FG:453:ALA:O	2.47	0.48
5:FH:330:VAL:HG22	5:FH:387:ILE:HG12	1.95	0.48
5:FH:380:GLU:OE1	5:FH:382:TRP:NE1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FI:406:ASN:HD22	5:FJ:206:GLY:HA3	1.78	0.48
5:FI:619:ASP:OD1	5:FI:619:ASP:N	2.44	0.48
5:FK:365:VAL:HG21	5:FK:373:VAL:HB	1.96	0.48
1:AD:342:GLN:OE1	1:AD:425:TYR:OH	2.27	0.48
1:BB:242:MET:HE3	1:BB:245:HIS:HB2	1.96	0.48
1:BB:380:SER:OG	1:BB:381:ALA:N	2.46	0.48
1:CB:304:TYR:OH	1:CB:423:TYR:O	2.30	0.48
1:CD:80:ARG:HD2	2:Cd:110:LEU:HG	1.95	0.48
1:CE:18:GLY:O	1:DC:209:HIS:NE2	2.44	0.48
1:DC:75:ILE:HG21	1:DD:40:MET:HE3	1.96	0.48
1:DE:21:SER:OG	1:DE:22:ASP:N	2.46	0.48
1:DF:62:ARG:HH21	1:DF:436:PRO:HD2	1.79	0.48
1:DF:409:ARG:O	1:DF:411:LYS:NZ	2.36	0.48
2:De:99:ILE:HG12	2:De:121:GLU:HG3	1.95	0.48
1:ED:144:GLY:HA2	2:Ed:281:VAL:HG11	1.96	0.48
5:FB:50:ASN:ND2	5:FB:432:ASP:OD1	2.46	0.48
5:FG:693:ALA:HA	5:FG:696:GLU:HG2	1.95	0.48
7:GJ:109:TYR:HA	7:GJ:130:CYS:HB2	1.96	0.48
8:GK:484:SER:H	8:GK:539:GLN:HE22	1.61	0.48
1:AA:338:ARG:NH2	1:AF:318:GLU:OE1	2.47	0.48
1:AE:184:SER:OG	1:AF:206:ARG:NH1	2.46	0.48
1:BC:80:ARG:NH2	1:BC:115:GLU:OE1	2.44	0.48
2:Cd:104:PHE:HB2	2:Cd:116:TYR:HB3	1.94	0.48
1:DF:48:ARG:NH1	1:DF:405:ASP:O	2.47	0.48
1:EB:71:TYR:HE2	1:EC:35:LYS:HE3	1.79	0.48
1:ED:404:TYR:OH	1:ED:426:ASP:OD2	2.26	0.48
5:FF:402:TYR:OH	5:FF:592:THR:OG1	2.30	0.48
5:FH:41:ARG:O	5:FH:426:ARG:NH1	2.47	0.48
5:FI:147:LYS:HA	5:FI:150:LYS:HG2	1.96	0.48
7:GC:132:LYS:HE2	7:GC:136:GLY:HA2	1.96	0.48
1:AA:438:ILE:HD13	1:AA:488:VAL:HG22	1.96	0.47
1:AD:9:GLN:NE2	3:Ag:89:ASN:O	2.47	0.47
1:AD:197:SER:OG	2:Bb:265:ASN:OD1	2.29	0.47
1:AF:48:ARG:NH1	1:AF:405:ASP:O	2.46	0.47
4:Ai:2:LYS:HD2	4:Aj:9:ILE:HD12	1.96	0.47
1:BA:319:LEU:O	1:BA:323:LYS:N	2.45	0.47
1:BC:414:HIS:CD2	1:BC:416:MET:H	2.32	0.47
2:Cb:140:SER:O	2:Cb:144:ASN:ND2	2.40	0.47
2:Ce:158:TYR:HB2	2:Ce:189:ILE:HB	1.96	0.47
2:Ce:281:VAL:HG22	2:Ce:305:VAL:HG12	1.95	0.47
1:DD:317:TYR:O	1:DD:321:ALA:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Db:99:ILE:HG12	2:Db:121:GLU:HG2	1.96	0.47
2:Db:278:VAL:HG23	2:Db:308:ASP:HB3	1.95	0.47
1:EA:272:LEU:HD11	2:Ea:151:SER:HA	1.96	0.47
1:EB:180:GLU:OE2	1:EC:282:SER:OG	2.30	0.47
1:ED:47:TYR:HB2	1:ED:407:PRO:HG2	1.95	0.47
5:FC:87:MET:HE1	5:FC:431:VAL:HG13	1.96	0.47
5:FI:489:ASP:HB3	5:FI:492:LYS:HG3	1.96	0.47
6:FS:208:ASN:ND2	6:FS:228:GLY:O	2.45	0.47
7:FZ:109:TYR:HA	7:FZ:130:CYS:HB2	1.96	0.47
8:GN:492:ASP:OD2	8:GN:545:ARG:NH1	2.47	0.47
8:GS:475:GLU:HG2	8:GS:484:SER:HA	1.96	0.47
8:GT:475:GLU:HG2	8:GT:485:ASP:H	1.78	0.47
1:AE:4:LYS:HD2	2:Bb:196:PRO:HG2	1.95	0.47
1:BD:199:ARG:HH22	1:BE:33:PRO:HG3	1.79	0.47
1:BD:210:LYS:HD3	1:BD:477:VAL:HG22	1.96	0.47
1:BD:359:LEU:HA	1:BE:361:ASN:HB2	1.94	0.47
1:BE:406:ASP:O	1:BE:410:ASN:ND2	2.46	0.47
1:CA:389:LYS:HB2	1:CB:382:GLY:HA3	1.96	0.47
1:CA:489:LEU:HD11	1:CB:39:LEU:HB3	1.95	0.47
1:EA:326:MET:HE1	1:EB:400:VAL:HG21	1.96	0.47
1:ED:189:ASP:O	1:ED:191:ARG:NH1	2.48	0.47
2:Ed:57:ILE:HD11	2:Ed:302:ILE:HD12	1.96	0.47
5:FA:125:GLU:OE1	5:FA:618:ILE:HG23	2.14	0.47
5:FG:400:ILE:HG23	5:FG:595:VAL:HG21	1.97	0.47
6:FP:66:CYS:HB3	6:FP:116:ARG:HH12	1.78	0.47
6:FQ:174:PRO:HG3	8:IN:239:GLN:HB3	1.97	0.47
6:FW:68:LEU:HD21	6:FW:71:ILE:HG13	1.96	0.47
7:GA:104:GLN:NE2	7:GB:75:GLU:O	2.40	0.47
7:GB:42:GLN:OE1	8:IN:225:ASN:ND2	2.47	0.47
1:AA:229:ASN:ND2	1:AA:250:GLU:OE2	2.48	0.47
1:AD:122:GLU:OE2	1:AE:258:TYR:OH	2.28	0.47
2:Bb:216:ILE:O	2:Bb:216:ILE:HG13	2.14	0.47
1:CA:338:ARG:NH2	1:CF:318:GLU:OE1	2.37	0.47
1:CC:79:ARG:NH2	1:CD:406:ASP:OD2	2.48	0.47
1:CD:310:LYS:NZ	2:Cd:97:ASN:O	2.48	0.47
1:DD:66:ASP:OD1	1:DD:66:ASP:N	2.46	0.47
2:Db:30:ILE:HD11	2:Db:43:PHE:HB3	1.96	0.47
1:EA:400:VAL:HG21	1:EB:374:LEU:HD11	1.97	0.47
1:EB:207:ILE:HG22	1:EB:480:ARG:HB2	1.95	0.47
1:EC:61:THR:CB	5:FD:269:ILE:HG22	2.44	0.47
5:FA:221:PHE:HE2	5:FA:236:ILE:HD12	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FK:412:HIS:ND1	5:FK:413:PHE:O	2.40	0.47
7:GD:35:TYR:OH	7:GD:202:GLU:OE1	2.22	0.47
1:AA:122:GLU:OE2	1:AB:258:TYR:OH	2.29	0.47
1:AD:304:TYR:OH	1:AD:423:TYR:O	2.33	0.47
1:AF:323:LYS:HB2	1:AF:324:LEU:HD12	1.97	0.47
3:Ag:33:LEU:HD23	3:Ag:51:LYS:HB3	1.96	0.47
1:BA:35:LYS:NZ	1:BF:73:ASP:OD2	2.48	0.47
1:BB:301:THR:O	2:Bb:118:LYS:NZ	2.37	0.47
1:BB:489:LEU:HD21	1:BC:39:LEU:HD22	1.96	0.47
1:BD:252:GLU:OE1	1:BD:480:ARG:NH1	2.47	0.47
3:Bg:51:LYS:NZ	3:Bh:84:ILE:O	2.47	0.47
1:CA:266:GLY:O	1:CA:291:GLY:N	2.40	0.47
1:CB:112:VAL:HG12	1:CB:148:VAL:HG22	1.96	0.47
1:DB:490:ASP:HB3	1:DB:493:ARG:HG3	1.96	0.47
2:Dd:105:ARG:O	2:Dd:112:GLU:HA	2.13	0.47
1:ED:207:ILE:HG22	1:ED:480:ARG:HB2	1.97	0.47
5:FD:97:GLU:OE2	5:FD:547:ARG:NH1	2.34	0.47
5:FD:98:GLU:OE1	5:FD:185:ASN:ND2	2.44	0.47
5:FE:694:GLN:OE1	5:FE:695:LYS:NZ	2.47	0.47
5:FG:65:LEU:O	6:FU:232:TYR:HB2	2.15	0.47
5:FI:377:TRP:HB2	5:FJ:259:ILE:HD13	1.95	0.47
6:FO:174:PRO:HG3	8:IL:239:GLN:HB3	1.96	0.47
6:FX:12:VAL:HG22	7:FY:120:TYR:HB3	1.97	0.47
7:GF:63:LEU:HD12	7:GF:150:LEU:HB3	1.96	0.47
7:GG:36:ARG:NH1	7:GG:186:PRO:O	2.39	0.47
1:AC:303:TYR:HB2	3:Ag:80:ILE:HB	1.96	0.47
1:AC:329:ARG:NH1	1:AC:392:ASN:O	2.47	0.47
1:AC:400:VAL:HB	1:AD:373:ARG:HH22	1.79	0.47
1:AD:301:THR:HG22	1:AD:496:SER:HB2	1.96	0.47
4:Aj:19:VAL:HG11	4:Aj:26:MET:HE3	1.96	0.47
1:BC:453:GLN:HE21	1:BC:479:HIS:HE1	1.61	0.47
1:BD:47:TYR:HB2	1:BD:407:PRO:HG2	1.97	0.47
1:CC:363:SER:O	1:CD:369:LYS:NZ	2.44	0.47
1:CF:21:SER:OG	1:CF:22:ASP:N	2.46	0.47
1:DD:443:ILE:HB	1:DD:447:ASN:HB3	1.95	0.47
1:DF:53:ASP:OD1	1:DF:260:ASN:ND2	2.47	0.47
2:Dd:162:ALA:HB3	2:Dd:184:ASP:HB2	1.96	0.47
1:ED:43:LEU:O	1:ED:48:ARG:NH2	2.47	0.47
1:EF:335:THR:OG1	1:EF:336:GLY:N	2.47	0.47
2:Ea:244:ALA:HA	2:Ea:273:VAL:HG11	1.96	0.47
3:Eh:32:GLN:OE1	3:Eh:82:GLN:NE2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FG:221:PHE:HB2	5:FG:234:MET:HB3	1.95	0.47
5:FK:570:ILE:HG12	5:FL:93:VAL:HG22	1.96	0.47
6:FS:199:SER:HB3	6:FS:202:GLU:HG3	1.97	0.47
6:FT:20:HIS:HB3	6:FT:23:LEU:HD12	1.96	0.47
7:FZ:43:ARG:NH2	8:IL:225:ASN:OD1	2.47	0.47
1:BE:310:LYS:HA	1:BE:313:GLU:HG2	1.95	0.47
2:Bf:89:SER:OG	2:Bf:91:THR:O	2.32	0.47
1:CD:269:ASN:OD1	1:CD:269:ASN:N	2.47	0.47
1:DD:264:ALA:HA	1:DD:292:ILE:HG13	1.97	0.47
1:DD:380:SER:OG	1:DD:381:ALA:N	2.48	0.47
1:DF:55:PHE:O	1:DF:58:SER:OG	2.33	0.47
2:Db:107:TYR:CE2	2:Db:108:ILE:HG12	2.50	0.47
1:EA:224:ILE:HD12	1:EF:195:PRO:HD2	1.96	0.47
1:ED:252:GLU:OE2	1:ED:480:ARG:NH1	2.47	0.47
4:Ek:30:ASN:ND2	4:Ek:35:GLU:OE1	2.47	0.47
5:FA:570:ILE:HG12	5:FB:93:VAL:HG22	1.96	0.47
6:FM:122:ILE:HD12	6:FM:125:GLU:HB2	1.96	0.47
6:FP:44:LEU:HD22	6:FP:195:PHE:HB2	1.97	0.47
6:FT:68:LEU:HD21	6:FT:71:ILE:HG13	1.96	0.47
7:GC:50:GLN:NE2	7:GD:91:MET:SD	2.87	0.47
7:GC:218:LYS:NZ	7:GC:223:ASP:OD2	2.46	0.47
1:AC:330:LEU:HD11	1:AC:397:ARG:HG3	1.96	0.47
1:BB:270:ARG:NH2	1:BB:276:TYR:OH	2.48	0.47
1:BC:81:ASN:HD22	1:BD:411:LYS:HG2	1.78	0.47
1:BF:205:ILE:HD12	1:BF:258:TYR:HB3	1.96	0.47
2:Bd:201:MET:HB3	1:CC:11:LEU:HD23	1.97	0.47
2:Bf:120:GLY:HA3	2:Bf:141:LEU:HD23	1.97	0.47
3:Bh:35:VAL:HG22	3:Bh:49:MET:HG3	1.97	0.47
1:CB:366:VAL:HG23	1:CB:383:PHE:HB3	1.97	0.47
1:DA:144:GLY:HA2	2:Da:281:VAL:HG11	1.97	0.47
1:DA:376:SER:H	1:DE:395:ARG:NH2	2.12	0.47
1:DB:183:LEU:O	1:DC:282:SER:OG	2.26	0.47
1:DB:390:ALA:HB3	1:DB:394:VAL:HB	1.96	0.47
1:DC:311:LEU:HD13	3:Dg:79:ARG:HB2	1.95	0.47
1:DD:43:LEU:O	1:DD:48:ARG:NH2	2.48	0.47
2:Db:198:VAL:H	2:Db:202:MET:HB3	1.79	0.47
1:EA:244:MET:HA	1:EA:247:VAL:HG12	1.97	0.47
1:EB:122:GLU:OE2	1:EC:258:TYR:OH	2.26	0.47
1:EC:331:PHE:HE1	1:EC:430:ILE:HG23	1.79	0.47
1:ED:144:GLY:HA3	2:Ed:73:LEU:HD11	1.95	0.47
1:EF:137:LEU:HD21	1:EF:152:GLU:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Eb:79:ARG:NH1	2:Eb:234:THR:OG1	2.48	0.47
2:Ed:100:LEU:HD22	2:Ed:141:LEU:HD11	1.96	0.47
4:Ei:4:LEU:HB2	4:Ej:7:LEU:HB2	1.97	0.47
5:FA:58:LEU:HB2	5:FA:83:HIS:HB2	1.97	0.47
5:FA:163:ARG:NH2	5:FA:621:ASP:OD1	2.48	0.47
5:FC:579:ASP:HA	5:FC:582:LYS:HD3	1.96	0.47
5:FD:292:ILE:H	5:FD:310:LEU:HD21	1.78	0.47
5:FD:719:LYS:HE2	5:FE:718:GLN:HE22	1.80	0.47
5:FE:657:THR:HA	5:FE:686:ILE:HD13	1.96	0.47
5:FF:217:LYS:NZ	5:FF:239:ASP:OD1	2.38	0.47
5:FG:459:ILE:HB	5:FG:515:ILE:HB	1.96	0.47
6:FU:160:LYS:HD2	6:FU:181:GLN:HG2	1.96	0.47
7:GD:36:ARG:HG3	7:GD:187:ILE:HD12	1.96	0.47
7:GD:86:VAL:HG23	7:GD:132:LYS:HD2	1.97	0.47
2:Ad:101:ARG:HE	2:Ad:212:GLN:HB2	1.79	0.47
1:BD:186:LYS:HB2	1:BE:208:GLN:HG2	1.97	0.47
2:Bb:79:ARG:NH2	2:Bb:168:ASP:OD2	2.46	0.47
1:CE:116:ASP:OD1	1:CE:149:TYR:OH	2.31	0.47
2:Cf:100:LEU:HD21	2:Cf:211:PRO:HB3	1.96	0.47
4:Ci:1:MET:HB3	4:Ci:1:MET:HE2	1.77	0.47
1:EE:67:ASP:OD1	1:EE:67:ASP:N	2.44	0.47
5:FA:497:GLY:HA3	5:FA:503:LEU:HG	1.97	0.47
5:FB:498:ALA:HB1	5:FB:505:GLY:HA2	1.97	0.47
5:FD:291:MET:HA	5:FD:310:LEU:HD21	1.97	0.47
5:FE:196:GLU:HG2	5:FE:419:ILE:HD12	1.97	0.47
5:FL:272:GLY:HA2	5:FL:305:PHE:CE1	2.50	0.47
6:FN:83:LEU:HD22	6:FN:109:PRO:HB2	1.97	0.47
6:FO:216:ARG:NH1	6:FO:226:ASN:O	2.47	0.47
6:FS:199:SER:OG	6:FS:200:VAL:N	2.48	0.47
6:FT:75:ARG:HA	6:FT:82:ALA:HA	1.96	0.47
6:FV:174:PRO:HG3	8:IS:239:GLN:HG2	1.96	0.47
7:GC:36:ARG:NH2	7:GC:159:PHE:O	2.45	0.47
1:AA:392:ASN:ND2	1:AB:337:GLU:O	2.48	0.47
1:AB:116:ASP:OD1	1:AB:149:TYR:OH	2.32	0.47
1:AC:390:ALA:HB3	1:AC:394:VAL:HB	1.97	0.47
1:AD:59:PHE:O	1:AD:440:LYS:NZ	2.48	0.47
1:BA:382:GLY:HA3	1:BF:389:LYS:HB2	1.95	0.47
1:BB:81:ASN:OD1	2:Bb:112:GLU:HG3	2.15	0.47
1:BD:363:SER:OG	1:BE:361:ASN:ND2	2.42	0.47
1:BE:182:GLU:OE1	1:BF:284:ASN:ND2	2.47	0.47
1:BE:212:ALA:HB3	1:BE:215:LYS:HZ2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:122:GLU:OE2	1:CF:258:TYR:OH	2.30	0.47
1:CF:90:GLU:HB2	1:CF:108:PRO:O	2.15	0.47
2:Cb:107:TYR:CB	2:Cb:116:TYR:HB2	2.45	0.47
3:Cg:79:ARG:NH2	3:Cg:95:GLN:OE1	2.48	0.47
1:EB:62:ARG:NH1	1:EB:63:GLU:O	2.47	0.47
1:EF:215:LYS:HA	1:EF:218:LYS:HB2	1.97	0.47
1:EF:475:SER:OG	1:EF:476:ALA:N	2.47	0.47
2:Ea:215:THR:HB	2:Ea:222:ASP:HB3	1.97	0.47
5:FB:537:MET:HE2	5:FB:537:MET:HB3	1.79	0.47
5:FI:459:ILE:HB	5:FI:515:ILE:HB	1.97	0.47
6:FO:84:ARG:HG3	6:FO:85:ALA:H	1.80	0.47
7:GE:32:LEU:HD23	7:GE:199:VAL:HG21	1.96	0.47
8:GS:472:GLU:HG3	8:GS:474:GLY:H	1.79	0.47
1:AA:91:ASN:OD1	1:AA:91:ASN:N	2.44	0.47
1:AA:140:ALA:HB1	1:AA:147:ALA:HB1	1.96	0.47
2:Ab:197:TRP:NE1	2:Ab:245:ASP:OD2	2.42	0.47
2:Ab:223:ARG:O	2:Ab:224:LEU:C	2.54	0.47
1:BB:171:ARG:HB2	1:BC:411:LYS:HD3	1.97	0.47
1:BD:253:LEU:HD13	5:FJ:269:ILE:HG21	1.96	0.47
1:BF:77:SER:OG	1:BF:78:SER:N	2.48	0.47
1:CC:305:ASN:ND2	3:Cg:59:GLU:OE1	2.46	0.47
3:Ch:36:MET:HG2	3:Ch:80:ILE:HG12	1.97	0.47
1:DA:186:LYS:HB2	1:DB:208:GLN:HG2	1.97	0.47
1:DA:382:GLY:HA3	1:DF:389:LYS:HB2	1.97	0.47
2:Dd:79:ARG:NH1	2:Dd:234:THR:OG1	2.48	0.47
1:EA:329:ARG:NH1	1:EA:392:ASN:O	2.47	0.47
2:Ea:11:LEU:HD22	2:Ea:247:GLU:HG3	1.96	0.47
2:Ea:206:PHE:HZ	2:Ea:237:VAL:HG11	1.80	0.47
2:Ee:184:ASP:OD1	2:Ee:184:ASP:N	2.47	0.47
5:FH:676:GLN:HE22	5:FI:668:THR:HG21	1.80	0.47
5:FJ:196:GLU:HG2	5:FJ:419:ILE:HD12	1.97	0.47
5:FJ:354:GLU:OE1	8:GU:429:TRP:NE1	2.39	0.47
6:FM:8:VAL:HG23	6:FM:144:ILE:HG13	1.97	0.47
6:FU:8:VAL:HB	6:FU:12:VAL:HG21	1.97	0.47
7:GA:46:ASP:N	7:GA:46:ASP:OD1	2.46	0.47
7:GC:3:TYR:HB2	7:GC:181:GLU:HA	1.96	0.47
8:GT:477:VAL:HG22	8:GT:482:VAL:HG22	1.96	0.47
1:AD:433:MET:HG2	1:AD:435:GLN:HG3	1.97	0.46
2:Ad:140:SER:HA	2:Ad:143:LYS:HE2	1.97	0.46
2:Ae:97:ASN:ND2	2:Ae:121:GLU:OE2	2.42	0.46
1:BB:80:ARG:HD2	2:Bb:110:LEU:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Be:99:ILE:HB	2:Be:214:LEU:HD12	1.96	0.46
1:CC:220:LEU:HD21	1:CC:243:TRP:HB2	1.97	0.46
4:Cj:15:ASP:N	4:Cj:15:ASP:OD1	2.48	0.46
1:DB:424:ARG:NE	1:DB:426:ASP:OD2	2.43	0.46
1:DC:406:ASP:O	1:DC:410:ASN:ND2	2.48	0.46
5:FA:97:GLU:OE2	5:FA:547:ARG:NH1	2.36	0.46
5:FA:168:ASN:ND2	5:FA:670:SER:O	2.43	0.46
5:FA:536:GLU:OE2	5:FB:441:TYR:OH	2.31	0.46
5:FF:221:PHE:HB2	5:FF:234:MET:HB3	1.97	0.46
7:GH:36:ARG:HG3	7:GH:187:ILE:HD12	1.96	0.46
1:AA:406:ASP:OD1	1:AF:79:ARG:NH1	2.42	0.46
1:AC:360:ASP:OD1	1:AC:360:ASP:N	2.48	0.46
1:AE:8:PHE:CZ	1:BB:270:ARG:HD2	2.51	0.46
1:BB:244:MET:HE2	1:BB:459:PRO:HB2	1.98	0.46
1:BE:74:VAL:HA	1:BF:41:VAL:HG23	1.98	0.46
2:Bb:162:ALA:HB3	2:Bb:184:ASP:HB2	1.97	0.46
1:CA:81:ASN:HB3	1:CA:171:ARG:HB3	1.97	0.46
2:Cd:1:MET:HE2	2:Cd:1:MET:HB3	1.86	0.46
1:DD:448:GLU:HG2	1:DD:482:ALA:HB2	1.97	0.46
1:DE:335:THR:OG1	1:DE:336:GLY:N	2.48	0.46
2:Da:215:THR:HB	2:Da:222:ASP:HB2	1.96	0.46
1:EA:118:PHE:HA	1:EA:191:ARG:HH21	1.80	0.46
1:EE:132:TYR:HA	1:EE:157:ASN:HD21	1.80	0.46
1:EF:455:GLY:O	1:EF:466:ASN:ND2	2.34	0.46
2:Ea:24:LEU:HD21	2:Ea:31:VAL:HG13	1.96	0.46
5:FA:622:GLU:H	5:FA:622:GLU:HG2	1.45	0.46
5:FA:668:THR:HB	5:FL:112:PRO:HG2	1.97	0.46
5:FA:684:LYS:HA	5:FA:687:ARG:HG2	1.97	0.46
5:FD:253:VAL:O	5:FD:253:VAL:CG2	2.60	0.46
5:FF:406:ASN:HD22	5:FG:206:GLY:HA3	1.80	0.46
5:FF:459:ILE:HB	5:FF:515:ILE:HB	1.96	0.46
5:FF:489:ASP:HB3	5:FF:492:LYS:HG3	1.95	0.46
5:FG:282:GLU:H	5:FG:282:GLU:HG2	1.49	0.46
5:FH:41:ARG:HD2	5:FH:220:ILE:HD12	1.98	0.46
5:FH:99:SER:OG	5:FH:185:ASN:ND2	2.49	0.46
5:FI:725:ARG:O	5:FI:729:THR:OG1	2.24	0.46
6:FM:67:ASP:OD1	6:FM:67:ASP:N	2.41	0.46
1:AD:175:GLU:HG2	1:AE:409:ARG:HH12	1.81	0.46
2:Aa:158:TYR:HB3	2:Aa:168:ASP:HB2	1.96	0.46
2:Ae:154:LEU:HA	2:Ae:207:ILE:HD11	1.97	0.46
1:BE:193:THR:OG1	1:BF:229:ASN:OD1	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BE:296:THR:HG22	1:BE:488:VAL:HG11	1.97	0.46
1:CD:2:ALA:N	3:Cg:96:VAL:O	2.48	0.46
1:CD:304:TYR:OH	1:CD:423:TYR:O	2.32	0.46
1:DA:182:GLU:O	1:DB:284:ASN:ND2	2.48	0.46
1:DC:317:TYR:OH	1:DC:392:ASN:ND2	2.42	0.46
1:DF:320:SER:O	1:DF:329:ARG:NH2	2.47	0.46
2:Db:100:LEU:HB2	2:Db:225:TRP:HZ3	1.80	0.46
2:Ed:158:TYR:HB2	2:Ed:189:ILE:HB	1.97	0.46
2:Ee:153:PRO:O	2:Ee:195:GLN:NE2	2.44	0.46
5:FC:618:ILE:HD13	5:FC:618:ILE:H	1.77	0.46
5:FE:113:ASN:ND2	5:FF:674:GLU:OE2	2.47	0.46
5:FE:570:ILE:HG12	5:FF:93:VAL:HG22	1.97	0.46
5:FG:60:MET:SD	5:FG:63:LEU:HD21	2.55	0.46
5:FG:712:LYS:NZ	5:FG:713:GLU:OE1	2.48	0.46
5:FJ:219:ARG:NH1	5:FJ:238:GLU:OE1	2.44	0.46
6:FN:156:LEU:HB3	6:FN:184:TYR:HB2	1.97	0.46
6:FX:83:LEU:HD22	6:FX:109:PRO:HB2	1.97	0.46
7:GA:11:LEU:HD11	7:GA:25:PRO:HG3	1.97	0.46
7:GB:121:ASN:HB3	7:GB:124:LEU:HD12	1.97	0.46
2:Aa:260:GLY:HA2	2:Aa:266:ILE:HG21	1.97	0.46
2:Ad:255:GLY:HA2	1:BB:275:GLU:HA	1.97	0.46
2:Ae:63:LEU:N	2:Ae:285:HIS:O	2.49	0.46
1:CD:66:ASP:OD1	1:CE:34:GLN:NE2	2.49	0.46
1:CE:102:VAL:HG21	1:CE:166:LEU:HD12	1.96	0.46
1:CF:335:THR:OG1	1:CF:336:GLY:N	2.49	0.46
2:Ca:198:VAL:H	2:Ca:202:MET:HB3	1.79	0.46
2:Ce:197:TRP:NE1	2:Ce:245:ASP:OD2	2.38	0.46
1:DC:303:TYR:HB2	3:Dg:80:ILE:HB	1.96	0.46
1:DD:125:VAL:HB	1:DD:129:ASN:HA	1.97	0.46
1:EC:335:THR:OG1	1:EC:336:GLY:N	2.47	0.46
2:Ea:93:VAL:HG11	2:Ea:218:VAL:HG12	1.97	0.46
5:FA:267:ASP:HB2	5:FA:271:GLN:HB2	1.96	0.46
5:FA:277:MET:O	5:FA:279:ASN:ND2	2.49	0.46
5:FC:423:ASN:OD1	5:FD:212:ARG:NH2	2.48	0.46
5:FC:720:GLU:HA	5:FD:725:ARG:HH22	1.79	0.46
5:FD:543:ILE:HG23	5:FD:547:ARG:HD2	1.96	0.46
5:FE:221:PHE:HB2	5:FE:234:MET:HB3	1.97	0.46
5:FK:715:GLU:O	5:FK:719:LYS:NZ	2.39	0.46
5:FL:330:VAL:HG22	5:FL:387:ILE:HG12	1.96	0.46
5:FL:497:GLY:HA3	5:FL:503:LEU:HG	1.98	0.46
6:FW:75:ARG:HD2	6:FW:80:GLY:HA2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:GU:521:ASP:HB3	8:GU:524:SER:HB2	1.97	0.46
1:AA:489:LEU:HD11	1:AB:39:LEU:HD22	1.98	0.46
1:AB:191:ARG:HG3	1:EE:17:LYS:HA	1.97	0.46
1:AD:88:ARG:HB2	1:AD:110:TYR:HB2	1.96	0.46
1:BA:186:LYS:HB2	1:BB:208:GLN:HG2	1.97	0.46
1:BA:201:GLU:HG2	1:BA:202:TRP:H	1.80	0.46
1:BD:387:GLU:OE2	1:BD:397:ARG:NH1	2.48	0.46
1:BD:402:PRO:HB2	5:FJ:278:ASP:HB2	1.97	0.46
1:BE:10:MET:HE1	2:Bd:268:LYS:H	1.80	0.46
2:Bd:152:THR:OG1	2:Bd:195:GLN:OE1	2.34	0.46
1:CB:359:LEU:HA	1:CC:361:ASN:HB2	1.97	0.46
2:Cd:79:ARG:HH21	2:Cd:189:ILE:HD13	1.80	0.46
3:Cg:88:CYS:SG	3:Cg:89:ASN:N	2.86	0.46
1:DA:175:GLU:OE2	1:DB:409:ARG:NH1	2.48	0.46
1:DB:327:ASP:OD1	1:DB:327:ASP:N	2.49	0.46
1:EA:363:SER:OG	1:EB:361:ASN:ND2	2.48	0.46
2:Ed:1:MET:HB3	2:Ed:245:ASP:HB3	1.97	0.46
5:FA:170:LEU:HD22	5:FA:593:ALA:HB1	1.98	0.46
5:FC:412:HIS:ND1	5:FC:413:PHE:O	2.49	0.46
5:FC:720:GLU:O	5:FD:725:ARG:NH1	2.44	0.46
5:FD:718:GLN:HA	5:FD:721:GLU:HG3	1.96	0.46
5:FF:197:GLU:OE1	5:FF:420:TYR:OH	2.26	0.46
5:FL:489:ASP:HB3	5:FL:492:LYS:HG3	1.98	0.46
6:FQ:19:ARG:NH2	6:FR:29:GLU:OE2	2.49	0.46
6:FX:56:ASP:OD1	6:FX:56:ASP:N	2.44	0.46
7:GD:37:SER:OG	7:GD:160:GLU:O	2.34	0.46
8:GM:494:ARG:NH2	8:GM:501:GLY:O	2.48	0.46
1:AB:191:ARG:HD2	1:EE:17:LYS:HG3	1.98	0.46
1:AF:216:LEU:HD12	1:AF:459:PRO:HA	1.97	0.46
2:Bd:308:ASP:OD2	2:Bd:312:HIS:ND1	2.47	0.46
1:CA:329:ARG:NH2	1:CB:337:GLU:OE2	2.39	0.46
2:Cd:251:MET:SD	2:Cd:254:ARG:NH2	2.89	0.46
1:DF:111:LEU:HD12	1:DF:151:VAL:HG21	1.97	0.46
1:EC:181:LYS:HD3	1:ED:287:LYS:HD2	1.96	0.46
1:ED:323:LYS:HB3	1:EE:44:LEU:HG	1.97	0.46
1:ED:341:ILE:HA	1:ED:344:HIS:HB3	1.98	0.46
1:EE:309:LEU:HD22	1:EE:347:VAL:HA	1.98	0.46
1:EF:80:ARG:HD2	2:Ef:110:LEU:HD12	1.97	0.46
5:FC:114:ALA:HA	5:FD:609:SER:HB3	1.97	0.46
5:FD:544:SER:OG	5:FD:545:LYS:N	2.48	0.46
5:FE:436:PRO:HG3	6:FS:236:HIS:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FH:720:GLU:HB3	5:FI:718:GLN:HE21	1.80	0.46
5:FK:134:ILE:HA	5:FK:137:THR:HG22	1.97	0.46
5:FL:265:MET:HE3	5:FL:265:MET:HB2	1.84	0.46
5:FL:436:PRO:HG3	6:FN:236:HIS:HB2	1.98	0.46
6:FO:208:ASN:HB3	6:FO:230:LYS:HA	1.97	0.46
6:FS:84:ARG:HG3	6:FS:85:ALA:H	1.81	0.46
8:GM:459:GLN:HE22	8:GM:468:PRO:HA	1.80	0.46
1:BC:77:SER:HA	5:FJ:282:GLU:HG3	1.96	0.46
1:CB:271:ASN:HB3	1:CB:273:ASN:H	1.81	0.46
1:CC:358:VAL:N	1:CD:359:LEU:O	2.47	0.46
1:CD:275:GLU:OE1	2:Db:254:ARG:NH1	2.49	0.46
1:CE:389:LYS:HG2	1:CE:395:ARG:HG3	1.98	0.46
2:Db:84:LEU:N	2:Db:134:TYR:OH	2.42	0.46
1:EA:39:LEU:HD22	1:EF:489:LEU:HD21	1.98	0.46
1:EB:174:ILE:HG21	1:EB:191:ARG:HH22	1.80	0.46
2:Ea:252:GLY:HA3	2:Ea:259:ARG:HH21	1.80	0.46
2:Eb:57:ILE:HD11	2:Eb:302:ILE:HD12	1.98	0.46
2:Eb:129:THR:OG1	2:Eb:130:ALA:N	2.49	0.46
2:Ee:282:LEU:HD23	2:Ee:304:LEU:HD13	1.98	0.46
5:FB:97:GLU:OE2	5:FB:547:ARG:NH1	2.48	0.46
5:FB:396:ARG:NH2	8:GL:433:GLN:OE1	2.40	0.46
5:FD:45:ILE:HG23	5:FD:317:ASN:ND2	2.30	0.46
5:FF:87:MET:HE2	5:FF:438:ASN:HD22	1.81	0.46
5:FF:537:MET:HE2	5:FF:537:MET:HB3	1.80	0.46
5:FI:339:ARG:NH2	8:GS:521:ASP:OD2	2.48	0.46
8:GQ:477:VAL:HG22	8:GQ:482:VAL:HG22	1.98	0.46
8:GV:487:MET:HE1	8:GV:543:ARG:HE	1.79	0.46
8:IM:233:MET:HE3	8:IM:233:MET:HB2	1.77	0.46
1:AA:71:TYR:HB3	1:AA:199:ARG:HG2	1.97	0.46
1:AB:304:TYR:OH	1:AB:423:TYR:O	2.34	0.46
1:AE:122:GLU:OE2	1:AF:258:TYR:OH	2.31	0.46
4:Ak:30:ASN:ND2	4:Ak:35:GLU:OE1	2.48	0.46
1:BF:475:SER:OG	1:BF:476:ALA:N	2.49	0.46
2:Bb:11:LEU:O	2:Bb:254:ARG:NH2	2.37	0.46
2:Bd:256:ASP:HB3	2:Bd:267:ILE:HD11	1.97	0.46
1:CC:4:LYS:HG2	1:CC:9:GLN:HB3	1.97	0.46
1:CC:414:HIS:CD2	1:CC:416:MET:H	2.34	0.46
1:DB:329:ARG:NH1	1:DC:337:GLU:OE2	2.40	0.46
1:DF:277:MET:HE3	1:DF:277:MET:HB2	1.82	0.46
2:Df:79:ARG:HE	2:Df:189:ILE:HD13	1.81	0.46
1:EA:336:GLY:HA3	1:EA:422:SER:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ed:1:MET:HB2	2:Ed:203:PRO:HB3	1.98	0.46
2:Ed:184:ASP:OD1	2:Ed:184:ASP:N	2.48	0.46
4:Ej:26:MET:HG2	4:Ej:37:ILE:HD12	1.98	0.46
4:Ej:30:ASN:ND2	4:Ej:31:ASN:OD1	2.49	0.46
5:FA:405:LEU:HD21	5:FB:602:LYS:HB2	1.97	0.46
5:FB:134:ILE:HD12	5:FB:147:LYS:HD2	1.97	0.46
5:FD:709:GLN:HE22	5:FE:711:GLN:HG2	1.81	0.46
5:FE:404:ARG:NH1	5:FE:627:ASP:OD1	2.49	0.46
5:FF:570:ILE:HG12	5:FG:93:VAL:HG22	1.97	0.46
5:FF:729:THR:HA	5:FF:732:ILE:HG22	1.96	0.46
5:FG:436:PRO:HG3	6:FU:236:HIS:HB2	1.98	0.46
5:FK:372:GLU:HB2	8:GV:425:ALA:HB1	1.97	0.46
6:FM:74:VAL:HG22	6:FM:129:ILE:HG12	1.97	0.46
7:FZ:85:LYS:NZ	7:FZ:135:ASP:O	2.49	0.46
7:GE:178:CYS:SG	7:GE:179:LYS:N	2.89	0.46
7:GI:89:THR:HA	7:GI:159:PHE:HA	1.98	0.46
1:AF:130:GLN:O	1:AF:131:VAL:C	2.59	0.46
1:BC:425:TYR:HB2	1:BC:497:LEU:HB3	1.98	0.46
1:CD:273:ASN:HD21	2:Db:48:PRO:HB2	1.79	0.46
2:Cb:70:SER:HB2	2:Cb:278:VAL:HG12	1.97	0.46
2:Ce:186:ASN:OD1	2:Ce:186:ASN:N	2.49	0.46
1:DA:365:ARG:HB2	1:DB:369:LYS:HD3	1.97	0.46
1:DE:137:LEU:HD11	1:DE:152:GLU:HB3	1.97	0.46
1:DE:215:LYS:NZ	1:EC:20:THR:O	2.49	0.46
1:EA:302:MET:HE3	1:EA:302:MET:HB2	1.80	0.46
1:EB:137:LEU:HD11	1:EB:152:GLU:HB2	1.97	0.46
1:EE:128:LEU:HD23	1:EE:165:ARG:HD2	1.98	0.46
1:EF:292:ILE:HG12	1:EF:486:VAL:HG11	1.96	0.46
5:FA:103:PHE:HE2	5:FA:175:ILE:HD13	1.80	0.46
5:FA:190:ASP:OD2	5:FA:212:ARG:NH2	2.42	0.46
5:FC:663:ILE:HA	5:FC:666:LEU:HD12	1.97	0.46
6:FP:75:ARG:HA	6:FP:82:ALA:HA	1.96	0.46
6:FU:84:ARG:HG3	6:FU:85:ALA:H	1.81	0.46
6:FV:160:LYS:O	6:FV:164:THR:OG1	2.29	0.46
7:GE:109:TYR:HA	7:GE:130:CYS:HB2	1.98	0.46
7:GF:104:GLN:NE2	7:GG:75:GLU:O	2.45	0.46
1:BA:204:THR:HG23	1:BA:483:THR:HB	1.97	0.46
1:BB:434:ASP:OD1	1:BB:434:ASP:N	2.46	0.46
1:BE:219:LYS:HE3	1:BE:241:ASN:HD22	1.80	0.46
1:BF:414:HIS:HD2	1:BF:416:MET:H	1.63	0.46
4:Bj:28:TYR:OH	4:Bk:22:TYR:O	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:266:GLY:O	1:CC:291:GLY:N	2.48	0.46
1:DC:330:LEU:HD11	1:DC:397:ARG:HD3	1.96	0.46
1:DF:220:LEU:HD13	1:DF:226:MET:HG3	1.97	0.46
3:Dg:23:VAL:HG11	3:Dh:85:VAL:HG21	1.98	0.46
1:EB:77:SER:OG	2:Eb:111:SER:HB3	2.16	0.46
1:EB:430:ILE:HD11	1:EB:495:MET:HB3	1.98	0.46
1:EC:88:ARG:HB2	1:EC:110:TYR:HB2	1.97	0.46
5:FA:716:LEU:HD11	5:FB:718:GLN:HG2	1.98	0.46
5:FC:337:SER:OG	5:FC:338:LYS:N	2.49	0.46
5:FC:423:ASN:ND2	5:FD:214:ASN:OD1	2.43	0.46
5:FD:400:ILE:HG23	5:FD:595:VAL:HG21	1.98	0.46
5:FF:378:VAL:HG22	5:FF:409:SER:HB3	1.97	0.46
5:FF:723:ASN:HB3	5:FG:725:ARG:HH21	1.81	0.46
5:FI:19:LYS:HA	5:FI:22:ARG:HD2	1.98	0.46
6:FQ:86:MET:HE3	6:FQ:86:MET:HB2	1.80	0.46
7:GB:36:ARG:HG3	7:GB:187:ILE:HD12	1.98	0.46
7:GJ:115:MET:HE3	7:GJ:141:LYS:HB3	1.98	0.46
8:GM:430:LEU:HD13	8:GM:517:GLU:HA	1.97	0.46
2:Ad:11:LEU:O	2:Ad:254:ARG:NH2	2.49	0.45
1:BB:128:LEU:HD21	1:BC:503:GLN:HE21	1.81	0.45
1:BC:50:LYS:HE3	1:BC:232:SER:HB2	1.97	0.45
2:Ba:79:ARG:HB2	2:Ba:231:VAL:HB	1.97	0.45
1:CA:447:ASN:ND2	1:CA:483:THR:O	2.50	0.45
1:CB:270:ARG:NH2	1:CB:276:TYR:OH	2.49	0.45
1:CD:300:ASN:HB3	1:CD:495:MET:HG2	1.98	0.45
1:DE:219:LYS:HE2	1:DE:241:ASN:HB2	1.98	0.45
2:De:105:ARG:HB3	2:De:112:GLU:HG3	1.98	0.45
5:FD:315:ILE:H	5:FD:315:ILE:HG12	1.44	0.45
5:FE:405:LEU:HD21	5:FF:602:LYS:HB2	1.99	0.45
5:FF:330:VAL:HG22	5:FF:387:ILE:HG12	1.97	0.45
5:FH:617:GLU:H	5:FH:617:GLU:HG2	1.58	0.45
5:FK:567:SER:HB2	5:FL:549:GLY:HA2	1.97	0.45
6:FO:23:LEU:HB3	6:FO:26:LEU:HD12	1.98	0.45
6:FS:34:TYR:HB3	6:FS:158:ILE:HG12	1.98	0.45
6:FT:199:SER:HB3	6:FT:202:GLU:HG3	1.98	0.45
7:GF:91:MET:HE3	7:GF:91:MET:HB2	1.81	0.45
8:IK:226:ARG:HB3	8:IV:228:LEU:HD13	1.98	0.45
2:Ab:57:ILE:HD11	2:Ab:302:ILE:HD12	1.97	0.45
2:Ad:24:LEU:HD23	2:Ad:46:MET:HB2	1.98	0.45
2:Ad:63:LEU:HD12	2:Ad:285:HIS:HD2	1.80	0.45
1:BD:404:TYR:HB3	1:BD:422:SER:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BE:22:ASP:OD2	1:CC:214:ASN:ND2	2.49	0.45
1:BE:229:ASN:O	1:BE:249:TRP:NE1	2.45	0.45
2:Bd:118:LYS:HD2	2:Bd:118:LYS:HA	1.80	0.45
2:Be:278:VAL:HG13	2:Be:308:ASP:HB3	1.97	0.45
1:CA:144:GLY:HA2	2:Ca:281:VAL:HG11	1.98	0.45
3:Ch:98:THR:OG1	3:Ch:99:TYR:N	2.50	0.45
1:DD:389:LYS:N	1:DE:381:ALA:O	2.45	0.45
1:DD:402:PRO:HB3	5:FF:277:MET:HG3	1.98	0.45
1:EA:329:ARG:NH2	1:EB:337:GLU:OE2	2.48	0.45
1:EE:384:GLN:HE21	1:EF:375:HIS:HB2	1.81	0.45
2:Eb:197:TRP:NE1	2:Eb:245:ASP:OD2	2.43	0.45
5:FA:126:LEU:HD13	5:FA:159:TRP:HZ3	1.80	0.45
5:FC:734:ALA:HB1	5:FD:736:ILE:HG21	1.98	0.45
5:FD:28:TRP:CH2	5:FD:33:THR:HG21	2.51	0.45
5:FE:101:ARG:NH2	5:FE:572:GLU:OE1	2.36	0.45
5:FG:207:GLU:HG3	5:FG:601:ASN:HD21	1.81	0.45
5:FI:72:ILE:HG12	5:FI:79:ASP:HB3	1.97	0.45
7:GF:34:LYS:NZ	7:GF:161:ASP:OD1	2.47	0.45
8:GM:477:VAL:HG22	8:GM:482:VAL:HG22	1.97	0.45
8:IT:228:LEU:HD13	8:IU:226:ARG:HB3	1.98	0.45
1:AA:26:GLY:HA2	1:AA:31:GLN:HB2	1.99	0.45
1:AA:235:GLN:NE2	1:AF:193:THR:OG1	2.49	0.45
1:AF:88:ARG:HB2	1:AF:110:TYR:HB2	1.97	0.45
1:BA:73:ASP:OD1	1:BA:73:ASP:N	2.42	0.45
1:BF:335:THR:OG1	1:BF:336:GLY:N	2.49	0.45
1:CE:215:LYS:NZ	1:DC:20:THR:O	2.49	0.45
1:CF:317:TYR:O	1:CF:321:ALA:N	2.48	0.45
2:Cf:216:ILE:O	2:Cf:216:ILE:CG1	2.64	0.45
1:DC:433:MET:HE2	1:DC:435:GLN:HE21	1.81	0.45
2:Da:148:LYS:HE2	2:Da:150:GLU:HB2	1.98	0.45
1:EE:244:MET:HE2	1:EE:459:PRO:HB2	1.98	0.45
2:Ea:105:ARG:HB3	2:Ea:105:ARG:HH11	1.81	0.45
3:Eh:36:MET:HE1	3:Eh:62:LEU:HB2	1.98	0.45
5:FA:87:MET:HE2	5:FA:438:ASN:HD22	1.81	0.45
5:FA:423:ASN:OD1	5:FB:212:ARG:NH2	2.38	0.45
5:FD:727:ASN:HD22	5:FD:730:LYS:HE3	1.82	0.45
5:FE:198:ILE:HG12	5:FE:229:VAL:HG21	1.97	0.45
5:FF:412:HIS:ND1	5:FF:413:PHE:O	2.50	0.45
5:FF:653:LEU:HD13	5:FF:663:ILE:HG13	1.99	0.45
5:FI:616:MET:HE2	5:FI:616:MET:HB3	1.83	0.45
6:FT:8:VAL:HB	6:FT:12:VAL:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:GI:70:SER:OG	7:GI:71:GLY:N	2.49	0.45
7:GJ:36:ARG:HG3	7:GJ:187:ILE:HD12	1.97	0.45
8:GN:444:ILE:HD13	8:GN:471:VAL:HG21	1.98	0.45
1:AE:19:LEU:HD23	2:Bb:7:GLN:HA	1.97	0.45
1:AF:55:PHE:O	1:AF:58:SER:OG	2.34	0.45
2:Ab:129:THR:OG1	2:Ab:130:ALA:N	2.49	0.45
1:BB:454:TRP:CD2	1:BB:458:ASN:HB2	2.52	0.45
1:BE:102:VAL:HG21	1:BE:166:LEU:HD12	1.98	0.45
1:BE:220:LEU:HB3	1:CC:30:GLN:HB3	1.99	0.45
3:Bg:50:CYS:HB3	3:Bh:91:LEU:HD23	1.99	0.45
1:CD:244:MET:O	5:FH:287:VAL:HG23	2.17	0.45
1:DE:22:ASP:OD2	1:EC:214:ASN:ND2	2.44	0.45
2:Da:251:MET:SD	2:Da:254:ARG:NH2	2.89	0.45
1:EE:62:ARG:NH2	1:EE:435:GLN:OE1	2.48	0.45
1:EE:307:PHE:HZ	1:EE:312:LEU:HD22	1.82	0.45
2:Ef:105:ARG:HH21	2:Ef:208:PRO:HB2	1.80	0.45
5:FE:676:GLN:HE22	5:FF:668:THR:HG21	1.81	0.45
5:FG:190:ASP:OD2	5:FG:212:ARG:NH2	2.49	0.45
5:FI:423:ASN:ND2	5:FJ:214:ASN:OD1	2.48	0.45
5:FI:649:ALA:O	5:FI:653:LEU:N	2.45	0.45
5:FJ:9:ARG:NH2	5:FJ:11:MET:O	2.49	0.45
5:FJ:683:GLU:OE1	5:FK:661:SER:OG	2.32	0.45
6:FO:8:VAL:HB	6:FO:12:VAL:HG21	1.97	0.45
6:FP:198:PRO:HB2	6:FP:203:MET:HG2	1.96	0.45
6:FT:19:ARG:HH21	6:FU:30:THR:HA	1.81	0.45
7:GI:58:SER:HG	7:GI:98:TYR:HH	1.61	0.45
8:GN:515:SER:O	8:GN:515:SER:OG	2.34	0.45
8:GU:494:ARG:NH2	8:GU:501:GLY:O	2.45	0.45
1:AE:80:ARG:HD2	2:Ae:110:LEU:HD13	1.97	0.45
2:Aa:131:SER:OG	2:Aa:185:TYR:N	2.44	0.45
2:Aa:135:LYS:HD3	2:Aa:177:GLU:HG3	1.98	0.45
3:Ah:60:MET:O	3:Ah:64:SER:OG	2.30	0.45
1:BC:211:VAL:HG11	1:BC:244:MET:HE1	1.98	0.45
1:BD:48:ARG:NH2	5:FJ:3:ASP:OD2	2.49	0.45
1:BD:304:TYR:OH	1:BD:423:TYR:O	2.33	0.45
2:Be:63:LEU:N	2:Be:285:HIS:O	2.49	0.45
4:Cj:1:MET:N	4:Ck:9:ILE:O	2.49	0.45
1:DA:112:VAL:HG13	1:DA:148:VAL:HG12	1.99	0.45
1:DA:321:ALA:O	1:DB:48:ARG:NH2	2.43	0.45
1:DC:153:LEU:HD22	1:DC:157:ASN:HD22	1.81	0.45
1:DE:363:SER:OG	1:DF:361:ASN:ND2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DF:28:ILE:HG13	1:DF:30:GLN:HG2	1.98	0.45
1:EE:8:PHE:HB3	2:Ed:267:ILE:HD11	1.99	0.45
2:Eb:24:LEU:HB3	2:Eb:46:MET:HB2	1.98	0.45
2:Ee:129:THR:OG1	2:Ee:130:ALA:N	2.49	0.45
5:FA:214:ASN:HB3	5:FA:217:LYS:HB2	1.99	0.45
5:FE:266:PRO:O	5:FE:267:ASP:HB3	2.17	0.45
6:FS:86:MET:HB2	6:FS:86:MET:HE3	1.78	0.45
6:FV:19:ARG:NH2	6:FW:29:GLU:OE2	2.49	0.45
7:GG:42:GLN:NE2	8:IS:222:GLU:OE1	2.50	0.45
1:AA:425:TYR:HB2	1:AA:497:LEU:HB3	1.98	0.45
1:AC:52:LEU:HD11	1:AC:265:TRP:HE1	1.80	0.45
1:AD:79:ARG:O	2:Ad:111:SER:HA	2.17	0.45
1:AE:137:LEU:HD22	1:AE:152:GLU:HG2	1.98	0.45
2:Ab:129:THR:HG23	2:Ab:132:ASP:H	1.82	0.45
1:CE:229:ASN:ND2	1:CE:250:GLU:OE2	2.39	0.45
1:CF:40:MET:HE3	1:CF:40:MET:HB2	1.82	0.45
2:Cf:204:GLN:HE21	2:Cf:241:HIS:HB2	1.81	0.45
1:DC:74:VAL:HG12	1:DD:41:VAL:HB	1.98	0.45
3:Eg:36:MET:HB2	3:Eg:48:ALA:HB3	1.99	0.45
5:FL:698:LEU:HD12	5:FL:701:GLN:HE21	1.82	0.45
7:FY:107:ILE:HG23	7:FY:128:ILE:HB	1.99	0.45
1:AE:193:THR:OG1	1:AE:194:SER:N	2.49	0.45
1:AE:229:ASN:O	1:AE:249:TRP:NE1	2.40	0.45
1:AE:299:ALA:HB3	1:AE:491:PRO:HB2	1.99	0.45
1:AE:400:VAL:HG21	1:AF:374:LEU:HD21	1.98	0.45
1:BC:255:PHE:HE2	1:BC:448:GLU:HG2	1.81	0.45
1:BD:317:TYR:OH	1:BD:392:ASN:ND2	2.48	0.45
2:Bb:61:HIS:NE2	2:Bb:289:THR:OG1	2.49	0.45
1:CE:424:ARG:NH2	1:CE:426:ASP:OD2	2.49	0.45
2:Ca:13:VAL:HA	2:Ca:305:VAL:HG12	1.98	0.45
2:Cf:168:ASP:OD1	2:Cf:168:ASP:N	2.43	0.45
4:Cj:23:LYS:HB3	4:Cj:23:LYS:HE3	1.80	0.45
1:DD:310:LYS:HG2	2:Dd:99:ILE:HD12	1.98	0.45
1:DE:361:ASN:HD21	1:DE:367:VAL:H	1.65	0.45
4:Ej:7:LEU:HD23	4:Ej:19:VAL:HB	1.99	0.45
5:FB:36:ASN:HB2	5:FB:219:ARG:HG2	1.98	0.45
5:FI:111:ASN:ND2	5:FJ:169:GLU:O	2.39	0.45
5:FJ:423:ASN:ND2	5:FK:214:ASN:OD1	2.47	0.45
5:FK:345:LYS:NZ	5:FK:347:TYR:OH	2.41	0.45
5:FK:537:MET:HB3	5:FK:537:MET:HE2	1.77	0.45
6:FV:84:ARG:HG3	6:FV:84:ARG:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FY:31:LEU:HD21	7:GJ:9:MET:HE2	1.97	0.45
8:GV:462:VAL:O	8:GV:462:VAL:HG12	2.15	0.45
1:AA:220:LEU:HD22	1:AA:226:MET:HE3	1.99	0.45
1:AA:323:LYS:HB3	1:AB:44:LEU:HG	1.99	0.45
2:Af:155:VAL:HG23	2:Af:192:GLU:HA	1.99	0.45
3:Bg:36:MET:HB2	3:Bg:48:ALA:HB3	1.98	0.45
4:Bk:7:LEU:HG	4:Bk:19:VAL:HB	1.98	0.45
1:CE:73:ASP:HB2	1:CF:40:MET:HE2	1.98	0.45
2:Ca:79:ARG:NH1	2:Ca:234:THR:OG1	2.50	0.45
3:Cg:46:GLY:HA2	3:Cg:97:VAL:HG11	1.98	0.45
4:Cj:12:ASN:OD1	4:Cj:12:ASN:N	2.48	0.45
2:Df:105:ARG:HH21	2:Df:208:PRO:HB2	1.82	0.45
1:EC:77:SER:OG	5:FC:282:GLU:OE2	2.32	0.45
1:EC:229:ASN:OD1	1:EC:229:ASN:N	2.48	0.45
5:FE:257:LYS:H	5:FE:257:LYS:HG2	1.45	0.45
5:FG:214:ASN:HD22	5:FG:217:LYS:HE3	1.81	0.45
5:FH:86:ILE:HB	5:FH:534:LYS:HE3	1.98	0.45
5:FK:417:GLY:O	5:FK:584:ARG:NH2	2.44	0.45
6:FM:83:LEU:HD23	6:FM:83:LEU:N	2.31	0.45
6:FN:19:ARG:NH1	6:FO:33:GLN:OE1	2.50	0.45
6:FO:172:ILE:HD13	6:FO:172:ILE:HA	1.83	0.45
6:FQ:19:ARG:HE	6:FR:30:THR:HG23	1.81	0.45
7:FY:85:LYS:NZ	7:FY:135:ASP:O	2.42	0.45
8:GL:446:GLU:H	8:GL:473:GLN:HE21	1.65	0.45
8:IV:237:ALA:O	8:IV:240:ARG:NH2	2.50	0.45
1:AA:210:LYS:HA	1:AA:477:VAL:HG12	1.98	0.45
1:AB:406:ASP:OD1	1:AB:406:ASP:N	2.50	0.45
1:AB:412:ILE:HD12	1:AB:502:LEU:HD23	1.98	0.45
1:AB:499:PRO:HD2	1:AB:502:LEU:HD12	1.99	0.45
1:AC:11:LEU:HD23	2:Ed:201:MET:HB3	1.98	0.45
1:BC:38:ASN:OD1	1:BC:38:ASN:N	2.48	0.45
1:BD:129:ASN:ND2	1:BE:409:ARG:O	2.40	0.45
1:CA:205:ILE:HD12	1:CA:258:TYR:HB3	1.99	0.45
1:CC:118:PHE:HA	1:CC:191:ARG:HH21	1.81	0.45
1:CC:408:VAL:HG22	2:Cb:112:GLU:HB2	1.99	0.45
2:Ce:140:SER:O	2:Ce:144:ASN:ND2	2.50	0.45
1:DE:23:ASN:HD21	2:Eb:259:ARG:NH2	2.15	0.45
5:FA:602:LYS:HB3	5:FL:405:LEU:HD21	1.98	0.45
5:FB:424:ASP:OD2	5:FC:214:ASN:ND2	2.49	0.45
5:FB:680:GLU:HG2	5:FC:661:SER:HA	1.99	0.45
5:FG:116:SER:OG	5:FH:608:LEU:O	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FI:698:LEU:HD12	5:FI:701:GLN:HE21	1.82	0.45
6:FX:109:PRO:HB2	6:FX:122:ILE:HD11	1.99	0.45
7:GB:44:TYR:OH	7:GB:188:GLU:OE2	2.34	0.45
8:GN:494:ARG:HH22	8:GN:502:LYS:HA	1.81	0.45
1:AB:406:ASP:O	1:AB:410:ASN:ND2	2.49	0.45
2:Aa:282:LEU:HD23	2:Aa:304:LEU:HD12	1.98	0.45
1:BA:475:SER:OG	1:BA:476:ALA:N	2.46	0.45
2:Ba:70:SER:O	2:Ba:70:SER:OG	2.34	0.45
2:Bf:158:TYR:OH	2:Bf:235:LYS:NZ	2.44	0.45
1:CD:323:LYS:HB3	1:CE:44:LEU:HG	1.99	0.45
1:CE:142:MET:N	2:Ce:64:TYR:OH	2.45	0.45
2:Cb:292:ASN:ND2	2:Cb:294:SER:H	2.14	0.45
4:Cj:3:THR:HG22	4:Ck:8:LYS:HG2	1.97	0.45
1:DA:140:ALA:HB1	1:DA:147:ALA:HB1	1.99	0.45
1:DB:125:VAL:HG11	1:DB:130:GLN:H	1.82	0.45
2:Dd:3:ILE:O	1:EC:24:HIS:NE2	2.49	0.45
2:De:89:SER:OG	2:De:91:THR:O	2.27	0.45
3:Dh:33:LEU:HB2	3:Dh:83:VAL:HB	1.99	0.45
2:Ef:145:LEU:HD12	2:Ef:157:ILE:HD11	1.99	0.45
5:FF:214:ASN:HD22	5:FF:217:LYS:HE3	1.82	0.45
5:FJ:727:ASN:HD22	5:FK:725:ARG:HH21	1.64	0.45
6:FN:84:ARG:HG3	6:FN:85:ALA:H	1.82	0.45
6:FR:75:ARG:HA	6:FR:82:ALA:HA	1.99	0.45
6:FX:172:ILE:HD13	6:FX:172:ILE:HA	1.87	0.45
7:GB:216:ASN:N	7:GB:216:ASN:OD1	2.48	0.45
7:GD:198:LEU:HD23	7:GD:198:LEU:HA	1.87	0.45
8:GL:444:ILE:HD12	8:GL:471:VAL:HG11	1.98	0.45
1:AD:171:ARG:NH2	1:AE:411:LYS:O	2.50	0.44
2:Ab:35:ASP:HB3	1:EC:90:GLU:HG2	1.98	0.44
1:BA:393:GLY:O	1:BA:395:ARG:NH1	2.50	0.44
2:Ba:158:TYR:HB2	2:Ba:189:ILE:HB	1.99	0.44
2:Bf:155:VAL:HG23	2:Bf:192:GLU:HA	1.99	0.44
1:CA:438:ILE:HG12	1:CA:488:VAL:HG12	2.00	0.44
1:CE:81:ASN:ND2	1:CF:408:VAL:O	2.41	0.44
2:Ca:304:LEU:HD13	2:Ca:318:LEU:HD21	1.98	0.44
2:Cb:162:ALA:HB3	2:Cb:184:ASP:HB2	1.99	0.44
2:Ce:162:ALA:HB3	2:Ce:184:ASP:HB2	1.99	0.44
3:Cg:51:LYS:HD2	3:Ch:88:CYS:HA	1.99	0.44
1:DB:43:LEU:HD13	2:Da:108:ILE:O	2.18	0.44
1:DB:270:ARG:NH2	1:DB:276:TYR:OH	2.50	0.44
1:DF:80:ARG:HD2	2:Df:110:LEU:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Db:79:ARG:HH21	2:Db:189:ILE:HD12	1.81	0.44
3:Eg:53:ILE:O	3:Eg:54:ASN:ND2	2.49	0.44
5:FB:365:VAL:HG11	5:FB:373:VAL:HB	1.99	0.44
5:FF:48:LYS:NZ	5:FF:52:ASP:OD1	2.48	0.44
5:FF:456:TRP:NE1	6:FS:210:TRP:O	2.38	0.44
5:FH:489:ASP:OD1	6:FS:193:ASN:ND2	2.40	0.44
5:FH:503:LEU:HD22	5:FI:500:THR:HG22	1.99	0.44
5:FI:223:SER:O	5:FJ:327:ASN:ND2	2.35	0.44
5:FJ:396:ARG:NH2	8:GT:433:GLN:OE1	2.46	0.44
6:FO:71:ILE:HD12	6:FO:113:THR:HG21	1.98	0.44
6:FX:56:ASP:HB3	6:FX:126:LYS:HG2	2.00	0.44
7:GB:178:CYS:SG	7:GB:179:LYS:N	2.89	0.44
7:GC:89:THR:HA	7:GC:159:PHE:HA	1.99	0.44
8:GS:481:TYR:OH	8:GS:540:GLU:OE2	2.33	0.44
8:GS:515:SER:O	8:GS:515:SER:OG	2.34	0.44
1:AA:361:ASN:HD21	1:AA:367:VAL:HG22	1.83	0.44
1:AC:229:ASN:O	1:AC:249:TRP:NE1	2.42	0.44
1:AD:254:GLN:HA	1:AD:257:GLU:HG3	2.00	0.44
1:AD:263:MET:HG3	1:AD:484:LEU:HD13	1.98	0.44
2:Aa:15:LYS:HG3	2:Aa:28:GLY:HA3	2.00	0.44
2:Ab:67:ALA:HB2	2:Ab:282:LEU:HD13	1.99	0.44
1:BD:447:ASN:OD1	1:BD:447:ASN:N	2.49	0.44
1:CB:228:ARG:NE	1:CB:238:ASP:OD2	2.50	0.44
2:Cd:89:SER:OG	2:Cd:91:THR:O	2.33	0.44
1:DA:122:GLU:OE2	1:DB:258:TYR:OH	2.35	0.44
4:Di:10:SER:O	4:Di:20:TRP:NE1	2.41	0.44
1:ED:317:TYR:O	1:ED:321:ALA:N	2.50	0.44
5:FG:504:ALA:N	5:FH:499:SER:O	2.50	0.44
5:FI:489:ASP:OD1	6:FT:193:ASN:ND2	2.50	0.44
5:FJ:702:GLN:O	5:FJ:706:ALA:N	2.50	0.44
5:FL:153:ASP:HB2	5:FL:681:LYS:HD2	1.99	0.44
5:FL:354:GLU:OE1	8:GK:429:TRP:NE1	2.42	0.44
8:GO:444:ILE:HG22	8:GO:458:ILE:HD12	1.99	0.44
1:AD:199:ARG:NH1	2:Bb:258:TYR:OH	2.37	0.44
1:AD:300:ASN:HB3	1:AD:495:MET:HE3	1.98	0.44
2:Ad:293:GLU:OE1	1:BB:210:LYS:NZ	2.50	0.44
1:BD:301:THR:O	2:Bd:118:LYS:NZ	2.49	0.44
2:Ba:35:ASP:OD1	2:Ba:35:ASP:N	2.46	0.44
1:CB:122:GLU:OE2	1:CC:258:TYR:OH	2.35	0.44
2:Cd:107:TYR:HB2	2:Cd:116:TYR:HB2	1.99	0.44
2:Ce:131:SER:HB2	2:Ce:185:TYR:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:312:LEU:HD12	1:DB:497:LEU:HD22	1.98	0.44
1:DE:186:LYS:HB2	1:DF:208:GLN:HG2	1.99	0.44
5:FA:704:ILE:HA	5:FA:707:MET:HG3	1.99	0.44
5:FB:330:VAL:HG22	5:FB:387:ILE:HG12	1.98	0.44
5:FC:134:ILE:HD13	5:FC:151:LEU:HD21	2.00	0.44
5:FD:252:ASP:OD1	5:FD:252:ASP:N	2.44	0.44
5:FK:118:ILE:HG21	5:FL:605:GLN:HB3	1.98	0.44
5:FK:683:GLU:OE1	5:FL:661:SER:OG	2.32	0.44
6:FQ:75:ARG:HD2	6:FQ:80:GLY:HA2	1.99	0.44
6:FW:2:VAL:HA	6:FW:199:SER:HB3	1.99	0.44
2:Ab:108:ILE:HD12	1:EE:5:LEU:HB2	2.00	0.44
1:BB:438:ILE:HG23	1:BB:488:VAL:HG22	1.99	0.44
1:BE:17:LYS:HG3	1:CB:191:ARG:HD2	1.98	0.44
1:BF:181:LYS:HE2	1:BF:181:LYS:HB2	1.85	0.44
1:CB:292:ILE:HG13	1:CB:486:VAL:HG21	1.99	0.44
1:CD:85:VAL:HG23	1:CD:114:PRO:HD3	1.99	0.44
1:CD:153:LEU:HD13	1:CD:157:ASN:HB3	2.00	0.44
1:DC:425:TYR:HB2	1:DC:497:LEU:HB3	1.98	0.44
1:DE:144:GLY:HA2	2:De:281:VAL:HG11	1.97	0.44
1:EC:79:ARG:NH2	1:ED:257:GLU:OE2	2.50	0.44
1:EE:185:ARG:HD3	1:EF:281:LYS:HG2	1.99	0.44
5:FD:112:PRO:HG2	5:FE:668:THR:HB	2.00	0.44
5:FD:721:GLU:HA	5:FD:724:ILE:HG22	1.99	0.44
5:FL:273:ALA:HB2	5:FL:304:PHE:HE1	1.82	0.44
6:FX:13:ILE:HD12	6:FX:13:ILE:HA	1.90	0.44
6:FX:34:TYR:HD2	6:FX:158:ILE:HG23	1.80	0.44
7:GA:2:THR:HA	7:GA:184:GLU:HA	2.00	0.44
7:GD:94:ASN:ND2	7:GE:113:ASP:OD2	2.43	0.44
7:GF:98:TYR:HE1	7:GF:156:ASN:HB2	1.83	0.44
7:GI:121:ASN:HB3	7:GI:124:LEU:HD12	1.99	0.44
8:GM:475:GLU:HG2	8:GM:485:ASP:H	1.83	0.44
8:GP:487:MET:HE3	8:GP:487:MET:HB2	1.86	0.44
1:AA:324:LEU:HD11	1:AA:430:ILE:HG23	1.99	0.44
1:AB:185:ARG:HB2	1:AC:281:LYS:HE3	1.99	0.44
1:AB:216:LEU:HD13	1:AB:457:ARG:HB2	1.98	0.44
2:Ab:106:GLN:O	1:EE:2:ALA:N	2.50	0.44
1:BD:319:LEU:HD21	1:BD:430:ILE:HD13	1.99	0.44
2:Ba:256:ASP:OD1	2:Ba:256:ASP:N	2.45	0.44
1:CA:414:HIS:HD2	1:CA:416:MET:HB2	1.83	0.44
1:CD:279:PHE:HA	1:CD:285:ALA:HA	2.00	0.44
1:CF:309:LEU:HD22	1:CF:347:VAL:HG22	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:220:LEU:HD11	1:DA:243:TRP:HB2	1.98	0.44
1:DD:69:GLU:HG2	1:DD:201:GLU:HA	2.00	0.44
2:Da:68:THR:HG22	2:Da:70:SER:H	1.83	0.44
3:Eg:51:LYS:NZ	3:Eh:84:ILE:O	2.45	0.44
5:FC:200:GLN:HG3	5:FC:415:ILE:HG13	1.98	0.44
5:FC:493:GLU:OE2	6:FO:184:TYR:OH	2.31	0.44
5:FE:267:ASP:O	5:FE:267:ASP:OD1	2.36	0.44
5:FG:252:ASP:N	5:FG:252:ASP:OD1	2.43	0.44
5:FI:100:LYS:HB3	5:FI:100:LYS:HE3	1.79	0.44
5:FJ:201:CYS:SG	5:FJ:414:GLY:O	2.75	0.44
6:FT:58:LYS:HA	6:FT:58:LYS:HD3	1.83	0.44
6:FT:84:ARG:HG3	6:FT:85:ALA:H	1.82	0.44
6:FU:4:ASN:ND2	6:FV:115:GLY:O	2.46	0.44
1:AD:264:ALA:HA	1:AD:292:ILE:H	1.81	0.44
2:Aa:57:ILE:HD11	2:Aa:302:ILE:HD12	2.00	0.44
2:Ab:33:LYS:HE3	2:Ab:33:LYS:HB3	1.85	0.44
2:Ab:152:THR:OG1	2:Ab:195:GLN:OE1	2.36	0.44
1:BA:266:GLY:O	1:BA:291:GLY:N	2.47	0.44
1:BF:135:ARG:HB2	1:BF:154:MET:HG3	1.98	0.44
1:CA:392:ASN:HD22	1:CB:337:GLU:HG2	1.82	0.44
1:CB:428:TRP:HA	1:CB:494:THR:HG23	1.99	0.44
1:CB:466:ASN:HA	1:CB:467:PRO:HD3	1.87	0.44
1:CD:335:THR:OG1	1:CD:336:GLY:N	2.51	0.44
1:CE:310:LYS:HG3	2:Ce:99:ILE:HD12	1.98	0.44
1:DD:56:LEU:HD21	1:DD:264:ALA:HB2	1.99	0.44
1:DD:74:VAL:HB	1:DD:196:VAL:HG23	1.99	0.44
1:DD:186:LYS:HB2	1:DE:208:GLN:HG2	1.98	0.44
1:DE:267:THR:HG22	1:DE:294:GLU:HG3	2.00	0.44
2:De:85:ASP:OD1	2:De:85:ASP:N	2.49	0.44
2:De:119:TYR:O	2:De:144:ASN:ND2	2.50	0.44
1:EE:227:VAL:HA	1:EE:237:LYS:HA	2.00	0.44
2:Ea:35:ASP:N	2:Ea:35:ASP:OD1	2.46	0.44
5:FD:11:MET:HB2	5:FE:263:GLU:OE1	2.17	0.44
5:FE:29:ALA:HB2	5:FE:333:LEU:HD22	2.00	0.44
5:FG:458:SER:HB3	5:FG:514:MET:HE3	1.98	0.44
5:FJ:650:GLN:NE2	5:FJ:667:TYR:OH	2.48	0.44
5:FJ:681:LYS:HE2	5:FJ:681:LYS:HB3	1.82	0.44
6:FT:75:ARG:HG2	6:FT:128:ASP:HB2	1.98	0.44
7:FZ:70:SER:OG	7:FZ:71:GLY:N	2.51	0.44
7:GB:225:ARG:HD3	7:GB:225:ARG:HA	1.89	0.44
7:GJ:132:LYS:HE2	7:GJ:136:GLY:HA2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:262:ALA:HB3	1:AA:484:LEU:HD11	1.99	0.44
1:AC:363:SER:OG	1:AD:361:ASN:OD1	2.36	0.44
1:AD:387:GLU:HB3	1:AE:380:SER:HB2	2.00	0.44
2:Aa:285:HIS:ND1	2:Aa:300:LYS:O	2.51	0.44
1:BC:111:LEU:HD12	1:BC:151:VAL:HG21	1.99	0.44
1:BD:131:VAL:O	1:BD:157:ASN:ND2	2.51	0.44
2:Bd:110:LEU:HD13	1:CC:13:PHE:HB2	2.00	0.44
1:CB:443:ILE:HG21	1:CB:447:ASN:HD22	1.83	0.44
1:CD:291:GLY:O	1:CD:295:GLN:NE2	2.50	0.44
1:CF:145:THR:HG21	2:Cf:242:LEU:HD13	1.99	0.44
1:DB:153:LEU:HD11	1:DB:161:VAL:HG12	1.99	0.44
1:DC:21:SER:OG	1:DC:22:ASP:N	2.51	0.44
1:DE:419:VAL:HG12	1:DE:421:PHE:H	1.83	0.44
1:EB:489:LEU:HD21	1:EC:39:LEU:HD22	1.99	0.44
3:Eh:59:GLU:HG2	3:Eh:77:VAL:HG21	2.00	0.44
5:FB:683:GLU:HG3	5:FC:660:PHE:HB2	2.00	0.44
5:FD:29:ALA:HB2	5:FD:333:LEU:HD22	2.00	0.44
5:FH:77:ILE:HG12	6:FU:235:VAL:HG12	2.00	0.44
5:FI:221:PHE:HB2	5:FI:234:MET:HB3	1.99	0.44
5:FJ:727:ASN:HD21	5:FK:726:ASP:HA	1.81	0.44
8:GK:447:GLY:HA3	8:GK:458:ILE:HD11	2.00	0.44
8:GT:447:GLY:HA3	8:GT:458:ILE:HD11	1.98	0.44
8:GV:542:ALA:HA	8:GV:545:ARG:HG2	1.99	0.44
1:AF:442:LYS:HE2	1:AF:442:LYS:HB3	1.82	0.44
2:Ab:162:ALA:HB3	2:Ab:184:ASP:HB2	2.00	0.44
1:BB:319:LEU:HD21	1:BB:430:ILE:HD12	1.99	0.44
1:BD:309:LEU:HD21	1:BD:347:VAL:HG22	1.98	0.44
1:CA:296:THR:HB	1:CA:494:THR:HG21	2.00	0.44
1:CB:335:THR:OG1	1:CB:336:GLY:N	2.49	0.44
1:CC:116:ASP:HB2	1:CC:142:MET:HE1	1.99	0.44
1:CE:329:ARG:NH1	1:CE:392:ASN:O	2.46	0.44
2:Cf:107:TYR:HA	2:Cf:207:ILE:HD12	2.00	0.44
2:Cf:129:THR:OG1	2:Cf:130:ALA:N	2.51	0.44
1:DD:136:ILE:HG23	1:DD:149:TYR:HB3	1.98	0.44
2:Df:84:LEU:N	2:Df:134:TYR:OH	2.45	0.44
1:EE:174:ILE:HD12	1:EF:254:GLN:HE22	1.83	0.44
5:FF:8:PRO:O	5:FF:10:GLN:NE2	2.49	0.44
5:FL:725:ARG:HG3	5:FL:728:GLN:HE21	1.83	0.44
6:FP:149:ILE:HD11	6:FQ:41:ALA:HA	1.99	0.44
6:FS:122:ILE:HD12	6:FS:125:GLU:HB3	2.00	0.44
7:FZ:29:ILE:HG22	7:FZ:163:LYS:HD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FZ:179:LYS:HE2	7:FZ:181:GLU:HB2	2.00	0.44
7:GB:89:THR:HA	7:GB:159:PHE:HA	2.00	0.44
7:GE:57:GLN:HE22	7:GE:162:ALA:HA	1.82	0.44
1:AE:228:ARG:HE	1:AE:228:ARG:HB3	1.60	0.44
1:CC:80:ARG:HD2	1:CD:10:MET:HB3	1.99	0.44
1:CC:468:TYR:O	5:FI:290:ASN:ND2	2.40	0.44
1:DB:179:VAL:HG21	1:DC:481:MET:HE2	1.99	0.44
1:DB:503:GLN:NE2	2:Db:143:LYS:O	2.51	0.44
1:DC:434:ASP:HA	5:FF:266:PRO:HB3	2.00	0.44
1:EA:122:GLU:OE2	1:EB:258:TYR:OH	2.34	0.44
1:EA:217:ASN:HA	1:EA:242:MET:HE1	2.00	0.44
1:EB:481:MET:HE2	1:EB:481:MET:HB3	1.79	0.44
1:EE:141:ARG:HH21	2:Ee:66:LYS:HD3	1.82	0.44
5:FH:702:GLN:O	5:FH:706:ALA:N	2.45	0.44
5:FK:382:TRP:HA	5:FK:397:PRO:HA	1.99	0.44
6:FW:65:PRO:HG2	6:FW:68:LEU:HB2	2.00	0.44
7:GD:32:LEU:HD23	7:GD:199:VAL:HG21	2.00	0.44
7:GJ:1:MET:HE3	7:GJ:185:PHE:HB3	2.00	0.44
8:GT:484:SER:H	8:GT:539:GLN:HE22	1.66	0.44
8:GV:458:ILE:HG22	8:GV:460:ILE:HG22	1.99	0.44
1:AC:311:LEU:HD11	3:Ag:79:ARG:HD3	1.99	0.43
2:Ad:5:ILE:HG12	1:BC:24:HIS:HE1	1.82	0.43
2:Ad:257:ILE:HD13	1:BC:22:ASP:HB3	2.00	0.43
2:Ae:158:TYR:HB3	2:Ae:168:ASP:HB2	2.00	0.43
1:BC:62:ARG:NH1	1:BD:36:ALA:O	2.51	0.43
2:Bd:81:SER:OG	2:Bd:187:GLN:OE1	2.30	0.43
1:CA:203:THR:HG1	1:CA:289:GLY:H	1.64	0.43
1:CB:184:SER:O	1:CC:206:ARG:NH1	2.51	0.43
1:CB:211:VAL:HG11	1:CB:244:MET:HE1	2.00	0.43
2:Ce:145:LEU:HD22	2:Ce:155:VAL:HG22	2.00	0.43
1:DC:503:GLN:HB3	3:Dg:54:ASN:HD22	1.83	0.43
1:DD:215:LYS:HD2	1:DD:215:LYS:HA	1.82	0.43
2:Da:9:ARG:NH2	2:Da:283:ASP:OD1	2.51	0.43
2:Da:57:ILE:HD11	2:Da:302:ILE:HD12	2.00	0.43
2:Da:102:LEU:HD22	2:Da:145:LEU:HD11	2.00	0.43
1:EA:333:ILE:HG22	1:EA:427:ILE:HG12	1.99	0.43
1:ED:294:GLU:OE2	2:Ed:149:THR:OG1	2.36	0.43
3:Eh:37:GLU:HG3	3:Eh:79:ARG:HH21	1.82	0.43
3:Eh:52:ALA:HB1	3:Eh:57:GLN:HB3	1.99	0.43
5:FC:459:ILE:HB	5:FC:515:ILE:HB	1.99	0.43
5:FD:72:ILE:HB	5:FD:73:LYS:H	1.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FF:352:GLY:HA2	8:GQ:460:ILE:O	2.18	0.43
5:FI:683:GLU:HG3	5:FJ:660:PHE:HB2	2.00	0.43
5:FL:192:MET:HG2	5:FL:574:LEU:HD21	2.00	0.43
6:FU:75:ARG:HA	6:FU:82:ALA:HA	2.00	0.43
7:GB:39:LEU:HD21	7:GB:194:PRO:HB2	1.99	0.43
1:AE:323:LYS:HA	1:AF:46:PHE:H	1.83	0.43
1:DD:129:ASN:OD1	1:DD:129:ASN:N	2.52	0.43
2:Db:102:LEU:HD21	2:Db:190:ILE:HG21	2.00	0.43
2:Dd:319:ILE:O	2:Dd:323:ASN:ND2	2.39	0.43
1:EB:181:LYS:HD3	5:FD:299:ARG:HB2	1.99	0.43
1:EC:112:VAL:HG22	1:EC:148:VAL:HB	2.00	0.43
2:Ef:204:GLN:HE21	2:Ef:241:HIS:HB2	1.83	0.43
5:FC:77:ILE:HG12	6:FP:235:VAL:HG22	2.00	0.43
5:FF:416:VAL:HG11	5:FF:585:ALA:HA	2.00	0.43
5:FG:350:GLU:HA	8:GR:462:VAL:HG12	1.99	0.43
6:FN:19:ARG:HH21	6:FO:30:THR:HA	1.82	0.43
7:GH:86:VAL:HG21	7:GH:138:LEU:HB2	2.00	0.43
8:GO:447:GLY:HA3	8:GO:458:ILE:HD11	2.00	0.43
1:AB:184:SER:O	1:AC:206:ARG:NH1	2.52	0.43
1:AC:111:LEU:HD12	1:AC:151:VAL:HG21	2.00	0.43
1:AC:171:ARG:HB2	1:AD:411:LYS:HD2	2.00	0.43
1:BD:444:LYS:HB3	1:BD:444:LYS:HE2	1.71	0.43
1:BF:311:LEU:HD22	2:Bf:121:GLU:HG2	2.01	0.43
3:Bg:92:MET:HE3	3:Bh:49:MET:HG2	2.00	0.43
1:CD:243:TRP:HB2	5:FH:286:PHE:CD1	2.52	0.43
1:CE:128:LEU:HD23	1:CE:128:LEU:HA	1.84	0.43
4:Cj:28:TYR:OH	4:Ck:22:TYR:O	2.28	0.43
1:DA:269:ASN:OD1	1:DA:269:ASN:N	2.50	0.43
1:DE:207:ILE:HG22	1:DE:480:ARG:HB3	2.01	0.43
1:DF:425:TYR:HB2	1:DF:497:LEU:HB2	1.99	0.43
1:EE:314:ASP:OD2	2:Ee:101:ARG:NH1	2.52	0.43
1:EF:387:GLU:OE2	1:EF:397:ARG:NH1	2.43	0.43
2:Ea:30:ILE:HD11	2:Ea:43:PHE:HB3	2.01	0.43
2:Ed:220:GLY:HA3	4:Ei:1:MET:HE3	2.00	0.43
5:FG:337:SER:HB3	5:FG:382:TRP:CD1	2.53	0.43
5:FH:412:HIS:ND1	5:FH:413:PHE:O	2.51	0.43
5:FI:58:LEU:HB2	5:FI:83:HIS:HB2	2.00	0.43
5:FI:423:ASN:OD1	5:FJ:212:ARG:NH2	2.52	0.43
6:FW:7:TRP:HB3	6:FW:143:LEU:HG	2.00	0.43
7:GG:101:ASP:OD2	7:GH:79:TYR:OH	2.33	0.43
1:AA:44:LEU:HG	1:AF:323:LYS:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:51:SER:O	1:AB:51:SER:OG	2.33	0.43
1:AD:189:ASP:HB3	1:BC:17:LYS:HD3	2.00	0.43
1:AD:392:ASN:ND2	1:AE:337:GLU:O	2.44	0.43
2:Ad:201:MET:HB3	1:BC:11:LEU:HD23	2.01	0.43
1:BD:4:LYS:HB2	1:BD:4:LYS:HE3	1.82	0.43
1:BD:243:TRP:HB2	5:FJ:286:PHE:HD2	1.84	0.43
1:BF:128:LEU:HD23	1:BF:128:LEU:HA	1.89	0.43
4:Bi:19:VAL:HG21	4:Bj:7:LEU:HD22	2.00	0.43
1:CA:380:SER:OG	1:CF:387:GLU:OE1	2.31	0.43
1:CA:408:VAL:HG21	1:CF:79:ARG:HB3	2.00	0.43
1:CD:333:ILE:HB	1:CD:398:LEU:HD12	2.00	0.43
1:CD:404:TYR:O	1:CD:410:ASN:ND2	2.51	0.43
1:DD:47:TYR:HE2	1:DD:408:VAL:HG22	1.83	0.43
2:Dd:153:PRO:O	2:Dd:193:THR:OG1	2.30	0.43
1:EE:424:ARG:HE	1:EE:424:ARG:HB3	1.65	0.43
2:Ef:235:LYS:HE3	2:Ef:235:LYS:HB3	1.91	0.43
5:FA:241:TRP:O	5:FA:328:LEU:N	2.51	0.43
5:FA:633:ASP:OD2	5:FA:635:SER:OG	2.27	0.43
5:FJ:417:GLY:O	5:FJ:584:ARG:NH2	2.51	0.43
5:FL:22:ARG:HB3	5:FL:395:MET:HB3	1.99	0.43
5:FL:412:HIS:ND1	5:FL:413:PHE:O	2.52	0.43
6:FP:8:VAL:HB	6:FP:12:VAL:HG21	2.00	0.43
7:GJ:14:LEU:HA	7:GJ:204:ARG:HH12	1.83	0.43
1:AD:206:ARG:NH2	1:BC:472:ASP:O	2.51	0.43
1:AF:205:ILE:HD12	1:AF:258:TYR:HB3	2.00	0.43
1:BC:56:LEU:HD13	1:BC:263:MET:HE2	2.01	0.43
1:CA:229:ASN:OD1	1:CF:193:THR:OG1	2.35	0.43
1:CF:438:ILE:HG12	1:CF:488:VAL:HG13	1.99	0.43
2:Ca:57:ILE:HD11	2:Ca:302:ILE:HD12	2.01	0.43
2:Cb:11:LEU:O	2:Cb:254:ARG:NH2	2.41	0.43
1:DC:333:ILE:HG12	1:DC:427:ILE:HG13	2.00	0.43
1:DE:228:ARG:HE	1:DE:228:ARG:HB3	1.55	0.43
1:DF:129:ASN:OD1	1:DF:129:ASN:C	2.62	0.43
2:Db:79:ARG:NH1	2:Db:234:THR:OG1	2.51	0.43
2:Dd:256:ASP:OD1	2:Dd:269:THR:OG1	2.36	0.43
2:Dd:295:VAL:HG21	2:Ea:296:GLN:HA	2.01	0.43
2:De:138:ALA:HB1	2:De:171:VAL:HG11	2.00	0.43
2:Ed:108:ILE:HD13	2:Ed:108:ILE:HA	1.75	0.43
5:FA:702:GLN:O	5:FA:706:ALA:N	2.51	0.43
5:FD:306:ASP:HB3	5:FD:309:ASN:HD22	1.83	0.43
5:FE:104:ASP:OD1	5:FE:104:ASP:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FE:461:GLU:OE2	5:FF:512:LYS:NZ	2.37	0.43
5:FF:125:GLU:HG2	5:FF:618:ILE:HD12	2.01	0.43
5:FK:330:VAL:HG22	5:FK:387:ILE:HG12	2.00	0.43
5:FL:217:LYS:NZ	5:FL:239:ASP:OD1	2.41	0.43
6:FO:227:LEU:HD23	6:FP:87:THR:HG21	2.01	0.43
6:FR:12:VAL:HG22	7:GE:120:TYR:HB3	2.00	0.43
6:FV:8:VAL:HG22	6:FV:12:VAL:HG21	1.99	0.43
1:AB:275:GLU:HA	2:Ed:255:GLY:HA2	2.01	0.43
2:Aa:104:PHE:HE1	2:Aa:155:VAL:HG13	1.83	0.43
4:Aj:1:MET:N	4:Ak:9:ILE:O	2.51	0.43
1:BB:53:ASP:O	1:BB:57:ASN:N	2.50	0.43
1:BB:74:VAL:HG22	1:BC:41:VAL:HB	1.99	0.43
1:BB:282:SER:O	1:BB:282:SER:OG	2.32	0.43
2:Be:244:ALA:HA	2:Be:273:VAL:HG21	2.01	0.43
1:CA:73:ASP:OD1	1:CA:73:ASP:N	2.51	0.43
2:Ca:138:ALA:HB1	2:Ca:171:VAL:HG21	1.99	0.43
1:DA:362:ASN:O	1:DA:365:ARG:NH1	2.52	0.43
1:DB:16:TRP:HE1	1:DB:20:THR:HB	1.83	0.43
1:DC:108:PRO:HG3	2:Eb:56:LYS:HE2	2.00	0.43
1:DD:56:LEU:HD12	1:DD:440:LYS:HD3	2.01	0.43
1:DD:180:GLU:HG3	1:DE:284:ASN:HB2	2.01	0.43
1:DD:207:ILE:HG22	1:DD:480:ARG:HB2	1.99	0.43
2:Dd:258:TYR:OH	1:EB:68:ASN:OD1	2.32	0.43
2:De:153:PRO:HD2	2:De:196:PRO:HD3	2.01	0.43
1:EA:41:VAL:HB	1:EF:74:VAL:HG22	2.00	0.43
5:FA:609:SER:OG	5:FA:610:ASP:N	2.51	0.43
5:FH:536:GLU:OE2	5:FI:441:TYR:OH	2.30	0.43
5:FI:435:LYS:HB3	5:FI:435:LYS:HE2	1.84	0.43
6:FU:112:LYS:O	6:FU:119:PHE:N	2.39	0.43
7:GF:35:TYR:HA	7:GF:38:PHE:HB3	2.01	0.43
7:GF:216:ASN:OD1	7:GF:216:ASN:N	2.51	0.43
7:GJ:35:TYR:OH	7:GJ:202:GLU:OE1	2.32	0.43
8:GP:545:ARG:HE	8:GP:545:ARG:HB2	1.65	0.43
8:GR:447:GLY:HA3	8:GR:458:ILE:HD11	2.01	0.43
1:AC:359:LEU:HA	1:AD:361:ASN:HB2	2.00	0.43
1:AE:207:ILE:HG22	1:AE:480:ARG:HB3	2.01	0.43
2:Ab:100:LEU:HD23	2:Ab:141:LEU:HD11	2.01	0.43
2:Ad:60:LYS:HE2	2:Ad:60:LYS:HB2	1.89	0.43
2:Af:204:GLN:HE21	2:Af:241:HIS:HB2	1.84	0.43
1:BA:363:SER:O	1:BB:369:LYS:NZ	2.44	0.43
1:BC:140:ALA:HB1	1:BC:147:ALA:HB1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:446:ASP:O	1:CC:464:LYS:NZ	2.42	0.43
1:BE:55:PHE:O	1:BE:58:SER:OG	2.36	0.43
2:Bb:47:SER:OG	2:Bb:50:GLY:O	2.34	0.43
2:Bb:260:GLY:HA2	2:Bb:266:ILE:HG21	2.00	0.43
1:CE:269:ASN:HD22	1:CE:278:ASN:HB2	1.84	0.43
1:DE:5:LEU:HD12	2:Eb:108:ILE:HG21	1.99	0.43
1:EA:81:ASN:HB3	1:EA:171:ARG:HB3	1.99	0.43
1:EC:207:ILE:HG22	1:EC:480:ARG:HB2	2.01	0.43
1:ED:53:ASP:O	1:ED:57:ASN:N	2.43	0.43
2:Ed:119:TYR:O	2:Ed:144:ASN:ND2	2.50	0.43
2:Ef:94:ALA:HB3	4:Ej:32:GLY:HA3	2.01	0.43
5:FA:252:ASP:OD1	5:FA:252:ASP:N	2.49	0.43
5:FC:430:LEU:HD11	5:FC:574:LEU:HD11	1.99	0.43
5:FD:569:HIS:HE2	5:FE:100:LYS:HD2	1.83	0.43
5:FH:216:LEU:HB3	5:FH:314:GLY:HA2	2.01	0.43
5:FJ:241:TRP:HE3	5:FJ:246:VAL:HG12	1.82	0.43
5:FK:345:LYS:NZ	5:FK:372:GLU:OE2	2.46	0.43
6:FO:83:LEU:HD22	6:FO:109:PRO:HB2	2.00	0.43
6:FS:19:ARG:HH21	6:FT:30:THR:HA	1.84	0.43
7:GC:31:LEU:HD23	7:GC:31:LEU:HA	1.88	0.43
7:GD:107:ILE:HG23	7:GD:128:ILE:HB	2.01	0.43
8:GR:442:THR:O	8:GR:442:THR:OG1	2.35	0.43
1:AC:17:LYS:HE3	1:AC:17:LYS:HB3	1.88	0.43
1:AC:80:ARG:NH2	1:AC:115:GLU:OE2	2.52	0.43
2:Ad:259:ARG:HH22	1:BC:23:ASN:HB2	1.84	0.43
4:Ai:9:ILE:HD11	4:Ak:4:LEU:HD11	2.01	0.43
1:BA:194:SER:HA	1:BA:195:PRO:HD3	1.91	0.43
1:BC:88:ARG:NH1	1:BC:143:GLU:OE2	2.52	0.43
1:BC:238:ASP:OD1	1:BC:239:THR:N	2.52	0.43
1:BF:123:VAL:HG23	1:BF:178:PRO:HD3	2.01	0.43
1:CA:400:VAL:HG21	1:CB:374:LEU:HD11	2.00	0.43
2:Ca:158:TYR:HB3	2:Ca:168:ASP:HB2	2.00	0.43
3:Cg:99:TYR:HB3	3:Ch:102:VAL:HG23	2.01	0.43
1:DB:218:LYS:HD2	1:DB:218:LYS:HA	1.87	0.43
1:DB:321:ALA:O	1:DC:48:ARG:NH2	2.32	0.43
1:DB:499:PRO:HD2	1:DB:502:LEU:HD12	2.00	0.43
1:EB:300:ASN:HB3	1:EB:495:MET:HA	2.01	0.43
1:EC:302:MET:HE1	1:EC:315:ALA:HB1	2.01	0.43
1:ED:494:THR:HG23	9:ED:601:MG:MG	1.43	0.43
1:EF:134:PHE:HB3	1:EF:151:VAL:HG11	2.01	0.43
5:FD:517:THR:HB	5:FD:519:ILE:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FE:635:SER:OG	5:FE:636:ASN:N	2.51	0.43
5:FK:197:GLU:OE1	5:FK:420:TYR:OH	2.31	0.43
5:FL:337:SER:OG	5:FL:338:LYS:N	2.52	0.43
6:FS:25:ASP:OD1	6:FS:25:ASP:N	2.46	0.43
7:GA:107:ILE:HG23	7:GA:128:ILE:HB	2.00	0.43
8:GR:535:ILE:HA	8:GR:538:ALA:HB3	2.00	0.43
1:AD:355:THR:HG21	4:Ai:3:THR:H	1.84	0.43
1:BC:389:LYS:HB2	1:BD:382:GLY:HA3	1.99	0.43
1:BE:454:TRP:O	1:BE:470:SER:OG	2.37	0.43
2:Ba:57:ILE:HD11	2:Ba:302:ILE:HD12	2.01	0.43
2:Bb:67:ALA:HB2	2:Bb:282:LEU:HD13	2.01	0.43
2:Bd:295:VAL:HG23	2:Ca:297:LYS:HE3	2.00	0.43
1:CF:414:HIS:HD2	1:CF:416:MET:HB2	1.84	0.43
2:Ca:139:ILE:HD12	2:Ca:139:ILE:HA	1.89	0.43
2:Cb:136:LYS:NZ	2:Cb:177:GLU:OE2	2.50	0.43
1:DA:272:LEU:HD11	2:Da:151:SER:HA	2.01	0.43
1:DB:11:LEU:HD21	2:Da:264:PRO:HB3	2.01	0.43
1:DB:80:ARG:NH1	2:Db:110:LEU:HD22	2.34	0.43
1:DB:126:GLY:O	1:DC:411:LYS:NZ	2.45	0.43
1:DB:389:LYS:HB2	1:DC:382:GLY:HA3	2.01	0.43
1:DE:128:LEU:HD22	1:DE:165:ARG:HD2	2.01	0.43
1:DF:335:THR:OG1	1:DF:336:GLY:N	2.51	0.43
1:EB:389:LYS:HB2	1:EC:382:GLY:HA3	2.01	0.43
1:EC:339:GLY:O	1:EC:425:TYR:OH	2.34	0.43
2:Ef:89:SER:OG	2:Ef:91:THR:O	2.33	0.43
5:FF:43:SER:OG	5:FG:280:ILE:HG12	2.18	0.43
5:FJ:82:GLN:NE2	5:FJ:83:HIS:O	2.50	0.43
6:FS:160:LYS:O	6:FS:164:THR:OG1	2.35	0.43
6:FV:208:ASN:HB3	6:FV:230:LYS:HA	2.01	0.43
7:GD:89:THR:HA	7:GD:159:PHE:HA	2.01	0.43
7:GE:44:TYR:OH	7:GE:188:GLU:OE2	2.35	0.43
8:GV:458:ILE:O	8:GV:458:ILE:CG2	2.66	0.43
1:AD:11:LEU:O	1:AD:222:MET:N	2.47	0.43
1:AD:181:LYS:HG3	1:AD:182:GLU:HG3	2.01	0.43
2:Aa:105:ARG:NH1	2:Aa:105:ARG:HB3	2.33	0.43
1:BB:374:LEU:HD12	1:BF:392:ASN:HD22	1.83	0.43
1:BD:145:THR:HG21	2:Bd:242:LEU:HD22	2.01	0.43
1:BE:122:GLU:OE1	1:BE:191:ARG:NH2	2.51	0.43
1:BE:207:ILE:HG22	1:BE:480:ARG:HB3	2.01	0.43
2:Ba:129:THR:HG23	2:Ba:132:ASP:H	1.83	0.43
2:Bb:223:ARG:HE	2:Bb:223:ARG:HB3	1.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bb:285:HIS:ND1	2:Bb:300:LYS:O	2.52	0.43
2:Bd:105:ARG:HB2	2:Bd:208:PRO:HG2	2.00	0.43
2:Bd:255:GLY:HA2	1:CB:275:GLU:HA	2.01	0.43
1:CF:329:ARG:H	1:CF:329:ARG:HG2	1.52	0.43
1:DA:44:LEU:HG	1:DF:323:LYS:HB3	2.00	0.43
1:DB:128:LEU:HD13	1:DB:128:LEU:HA	1.86	0.43
1:DD:205:ILE:HG21	1:DD:258:TYR:HB3	2.00	0.43
1:DE:495:MET:HB3	1:DE:495:MET:HE2	1.75	0.43
2:De:118:LYS:HA	2:De:118:LYS:HD2	1.85	0.43
1:EB:329:ARG:NH2	1:EC:337:GLU:OE2	2.52	0.43
1:EB:503:GLN:OE1	2:Eb:173:SER:OG	2.36	0.43
1:EC:71:TYR:HE1	1:EC:199:ARG:HE	1.67	0.43
1:EC:311:LEU:HD11	3:Eg:79:ARG:HD3	2.01	0.43
1:EC:414:HIS:HD2	1:EC:416:MET:H	1.67	0.43
1:EC:448:GLU:OE1	1:EC:480:ARG:NH2	2.52	0.43
1:ED:309:LEU:HD11	1:ED:347:VAL:HG22	2.01	0.43
2:Ea:129:THR:OG1	2:Ea:130:ALA:N	2.52	0.43
2:Ea:316:ASN:ND2	2:Ea:333:LEU:O	2.39	0.43
2:Eb:24:LEU:HD21	2:Eb:31:VAL:HG23	2.00	0.43
2:Ed:108:ILE:O	2:Ed:108:ILE:CG2	2.62	0.43
5:FA:168:ASN:O	5:FA:172:ASN:N	2.44	0.43
5:FB:645:LEU:HD13	5:FB:675:LYS:HG3	2.00	0.43
5:FC:727:ASN:HD22	5:FD:729:THR:HG21	1.84	0.43
5:FE:52:ASP:HB3	5:FE:57:ARG:HB2	2.01	0.43
5:FF:62:ASP:OD2	5:FF:439:TYR:OH	2.33	0.43
5:FJ:117:GLU:HA	5:FJ:120:ASP:HB2	2.01	0.43
6:FN:64:LEU:HD21	6:FN:68:LEU:HD22	2.01	0.43
6:FQ:208:ASN:HB3	6:FQ:230:LYS:HA	2.01	0.43
7:GB:91:MET:HE3	7:GB:91:MET:HB2	1.79	0.43
7:GE:39:LEU:HD21	7:GE:194:PRO:HB2	2.00	0.43
7:GF:200:VAL:O	7:GF:204:ARG:N	2.52	0.43
7:GG:41:LYS:O	7:GG:45:SER:OG	2.31	0.43
1:AB:302:MET:HE2	1:AB:311:LEU:HD11	2.00	0.42
1:AC:471:PHE:HE1	1:AC:475:SER:HB2	1.83	0.42
2:Ad:291:SER:OG	2:Ad:292:ASN:N	2.50	0.42
2:Af:158:TYR:HB2	2:Af:189:ILE:HB	2.01	0.42
1:BA:338:ARG:NH2	1:BF:318:GLU:OE1	2.43	0.42
1:BC:88:ARG:HG3	1:BC:110:TYR:CB	2.47	0.42
1:BC:122:GLU:OE2	1:BD:258:TYR:OH	2.36	0.42
1:BE:153:LEU:HD13	1:BE:157:ASN:HD22	1.84	0.42
1:BF:214:ASN:OD1	1:BF:215:LYS:NZ	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bg:100:LYS:HA	3:Bg:100:LYS:HD3	1.77	0.42
1:CD:88:ARG:HB2	1:CD:110:TYR:HB2	2.01	0.42
2:Ca:145:LEU:HD22	2:Ca:155:VAL:HG22	2.00	0.42
1:DE:132:TYR:OH	1:DF:504:GLY:O	2.29	0.42
1:DF:304:TYR:OH	1:DF:423:TYR:O	2.30	0.42
1:EA:393:GLY:N	1:EC:374:LEU:O	2.52	0.42
2:Ee:197:TRP:NE1	2:Ee:245:ASP:OD2	2.40	0.42
5:FG:67:LEU:HA	5:FG:67:LEU:HD23	1.84	0.42
5:FH:75:ALA:HB1	6:FU:235:VAL:HG22	2.01	0.42
5:FI:166:ARG:NH2	5:FI:621:ASP:OD1	2.39	0.42
5:FJ:33:THR:O	5:FJ:219:ARG:NH2	2.52	0.42
5:FK:258:ASP:HB3	5:FK:391:ILE:HG12	2.01	0.42
5:FK:436:PRO:HG3	6:FM:236:HIS:HB2	2.01	0.42
6:FM:197:ILE:HA	6:FM:198:PRO:HD3	1.86	0.42
6:FT:26:LEU:HD23	6:FT:26:LEU:HA	1.88	0.42
6:FW:13:ILE:HD12	6:FW:13:ILE:HA	1.92	0.42
6:FW:34:TYR:HD2	6:FW:158:ILE:HG23	1.84	0.42
7:GC:125:ARG:HG2	7:GC:143:TRP:HB2	2.01	0.42
8:GO:459:GLN:HE21	8:GO:459:GLN:C	2.27	0.42
1:AC:17:LYS:O	2:Ed:4:SER:OG	2.31	0.42
2:Ae:104:PHE:HB2	2:Ae:116:TYR:HB3	2.01	0.42
1:BA:324:LEU:HD11	1:BA:430:ILE:HG23	2.00	0.42
1:BD:203:THR:HG23	1:BD:288:THR:HG22	2.02	0.42
1:BE:334:LYS:HD2	1:BE:428:TRP:HE1	1.84	0.42
1:BE:424:ARG:HG2	1:BE:498:ILE:HA	2.01	0.42
1:CC:140:ALA:HB1	1:CC:147:ALA:HB1	2.01	0.42
2:Cb:57:ILE:HD11	2:Cb:302:ILE:HD12	2.01	0.42
1:DA:376:SER:H	1:DE:395:ARG:HH22	1.66	0.42
2:Dd:24:LEU:HD21	2:Dd:31:VAL:HG23	2.01	0.42
2:De:102:LEU:HD21	2:De:190:ILE:HG21	2.01	0.42
2:De:153:PRO:O	2:De:195:GLN:NE2	2.43	0.42
3:Dg:41:THR:HA	4:Di:12:ASN:HD21	1.85	0.42
1:EA:50:LYS:NZ	1:EA:232:SER:OG	2.44	0.42
1:EB:257:GLU:O	1:EB:261:ASN:ND2	2.52	0.42
2:Ea:283:ASP:OD1	2:Ea:301:THR:OG1	2.37	0.42
5:FA:507:LEU:HD13	5:FB:491:PHE:CZ	2.54	0.42
5:FA:576:THR:HG22	5:FB:182:LEU:HD13	2.01	0.42
5:FD:22:ARG:HB3	5:FD:395:MET:HB3	2.00	0.42
5:FF:665:LYS:O	5:FF:669:SER:OG	2.35	0.42
5:FG:454:SER:O	5:FG:454:SER:OG	2.36	0.42
5:FH:87:MET:HE2	5:FH:438:ASN:HD22	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FK:196:GLU:HG2	5:FK:419:ILE:HG23	2.00	0.42
6:FN:86:MET:HE3	6:FN:86:MET:HB2	1.87	0.42
6:FP:141:LEU:HD23	6:FP:141:LEU:HA	1.90	0.42
7:GC:110:ILE:HD12	7:GC:114:ARG:HG2	2.01	0.42
1:AA:472:ASP:OD1	1:AA:472:ASP:N	2.43	0.42
1:AC:240:ALA:O	1:AC:246:TYR:OH	2.33	0.42
3:Ag:63:LYS:HB3	3:Ag:72:SER:HB2	2.02	0.42
1:BB:40:MET:HE2	1:BB:40:MET:HB3	1.96	0.42
1:BB:116:ASP:OD1	1:BB:149:TYR:OH	2.29	0.42
1:BB:163:ALA:O	1:BB:167:GLN:NE2	2.52	0.42
1:BB:182:GLU:HG2	1:BB:183:LEU:HD13	2.01	0.42
1:BD:206:ARG:NH2	1:CC:472:ASP:O	2.52	0.42
2:Bb:108:ILE:O	2:Bb:108:ILE:CG2	2.67	0.42
2:Bd:56:LYS:NZ	1:CA:152:GLU:OE1	2.42	0.42
2:Bd:100:LEU:HD22	2:Bd:141:LEU:HD11	1.99	0.42
2:Bf:242:LEU:O	2:Bf:246:LEU:N	2.51	0.42
1:CD:340:ALA:HA	1:CD:398:LEU:HD21	2.00	0.42
2:Cb:157:ILE:HG13	2:Cb:171:VAL:HG23	2.01	0.42
1:DD:184:SER:OG	1:DD:185:ARG:N	2.52	0.42
2:Db:59:LEU:HD22	2:Db:328:LEU:HD21	2.01	0.42
1:EA:248:ASP:HA	1:EA:251:VAL:HG12	2.01	0.42
1:EB:220:LEU:HD11	1:EB:243:TRP:HB2	2.01	0.42
1:EF:217:ASN:HA	1:EF:242:MET:HE1	2.00	0.42
2:Ea:20:ASN:OD1	2:Ea:20:ASN:N	2.52	0.42
2:Ed:155:VAL:HG12	2:Ed:192:GLU:HA	2.00	0.42
2:Ed:309:ASP:N	2:Ed:309:ASP:OD1	2.50	0.42
5:FD:436:PRO:HG3	6:FR:236:HIS:HB2	2.00	0.42
5:FG:78:PRO:HG2	5:FG:80:ARG:HH21	1.84	0.42
5:FI:163:ARG:HB3	5:FI:630:LEU:HD11	2.00	0.42
5:FK:158:GLU:HG3	5:FK:160:GLN:HG2	2.00	0.42
5:FL:660:PHE:HA	5:FL:663:ILE:HG22	2.02	0.42
6:FM:26:LEU:HD23	6:FM:26:LEU:HA	1.90	0.42
6:FT:74:VAL:HG22	6:FT:129:ILE:HG12	2.01	0.42
7:FZ:36:ARG:HG3	7:FZ:187:ILE:HD12	2.01	0.42
7:GI:216:ASN:OD1	7:GI:216:ASN:N	2.52	0.42
1:AB:417:GLY:O	1:AB:423:TYR:OH	2.33	0.42
1:AD:171:ARG:HB2	1:AE:411:LYS:HG2	2.01	0.42
2:Af:139:ILE:HD11	2:Af:180:LEU:HD12	2.02	0.42
1:BA:335:THR:OG1	1:BA:336:GLY:N	2.50	0.42
1:BD:74:VAL:HG22	1:BE:41:VAL:HB	2.01	0.42
1:BF:261:ASN:HD22	1:BF:265:TRP:CD1	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bh:32:GLN:OE1	3:Bh:82:GLN:NE2	2.52	0.42
1:CA:329:ARG:NH1	1:CA:392:ASN:O	2.50	0.42
2:Cb:181:THR:O	2:Cb:181:THR:OG1	2.35	0.42
2:Ce:169:VAL:HA	2:Ce:170:PRO:HD3	1.89	0.42
1:DA:111:LEU:HD12	1:DA:151:VAL:HG21	2.01	0.42
1:DC:85:VAL:HG23	1:DC:114:PRO:HD3	2.00	0.42
1:DE:321:ALA:O	1:DF:48:ARG:NH2	2.52	0.42
2:Dd:4:SER:OG	1:EC:17:LYS:O	2.29	0.42
1:EB:124:ILE:HD13	1:EB:136:ILE:HD11	2.02	0.42
1:EF:390:ALA:N	1:EF:394:VAL:O	2.52	0.42
5:FA:98:GLU:OE1	5:FA:185:ASN:ND2	2.53	0.42
5:FA:166:ARG:NH2	5:FA:625:GLU:OE2	2.47	0.42
5:FD:170:LEU:HD21	5:FD:597:LEU:HD21	2.00	0.42
5:FE:260:LYS:HE2	5:FE:260:LYS:HB2	1.40	0.42
5:FI:166:ARG:HH22	5:FI:621:ASP:CG	2.23	0.42
5:FK:463:ASP:OD2	5:FL:490:SER:OG	2.34	0.42
6:FR:21:PRO:HB2	7:GD:50:GLN:HG2	2.01	0.42
6:FX:64:LEU:HG	6:FX:68:LEU:HD13	2.01	0.42
7:FZ:104:GLN:HE22	7:GA:76:GLY:HA3	1.82	0.42
7:GJ:168:MET:HE2	7:GJ:168:MET:HB3	1.85	0.42
8:GT:503:THR:O	8:GT:507:ALA:N	2.52	0.42
1:AA:400:VAL:HG21	1:AB:374:LEU:HD21	2.01	0.42
1:AE:5:LEU:HB2	2:Bb:108:ILE:HG21	2.02	0.42
2:Ab:56:LYS:HE2	1:EC:108:PRO:HG3	2.01	0.42
1:BB:88:ARG:HG3	1:BB:94:VAL:HA	2.01	0.42
1:BE:8:PHE:CZ	1:CB:270:ARG:HD2	2.55	0.42
1:BE:453:GLN:HB3	1:BE:477:VAL:HG22	2.02	0.42
1:CE:124:ILE:HG13	1:CE:134:PHE:HB2	2.01	0.42
4:Ci:26:MET:HB2	4:Ck:37:ILE:HD13	2.01	0.42
1:DA:346:GLU:O	1:DA:350:THR:OG1	2.34	0.42
2:De:129:THR:OG1	2:De:130:ALA:N	2.52	0.42
3:Dg:86:PRO:HD2	3:Dh:51:LYS:HD2	2.01	0.42
1:EA:74:VAL:HG22	1:EB:41:VAL:HB	2.01	0.42
1:EA:319:LEU:HD22	1:EA:495:MET:HE2	2.01	0.42
1:EA:409:ARG:HH21	1:EF:129:ASN:HD22	1.68	0.42
1:EE:117:TRP:NE1	1:EE:191:ARG:HD3	2.35	0.42
2:Ea:3:ILE:HD12	2:Ea:9:ARG:HH11	1.84	0.42
2:Ea:18:LYS:HD3	2:Ea:18:LYS:HA	1.84	0.42
5:FA:735:GLN:O	5:FA:738:SER:OG	2.38	0.42
5:FB:148:LEU:O	5:FB:152:ASN:N	2.53	0.42
5:FB:594:LYS:HA	5:FB:597:LEU:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FD:310:LEU:HA	5:FD:310:LEU:HD23	1.81	0.42
5:FF:707:MET:HA	5:FF:710:GLN:HG3	2.00	0.42
5:FG:57:ARG:NH2	5:FG:281:ASP:O	2.52	0.42
5:FH:78:PRO:HG2	6:FU:232:TYR:HA	2.01	0.42
5:FI:702:GLN:O	5:FI:706:ALA:N	2.51	0.42
5:FK:448:LEU:HD13	5:FK:526:GLN:HB2	2.01	0.42
6:FU:86:MET:HE3	6:FU:86:MET:HB2	1.84	0.42
6:FU:216:ARG:NH1	6:FU:219:GLU:OE2	2.53	0.42
7:GE:91:MET:HB2	7:GE:91:MET:HE3	1.82	0.42
7:GG:96:ARG:NH2	7:GG:102:PHE:O	2.52	0.42
8:IU:238:LYS:NZ	8:IV:234:SER:OG	2.52	0.42
1:AB:180:GLU:H	1:AB:180:GLU:HG2	1.55	0.42
1:AD:16:TRP:HE1	1:AD:224:ILE:HD11	1.83	0.42
1:AD:136:ILE:HG23	1:AD:149:TYR:HB3	2.01	0.42
1:AF:124:ILE:HG13	1:AF:134:PHE:HB2	2.01	0.42
1:BE:4:LYS:O	2:Cb:151:SER:OG	2.29	0.42
2:Bf:198:VAL:HG23	2:Bf:202:MET:HB2	2.01	0.42
1:DE:363:SER:O	1:DF:369:LYS:NZ	2.42	0.42
1:EC:174:ILE:O	1:ED:409:ARG:NH1	2.32	0.42
1:EC:446:ASP:O	5:FD:284:TYR:O	2.38	0.42
2:Ea:57:ILE:HD11	2:Ea:302:ILE:HD12	2.01	0.42
2:Ea:184:ASP:N	2:Ea:184:ASP:OD1	2.53	0.42
5:FA:233:ASP:OD2	5:FB:244:GLY:N	2.52	0.42
5:FF:572:GLU:OE1	5:FG:99:SER:OG	2.36	0.42
5:FJ:459:ILE:HB	5:FJ:515:ILE:HB	2.02	0.42
5:FJ:713:GLU:HA	5:FJ:716:LEU:HB3	1.99	0.42
5:FK:683:GLU:OE2	5:FL:659:SER:OG	2.34	0.42
6:FS:17:LEU:HD13	6:FS:26:LEU:HD13	2.01	0.42
6:FW:83:LEU:HD22	6:FW:109:PRO:HG2	2.02	0.42
7:GF:11:LEU:HD11	7:GF:25:PRO:HG3	2.02	0.42
8:IM:243:SER:OG	8:IM:244:LEU:N	2.47	0.42
1:AE:69:GLU:OE2	1:AE:199:ARG:NH2	2.52	0.42
1:AF:133:PRO:HB2	1:AF:154:MET:HB2	2.01	0.42
1:AF:454:TRP:CD2	1:AF:458:ASN:HB2	2.55	0.42
2:Aa:85:ASP:OD1	2:Aa:85:ASP:N	2.49	0.42
3:Ag:83:VAL:HG11	3:Ag:93:ALA:HB2	2.02	0.42
1:BA:454:TRP:HA	1:BA:476:ALA:HA	2.02	0.42
1:BD:50:LYS:HD2	1:BD:406:ASP:HA	2.02	0.42
1:BD:383:PHE:HB2	1:BE:379:LEU:HD13	2.01	0.42
1:BE:464:LYS:HG2	1:CB:449:TYR:HE1	1.85	0.42
2:Be:136:LYS:HB2	2:Be:136:LYS:HE2	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:479:HIS:HE1	1:CF:186:LYS:HD3	1.84	0.42
1:CB:88:ARG:HG3	1:CB:94:VAL:HA	2.01	0.42
1:CB:263:MET:HG3	1:CB:484:LEU:HD13	2.01	0.42
1:DF:490:ASP:HB3	1:DF:493:ARG:HG3	2.01	0.42
2:Ed:107:TYR:HA	2:Ed:207:ILE:HD13	2.02	0.42
4:Ej:4:LEU:N	4:Ek:7:LEU:O	2.51	0.42
5:FA:583:LYS:NZ	5:FA:587:GLU:OE2	2.52	0.42
5:FC:10:GLN:HE22	5:FC:335:TRP:HE1	1.67	0.42
5:FD:307:PRO:O	5:FD:312:THR:OG1	2.35	0.42
5:FE:689:ARG:HA	5:FE:692:GLN:HG3	2.01	0.42
5:FI:617:GLU:H	5:FI:617:GLU:HG2	1.67	0.42
5:FK:719:LYS:HB3	5:FK:719:LYS:HE3	1.82	0.42
6:FP:19:ARG:HH21	6:FQ:30:THR:HA	1.84	0.42
6:FQ:75:ARG:HA	6:FQ:82:ALA:HA	2.01	0.42
6:FX:86:MET:HE3	6:FX:86:MET:HB2	1.83	0.42
7:GH:109:TYR:HA	7:GH:130:CYS:HB2	2.00	0.42
8:GP:447:GLY:HA3	8:GP:458:ILE:HD11	2.02	0.42
1:AC:29:PHE:HZ	2:Ed:201:MET:HG2	1.84	0.42
1:AE:88:ARG:HG3	1:AE:110:TYR:HB2	2.01	0.42
1:AF:133:PRO:HD2	1:AF:154:MET:O	2.20	0.42
1:AF:455:GLY:O	1:AF:466:ASN:ND2	2.40	0.42
2:Ab:24:LEU:HD21	2:Ab:31:VAL:HG23	2.02	0.42
1:BA:235:GLN:NE2	1:BF:77:SER:O	2.52	0.42
1:BC:73:ASP:OD1	1:BC:73:ASP:N	2.47	0.42
1:BC:449:TYR:HB3	5:FL:303:TYR:HD2	1.85	0.42
1:BE:309:LEU:HD22	1:BE:347:VAL:HA	2.01	0.42
2:Bd:309:ASP:N	2:Bd:309:ASP:OD1	2.53	0.42
4:Bj:19:VAL:HG11	4:Bj:26:MET:HE3	2.02	0.42
1:CE:5:LEU:HB2	2:Db:108:ILE:HG13	2.01	0.42
2:Ca:186:ASN:OD1	2:Ca:186:ASN:N	2.53	0.42
2:Cd:129:THR:OG1	2:Cd:130:ALA:N	2.52	0.42
1:DC:390:ALA:N	1:DC:394:VAL:O	2.50	0.42
1:DE:16:TRP:HE1	1:DE:20:THR:HB	1.84	0.42
3:Dh:36:MET:HE1	3:Dh:62:LEU:HB2	2.02	0.42
1:EA:26:GLY:HA2	1:EA:31:GLN:HB2	2.00	0.42
1:EB:154:MET:HE2	1:EB:154:MET:HB3	1.98	0.42
1:EB:390:ALA:HB3	1:EB:394:VAL:HB	2.01	0.42
4:Ei:16:ILE:H	4:Ei:16:ILE:HG12	1.66	0.42
5:FA:671:SER:HB2	5:FA:674:GLU:HB2	2.01	0.42
5:FF:107:VAL:O	5:FF:168:ASN:ND2	2.52	0.42
5:FF:241:TRP:HE3	5:FF:246:VAL:HG12	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FH:365:VAL:HG11	5:FH:373:VAL:HB	2.02	0.42
5:FI:625:GLU:O	5:FI:626:ALA:C	2.58	0.42
5:FJ:223:SER:O	5:FK:327:ASN:ND2	2.53	0.42
5:FJ:412:HIS:ND1	5:FJ:413:PHE:O	2.52	0.42
5:FL:273:ALA:HB2	5:FL:304:PHE:CE1	2.54	0.42
6:FP:19:ARG:NH2	6:FQ:29:GLU:OE2	2.53	0.42
6:FP:65:PRO:HG2	6:FP:68:LEU:HD12	2.01	0.42
6:FP:172:ILE:HD13	6:FP:172:ILE:HA	1.91	0.42
6:FS:18:LEU:HD22	6:FS:24:THR:HA	2.01	0.42
6:FU:84:ARG:HE	6:FU:108:GLU:HG2	1.84	0.42
6:FX:7:TRP:HB3	6:FX:143:LEU:HG	2.01	0.42
6:FX:149:ILE:HD12	6:FX:194:GLU:HG3	2.02	0.42
8:GL:503:THR:HB	8:GL:506:LYS:HB2	2.02	0.42
8:GS:477:VAL:HG22	8:GS:482:VAL:HG22	2.00	0.42
1:AB:373:ARG:HD2	1:AF:326:MET:HG2	2.02	0.42
1:AC:390:ALA:N	1:AC:394:VAL:O	2.52	0.42
2:Ab:215:THR:OG1	2:Ab:222:ASP:HB3	2.19	0.42
2:Ae:222:ASP:OD1	2:Ae:222:ASP:N	2.50	0.42
1:BA:312:LEU:HD13	1:BA:497:LEU:HD22	2.01	0.42
1:BB:279:PHE:HA	1:BB:285:ALA:HA	2.02	0.42
2:Ba:109:GLY:HA3	2:Ba:114:ASP:OD2	2.20	0.42
3:Bh:30:ALA:HA	3:Bh:51:LYS:HE2	2.02	0.42
1:CB:404:TYR:OH	1:CB:426:ASP:OD2	2.27	0.42
1:CC:136:ILE:HG23	1:CC:149:TYR:HB3	2.01	0.42
1:CD:205:ILE:HG21	1:CD:258:TYR:HB3	2.01	0.42
1:CD:499:PRO:HD2	1:CD:502:LEU:HD12	2.01	0.42
1:CE:227:VAL:HB	1:CE:235:GLN:HB3	2.02	0.42
2:Ca:110:LEU:HD12	2:Ca:110:LEU:HA	1.80	0.42
2:Cd:24:LEU:HD21	2:Cd:31:VAL:HG13	2.02	0.42
1:DD:271:ASN:HD22	1:DD:275:GLU:HB2	1.84	0.42
1:DE:7:LYS:HE2	1:DE:7:LYS:HB2	1.83	0.42
1:DF:196:VAL:HG12	1:DF:197:SER:H	1.85	0.42
2:Da:93:VAL:HG21	2:Da:218:VAL:HG12	2.02	0.42
1:EA:413:LEU:HD22	2:Ef:210:THR:HG21	2.01	0.42
5:FA:92:ASN:HA	5:FA:95:ARG:HG2	2.02	0.42
5:FD:126:LEU:HD22	5:FD:159:TRP:HZ3	1.85	0.42
5:FD:163:ARG:NH1	5:FD:625:GLU:OE2	2.53	0.42
5:FG:126:LEU:HD13	5:FG:159:TRP:HZ3	1.84	0.42
5:FH:107:VAL:HG22	5:FH:632:VAL:HG22	2.00	0.42
5:FH:217:LYS:NZ	5:FH:239:ASP:OD1	2.42	0.42
5:FH:328:LEU:HD22	5:FH:387:ILE:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FS:197:ILE:HA	6:FS:198:PRO:HD3	1.88	0.42
7:FZ:128:ILE:HA	7:FZ:142:SER:HB2	2.02	0.42
7:GB:33:VAL:HG13	7:GB:162:ALA:H	1.85	0.42
7:GH:121:ASN:HB3	7:GH:124:LEU:HD12	2.02	0.42
8:GU:459:GLN:HE22	8:GU:462:VAL:HG22	1.85	0.42
2:Af:84:LEU:N	2:Af:134:TYR:OH	2.48	0.42
2:Af:242:LEU:O	2:Af:246:LEU:N	2.51	0.42
2:Ba:9:ARG:HE	2:Ba:303:THR:HG21	1.84	0.42
1:CA:333:ILE:HG22	1:CA:427:ILE:HG13	2.01	0.42
1:CB:135:ARG:HB2	1:CB:154:MET:HG3	2.00	0.42
1:CF:79:ARG:HA	1:CF:79:ARG:HD3	1.83	0.42
1:EB:273:ASN:ND2	1:EB:275:GLU:OE2	2.46	0.42
1:EC:50:LYS:HD2	1:EC:53:ASP:HB3	2.02	0.42
1:EE:168:GLN:NE2	2:Ee:76:LYS:O	2.50	0.42
5:FB:190:ASP:OD2	5:FB:212:ARG:NH2	2.42	0.42
5:FE:190:ASP:OD2	5:FE:212:ARG:NH2	2.53	0.42
5:FL:29:ALA:HB2	5:FL:333:LEU:HD22	2.02	0.42
6:FM:135:MET:HG2	6:FM:143:LEU:HD23	2.01	0.42
6:FR:64:LEU:HG	6:FR:68:LEU:HD13	2.01	0.42
6:FS:137:ASP:OD1	6:FS:137:ASP:N	2.52	0.42
6:FT:1:MET:HE2	6:FT:3:ASN:HB2	2.01	0.42
7:GH:63:LEU:HD12	7:GH:150:LEU:HB3	2.02	0.42
1:AA:406:ASP:HA	1:AA:407:PRO:HD3	1.92	0.41
1:AC:72:TRP:HB3	1:AD:36:ALA:HB3	2.02	0.41
1:AC:416:MET:HE3	1:AC:416:MET:HB3	1.99	0.41
1:AE:348:LEU:HA	1:AE:351:VAL:HG12	2.01	0.41
1:AF:252:GLU:HA	1:AF:480:ARG:HH12	1.85	0.41
2:Aa:168:ASP:OD1	2:Aa:168:ASP:N	2.45	0.41
3:Ag:92:MET:HE2	3:Ah:51:LYS:HB2	2.02	0.41
1:BA:400:VAL:HG11	1:BF:326:MET:HE1	2.02	0.41
2:Ba:131:SER:OG	2:Ba:185:TYR:N	2.50	0.41
2:Ba:158:TYR:HB3	2:Ba:168:ASP:HB3	2.01	0.41
2:Ba:322:ILE:O	2:Ba:326:SER:OG	2.36	0.41
1:CD:16:TRP:HZ2	1:CD:224:ILE:HG13	1.85	0.41
1:CD:66:ASP:OD1	1:CD:66:ASP:N	2.52	0.41
1:CE:186:LYS:HG2	1:CF:479:HIS:CE1	2.55	0.41
1:CE:282:SER:O	1:CE:282:SER:OG	2.31	0.41
1:CE:321:ALA:O	1:CF:48:ARG:NH2	2.53	0.41
1:CF:339:GLY:O	1:CF:425:TYR:OH	2.37	0.41
1:DD:392:ASN:H	1:DE:384:GLN:HE22	1.68	0.41
1:EC:442:LYS:HE3	1:EC:442:LYS:HB3	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ED:359:LEU:HD21	1:EE:367:VAL:HG21	2.01	0.41
2:Ea:17:LEU:HD11	2:Ea:32:PRO:HD3	2.02	0.41
2:Eb:142:ALA:HB2	2:Eb:157:ILE:HD11	2.02	0.41
4:Ej:21:LEU:HD23	4:Ej:21:LEU:HA	1.92	0.41
5:FA:79:ASP:N	5:FA:79:ASP:OD1	2.50	0.41
5:FC:652:ALA:HB1	5:FC:658:LEU:HD13	2.01	0.41
5:FH:707:MET:HA	5:FH:710:GLN:HG3	2.01	0.41
5:FL:142:ASP:OD1	5:FL:142:ASP:N	2.53	0.41
5:FL:339:ARG:HG2	5:FL:341:ILE:HG23	2.01	0.41
6:FO:137:ASP:N	6:FO:137:ASP:OD1	2.52	0.41
6:FR:172:ILE:HD13	6:FR:172:ILE:HA	1.92	0.41
6:FT:25:ASP:OD1	6:FT:25:ASP:N	2.48	0.41
7:FZ:3:TYR:HB2	7:FZ:181:GLU:HA	2.02	0.41
7:FZ:35:TYR:OH	7:FZ:202:GLU:OE1	2.23	0.41
7:FZ:122:LYS:HA	7:FZ:125:ARG:HD2	2.02	0.41
8:GP:446:GLU:H	8:GP:473:GLN:HG3	1.84	0.41
8:GU:472:GLU:HG3	8:GU:474:GLY:H	1.85	0.41
1:AD:189:ASP:O	1:AD:191:ARG:NH1	2.50	0.41
2:Ad:193:THR:OG1	2:Ad:194:GLU:N	2.54	0.41
1:BB:144:GLY:HA2	2:Bb:281:VAL:HG11	2.02	0.41
1:BC:304:TYR:OH	1:BC:423:TYR:O	2.33	0.41
1:BD:144:GLY:HA2	2:Bd:281:VAL:HG11	2.01	0.41
1:BD:318:GLU:OE1	1:BE:338:ARG:NH2	2.46	0.41
3:Bg:40:VAL:N	3:Bg:44:GLY:O	2.53	0.41
1:CA:45:ALA:HA	1:CF:323:LYS:HA	2.03	0.41
1:CA:120:ASP:OD1	1:CA:120:ASP:N	2.49	0.41
1:CC:63:GLU:H	1:CC:63:GLU:HG2	1.68	0.41
1:CC:296:THR:HG21	1:CC:428:TRP:HZ3	1.85	0.41
1:CD:392:ASN:H	1:CE:384:GLN:HE22	1.68	0.41
1:CF:308:SER:HB3	1:CF:311:LEU:HD23	2.01	0.41
1:CF:390:ALA:N	1:CF:394:VAL:O	2.53	0.41
2:Ca:42:TYR:HE2	2:Ca:44:GLN:HE21	1.67	0.41
1:DA:125:VAL:HB	1:DA:129:ASN:HA	2.01	0.41
1:DD:47:TYR:HB2	1:DD:407:PRO:HG2	2.01	0.41
1:DF:438:ILE:HG12	1:DF:488:VAL:HG13	2.01	0.41
2:Db:33:LYS:HE3	2:Db:33:LYS:HB3	1.84	0.41
2:Dd:247:GLU:HG2	2:Dd:251:MET:HG2	2.01	0.41
2:Df:154:LEU:HD23	2:Df:154:LEU:HA	1.91	0.41
1:EB:159:GLN:HG3	3:Eg:26:ALA:HA	2.01	0.41
1:EF:339:GLY:O	1:EF:425:TYR:OH	2.36	0.41
2:Eb:43:PHE:H	2:Eb:54:SER:HB2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Eg:41:THR:HA	4:Ei:12:ASN:HD21	1.84	0.41
4:Ei:19:VAL:HG11	4:Ei:26:MET:HE3	2.03	0.41
5:FD:92:ASN:HA	5:FD:95:ARG:HG2	2.02	0.41
5:FD:423:ASN:OD1	5:FE:212:ARG:NH2	2.54	0.41
5:FE:84:TYR:OH	5:FE:449:ASN:ND2	2.53	0.41
5:FF:153:ASP:OD1	5:FF:153:ASP:N	2.52	0.41
5:FI:463:ASP:OD2	5:FJ:490:SER:OG	2.35	0.41
6:FT:83:LEU:HG	6:FT:109:PRO:HB2	2.01	0.41
6:FU:13:ILE:HD12	6:FU:16:ARG:HD3	2.02	0.41
7:GC:91:MET:HE3	7:GC:91:MET:HB2	1.82	0.41
7:GE:31:LEU:HD23	7:GE:31:LEU:HA	1.90	0.41
7:GE:89:THR:HA	7:GE:159:PHE:HA	2.02	0.41
7:GH:51:ILE:HG21	7:GH:158:ILE:HD11	2.02	0.41
8:GR:515:SER:O	8:GR:515:SER:OG	2.35	0.41
1:AA:218:LYS:H	1:AA:242:MET:HE1	1.85	0.41
1:AB:122:GLU:HG3	1:AB:177:ALA:HB2	2.01	0.41
1:AC:312:LEU:HD21	1:AC:333:ILE:HD11	2.02	0.41
1:AE:469:MET:O	1:BB:470:SER:OG	2.31	0.41
2:Af:216:ILE:HG12	2:Af:225:TRP:HB3	2.02	0.41
1:BA:112:VAL:HG22	1:BA:148:VAL:HG12	2.03	0.41
1:CC:10:MET:HG2	2:Cb:265:ASN:HA	2.01	0.41
2:Ce:251:MET:SD	2:Ce:254:ARG:NH2	2.93	0.41
1:DA:206:ARG:HB2	1:DF:179:VAL:HG11	2.02	0.41
1:DB:195:PRO:HG2	1:DC:224:ILE:HB	2.03	0.41
1:DB:490:ASP:OD2	1:DB:492:THR:OG1	2.38	0.41
1:DD:3:GLY:HA3	3:Dg:95:GLN:HA	2.02	0.41
2:Db:100:LEU:HD23	2:Db:141:LEU:HD11	2.01	0.41
1:EC:333:ILE:O	1:EC:399:ASP:N	2.53	0.41
5:FA:707:MET:HA	5:FA:710:GLN:HG3	2.01	0.41
5:FB:104:ASP:H	5:FB:634:ASN:ND2	2.18	0.41
5:FE:343:LYS:HE2	5:FE:376:PHE:HE2	1.85	0.41
5:FE:535:MET:HE2	5:FE:535:MET:HB3	1.98	0.41
5:FK:493:GLU:OE2	6:FW:184:TYR:OH	2.32	0.41
5:FL:729:THR:O	5:FL:733:ILE:HG12	2.20	0.41
6:FM:49:VAL:HG11	6:FM:135:MET:HE3	2.02	0.41
6:FV:83:LEU:HG	6:FV:109:PRO:HB2	2.03	0.41
6:FX:3:ASN:ND2	6:FX:194:GLU:OE2	2.52	0.41
7:GF:33:VAL:HG21	7:GF:163:LYS:HB2	2.02	0.41
7:GG:198:LEU:HD23	7:GG:198:LEU:HA	1.90	0.41
8:GS:463:ASP:H	8:GS:467:ALA:HA	1.86	0.41
1:AC:380:SER:OG	1:AC:381:ALA:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:249:PHE:HA	2:Ab:259:ARG:HH22	1.86	0.41
2:Ad:100:LEU:HB2	2:Ad:225:TRP:HZ2	1.85	0.41
2:Ad:110:LEU:HD21	1:BC:13:PHE:HB3	2.01	0.41
1:BA:207:ILE:HD12	1:BF:188:GLY:HA3	2.03	0.41
1:BB:321:ALA:O	1:BC:48:ARG:NH2	2.41	0.41
1:BC:108:PRO:HG3	2:Cb:56:LYS:HE2	2.02	0.41
1:BF:211:VAL:HG11	1:BF:244:MET:HE1	2.03	0.41
2:Bb:152:THR:OG1	2:Bb:195:GLN:OE1	2.38	0.41
1:CA:194:SER:HA	1:CA:195:PRO:HD3	1.92	0.41
1:CA:206:ARG:HG3	1:CA:481:MET:HB2	2.02	0.41
1:CC:206:ARG:HH21	1:CC:479:HIS:CD2	2.38	0.41
1:CF:330:LEU:HD11	1:CF:397:ARG:HD3	2.02	0.41
2:Ce:6:ASN:ND2	2:Ce:299:GLU:OE1	2.53	0.41
2:Ce:81:SER:OG	2:Ce:229:THR:OG1	2.36	0.41
1:EC:272:LEU:HD11	3:Eg:30:ALA:HB2	2.03	0.41
1:EF:218:LYS:HA	1:EF:218:LYS:HD2	1.90	0.41
4:Ei:9:ILE:HD11	4:Ek:4:LEU:HD11	2.02	0.41
5:FC:78:PRO:HG2	6:FP:232:TYR:HA	2.03	0.41
5:FC:709:GLN:HE22	5:FD:711:GLN:HB3	1.84	0.41
5:FF:406:ASN:ND2	8:GQ:434:GLY:O	2.53	0.41
5:FL:126:LEU:HD13	5:FL:159:TRP:HZ3	1.85	0.41
6:FO:34:TYR:HD2	6:FO:158:ILE:HG23	1.85	0.41
6:FO:68:LEU:HD21	6:FO:71:ILE:HG13	2.01	0.41
6:FP:83:LEU:HD22	6:FP:109:PRO:HG2	2.02	0.41
6:FP:197:ILE:HA	6:FP:198:PRO:HD3	1.93	0.41
7:FY:91:MET:HE3	7:FY:91:MET:HB2	1.88	0.41
7:FZ:11:LEU:HD11	7:FZ:25:PRO:HG3	2.03	0.41
7:GF:39:LEU:HD21	7:GF:198:LEU:HD12	2.02	0.41
1:AA:265:TRP:CD1	1:AA:409:ARG:HH12	2.38	0.41
1:AC:18:GLY:O	1:EE:209:HIS:NE2	2.44	0.41
1:AD:493:ARG:HG2	1:AE:44:LEU:HD22	2.03	0.41
1:AE:180:GLU:OE2	1:AF:282:SER:OG	2.37	0.41
1:AF:135:ARG:HB2	1:AF:154:MET:HG3	2.03	0.41
2:Aa:68:THR:HA	2:Aa:69:PRO:HD3	1.89	0.41
1:BC:79:ARG:HB3	1:BD:408:VAL:HG21	2.02	0.41
2:Ba:222:ASP:OD1	2:Ba:222:ASP:N	2.46	0.41
2:Bd:41:LEU:HD13	2:Bd:326:SER:HB3	2.02	0.41
2:Bf:88:VAL:HG23	2:Bf:218:VAL:HG21	2.03	0.41
1:CA:22:ASP:HB3	1:CA:25:LEU:HB3	2.01	0.41
1:CC:470:SER:OG	5:FI:291:MET:O	2.28	0.41
1:CE:8:PHE:CE1	1:DB:270:ARG:HD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:228:ARG:HE	1:CE:228:ARG:HB3	1.53	0.41
2:Ca:62:VAL:HG21	2:Ca:328:LEU:HD21	2.01	0.41
2:Cf:84:LEU:N	2:Cf:134:TYR:OH	2.52	0.41
4:Ci:26:MET:HB2	4:Ck:37:ILE:HG21	2.02	0.41
1:DA:489:LEU:HD21	1:DB:39:LEU:HB3	2.02	0.41
1:DD:296:THR:HG21	1:DD:428:TRP:HZ3	1.84	0.41
1:DE:276:TYR:HB2	1:DE:285:ALA:HB1	2.03	0.41
1:DE:365:ARG:HD3	1:DE:365:ARG:HA	1.88	0.41
2:Df:95:GLY:H	4:Dj:32:GLY:HA3	1.85	0.41
1:EA:207:ILE:HD12	1:EF:188:GLY:HA3	2.02	0.41
1:EA:244:MET:HE2	1:EA:459:PRO:HB2	2.01	0.41
1:EA:331:PHE:HD1	1:EA:427:ILE:HG21	1.86	0.41
1:EC:175:GLU:O	1:ED:261:ASN:ND2	2.50	0.41
1:EF:269:ASN:OD1	1:EF:269:ASN:N	2.52	0.41
2:Ea:62:VAL:HG21	2:Ea:328:LEU:HD21	2.02	0.41
5:FA:721:GLU:HA	5:FA:724:ILE:HG12	2.02	0.41
5:FB:22:ARG:HB3	5:FB:395:MET:HB3	2.03	0.41
5:FB:436:PRO:HG3	6:FP:236:HIS:HB2	2.02	0.41
5:FC:413:PHE:HB2	5:FC:415:ILE:HD12	2.01	0.41
5:FG:5:LEU:HA	5:FG:5:LEU:HD12	1.79	0.41
5:FI:45:ILE:HD11	5:FI:287:VAL:HG11	2.02	0.41
5:FI:133:MET:HE1	5:FI:614:ARG:HH11	1.85	0.41
5:FJ:148:LEU:HG	5:FJ:152:ASN:HD21	1.85	0.41
5:FL:496:ILE:O	5:FL:500:THR:OG1	2.30	0.41
6:FX:197:ILE:HA	6:FX:198:PRO:HD3	1.90	0.41
8:GO:444:ILE:HD12	8:GO:471:VAL:HG11	2.03	0.41
8:GQ:447:GLY:HA3	8:GQ:458:ILE:HD11	2.03	0.41
8:GS:494:ARG:HH22	8:GS:502:LYS:HA	1.84	0.41
8:GV:463:ASP:OD1	8:GV:463:ASP:N	2.54	0.41
1:AA:134:PHE:HB3	1:AA:151:VAL:HG11	2.02	0.41
1:AA:360:ASP:O	1:AA:364:THR:OG1	2.31	0.41
1:AD:383:PHE:HB2	1:AE:379:LEU:HD13	2.03	0.41
1:AE:430:ILE:HD13	1:AE:430:ILE:HA	1.96	0.41
1:AF:40:MET:HE2	1:AF:40:MET:HB3	1.85	0.41
1:AF:65:GLU:HA	1:AF:444:LYS:HG2	2.02	0.41
2:Aa:107:TYR:C	2:Aa:109:GLY:N	2.77	0.41
1:BA:125:VAL:HG13	1:BA:175:GLU:HG3	2.02	0.41
1:BB:361:ASN:HD21	1:BB:367:VAL:N	2.14	0.41
1:BE:228:ARG:HE	1:BE:228:ARG:HB3	1.64	0.41
1:BE:368:GLU:O	1:BE:380:SER:OG	2.30	0.41
2:Ba:162:ALA:HB3	2:Ba:184:ASP:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bf:100:LEU:HD21	2:Bf:211:PRO:HB3	2.03	0.41
1:CA:139:ASP:OD1	1:CA:139:ASP:N	2.53	0.41
2:Cf:68:THR:HG21	2:Cf:73:LEU:HD21	2.03	0.41
1:DC:107:SER:OG	2:Eb:42:TYR:OH	2.31	0.41
1:DC:333:ILE:HG21	1:DC:425:TYR:HD2	1.85	0.41
1:DD:271:ASN:HB3	1:DD:273:ASN:H	1.84	0.41
3:Dh:45:LYS:HD3	3:Dh:95:GLN:HG2	2.03	0.41
4:Dj:21:LEU:HD23	4:Dj:21:LEU:HA	1.92	0.41
1:EA:116:ASP:HB3	2:Ea:4:SER:HB2	2.02	0.41
1:EA:320:SER:HB2	1:EA:329:ARG:HG2	2.03	0.41
1:EA:409:ARG:NH2	1:EF:129:ASN:HD22	2.18	0.41
1:EB:320:SER:HB2	1:EB:329:ARG:HG2	2.02	0.41
1:EC:23:ASN:OD1	1:EC:23:ASN:N	2.54	0.41
1:ED:409:ARG:HE	1:ED:409:ARG:HB2	1.67	0.41
2:Ea:213:PHE:HB2	2:Ea:224:LEU:HG	2.02	0.41
2:Ef:158:TYR:HB3	2:Ef:168:ASP:HB2	2.03	0.41
5:FC:378:VAL:HG22	5:FC:409:SER:HB2	2.02	0.41
6:FM:25:ASP:OD1	6:FM:25:ASP:N	2.49	0.41
6:FN:209:MET:HE3	6:FN:210:TRP:HE3	1.86	0.41
6:FO:197:ILE:HA	6:FO:198:PRO:HD3	1.91	0.41
6:FP:71:ILE:HD12	6:FP:113:THR:HG21	2.01	0.41
6:FV:36:LEU:O	6:FV:40:SER:OG	2.37	0.41
6:FX:8:VAL:HG22	6:FX:12:VAL:HG21	2.01	0.41
7:GB:1:MET:HE3	7:GB:185:PHE:HB3	2.02	0.41
8:GV:444:ILE:HD13	8:GV:460:ILE:CG2	2.39	0.41
1:AB:269:ASN:HD22	1:AB:278:ASN:HB2	1.84	0.41
1:AD:145:THR:HG21	2:Ad:242:LEU:HD22	2.03	0.41
2:Af:119:TYR:O	2:Af:144:ASN:ND2	2.54	0.41
1:BD:275:GLU:OE1	2:Cb:254:ARG:NH1	2.53	0.41
1:BE:185:ARG:HD3	1:BF:281:LYS:HG2	2.03	0.41
1:BE:425:TYR:HB2	1:BE:497:LEU:HB2	2.02	0.41
1:CA:158:THR:HG22	1:CB:277:MET:HE1	2.03	0.41
1:CE:398:LEU:HD23	1:CE:398:LEU:HA	1.92	0.41
1:DB:66:ASP:OD1	1:DB:66:ASP:N	2.52	0.41
1:DC:311:LEU:HD22	3:Dg:79:ARG:HD3	2.02	0.41
1:DE:69:GLU:OE1	1:DE:199:ARG:NH2	2.54	0.41
3:Dg:63:LYS:HB3	3:Dg:72:SER:HB2	2.02	0.41
1:EA:427:ILE:HD12	1:EA:495:MET:HE3	2.02	0.41
1:EB:185:ARG:HE	5:FD:295:GLU:HG2	1.85	0.41
1:EB:341:ILE:HG22	1:EB:345:LYS:HE3	2.03	0.41
1:EF:332:VAL:HG22	1:EF:397:ARG:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FC:683:GLU:OE1	5:FD:661:SER:N	2.54	0.41
5:FG:437:TYR:CE2	5:FG:540:VAL:HG21	2.55	0.41
5:FJ:493:GLU:OE1	6:FU:190:GLN:NE2	2.41	0.41
6:FQ:66:CYS:SG	6:FQ:116:ARG:NH1	2.89	0.41
7:GA:37:SER:OG	7:GA:160:GLU:O	2.33	0.41
7:GF:89:THR:HG23	7:GF:157:ALA:HB1	2.03	0.41
8:GR:494:ARG:NH2	8:GR:501:GLY:O	2.51	0.41
1:AE:220:LEU:HB2	1:AE:222:MET:HE2	2.02	0.41
1:AF:335:THR:OG1	1:AF:336:GLY:N	2.53	0.41
2:Ad:106:GLN:NE2	2:Ad:110:LEU:O	2.50	0.41
2:Bd:148:LYS:HA	2:Bd:148:LYS:HD3	1.83	0.41
2:Bf:158:TYR:HB2	2:Bf:189:ILE:HB	2.02	0.41
1:DC:309:LEU:HB2	1:DC:346:GLU:HG3	2.03	0.41
2:De:104:PHE:HB2	2:De:116:TYR:HB3	2.03	0.41
2:De:285:HIS:ND1	2:De:300:LYS:O	2.54	0.41
1:EA:412:ILE:HD12	1:EA:502:LEU:HD23	2.03	0.41
1:EB:119:ALA:HB3	1:EB:122:GLU:HG3	2.03	0.41
1:ED:12:GLY:HA2	1:ED:221:ALA:HA	2.03	0.41
1:EF:307:PHE:HZ	1:EF:312:LEU:HD22	1.86	0.41
2:Ed:15:LYS:HD3	2:Ed:28:GLY:HA3	2.02	0.41
3:Eg:31:MET:HE2	3:Eg:31:MET:HB3	1.82	0.41
4:Ek:27:LYS:HB3	4:Ek:34:TRP:HB3	2.02	0.41
5:FC:92:ASN:HA	5:FC:95:ARG:HG2	2.02	0.41
5:FD:496:ILE:O	5:FD:500:THR:OG1	2.31	0.41
5:FF:381:ALA:H	5:FF:401:GLN:HE22	1.69	0.41
5:FJ:22:ARG:HB3	5:FJ:395:MET:HB3	2.03	0.41
5:FJ:163:ARG:HB3	5:FJ:630:LEU:HD11	2.02	0.41
5:FK:178:TYR:OH	5:FK:207:GLU:OE2	2.38	0.41
5:FK:447:ARG:HH11	5:FK:447:ARG:HD3	1.74	0.41
5:FK:676:GLN:HE22	5:FL:668:THR:HG21	1.86	0.41
6:FR:71:ILE:HD12	6:FR:113:THR:HG21	2.02	0.41
6:FR:160:LYS:HD2	6:FR:181:GLN:HG2	2.03	0.41
7:GA:6:LEU:HD12	7:GA:6:LEU:HA	1.91	0.41
7:GA:81:ARG:NH1	7:GA:82:SER:O	2.54	0.41
1:AD:253:LEU:HD21	5:FA:280:ILE:HD12	2.02	0.41
1:AE:68:ASN:ND2	1:AF:32:ALA:O	2.54	0.41
1:AF:266:GLY:O	1:AF:291:GLY:N	2.54	0.41
2:Ab:249:PHE:O	1:EE:23:ASN:ND2	2.45	0.41
2:Af:107:TYR:CD2	2:Af:108:ILE:HG12	2.56	0.41
1:BA:215:LYS:HE3	1:BA:243:TRP:CD1	2.56	0.41
1:BA:411:LYS:HE2	1:BA:411:LYS:HB2	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:77:SER:OG	1:BB:78:SER:N	2.53	0.41
1:BC:186:LYS:HB2	1:BD:208:GLN:HG2	2.03	0.41
1:BE:189:ASP:O	1:BE:191:ARG:NH1	2.52	0.41
1:BE:194:SER:HA	1:BE:195:PRO:HD3	1.88	0.41
1:BF:107:SER:HA	1:BF:108:PRO:HD3	1.92	0.41
1:BF:224:ILE:HD13	1:BF:224:ILE:HA	1.97	0.41
2:Ba:104:PHE:HE1	2:Ba:155:VAL:HG13	1.86	0.41
2:Bb:100:LEU:HB2	2:Bb:225:TRP:HZ3	1.86	0.41
2:Bb:309:ASP:OD1	2:Bb:309:ASP:N	2.51	0.41
3:Bh:31:MET:HG3	3:Bh:53:ILE:HG22	2.01	0.41
1:CA:38:ASN:O	1:CF:435:GLN:NE2	2.54	0.41
1:CE:229:ASN:O	1:CE:249:TRP:NE1	2.40	0.41
1:CE:424:ARG:HE	1:CE:424:ARG:HB3	1.71	0.41
1:CF:129:ASN:C	1:CF:130:GLN:HG3	2.45	0.41
2:Cd:232:THR:HA	2:Cd:233:PRO:HD3	1.95	0.41
4:Cj:4:LEU:N	4:Ck:7:LEU:O	2.53	0.41
1:DB:333:ILE:HG12	1:DB:427:ILE:HG12	2.02	0.41
1:DD:168:GLN:HE22	2:Dd:76:LYS:HB2	1.85	0.41
2:Dd:41:LEU:HD13	2:Dd:326:SER:HB3	2.02	0.41
1:ED:392:ASN:ND2	1:ED:337:GLU:HG2	2.36	0.41
1:ED:55:PHE:O	1:ED:58:SER:OG	2.37	0.41
1:ED:387:GLU:HG3	1:EE:370:VAL:HG21	2.03	0.41
1:EF:442:LYS:HB2	1:EF:442:LYS:HE2	1.92	0.41
2:Ea:7:GLN:HE21	2:Ea:7:GLN:HB3	1.69	0.41
2:Ea:76:LYS:HG2	2:Ea:236:THR:HG22	2.03	0.41
2:Eb:1:MET:HG2	2:Eb:245:ASP:HB3	2.01	0.41
2:Eb:129:THR:HG23	2:Eb:132:ASP:H	1.85	0.41
2:Eb:158:TYR:HB3	2:Eb:168:ASP:HB3	2.02	0.41
2:Ee:214:LEU:HD23	2:Ee:214:LEU:HA	1.89	0.41
3:Eh:68:TYR:HB2	3:Eh:75:TYR:CZ	2.56	0.41
5:FA:191:ALA:HB1	5:FA:420:TYR:CE2	2.56	0.41
5:FA:668:THR:HG21	5:FL:676:GLN:HE22	1.86	0.41
5:FC:82:GLN:HE22	6:FP:236:HIS:HB2	1.86	0.41
5:FE:700:ALA:HA	5:FE:703:GLN:HG3	2.02	0.41
5:FF:207:GLU:HG3	5:FF:601:ASN:HD21	1.85	0.41
5:FF:447:ARG:NH2	6:FT:212:GLN:O	2.51	0.41
5:FF:723:ASN:HD22	5:FG:725:ARG:HH21	1.69	0.41
5:FG:468:PRO:HB3	6:FR:197:ILE:HD13	2.03	0.41
5:FH:348:ASP:OD2	5:FH:351:THR:OG1	2.37	0.41
5:FK:72:ILE:HG12	5:FK:79:ASP:HB3	2.02	0.41
5:FK:170:LEU:HD22	5:FK:593:ALA:HB1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FK:454:SER:O	5:FK:454:SER:OG	2.36	0.41
5:FL:725:ARG:HA	5:FL:728:GLN:HG3	2.03	0.41
6:FR:20:HIS:CD2	6:FR:159:LYS:HE3	2.56	0.41
6:FR:86:MET:HE3	6:FR:86:MET:HB2	1.93	0.41
6:FV:68:LEU:HD21	6:FV:71:ILE:HG13	2.01	0.41
6:FV:84:ARG:O	6:FV:110:SER:HA	2.21	0.41
7:GB:3:TYR:HB2	7:GB:181:GLU:HA	2.03	0.41
8:GL:445:ASN:OD1	8:GL:445:ASN:N	2.52	0.41
8:GL:503:THR:HG22	8:GL:505:ALA:H	1.86	0.41
1:AA:369:LYS:HE3	1:AA:369:LYS:HB2	1.91	0.41
1:AB:282:SER:O	1:AB:282:SER:OG	2.38	0.41
1:BC:195:PRO:HG3	1:BD:40:MET:HE1	2.02	0.41
1:BF:28:ILE:O	1:BF:30:GLN:NE2	2.47	0.41
2:Bd:84:LEU:N	2:Bd:134:TYR:OH	2.47	0.41
1:CB:125:VAL:HB	1:CB:129:ASN:HA	2.02	0.41
1:CC:79:ARG:HD3	1:CD:49:GLY:HA3	2.03	0.41
1:CC:164:GLU:H	1:CC:164:GLU:HG2	1.72	0.41
1:CD:453:GLN:OE1	1:CD:479:HIS:NE2	2.44	0.41
3:Cg:89:ASN:OD1	3:Ch:30:ALA:N	2.54	0.41
1:DE:17:LYS:HG3	1:EB:191:ARG:HD2	2.02	0.41
1:DE:203:THR:HB	1:DE:289:GLY:H	1.86	0.41
1:DE:266:GLY:O	1:DE:291:GLY:N	2.51	0.41
2:Dd:110:LEU:HD12	2:Dd:110:LEU:HA	1.81	0.41
1:EC:205:ILE:HD11	1:EC:259:LYS:HG3	2.03	0.41
1:EC:271:ASN:HB2	1:EC:277:MET:HE1	2.03	0.41
1:ED:85:VAL:HG23	1:ED:114:PRO:HD3	2.03	0.41
1:EE:80:ARG:NH2	1:EE:115:GLU:OE2	2.54	0.41
2:Eb:100:LEU:HD23	2:Eb:141:LEU:HD11	2.03	0.41
5:FA:680:GLU:HG2	5:FB:661:SER:HA	2.03	0.41
5:FC:461:GLU:OE2	5:FD:512:LYS:NZ	2.42	0.41
5:FD:122:LYS:NZ	5:FE:606:TYR:OH	2.38	0.41
5:FH:272:GLY:O	5:FH:273:ALA:HB3	2.21	0.41
5:FJ:569:HIS:CD2	5:FK:100:LYS:HD2	2.55	0.41
6:FN:197:ILE:HA	6:FN:198:PRO:HD3	1.88	0.41
6:FX:75:ARG:HD2	6:FX:80:GLY:HA2	2.02	0.41
7:GC:34:LYS:HD3	7:GC:34:LYS:HA	1.88	0.41
7:GE:1:MET:HE1	7:GE:6:LEU:HD13	2.03	0.41
7:GG:36:ARG:HG3	7:GG:187:ILE:HD12	2.03	0.41
7:GI:213:GLU:HG3	7:GJ:218:LYS:HE3	2.02	0.41
8:GK:471:VAL:HG13	8:GK:475:GLU:HB2	2.03	0.41
8:GQ:475:GLU:HG2	8:GQ:485:ASP:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:199:ARG:NH1	2:Ed:265:ASN:O	2.42	0.40
1:AB:263:MET:HE2	1:AB:440:LYS:HB3	2.03	0.40
2:Aa:41:LEU:HD13	2:Aa:326:SER:HB2	2.04	0.40
2:Ab:101:ARG:HE	2:Ab:212:GLN:HB2	1.85	0.40
1:BA:180:GLU:HG3	1:BB:284:ASN:HB2	2.03	0.40
1:BE:156:GLY:HA2	1:BF:277:MET:HE1	2.03	0.40
1:BE:472:ASP:OD2	2:Bd:294:SER:OG	2.29	0.40
2:Ba:1:MET:HB3	2:Ba:203:PRO:HB3	2.02	0.40
2:Ba:18:LYS:NZ	2:Ba:23:ALA:O	2.42	0.40
2:Bd:108:ILE:HD13	1:CC:5:LEU:HG	2.02	0.40
1:CC:7:LYS:HA	1:CC:7:LYS:HD3	1.94	0.40
1:CC:50:LYS:HE3	1:CC:50:LYS:HB3	1.89	0.40
1:CE:335:THR:OG1	1:CE:336:GLY:N	2.54	0.40
4:Cj:26:MET:HG2	4:Cj:37:ILE:HD12	2.03	0.40
1:DA:189:ASP:O	1:DA:191:ARG:NH1	2.54	0.40
1:DB:314:ASP:OD2	2:Db:101:ARG:NH1	2.54	0.40
1:DC:190:VAL:HG21	1:DD:251:VAL:HG22	2.03	0.40
1:DD:198:MET:HE3	1:EC:6:GLY:HA3	2.02	0.40
2:Da:20:ASN:ND2	2:Da:21:THR:O	2.53	0.40
2:Dd:57:ILE:HG12	2:Dd:286:TYR:CZ	2.56	0.40
5:FA:206:GLY:HA3	5:FL:406:ASN:HD22	1.86	0.40
5:FC:735:GLN:O	5:FC:738:SER:OG	2.38	0.40
5:FF:22:ARG:HB3	5:FF:395:MET:HB3	2.03	0.40
6:FS:18:LEU:HD12	7:GF:114:ARG:HA	2.02	0.40
6:FV:64:LEU:HG	6:FV:68:LEU:HD13	2.02	0.40
8:GO:460:ILE:HD12	8:GO:460:ILE:O	2.21	0.40
1:AD:63:GLU:HB3	1:AD:442:LYS:HE3	2.03	0.40
1:AD:297:GLU:OE2	1:AD:424:ARG:NH2	2.53	0.40
1:AD:389:LYS:NZ	1:AE:380:SER:OG	2.55	0.40
2:Ad:27:ALA:HB1	2:Ad:48:PRO:HG3	2.03	0.40
2:Af:198:VAL:HG23	2:Af:202:MET:HB2	2.04	0.40
3:Ah:84:ILE:HD12	3:Ah:84:ILE:HA	1.98	0.40
2:Ba:110:LEU:HD12	2:Ba:110:LEU:HA	1.96	0.40
3:Bh:63:LYS:O	3:Bh:72:SER:OG	2.32	0.40
1:CD:293:PHE:HA	1:CD:296:THR:HG22	2.03	0.40
2:Ca:81:SER:OG	2:Ca:187:GLN:NE2	2.53	0.40
2:Ce:119:TYR:O	2:Ce:144:ASN:ND2	2.55	0.40
2:Cf:232:THR:HA	2:Cf:233:PRO:HD3	1.94	0.40
1:DA:331:PHE:HB3	1:DA:427:ILE:HD13	2.02	0.40
1:DC:118:PHE:HA	1:DC:191:ARG:HH21	1.87	0.40
1:DD:301:THR:O	2:Dd:118:LYS:NZ	2.48	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DD:413:LEU:H	3:Dh:69:ASN:HB2	1.85	0.40
1:DF:112:VAL:HG22	1:DF:148:VAL:HG22	2.02	0.40
1:EA:409:ARG:NH1	1:EF:175:GLU:OE1	2.54	0.40
1:EB:136:ILE:HG12	1:EB:151:VAL:HG12	2.02	0.40
1:ED:122:GLU:OE2	1:ED:191:ARG:NH2	2.53	0.40
2:Ee:158:TYR:HB2	2:Ee:189:ILE:HB	2.02	0.40
5:FA:90:LYS:NZ	5:FA:548:GLU:OE2	2.36	0.40
5:FA:166:ARG:HG3	5:FA:612:SER:HB3	2.04	0.40
5:FD:247:ILE:O	5:FD:251:TYR:HB3	2.20	0.40
5:FG:569:HIS:CD2	5:FH:100:LYS:HD2	2.56	0.40
5:FH:275:ASP:O	5:FH:276:GLN:HB2	2.20	0.40
6:FO:84:ARG:NH1	6:FO:85:ALA:O	2.55	0.40
6:FT:10:LEU:HD11	6:FT:142:PRO:HD2	2.03	0.40
6:FW:156:LEU:HB3	6:FW:184:TYR:HB2	2.02	0.40
6:FX:23:LEU:HD22	6:FX:26:LEU:HD11	2.03	0.40
7:GC:14:LEU:HA	7:GC:204:ARG:HH12	1.85	0.40
7:GE:3:TYR:HB2	7:GE:181:GLU:HA	2.04	0.40
8:GM:517:GLU:H	8:GM:517:GLU:HG2	1.72	0.40
1:AA:86:GLU:H	1:AA:112:VAL:HB	1.87	0.40
1:AA:171:ARG:NH2	1:AB:407:PRO:O	2.54	0.40
1:AC:414:HIS:CD2	1:AC:416:MET:H	2.39	0.40
2:Ad:1:MET:HE2	2:Ad:245:ASP:HB3	2.03	0.40
1:BB:205:ILE:HD12	1:BB:258:TYR:HB3	2.03	0.40
1:BB:368:GLU:OE2	1:BC:377:ASN:ND2	2.53	0.40
1:BC:86:GLU:OE2	1:BC:88:ARG:HD2	2.21	0.40
1:BC:136:ILE:HG23	1:BC:149:TYR:HB3	2.04	0.40
1:BD:215:LYS:HD2	1:BD:215:LYS:HA	1.85	0.40
1:BE:333:ILE:O	1:BE:399:ASP:N	2.55	0.40
3:Bh:31:MET:HE2	3:Bh:31:MET:HB3	1.94	0.40
1:CA:39:LEU:HB3	1:CF:489:LEU:HD21	2.03	0.40
1:CA:286:ILE:HG12	1:CF:180:GLU:HG3	2.02	0.40
1:CB:119:ALA:HB3	1:CB:122:GLU:HG3	2.03	0.40
1:CD:211:VAL:HG22	1:CD:247:VAL:HG11	2.02	0.40
1:CF:65:GLU:HA	1:CF:444:LYS:HG2	2.03	0.40
1:CF:310:LYS:HD2	2:Cf:99:ILE:HD13	2.03	0.40
2:Ca:68:THR:HA	2:Ca:69:PRO:HD3	1.87	0.40
2:Cd:201:MET:HB3	1:DC:11:LEU:HD23	2.02	0.40
2:Cf:221:GLU:OE2	4:Ck:12:ASN:ND2	2.54	0.40
1:DA:406:ASP:HA	1:DA:407:PRO:HD3	1.88	0.40
2:Dd:217:THR:O	2:Dd:217:THR:OG1	2.37	0.40
4:Di:19:VAL:HG21	4:Dj:7:LEU:HD22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:76:GLY:HA2	1:EB:43:LEU:HD12	2.03	0.40
1:ED:310:LYS:HD3	2:Ed:99:ILE:HD12	2.03	0.40
2:Ea:274:ASP:HA	2:Ea:275:PRO:HD3	1.96	0.40
2:Ed:106:GLN:NE2	2:Ed:112:GLU:OE2	2.44	0.40
5:FB:153:ASP:OD1	5:FB:153:ASP:N	2.47	0.40
5:FG:62:ASP:OD2	5:FG:439:TYR:OH	2.33	0.40
5:FG:296:ILE:HD12	5:FG:303:TYR:HB3	2.02	0.40
5:FH:576:THR:HG22	5:FI:182:LEU:HD13	2.03	0.40
5:FH:618:ILE:HD13	5:FH:618:ILE:N	2.36	0.40
5:FJ:635:SER:OG	5:FJ:636:ASN:N	2.54	0.40
5:FK:379:ASN:ND2	5:FL:248:ASP:OD1	2.54	0.40
6:FT:18:LEU:HD12	7:GG:114:ARG:HA	2.02	0.40
7:FZ:91:MET:HE3	7:FZ:91:MET:HB2	1.92	0.40
1:AA:292:ILE:HG12	1:AA:438:ILE:HD11	2.04	0.40
2:Ad:232:THR:HA	2:Ad:233:PRO:HD3	1.92	0.40
3:Ag:36:MET:HB2	3:Ag:48:ALA:HB3	2.03	0.40
1:BA:40:MET:HB3	1:BA:40:MET:HE3	1.86	0.40
2:Bb:110:LEU:H	2:Bb:110:LEU:HG	1.71	0.40
1:CA:77:SER:OG	1:CA:78:SER:N	2.54	0.40
1:CC:319:LEU:HD11	1:CC:430:ILE:HD13	2.04	0.40
1:CD:493:ARG:HG2	1:CE:44:LEU:HD22	2.04	0.40
1:CF:207:ILE:HG22	1:CF:480:ARG:HB2	2.03	0.40
2:Cb:145:LEU:HD22	2:Cb:155:VAL:HG22	2.04	0.40
2:Cd:118:LYS:HD2	2:Cd:118:LYS:HA	1.89	0.40
2:Cd:284:ILE:HB	2:Cd:302:ILE:HG23	2.02	0.40
1:DA:153:LEU:HD22	1:DA:157:ASN:HD22	1.87	0.40
1:DA:401:ASP:HB3	1:DA:404:TYR:HD2	1.87	0.40
1:DB:81:ASN:HD21	1:DB:171:ARG:HE	1.69	0.40
1:DB:145:THR:HG21	2:Db:1:MET:HE1	2.04	0.40
1:DB:185:ARG:HB3	1:DC:281:LYS:HE3	2.03	0.40
1:DB:390:ALA:N	1:DB:394:VAL:O	2.55	0.40
1:DC:194:SER:HB3	1:DD:222:MET:HG2	2.03	0.40
1:DD:450:ARG:O	1:EC:465:GLY:HA2	2.21	0.40
2:Db:31:VAL:HG12	2:Db:33:LYS:HG2	2.03	0.40
2:Db:81:SER:OG	2:Db:187:GLN:OE1	2.29	0.40
1:EA:469:MET:N	1:EA:469:MET:SD	2.94	0.40
1:EB:442:LYS:NZ	1:EB:447:ASN:OD1	2.54	0.40
1:EC:444:LYS:HB3	5:FD:283:ARG:HD2	2.04	0.40
5:FC:80:ARG:HB3	6:FP:235:VAL:HG21	2.04	0.40
5:FD:269:ILE:HD11	5:FD:324:LEU:CA	2.52	0.40
5:FE:112:PRO:HG2	5:FF:668:THR:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FI:261:TYR:HB3	5:FI:391:ILE:HD11	2.04	0.40
5:FJ:454:SER:OG	6:FW:211:ASN:OD1	2.39	0.40
5:FJ:727:ASN:HD22	5:FK:725:ARG:NH2	2.18	0.40
5:FK:337:SER:HB3	5:FK:382:TRP:CD1	2.56	0.40
6:FM:48:TYR:HB3	6:FM:132:LYS:HB3	2.02	0.40
7:FZ:188:GLU:HG3	7:FZ:191:LEU:HB2	2.04	0.40
7:GI:11:LEU:HD11	7:GI:25:PRO:HG3	2.03	0.40
8:GL:459:GLN:NE2	8:GL:461:GLY:O	2.53	0.40
1:AB:84:LEU:HD11	1:AB:111:LEU:HB3	2.03	0.40
2:Af:217:THR:HA	2:Af:221:GLU:O	2.22	0.40
1:BA:44:LEU:HD21	1:BF:493:ARG:NE	2.36	0.40
1:BA:361:ASN:HB2	1:BF:359:LEU:HA	2.03	0.40
1:BD:77:SER:OG	1:BD:78:SER:N	2.54	0.40
1:BD:366:VAL:HG23	1:BD:367:VAL:HG23	2.03	0.40
1:BE:133:PRO:HB2	1:BE:154:MET:HB3	2.03	0.40
1:CC:106:THR:O	2:Db:56:LYS:NZ	2.48	0.40
2:Ca:106:GLN:HA	2:Ca:111:SER:O	2.20	0.40
1:DE:50:LYS:HA	1:DE:50:LYS:HD2	1.81	0.40
2:Db:242:LEU:HD23	2:Db:242:LEU:HA	1.96	0.40
2:Dd:48:PRO:HG3	2:Dd:272:LEU:HD21	2.03	0.40
3:Dg:96:VAL:HG21	3:Dh:68:TYR:HE2	1.86	0.40
1:EB:74:VAL:HB	1:EB:196:VAL:HG23	2.03	0.40
1:EC:184:SER:OG	1:ED:206:ARG:NH1	2.42	0.40
2:Eb:312:HIS:O	2:Eb:316:ASN:ND2	2.55	0.40
3:Eh:37:GLU:OE2	3:Eh:94:GLU:N	2.55	0.40
5:FA:713:GLU:HA	5:FA:716:LEU:HB3	2.03	0.40
5:FC:569:HIS:CD2	5:FD:100:LYS:HD2	2.57	0.40
5:FG:732:ILE:HA	5:FG:735:GLN:HG3	2.03	0.40
6:FO:78:LYS:HA	6:FP:96:HIS:HB3	2.04	0.40
6:FW:29:GLU:OE2	7:GI:114:ARG:NH2	2.38	0.40
6:FW:222:ARG:NH1	6:FW:226:ASN:OD1	2.54	0.40
7:FZ:106:GLU:OE1	7:GA:117:TYR:OH	2.35	0.40
7:FZ:216:ASN:OD1	7:FZ:216:ASN:N	2.52	0.40
7:GF:203:LEU:O	7:GF:207:GLU:HB2	2.22	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	AA	482/504 (96%)	466 (97%)	16 (3%)	0	100	100
1	AB	501/504 (99%)	479 (96%)	22 (4%)	0	100	100
1	AC	501/504 (99%)	484 (97%)	17 (3%)	0	100	100
1	AD	446/504 (88%)	426 (96%)	20 (4%)	0	100	100
1	AE	501/504 (99%)	488 (97%)	13 (3%)	0	100	100
1	AF	501/504 (99%)	485 (97%)	16 (3%)	0	100	100
1	BA	483/504 (96%)	472 (98%)	11 (2%)	0	100	100
1	BB	501/504 (99%)	478 (95%)	23 (5%)	0	100	100
1	BC	501/504 (99%)	482 (96%)	19 (4%)	0	100	100
1	BD	446/504 (88%)	427 (96%)	19 (4%)	0	100	100
1	BE	501/504 (99%)	488 (97%)	13 (3%)	0	100	100
1	BF	501/504 (99%)	481 (96%)	20 (4%)	0	100	100
1	CA	199/504 (40%)	197 (99%)	2 (1%)	0	100	100
1	CB	75/504 (15%)	70 (93%)	5 (7%)	0	100	100
1	CC	478/504 (95%)	457 (96%)	21 (4%)	0	100	100
1	CD	309/504 (61%)	295 (96%)	14 (4%)	0	100	100
1	CE	143/504 (28%)	137 (96%)	6 (4%)	0	100	100
1	CF	26/504 (5%)	24 (92%)	2 (8%)	0	100	100
1	DA	148/504 (29%)	147 (99%)	1 (1%)	0	100	100
1	DB	294/504 (58%)	282 (96%)	12 (4%)	0	100	100
1	DC	226/504 (45%)	220 (97%)	6 (3%)	0	100	100
1	DD	331/504 (66%)	319 (96%)	12 (4%)	0	100	100
1	DE	472/504 (94%)	453 (96%)	19 (4%)	0	100	100
1	DF	487/504 (97%)	471 (97%)	16 (3%)	0	100	100
1	EA	283/504 (56%)	274 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EB	344/504 (68%)	336 (98%)	8 (2%)	0	100	100
1	EC	501/504 (99%)	474 (95%)	27 (5%)	0	100	100
1	ED	446/504 (88%)	427 (96%)	19 (4%)	0	100	100
1	EE	501/504 (99%)	486 (97%)	15 (3%)	0	100	100
1	EF	353/504 (70%)	337 (96%)	16 (4%)	0	100	100
2	Aa	331/333 (99%)	315 (95%)	16 (5%)	0	100	100
2	Ab	331/333 (99%)	308 (93%)	23 (7%)	0	100	100
2	Ad	331/333 (99%)	313 (95%)	18 (5%)	0	100	100
2	Ae	261/333 (78%)	248 (95%)	13 (5%)	0	100	100
2	Af	183/333 (55%)	175 (96%)	8 (4%)	0	100	100
2	Ba	331/333 (99%)	310 (94%)	21 (6%)	0	100	100
2	Bb	331/333 (99%)	313 (95%)	17 (5%)	1 (0%)	36	64
2	Bd	317/333 (95%)	295 (93%)	22 (7%)	0	100	100
2	Be	59/333 (18%)	56 (95%)	3 (5%)	0	100	100
2	Bf	24/333 (7%)	24 (100%)	0	0	100	100
2	Cb	174/333 (52%)	163 (94%)	11 (6%)	0	100	100
2	Cd	216/333 (65%)	205 (95%)	11 (5%)	0	100	100
2	Da	150/333 (45%)	142 (95%)	8 (5%)	0	100	100
2	Db	133/333 (40%)	126 (95%)	7 (5%)	0	100	100
2	Dd	95/333 (28%)	90 (95%)	5 (5%)	0	100	100
2	De	125/333 (38%)	120 (96%)	5 (4%)	0	100	100
2	Df	99/333 (30%)	94 (95%)	5 (5%)	0	100	100
2	Ea	191/333 (57%)	179 (94%)	12 (6%)	0	100	100
2	Eb	331/333 (99%)	308 (93%)	23 (7%)	0	100	100
2	Ed	331/333 (99%)	315 (95%)	16 (5%)	0	100	100
2	Ee	261/333 (78%)	247 (95%)	14 (5%)	0	100	100
2	Ef	183/333 (55%)	171 (93%)	12 (7%)	0	100	100
3	Ag	80/104 (77%)	76 (95%)	4 (5%)	0	100	100
3	Ah	71/104 (68%)	64 (90%)	7 (10%)	0	100	100
3	Bg	17/104 (16%)	15 (88%)	2 (12%)	0	100	100
3	Dg	79/104 (76%)	75 (95%)	4 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Dh	48/104 (46%)	46 (96%)	2 (4%)	0	100	100
3	Eg	80/104 (77%)	77 (96%)	3 (4%)	0	100	100
3	Eh	71/104 (68%)	66 (93%)	5 (7%)	0	100	100
4	Ai	36/97 (37%)	35 (97%)	1 (3%)	0	100	100
4	Aj	36/97 (37%)	34 (94%)	2 (6%)	0	100	100
4	Ak	36/97 (37%)	32 (89%)	3 (8%)	1 (3%)	4	23
4	Bk	10/97 (10%)	9 (90%)	1 (10%)	0	100	100
4	Cj	4/97 (4%)	4 (100%)	0	0	100	100
4	Di	25/97 (26%)	24 (96%)	1 (4%)	0	100	100
4	Dj	36/97 (37%)	35 (97%)	1 (3%)	0	100	100
4	Dk	36/97 (37%)	33 (92%)	3 (8%)	0	100	100
4	Ei	36/97 (37%)	34 (94%)	2 (6%)	0	100	100
4	Ej	36/97 (37%)	35 (97%)	1 (3%)	0	100	100
4	Ek	36/97 (37%)	33 (92%)	3 (8%)	0	100	100
5	FA	678/806 (84%)	657 (97%)	21 (3%)	0	100	100
5	FB	666/806 (83%)	647 (97%)	19 (3%)	0	100	100
5	FC	674/806 (84%)	658 (98%)	16 (2%)	0	100	100
5	FD	697/806 (86%)	662 (95%)	34 (5%)	1 (0%)	48	78
5	FE	652/806 (81%)	634 (97%)	18 (3%)	0	100	100
5	FF	676/806 (84%)	658 (97%)	18 (3%)	0	100	100
5	FG	668/806 (83%)	643 (96%)	25 (4%)	0	100	100
5	FH	679/806 (84%)	656 (97%)	21 (3%)	2 (0%)	36	64
5	FI	684/806 (85%)	669 (98%)	15 (2%)	0	100	100
5	FJ	690/806 (86%)	672 (97%)	18 (3%)	0	100	100
5	FK	661/806 (82%)	636 (96%)	25 (4%)	0	100	100
5	FL	669/806 (83%)	645 (96%)	24 (4%)	0	100	100
6	FM	222/236 (94%)	215 (97%)	7 (3%)	0	100	100
6	FN	222/236 (94%)	208 (94%)	14 (6%)	0	100	100
6	FO	222/236 (94%)	211 (95%)	11 (5%)	0	100	100
6	FP	222/236 (94%)	212 (96%)	10 (4%)	0	100	100
6	FQ	222/236 (94%)	208 (94%)	14 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	FR	222/236 (94%)	209 (94%)	13 (6%)	0	100	100
6	FS	225/236 (95%)	214 (95%)	11 (5%)	0	100	100
6	FT	222/236 (94%)	211 (95%)	11 (5%)	0	100	100
6	FU	222/236 (94%)	210 (95%)	12 (5%)	0	100	100
6	FV	222/236 (94%)	213 (96%)	9 (4%)	0	100	100
6	FW	222/236 (94%)	210 (95%)	12 (5%)	0	100	100
6	FX	222/236 (94%)	214 (96%)	8 (4%)	0	100	100
7	FY	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
7	FZ	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
7	GA	223/225 (99%)	210 (94%)	13 (6%)	0	100	100
7	GB	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
7	GC	223/225 (99%)	217 (97%)	6 (3%)	0	100	100
7	GD	223/225 (99%)	219 (98%)	4 (2%)	0	100	100
7	GE	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
7	GF	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
7	GG	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
7	GH	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
7	GI	223/225 (99%)	217 (97%)	6 (3%)	0	100	100
7	GJ	223/225 (99%)	210 (94%)	13 (6%)	0	100	100
8	GK	122/842 (14%)	117 (96%)	5 (4%)	0	100	100
8	GL	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GM	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GN	122/842 (14%)	112 (92%)	10 (8%)	0	100	100
8	GO	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GP	122/842 (14%)	120 (98%)	1 (1%)	1 (1%)	16	46
8	GQ	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GR	122/842 (14%)	112 (92%)	10 (8%)	0	100	100
8	GS	122/842 (14%)	117 (96%)	5 (4%)	0	100	100
8	GT	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GU	122/842 (14%)	114 (93%)	8 (7%)	0	100	100
8	GV	122/842 (14%)	115 (94%)	7 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	IK	30/842 (4%)	25 (83%)	5 (17%)	0	100	100
8	IL	30/842 (4%)	29 (97%)	1 (3%)	0	100	100
8	IM	30/842 (4%)	25 (83%)	5 (17%)	0	100	100
8	IN	30/842 (4%)	27 (90%)	3 (10%)	0	100	100
8	IO	30/842 (4%)	26 (87%)	4 (13%)	0	100	100
8	IP	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
8	IQ	30/842 (4%)	26 (87%)	4 (13%)	0	100	100
8	IR	30/842 (4%)	27 (90%)	3 (10%)	0	100	100
8	IS	30/842 (4%)	29 (97%)	1 (3%)	0	100	100
8	IT	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
8	IU	30/842 (4%)	27 (90%)	3 (10%)	0	100	100
8	IV	30/842 (4%)	27 (90%)	3 (10%)	0	100	100
All	All	32303/59653 (54%)	30962 (96%)	1335 (4%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	FH	266	PRO
5	FH	276	GLN
5	FD	267	ASP
2	Bb	107	TYR
8	GP	426	PHE
4	Ak	14	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	412/427 (96%)	409 (99%)	3 (1%)	76	76
1	AB	426/427 (100%)	425 (100%)	1 (0%)	87	84
1	AC	426/427 (100%)	426 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AD	387/427 (91%)	387 (100%)	0	100	100
1	AE	426/427 (100%)	425 (100%)	1 (0%)	87	84
1	AF	426/427 (100%)	424 (100%)	2 (0%)	81	78
1	BA	413/427 (97%)	410 (99%)	3 (1%)	76	76
1	BB	426/427 (100%)	426 (100%)	0	100	100
1	BC	426/427 (100%)	423 (99%)	3 (1%)	76	76
1	BD	387/427 (91%)	387 (100%)	0	100	100
1	BE	426/427 (100%)	423 (99%)	3 (1%)	76	76
1	BF	426/427 (100%)	425 (100%)	1 (0%)	87	84
1	CA	411/427 (96%)	407 (99%)	4 (1%)	68	72
1	CB	426/427 (100%)	426 (100%)	0	100	100
1	CC	426/427 (100%)	426 (100%)	0	100	100
1	CD	383/427 (90%)	379 (99%)	4 (1%)	68	72
1	CE	426/427 (100%)	426 (100%)	0	100	100
1	CF	426/427 (100%)	418 (98%)	8 (2%)	50	64
1	DA	413/427 (97%)	404 (98%)	9 (2%)	45	62
1	DB	426/427 (100%)	425 (100%)	1 (0%)	87	84
1	DC	426/427 (100%)	425 (100%)	1 (0%)	87	84
1	DD	387/427 (91%)	386 (100%)	1 (0%)	86	81
1	DE	426/427 (100%)	425 (100%)	1 (0%)	87	84
1	DF	426/427 (100%)	420 (99%)	6 (1%)	59	68
1	EA	413/427 (97%)	409 (99%)	4 (1%)	68	72
1	EB	426/427 (100%)	424 (100%)	2 (0%)	81	78
1	EC	426/427 (100%)	418 (98%)	8 (2%)	50	64
1	ED	387/427 (91%)	385 (100%)	2 (0%)	81	78
1	EE	426/427 (100%)	421 (99%)	5 (1%)	63	70
1	EF	426/427 (100%)	422 (99%)	4 (1%)	70	73
2	Aa	275/275 (100%)	273 (99%)	2 (1%)	76	76
2	Ab	275/275 (100%)	270 (98%)	5 (2%)	51	65
2	Ad	275/275 (100%)	270 (98%)	5 (2%)	51	65
2	Ae	225/275 (82%)	224 (100%)	1 (0%)	84	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Af	157/275 (57%)	151 (96%)	6 (4%)	29	51
2	Ba	275/275 (100%)	272 (99%)	3 (1%)	65	71
2	Bb	275/275 (100%)	268 (98%)	7 (2%)	42	59
2	Bd	275/275 (100%)	275 (100%)	0	100	100
2	Be	224/275 (82%)	223 (100%)	1 (0%)	84	79
2	Bf	157/275 (57%)	149 (95%)	8 (5%)	21	46
2	Ca	275/275 (100%)	273 (99%)	2 (1%)	76	76
2	Cb	275/275 (100%)	266 (97%)	9 (3%)	33	54
2	Cd	275/275 (100%)	270 (98%)	5 (2%)	51	65
2	Ce	225/275 (82%)	221 (98%)	4 (2%)	51	65
2	Cf	157/275 (57%)	150 (96%)	7 (4%)	24	48
2	Da	275/275 (100%)	275 (100%)	0	100	100
2	Db	275/275 (100%)	270 (98%)	5 (2%)	51	65
2	Dd	275/275 (100%)	271 (98%)	4 (2%)	57	66
2	De	225/275 (82%)	225 (100%)	0	100	100
2	Df	157/275 (57%)	155 (99%)	2 (1%)	61	69
2	Ea	275/275 (100%)	271 (98%)	4 (2%)	57	66
2	Eb	275/275 (100%)	273 (99%)	2 (1%)	76	76
2	Ed	275/275 (100%)	271 (98%)	4 (2%)	57	66
2	Ee	225/275 (82%)	222 (99%)	3 (1%)	61	69
2	Ef	157/275 (57%)	153 (98%)	4 (2%)	42	59
3	Ag	68/86 (79%)	66 (97%)	2 (3%)	37	56
3	Ah	62/86 (72%)	62 (100%)	0	100	100
3	Bg	68/86 (79%)	68 (100%)	0	100	100
3	Bh	62/86 (72%)	62 (100%)	0	100	100
3	Cg	68/86 (79%)	67 (98%)	1 (2%)	57	66
3	Ch	62/86 (72%)	62 (100%)	0	100	100
3	Dg	68/86 (79%)	68 (100%)	0	100	100
3	Dh	62/86 (72%)	62 (100%)	0	100	100
3	Eg	68/86 (79%)	68 (100%)	0	100	100
3	Eh	62/86 (72%)	62 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Ai	34/78 (44%)	34 (100%)	0	100	100
4	Aj	34/78 (44%)	34 (100%)	0	100	100
4	Ak	34/78 (44%)	34 (100%)	0	100	100
4	Bi	34/78 (44%)	34 (100%)	0	100	100
4	Bj	34/78 (44%)	34 (100%)	0	100	100
4	Bk	34/78 (44%)	34 (100%)	0	100	100
4	Ci	34/78 (44%)	34 (100%)	0	100	100
4	Cj	34/78 (44%)	33 (97%)	1 (3%)	37	56
4	Ck	34/78 (44%)	34 (100%)	0	100	100
4	Di	34/78 (44%)	33 (97%)	1 (3%)	37	56
4	Dj	34/78 (44%)	34 (100%)	0	100	100
4	Dk	34/78 (44%)	34 (100%)	0	100	100
4	Ei	34/78 (44%)	34 (100%)	0	100	100
4	Ej	34/78 (44%)	34 (100%)	0	100	100
4	Ek	34/78 (44%)	34 (100%)	0	100	100
5	FA	615/714 (86%)	608 (99%)	7 (1%)	65	71
5	FB	607/714 (85%)	599 (99%)	8 (1%)	61	69
5	FC	613/714 (86%)	608 (99%)	5 (1%)	73	74
5	FD	629/714 (88%)	619 (98%)	10 (2%)	55	66
5	FE	591/714 (83%)	585 (99%)	6 (1%)	68	72
5	FF	612/714 (86%)	604 (99%)	8 (1%)	61	69
5	FG	610/714 (85%)	599 (98%)	11 (2%)	51	65
5	FH	614/714 (86%)	593 (97%)	21 (3%)	32	53
5	FI	620/714 (87%)	606 (98%)	14 (2%)	44	61
5	FJ	623/714 (87%)	619 (99%)	4 (1%)	78	77
5	FK	600/714 (84%)	598 (100%)	2 (0%)	86	81
5	FL	608/714 (85%)	598 (98%)	10 (2%)	55	66
6	FM	206/215 (96%)	203 (98%)	3 (2%)	57	66
6	FN	206/215 (96%)	200 (97%)	6 (3%)	37	56
6	FO	206/215 (96%)	203 (98%)	3 (2%)	57	66
6	FP	206/215 (96%)	202 (98%)	4 (2%)	50	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	FQ	206/215 (96%)	206 (100%)	0	100	100
6	FR	206/215 (96%)	205 (100%)	1 (0%)	81	78
6	FS	209/215 (97%)	208 (100%)	1 (0%)	81	78
6	FT	206/215 (96%)	205 (100%)	1 (0%)	81	78
6	FU	206/215 (96%)	206 (100%)	0	100	100
6	FV	206/215 (96%)	204 (99%)	2 (1%)	68	72
6	FW	206/215 (96%)	204 (99%)	2 (1%)	68	72
6	FX	206/215 (96%)	203 (98%)	3 (2%)	57	66
7	FY	208/208 (100%)	206 (99%)	2 (1%)	68	72
7	FZ	208/208 (100%)	208 (100%)	0	100	100
7	GA	208/208 (100%)	206 (99%)	2 (1%)	68	72
7	GB	208/208 (100%)	207 (100%)	1 (0%)	81	78
7	GC	208/208 (100%)	207 (100%)	1 (0%)	81	78
7	GD	208/208 (100%)	208 (100%)	0	100	100
7	GE	208/208 (100%)	207 (100%)	1 (0%)	81	78
7	GF	208/208 (100%)	208 (100%)	0	100	100
7	GG	208/208 (100%)	206 (99%)	2 (1%)	68	72
7	GH	208/208 (100%)	208 (100%)	0	100	100
7	GI	208/208 (100%)	207 (100%)	1 (0%)	81	78
7	GJ	208/208 (100%)	208 (100%)	0	100	100
8	GK	100/644 (16%)	100 (100%)	0	100	100
8	GL	100/644 (16%)	100 (100%)	0	100	100
8	GM	100/644 (16%)	100 (100%)	0	100	100
8	GN	100/644 (16%)	99 (99%)	1 (1%)	68	72
8	GO	100/644 (16%)	97 (97%)	3 (3%)	36	56
8	GP	100/644 (16%)	98 (98%)	2 (2%)	48	63
8	GQ	100/644 (16%)	99 (99%)	1 (1%)	68	72
8	GR	100/644 (16%)	100 (100%)	0	100	100
8	GS	100/644 (16%)	99 (99%)	1 (1%)	68	72
8	GT	100/644 (16%)	100 (100%)	0	100	100
8	GU	100/644 (16%)	98 (98%)	2 (2%)	48	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	GV	100/644 (16%)	97 (97%)	3 (3%)	36	56
8	IK	26/644 (4%)	26 (100%)	0	100	100
8	IL	26/644 (4%)	26 (100%)	0	100	100
8	IM	26/644 (4%)	26 (100%)	0	100	100
8	IN	26/644 (4%)	26 (100%)	0	100	100
8	IO	26/644 (4%)	25 (96%)	1 (4%)	29	51
8	IP	26/644 (4%)	26 (100%)	0	100	100
8	IQ	26/644 (4%)	26 (100%)	0	100	100
8	IR	26/644 (4%)	26 (100%)	0	100	100
8	IS	26/644 (4%)	24 (92%)	2 (8%)	12	36
8	IT	26/644 (4%)	26 (100%)	0	100	100
8	IU	26/644 (4%)	26 (100%)	0	100	100
8	IV	26/644 (4%)	26 (100%)	0	100	100
All	All	33532/50815 (66%)	33199 (99%)	333 (1%)	65	72

All (333) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	91	ASN
1	AA	129	ASN
1	AA	130	GLN
1	AB	148	VAL
1	AE	332	VAL
1	AF	44	LEU
1	AF	131	VAL
2	Aa	108	ILE
2	Aa	295	VAL
2	Ab	207	ILE
2	Ab	219	ASP
2	Ab	221	GLU
2	Ab	223	ARG
2	Ab	329	THR
2	Ad	106	GLN
2	Ad	108	ILE
2	Ad	110	LEU
2	Ad	112	GLU
2	Ad	172	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Ae	222	ASP
2	Af	122	VAL
2	Af	198	VAL
2	Af	218	VAL
2	Af	219	ASP
2	Af	221	GLU
2	Af	222	ASP
3	Ag	89	ASN
3	Ag	97	VAL
1	BA	129	ASN
1	BA	130	GLN
1	BA	148	VAL
1	BC	88	ARG
1	BC	91	ASN
1	BC	449	TYR
1	BE	125	VAL
1	BE	158	THR
1	BE	356	THR
1	BF	56	LEU
2	Ba	108	ILE
2	Ba	145	LEU
2	Ba	295	VAL
2	Bb	108	ILE
2	Bb	110	LEU
2	Bb	113	GLU
2	Bb	216	ILE
2	Bb	217	THR
2	Bb	218	VAL
2	Bb	223	ARG
2	Be	149	THR
2	Bf	88	VAL
2	Bf	172	THR
2	Bf	198	VAL
2	Bf	217	THR
2	Bf	218	VAL
2	Bf	219	ASP
2	Bf	221	GLU
2	Bf	223	ARG
1	CA	129	ASN
1	CA	131	VAL
1	CA	190	VAL
1	CA	419	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CD	5	LEU
1	CD	7	LYS
1	CD	332	VAL
1	CD	367	VAL
1	CF	88	ARG
1	CF	91	ASN
1	CF	93	VAL
1	CF	95	VAL
1	CF	127	ASN
1	CF	130	GLN
1	CF	190	VAL
1	CF	196	VAL
2	Ca	31	VAL
2	Ca	108	ILE
2	Cb	105	ARG
2	Cb	108	ILE
2	Cb	169	VAL
2	Cb	172	THR
2	Cb	183	THR
2	Cb	218	VAL
2	Cb	222	ASP
2	Cb	224	LEU
2	Cb	231	VAL
2	Cd	106	GLN
2	Cd	108	ILE
2	Cd	111	SER
2	Cd	112	GLU
2	Cd	265	ASN
2	Ce	8	VAL
2	Ce	129	THR
2	Ce	168	ASP
2	Ce	266	ILE
2	Cf	147	ASN
2	Cf	198	VAL
2	Cf	215	THR
2	Cf	218	VAL
2	Cf	219	ASP
2	Cf	222	ASP
2	Cf	223	ARG
3	Cg	97	VAL
4	Cj	12	ASN
1	DA	21	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DA	22	ASP
1	DA	23	ASN
1	DA	129	ASN
1	DA	130	GLN
1	DA	131	VAL
1	DA	135	ARG
1	DA	239	THR
1	DA	252	GLU
1	DB	239	THR
1	DC	356	THR
1	DD	412	ILE
1	DE	367	VAL
1	DF	88	ARG
1	DF	90	GLU
1	DF	91	ASN
1	DF	129	ASN
1	DF	130	GLN
1	DF	196	VAL
2	Db	108	ILE
2	Db	111	SER
2	Db	169	VAL
2	Db	218	VAL
2	Db	295	VAL
2	Dd	110	LEU
2	Dd	172	THR
2	Dd	177	GLU
2	Dd	218	VAL
2	Df	218	VAL
2	Df	222	ASP
4	Di	3	THR
1	EA	128	LEU
1	EA	130	GLN
1	EA	179	VAL
1	EA	396	VAL
1	EB	11	LEU
1	EB	193	THR
1	EC	63	GLU
1	EC	66	ASP
1	EC	69	GLU
1	EC	70	TYR
1	EC	158	THR
1	EC	180	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	EC	229	ASN
1	EC	442	LYS
1	ED	408	VAL
1	ED	432	THR
1	EE	88	ARG
1	EE	89	ASP
1	EE	91	ASN
1	EE	93	VAL
1	EE	335	THR
1	EF	41	VAL
1	EF	128	LEU
1	EF	130	GLN
1	EF	229	ASN
2	Ea	105	ARG
2	Ea	106	GLN
2	Ea	108	ILE
2	Ea	111	SER
2	Eb	189	ILE
2	Eb	218	VAL
2	Ed	31	VAL
2	Ed	108	ILE
2	Ed	230	VAL
2	Ed	309	ASP
2	Ee	8	VAL
2	Ee	77	LEU
2	Ee	88	VAL
2	Ef	218	VAL
2	Ef	221	GLU
2	Ef	222	ASP
2	Ef	223	ARG
5	FA	180	ILE
5	FA	223	SER
5	FA	226	SER
5	FA	512	LYS
5	FA	618	ILE
5	FA	619	ASP
5	FA	622	GLU
5	FB	39	LEU
5	FB	139	ILE
5	FB	142	ASP
5	FB	201	CYS
5	FB	253	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	FB	295	GLU
5	FB	420	TYR
5	FB	588	CYS
5	FC	230	GLU
5	FC	378	VAL
5	FC	588	CYS
5	FC	618	ILE
5	FC	619	ASP
5	FD	35	PHE
5	FD	201	CYS
5	FD	253	VAL
5	FD	267	ASP
5	FD	290	ASN
5	FD	315	ILE
5	FD	318	SER
5	FD	324	LEU
5	FD	519	ILE
5	FD	639	GLN
5	FE	180	ILE
5	FE	201	CYS
5	FE	257	LYS
5	FE	260	LYS
5	FE	378	VAL
5	FE	588	CYS
5	FF	39	LEU
5	FF	237	LEU
5	FF	253	VAL
5	FF	277	MET
5	FF	378	VAL
5	FF	519	ILE
5	FF	616	MET
5	FF	619	ASP
5	FG	4	PHE
5	FG	5	LEU
5	FG	9	ARG
5	FG	59	HIS
5	FG	64	GLU
5	FG	65	LEU
5	FG	66	VAL
5	FG	282	GLU
5	FG	283	ARG
5	FG	298	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	FG	378	VAL
5	FH	139	ILE
5	FH	142	ASP
5	FH	263	GLU
5	FH	265	MET
5	FH	266	PRO
5	FH	267	ASP
5	FH	268	TYR
5	FH	271	GLN
5	FH	274	VAL
5	FH	275	ASP
5	FH	276	GLN
5	FH	288	ASN
5	FH	315	ILE
5	FH	317	ASN
5	FH	318	SER
5	FH	533	ILE
5	FH	564	THR
5	FH	616	MET
5	FH	618	ILE
5	FH	619	ASP
5	FH	622	GLU
5	FI	36	ASN
5	FI	37	TYR
5	FI	38	SER
5	FI	41	ARG
5	FI	77	ILE
5	FI	180	ILE
5	FI	201	CYS
5	FI	298	VAL
5	FI	328	LEU
5	FI	393	VAL
5	FI	588	CYS
5	FI	617	GLU
5	FI	619	ASP
5	FI	622	GLU
5	FJ	201	CYS
5	FJ	364	VAL
5	FJ	588	CYS
5	FJ	686	ILE
5	FK	5	LEU
5	FK	78	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	FL	201	CYS
5	FL	269	ILE
5	FL	297	THR
5	FL	299	ARG
5	FL	320	LEU
5	FL	517	THR
5	FL	588	CYS
5	FL	617	GLU
5	FL	619	ASP
5	FL	657	THR
6	FM	83	LEU
6	FM	84	ARG
6	FM	86	MET
6	FN	8	VAL
6	FN	83	LEU
6	FN	94	PRO
6	FN	95	THR
6	FN	96	HIS
6	FN	125	GLU
6	FO	56	ASP
6	FO	137	ASP
6	FO	172	ILE
6	FP	84	ARG
6	FP	87	THR
6	FP	120	THR
6	FP	172	ILE
6	FR	15	ASP
6	FS	137	ASP
6	FT	233	ILE
6	FV	84	ARG
6	FV	87	THR
6	FW	83	LEU
6	FW	84	ARG
6	FX	15	ASP
6	FX	125	GLU
6	FX	137	ASP
7	FY	19	ASP
7	FY	51	ILE
7	GA	130	CYS
7	GA	170	CYS
7	GB	135	ASP
7	GC	117	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	GE	170	CYS
7	GG	51	ILE
7	GG	118	VAL
7	GI	130	CYS
8	GN	493	ILE
8	GO	459	GLN
8	GO	460	ILE
8	GO	471	VAL
8	GP	426	PHE
8	GP	471	VAL
8	GQ	471	VAL
8	GS	471	VAL
8	GU	471	VAL
8	GU	503	THR
8	GV	454	PRO
8	GV	459	GLN
8	GV	471	VAL
8	IO	242	THR
8	IS	243	SER
8	IS	245	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (699) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	42	GLN
1	AA	57	ASN
1	AA	101	ASN
1	AA	229	ASN
1	AA	235	GLN
1	AA	278	ASN
1	AA	342	GLN
1	AA	344	HIS
1	AA	361	ASN
1	AA	377	ASN
1	AA	458	ASN
1	AA	463	GLN
1	AB	9	GLN
1	AB	24	HIS
1	AB	271	ASN
1	AB	295	GLN
1	AB	342	GLN
1	AB	377	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AB	410	ASN
1	AB	458	ASN
1	AC	31	GLN
1	AC	42	GLN
1	AC	254	GLN
1	AC	273	ASN
1	AC	284	ASN
1	AC	342	GLN
1	AC	410	ASN
1	AC	414	HIS
1	AC	435	GLN
1	AC	458	ASN
1	AC	479	HIS
1	AD	98	ASN
1	AD	167	GLN
1	AD	200	ASN
1	AD	214	ASN
1	AD	217	ASN
1	AD	254	GLN
1	AD	278	ASN
1	AD	295	GLN
1	AD	361	ASN
1	AD	377	ASN
1	AD	410	ASN
1	AD	414	HIS
1	AD	435	GLN
1	AE	9	GLN
1	AE	14	GLN
1	AE	129	ASN
1	AE	214	ASN
1	AE	245	HIS
1	AE	278	ASN
1	AE	284	ASN
1	AE	361	ASN
1	AE	377	ASN
1	AE	384	GLN
1	AF	24	HIS
1	AF	42	GLN
1	AF	57	ASN
1	AF	91	ASN
1	AF	101	ASN
1	AF	168	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AF	245	HIS
1	AF	410	ASN
1	AF	463	GLN
2	Aa	7	GLN
2	Aa	97	ASN
2	Aa	115	GLN
2	Ab	20	ASN
2	Ab	75	HIS
2	Ab	147	ASN
2	Ab	195	GLN
2	Ab	212	GLN
2	Ad	7	GLN
2	Ad	75	HIS
2	Ad	96	GLN
2	Ad	156	ASN
2	Ad	285	HIS
2	Ad	316	ASN
2	Ae	97	ASN
2	Ae	115	GLN
2	Ae	316	ASN
2	Af	144	ASN
2	Af	204	GLN
3	Ag	32	GLN
3	Ag	54	ASN
3	Ah	57	GLN
4	Ai	12	ASN
1	BA	38	ASN
1	BA	42	GLN
1	BA	57	ASN
1	BA	68	ASN
1	BA	130	GLN
1	BA	159	GLN
1	BA	261	ASN
1	BA	278	ASN
1	BA	284	ASN
1	BA	300	ASN
1	BA	344	HIS
1	BA	392	ASN
1	BA	479	HIS
1	BB	31	GLN
1	BB	42	GLN
1	BB	98	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BB	159	GLN
1	BB	241	ASN
1	BB	245	HIS
1	BB	271	ASN
1	BB	361	ASN
1	BB	377	ASN
1	BB	392	ASN
1	BB	410	ASN
1	BC	34	GLN
1	BC	57	ASN
1	BC	91	ASN
1	BC	168	GLN
1	BC	260	ASN
1	BC	273	ASN
1	BC	361	ASN
1	BC	414	HIS
1	BC	466	ASN
1	BC	479	HIS
1	BC	503	GLN
1	BD	159	GLN
1	BD	167	GLN
1	BD	245	HIS
1	BD	254	GLN
1	BD	278	ASN
1	BE	14	GLN
1	BE	15	HIS
1	BE	98	ASN
1	BE	130	GLN
1	BE	200	ASN
1	BE	229	ASN
1	BE	245	HIS
1	BE	377	ASN
1	BE	384	GLN
1	BE	410	ASN
1	BF	14	GLN
1	BF	42	GLN
1	BF	57	ASN
1	BF	68	ASN
1	BF	261	ASN
1	BF	284	ASN
1	BF	295	GLN
1	BF	342	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BF	392	ASN
1	BF	414	HIS
1	BF	435	GLN
2	Ba	44	GLN
2	Ba	115	GLN
2	Ba	186	ASN
2	Ba	204	GLN
2	Bb	212	GLN
2	Bb	241	HIS
2	Bd	6	ASN
2	Bd	96	GLN
2	Bd	316	ASN
2	Bd	323	ASN
2	Be	187	GLN
2	Be	195	GLN
3	Bg	89	ASN
3	Bh	82	GLN
4	Bi	12	ASN
4	Bk	17	ASN
1	CA	42	GLN
1	CA	57	ASN
1	CA	129	ASN
1	CA	271	ASN
1	CA	278	ASN
1	CA	300	ASN
1	CA	342	GLN
1	CA	479	HIS
1	CB	23	ASN
1	CB	34	GLN
1	CB	159	GLN
1	CB	295	GLN
1	CB	342	GLN
1	CB	377	ASN
1	CB	392	ASN
1	CB	447	ASN
1	CB	458	ASN
1	CB	466	ASN
1	CC	14	GLN
1	CC	30	GLN
1	CC	31	GLN
1	CC	42	GLN
1	CC	129	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CC	157	ASN
1	CC	168	GLN
1	CC	261	ASN
1	CC	295	GLN
1	CC	342	GLN
1	CC	362	ASN
1	CC	410	ASN
1	CC	414	HIS
1	CC	479	HIS
1	CD	38	ASN
1	CD	167	GLN
1	CD	273	ASN
1	CD	361	ASN
1	CD	377	ASN
1	CD	410	ASN
1	CE	9	GLN
1	CE	14	GLN
1	CE	34	GLN
1	CE	101	ASN
1	CE	229	ASN
1	CE	254	GLN
1	CE	273	ASN
1	CE	284	ASN
1	CE	295	GLN
1	CE	371	GLN
1	CE	377	ASN
1	CE	384	GLN
1	CE	458	ASN
1	CE	479	HIS
1	CF	14	GLN
1	CF	42	GLN
1	CF	101	ASN
1	CF	130	GLN
1	CF	168	GLN
1	CF	214	ASN
1	CF	235	GLN
1	CF	245	HIS
1	CF	278	ASN
1	CF	392	ASN
1	CF	414	HIS
2	Ca	96	GLN
2	Ca	115	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Ca	187	GLN
2	Ca	204	GLN
2	Cb	75	HIS
2	Cb	97	ASN
2	Cb	156	ASN
2	Cb	212	GLN
2	Cb	292	ASN
2	Cb	323	ASN
2	Cd	156	ASN
2	Cd	285	HIS
2	Cd	292	ASN
2	Cd	323	ASN
2	Ce	97	ASN
2	Ce	204	GLN
2	Cf	144	ASN
2	Cf	195	GLN
2	Cf	204	GLN
3	Cg	89	ASN
3	Ch	57	GLN
3	Ch	82	GLN
3	Ch	89	ASN
4	Ci	31	ASN
1	DA	42	GLN
1	DA	68	ASN
1	DA	342	GLN
1	DB	245	HIS
1	DB	271	ASN
1	DB	284	ASN
1	DB	295	GLN
1	DB	377	ASN
1	DB	392	ASN
1	DB	410	ASN
1	DC	14	GLN
1	DC	31	GLN
1	DC	42	GLN
1	DC	91	ASN
1	DC	129	ASN
1	DC	130	GLN
1	DC	168	GLN
1	DC	261	ASN
1	DC	342	GLN
1	DC	414	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DC	435	GLN
1	DC	447	ASN
1	DC	466	ASN
1	DD	101	ASN
1	DD	159	GLN
1	DD	167	GLN
1	DD	214	ASN
1	DD	254	GLN
1	DD	503	GLN
1	DE	14	GLN
1	DE	23	ASN
1	DE	38	ASN
1	DE	127	ASN
1	DE	129	ASN
1	DE	241	ASN
1	DE	261	ASN
1	DE	278	ASN
1	DE	284	ASN
1	DE	295	GLN
1	DE	361	ASN
1	DE	377	ASN
1	DE	384	GLN
1	DE	435	GLN
1	DE	458	ASN
1	DF	91	ASN
1	DF	245	HIS
1	DF	278	ASN
1	DF	342	GLN
1	DF	377	ASN
1	DF	392	ASN
2	Da	75	HIS
2	Da	97	ASN
2	Da	187	GLN
2	Da	265	ASN
2	Db	10	GLN
2	Db	61	HIS
2	Db	204	GLN
2	Db	316	ASN
2	Dd	20	ASN
2	Dd	96	GLN
2	Dd	97	ASN
2	Dd	292	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	De	156	ASN
2	De	212	GLN
2	Df	187	GLN
2	Df	204	GLN
3	Dg	32	GLN
3	Dg	57	GLN
3	Dg	89	ASN
3	Dh	56	GLN
3	Dh	82	GLN
4	Di	12	ASN
4	Dj	30	ASN
4	Dj	31	ASN
4	Dk	12	ASN
4	Dk	17	ASN
1	EA	24	HIS
1	EA	31	GLN
1	EA	34	GLN
1	EA	57	ASN
1	EA	130	GLN
1	EA	157	ASN
1	EA	168	GLN
1	EA	214	ASN
1	EA	229	ASN
1	EA	254	GLN
1	EA	260	ASN
1	EA	261	ASN
1	EA	295	GLN
1	EA	300	ASN
1	EA	435	GLN
1	EA	463	GLN
1	EB	9	GLN
1	EB	91	ASN
1	EB	168	GLN
1	EB	245	HIS
1	EB	305	ASN
1	EB	361	ASN
1	EB	410	ASN
1	EC	14	GLN
1	EC	38	ASN
1	EC	98	ASN
1	EC	168	GLN
1	EC	261	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	EC	300	ASN
1	EC	362	ASN
1	EC	414	HIS
1	EC	447	ASN
1	EC	466	ASN
1	ED	167	GLN
1	ED	200	ASN
1	ED	217	ASN
1	ED	271	ASN
1	ED	284	ASN
1	ED	305	ASN
1	ED	414	HIS
1	ED	435	GLN
1	EE	9	GLN
1	EE	14	GLN
1	EE	81	ASN
1	EE	98	ASN
1	EE	129	ASN
1	EE	157	ASN
1	EE	261	ASN
1	EE	278	ASN
1	EE	284	ASN
1	EE	300	ASN
1	EE	305	ASN
1	EE	377	ASN
1	EE	384	GLN
1	EE	458	ASN
1	EE	479	HIS
1	EF	68	ASN
1	EF	129	ASN
1	EF	159	GLN
1	EF	245	HIS
1	EF	254	GLN
1	EF	261	ASN
1	EF	278	ASN
1	EF	295	GLN
1	EF	300	ASN
1	EF	392	ASN
1	EF	414	HIS
1	EF	463	GLN
1	EF	479	HIS
2	Ea	7	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Ea	44	GLN
2	Ea	75	HIS
2	Ea	96	GLN
2	Ea	106	GLN
2	Ea	187	GLN
2	Eb	156	ASN
2	Eb	316	ASN
2	Ed	20	ASN
2	Ed	96	GLN
2	Ed	156	ASN
2	Ed	186	ASN
2	Ed	265	ASN
2	Ed	323	ASN
2	Ee	106	GLN
2	Ee	115	GLN
2	Ee	144	ASN
2	Ee	312	HIS
2	Ee	316	ASN
2	Ef	156	ASN
2	Ef	186	ASN
2	Ef	195	GLN
2	Ef	204	GLN
3	Eg	54	ASN
3	Eg	57	GLN
3	Eh	32	GLN
3	Eh	82	GLN
4	Ei	12	ASN
4	Ei	17	ASN
4	Ej	17	ASN
4	Ej	30	ASN
5	FA	82	GLN
5	FA	185	ASN
5	FA	366	ASN
5	FA	401	GLN
5	FA	438	ASN
5	FA	449	ASN
5	FA	455	ASN
5	FA	484	HIS
5	FA	508	ASN
5	FA	526	GLN
5	FA	639	GLN
5	FA	650	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	FA	676	GLN
5	FA	723	ASN
5	FB	152	ASN
5	FB	401	GLN
5	FB	406	ASN
5	FB	438	ASN
5	FB	524	GLN
5	FB	634	ASN
5	FB	639	GLN
5	FB	676	GLN
5	FB	685	GLN
5	FB	701	GLN
5	FC	10	GLN
5	FC	31	GLN
5	FC	128	GLN
5	FC	200	GLN
5	FC	288	ASN
5	FC	484	HIS
5	FC	508	ASN
5	FC	524	GLN
5	FC	601	ASN
5	FC	634	ASN
5	FC	656	GLN
5	FC	702	GLN
5	FC	709	GLN
5	FC	711	GLN
5	FC	718	GLN
5	FC	727	ASN
5	FD	46	HIS
5	FD	200	GLN
5	FD	309	ASN
5	FD	317	ASN
5	FD	484	HIS
5	FD	518	ASN
5	FD	528	ASN
5	FD	676	GLN
5	FD	685	GLN
5	FD	709	GLN
5	FD	727	ASN
5	FD	728	GLN
5	FE	10	GLN
5	FE	128	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	FE	172	ASN
5	FE	200	GLN
5	FE	366	ASN
5	FE	401	GLN
5	FE	449	ASN
5	FE	518	ASN
5	FE	524	GLN
5	FE	546	GLN
5	FE	676	GLN
5	FE	685	GLN
5	FE	697	GLN
5	FE	710	GLN
5	FE	723	ASN
5	FE	735	GLN
5	FF	6	ASN
5	FF	92	ASN
5	FF	152	ASN
5	FF	200	GLN
5	FF	271	GLN
5	FF	357	ASN
5	FF	401	GLN
5	FF	406	ASN
5	FF	407	ASN
5	FF	438	ASN
5	FF	601	ASN
5	FF	634	ASN
5	FF	709	GLN
5	FF	723	ASN
5	FF	728	GLN
5	FG	82	GLN
5	FG	200	GLN
5	FG	401	GLN
5	FG	438	ASN
5	FG	455	ASN
5	FG	546	GLN
5	FG	566	GLN
5	FG	634	ASN
5	FG	639	GLN
5	FG	676	GLN
5	FG	728	GLN
5	FH	30	ASN
5	FH	111	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	FH	200	GLN
5	FH	288	ASN
5	FH	317	ASN
5	FH	389	ASN
5	FH	546	GLN
5	FH	676	GLN
5	FH	718	GLN
5	FH	723	ASN
5	FI	10	GLN
5	FI	36	ASN
5	FI	200	GLN
5	FI	389	ASN
5	FI	449	ASN
5	FI	634	ASN
5	FI	639	GLN
5	FI	643	GLN
5	FI	676	GLN
5	FI	697	GLN
5	FI	701	GLN
5	FI	727	ASN
5	FI	728	GLN
5	FJ	10	GLN
5	FJ	30	ASN
5	FJ	31	GLN
5	FJ	168	ASN
5	FJ	271	GLN
5	FJ	279	ASN
5	FJ	389	ASN
5	FJ	401	GLN
5	FJ	484	HIS
5	FJ	518	ASN
5	FJ	526	GLN
5	FJ	634	ASN
5	FJ	650	GLN
5	FJ	690	GLN
5	FJ	718	GLN
5	FJ	727	ASN
5	FJ	737	GLN
5	FK	55	ASN
5	FK	185	ASN
5	FK	200	GLN
5	FK	406	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	FK	508	ASN
5	FK	650	GLN
5	FK	676	GLN
5	FK	709	GLN
5	FK	723	ASN
5	FL	31	GLN
5	FL	200	GLN
5	FL	227	ASN
5	FL	327	ASN
5	FL	401	GLN
5	FL	508	ASN
5	FL	634	ASN
5	FL	701	GLN
5	FL	702	GLN
5	FL	718	GLN
5	FL	728	GLN
6	FM	3	ASN
6	FM	6	ASN
6	FM	46	ASN
6	FM	181	GLN
6	FM	236	HIS
6	FN	46	ASN
6	FN	77	HIS
6	FN	178	ASN
6	FN	192	ASN
6	FO	46	ASN
6	FO	96	HIS
6	FP	27	ASN
6	FP	46	ASN
6	FP	114	GLN
6	FP	193	ASN
6	FP	236	HIS
6	FQ	3	ASN
6	FQ	46	ASN
6	FQ	190	GLN
6	FQ	236	HIS
6	FR	3	ASN
6	FR	211	ASN
6	FS	46	ASN
6	FS	236	HIS
6	FT	27	ASN
6	FT	192	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	FU	3	ASN
6	FU	27	ASN
6	FU	46	ASN
6	FU	72	ASN
6	FU	114	GLN
6	FU	192	ASN
6	FV	46	ASN
6	FV	77	HIS
6	FV	91	ASN
6	FV	192	ASN
6	FW	3	ASN
6	FW	96	HIS
6	FW	147	ASN
6	FX	27	ASN
6	FX	46	ASN
6	FX	190	GLN
7	FY	144	ASN
7	FZ	104	GLN
7	FZ	144	ASN
7	FZ	146	GLN
7	GA	144	ASN
7	GB	156	ASN
7	GC	4	ASN
7	GC	50	GLN
7	GD	50	GLN
7	GD	104	GLN
7	GE	42	GLN
7	GE	57	GLN
7	GE	104	GLN
7	GF	126	ASN
7	GF	144	ASN
7	GF	146	GLN
7	GG	104	GLN
7	GG	144	ASN
7	GH	42	GLN
7	GH	104	GLN
7	GH	156	ASN
7	GI	42	GLN
7	GI	126	ASN
7	GI	156	ASN
7	GJ	42	GLN
7	GJ	104	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	GK	431	ASN
8	GK	453	ASN
8	GK	469	ASN
8	GK	539	GLN
8	GK	544	GLN
8	GL	431	ASN
8	GL	456	GLN
8	GL	459	GLN
8	GL	469	ASN
8	GL	473	GLN
8	GM	431	ASN
8	GM	445	ASN
8	GN	539	GLN
8	GO	431	ASN
8	GO	453	ASN
8	GO	459	GLN
8	GP	469	ASN
8	GP	529	GLN
8	GQ	431	ASN
8	GQ	445	ASN
8	GQ	450	HIS
8	GQ	544	GLN
8	GR	453	ASN
8	GR	473	GLN
8	GR	539	GLN
8	GS	431	ASN
8	GS	450	HIS
8	GS	544	GLN
8	GT	431	ASN
8	GT	469	ASN
8	GT	473	GLN
8	GU	431	ASN
8	GU	459	GLN
8	GU	544	GLN
8	GV	431	ASN
8	GV	459	GLN
8	GV	520	ASN
8	IK	229	ASN
8	IK	231	GLN
8	IL	229	ASN
8	IM	231	GLN
8	IN	225	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	IN	231	GLN
8	IP	231	GLN
8	IQ	231	GLN
8	IR	225	ASN
8	IR	239	GLN
8	IS	231	GLN
8	IT	231	GLN
8	IV	225	ASN
8	IV	231	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 27 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

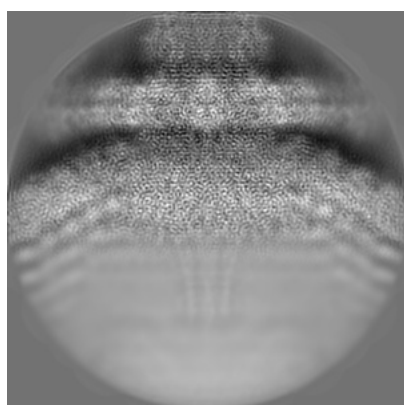
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14091. These allow visual inspection of the internal detail of the map and identification of artifacts.

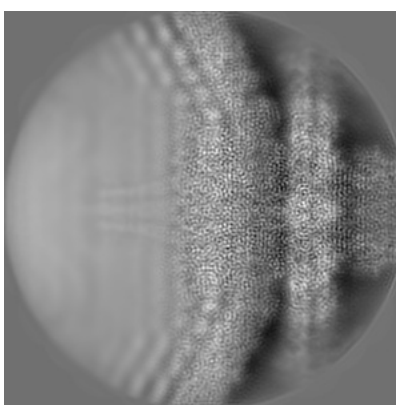
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

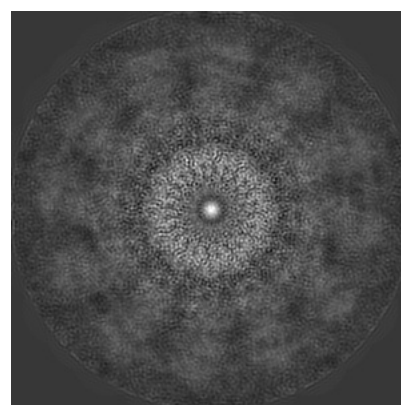
6.1.1 Primary map



X



Y

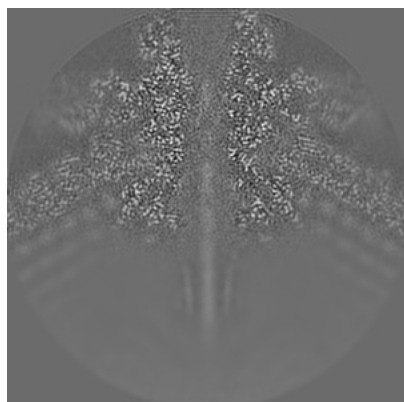


Z

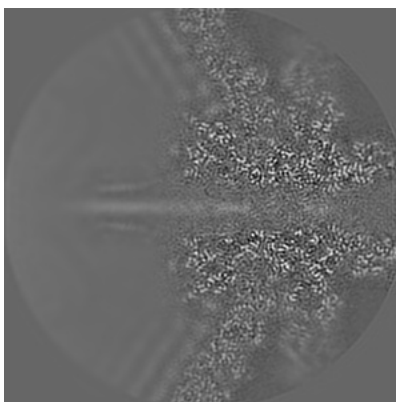
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

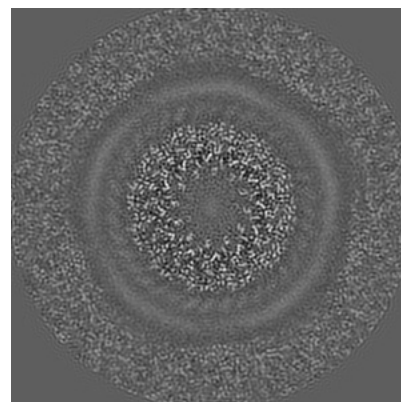
6.2.1 Primary map



X Index: 143



Y Index: 143

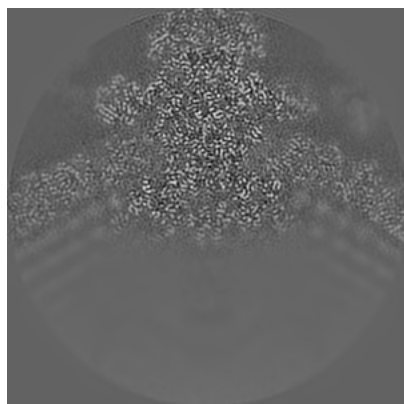


Z Index: 143

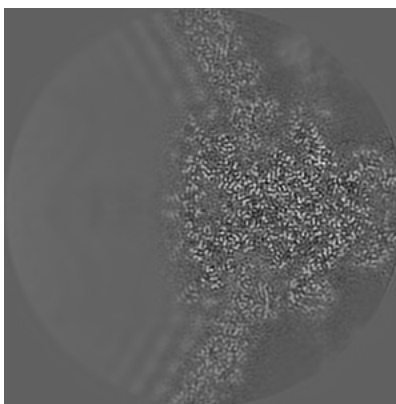
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

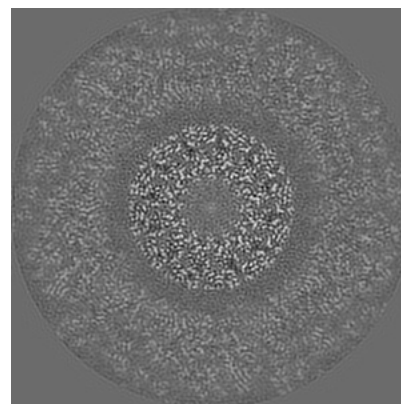
6.3.1 Primary map



X Index: 166



Y Index: 121

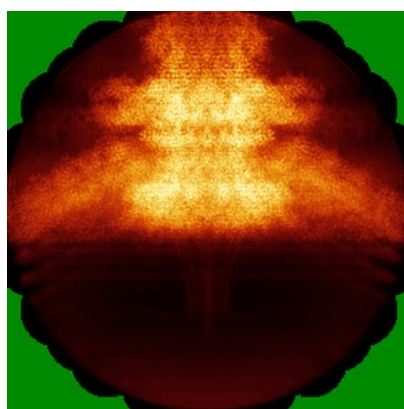


Z Index: 158

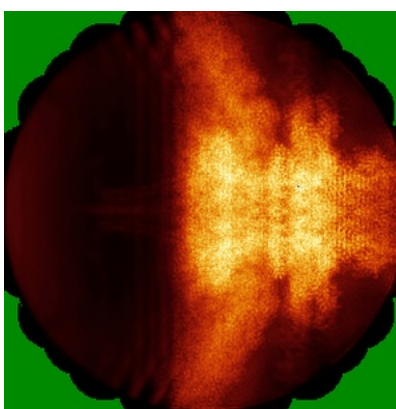
The images above show the largest variance slices of the map in three orthogonal directions.

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

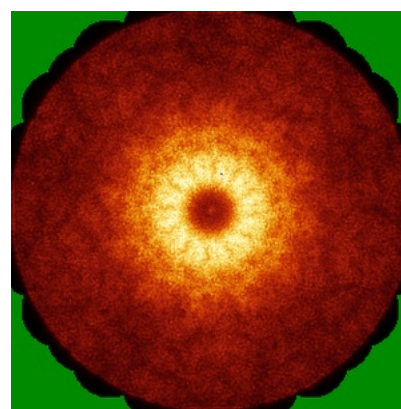
6.4.1 Primary map



X



Y

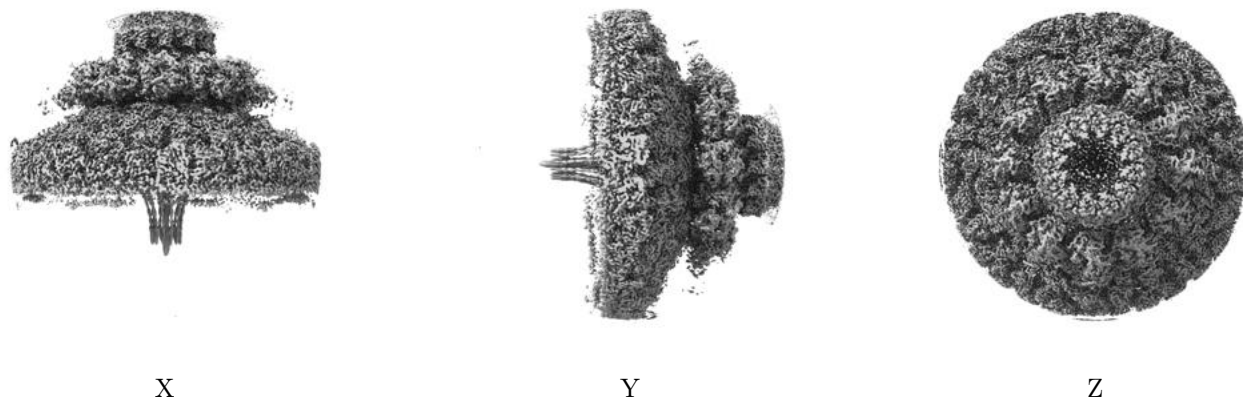


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

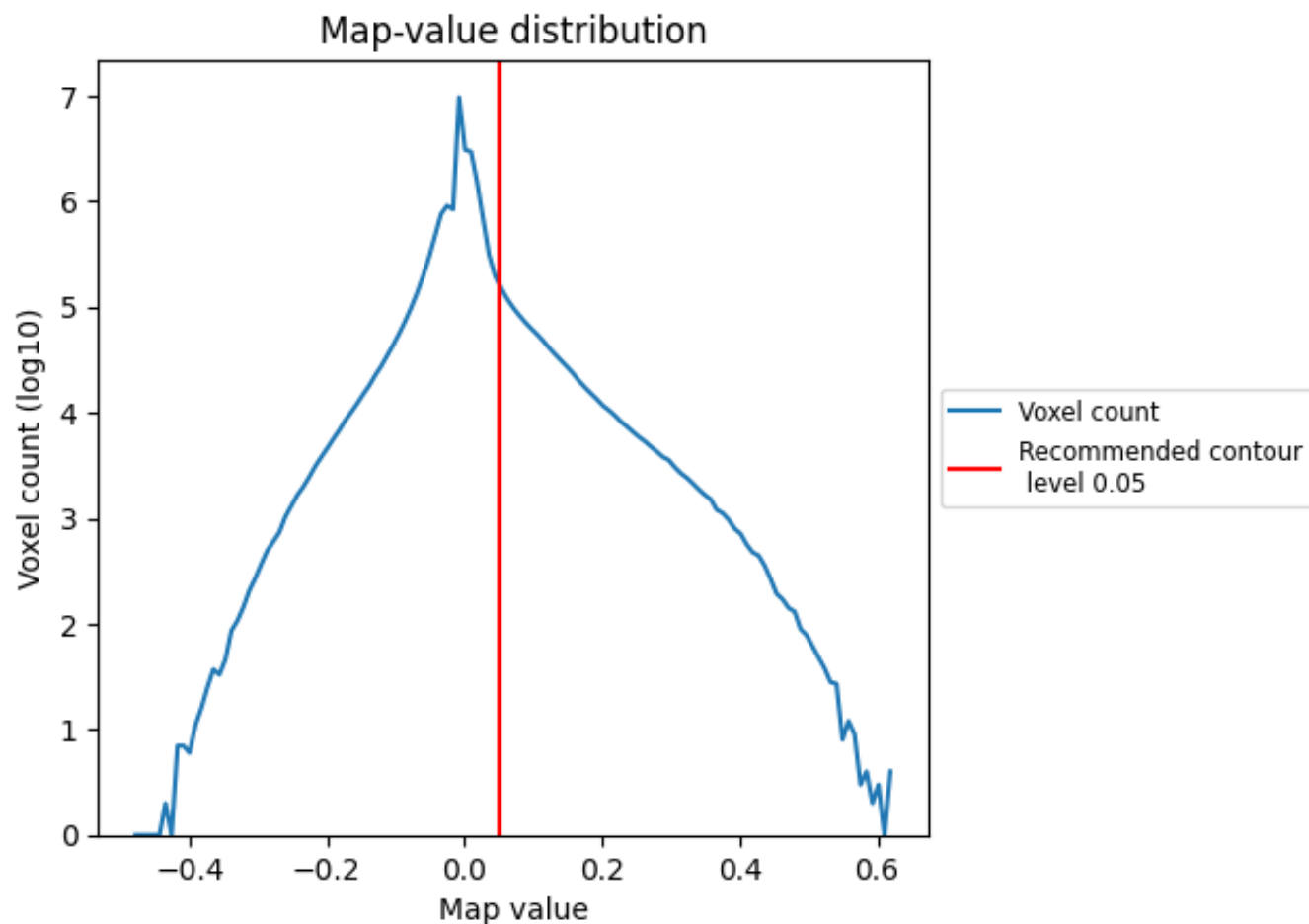
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

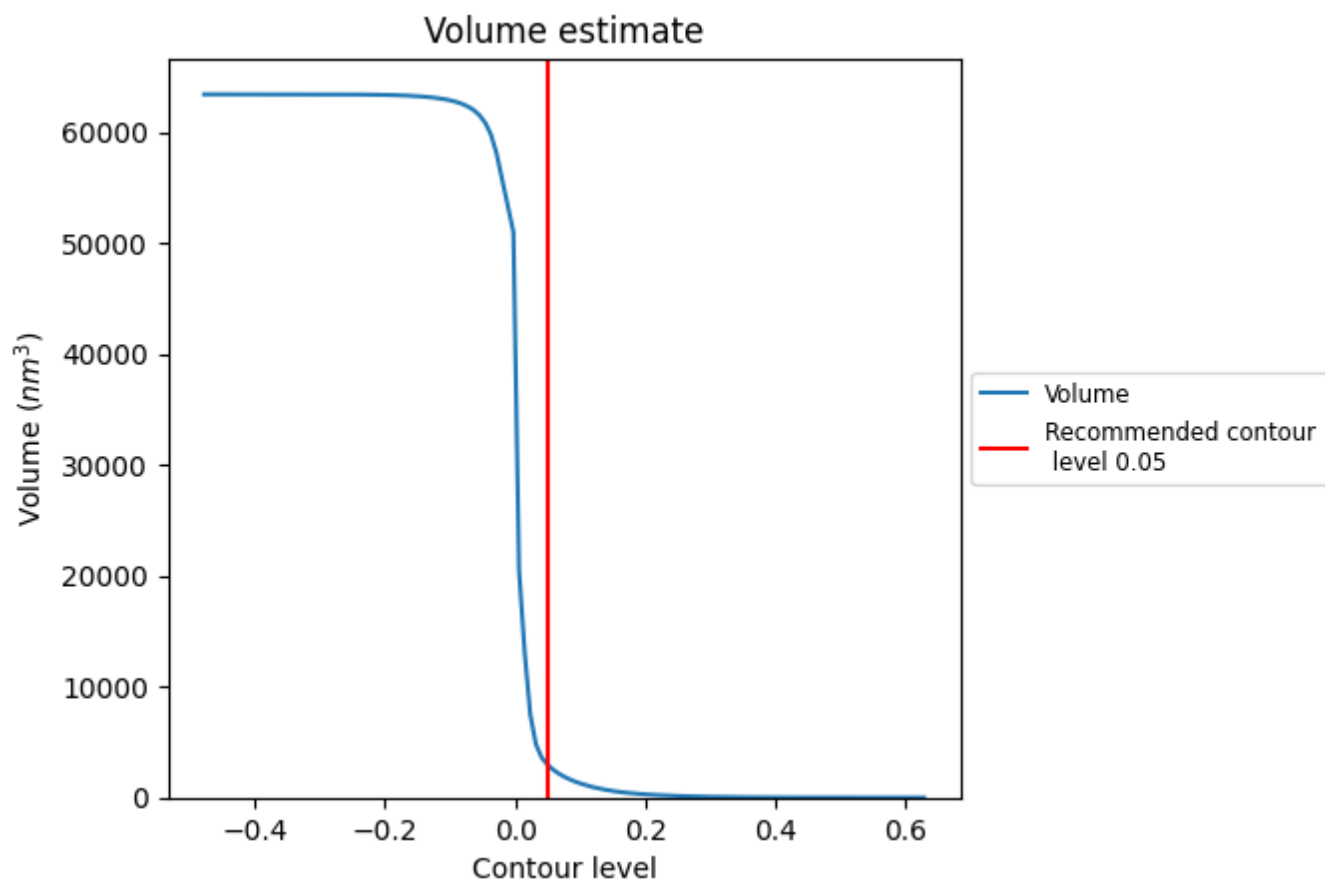
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

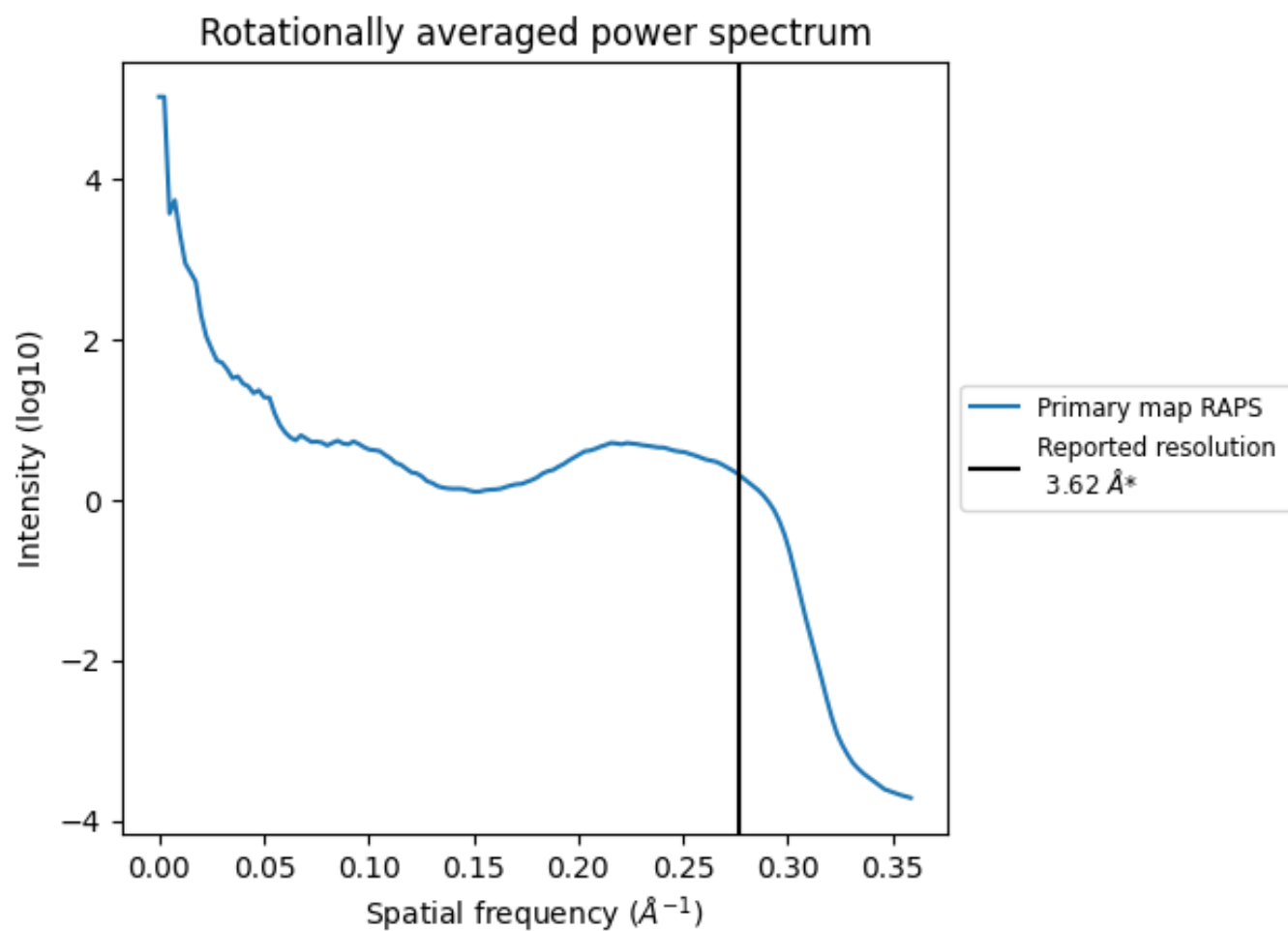
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2949 nm^3 ; this corresponds to an approximate mass of 2664 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 ⓘ

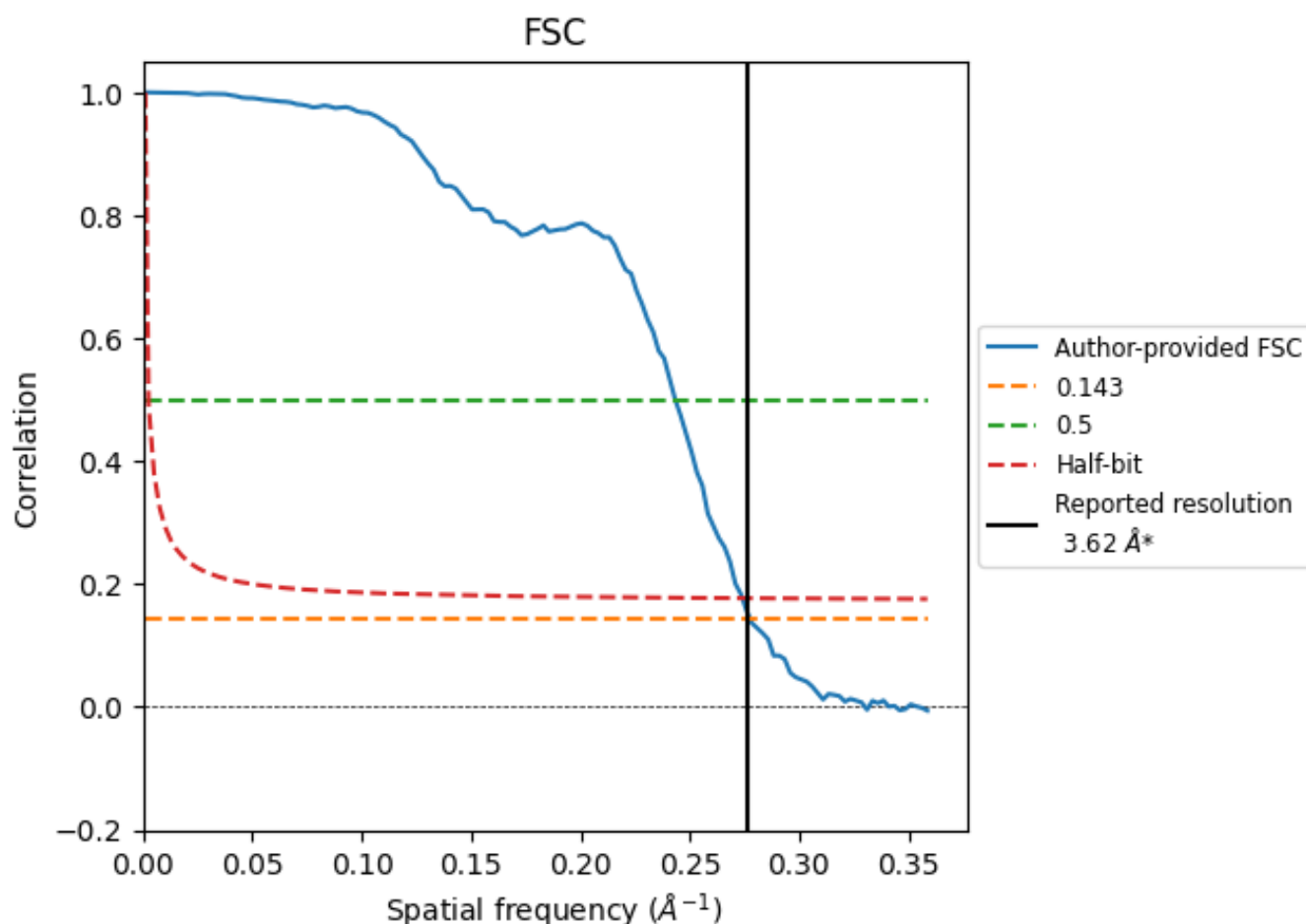


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

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 0.276 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

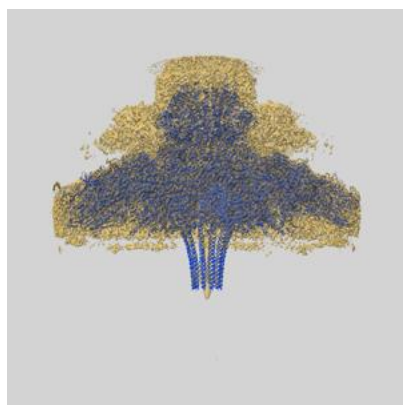
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.60	4.11	3.65
Unmasked-calculated*	-	-	-

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

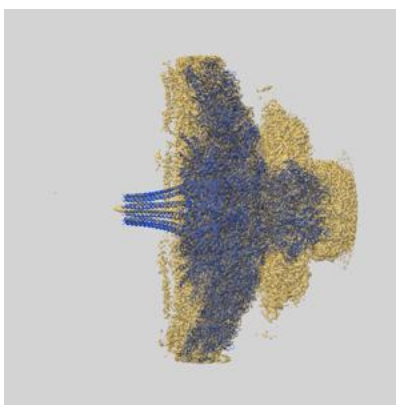
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14091 and PDB model 7QOI. Per-residue inclusion information can be found in section [3](#) on page [18](#).

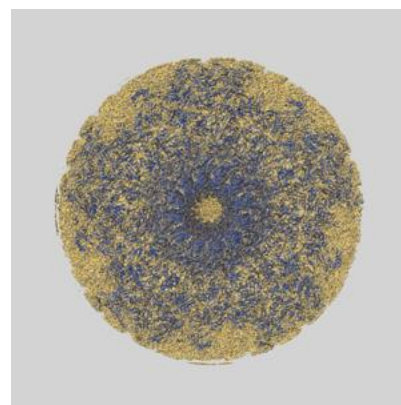
9.1 Map-model overlay [i](#)



X



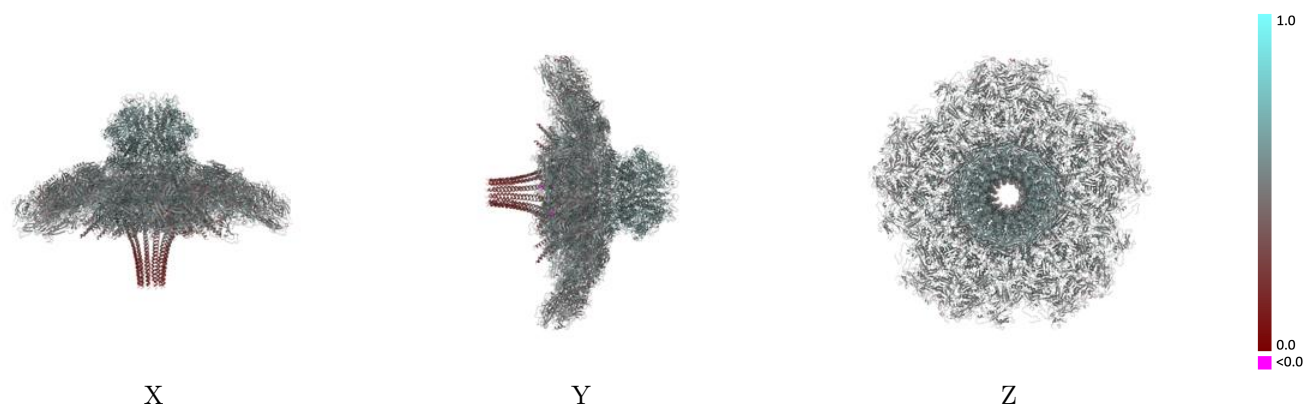
Y



Z

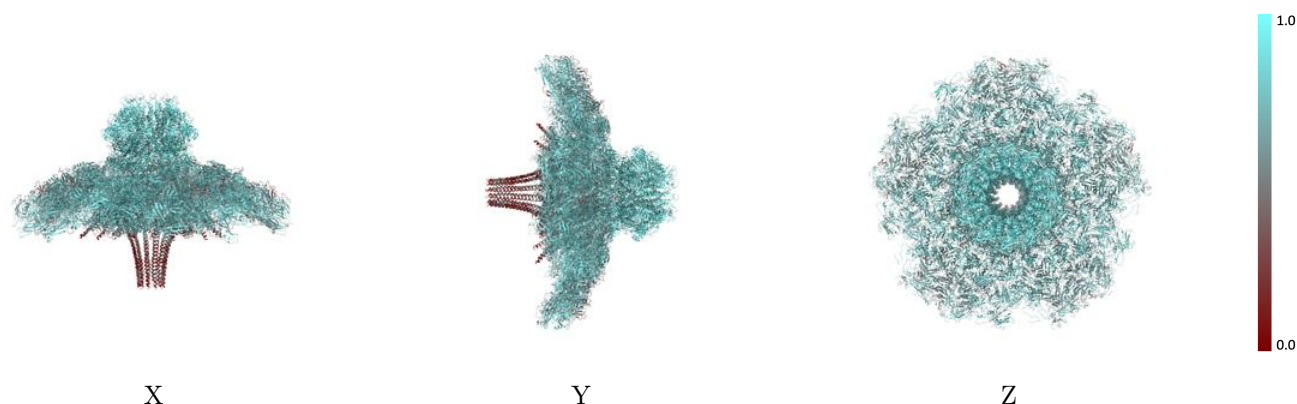
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



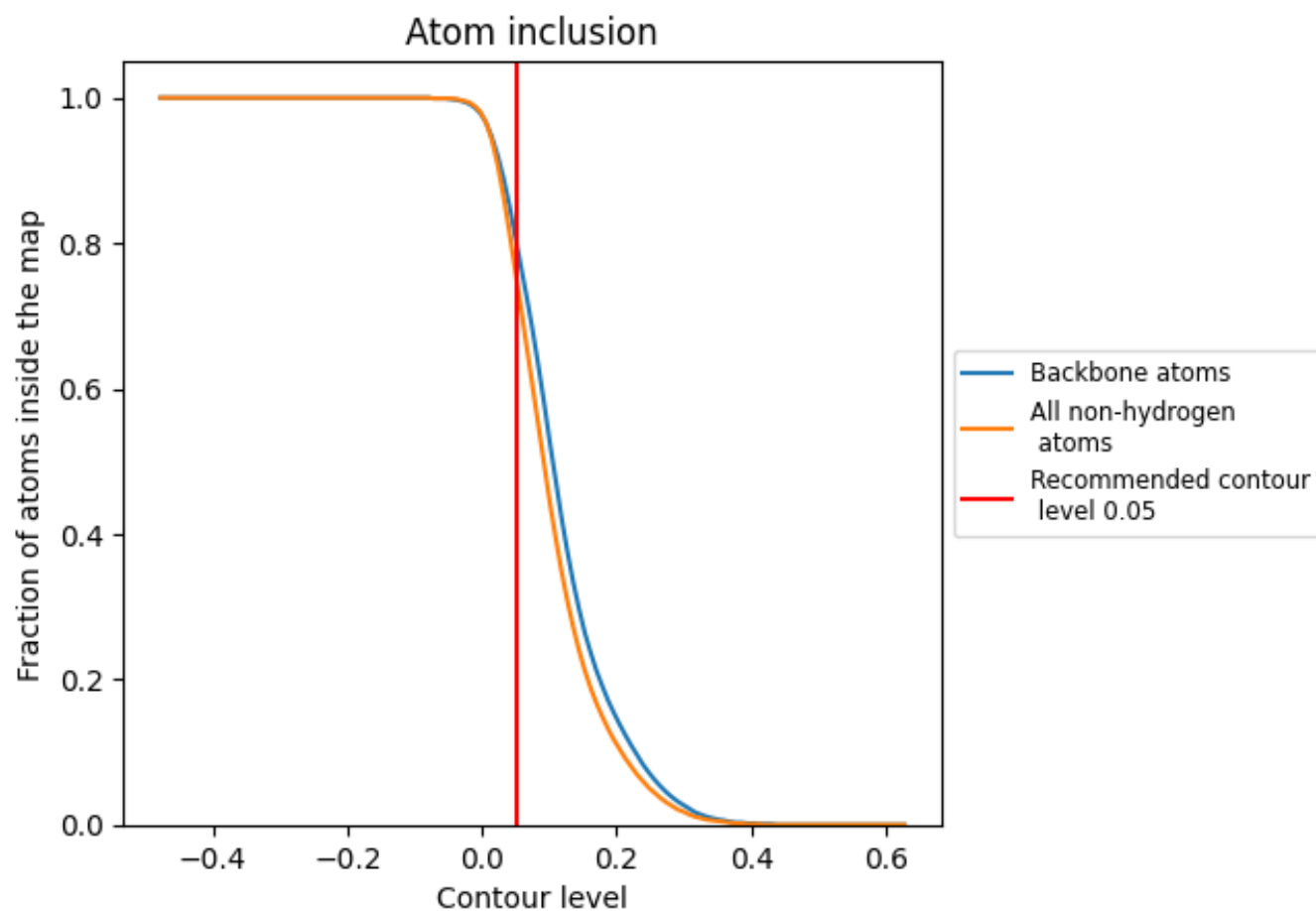
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.5050
AA	 0.7010	 0.4810
AB	 0.7480	 0.5010
AC	 0.7830	 0.5100
AD	 0.7680	 0.4980
AE	 0.7460	 0.4960
AF	 0.6950	 0.4760
Aa	 0.7240	 0.4850
Ab	 0.7370	 0.4910
Ad	 0.7280	 0.4950
Ae	 0.6870	 0.4820
Af	 0.5810	 0.4460
Ag	 0.7510	 0.4960
Ah	 0.7410	 0.4970
Ai	 0.6480	 0.4900
Aj	 0.6220	 0.4830
Ak	 0.6120	 0.4880
BA	 0.7130	 0.4870
BB	 0.7580	 0.5050
BC	 0.7880	 0.5130
BD	 0.7660	 0.5010
BE	 0.7430	 0.4960
BF	 0.7000	 0.4820
Ba	 0.7040	 0.4860
Bb	 0.7530	 0.5030
Bd	 0.7310	 0.4950
Be	 0.6590	 0.4590
Bf	 0.6070	 0.4570
Bg	 0.7760	 0.5030
Bh	 0.7330	 0.4980
Bi	 0.6580	 0.4920
Bj	 0.5620	 0.4810
Bk	 0.6150	 0.4780
CA	 0.7180	 0.4900
CB	 0.7610	 0.5010



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
CC	 0.7860	 0.5080
CD	 0.7660	 0.5030
CE	 0.7450	 0.5020
CF	 0.7030	 0.4830
Ca	 0.7100	 0.4860
Cb	 0.7470	 0.5020
Cd	 0.7260	 0.4910
Ce	 0.6490	 0.4730
Cf	 0.6140	 0.4430
Cg	 0.7610	 0.5020
Ch	 0.7460	 0.5030
Ci	 0.5790	 0.4840
Cj	 0.6220	 0.4810
Ck	 0.5950	 0.4710
DA	 0.7080	 0.4910
DB	 0.7510	 0.5010
DC	 0.7880	 0.5100
DD	 0.7520	 0.4960
DE	 0.7480	 0.4990
DF	 0.7140	 0.4890
Da	 0.6930	 0.4840
Db	 0.7350	 0.5020
Dd	 0.7200	 0.4880
De	 0.6810	 0.4800
Df	 0.6250	 0.4580
Dg	 0.7500	 0.4920
Dh	 0.7480	 0.4860
Di	 0.6120	 0.4720
Dj	 0.5790	 0.4800
Dk	 0.5790	 0.4860
EA	 0.7230	 0.4910
EB	 0.7710	 0.5040
EC	 0.7870	 0.5080
ED	 0.7830	 0.5040
EE	 0.7510	 0.5010
EF	 0.7000	 0.4780
Ea	 0.6960	 0.4830
Eb	 0.7530	 0.5040
Ed	 0.7370	 0.4940
Ee	 0.6820	 0.4790
Ef	 0.6090	 0.4530
Eg	 0.7640	 0.4950

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Eh	 0.7550	 0.4960
Ei	 0.5130	 0.4500
Ej	 0.4700	 0.4560
Ek	 0.5660	 0.4720
FA	 0.7890	 0.5170
FB	 0.7830	 0.5150
FC	 0.7830	 0.5170
FD	 0.7810	 0.5120
FE	 0.7820	 0.5120
FF	 0.7890	 0.5180
FG	 0.7840	 0.5140
FH	 0.7880	 0.5180
FI	 0.7870	 0.5180
FJ	 0.7820	 0.5160
FK	 0.7980	 0.5180
FL	 0.7850	 0.5110
FM	 0.9040	 0.5640
FN	 0.8910	 0.5560
FO	 0.8790	 0.5540
FP	 0.8830	 0.5570
FQ	 0.8920	 0.5610
FR	 0.8910	 0.5620
FS	 0.8970	 0.5610
FT	 0.8920	 0.5630
FU	 0.8810	 0.5560
FV	 0.8870	 0.5590
FW	 0.8990	 0.5630
FX	 0.8950	 0.5580
FY	 0.8710	 0.5470
FZ	 0.8860	 0.5540
GA	 0.8860	 0.5510
GB	 0.8830	 0.5500
GC	 0.8880	 0.5550
GD	 0.8770	 0.5510
GE	 0.8830	 0.5510
GF	 0.8850	 0.5520
GG	 0.8820	 0.5510
GH	 0.8840	 0.5500
GI	 0.8810	 0.5510
GJ	 0.8770	 0.5460
GK	 0.6080	 0.4640
GL	 0.6380	 0.4750

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
GM	 0.6270	 0.4660
GN	 0.6050	 0.4620
GO	 0.5980	 0.4550
GP	 0.5950	 0.4650
GQ	 0.6120	 0.4620
GR	 0.5980	 0.4720
GS	 0.6160	 0.4700
GT	 0.5950	 0.4580
GU	 0.5770	 0.4550
GV	 0.6220	 0.4760
IK	 0.7310	 0.5020
IL	 0.7220	 0.5000
IM	 0.7390	 0.4880
IN	 0.7220	 0.5140
IO	 0.7140	 0.5060
IP	 0.7350	 0.5050
IQ	 0.7220	 0.5080
IR	 0.7960	 0.5280
IS	 0.8330	 0.5290
IT	 0.7430	 0.5040
IU	 0.7550	 0.4960
IV	 0.7630	 0.5020