



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:02 PM UTC

PDB ID : 1S0V / pdb_00001s0v
Title : Structural basis for substrate selection by T7 RNA polymerase
Authors : Temiakov, D.; Patlan, V.; Anikin, M.; McAllister, W.T.; Yokoyama, S.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-01-05
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

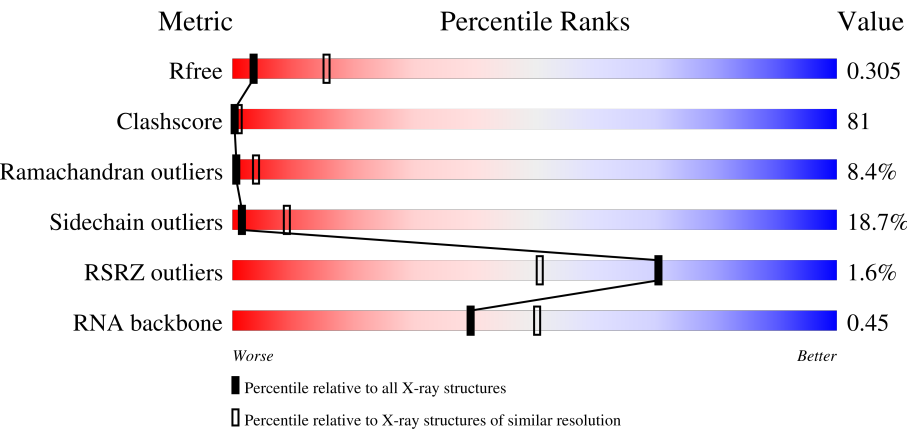
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	18	11% 44% 6% 33% 6%
1	H	18	17% 22% 33% 22% 6%
1	K	18	50% 28% 17% 6%
1	N	18	61% 22% 11% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	12	
2	I	12	
2	L	12	
2	O	12	
3	G	10	
3	J	10	
3	M	10	
3	P	10	
4	A	883	
4	B	883	
4	C	883	
4	D	883	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	APC	A	2000	-	-	X	-
6	APC	B	2001	-	-	X	-
6	APC	C	2002	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 30899 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA chain called 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			
1	H	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			
1	K	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			
1	N	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			

- Molecule 2 is a RNA chain called 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
2	I	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
2	L	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
2	O	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			

- Molecule 3 is a DNA chain called 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
3	J	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
3	M	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			

- Molecule 4 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
4	B	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
4	C	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
4	D	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			

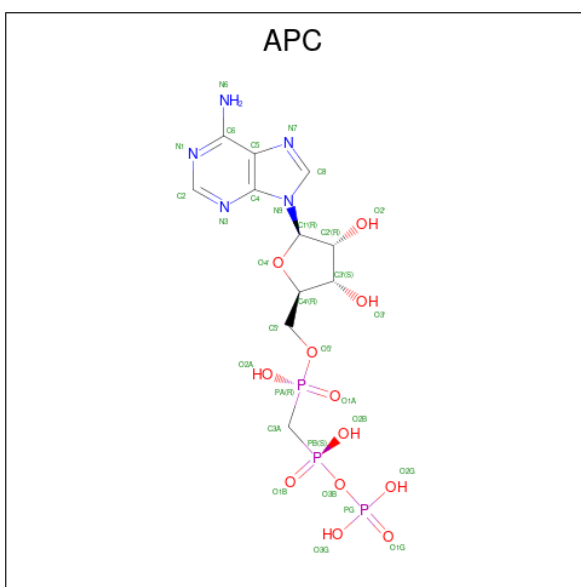
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	497	LEU	-	insertion	UNP P00573
B	497	LEU	-	insertion	UNP P00573
C	497	LEU	-	insertion	UNP P00573
D	497	LEU	-	insertion	UNP P00573

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	B	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		
5	D	2	Total	Mg	0	0
			2	2		

- Molecule 6 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
6	B	1	Total 31	C 11	N 5	O 12	P 3	0	0
6	C	1	Total 31	C 11	N 5	O 12	P 3	0	0
6	D	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	39	Total O 39 39	0	0
7	F	9	Total O 9 9	0	0
7	G	9	Total O 9 9	0	0
7	H	19	Total O 19 19	0	0
7	I	14	Total O 14 14	0	0
7	J	13	Total O 13 13	0	0
7	K	20	Total O 20 20	0	0
7	L	8	Total O 8 8	0	0

Continued on next page...

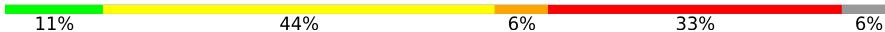
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	10	Total 10	O 10	0	0
7	N	14	Total 14	O 14	0	0
7	O	15	Total 15	O 15	0	0
7	P	6	Total 6	O 6	0	0
7	A	237	Total 237	O 237	0	0
7	B	212	Total 212	O 212	0	0
7	C	201	Total 201	O 201	0	0
7	D	173	Total 173	O 173	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

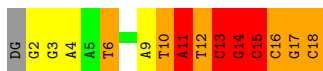
- Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain E: 



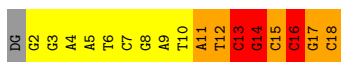
- Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain H: 



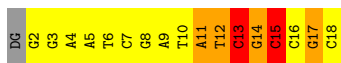
- Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain K: 



- Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain N: 



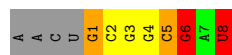
- Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain F: 



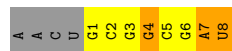
- Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain I: 



• Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain L: 

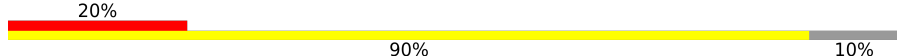


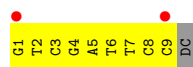
• Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain O: 



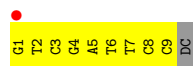
• Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

Chain G: 

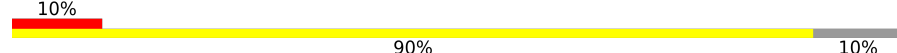


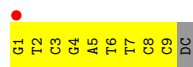
• Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

Chain J: 



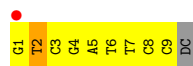
• Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

Chain M: 

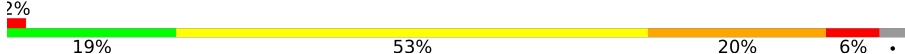


• Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

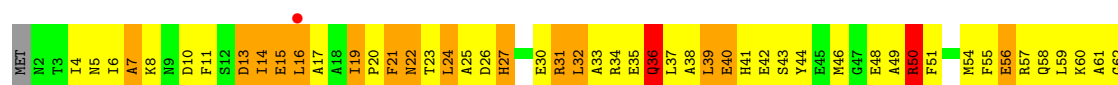
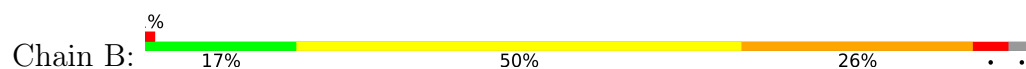
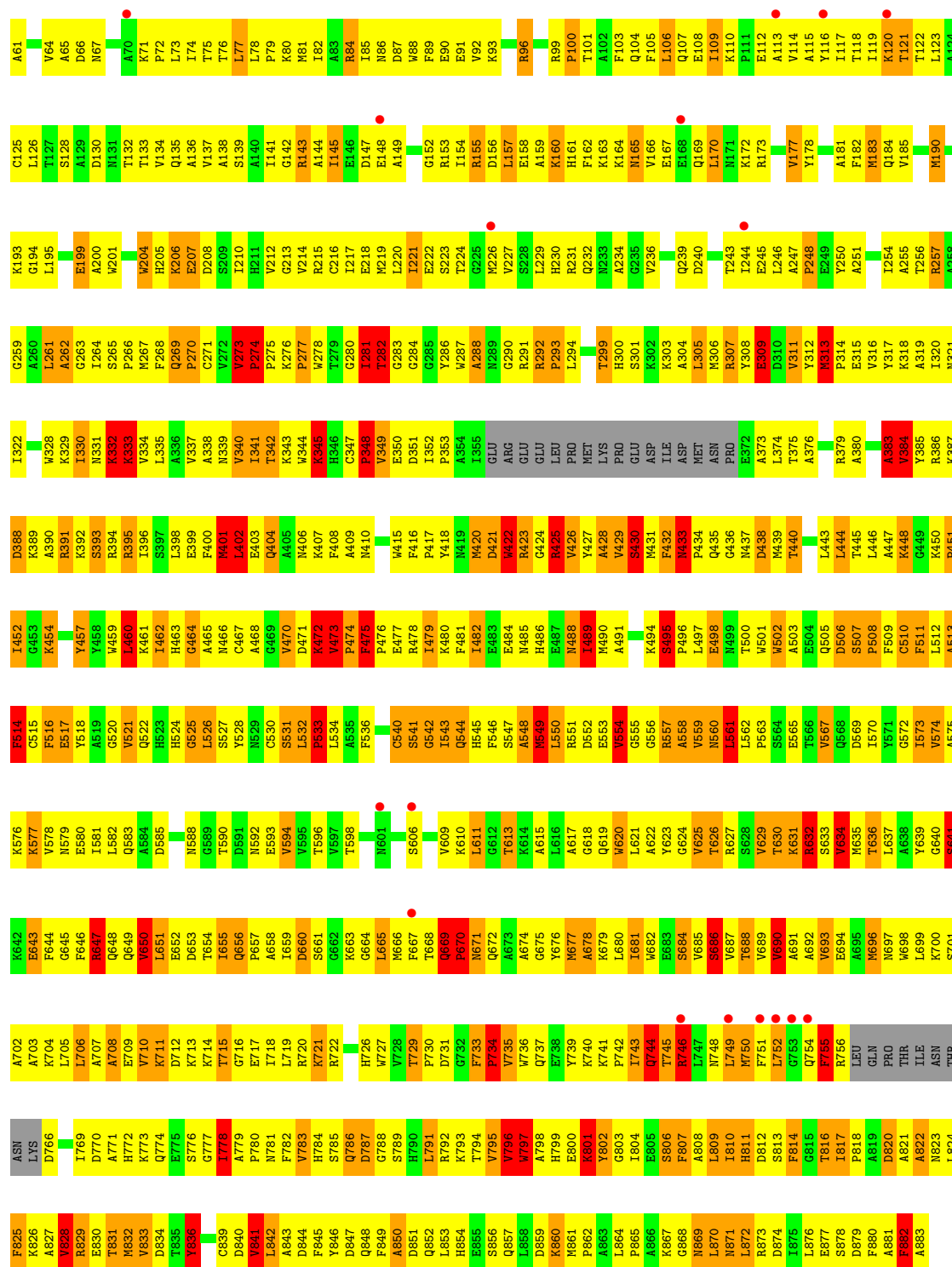
Chain P: 

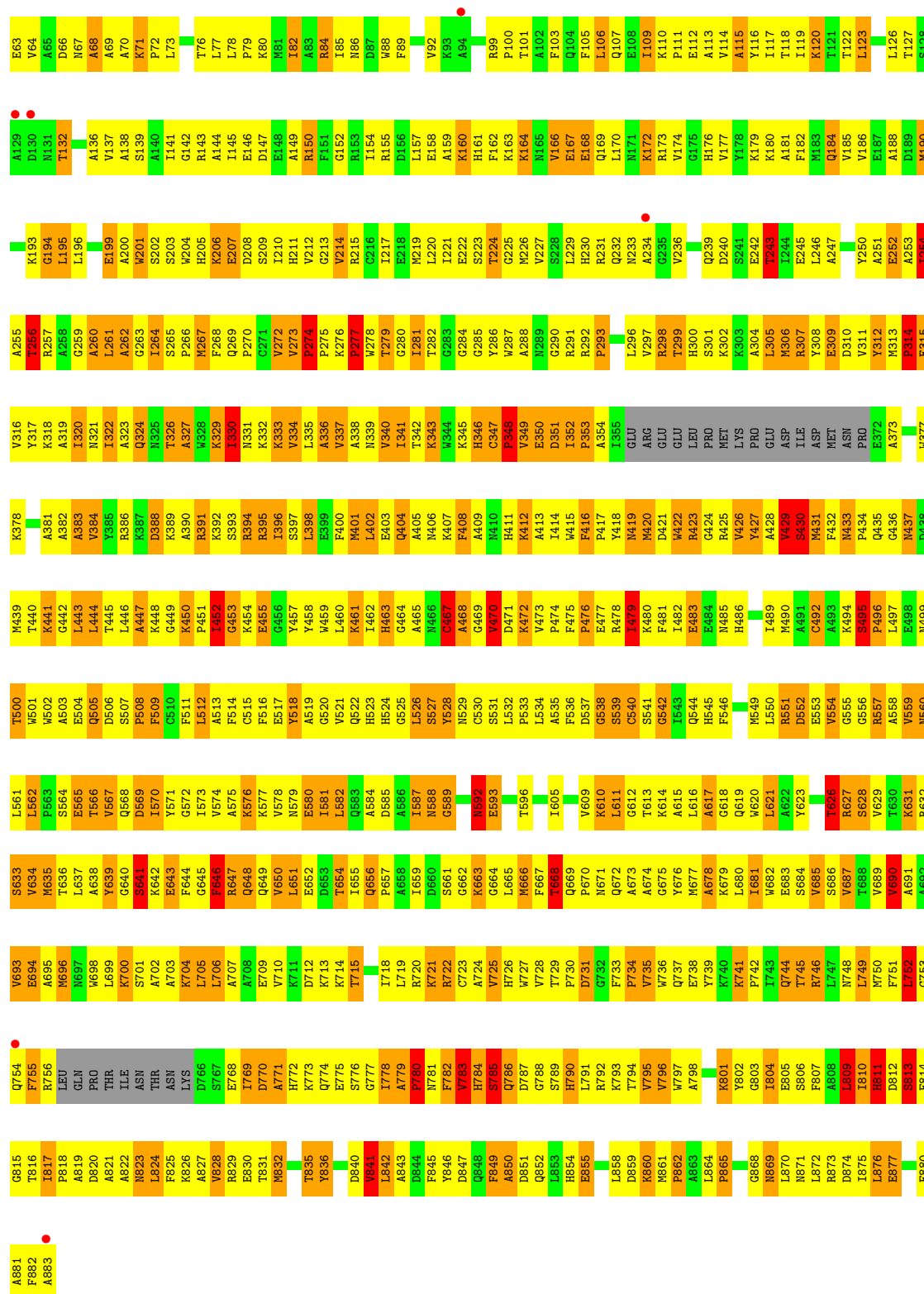


• Molecule 4: DNA-directed RNA polymerase

Chain A: 







● Molecule 4: DNA-directed RNA polymerase





E830	E831	M832	V833	D834	T835	V836	E837	D840	V841	D842	A843	D844	F845	Y846	D847	F848	F849	A850	D851	Q852	L853	H854	E855	S856	Q857	L858	D859	K860	M861	P862	A863	L864	P865	G868	N869	L870	N871	R872	R873	D874	L875	L876	E877	S878	D879	F880	A881	F882	A883	N823	L824	F825	K826	A827	V828	R829	L706	E709	V710	K711	D712	K713	L714	T715	V716	L717	E718	L719	R720	K721	R722	C723	A724	W725	H726	R727	D728	S729	L730	R731	D732	F733	P734	W735	L736	E737	Y738	K739	G740	K741	L742	P743	L744	L745	L746	L747	L748	L749	W750	F751	L752	G753	G754	A692	F755	R756	LEU	GLN	PRD	THR	TLE	L824	F825	K826	A702	A703	LYS	D766	S641	K642	E643	F646	K647	Q648	Q649	V650	L651	E652	D653	T654	L655	D660	S661	G662	K663	G664	L665	M666	F667	T668	Q669	P670	M671	Q672	Y676	M677	A678	K679	L680	L681	T681	W682	E683	S684	V685	S686	Q619	W620	L621	A622	Y623	G624	V625	W629	T630	K631	R632	S633	W634	M635	Y639	G640	Q568	D569	I570	Y571	G572	I573	W574	A575	F576	C577	W578	N579	E580	I581	L582	Q583	A584	D585	A586	I587	N588	G589	T590	D591	N592	E593	V594	N601	S606	W609	K610	L611	G612	T613	K614	L616	M549	L550	R551	D552	E553	W554	G555	G556	R557	V558	N559	N560	L561	L562	V563	S564	V567	T445	L446	K447	K448	G449	F451	P451	G452	L453	R394	K395	L454	E455	F456	S396	E397	L398	E399	F400	A336	K461	I462	A465	M466	C467	A468	V470	D471	D472	A473	P474	A475	E476	E477	R478	I479	K480	F481	L482	E483	E484	M485	H486	E487	M488	I489	M490	L491	C492	K493	K494	S495	P496	L497	E498	N499	T500	M439	F501	W502	S503	E504	Q505	A381	V384	K387	F326	A327	R391	R394	K395	L402	E403	Q404	A405	N406	K407	F408	A409	M410	H411	A412	A413	E414	W415	F416	P417	Y418	N419	M420	D421	K422	R423	G424	R425	V426	Y427	A428	V429	S430	M431	F432	N433	O434	Q435	G436	N437	D438	N439	T537	K437	L374	T375	V316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373	P314	D315	T316	V317	K318	A319	L444	A380	N321	I322	A323	Q324	G263	L264	S265	P266	M267	F268	Q269	K332	K333	V334	L335	V273	P274	P275	K276	P277	W278	G286	Y287	A288	R291	R292	P293	L294	A295	L296	V297	R298	T299	H300	S301	K302	A303	K304	PRD	GLU	ASP	ASP	ASP	ASN	PRD	E372	A373
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.13Å 87.70Å 206.53Å 91.93° 91.02° 110.66°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 83.3 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.307 0.255 , 0.305	Depositor DCC
R_{free} test set	4474 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 110.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	30899	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: APC, 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	E	0.90	0/388	1.58	11/597 (1.8%)
1	H	0.79	0/388	1.47	8/597 (1.3%)
1	K	0.82	1/388 (0.3%)	1.33	5/597 (0.8%)
1	N	0.68	0/388	1.32	8/597 (1.3%)
2	F	1.44	0/191	1.96	11/297 (3.7%)
2	I	1.35	0/191	1.53	5/297 (1.7%)
2	L	1.02	0/191	1.30	3/297 (1.0%)
2	O	0.90	0/191	1.26	3/297 (1.0%)
3	G	0.54	0/199	0.88	0/305
3	J	0.49	0/199	0.93	0/305
3	M	0.51	0/199	0.92	0/305
3	P	0.57	0/199	1.00	0/305
4	A	1.47	67/6897 (1.0%)	1.56	105/9329 (1.1%)
4	B	1.49	62/6897 (0.9%)	1.51	86/9329 (0.9%)
4	C	1.19	22/6897 (0.3%)	1.33	39/9329 (0.4%)
4	D	1.14	22/6897 (0.3%)	1.29	45/9329 (0.5%)
All	All	1.29	174/30700 (0.6%)	1.42	329/42112 (0.8%)

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	E	0	6
1	H	0	9
1	K	0	6
1	N	0	4
2	F	0	4
2	I	0	2
2	L	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	3
3	P	0	1
4	A	0	1
4	B	0	1
4	D	0	1
All	All	0	39

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	482	ILE	CA-CB	-14.20	1.37	1.54
4	B	330	ILE	CA-CB	-11.59	1.38	1.54
4	A	313	MET	SD-CE	10.49	2.05	1.79
4	B	588	ASN	CA-C	-9.75	1.48	1.53
4	A	384	VAL	CA-CB	-9.42	1.41	1.54
4	B	795	VAL	CA-CB	-8.80	1.44	1.54
4	A	498	GLU	CA-C	-8.72	1.41	1.52
4	A	341	ILE	CA-CB	-8.69	1.44	1.54
4	D	609	VAL	CA-CB	8.67	1.64	1.54
4	A	514	PHE	CA-C	-8.48	1.42	1.52
4	C	401	MET	SD-CE	8.45	2.00	1.79
4	A	433	ASN	N-CA	-8.37	1.40	1.46
4	A	513	ALA	CA-C	-8.35	1.42	1.52
4	B	778	ILE	CA-CB	-8.14	1.45	1.54
4	B	326	THR	CA-CB	8.04	1.67	1.53
4	A	696	MET	SD-CE	7.78	1.99	1.79
4	A	808	ALA	CA-CB	-7.67	1.41	1.53
4	A	479	ILE	CA-CB	-7.67	1.43	1.54
4	A	502	TRP	CB-CG	-7.65	1.26	1.50
4	A	337	VAL	CA-CB	-7.54	1.45	1.54
4	A	383	ALA	CA-C	-7.47	1.42	1.52
4	A	460	LEU	CA-C	-7.44	1.42	1.52
4	D	500	THR	CA-CB	7.42	1.66	1.53
4	B	783	VAL	CA-CB	-7.40	1.46	1.54
4	B	340	VAL	CA-CB	-7.33	1.47	1.55
4	C	306	MET	SD-CE	7.29	1.97	1.79
4	B	384	VAL	CA-CB	-7.27	1.44	1.54
4	C	549	MET	SD-CE	7.21	1.97	1.79
4	C	217	ILE	CA-CB	-7.21	1.46	1.54
4	D	19	ILE	CA-CB	7.06	1.63	1.54
4	B	507	SER	CA-C	-6.98	1.45	1.52
4	B	499	ASN	CA-C	-6.94	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	274	PRO	CA-C	6.93	1.58	1.52
4	A	502	TRP	CA-C	-6.91	1.44	1.52
4	C	735	VAL	CA-CB	6.85	1.64	1.54
4	B	310	ASP	CB-CG	6.84	1.69	1.52
4	B	401	MET	SD-CE	6.78	1.96	1.79
4	A	718	ILE	CA-CB	-6.75	1.45	1.54
4	C	4	ILE	CA-CB	6.68	1.63	1.54
4	B	559	VAL	CA-CB	6.67	1.63	1.54
4	C	490	MET	SD-CE	6.65	1.96	1.79
4	A	549	MET	SD-CE	6.63	1.96	1.79
4	D	273	VAL	CA-CB	-6.63	1.49	1.55
4	B	420	MET	SD-CE	6.62	1.96	1.79
4	C	19	ILE	CA-CB	6.61	1.62	1.54
4	A	311	VAL	CA-CB	-6.59	1.46	1.54
4	D	373	ALA	CA-C	6.58	1.57	1.52
4	B	696	MET	SD-CE	6.57	1.96	1.79
4	D	490	MET	SD-CE	6.56	1.96	1.79
4	B	82	ILE	CA-CB	6.55	1.61	1.54
4	A	778	ILE	CA-CB	6.54	1.63	1.54
4	B	499	ASN	CA-CB	-6.52	1.44	1.52
4	A	421	ASP	CA-C	-6.49	1.44	1.52
4	D	778	ILE	CA-CB	-6.43	1.45	1.54
4	A	352	ILE	CA-CB	-6.37	1.49	1.54
4	B	429	VAL	CA-C	6.34	1.61	1.52
4	C	605	ILE	CA-CB	6.31	1.61	1.54
4	B	336	ALA	CA-CB	-6.29	1.43	1.53
4	B	635	MET	CG-SD	6.28	1.96	1.80
4	C	574	VAL	CA-CB	-6.26	1.47	1.54
4	A	558	ALA	CA-CB	-6.26	1.43	1.53
4	A	514	PHE	C-O	-6.21	1.16	1.24
4	C	313	MET	SD-CE	6.20	1.95	1.79
4	A	384	VAL	N-CA	-6.19	1.38	1.46
4	A	428	ALA	CA-CB	-6.18	1.43	1.53
4	A	426	VAL	CA-CB	-6.17	1.46	1.54
4	B	331	ASN	N-CA	6.17	1.54	1.46
4	B	629	VAL	CA-CB	-6.09	1.46	1.54
4	B	725	VAL	CA-CB	-6.09	1.47	1.54
4	D	735	VAL	CA-CB	6.03	1.64	1.54
4	A	470	VAL	CA-CB	-6.00	1.47	1.53
4	A	514	PHE	CA-CB	-5.99	1.44	1.53
4	A	796	VAL	CA-CB	5.96	1.62	1.54
4	D	320	ILE	CA-CB	-5.96	1.48	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	352	ILE	CA-C	-5.96	1.47	1.52
4	B	341	ILE	CA-CB	-5.94	1.47	1.54
4	A	273	VAL	CA-C	-5.94	1.46	1.52
4	B	782	PHE	CA-C	5.92	1.60	1.52
4	A	341	ILE	N-CA	-5.89	1.40	1.46
4	A	681	ILE	CA-CB	-5.88	1.46	1.54
4	A	810	ILE	CA-CB	-5.88	1.46	1.54
4	A	109	ILE	CA-CB	5.87	1.61	1.54
4	A	349	VAL	N-CA	-5.87	1.39	1.46
4	C	725	VAL	CA-CB	-5.85	1.46	1.54
4	B	470	VAL	CA-CB	-5.84	1.46	1.54
4	B	433	ASN	CA-C	-5.83	1.45	1.52
4	A	311	VAL	CA-C	-5.77	1.45	1.52
4	B	479	ILE	CA-CB	-5.74	1.46	1.54
4	A	340	VAL	CA-C	-5.72	1.45	1.52
4	A	271	CYS	CA-C	-5.71	1.46	1.52
4	A	433	ASN	C-O	-5.71	1.19	1.24
4	D	439	MET	SD-CE	5.70	1.93	1.79
4	C	473	VAL	CA-C	5.69	1.58	1.52
4	A	273	VAL	CA-CB	-5.68	1.46	1.54
4	A	502	TRP	CA-CB	-5.67	1.44	1.53
4	A	532	LEU	CA-C	5.67	1.59	1.52
4	B	641	SER	CA-C	-5.67	1.45	1.52
4	A	348	PRO	CA-C	-5.66	1.44	1.52
4	B	468	ALA	CA-C	-5.64	1.45	1.52
4	C	649	GLN	CA-C	5.63	1.59	1.52
4	B	778	ILE	N-CA	-5.61	1.40	1.46
4	A	488	ASN	CA-C	-5.60	1.45	1.52
4	B	433	ASN	C-O	-5.60	1.17	1.24
4	B	462	ILE	CA-C	-5.60	1.45	1.52
4	A	636	THR	CA-CB	5.59	1.62	1.54
4	D	311	VAL	CA-CB	-5.59	1.47	1.54
4	B	190	MET	SD-CE	5.56	1.93	1.79
4	C	429	VAL	CA-CB	-5.56	1.47	1.54
4	C	400	PHE	CA-C	-5.55	1.46	1.52
4	A	634	VAL	CA-CB	5.51	1.62	1.54
4	B	256	THR	CA-CB	5.51	1.62	1.53
4	A	425	ARG	CA-C	5.50	1.60	1.52
4	C	813	SER	CA-C	5.50	1.58	1.52
4	A	533	PRO	C-O	-5.48	1.16	1.24
4	A	729	THR	CA-C	-5.46	1.47	1.53
4	C	256	THR	CA-CB	5.44	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	236	VAL	CA-CB	5.44	1.62	1.54
1	K	14	DG	C5-C6	-5.44	1.31	1.42
4	B	646	PHE	CA-CB	-5.41	1.44	1.53
4	A	282	THR	CA-CB	-5.41	1.46	1.53
4	A	333	LYS	CA-C	5.40	1.59	1.52
4	A	460	LEU	C-O	-5.36	1.17	1.24
4	A	402	LEU	CA-CB	-5.34	1.44	1.53
4	B	404	GLN	CA-CB	-5.33	1.44	1.53
4	C	828	VAL	CA-CB	-5.33	1.48	1.54
4	A	557	ARG	CA-C	-5.32	1.45	1.52
4	B	416	PHE	CA-CB	-5.30	1.43	1.54
4	B	635	MET	SD-CE	5.30	1.92	1.79
4	A	558	ALA	CA-C	-5.29	1.46	1.52
4	B	243	THR	CA-CB	5.28	1.63	1.54
4	D	693	VAL	CA-CB	-5.28	1.47	1.54
4	A	548	ALA	CA-C	5.26	1.59	1.52
4	B	333	LYS	CA-C	5.26	1.59	1.52
4	D	274	PRO	CA-C	5.26	1.57	1.52
4	B	349	VAL	CA-CB	-5.24	1.47	1.54
4	A	797	TRP	CA-C	-5.24	1.45	1.52
4	A	340	VAL	CA-CB	-5.20	1.47	1.54
4	B	581	ILE	CA-CB	-5.19	1.47	1.54
4	B	341	ILE	CA-C	-5.19	1.46	1.52
4	B	635	MET	CA-CB	5.18	1.61	1.53
4	C	384	VAL	CA-CB	-5.18	1.48	1.54
4	B	306	MET	SD-CE	5.18	1.92	1.79
4	A	467	CYS	CB-SG	-5.17	1.64	1.81
4	A	598	THR	CA-CB	5.17	1.60	1.53
4	B	811	HIS	CA-CB	-5.15	1.44	1.53
4	B	463	HIS	CA-C	-5.15	1.45	1.52
4	B	346	HIS	CA-CB	-5.15	1.45	1.53
4	D	331	ASN	CA-CB	5.14	1.59	1.53
4	B	320	ILE	CA-CB	-5.14	1.48	1.54
4	A	19	ILE	CA-CB	5.13	1.60	1.54
4	B	338	ALA	CA-CB	-5.13	1.45	1.53
4	A	394	ARG	CA-C	-5.13	1.45	1.52
4	D	331	ASN	N-CA	5.11	1.52	1.46
4	B	309	GLU	CA-C	-5.11	1.46	1.52
4	B	16	LEU	CA-C	5.10	1.59	1.52
4	C	237	VAL	CA-CB	5.09	1.60	1.54
4	B	626	THR	CA-CB	-5.08	1.44	1.53
4	D	410	ASN	CA-C	5.08	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	429	VAL	CA-CB	-5.07	1.47	1.54
4	D	46	MET	SD-CE	5.05	1.92	1.79
4	A	342	THR	CA-C	5.05	1.59	1.52
4	B	835	THR	CA-C	5.05	1.59	1.52
4	B	329	LYS	CA-C	-5.05	1.46	1.52
4	B	352	ILE	CA-CB	-5.05	1.47	1.54
4	B	430	SER	CA-C	-5.04	1.46	1.52
4	B	327	ALA	CA-CB	-5.04	1.46	1.53
4	D	109	ILE	CA-CB	5.03	1.60	1.54
4	B	813	SER	CA-C	5.03	1.58	1.52
4	A	507	SER	CA-C	-5.02	1.46	1.52
4	D	127	THR	CA-CB	5.02	1.59	1.52
4	A	686	SER	CA-C	5.01	1.59	1.52
4	B	347	CYS	C-O	-5.01	1.19	1.24
4	D	613	THR	CA-CB	5.01	1.61	1.53
4	C	429	VAL	N-CA	-5.01	1.40	1.46

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	450	LYS	CA-C-N	-20.23	98.14	119.99
4	A	450	LYS	C-N-CA	-20.23	98.14	119.99
4	B	347	CYS	CA-C-N	12.36	135.29	119.84
4	B	347	CYS	C-N-CA	12.36	135.29	119.84
2	F	8	U	C1'-C2'-O2'	12.30	126.85	108.40
4	C	433	ASN	CA-C-N	12.27	135.18	119.84
4	C	433	ASN	C-N-CA	12.27	135.18	119.84
1	E	18	DC	C2'-C3'-O3'	-11.80	93.81	111.50
4	A	475	PHE	CA-C-N	-11.54	106.97	118.97
4	A	475	PHE	C-N-CA	-11.54	106.97	118.97
4	A	352	ILE	CA-C-N	10.84	133.39	119.84
4	A	352	ILE	C-N-CA	10.84	133.39	119.84
4	C	507	SER	CA-C-N	10.76	133.29	119.84
4	C	507	SER	C-N-CA	10.76	133.29	119.84
4	A	269	GLN	CA-C-N	-10.74	106.41	119.84
4	A	269	GLN	C-N-CA	-10.74	106.41	119.84
1	E	13	DC	C5'-C4'-O4'	-10.49	93.67	109.40
4	D	433	ASN	CA-C-N	10.17	129.93	119.56
4	D	433	ASN	C-N-CA	10.17	129.93	119.56
4	D	352	ILE	CA-C-N	10.15	132.52	119.84
4	D	352	ILE	C-N-CA	10.15	132.52	119.84
4	B	562	LEU	CA-C-N	10.10	132.47	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	562	LEU	C-N-CA	10.10	132.47	119.84
2	F	8	U	C3'-C2'-O2'	9.53	124.99	110.70
4	A	507	SER	CA-C-N	9.43	131.62	119.84
4	A	507	SER	C-N-CA	9.43	131.62	119.84
4	A	432	PHE	CA-C-N	-9.39	110.44	123.96
4	A	432	PHE	C-N-CA	-9.39	110.44	123.96
1	H	13	DC	N1-C1'-C2'	-9.32	99.52	113.50
4	C	347	CYS	CA-C-N	9.18	131.31	119.84
4	C	347	CYS	C-N-CA	9.18	131.31	119.84
4	D	733	PHE	CA-C-N	9.10	131.21	119.84
4	D	733	PHE	C-N-CA	9.10	131.21	119.84
1	H	18	DC	C2'-C3'-O3'	-9.03	97.96	111.50
4	A	733	PHE	CA-C-N	8.93	131.00	119.84
4	A	733	PHE	C-N-CA	8.93	131.00	119.84
4	C	352	ILE	CA-C-N	8.91	130.97	119.84
4	C	352	ILE	C-N-CA	8.91	130.97	119.84
2	F	8	U	C4'-C3'-O3'	8.87	126.30	113.00
4	B	741	LYS	CA-C-N	-8.85	111.76	120.52
4	B	741	LYS	C-N-CA	-8.85	111.76	120.52
1	H	15	DC	N1-C1'-C2'	-8.82	100.26	113.50
4	B	433	ASN	CA-C-N	8.79	129.53	120.04
4	B	433	ASN	C-N-CA	8.79	129.53	120.04
1	H	14	DG	N9-C1'-C2'	-8.65	100.52	113.50
4	A	433	ASN	CA-C-N	8.60	130.59	119.84
4	A	433	ASN	C-N-CA	8.60	130.59	119.84
4	A	513	ALA	O-C-N	8.56	130.89	122.07
4	D	495	SER	CA-C-N	8.38	127.68	118.97
4	D	495	SER	C-N-CA	8.38	127.68	118.97
4	D	817	ILE	CA-C-N	8.35	128.84	119.32
4	D	817	ILE	C-N-CA	8.35	128.84	119.32
4	B	426	VAL	CB-CA-C	-8.32	101.34	111.08
4	B	340	VAL	CA-C-N	-8.29	109.94	120.56
4	B	340	VAL	C-N-CA	-8.29	109.94	120.56
4	A	470	VAL	CB-CA-C	-8.16	100.88	111.25
4	D	247	ALA	CA-C-N	8.13	128.90	119.47
4	D	247	ALA	C-N-CA	8.13	128.90	119.47
1	N	11	DA	N9-C1'-C2'	-8.07	101.39	113.50
2	O	8	U	C1'-C2'-O2'	8.01	120.41	108.40
2	F	4	G	O4'-C4'-C3'	-7.96	96.04	104.00
4	A	473	VAL	CA-C-N	7.85	129.65	119.84
4	A	473	VAL	C-N-CA	7.85	129.65	119.84
1	K	12	DT	C4'-C3'-O3'	7.81	121.71	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	350	GLU	CA-C-N	-7.79	110.56	123.33
4	B	350	GLU	C-N-CA	-7.79	110.56	123.33
4	A	342	THR	CA-C-N	-7.76	109.77	122.65
4	A	342	THR	C-N-CA	-7.76	109.77	122.65
4	A	801	LYS	CA-C-N	-7.71	111.76	122.93
4	A	801	LYS	C-N-CA	-7.71	111.76	122.93
1	E	17	DG	C5'-C4'-C3'	-7.65	103.43	114.90
1	E	16	DC	N1-C1'-C2'	-7.59	102.11	113.50
4	A	495	SER	CA-C-N	7.57	127.10	118.85
4	A	495	SER	C-N-CA	7.57	127.10	118.85
2	F	5	C	C3'-C2'-O2'	-7.56	99.36	110.70
4	D	639	TYR	CA-C-N	-7.50	115.35	123.30
4	D	639	TYR	C-N-CA	-7.50	115.35	123.30
4	B	330	ILE	CB-CA-C	-7.49	99.01	111.29
4	A	497	LEU	CA-C-N	-7.41	111.01	122.49
4	A	497	LEU	C-N-CA	-7.41	111.01	122.49
4	A	340	VAL	CA-C-N	-7.28	111.21	120.60
4	A	340	VAL	C-N-CA	-7.28	111.21	120.60
4	A	482	ILE	CB-CA-C	-7.26	102.52	112.04
4	A	443	LEU	N-CA-C	-7.21	104.52	113.38
2	I	8	U	C2'-C3'-O3'	7.17	124.46	113.70
1	N	13	DC	N1-C1'-C2'	-7.13	102.80	113.50
4	A	828	VAL	CB-CA-C	-7.10	102.93	111.81
1	H	18	DC	C4'-C3'-O3'	7.04	120.56	110.00
4	B	340	VAL	CB-CA-C	-7.03	103.50	111.80
4	B	447	ALA	CA-C-N	-7.02	113.15	123.11
4	B	447	ALA	C-N-CA	-7.02	113.15	123.11
4	B	202	SER	N-CA-C	-7.01	103.57	111.07
4	C	817	ILE	CA-C-N	6.99	126.81	119.05
4	C	817	ILE	C-N-CA	6.99	126.81	119.05
4	D	38	ALA	CA-C-N	6.98	129.51	120.44
4	D	38	ALA	C-N-CA	6.98	129.51	120.44
1	E	15	DC	N1-C1'-C2'	-6.97	103.04	113.50
4	B	177	VAL	CB-CA-C	-6.93	102.95	112.02
4	A	348	PRO	CA-C-N	-6.92	109.52	121.97
4	A	348	PRO	C-N-CA	-6.92	109.52	121.97
4	B	453	GLY	CA-C-O	-6.83	117.78	122.22
4	B	779	ALA	CA-C-N	6.82	128.37	119.84
4	B	779	ALA	C-N-CA	6.82	128.37	119.84
4	D	532	LEU	CA-C-N	6.81	128.36	119.84
4	D	532	LEU	C-N-CA	6.81	128.36	119.84
4	C	650	VAL	CA-C-N	6.72	131.45	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	650	VAL	C-N-CA	6.72	131.45	120.63
4	B	650	VAL	CB-CA-C	-6.65	101.85	112.16
1	K	18	DC	C2'-C3'-O3'	-6.64	101.54	111.50
4	B	352	ILE	CA-C-N	6.62	128.12	119.84
4	B	352	ILE	C-N-CA	6.62	128.12	119.84
4	C	574	VAL	CB-CA-C	-6.62	103.37	112.04
4	B	771	ALA	CA-C-N	-6.60	111.94	120.65
4	B	771	ALA	C-N-CA	-6.60	111.94	120.65
4	A	472	LYS	CA-C-O	6.56	126.13	119.97
4	A	501	TRP	CA-C-N	-6.54	111.74	120.63
4	A	501	TRP	C-N-CA	-6.54	111.74	120.63
4	C	281	ILE	CA-C-N	-6.47	109.93	123.20
4	C	281	ILE	C-N-CA	-6.47	109.93	123.20
4	A	750	MET	CA-C-N	-6.44	114.78	122.44
4	A	750	MET	C-N-CA	-6.44	114.78	122.44
4	B	528	TYR	CA-C-N	-6.38	114.28	122.77
4	B	528	TYR	C-N-CA	-6.38	114.28	122.77
4	C	473	VAL	N-CA-CB	-6.36	102.30	111.21
2	F	7	A	C5'-C4'-C3'	-6.36	106.46	116.00
4	B	309	GLU	CA-C-N	-6.35	112.52	123.25
4	B	309	GLU	C-N-CA	-6.35	112.52	123.25
4	B	780	PRO	CA-C-N	-6.35	111.68	120.38
4	B	780	PRO	C-N-CA	-6.35	111.68	120.38
4	D	507	SER	CA-C-N	6.34	127.77	119.84
4	D	507	SER	C-N-CA	6.34	127.77	119.84
4	A	532	LEU	CA-C-N	6.33	127.75	119.84
4	A	532	LEU	C-N-CA	6.33	127.75	119.84
4	B	635	MET	CA-CB-CG	6.33	126.75	114.10
4	B	348	PRO	CA-C-N	-6.30	110.62	121.97
4	B	348	PRO	C-N-CA	-6.30	110.62	121.97
2	F	6	G	O4'-C4'-C3'	-6.29	97.71	104.00
2	I	6	G	C1'-C2'-O2'	6.29	117.83	108.40
2	F	7	A	C1'-C2'-O2'	6.25	117.77	108.40
4	A	870	LEU	CA-C-N	-6.23	113.44	123.23
4	A	870	LEU	C-N-CA	-6.23	113.44	123.23
4	D	269	GLN	CA-C-N	-6.23	114.32	120.98
4	D	269	GLN	C-N-CA	-6.23	114.32	120.98
4	C	807	PHE	N-CA-C	6.21	119.60	109.59
4	A	467	CYS	CA-C-N	-6.17	112.92	122.49
4	A	467	CYS	C-N-CA	-6.17	112.92	122.49
1	N	18	DC	C2'-C3'-O3'	-6.17	102.25	111.50
4	A	395	ARG	CA-C-N	-6.16	111.68	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	395	ARG	C-N-CA	-6.16	111.68	120.42
4	A	715	THR	N-CA-C	-6.12	107.05	114.75
4	B	538	GLY	CA-C-O	-6.11	116.02	121.64
1	H	14	DG	C5'-C4'-O4'	-6.10	100.25	109.40
1	N	15	DC	N1-C1'-C2'	-6.10	104.36	113.50
1	E	16	DC	C5'-C4'-C3'	-6.09	105.76	114.90
1	E	14	DG	N9-C1'-C2'	-6.07	104.39	113.50
2	I	8	U	O4'-C4'-C3'	-6.04	97.96	104.00
4	B	495	SER	CA-C-N	6.04	127.39	119.84
4	B	495	SER	C-N-CA	6.04	127.39	119.84
4	B	576	LYS	N-CA-C	-6.02	104.41	110.97
4	A	489	ILE	CB-CA-C	-6.01	101.43	111.29
4	B	450	LYS	CA-C-N	-6.00	112.33	119.84
4	B	450	LYS	C-N-CA	-6.00	112.33	119.84
4	A	554	VAL	CB-CA-C	-6.00	104.31	111.81
4	A	282	THR	N-CA-C	5.96	116.15	108.34
4	A	494	LYS	O-C-N	5.95	128.21	122.03
2	L	4	G	C2'-C3'-O3'	-5.93	104.81	113.70
4	B	659	ILE	CB-CA-C	-5.92	104.30	111.88
4	A	809	LEU	N-CA-C	5.92	118.17	108.52
4	B	429	VAL	N-CA-C	5.92	116.70	110.72
1	K	16	DC	N1-C1'-C2'	-5.91	104.64	113.50
4	B	566	THR	CA-C-N	-5.90	115.49	122.93
4	B	566	THR	C-N-CA	-5.90	115.49	122.93
4	C	340	VAL	CA-C-N	-5.89	111.37	121.97
4	C	340	VAL	C-N-CA	-5.89	111.37	121.97
4	D	775	GLU	CA-C-N	5.89	128.65	120.29
4	D	775	GLU	C-N-CA	5.89	128.65	120.29
4	B	517	GLU	CA-C-N	-5.84	112.69	120.63
4	B	517	GLU	C-N-CA	-5.84	112.69	120.63
4	A	341	ILE	O-C-N	-5.82	116.12	121.94
4	B	639	TYR	N-CA-C	-5.82	105.37	112.88
1	N	12	DT	C4'-C3'-O3'	5.81	118.71	110.00
4	A	836	TYR	CA-CB-CG	-5.81	103.45	113.90
4	B	565	GLU	N-CA-C	-5.80	106.03	113.23
4	A	655	ILE	CB-CA-C	-5.80	104.55	111.97
4	C	655	ILE	CB-CA-C	-5.79	103.48	111.65
1	E	12	DT	C6-N1-C1'	5.79	128.03	119.35
4	A	650	VAL	CA-C-N	5.75	129.44	120.82
4	A	650	VAL	C-N-CA	5.75	129.44	120.82
4	A	629	VAL	N-CA-C	-5.72	107.16	112.83
1	E	17	DG	N9-C1'-C2'	-5.71	104.93	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	82	ILE	CB-CA-C	-5.69	104.60	111.88
4	A	513	ALA	CA-C-N	5.64	128.31	120.63
4	A	513	ALA	C-N-CA	5.64	128.31	120.63
4	D	725	VAL	N-CA-CB	-5.64	104.79	111.90
4	B	809	LEU	N-CA-C	5.62	118.38	109.50
4	C	783	VAL	CB-CA-C	-5.61	104.56	112.14
4	B	312	TYR	CA-C-N	-5.60	116.37	123.15
4	B	312	TYR	C-N-CA	-5.60	116.37	123.15
1	H	15	DC	C2'-C3'-O3'	-5.59	103.11	111.50
4	B	570	ILE	CB-CA-C	-5.59	102.12	111.29
4	C	119	ILE	CB-CA-C	-5.59	104.72	111.88
4	D	264	ILE	CB-CA-C	-5.59	105.76	112.19
4	A	880	PHE	N-CA-C	5.57	120.14	113.23
4	A	460	LEU	CB-CG-CD1	-5.57	93.98	110.70
2	F	8	U	N1-C1'-C2'	-5.56	103.66	112.00
4	B	201	TRP	N-CA-C	-5.54	107.16	114.31
4	C	419	ASN	CB-CA-C	-5.53	104.46	113.37
4	C	429	VAL	CB-CA-C	-5.53	104.64	111.94
4	B	444	LEU	CA-CB-CG	-5.53	96.96	116.30
4	B	559	VAL	CA-C-N	5.52	131.23	122.61
4	B	559	VAL	C-N-CA	5.52	131.23	122.61
4	B	40	GLU	CA-C-N	-5.52	113.12	120.79
4	B	40	GLU	C-N-CA	-5.52	113.12	120.79
4	D	791	LEU	CA-CB-CG	5.49	135.52	116.30
2	L	4	G	C1'-C2'-O2'	5.49	116.63	108.40
4	A	822	ALA	CA-C-N	5.49	128.09	120.63
4	A	822	ALA	C-N-CA	5.49	128.09	120.63
4	A	841	VAL	CB-CA-C	-5.44	102.37	111.29
4	B	174	VAL	N-CA-C	5.43	115.41	107.37
4	A	425	ARG	NE-CZ-NH1	-5.43	116.07	121.50
4	A	561	LEU	N-CA-C	-5.43	105.02	111.69
4	C	714	LYS	N-CA-C	-5.42	105.32	113.89
4	B	22	ASN	N-CA-C	-5.42	106.37	112.87
4	A	420	MET	CA-C-N	-5.42	112.88	122.74
4	A	420	MET	C-N-CA	-5.42	112.88	122.74
4	C	427	TYR	CA-C-N	-5.41	112.41	121.39
4	C	427	TYR	C-N-CA	-5.41	112.41	121.39
4	B	668	THR	CA-C-N	-5.40	113.78	123.08
4	B	668	THR	C-N-CA	-5.40	113.78	123.08
4	C	729	THR	CA-C-N	5.40	126.59	119.84
4	C	729	THR	C-N-CA	5.40	126.59	119.84
4	C	428	ALA	CA-C-N	-5.39	114.30	120.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	428	ALA	C-N-CA	-5.39	114.30	120.88
4	A	341	ILE	CA-C-N	-5.39	111.98	120.60
4	A	341	ILE	C-N-CA	-5.39	111.98	120.60
4	A	807	PHE	CA-C-N	5.38	130.92	123.07
4	A	807	PHE	C-N-CA	5.38	130.92	123.07
1	K	13	DC	N1-C1'-C2'	-5.37	105.45	113.50
4	A	684	SER	CA-C-N	-5.36	112.66	121.34
4	A	684	SER	C-N-CA	-5.36	112.66	121.34
4	D	450	LYS	CA-C-N	-5.36	113.64	120.23
4	D	450	LYS	C-N-CA	-5.36	113.64	120.23
4	B	518	TYR	N-CA-C	-5.36	105.09	111.03
4	B	443	LEU	O-C-N	-5.34	116.37	122.08
4	B	634	VAL	CB-CA-C	-5.33	103.89	112.16
4	A	281	ILE	CA-C-N	-5.33	113.64	122.39
4	A	281	ILE	C-N-CA	-5.33	113.64	122.39
4	A	729	THR	CA-C-N	5.33	126.50	119.84
4	A	729	THR	C-N-CA	5.33	126.50	119.84
4	A	500	THR	CA-C-N	-5.33	111.83	120.72
4	A	500	THR	C-N-CA	-5.33	111.83	120.72
4	C	154	ILE	CB-CA-C	-5.33	105.00	111.87
4	B	694	GLU	CA-C-N	5.32	128.15	120.38
4	B	694	GLU	C-N-CA	5.32	128.15	120.38
4	B	790	HIS	O-C-N	5.31	127.76	122.08
4	B	468	ALA	O-C-N	5.31	127.55	122.03
4	C	341	ILE	CA-C-N	-5.31	112.77	122.38
4	C	341	ILE	C-N-CA	-5.31	112.77	122.38
4	A	443	LEU	CA-C-O	5.30	125.19	119.15
4	A	807	PHE	N-CA-C	5.30	118.22	109.85
4	D	117	ILE	CB-CA-C	-5.29	105.04	111.87
4	B	496	PRO	CA-C-N	-5.29	110.71	121.18
4	B	496	PRO	C-N-CA	-5.29	110.71	121.18
4	B	715	THR	N-CA-C	-5.29	108.09	114.75
4	A	795	VAL	CB-CA-C	-5.29	104.93	111.70
4	D	418	TYR	N-CA-C	5.28	117.00	108.34
4	D	492	CYS	CA-CB-SG	-5.26	102.29	114.40
4	C	19	ILE	CA-C-N	-5.24	116.35	121.65
4	C	19	ILE	C-N-CA	-5.24	116.35	121.65
4	B	467	CYS	N-CA-C	-5.23	107.03	113.41
4	C	92	VAL	CB-CA-C	-5.22	104.98	110.62
4	A	460	LEU	CB-CG-CD2	5.22	126.35	110.70
4	B	416	PHE	CB-CA-C	-5.22	101.05	108.88
4	A	422	TRP	CA-C-N	-5.21	114.47	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	422	TRP	C-N-CA	-5.21	114.47	122.60
4	D	347	CYS	CA-C-N	5.20	126.34	119.84
4	D	347	CYS	C-N-CA	5.20	126.34	119.84
1	N	13	DC	C5'-C4'-C3'	-5.19	107.12	114.90
2	L	7	A	C5'-C4'-C3'	-5.18	108.22	116.00
1	N	15	DC	C2'-C3'-O3'	-5.17	103.75	111.50
4	C	273	VAL	CA-C-N	-5.16	115.06	120.38
4	C	273	VAL	C-N-CA	-5.16	115.06	120.38
2	F	3	G	C5'-C4'-C3'	5.15	123.73	116.00
4	A	871	ASN	CB-CA-C	-5.15	102.65	111.41
4	A	507	SER	C-N-CD	-5.14	103.93	125.00
4	A	445	THR	CA-C-N	5.14	129.01	120.94
4	A	445	THR	C-N-CA	5.14	129.01	120.94
2	O	8	U	C3'-C2'-O2'	5.13	118.40	110.70
4	B	817	ILE	CA-C-N	5.13	126.26	119.84
4	B	817	ILE	C-N-CA	5.13	126.26	119.84
4	A	577	LYS	CA-C-N	-5.12	114.07	121.65
4	A	577	LYS	C-N-CA	-5.12	114.07	121.65
4	D	511	PHE	CA-C-N	5.12	127.40	120.44
4	D	511	PHE	C-N-CA	5.12	127.40	120.44
4	D	348	PRO	CA-C-N	-5.12	112.76	121.97
4	D	348	PRO	C-N-CA	-5.12	112.76	121.97
2	F	6	G	OP1-P-O3'	-5.10	92.69	108.00
4	D	310	ASP	CA-C-N	-5.10	114.43	122.64
4	D	310	ASP	C-N-CA	-5.10	114.43	122.64
4	A	443	LEU	CA-C-N	-5.09	115.88	123.11
4	A	443	LEU	C-N-CA	-5.09	115.88	123.11
4	A	332	LYS	CA-C-N	-5.09	113.70	120.63
4	A	332	LYS	C-N-CA	-5.09	113.70	120.63
1	E	12	DT	C2-N1-C1'	-5.09	111.71	119.35
1	K	13	DC	C4'-C3'-O3'	5.09	117.63	110.00
4	A	498	GLU	N-CA-C	-5.08	106.49	113.30
4	B	383	ALA	N-CA-C	-5.08	107.21	113.41
4	B	835	THR	N-CA-C	5.08	117.20	111.11
4	B	201	TRP	CA-C-O	5.07	124.40	118.77
1	N	11	DA	C4'-C3'-O3'	5.07	117.60	110.00
1	H	11	DA	C4'-C3'-O3'	5.07	117.60	110.00
2	I	1	G	O5'-C5'-C4'	-5.07	103.90	111.50
1	E	11	DA	C5'-C4'-C3'	-5.06	107.31	114.90
4	D	82	ILE	CB-CA-C	-5.06	105.22	111.70
4	D	320	ILE	CB-CA-C	-5.05	105.23	111.70
4	D	807	PHE	N-CA-C	5.05	117.68	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	8	U	C2'-C3'-O3'	5.04	121.26	113.70
4	A	444	LEU	N-CA-C	5.04	116.91	107.99
4	A	451	PRO	CB-CA-C	5.04	117.95	110.85
4	B	509	PHE	CA-C-N	-5.04	112.32	121.14
4	B	509	PHE	C-N-CA	-5.04	112.32	121.14
4	B	427	TYR	CA-C-N	-5.04	115.77	122.72
4	B	427	TYR	C-N-CA	-5.04	115.77	122.72
4	A	335	LEU	CA-C-N	-5.03	109.75	121.52
4	A	335	LEU	C-N-CA	-5.03	109.75	121.52
4	A	532	LEU	N-CA-C	5.03	116.89	109.50
2	I	8	U	C4'-C3'-O3'	-5.02	105.47	113.00
4	D	586	ALA	CA-C-N	5.00	126.99	120.88
4	D	586	ALA	C-N-CA	5.00	126.99	120.88

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	836	TYR	Sidechain
4	B	836	TYR	Sidechain
4	D	518	TYR	Sidechain
1	E	11	DA	Sidechain
1	E	12	DT	Sidechain
1	E	13	DC	Sidechain
1	E	14	DG	Sidechain
1	E	16	DC	Sidechain
1	E	17	DG	Sidechain
2	F	3	G	Sidechain
2	F	6	G	Sidechain
2	F	7	A	Sidechain
2	F	8	U	Sidechain
1	H	10	DT	Sidechain
1	H	11	DA	Sidechain
1	H	12	DT	Sidechain
1	H	13	DC	Sidechain
1	H	14	DG	Sidechain
1	H	15	DC	Sidechain
1	H	16	DC	Sidechain
1	H	17	DG	Sidechain
1	H	6	DT	Sidechain
2	I	5	C	Sidechain
2	I	6	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	K	11	DA	Sidechain
1	K	13	DC	Sidechain
1	K	14	DG	Sidechain
1	K	15	DC	Sidechain
1	K	16	DC	Sidechain
1	K	17	DG	Sidechain
2	L	8	U	Sidechain
1	N	13	DC	Sidechain
1	N	14	DG	Sidechain
1	N	15	DC	Sidechain
1	N	17	DG	Sidechain
2	O	4	G	Sidechain
2	O	6	G	Sidechain
2	O	8	U	Sidechain
3	P	2	DT	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	346	0	190	29	0
1	H	346	0	192	67	0
1	K	346	0	190	57	0
1	N	346	0	192	38	0
2	F	171	0	89	10	0
2	I	171	0	89	11	0
2	L	171	0	89	14	0
2	O	171	0	89	5	0
3	G	179	0	104	13	0
3	J	179	0	104	17	0
3	M	179	0	104	13	0
3	P	179	0	104	8	0
4	A	6746	0	6708	1223	0
4	B	6746	0	6708	1254	0
4	C	6746	0	6708	1071	0
4	D	6746	0	6708	948	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	F	1	0	0	0	0
6	A	31	0	13	16	0
6	B	31	0	13	10	0
6	C	31	0	14	18	0
6	D	31	0	13	8	0
7	A	237	0	0	84	0
7	B	212	0	0	68	0
7	C	201	0	0	70	0
7	D	173	0	0	53	0
7	E	39	0	0	1	0
7	F	9	0	0	1	0
7	G	9	0	0	1	0
7	H	19	0	0	9	0
7	I	14	0	0	4	0
7	J	13	0	0	0	0
7	K	20	0	0	7	0
7	L	8	0	0	0	0
7	M	10	0	0	2	0
7	N	14	0	0	3	0
7	O	15	0	0	2	0
7	P	6	0	0	2	0
All	All	30899	0	28421	4707	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 81.

All (4707) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:313:MET:CE	4:A:313:MET:SD	2.05	1.44
4:C:631:LYS:NZ	6:C:2002:APC:H3A2	1.52	1.22
2:F:1:G:H5"	7:F:3008:HOH:O	1.40	1.19
4:A:631:LYS:NZ	6:A:2000:APC:H3A2	1.58	1.18
4:A:546:PHE:CE1	4:A:783:VAL:HG22	1.78	1.16
4:A:631:LYS:HZ1	6:A:2000:APC:H3A2	0.97	1.13
4:A:281:ILE:HG22	4:A:282:THR:HG23	1.20	1.13
4:D:720:ARG:HG2	4:D:720:ARG:HH11	0.95	1.12
4:B:59:LEU:HD23	4:B:64:VAL:HG22	1.17	1.12
4:A:109:ILE:HD13	4:A:145:ILE:HG22	1.31	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:471:ASP:OD1	4:A:472:LYS:HD2	1.47	1.11
1:K:12:DT:H2''	1:K:13:DC:H5'	1.16	1.11
4:A:722:ARG:HB2	4:A:769:ILE:HD13	1.27	1.11
4:C:281:ILE:HG22	4:C:282:THR:HG22	1.18	1.11
4:A:804:ILE:HG12	4:A:820:ASP:HB3	1.33	1.10
4:B:452:ILE:CG2	4:B:453:GLY:H	1.64	1.10
1:N:12:DT:H2''	1:N:13:DC:H5'	1.33	1.10
4:A:647:ARG:HD2	4:A:675:GLY:HA2	1.34	1.10
4:B:816:THR:HG22	4:B:817:ILE:H	1.09	1.09
4:A:560:ASN:O	4:A:881:ALA:HB2	1.50	1.09
4:D:36:GLN:OE1	4:D:273:VAL:HG22	1.52	1.09
4:C:158:GLU:HG2	4:C:195:LEU:HD22	1.10	1.08
4:A:871:ASN:HD21	4:A:873:ARG:HB2	1.08	1.08
4:D:718:ILE:H	4:D:718:ILE:HD12	1.11	1.08
4:C:556:GLY:HA2	4:C:561:LEU:HD22	1.35	1.08
4:B:435:GLN:HG2	4:B:810:ILE:HG23	1.36	1.07
4:B:549:MET:HE2	4:B:841:VAL:HG21	1.26	1.07
4:C:19:ILE:HG12	4:C:20:PRO:HD2	1.30	1.07
1:E:12:DT:H2''	1:E:13:DC:H5'	1.37	1.06
4:B:706:LEU:HD21	4:B:849:PHE:HB2	1.33	1.06
4:B:720:ARG:HG2	4:B:720:ARG:HH11	1.19	1.06
4:B:433:ASN:HB2	4:B:434:PRO:HD3	1.34	1.06
1:H:13:DC:H2''	1:H:14:DG:H5'	1.32	1.05
4:B:433:ASN:HB2	4:B:434:PRO:CD	1.87	1.05
4:D:512:LEU:HA	4:D:515:CYS:SG	1.97	1.05
4:C:333:LYS:HB3	4:C:516:PHE:CE2	1.91	1.05
4:C:536:PHE:HB3	4:C:882:PHE:HB3	1.35	1.05
4:B:473:VAL:HG13	4:B:474:PRO:HD2	1.36	1.04
4:B:623:TYR:HA	4:B:666:MET:HE2	1.33	1.04
1:H:9:DA:H5''	7:H:484:HOH:O	1.57	1.04
4:A:281:ILE:HG22	4:A:282:THR:CG2	1.86	1.03
4:B:829:ARG:HH22	4:B:882:PHE:HA	1.16	1.03
4:C:158:GLU:HG2	4:C:195:LEU:CD2	1.89	1.03
4:D:120:LYS:HG3	4:D:752:LEU:HD21	1.38	1.03
4:A:16:LEU:HD13	4:A:38:ALA:HB2	1.41	1.02
4:B:268:PHE:HB3	4:B:286:TYR:OH	1.59	1.02
4:B:829:ARG:NH2	4:B:882:PHE:HA	1.73	1.02
4:C:792:ARG:O	4:C:796:VAL:HG23	1.59	1.02
4:B:398:LEU:HD21	4:B:439:MET:HE1	1.42	1.01
4:C:54:MET:O	4:C:58:GLN:HG2	1.58	1.01
4:D:737:GLN:HE22	4:D:778:ILE:HA	1.23	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:794:THR:OG1	4:A:831:THR:HG21	1.58	1.01
1:E:12:DT:H2''	1:E:13:DC:C5'	1.90	1.01
4:A:829:ARG:HH11	4:A:829:ARG:HG3	1.18	1.01
4:B:751:PHE:HB3	4:B:752:LEU:HD12	1.36	1.01
4:A:688:THR:HG22	4:A:689:VAL:HG13	1.41	1.01
4:C:342:THR:HG22	4:C:348:PRO:HG2	1.40	1.00
4:D:560:ASN:O	4:D:881:ALA:HB2	1.60	1.00
4:D:794:THR:OG1	4:D:831:THR:HG21	1.58	1.00
4:A:304:ALA:O	4:A:307:ARG:HG3	1.62	1.00
4:C:437:ASN:H	4:C:437:ASN:HD22	1.10	1.00
4:C:457:TYR:CD1	4:C:521:VAL:HG11	1.97	1.00
4:B:418:TYR:HE2	4:B:428:ALA:HB2	1.27	1.00
4:C:651:LEU:HD13	4:C:651:LEU:O	1.61	1.00
4:A:690:VAL:HG23	7:A:3200:HOH:O	1.61	0.99
4:A:687:VAL:HG23	7:A:3114:HOH:O	1.61	0.99
4:A:786:GLN:HE21	4:A:786:GLN:HA	1.27	0.99
4:D:198:GLY:HA3	7:D:3152:HOH:O	1.61	0.99
4:A:841:VAL:HG12	7:A:3070:HOH:O	1.60	0.99
4:C:84:ARG:HH12	4:C:87:ASP:HB2	1.27	0.99
4:B:669:GLN:HG2	4:B:672:GLN:HG3	1.45	0.98
4:A:154:ILE:HG23	4:A:190:MET:HE2	1.43	0.98
4:D:790:HIS:HE1	4:D:831:THR:HG23	1.28	0.98
4:A:463:HIS:HA	4:A:466:ASN:HD22	1.27	0.98
4:C:281:ILE:HG22	4:C:282:THR:CG2	1.92	0.98
4:B:42:GLU:HG2	4:B:46:MET:HE2	1.46	0.98
4:D:32:LEU:H	4:D:32:LEU:HD12	1.29	0.97
4:A:280:GLY:HA2	4:A:317:TYR:OH	1.62	0.97
4:B:11:PHE:HB3	4:B:41:HIS:HE1	1.28	0.97
4:A:169:GLN:O	4:A:173:ARG:HG2	1.65	0.97
4:B:14:ILE:HD12	4:B:14:ILE:H	1.28	0.97
4:B:452:ILE:HG23	4:B:453:GLY:N	1.57	0.97
4:C:423:ARG:HH11	4:C:423:ARG:HB2	1.26	0.97
4:C:551:ARG:NE	4:C:872:LEU:HD21	1.80	0.96
4:B:84:ARG:HD2	4:B:219:MET:HG2	1.47	0.96
4:B:407:LYS:HG2	4:B:408:PHE:CE2	2.00	0.96
4:A:562:LEU:HD21	4:A:870:LEU:CD1	1.94	0.96
4:C:631:LYS:HZ1	6:C:2002:APC:H3A2	1.28	0.96
4:C:249:GLU:H	4:C:249:GLU:CD	1.73	0.95
4:A:80:LYS:HE2	4:A:223:SER:O	1.66	0.95
4:B:59:LEU:HD23	4:B:64:VAL:CG2	1.95	0.95
4:A:308:TYR:HE2	4:A:734:PRO:HG2	1.29	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:DC:H2''	1:K:16:DC:O5'	1.64	0.95
4:A:379:ARG:HD3	4:A:660:ASP:OD2	1.66	0.95
4:C:92:VAL:HG12	4:C:99:ARG:HG3	1.44	0.95
4:C:338:ALA:HB2	4:C:509:PHE:HE1	1.28	0.95
4:D:623:TYR:HA	4:D:666:MET:HE2	1.46	0.95
4:A:404:GLN:HE21	4:A:404:GLN:HA	1.30	0.95
4:C:706:LEU:HD22	4:C:725:VAL:HG13	1.49	0.94
4:A:546:PHE:HE1	4:A:783:VAL:HG22	1.28	0.94
4:C:341:ILE:HD12	4:C:348:PRO:HB3	1.49	0.94
1:K:12:DT:H2''	1:K:13:DC:C5'	1.96	0.94
4:B:505:GLN:N	4:B:505:GLN:NE2	2.14	0.94
4:A:544:GLN:HG2	4:A:559:VAL:HG21	1.47	0.94
4:C:133:THR:HA	4:C:243:THR:HG22	1.49	0.94
4:D:16:LEU:HD13	4:D:38:ALA:HB2	1.50	0.94
4:C:629:VAL:HG22	4:C:654:THR:HG21	1.50	0.93
4:B:490:MET:SD	4:B:522:GLN:HG3	2.07	0.93
4:B:430:SER:O	4:B:431:MET:C	2.09	0.93
4:C:236:VAL:HB	4:C:239:GLN:HB2	1.49	0.93
1:H:15:DC:H2''	1:H:16:DC:O5'	1.66	0.93
4:A:421:ASP:OD2	4:A:425:ARG:HB2	1.67	0.93
4:A:105:PHE:HB3	4:A:204:TRP:HZ2	1.34	0.93
4:C:404:GLN:HG2	4:C:432:PHE:CG	2.04	0.93
4:C:632:ARG:HH22	6:C:2002:APC:H5'1	1.31	0.93
4:B:116:TYR:OH	4:B:752:LEU:HD22	1.69	0.93
2:I:4:G:H2'	2:I:5:C:H6	1.33	0.93
4:B:492:CYS:O	4:B:496:PRO:HD3	1.68	0.93
4:A:154:ILE:HG23	4:A:190:MET:CE	1.99	0.92
4:A:457:TYR:CZ	4:A:461:LYS:HD3	2.05	0.92
4:A:457:TYR:CE2	4:A:461:LYS:HD3	2.03	0.92
4:C:457:TYR:CE1	4:C:521:VAL:HG11	2.04	0.92
4:D:380:ALA:O	4:D:384:VAL:HG23	1.69	0.92
4:C:281:ILE:CG2	4:C:282:THR:HG22	2.00	0.92
4:D:264:ILE:HG23	4:D:292:ARG:HB2	1.52	0.92
1:H:13:DC:H2''	1:H:14:DG:C5'	1.99	0.92
4:D:718:ILE:HD12	4:D:718:ILE:N	1.85	0.92
4:A:85:ILE:HG12	4:A:219:MET:SD	2.10	0.92
4:C:778:ILE:HG23	4:C:779:ALA:N	1.83	0.92
4:C:334:VAL:HG21	4:C:513:ALA:HB2	1.49	0.92
4:A:5:ASN:HD21	4:A:7:ALA:HB3	1.34	0.91
4:A:871:ASN:HD21	4:A:873:ARG:CB	1.83	0.91
4:C:333:LYS:HD3	4:C:516:PHE:HD2	1.34	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:810:ILE:HB	4:D:813:SER:OG	1.70	0.91
4:A:828:VAL:HG23	4:A:829:ARG:H	1.33	0.91
4:B:11:PHE:HB3	4:B:41:HIS:CE1	2.05	0.91
4:B:571:TYR:OH	4:B:635:MET:HE3	1.70	0.91
4:C:556:GLY:CA	4:C:561:LEU:HD22	2.00	0.91
4:A:280:GLY:O	4:A:282:THR:N	2.04	0.91
4:B:706:LEU:HD11	4:B:849:PHE:CD2	2.05	0.91
4:C:560:ASN:O	4:C:881:ALA:HB2	1.70	0.91
4:A:341:ILE:HD12	4:A:348:PRO:HB3	1.49	0.91
4:A:502:TRP:CD2	4:A:512:LEU:HD13	2.06	0.91
4:B:646:PHE:O	4:B:650:VAL:HG23	1.69	0.91
4:D:718:ILE:H	4:D:718:ILE:CD1	1.84	0.91
4:A:825:PHE:CE1	4:A:829:ARG:NH1	2.39	0.91
4:D:552:ASP:HB2	4:D:691:ALA:HB2	1.53	0.91
4:D:720:ARG:HG2	4:D:720:ARG:NH1	1.74	0.91
4:B:85:ILE:HG12	4:B:219:MET:SD	2.11	0.90
4:B:448:LYS:HD2	7:B:3017:HOH:O	1.70	0.90
4:A:103:PHE:O	4:A:107:GLN:HG3	1.71	0.90
6:A:2000:APC:H4'	7:A:3238:HOH:O	1.70	0.90
4:A:423:ARG:NH2	4:A:784:HIS:ND1	2.18	0.90
4:C:751:PHE:HB3	4:C:752:LEU:HD12	1.51	0.90
4:A:294:LEU:HD13	4:A:429:VAL:HG21	1.52	0.90
4:A:829:ARG:HH11	4:A:829:ARG:CG	1.84	0.90
4:C:460:LEU:HA	4:C:534:LEU:HD21	1.54	0.90
4:B:137:VAL:HG12	4:B:217:ILE:HD11	1.54	0.90
4:A:464:GLY:HA3	4:A:514:PHE:CE2	2.07	0.90
4:C:536:PHE:HB3	4:C:882:PHE:CB	2.01	0.90
4:D:273:VAL:HA	4:D:415:TRP:CZ3	2.06	0.90
4:A:204:TRP:CH2	4:A:212:VAL:HG21	2.06	0.90
4:B:702:ALA:HB1	4:B:849:PHE:CE2	2.07	0.90
4:C:551:ARG:HH21	4:C:872:LEU:HD11	1.37	0.90
4:A:452:ILE:HG22	4:A:528:TYR:O	1.72	0.89
4:B:163:LYS:NZ	4:B:166:VAL:HB	1.87	0.89
3:P:9:DC:H4'	7:P:872:HOH:O	1.72	0.89
4:B:793:LYS:HA	7:B:3141:HOH:O	1.71	0.89
4:D:473:VAL:HG22	4:D:477:GLU:HG3	1.54	0.89
4:B:296:LEU:O	4:B:296:LEU:HG	1.69	0.89
4:C:333:LYS:HB3	4:C:516:PHE:CD2	2.07	0.89
4:B:571:TYR:CE2	4:B:631:LYS:HG3	2.08	0.89
4:C:452:ILE:HD11	4:C:457:TYR:HA	1.52	0.89
4:A:881:ALA:O	4:A:882:PHE:C	2.14	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:96:ARG:HB3	7:C:3133:HOH:O	1.72	0.89
4:D:864:LEU:HA	7:D:3079:HOH:O	1.72	0.89
1:E:11:DA:H2'	1:E:12:DT:H71	1.54	0.89
4:D:854:HIS:CD2	4:D:856:SER:H	1.90	0.89
4:B:77:LEU:HD12	4:B:224:THR:HG21	1.55	0.88
4:B:236:VAL:HB	4:B:239:GLN:HB2	1.54	0.88
4:C:109:ILE:HD11	4:C:149:ALA:HB2	1.54	0.88
4:B:585:ASP:O	4:B:614:LYS:HA	1.73	0.88
4:B:452:ILE:HG23	4:B:453:GLY:H	0.76	0.88
4:C:421:ASP:O	4:C:423:ARG:N	2.07	0.88
4:B:231:ARG:HG2	4:B:234:ALA:HB2	1.55	0.88
1:H:12:DT:C4'	4:B:423:ARG:HE	1.86	0.88
4:A:546:PHE:HD2	4:A:692:ALA:HA	1.39	0.88
4:A:105:PHE:HB3	4:A:204:TRP:CZ2	2.09	0.88
4:A:563:PRO:HB3	4:A:878:SER:HA	1.55	0.88
4:B:110:LYS:HD3	4:B:111:PRO:HD2	1.55	0.88
4:B:695:ALA:O	4:B:699:LEU:HD13	1.72	0.88
4:D:231:ARG:HG2	4:D:234:ALA:HB2	1.53	0.88
4:A:452:ILE:HD11	4:A:457:TYR:HB2	1.55	0.88
4:C:221:ILE:HG12	4:C:227:VAL:HG23	1.55	0.87
1:N:7:DC:H2''	1:N:8:DG:O5'	1.73	0.87
4:B:264:ILE:HG23	4:B:292:ARG:HB2	1.56	0.87
1:N:2:DG:H2''	1:N:3:DG:H8	1.40	0.87
4:B:437:ASN:C	4:B:437:ASN:HD22	1.81	0.87
4:C:42:GLU:HG2	4:C:46:MET:HE2	1.53	0.87
1:E:12:DT:C2'	1:E:13:DC:H5'	2.04	0.87
4:A:155:ARG:HB2	4:A:163:LYS:HE3	1.55	0.87
4:B:881:ALA:O	4:B:882:PHE:C	2.14	0.87
4:D:333:LYS:HB3	4:D:516:PHE:CE2	2.10	0.87
4:C:437:ASN:H	4:C:437:ASN:ND2	1.70	0.87
4:A:308:TYR:O	4:A:311:VAL:HG23	1.75	0.87
4:B:829:ARG:HG3	4:B:829:ARG:HH11	1.38	0.87
4:B:420:MET:HA	4:B:425:ARG:O	1.75	0.87
4:A:231:ARG:HG2	4:A:234:ALA:HB2	1.54	0.87
4:A:871:ASN:ND2	4:A:873:ARG:HB2	1.90	0.86
4:B:118:THR:HG23	4:B:141:ILE:HD13	1.55	0.86
4:B:549:MET:HE2	4:B:841:VAL:CG2	2.05	0.86
1:H:2:DG:H2''	1:H:3:DG:C8	2.10	0.86
4:B:408:PHE:HD1	4:B:414:ILE:HG21	1.40	0.86
4:D:536:PHE:HB3	4:D:882:PHE:HB3	1.57	0.86
4:C:84:ARG:O	4:C:84:ARG:HD3	1.75	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:89:PHE:O	4:D:93:LYS:HG3	1.74	0.86
4:D:437:ASN:ND2	4:D:440:THR:H	1.73	0.86
4:D:39:LEU:HD23	7:D:3105:HOH:O	1.74	0.86
4:D:204:TRP:HE3	7:D:3053:HOH:O	1.56	0.86
4:D:724:ALA:HB2	4:D:738:GLU:HG3	1.57	0.86
4:A:383:ALA:O	4:A:385:TYR:N	2.08	0.86
4:C:635:MET:HE2	6:C:2002:APC:H8	1.57	0.86
4:B:300:HIS:HE2	4:B:422:TRP:HZ3	1.21	0.86
4:C:249:GLU:CD	4:C:249:GLU:N	2.31	0.86
4:C:828:VAL:HG23	4:C:829:ARG:H	1.40	0.86
4:D:137:VAL:O	4:D:141:ILE:HG13	1.75	0.86
4:A:791:LEU:HD11	4:A:809:LEU:HD22	1.55	0.86
4:C:317:TYR:O	4:C:321:ASN:ND2	2.07	0.86
4:C:574:VAL:O	4:C:578:VAL:HG23	1.75	0.86
4:B:706:LEU:HD21	4:B:849:PHE:CB	2.05	0.86
4:C:570:ILE:HA	4:C:573:ILE:CG2	2.05	0.86
4:D:308:TYR:HE2	4:D:734:PRO:HG2	1.39	0.86
4:A:109:ILE:HD11	4:A:145:ILE:O	1.76	0.85
4:C:84:ARG:NH1	4:C:87:ASP:HB2	1.91	0.85
4:C:845:PHE:O	4:C:848:GLN:HB2	1.75	0.85
4:B:463:HIS:CB	4:B:534:LEU:HD22	2.06	0.85
4:C:690:VAL:O	4:C:693:VAL:HB	1.76	0.85
4:B:408:PHE:N	4:B:408:PHE:HD2	1.72	0.85
4:D:804:ILE:HG23	4:D:816:THR:HG21	1.57	0.85
4:A:647:ARG:CD	4:A:675:GLY:HA2	2.05	0.85
1:N:12:DT:H2''	1:N:13:DC:C5'	2.06	0.85
4:B:737:GLN:HE21	4:B:739:TYR:HE2	1.22	0.85
4:C:338:ALA:O	4:C:340:VAL:N	2.10	0.85
3:P:1:DG:H1'	3:P:2:DT:H71	1.56	0.85
4:C:227:VAL:HB	4:C:244:ILE:HD12	1.58	0.85
4:C:276:LYS:HE2	7:C:3084:HOH:O	1.76	0.85
4:A:59:LEU:HA	4:A:64:VAL:CG2	2.06	0.85
4:A:801:LYS:C	4:A:801:LYS:HD3	2.01	0.85
4:B:37:LEU:H	4:B:37:LEU:HD12	1.42	0.85
4:C:404:GLN:HA	4:C:404:GLN:HE21	1.39	0.85
4:D:117:ILE:HG21	4:D:145:ILE:HD13	1.58	0.85
4:A:386:ARG:O	4:A:389:LYS:N	2.09	0.85
4:A:574:VAL:HG11	4:A:685:VAL:HG12	1.56	0.85
4:B:333:LYS:O	4:B:337:VAL:HG23	1.77	0.85
4:B:111:PRO:HG2	4:B:112:GLU:OE1	1.77	0.84
4:D:705:LEU:HB3	4:D:857:GLN:NE2	1.92	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:46:MET:HE1	4:B:269:GLN:NE2	1.91	0.84
4:B:473:VAL:HG13	4:B:474:PRO:CD	2.07	0.84
4:A:256:THR:HG23	7:A:3067:HOH:O	1.77	0.84
4:A:505:GLN:O	4:A:507:SER:N	2.10	0.84
4:C:232:GLN:HB2	4:C:241:SER:O	1.77	0.84
4:B:423:ARG:HG3	4:B:781:ASN:HD22	1.40	0.84
4:C:452:ILE:HD11	4:C:457:TYR:CA	2.07	0.84
4:C:158:GLU:CG	4:C:195:LEU:HD22	2.01	0.84
1:H:9:DA:N6	3:J:1:DG:N2	2.26	0.84
4:A:216:CYS:HA	4:A:219:MET:HE3	1.60	0.84
4:C:92:VAL:CG1	4:C:99:ARG:HG3	2.06	0.84
4:C:278:TRP:CE3	4:C:284:GLY:HA3	2.13	0.84
4:A:727:TRP:CE2	4:A:735:VAL:HG11	2.12	0.84
4:C:559:VAL:HG23	4:C:561:LEU:HD13	1.58	0.84
4:A:452:ILE:HD11	4:A:457:TYR:CA	2.07	0.84
4:B:17:ALA:HA	7:B:3012:HOH:O	1.78	0.84
4:B:168:GLU:O	4:B:172:LYS:HG2	1.77	0.84
4:B:770:ASP:C	4:B:770:ASP:OD1	2.21	0.84
4:A:721:LYS:HD3	4:A:722:ARG:H	1.41	0.84
4:B:632:ARG:HD2	6:B:2001:APC:HN61	1.43	0.84
4:B:728:VAL:HG22	4:B:734:PRO:HA	1.60	0.84
4:B:201:TRP:HB3	7:B:3009:HOH:O	1.78	0.83
4:C:423:ARG:HB2	4:C:423:ARG:NH1	1.93	0.83
4:A:816:THR:HG22	4:A:817:ILE:H	1.43	0.83
4:C:636:THR:HG22	4:C:639:TYR:HD2	1.41	0.83
4:A:646:PHE:O	4:A:650:VAL:HG23	1.78	0.83
4:A:731:ASP:OD1	4:A:792:ARG:NH2	2.11	0.83
4:A:720:ARG:HG2	4:A:720:ARG:HH11	1.42	0.83
4:B:574:VAL:HG21	4:B:685:VAL:HG12	1.57	0.83
4:B:339:ASN:O	4:B:343:LYS:CD	2.26	0.83
4:B:432:PHE:HE2	4:B:444:LEU:HD21	1.40	0.83
4:B:505:GLN:N	4:B:505:GLN:HE21	1.75	0.83
4:C:275:PRO:HG2	4:C:324:GLN:HG2	1.61	0.83
4:C:861:MET:HE3	4:C:862:PRO:HD2	1.60	0.83
4:A:386:ARG:HD2	7:A:3138:HOH:O	1.76	0.83
4:A:574:VAL:O	4:A:578:VAL:HG23	1.76	0.83
4:C:437:ASN:HD22	4:C:437:ASN:N	1.72	0.83
4:D:744:GLN:HA	4:D:756:ARG:CZ	2.08	0.83
4:A:66:ASP:OD2	4:A:752:LEU:HD23	1.79	0.83
4:A:833:VAL:HG13	4:A:872:LEU:HB3	1.58	0.83
4:C:404:GLN:HG2	4:C:432:PHE:CB	2.09	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:551:ARG:HE	4:C:872:LEU:HD21	1.42	0.83
4:C:728:VAL:HG22	4:C:734:PRO:HA	1.59	0.83
4:B:691:ALA:O	4:B:694:GLU:HB2	1.79	0.83
4:A:280:GLY:HA2	4:A:317:TYR:CZ	2.13	0.82
4:B:172:LYS:HB3	4:B:172:LYS:NZ	1.93	0.82
4:B:122:THR:HG21	4:B:226:MET:CE	2.09	0.82
4:D:59:LEU:HD23	4:D:64:VAL:HG22	1.59	0.82
4:D:329:LYS:HG2	4:D:445:THR:O	1.78	0.82
4:D:778:ILE:HG23	4:D:779:ALA:N	1.93	0.82
4:B:846:TYR:HA	4:B:849:PHE:HE1	1.42	0.82
4:C:582:LEU:HB3	4:C:621:LEU:HD21	1.62	0.82
4:C:663:LYS:HD3	4:C:664:GLY:H	1.45	0.82
4:A:881:ALA:O	4:A:882:PHE:O	1.98	0.82
4:D:668:THR:HG22	4:D:669:GLN:HE21	1.45	0.82
1:E:14:DG:H2'	1:E:15:DC:C6	2.15	0.82
4:A:278:TRP:CE3	4:A:284:GLY:HA3	2.15	0.82
4:B:345:LYS:NZ	4:B:351:ASP:H	1.77	0.82
4:B:574:VAL:O	4:B:574:VAL:CG1	2.26	0.82
4:C:308:TYR:O	4:C:311:VAL:HG23	1.79	0.82
4:D:490:MET:HE1	4:D:523:HIS:NE2	1.94	0.82
4:D:828:VAL:HB	4:D:883:ALA:HA	1.61	0.82
4:B:298:ARG:HG3	4:B:420:MET:O	1.78	0.82
4:B:574:VAL:O	4:B:574:VAL:HG12	1.76	0.82
4:C:579:ASN:HA	4:C:582:LEU:HD12	1.62	0.82
4:C:169:GLN:O	4:C:173:ARG:HG2	1.80	0.82
4:D:275:PRO:HG2	4:D:324:GLN:HG2	1.61	0.82
4:D:470:VAL:HG12	4:D:473:VAL:HG11	1.61	0.82
4:A:486:HIS:HD2	4:A:518:TYR:CE1	1.98	0.82
1:N:10:DT:H5'	4:D:641:SER:CA	2.09	0.82
4:A:512:LEU:HG	4:A:516:PHE:HE1	1.43	0.82
4:B:231:ARG:HD2	4:B:240:ASP:OD2	1.80	0.82
4:B:408:PHE:N	4:B:408:PHE:CD2	2.47	0.82
4:A:19:ILE:HG13	7:A:3121:HOH:O	1.78	0.81
4:B:264:ILE:C	4:B:266:PRO:HD3	2.05	0.81
4:C:236:VAL:CB	4:C:239:GLN:HB2	2.10	0.81
4:D:486:HIS:HA	4:D:489:ILE:HD12	1.59	0.81
4:B:229:LEU:HD11	4:B:242:GLU:HG2	1.61	0.81
4:D:342:THR:HG22	4:D:348:PRO:HG2	1.62	0.81
1:H:13:DC:O4'	4:B:427:TYR:HE2	1.60	0.81
4:A:421:ASP:OD1	4:A:423:ARG:HD3	1.79	0.81
4:D:541:SER:HA	4:D:544:GLN:NE2	1.95	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:870:LEU:HD22	4:D:872:LEU:HD23	1.62	0.81
2:I:4:G:H2'	2:I:5:C:C6	2.16	0.81
4:C:231:ARG:HG2	4:C:234:ALA:HB2	1.63	0.81
4:C:271:CYS:SG	4:C:417:PRO:HD3	2.20	0.81
4:B:51:PHE:O	4:B:51:PHE:CD2	2.34	0.81
4:C:550:LEU:HD21	4:C:865:PRO:HG2	1.62	0.81
4:D:308:TYR:CE2	4:D:734:PRO:HG2	2.14	0.81
4:A:401:MET:O	4:A:403:GLU:N	2.14	0.81
4:D:16:LEU:HD22	4:D:38:ALA:HA	1.61	0.81
4:D:699:LEU:O	4:D:778:ILE:HG21	1.80	0.81
4:B:632:ARG:O	4:B:636:THR:HG23	1.79	0.81
4:B:742:PRO:HB3	4:B:744:GLN:OE1	1.81	0.81
4:A:583:GLN:HB2	7:A:3056:HOH:O	1.79	0.81
4:D:80:LYS:HD3	4:D:224:THR:HB	1.62	0.81
4:A:184:GLN:HG3	7:A:3137:HOH:O	1.81	0.81
4:B:398:LEU:CD2	4:B:439:MET:HE1	2.11	0.81
4:B:587:ILE:HG22	4:B:588:ASN:ND2	1.96	0.81
4:D:551:ARG:HB2	4:D:868:GLY:H	1.45	0.81
4:A:303:LYS:HD2	7:D:3155:HOH:O	1.81	0.80
4:B:470:VAL:O	4:B:470:VAL:HG12	1.81	0.80
4:C:291:ARG:HG3	7:C:3104:HOH:O	1.81	0.80
4:C:610:LYS:HE3	7:C:3172:HOH:O	1.80	0.80
4:D:871:ASN:HD21	4:D:873:ARG:HB2	1.46	0.80
4:A:280:GLY:HA2	4:A:317:TYR:CE1	2.16	0.80
4:B:275:PRO:HD2	7:B:3116:HOH:O	1.81	0.80
4:D:286:TYR:CE1	4:D:417:PRO:HG3	2.15	0.80
4:B:126:LEU:HD13	4:B:246:LEU:HB2	1.61	0.80
4:B:869:ASN:N	4:B:869:ASN:ND2	2.28	0.80
4:A:15:GLU:HB3	4:A:19:ILE:HG12	1.63	0.80
4:D:840:ASP:O	4:D:842:LEU:N	2.14	0.80
4:A:669:GLN:HG2	4:A:672:GLN:HE21	1.47	0.80
4:A:278:TRP:CZ3	4:A:284:GLY:HA3	2.17	0.80
4:A:624:GLY:HA3	7:A:3045:HOH:O	1.79	0.80
4:D:582:LEU:HD11	4:D:625:VAL:HG21	1.62	0.80
4:A:502:TRP:CG	4:A:512:LEU:HD13	2.16	0.80
4:B:158:GLU:HA	4:B:195:LEU:HD13	1.63	0.80
4:C:631:LYS:CE	6:C:2002:APC:H3A2	2.11	0.80
4:D:448:LYS:NZ	4:D:806:SER:HB3	1.96	0.80
1:H:6:DT:C6	1:H:6:DT:H5'	2.16	0.80
4:A:802:TYR:O	4:A:804:ILE:N	2.13	0.80
4:B:537:ASP:H	4:B:882:PHE:HD2	1.28	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:669:GLN:CG	4:B:672:GLN:HG3	2.11	0.80
4:C:211:HIS:O	4:C:214:VAL:HG23	1.81	0.80
4:D:552:ASP:OD1	4:D:555:GLY:N	2.11	0.80
4:C:155:ARG:HB2	4:C:163:LYS:HZ2	1.47	0.80
7:I:777:HOH:O	4:B:386:ARG:HD3	1.82	0.79
1:N:2:DG:H2''	1:N:3:DG:C8	2.16	0.79
4:C:631:LYS:HZ3	6:C:2002:APC:H3A2	1.44	0.79
4:D:14:ILE:H	4:D:14:ILE:HD12	1.45	0.79
4:D:281:ILE:HG22	4:D:282:THR:HG22	1.62	0.79
4:D:489:ILE:O	4:D:492:CYS:SG	2.40	0.79
4:A:15:GLU:HG3	4:A:18:ALA:H	1.45	0.79
4:A:478:ARG:HH12	4:A:882:PHE:HZ	1.29	0.79
4:A:610:LYS:O	4:A:610:LYS:HG2	1.79	0.79
4:C:214:VAL:HA	4:C:217:ILE:HD12	1.65	0.79
4:D:125:CYS:O	4:D:128:SER:HB3	1.81	0.79
4:D:490:MET:O	4:D:493:ALA:HB3	1.81	0.79
4:A:462:ILE:HG12	4:A:479:ILE:HD11	1.64	0.79
4:B:881:ALA:O	4:B:883:ALA:OXT	1.99	0.79
4:A:157:LEU:HB3	7:A:3133:HOH:O	1.80	0.79
4:A:452:ILE:HD11	4:A:457:TYR:CB	2.13	0.79
4:A:526:LEU:HD12	4:A:526:LEU:N	1.97	0.79
4:C:78:LEU:N	4:C:79:PRO:HD2	1.97	0.79
4:D:804:ILE:HG12	4:D:820:ASP:HB3	1.63	0.79
1:H:14:DG:H2''	1:H:15:DC:C5'	2.13	0.79
4:A:119:ILE:O	4:A:123:LEU:HD12	1.81	0.79
4:A:342:THR:HG21	4:A:398:LEU:HD21	1.61	0.79
4:D:860:LYS:HD2	4:D:860:LYS:O	1.83	0.79
4:A:806:SER:O	4:A:816:THR:HG23	1.82	0.79
4:B:475:PHE:O	4:B:476:PRO:C	2.23	0.79
4:B:748:ASN:ND2	4:B:751:PHE:HB2	1.98	0.79
4:C:19:ILE:HD13	7:C:3117:HOH:O	1.83	0.79
4:C:59:LEU:HD22	4:C:64:VAL:HG13	1.65	0.79
4:C:158:GLU:HA	4:C:195:LEU:HD13	1.63	0.79
4:D:139:SER:HB2	4:D:210:ILE:CD1	2.13	0.79
4:C:396:ILE:HG22	7:C:3188:HOH:O	1.82	0.79
4:C:299:THR:HG22	4:C:300:HIS:N	1.98	0.79
4:A:291:ARG:HB2	7:A:3193:HOH:O	1.83	0.79
4:B:390:ALA:C	4:B:392:LYS:H	1.87	0.79
4:C:220:LEU:HD21	4:C:226:MET:HE2	1.64	0.79
4:A:452:ILE:HD11	4:A:457:TYR:HA	1.65	0.78
4:C:47:GLY:HA3	4:C:265:SER:O	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:563:PRO:HB3	4:C:877:GLU:O	1.82	0.78
4:A:16:LEU:HD13	4:A:38:ALA:CB	2.13	0.78
4:B:24:LEU:HD13	4:B:37:LEU:HD11	1.62	0.78
4:B:712:ASP:HB3	7:B:3078:HOH:O	1.84	0.78
4:B:814:PHE:HB3	4:B:824:LEU:HD21	1.65	0.78
4:D:302:LYS:HE3	4:D:306:MET:HE2	1.62	0.78
4:D:475:PHE:HE2	4:D:879:ASP:HB3	1.48	0.78
4:A:871:ASN:HB3	4:A:874:ASP:OD2	1.83	0.78
4:B:816:THR:CG2	4:B:817:ILE:H	1.89	0.78
4:A:133:THR:HA	4:A:243:THR:HG22	1.65	0.78
4:B:449:GLY:HA3	4:B:529:ASN:ND2	1.99	0.78
4:B:816:THR:HG22	4:B:817:ILE:N	1.91	0.78
4:C:404:GLN:HG2	4:C:432:PHE:HB2	1.65	0.78
4:C:778:ILE:CG2	4:C:779:ALA:N	2.46	0.78
4:D:806:SER:O	4:D:816:THR:HG23	1.81	0.78
4:A:748:ASN:ND2	4:A:751:PHE:H	1.82	0.78
4:C:505:GLN:O	4:C:508:PRO:HD3	1.82	0.78
1:K:11:DA:C8	4:C:639:TYR:HB3	2.18	0.78
4:A:546:PHE:CE1	4:A:783:VAL:CG2	2.63	0.78
4:A:791:LEU:CD1	4:A:809:LEU:HD22	2.14	0.78
4:B:446:LEU:HD12	4:B:817:ILE:HG23	1.64	0.78
4:C:84:ARG:HA	4:C:84:ARG:HH11	1.47	0.78
4:D:881:ALA:O	4:D:882:PHE:C	2.27	0.78
4:A:44:TYR:OH	4:A:292:ARG:HB3	1.83	0.78
4:A:475:PHE:O	4:A:479:ILE:HG12	1.84	0.78
4:D:427:TYR:HA	4:D:435:GLN:HE22	1.48	0.78
4:B:869:ASN:N	4:B:869:ASN:HD22	1.81	0.78
4:C:448:LYS:HE3	4:C:806:SER:OG	1.84	0.78
4:D:323:ALA:O	4:D:325:ASN:N	2.16	0.78
4:A:60:LYS:HZ1	4:A:61:ALA:HB2	1.49	0.78
4:A:546:PHE:CZ	4:A:783:VAL:HG22	2.19	0.78
4:A:562:LEU:HD21	4:A:870:LEU:HD12	1.65	0.78
4:A:860:LYS:HD2	4:A:860:LYS:O	1.84	0.78
4:C:70:ALA:C	4:C:72:PRO:HD2	2.09	0.78
4:C:545:HIS:O	4:C:549:MET:HG2	1.84	0.78
4:D:454:LYS:HG3	4:D:455:GLU:H	1.48	0.78
1:N:15:DC:C2	1:N:16:DC:C5	2.72	0.77
4:B:345:LYS:HZ1	4:B:351:ASP:H	1.27	0.77
4:D:475:PHE:CE2	4:D:879:ASP:HB3	2.19	0.77
4:B:423:ARG:HH12	4:B:784:HIS:HB3	1.48	0.77
4:B:274:PRO:HD3	4:B:415:TRP:CZ3	2.19	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:706:LEU:HD22	4:C:725:VAL:HG22	1.67	0.77
4:A:727:TRP:HA	4:A:848:GLN:HE21	1.46	0.77
4:B:80:LYS:O	4:B:223:SER:HB2	1.83	0.77
4:B:549:MET:HE1	4:B:782:PHE:HE2	1.49	0.77
4:D:159:ALA:O	4:D:163:LYS:HB2	1.84	0.77
1:H:2:DG:H2''	1:H:3:DG:H8	1.48	0.77
2:O:4:G:O2'	2:O:5:C:H5'	1.85	0.77
4:B:631:LYS:HE2	6:B:2001:APC:H3A2	1.67	0.77
4:C:460:LEU:HG	4:C:460:LEU:O	1.84	0.77
4:B:233:ASN:HD22	4:B:239:GLN:NE2	1.82	0.77
4:B:273:VAL:O	4:B:274:PRO:O	2.02	0.77
4:C:181:ALA:O	4:C:185:VAL:HG22	1.85	0.77
4:D:563:PRO:HB2	7:D:3032:HOH:O	1.85	0.77
4:A:468:ALA:HB2	4:A:511:PHE:CE1	2.20	0.77
4:D:57:ARG:O	4:D:60:LYS:HB3	1.85	0.77
4:A:141:ILE:HG22	4:A:145:ILE:HD11	1.66	0.77
4:A:664:GLY:HA2	4:A:667:PHE:HD2	1.50	0.77
4:B:407:LYS:HG2	4:B:408:PHE:CD2	2.19	0.77
4:B:489:ILE:HG22	4:B:515:CYS:HB3	1.67	0.77
4:B:663:LYS:HG2	4:B:664:GLY:H	1.49	0.77
4:C:81:MET:O	4:C:85:ILE:HG13	1.85	0.77
4:C:275:PRO:HB2	4:C:324:GLN:OE1	1.85	0.77
4:D:51:PHE:CE2	4:D:55:PHE:HB2	2.20	0.77
4:D:55:PHE:CZ	4:D:59:LEU:HD21	2.20	0.77
4:D:720:ARG:HH11	4:D:720:ARG:CG	1.86	0.77
1:H:14:DG:H2''	1:H:15:DC:H5'	1.67	0.77
4:B:5:ASN:HD22	4:B:8:LYS:HG3	1.49	0.77
4:C:337:VAL:HG21	4:C:512:LEU:HD21	1.66	0.77
4:C:433:ASN:CA	7:C:3164:HOH:O	2.33	0.77
1:K:11:DA:H2'	1:K:12:DT:C7	2.14	0.76
4:A:825:PHE:CZ	4:A:829:ARG:NH2	2.52	0.76
4:D:744:GLN:HA	4:D:756:ARG:NE	2.00	0.76
4:C:401:MET:O	4:C:404:GLN:HB3	1.85	0.76
4:C:516:PHE:O	4:C:519:ALA:HB3	1.84	0.76
4:D:95:LYS:HD3	7:D:3062:HOH:O	1.85	0.76
4:A:84:ARG:C	4:A:84:ARG:HD3	2.10	0.76
4:A:210:ILE:O	4:A:214:VAL:HG23	1.85	0.76
4:A:390:ALA:O	4:A:392:LYS:N	2.18	0.76
4:A:495:SER:HA	7:A:3203:HOH:O	1.85	0.76
4:B:582:LEU:HB3	4:B:621:LEU:HD11	1.65	0.76
4:C:55:PHE:O	4:C:58:GLN:HB2	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:473:VAL:N	4:D:567:VAL:HG21	2.00	0.76
4:A:281:ILE:CG1	4:A:309:GLU:HA	2.15	0.76
4:A:87:ASP:O	4:A:91:GLU:HG3	1.85	0.76
4:B:423:ARG:CG	4:B:781:ASN:HD22	1.98	0.76
4:D:651:LEU:O	4:D:651:LEU:HD13	1.85	0.76
4:B:163:LYS:HZ3	4:B:166:VAL:HB	1.47	0.76
4:B:690:VAL:O	4:B:693:VAL:HG23	1.84	0.76
4:A:512:LEU:HG	4:A:516:PHE:CE1	2.21	0.76
4:B:784:HIS:O	4:B:786:GLN:N	2.18	0.76
4:B:790:HIS:HE1	4:B:831:THR:HG23	1.50	0.76
4:A:92:VAL:HG11	4:A:100:PRO:HD2	1.66	0.76
4:B:418:TYR:CD2	4:B:428:ALA:HA	2.21	0.76
4:A:454:LYS:N	4:A:526:LEU:HD23	2.00	0.76
4:C:15:GLU:HG3	4:C:18:ALA:H	1.49	0.76
4:C:40:GLU:CD	4:C:286:TYR:HB3	2.10	0.76
4:C:744:GLN:CB	7:C:3076:HOH:O	2.34	0.76
4:A:548:ALA:O	4:A:550:LEU:N	2.18	0.76
4:C:778:ILE:CG2	4:C:779:ALA:H	1.99	0.76
4:D:790:HIS:CE1	4:D:831:THR:HG23	2.16	0.76
4:A:464:GLY:HA3	4:A:514:PHE:CZ	2.21	0.75
4:B:268:PHE:HB3	4:B:286:TYR:HH	1.49	0.75
4:C:308:TYR:OH	4:C:734:PRO:O	2.05	0.75
4:D:540:CYS:O	4:D:542:GLY:N	2.18	0.75
4:D:772:HIS:O	4:D:773:LYS:C	2.28	0.75
4:A:84:ARG:HD3	4:A:84:ARG:O	1.87	0.75
4:A:668:THR:HG22	4:A:669:GLN:OE1	1.86	0.75
4:A:825:PHE:CE1	4:A:829:ARG:CZ	2.68	0.75
4:A:290:GLY:O	4:A:293:PRO:HD3	1.86	0.75
4:C:308:TYR:OH	4:C:733:PHE:HE2	1.69	0.75
4:C:400:PHE:CE1	4:C:431:MET:HE2	2.22	0.75
4:D:228:SER:HB3	7:D:3168:HOH:O	1.86	0.75
4:A:457:TYR:HD1	4:A:521:VAL:HG21	1.52	0.75
4:A:816:THR:OG1	4:A:824:LEU:HD22	1.87	0.75
4:C:299:THR:HG22	4:C:300:HIS:H	1.51	0.75
4:D:829:ARG:HH11	4:D:829:ARG:HG3	1.51	0.75
4:C:155:ARG:HB2	4:C:163:LYS:NZ	2.00	0.75
4:D:141:ILE:O	4:D:145:ILE:HG12	1.87	0.75
4:B:719:LEU:HD23	4:B:854:HIS:NE2	2.01	0.75
4:C:5:ASN:HD21	4:C:7:ALA:HB3	1.50	0.75
4:D:465:ALA:CB	4:D:478:ARG:HB3	2.16	0.75
4:D:871:ASN:ND2	4:D:873:ARG:HB2	2.00	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:280:GLY:CA	4:A:317:TYR:OH	2.35	0.75
4:B:391:ARG:HG3	7:B:3101:HOH:O	1.86	0.75
4:B:463:HIS:HB2	4:B:534:LEU:HD22	1.68	0.75
4:C:539:SER:HA	7:C:3124:HOH:O	1.86	0.75
4:D:297:VAL:HG12	4:D:299:THR:HG22	1.68	0.75
4:A:273:VAL:CG2	4:A:273:VAL:O	2.35	0.75
4:A:463:HIS:HA	4:A:466:ASN:ND2	2.01	0.75
1:N:10:DT:H5'	4:D:641:SER:N	2.02	0.75
4:B:868:GLY:C	4:B:869:ASN:HD22	1.95	0.75
4:C:400:PHE:CZ	4:C:431:MET:HE2	2.21	0.75
4:D:36:GLN:CD	4:D:273:VAL:HG22	2.12	0.75
4:D:435:GLN:HB3	4:D:810:ILE:HG12	1.69	0.75
4:A:544:GLN:CG	4:A:559:VAL:HG21	2.16	0.74
1:H:15:DC:H2''	1:H:16:DC:C5'	2.18	0.74
7:I:777:HOH:O	4:B:386:ARG:CD	2.33	0.74
4:A:486:HIS:CD2	4:A:518:TYR:HE1	2.06	0.74
4:B:55:PHE:CD2	4:B:55:PHE:O	2.40	0.74
4:C:810:ILE:O	4:C:810:ILE:HG22	1.86	0.74
4:A:514:PHE:HD1	4:A:515:CYS:N	1.85	0.74
4:A:793:LYS:O	4:A:796:VAL:HG23	1.86	0.74
4:B:56:GLU:OE1	4:B:57:ARG:HA	1.87	0.74
4:B:647:ARG:O	4:B:648:GLN:C	2.31	0.74
4:C:4:ILE:HD12	4:C:256:THR:HG23	1.69	0.74
4:C:324:GLN:HE21	4:C:418:TYR:H	1.36	0.74
4:D:454:LYS:HG3	4:D:455:GLU:N	2.03	0.74
4:A:825:PHE:CE1	4:A:829:ARG:NH2	2.55	0.74
4:B:92:VAL:HA	7:B:3193:HOH:O	1.88	0.74
4:B:871:ASN:HB3	4:B:874:ASP:OD2	1.88	0.74
4:D:351:ASP:HA	7:D:3124:HOH:O	1.86	0.74
4:B:143:ARG:O	4:B:146:GLU:HB3	1.86	0.74
4:C:109:ILE:CD1	4:C:149:ALA:HB2	2.17	0.74
4:C:141:ILE:O	4:C:145:ILE:HG12	1.86	0.74
4:A:77:LEU:HD23	4:A:119:ILE:HD12	1.70	0.74
4:A:418:TYR:HD2	4:A:426:VAL:CG1	2.01	0.74
4:B:651:LEU:HD22	4:B:651:LEU:O	1.86	0.74
4:C:749:LEU:HD12	4:C:750:MET:HG2	1.69	0.74
4:A:275:PRO:HD2	7:A:3206:HOH:O	1.88	0.74
4:B:71:LYS:N	4:B:72:PRO:HD2	2.03	0.74
4:B:846:TYR:HA	4:B:849:PHE:CE1	2.23	0.74
4:B:855:GLU:O	4:B:858:LEU:HD12	1.87	0.74
4:C:84:ARG:HH12	4:C:87:ASP:CB	2.00	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:116:TYR:OH	4:A:752:LEU:HD22	1.88	0.74
4:C:706:LEU:CD2	4:C:725:VAL:HG13	2.18	0.74
4:A:60:LYS:O	4:A:60:LYS:HG2	1.86	0.74
4:A:118:THR:O	4:A:122:THR:OG1	2.03	0.74
4:A:395:ARG:HG3	4:A:395:ARG:O	1.88	0.74
4:B:537:ASP:O	4:B:882:PHE:HB2	1.87	0.74
4:B:663:LYS:CG	4:B:664:GLY:H	2.00	0.74
4:C:738:GLU:HA	4:C:774:GLN:HE22	1.53	0.74
4:C:744:GLN:HB3	4:C:756:ARG:HB3	1.70	0.74
4:D:250:TYR:O	4:D:254:ILE:HG13	1.88	0.74
4:A:236:VAL:HG11	4:A:239:GLN:CD	2.13	0.73
4:B:46:MET:HE1	4:B:269:GLN:HE22	1.50	0.73
4:B:122:THR:HG21	4:B:226:MET:HE2	1.67	0.73
4:B:172:LYS:HB3	4:B:172:LYS:HZ2	1.52	0.73
4:B:636:THR:HG21	4:B:649:GLN:HE22	1.53	0.73
4:C:656:GLN:N	4:C:657:PRO:HD2	2.02	0.73
4:D:663:LYS:HG2	4:D:664:GLY:H	1.52	0.73
1:H:12:DT:H4'	4:B:423:ARG:HE	1.52	0.73
4:B:780:PRO:HA	4:B:783:VAL:HG23	1.70	0.73
4:C:866:ALA:HB2	7:C:3189:HOH:O	1.86	0.73
4:C:850:ALA:O	4:C:853:LEU:HG	1.89	0.73
4:A:402:LEU:HG	4:A:439:MET:HE1	1.69	0.73
4:B:226:MET:O	4:B:247:ALA:HB2	1.88	0.73
4:B:278:TRP:CE3	4:B:284:GLY:HA3	2.23	0.73
4:B:557:ARG:O	4:B:557:ARG:HG2	1.86	0.73
4:B:662:GLY:O	4:B:663:LYS:O	2.06	0.73
4:C:655:ILE:HD12	4:C:674:ALA:HB2	1.69	0.73
4:C:492:CYS:HA	7:C:3071:HOH:O	1.89	0.73
4:C:744:GLN:HB2	7:C:3076:HOH:O	1.89	0.73
4:D:457:TYR:CE1	4:D:521:VAL:HG11	2.23	0.73
1:K:13:DC:H2''	1:K:14:DG:C5'	2.18	0.73
4:A:100:PRO:HG2	4:A:103:PHE:HB2	1.69	0.73
4:A:380:ALA:O	4:A:384:VAL:HG23	1.87	0.73
4:C:210:ILE:O	4:C:214:VAL:HG22	1.89	0.73
4:C:636:THR:HG22	4:C:639:TYR:CD2	2.22	0.73
4:C:778:ILE:HG23	4:C:779:ALA:H	1.51	0.73
4:D:417:PRO:O	4:D:429:VAL:HG23	1.87	0.73
4:D:457:TYR:CD1	4:D:521:VAL:HG11	2.24	0.73
4:A:562:LEU:HD21	4:A:870:LEU:HD11	1.69	0.73
4:A:668:THR:HG22	4:A:669:GLN:CD	2.14	0.73
4:C:337:VAL:HG12	4:C:338:ALA:N	2.03	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:54:MET:O	4:A:58:GLN:HG2	1.89	0.73
4:B:233:ASN:HD22	4:B:239:GLN:CD	1.97	0.73
4:C:281:ILE:HG12	4:C:309:GLU:HA	1.70	0.73
4:D:14:ILE:CG2	4:D:288:ALA:HB1	2.19	0.73
1:K:13:DC:H2''	1:K:14:DG:O5'	1.89	0.73
4:B:748:ASN:ND2	4:B:751:PHE:H	1.86	0.73
4:D:330:ILE:HG13	4:D:408:PHE:O	1.88	0.73
1:K:11:DA:H2'	1:K:12:DT:H72	1.69	0.73
4:A:138:ALA:O	4:A:213:GLY:HA3	1.89	0.73
4:A:281:ILE:CG2	4:A:282:THR:HG23	2.11	0.73
4:B:291:ARG:HB2	7:B:3037:HOH:O	1.89	0.73
4:C:739:TYR:HB2	4:C:774:GLN:OE1	1.89	0.73
2:I:1:G:H5''	7:I:873:HOH:O	1.89	0.72
4:C:269:GLN:O	4:C:430:SER:HB3	1.88	0.72
4:D:278:TRP:HB2	4:D:321:ASN:HD21	1.53	0.72
4:A:514:PHE:CD1	4:A:515:CYS:N	2.57	0.72
4:A:736:TRP:HB2	7:A:3116:HOH:O	1.88	0.72
4:C:728:VAL:HG22	4:C:734:PRO:CA	2.19	0.72
4:D:833:VAL:CG2	4:D:875:ILE:HB	2.19	0.72
4:A:428:ALA:H	4:A:435:GLN:HE22	1.34	0.72
4:A:829:ARG:HG3	4:A:829:ARG:NH1	1.98	0.72
4:B:418:TYR:HE2	4:B:428:ALA:CB	2.01	0.72
4:B:801:LYS:C	4:B:801:LYS:HD3	2.13	0.72
4:A:59:LEU:HA	4:A:64:VAL:HG22	1.70	0.72
4:B:119:ILE:O	4:B:122:THR:HB	1.88	0.72
4:B:395:ARG:O	4:B:398:LEU:N	2.22	0.72
4:B:454:LYS:HE2	7:B:3020:HOH:O	1.88	0.72
4:C:423:ARG:NH2	4:C:784:HIS:ND1	2.37	0.72
4:D:39:LEU:HD22	4:D:272:VAL:CG2	2.19	0.72
2:F:1:G:H2'	2:F:2:C:C6	2.24	0.72
4:B:552:ASP:C	4:B:552:ASP:OD1	2.32	0.72
4:D:272:VAL:O	4:D:415:TRP:HZ3	1.72	0.72
4:D:472:LYS:HA	4:D:567:VAL:HG11	1.71	0.72
4:D:505:GLN:N	4:D:505:GLN:NE2	2.37	0.72
4:B:122:THR:CG2	4:B:226:MET:HE1	2.19	0.72
4:B:339:ASN:O	4:B:343:LYS:HD2	1.88	0.72
4:A:42:GLU:HG2	4:A:46:MET:HE2	1.70	0.72
4:A:113:ALA:O	4:A:117:ILE:HG13	1.89	0.72
4:B:268:PHE:CB	4:B:286:TYR:OH	2.35	0.72
4:B:314:PRO:O	4:B:316:VAL:N	2.23	0.72
4:B:567:VAL:HG13	4:B:880:PHE:CG	2.25	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:423:ARG:HD2	4:C:781:ASN:ND2	2.03	0.72
4:D:328:TRP:O	4:D:414:ILE:N	2.20	0.72
1:H:3:DG:N3	7:H:1116:HOH:O	2.22	0.72
4:B:432:PHE:CE2	4:B:444:LEU:HD21	2.23	0.72
4:B:578:VAL:HG22	4:B:680:LEU:HB3	1.72	0.72
4:B:620:TRP:CE2	4:B:677:MET:HE2	2.25	0.72
4:C:459:TRP:HB3	4:C:534:LEU:HD13	1.70	0.72
4:D:327:ALA:HB2	4:D:415:TRP:NE1	2.05	0.72
4:D:448:LYS:CE	4:D:806:SER:HB3	2.19	0.72
4:D:593:GLU:O	4:D:610:LYS:N	2.19	0.72
4:A:182:PHE:O	4:A:185:VAL:HG22	1.90	0.72
4:A:423:ARG:NH2	4:A:784:HIS:HB3	2.05	0.72
4:B:281:ILE:CD1	4:B:309:GLU:HA	2.20	0.72
4:B:505:GLN:HE21	4:B:505:GLN:H	1.36	0.72
4:B:741:LYS:HB2	4:B:770:ASP:HB2	1.70	0.72
4:C:420:MET:HA	4:C:425:ARG:O	1.89	0.72
4:D:766:ASP:HB3	7:D:3085:HOH:O	1.88	0.72
4:A:502:TRP:CE2	4:A:512:LEU:HD13	2.25	0.71
4:B:471:ASP:O	4:B:472:LYS:HD2	1.90	0.71
4:C:335:LEU:HD21	4:C:339:ASN:HD22	1.55	0.71
4:C:402:LEU:HG	4:C:439:MET:HE3	1.71	0.71
4:A:421:ASP:O	4:A:423:ARG:N	2.22	0.71
4:B:300:HIS:NE2	4:B:422:TRP:CZ3	2.56	0.71
4:C:78:LEU:HG	4:C:78:LEU:O	1.88	0.71
4:C:247:ALA:HB1	4:C:249:GLU:OE1	1.90	0.71
4:D:352:ILE:HD12	4:D:352:ILE:N	2.05	0.71
4:D:443:LEU:N	4:D:443:LEU:HD23	2.04	0.71
1:E:15:DC:H2''	1:E:16:DC:H5'	1.71	0.71
4:B:281:ILE:HD13	4:B:309:GLU:HA	1.72	0.71
4:C:77:LEU:C	4:C:79:PRO:HD2	2.15	0.71
4:C:291:ARG:HB2	7:C:3192:HOH:O	1.89	0.71
4:C:433:ASN:OD1	4:C:435:GLN:N	2.21	0.71
4:C:663:LYS:CD	4:C:664:GLY:H	2.03	0.71
4:C:797:TRP:CZ2	4:C:801:LYS:HG3	2.26	0.71
4:B:423:ARG:CG	4:B:781:ASN:ND2	2.53	0.71
4:B:609:VAL:O	4:B:611:LEU:N	2.23	0.71
4:C:551:ARG:HD2	7:C:3087:HOH:O	1.91	0.71
4:A:666:MET:N	4:A:666:MET:SD	2.64	0.71
4:B:236:VAL:HG21	4:B:239:GLN:NE2	2.06	0.71
4:B:274:PRO:HD3	4:B:415:TRP:CH2	2.25	0.71
4:B:454:LYS:HB2	7:B:3020:HOH:O	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:557:ARG:HB2	4:C:562:LEU:HD12	1.70	0.71
4:A:5:ASN:ND2	4:A:7:ALA:HB3	2.06	0.71
4:A:457:TYR:CE1	4:A:521:VAL:HG11	2.25	0.71
4:A:669:GLN:O	4:A:670:PRO:C	2.33	0.71
4:B:308:TYR:CE2	4:B:734:PRO:HG2	2.25	0.71
4:B:617:ALA:HB2	4:B:676:TYR:OH	1.91	0.71
4:D:541:SER:HA	4:D:544:GLN:HE21	1.53	0.71
4:A:351:ASP:HA	7:A:3222:HOH:O	1.89	0.71
4:A:548:ALA:C	4:A:550:LEU:H	1.97	0.71
4:B:100:PRO:HG2	4:B:103:PHE:HB2	1.71	0.71
4:C:338:ALA:C	4:C:340:VAL:N	2.46	0.71
4:C:338:ALA:C	4:C:340:VAL:H	1.96	0.71
4:D:231:ARG:CG	4:D:234:ALA:HB2	2.21	0.71
1:H:14:DG:H2''	1:H:15:DC:O5'	1.90	0.71
4:A:423:ARG:NH2	4:A:784:HIS:CG	2.59	0.71
4:B:11:PHE:CZ	4:B:44:TYR:HB3	2.24	0.71
4:B:564:SER:OG	4:B:566:THR:N	2.20	0.71
4:C:201:TRP:O	4:C:204:TRP:HB2	1.90	0.71
4:C:828:VAL:O	4:C:831:THR:HG22	1.89	0.71
4:D:257:ARG:O	4:D:261:LEU:HB2	1.91	0.71
4:D:324:GLN:HG3	4:D:417:PRO:HA	1.73	0.71
4:A:540:CYS:O	4:A:541:SER:C	2.33	0.71
4:A:720:ARG:HG2	4:A:720:ARG:NH1	2.03	0.71
4:B:816:THR:HG21	4:B:820:ASP:HB3	1.73	0.71
4:D:269:GLN:HE22	4:D:407:LYS:HE2	1.56	0.71
4:A:109:ILE:CD1	4:A:145:ILE:O	2.39	0.71
4:A:643:GLU:HB2	7:A:3076:HOH:O	1.90	0.71
4:A:828:VAL:HB	4:A:883:ALA:HA	1.73	0.71
4:B:390:ALA:O	4:B:393:SER:N	2.24	0.71
4:C:629:VAL:HG11	4:C:677:MET:HE3	1.71	0.71
4:D:435:GLN:HA	4:D:810:ILE:HD11	1.72	0.71
4:A:60:LYS:O	4:A:60:LYS:NZ	2.18	0.70
4:A:161:HIS:O	4:A:164:LYS:HG2	1.90	0.70
4:A:786:GLN:OE1	4:A:841:VAL:HG11	1.91	0.70
4:B:213:GLY:O	4:B:217:ILE:HG13	1.91	0.70
4:C:553:GLU:HA	4:C:870:LEU:HD12	1.73	0.70
4:C:861:MET:HE3	4:C:862:PRO:CD	2.21	0.70
4:D:116:TYR:OH	4:D:752:LEU:HD22	1.90	0.70
4:D:428:ALA:H	4:D:435:GLN:NE2	1.89	0.70
4:A:633:SER:HB2	7:A:3199:HOH:O	1.91	0.70
4:A:810:ILE:HB	4:A:813:SER:HB3	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:849:PHE:O	4:B:852:GLN:N	2.22	0.70
4:C:120:LYS:HG3	4:C:752:LEU:HD11	1.74	0.70
4:C:553:GLU:CD	4:C:553:GLU:H	1.99	0.70
4:A:827:ALA:O	4:A:830:GLU:HB2	1.91	0.70
4:B:312:TYR:HA	7:B:3069:HOH:O	1.89	0.70
4:B:645:GLY:O	4:B:647:ARG:N	2.24	0.70
4:C:338:ALA:HB2	4:C:509:PHE:CE1	2.20	0.70
4:D:264:ILE:CG2	4:D:292:ARG:HB2	2.21	0.70
4:D:810:ILE:HG22	4:D:810:ILE:O	1.89	0.70
4:A:89:PHE:HA	4:A:103:PHE:CE1	2.26	0.70
4:A:158:GLU:HG2	4:A:195:LEU:HD23	1.74	0.70
4:A:281:ILE:HG12	4:A:309:GLU:HA	1.73	0.70
4:A:720:ARG:O	4:A:721:LYS:O	2.09	0.70
4:B:475:PHE:O	4:B:477:GLU:N	2.25	0.70
4:B:777:GLY:O	4:B:780:PRO:HD2	1.92	0.70
4:D:29:GLY:HA2	7:D:3080:HOH:O	1.91	0.70
4:A:480:LYS:O	4:A:484:GLU:HG3	1.91	0.70
4:B:273:VAL:O	4:B:274:PRO:C	2.32	0.70
4:C:40:GLU:OE2	4:C:286:TYR:HD1	1.74	0.70
4:C:67:ASN:O	4:C:69:ALA:N	2.25	0.70
4:C:340:VAL:O	4:C:341:ILE:C	2.33	0.70
4:C:572:GLY:O	4:C:575:ALA:HB3	1.91	0.70
4:D:221:ILE:HG12	4:D:227:VAL:HG23	1.73	0.70
1:E:12:DT:H2"	1:E:13:DC:H5"	1.71	0.70
4:C:330:ILE:HG13	4:C:408:PHE:O	1.91	0.70
4:D:306:MET:O	4:D:308:TYR:N	2.25	0.70
4:D:432:PHE:CE1	4:D:444:LEU:HD11	2.26	0.70
4:D:739:TYR:OH	4:D:781:ASN:OD1	2.10	0.70
4:A:78:LEU:N	4:A:79:PRO:HD2	2.06	0.70
4:A:433:ASN:C	4:A:433:ASN:OD1	2.34	0.70
4:A:525:GLY:O	4:A:527:SER:N	2.24	0.70
4:B:159:ALA:O	4:B:160:LYS:C	2.32	0.70
4:B:326:THR:HA	7:B:3162:HOH:O	1.90	0.70
4:C:333:LYS:HD3	4:C:516:PHE:CD2	2.22	0.70
4:C:703:ALA:HB2	4:C:778:ILE:HG12	1.73	0.70
4:D:268:PHE:CD2	4:D:429:VAL:HG12	2.26	0.70
4:A:4:ILE:HD12	7:A:3067:HOH:O	1.92	0.70
4:A:16:LEU:HA	4:A:37:LEU:HD22	1.73	0.70
4:B:632:ARG:HD3	6:B:2001:APC:N7	2.07	0.70
4:C:105:PHE:HE1	4:C:208:ASP:HB3	1.56	0.70
4:D:14:ILE:HG23	4:D:288:ALA:HB1	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:611:LEU:HD12	4:A:669:GLN:HB2	1.74	0.70
4:A:647:ARG:HG3	4:A:674:ALA:O	1.92	0.70
4:B:390:ALA:C	4:B:392:LYS:N	2.46	0.70
4:C:270:PRO:HG3	4:C:430:SER:OG	1.92	0.70
4:D:402:LEU:HD23	4:D:443:LEU:CD1	2.22	0.70
2:I:1:G:H2'	2:I:2:C:C6	2.27	0.70
4:A:632:ARG:O	4:A:633:SER:C	2.34	0.70
4:B:416:PHE:CE1	4:B:433:ASN:HA	2.26	0.70
4:B:544:GLN:HG3	4:B:561:LEU:HD11	1.74	0.70
4:B:557:ARG:HD3	7:B:3119:HOH:O	1.91	0.70
4:B:734:PRO:HG2	4:B:734:PRO:O	1.91	0.70
4:C:551:ARG:CG	4:C:551:ARG:HH11	2.05	0.70
4:D:882:PHE:O	4:D:883:ALA:HB3	1.92	0.70
1:K:11:DA:C2	1:K:12:DT:C4	2.80	0.69
4:A:746:ARG:HH12	4:A:754:GLN:H	1.37	0.69
4:B:298:ARG:HE	4:B:419:ASN:HB3	1.57	0.69
4:B:540:CYS:O	4:B:541:SER:C	2.35	0.69
4:B:788:GLY:O	4:B:792:ARG:HG3	1.92	0.69
4:D:71:LYS:HD3	7:D:3030:HOH:O	1.92	0.69
4:D:779:ALA:O	4:D:783:VAL:HG22	1.90	0.69
4:A:273:VAL:O	4:A:273:VAL:HG23	1.91	0.69
4:B:308:TYR:HA	4:B:311:VAL:CG2	2.21	0.69
4:D:340:VAL:O	4:D:341:ILE:C	2.35	0.69
4:A:721:LYS:HD3	4:A:722:ARG:N	2.07	0.69
4:B:278:TRP:HA	7:B:3014:HOH:O	1.92	0.69
4:C:322:ILE:HG13	7:C:3131:HOH:O	1.91	0.69
4:C:570:ILE:O	4:C:574:VAL:HG23	1.93	0.69
4:D:324:GLN:HG2	4:D:324:GLN:O	1.91	0.69
4:D:471:ASP:O	4:D:472:LYS:HD2	1.92	0.69
4:A:14:ILE:HD12	4:A:14:ILE:N	2.07	0.69
4:A:19:ILE:HG23	4:A:20:PRO:HD2	1.73	0.69
4:A:275:PRO:HD3	4:A:415:TRP:HB3	1.74	0.69
4:B:307:ARG:HD3	4:B:736:TRP:CE3	2.28	0.69
4:B:824:LEU:O	4:B:828:VAL:HG23	1.92	0.69
4:D:573:ILE:HA	4:D:576:LYS:HD2	1.73	0.69
4:A:452:ILE:CD1	4:A:457:TYR:HB2	2.22	0.69
4:A:421:ASP:O	4:A:422:TRP:C	2.31	0.69
4:B:449:GLY:C	4:B:529:ASN:HD21	2.01	0.69
4:B:473:VAL:CG1	4:B:477:GLU:HB2	2.23	0.69
4:C:29:GLY:HA3	7:C:3129:HOH:O	1.93	0.69
4:B:512:LEU:O	4:B:515:CYS:N	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:829:ARG:NH2	4:B:882:PHE:CA	2.54	0.69
4:D:158:GLU:HA	4:D:195:LEU:HD22	1.75	0.69
4:D:471:ASP:C	4:D:472:LYS:HD2	2.17	0.69
1:H:12:DT:H4'	4:B:423:ARG:NE	2.08	0.69
1:K:7:DC:H2''	1:K:8:DG:O5'	1.91	0.69
4:A:6:ILE:O	4:A:8:LYS:N	2.22	0.69
4:A:474:PRO:HG2	4:A:477:GLU:HG3	1.75	0.69
4:A:700:LYS:NZ	7:A:3017:HOH:O	2.25	0.69
4:B:264:ILE:O	4:B:266:PRO:HD3	1.92	0.69
4:B:418:TYR:CE2	4:B:428:ALA:HB2	2.18	0.69
4:B:663:LYS:CE	4:B:666:MET:HE1	2.23	0.69
4:C:25:ALA:HA	4:C:29:GLY:O	1.92	0.69
4:C:308:TYR:HE2	4:C:734:PRO:HG2	1.57	0.69
4:C:801:LYS:HD3	4:C:801:LYS:C	2.17	0.69
4:D:120:LYS:HD2	4:D:752:LEU:HD11	1.73	0.69
4:D:206:LYS:HD3	4:D:206:LYS:H	1.57	0.69
4:D:210:ILE:O	4:D:214:VAL:HG23	1.93	0.69
4:D:274:PRO:HD3	4:D:415:TRP:CH2	2.27	0.69
4:D:657:PRO:O	4:D:661:SER:HB2	1.92	0.69
4:B:132:THR:HG21	7:B:3161:HOH:O	1.92	0.69
4:B:390:ALA:O	4:B:392:LYS:N	2.25	0.69
4:B:423:ARG:HH12	4:B:784:HIS:CB	2.06	0.69
4:D:337:VAL:HG21	4:D:512:LEU:HD21	1.74	0.69
1:H:3:DG:N2	7:H:948:HOH:O	2.25	0.69
4:A:311:VAL:HG12	4:A:312:TYR:N	2.08	0.69
4:A:526:LEU:CD1	4:A:526:LEU:H	2.06	0.69
4:A:665:LEU:H	4:A:665:LEU:HD12	1.58	0.69
4:B:247:ALA:HB3	4:B:250:TYR:HB2	1.76	0.69
4:B:452:ILE:CG2	4:B:453:GLY:N	2.33	0.69
4:D:333:LYS:NZ	4:D:516:PHE:HB3	2.08	0.69
4:A:308:TYR:CE2	4:A:734:PRO:HG2	2.21	0.68
4:B:109:ILE:HD12	4:B:109:ILE:N	2.08	0.68
4:B:308:TYR:HA	4:B:311:VAL:HG23	1.75	0.68
4:C:428:ALA:H	4:C:435:GLN:NE2	1.90	0.68
4:D:390:ALA:HB1	4:D:394:ARG:HH21	1.58	0.68
4:D:470:VAL:HG12	4:D:473:VAL:CG1	2.23	0.68
4:A:275:PRO:HD3	4:A:415:TRP:CB	2.22	0.68
4:C:631:LYS:HZ1	6:C:2002:APC:C3A	2.05	0.68
4:A:4:ILE:HD11	4:A:256:THR:OG1	1.92	0.68
4:A:59:LEU:HD23	4:A:64:VAL:CG2	2.23	0.68
4:A:236:VAL:HG11	4:A:239:GLN:CG	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:404:GLN:HA	4:A:404:GLN:NE2	2.08	0.68
4:C:840:ASP:O	4:C:842:LEU:N	2.27	0.68
4:D:433:ASN:HB2	4:D:434:PRO:CD	2.23	0.68
4:B:571:TYR:HE1	7:B:3067:HOH:O	1.75	0.68
4:D:402:LEU:HG	4:D:439:MET:HE1	1.74	0.68
4:B:261:LEU:O	4:B:263:GLY:N	2.27	0.68
4:B:301:SER:O	4:B:304:ALA:N	2.27	0.68
4:C:335:LEU:HD11	4:C:406:ASN:OD1	1.94	0.68
4:A:11:PHE:CE1	4:A:44:TYR:HB3	2.29	0.68
4:B:840:ASP:O	4:B:842:LEU:N	2.27	0.68
4:A:551:ARG:HB2	4:A:868:GLY:H	1.58	0.68
4:B:31:ARG:HB3	4:B:31:ARG:HH11	1.59	0.68
4:B:720:ARG:HG2	4:B:720:ARG:NH1	1.92	0.68
4:B:730:PRO:CD	4:B:786:GLN:HE21	2.06	0.68
4:B:801:LYS:HD3	4:B:801:LYS:O	1.94	0.68
4:D:55:PHE:HA	4:D:58:GLN:HG3	1.75	0.68
4:D:326:THR:O	4:D:415:TRP:HD1	1.76	0.68
4:D:437:ASN:HD21	4:D:440:THR:H	1.41	0.68
1:E:12:DT:H5"	4:A:422:TRP:CH2	2.29	0.68
4:A:81:MET:HE2	4:A:220:LEU:HD13	1.75	0.68
4:A:486:HIS:CD2	4:A:518:TYR:CE1	2.80	0.68
4:A:655:ILE:HD12	4:A:674:ALA:HB2	1.76	0.68
4:B:301:SER:O	4:B:304:ALA:HB3	1.94	0.68
4:B:354:ALA:HA	7:B:3118:HOH:O	1.94	0.68
4:C:17:ALA:HB2	7:C:3201:HOH:O	1.92	0.68
4:C:40:GLU:OE1	4:C:286:TYR:HB3	1.92	0.68
4:C:432:PHE:CZ	4:C:444:LEU:HD21	2.28	0.68
4:C:465:ALA:O	4:C:470:VAL:HG23	1.94	0.68
4:D:433:ASN:HB2	4:D:434:PRO:HD2	1.74	0.68
4:B:564:SER:OG	4:B:565:GLU:N	2.25	0.68
4:B:706:LEU:HD11	4:B:849:PHE:HD2	1.58	0.68
4:D:233:ASN:HD22	4:D:239:GLN:NE2	1.92	0.68
4:A:552:ASP:OD2	7:A:3223:HOH:O	2.10	0.68
4:C:134:VAL:HG12	4:C:242:GLU:O	1.94	0.68
4:C:159:ALA:O	4:C:163:LYS:HB2	1.93	0.68
4:C:173:ARG:CZ	4:C:182:PHE:HB2	2.23	0.68
4:C:881:ALA:O	4:C:882:PHE:C	2.37	0.68
4:A:383:ALA:C	4:A:385:TYR:N	2.52	0.67
4:A:404:GLN:HE21	4:A:404:GLN:CA	2.02	0.67
4:B:299:THR:HG21	4:B:305:LEU:HA	1.76	0.67
4:C:146:GLU:OE2	4:C:201:TRP:HB3	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:340:VAL:O	4:C:342:THR:N	2.27	0.67
4:C:475:PHE:CE2	4:C:879:ASP:HB3	2.29	0.67
4:C:785:SER:HA	7:C:3159:HOH:O	1.93	0.67
4:D:55:PHE:CE1	4:D:59:LEU:HD21	2.30	0.67
4:D:100:PRO:HG2	4:D:103:PHE:CB	2.23	0.67
4:D:161:HIS:O	4:D:164:LYS:HG2	1.94	0.67
4:A:631:LYS:NZ	6:A:2000:APC:C3A	2.49	0.67
4:A:748:ASN:HD22	4:A:751:PHE:H	1.40	0.67
4:B:418:TYR:HD2	4:B:428:ALA:HA	1.59	0.67
4:D:333:LYS:HB3	4:D:516:PHE:CD2	2.28	0.67
4:D:718:ILE:HD12	7:D:3025:HOH:O	1.94	0.67
4:D:829:ARG:HG3	4:D:829:ARG:NH1	2.07	0.67
4:A:280:GLY:O	4:A:281:ILE:C	2.35	0.67
4:A:526:LEU:N	4:A:526:LEU:CD1	2.57	0.67
4:A:744:GLN:HA	4:A:756:ARG:NH2	2.09	0.67
4:C:50:ARG:HG2	4:C:50:ARG:NH1	2.07	0.67
4:C:317:TYR:C	4:C:321:ASN:ND2	2.52	0.67
4:C:866:ALA:HB1	7:C:3057:HOH:O	1.94	0.67
1:H:12:DT:O4'	4:B:423:ARG:NH2	2.27	0.67
1:N:14:DG:N7	7:N:81:HOH:O	2.27	0.67
4:A:78:LEU:HD21	4:A:116:TYR:HB2	1.74	0.67
4:A:423:ARG:NH2	4:A:784:HIS:CB	2.58	0.67
4:A:464:GLY:CA	4:A:514:PHE:CE2	2.78	0.67
4:A:551:ARG:NH2	4:A:872:LEU:HD11	2.10	0.67
4:B:269:GLN:NE2	4:B:407:LYS:NZ	2.42	0.67
4:B:418:TYR:HD2	4:B:427:TYR:O	1.78	0.67
4:C:32:LEU:HB2	7:C:3157:HOH:O	1.94	0.67
4:C:475:PHE:HE2	4:C:879:ASP:HB3	1.58	0.67
4:D:330:ILE:HD11	4:D:405:ALA:HA	1.75	0.67
4:D:855:GLU:O	4:D:858:LEU:HD12	1.94	0.67
4:A:495:SER:HB3	4:A:498:GLU:HG3	1.77	0.67
4:A:510:CYS:O	4:A:513:ALA:N	2.26	0.67
4:A:630:THR:O	7:A:3199:HOH:O	2.12	0.67
4:C:2:ASN:O	7:C:3169:HOH:O	2.11	0.67
4:C:59:LEU:CD2	4:C:64:VAL:HG13	2.24	0.67
4:A:109:ILE:HG13	4:A:149:ALA:HB2	1.75	0.67
4:A:428:ALA:HB3	4:A:433:ASN:HD22	1.57	0.67
4:B:449:GLY:HA3	4:B:529:ASN:HD21	1.58	0.67
4:B:829:ARG:HG3	4:B:829:ARG:NH1	2.05	0.67
4:C:24:LEU:HD21	4:C:287:TRP:CE2	2.29	0.67
4:C:330:ILE:CG1	4:C:408:PHE:O	2.43	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:303:LYS:HG3	4:D:304:ALA:N	2.10	0.67
4:A:716:GLY:HA3	7:A:3184:HOH:O	1.93	0.67
4:A:802:TYR:CD2	4:A:802:TYR:N	2.61	0.67
4:A:849:PHE:HD2	4:A:853:LEU:HD21	1.60	0.67
4:B:794:THR:OG1	4:B:831:THR:HG21	1.92	0.67
4:C:632:ARG:NH2	6:C:2002:APC:H5'1	2.08	0.67
4:D:778:ILE:CG2	4:D:779:ALA:N	2.57	0.67
4:D:797:TRP:HE1	4:D:802:TYR:HE2	1.41	0.67
4:A:518:TYR:O	4:A:518:TYR:CD1	2.48	0.67
4:B:569:ASP:CG	4:B:627:ARG:HH21	2.02	0.67
4:C:279:THR:HG22	7:C:3038:HOH:O	1.95	0.67
4:C:534:LEU:HD12	4:C:821:ALA:CB	2.25	0.67
4:D:19:ILE:HD12	4:D:20:PRO:HD2	1.77	0.67
4:D:540:CYS:O	4:D:541:SER:C	2.37	0.67
4:D:656:GLN:N	4:D:657:PRO:HD2	2.10	0.67
4:D:769:ILE:H	4:D:769:ILE:HD12	1.60	0.67
4:A:746:ARG:HG3	4:A:756:ARG:HB2	1.77	0.67
4:A:823:ASN:O	4:A:824:LEU:C	2.36	0.67
4:B:64:VAL:HG21	4:B:127:THR:HG21	1.76	0.67
4:B:77:LEU:CD1	4:B:224:THR:HG21	2.25	0.67
4:B:180:LYS:HG3	4:B:750:MET:HE1	1.76	0.67
4:B:423:ARG:CB	4:B:423:ARG:HH11	2.08	0.67
4:B:449:GLY:CA	4:B:529:ASN:HD21	2.08	0.67
4:C:9:ASN:HA	4:C:12:SER:HB3	1.76	0.67
4:C:308:TYR:CZ	4:C:733:PHE:HE2	2.12	0.67
4:C:349:VAL:HG11	4:C:508:PRO:HG3	1.77	0.67
4:A:428:ALA:HB3	4:A:433:ASN:ND2	2.09	0.67
4:A:843:ALA:O	4:A:846:TYR:N	2.27	0.67
4:B:254:ILE:HG22	4:B:255:ALA:N	2.10	0.67
4:B:720:ARG:HH11	4:B:720:ARG:CG	2.03	0.67
4:C:707:ALA:O	4:C:722:ARG:HB3	1.95	0.67
4:A:786:GLN:HE21	4:A:786:GLN:CA	2.03	0.66
4:B:345:LYS:HZ1	4:B:351:ASP:N	1.94	0.66
4:C:105:PHE:CE1	4:C:208:ASP:HB3	2.30	0.66
4:C:443:LEU:O	4:C:444:LEU:HD23	1.95	0.66
4:C:460:LEU:HA	4:C:534:LEU:CD2	2.24	0.66
4:D:39:LEU:HD22	4:D:272:VAL:HG23	1.76	0.66
4:D:272:VAL:O	4:D:415:TRP:CZ3	2.47	0.66
4:A:46:MET:HG2	7:A:3162:HOH:O	1.94	0.66
4:B:671:ASN:O	4:B:674:ALA:HB3	1.96	0.66
4:B:850:ALA:O	4:B:852:GLN:N	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:706:LEU:HD22	4:C:725:VAL:CG1	2.24	0.66
4:B:35:GLU:O	4:B:38:ALA:HB3	1.96	0.66
4:B:731:ASP:HB3	4:B:789:SER:OG	1.96	0.66
4:D:89:PHE:HZ	4:D:106:LEU:HB3	1.60	0.66
4:D:269:GLN:HG2	4:D:408:PHE:HZ	1.59	0.66
4:A:881:ALA:O	4:A:883:ALA:OXT	2.14	0.66
4:C:551:ARG:CD	4:C:872:LEU:HD21	2.24	0.66
4:D:109:ILE:HD13	4:D:114:VAL:HG22	1.76	0.66
4:D:744:GLN:HG2	4:D:756:ARG:HB3	1.75	0.66
4:D:829:ARG:HH22	4:D:882:PHE:HA	1.61	0.66
4:A:308:TYR:OH	4:A:734:PRO:O	2.14	0.66
4:A:828:VAL:HG23	4:A:829:ARG:N	2.06	0.66
4:B:424:GLY:O	4:B:792:ARG:NH1	2.29	0.66
4:C:50:ARG:HG2	4:C:50:ARG:HH11	1.60	0.66
4:C:50:ARG:HH11	4:C:50:ARG:CG	2.08	0.66
4:C:105:PHE:O	4:C:107:GLN:N	2.29	0.66
4:D:84:ARG:O	4:D:84:ARG:HD3	1.94	0.66
4:D:275:PRO:HD2	7:D:3108:HOH:O	1.94	0.66
4:D:560:ASN:OD1	4:D:568:GLN:HB2	1.95	0.66
4:A:418:TYR:HD2	4:A:426:VAL:HG12	1.60	0.66
4:A:574:VAL:HG11	4:A:685:VAL:CG1	2.25	0.66
4:A:769:ILE:H	4:A:769:ILE:HD12	1.60	0.66
4:B:437:ASN:HB2	7:B:3149:HOH:O	1.95	0.66
4:A:30:GLU:HB3	4:A:34:ARG:NH2	2.10	0.66
4:A:44:TYR:CE2	4:A:266:PRO:HB3	2.31	0.66
4:A:157:LEU:HD23	7:A:3133:HOH:O	1.95	0.66
4:B:525:GLY:O	4:B:527:SER:N	2.28	0.66
4:C:36:GLN:HG3	4:C:273:VAL:HG22	1.78	0.66
4:C:286:TYR:CZ	4:C:417:PRO:HG3	2.31	0.66
4:C:553:GLU:HG2	4:C:554:VAL:H	1.60	0.66
4:C:562:LEU:HD21	4:C:870:LEU:HG	1.77	0.66
4:C:605:ILE:HG23	7:C:3098:HOH:O	1.96	0.66
4:D:402:LEU:HD23	4:D:443:LEU:HD11	1.77	0.66
4:A:119:ILE:O	4:A:122:THR:HB	1.95	0.66
4:A:459:TRP:HE1	4:A:822:ALA:HA	1.61	0.66
4:A:463:HIS:HD2	7:A:3167:HOH:O	1.77	0.66
4:A:485:ASN:HB3	4:A:488:ASN:HD22	1.61	0.66
4:A:869:ASN:N	4:A:869:ASN:ND2	2.44	0.66
4:B:336:ALA:O	4:B:340:VAL:HG23	1.95	0.66
4:B:485:ASN:O	4:B:486:HIS:C	2.39	0.66
4:B:616:LEU:O	4:B:619:GLN:N	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:THR:O	4:D:27:HIS:HB2	1.96	0.66
4:D:337:VAL:O	4:D:341:ILE:HG12	1.96	0.66
4:D:422:TRP:CD1	4:D:422:TRP:C	2.74	0.66
4:D:574:VAL:O	4:D:578:VAL:HG23	1.95	0.66
4:A:281:ILE:HD11	4:A:309:GLU:N	2.11	0.66
4:A:459:TRP:O	4:A:460:LEU:C	2.36	0.66
4:A:563:PRO:HB3	4:A:877:GLU:O	1.96	0.66
4:B:623:TYR:CA	4:B:666:MET:HE2	2.18	0.66
4:B:825:PHE:O	4:B:829:ARG:NH1	2.29	0.66
4:D:425:ARG:HB3	4:D:427:TYR:HE1	1.61	0.66
1:K:12:DT:C2	1:K:13:DC:C5	2.83	0.66
4:B:291:ARG:CG	7:B:3037:HOH:O	2.44	0.66
4:B:475:PHE:HA	4:B:478:ARG:HD2	1.78	0.66
4:B:730:PRO:CD	4:B:786:GLN:NE2	2.59	0.66
4:A:80:LYS:HD3	4:A:224:THR:HG22	1.76	0.65
4:B:173:ARG:HH11	4:B:182:PHE:HD1	1.44	0.65
4:B:536:PHE:HB3	4:B:882:PHE:HB3	1.76	0.65
4:A:475:PHE:HD2	7:A:3202:HOH:O	1.79	0.65
4:A:737:GLN:O	4:A:774:GLN:NE2	2.29	0.65
4:B:37:LEU:HD12	4:B:37:LEU:N	2.09	0.65
4:B:639:TYR:HE1	7:B:3084:HOH:O	1.79	0.65
4:B:726:HIS:CD2	4:B:735:VAL:O	2.49	0.65
4:C:182:PHE:O	4:C:186:VAL:HG23	1.97	0.65
4:C:551:ARG:HH11	4:C:551:ARG:HG3	1.61	0.65
4:D:718:ILE:CD1	7:D:3025:HOH:O	2.43	0.65
4:B:330:ILE:HD12	4:B:405:ALA:HB1	1.78	0.65
4:B:428:ALA:H	4:B:435:GLN:HE22	1.43	0.65
4:C:551:ARG:NH2	4:C:872:LEU:HD11	2.11	0.65
4:D:106:LEU:HA	4:D:109:ILE:HD11	1.78	0.65
4:D:252:GLU:O	4:D:255:ALA:HB3	1.97	0.65
4:D:508:PRO:O	4:D:511:PHE:N	2.29	0.65
4:D:553:GLU:OE1	4:D:869:ASN:HB2	1.97	0.65
4:D:629:VAL:HG13	4:D:654:THR:HG21	1.77	0.65
4:A:24:LEU:HD21	4:A:287:TRP:CE2	2.31	0.65
4:A:668:THR:HG22	4:A:669:GLN:NE2	2.11	0.65
4:B:780:PRO:HD2	4:B:781:ASN:H	1.61	0.65
4:C:64:VAL:HG21	4:C:127:THR:HG21	1.77	0.65
4:C:298:ARG:HB2	4:C:421:ASP:HA	1.79	0.65
4:D:796:VAL:HA	7:D:3013:HOH:O	1.96	0.65
1:E:5:DA:C2	3:G:7:DT:O2	2.50	0.65
4:A:3:THR:HB	4:A:52:ARG:NH1	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:236:VAL:HG21	4:B:239:GLN:HE21	1.60	0.65
4:B:266:PRO:HG2	4:B:268:PHE:CZ	2.31	0.65
4:B:552:ASP:OD1	4:B:552:ASP:O	2.14	0.65
4:B:705:LEU:O	4:B:707:ALA:N	2.29	0.65
4:B:790:HIS:CE1	4:B:831:THR:HG23	2.30	0.65
4:C:631:LYS:O	4:C:632:ARG:C	2.37	0.65
4:C:788:GLY:C	4:C:792:ARG:NH1	2.54	0.65
4:D:236:VAL:HG21	4:D:239:GLN:NE2	2.11	0.65
1:N:16:DC:H2''	1:N:17:DG:O5'	1.97	0.65
4:A:141:ILE:O	4:A:145:ILE:HG12	1.96	0.65
4:A:292:ARG:H	4:A:293:PRO:HD3	1.62	0.65
4:B:257:ARG:HG2	4:B:257:ARG:HH11	1.60	0.65
4:B:728:VAL:O	7:B:3081:HOH:O	2.15	0.65
4:C:631:LYS:HE2	4:C:635:MET:SD	2.36	0.65
4:D:9:ASN:HA	4:D:12:SER:HB2	1.79	0.65
3:G:7:DT:H2''	3:G:8:DC:C6	2.31	0.65
1:K:13:DC:H2''	1:K:14:DG:H5'	1.78	0.65
4:B:446:LEU:HD12	4:B:817:ILE:CG2	2.27	0.65
4:C:42:GLU:CG	4:C:46:MET:HE2	2.27	0.65
4:C:551:ARG:NH2	4:C:836:TYR:O	2.30	0.65
4:D:109:ILE:HG12	4:D:145:ILE:HG22	1.79	0.65
4:D:475:PHE:N	4:D:476:PRO:HD2	2.11	0.65
4:A:390:ALA:C	4:A:392:LYS:N	2.52	0.65
4:B:119:ILE:HD13	4:B:119:ILE:N	2.11	0.65
4:C:651:LEU:HD13	4:C:651:LEU:C	2.22	0.65
4:D:218:GLU:O	4:D:222:GLU:HB2	1.95	0.65
4:D:428:ALA:H	4:D:435:GLN:HE21	1.43	0.65
4:A:19:ILE:CG2	7:A:3120:HOH:O	2.45	0.65
4:A:221:ILE:HG23	4:A:227:VAL:O	1.97	0.65
4:A:610:LYS:O	4:A:611:LEU:C	2.38	0.65
4:A:744:GLN:HA	4:A:756:ARG:CZ	2.27	0.65
4:A:793:LYS:HA	4:A:796:VAL:CG2	2.27	0.65
4:B:14:ILE:HD12	4:B:14:ILE:N	2.08	0.65
4:B:631:LYS:CE	6:B:2001:APC:H3A2	2.26	0.65
4:B:807:PHE:HA	4:B:815:GLY:O	1.96	0.65
4:C:175:GLY:O	4:C:176:HIS:C	2.37	0.65
4:C:474:PRO:HB2	4:C:476:PRO:HD2	1.78	0.65
1:K:17:DG:H2''	1:K:18:DC:C5	2.32	0.65
4:A:16:LEU:HD22	4:A:38:ALA:HA	1.77	0.65
4:B:122:THR:HG21	4:B:226:MET:HE1	1.78	0.65
4:B:296:LEU:O	4:B:296:LEU:CG	2.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:398:LEU:HD23	4:B:398:LEU:C	2.21	0.65
4:C:163:LYS:HB3	4:C:164:LYS:HZ3	1.62	0.65
4:C:346:HIS:HA	4:C:395:ARG:HH11	1.61	0.65
4:C:595:VAL:HG21	7:C:3085:HOH:O	1.97	0.65
4:D:737:GLN:NE2	4:D:778:ILE:HA	2.06	0.65
4:A:26:ASP:HB2	7:A:3183:HOH:O	1.97	0.64
4:B:138:ALA:HB2	4:B:214:VAL:HG13	1.79	0.64
4:B:435:GLN:CG	4:B:810:ILE:HG23	2.20	0.64
4:B:559:VAL:HG23	4:B:559:VAL:O	1.98	0.64
4:C:727:TRP:CE3	4:C:735:VAL:HG13	2.32	0.64
4:D:564:SER:O	7:D:3040:HOH:O	2.14	0.64
4:A:40:GLU:HG2	4:A:286:TYR:HD1	1.62	0.64
4:B:33:ALA:O	4:B:37:LEU:HD13	1.97	0.64
4:B:281:ILE:CG2	4:B:282:THR:HG23	2.27	0.64
4:B:828:VAL:CG1	4:B:883:ALA:HA	2.28	0.64
4:D:134:VAL:H	4:D:243:THR:HA	1.62	0.64
4:D:426:VAL:HG21	4:D:791:LEU:HD21	1.78	0.64
4:A:50:ARG:NH1	4:A:50:ARG:HG2	2.11	0.64
4:A:78:LEU:N	4:A:79:PRO:CD	2.60	0.64
4:A:689:VAL:O	4:A:690:VAL:C	2.39	0.64
4:A:817:ILE:HB	4:A:818:PRO:HD2	1.79	0.64
4:B:780:PRO:O	4:B:781:ASN:C	2.35	0.64
4:C:746:ARG:HD3	4:C:755:PHE:O	1.97	0.64
4:C:837:GLU:CG	4:C:872:LEU:HD12	2.27	0.64
1:E:14:DG:H2'	1:E:15:DC:C5	2.31	0.64
4:B:37:LEU:H	4:B:37:LEU:CD1	2.10	0.64
4:B:58:GLN:HG3	4:B:67:ASN:HD22	1.63	0.64
4:B:275:PRO:O	4:B:277:PRO:HD3	1.97	0.64
4:B:702:ALA:O	4:B:706:LEU:HD12	1.96	0.64
4:C:342:THR:HG22	4:C:348:PRO:CG	2.24	0.64
4:D:269:GLN:HG2	4:D:408:PHE:CZ	2.33	0.64
4:D:326:THR:O	4:D:415:TRP:CD1	2.50	0.64
4:D:402:LEU:CD2	4:D:443:LEU:HD11	2.28	0.64
4:D:438:ASP:OD2	4:D:508:PRO:HG2	1.97	0.64
4:D:471:ASP:OD1	4:D:472:LYS:HD3	1.97	0.64
4:A:274:PRO:HG3	4:A:415:TRP:CE2	2.32	0.64
4:A:476:PRO:O	4:A:479:ILE:N	2.28	0.64
4:B:473:VAL:CG1	4:B:474:PRO:N	2.59	0.64
4:C:433:ASN:HA	7:C:3164:HOH:O	1.93	0.64
4:C:514:PHE:CG	4:C:514:PHE:O	2.47	0.64
4:A:50:ARG:NE	4:A:267:MET:HE3	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:257:ARG:HG2	4:A:257:ARG:HH11	1.62	0.64
4:B:21:PHE:C	4:B:23:THR:H	2.05	0.64
4:B:231:ARG:CG	4:B:234:ALA:HB2	2.27	0.64
4:B:486:HIS:CE1	4:B:490:MET:HG3	2.32	0.64
4:B:861:MET:O	4:B:862:PRO:C	2.40	0.64
2:F:7:A:H2'	2:F:8:U:H6	1.62	0.64
4:B:423:ARG:NH1	4:B:784:HIS:HB3	2.13	0.64
4:B:446:LEU:HB2	4:B:531:SER:O	1.98	0.64
4:B:720:ARG:NH1	4:B:720:ARG:CG	2.59	0.64
4:B:779:ALA:N	4:B:780:PRO:CD	2.60	0.64
4:C:475:PHE:N	4:C:476:PRO:HD2	2.13	0.64
4:D:135:GLN:HG3	7:D:3160:HOH:O	1.97	0.64
4:D:439:MET:HE3	4:D:443:LEU:HD11	1.80	0.64
4:D:572:GLY:O	4:D:575:ALA:N	2.30	0.64
4:A:545:HIS:CE1	4:A:787:ASP:HA	2.33	0.64
4:B:5:ASN:ND2	4:B:7:ALA:N	2.46	0.64
4:B:122:THR:CG2	4:B:226:MET:CE	2.74	0.64
4:B:492:CYS:SG	4:B:502:TRP:CD1	2.90	0.64
4:B:751:PHE:C	4:B:752:LEU:HD12	2.23	0.64
4:C:850:ALA:C	4:C:852:GLN:H	2.06	0.64
4:D:281:ILE:HD12	4:D:317:TYR:OH	1.96	0.64
4:A:10:ASP:O	4:A:13:ASP:HB2	1.98	0.64
4:A:502:TRP:CD1	4:A:512:LEU:CD1	2.81	0.64
4:B:469:GLY:O	4:B:471:ASP:N	2.31	0.64
4:D:161:HIS:HE1	7:D:3114:HOH:O	1.80	0.64
4:D:273:VAL:C	4:D:415:TRP:CE3	2.76	0.64
4:D:421:ASP:O	4:D:423:ARG:N	2.31	0.64
4:C:423:ARG:HE	4:C:781:ASN:HD22	1.45	0.64
4:C:744:GLN:HB3	7:C:3076:HOH:O	1.96	0.64
4:D:311:VAL:HG12	4:D:312:TYR:N	2.13	0.64
4:D:734:PRO:HG2	4:D:734:PRO:O	1.97	0.64
1:K:17:DG:H2''	1:K:18:DC:C6	2.33	0.63
4:A:582:LEU:HD11	4:A:625:VAL:HG21	1.78	0.63
4:B:5:ASN:HD21	4:B:7:ALA:N	1.95	0.63
4:B:433:ASN:CB	4:B:434:PRO:CD	2.63	0.63
4:B:751:PHE:HB3	4:B:752:LEU:CD1	2.19	0.63
4:C:292:ARG:N	4:C:293:PRO:HD3	2.13	0.63
4:C:423:ARG:HD2	4:C:781:ASN:CB	2.27	0.63
4:B:217:ILE:O	4:B:221:ILE:HG13	1.98	0.63
4:C:424:GLY:HA3	7:C:3159:HOH:O	1.98	0.63
4:A:634:VAL:HG23	4:A:685:VAL:HG11	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:335:LEU:HD21	4:C:339:ASN:ND2	2.13	0.63
4:C:728:VAL:HG13	4:C:733:PHE:C	2.24	0.63
4:D:273:VAL:CA	4:D:415:TRP:CZ3	2.82	0.63
4:D:479:ILE:HG22	4:D:483:GLU:CD	2.23	0.63
4:D:804:ILE:CG2	4:D:816:THR:HG21	2.29	0.63
4:B:113:ALA:O	4:B:117:ILE:HG13	1.98	0.63
4:B:463:HIS:HB3	4:B:534:LEU:HD22	1.79	0.63
4:B:537:ASP:N	4:B:882:PHE:HD2	1.96	0.63
4:C:881:ALA:O	4:C:883:ALA:N	2.31	0.63
4:C:882:PHE:H	4:C:882:PHE:HD1	1.44	0.63
4:D:10:ASP:O	4:D:13:ASP:HB3	1.98	0.63
4:D:550:LEU:HD21	4:D:865:PRO:HG2	1.81	0.63
4:D:649:GLN:HA	4:D:652:GLU:OE2	1.98	0.63
4:B:777:GLY:O	4:B:781:ASN:HB2	1.98	0.63
4:C:423:ARG:NE	4:C:781:ASN:HD22	1.96	0.63
4:A:48:GLU:O	4:A:49:ALA:C	2.42	0.63
4:A:92:VAL:HG12	4:A:99:ARG:HG3	1.80	0.63
4:B:51:PHE:CE2	4:B:55:PHE:HD1	2.16	0.63
4:B:860:LYS:HD2	4:B:860:LYS:O	1.99	0.63
4:D:278:TRP:HB2	4:D:321:ASN:ND2	2.13	0.63
4:D:432:PHE:HE1	4:D:440:THR:HG23	1.64	0.63
4:D:475:PHE:O	4:D:476:PRO:C	2.37	0.63
4:D:552:ASP:CB	4:D:691:ALA:HB2	2.28	0.63
4:A:65:ALA:HB3	4:A:120:LYS:HE3	1.79	0.63
4:A:871:ASN:ND2	4:A:871:ASN:O	2.32	0.63
4:C:530:CYS:SG	4:C:818:PRO:HG2	2.39	0.63
4:C:552:ASP:OD1	4:C:555:GLY:N	2.27	0.63
4:D:141:ILE:HG22	4:D:145:ILE:HD11	1.80	0.63
4:D:274:PRO:HD3	4:D:415:TRP:CZ3	2.33	0.63
4:D:446:LEU:O	4:D:531:SER:HB2	1.99	0.63
1:H:12:DT:C4'	4:B:423:ARG:NE	2.59	0.63
4:A:446:LEU:O	4:A:531:SER:HB2	1.99	0.63
4:A:472:LYS:HA	4:A:567:VAL:HG11	1.81	0.63
4:A:716:GLY:CA	7:A:3184:HOH:O	2.47	0.63
4:B:14:ILE:H	4:B:14:ILE:CD1	2.03	0.63
4:B:281:ILE:HG22	4:B:282:THR:HG23	1.80	0.63
4:B:329:LYS:HD3	4:B:447:ALA:HA	1.78	0.63
4:B:549:MET:HG2	4:B:836:TYR:HE1	1.63	0.63
4:B:830:GLU:HA	4:B:876:LEU:HD21	1.80	0.63
4:C:296:LEU:HG	4:C:296:LEU:O	1.99	0.63
4:D:95:LYS:HB2	4:D:95:LYS:NZ	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:DC:H2''	1:E:17:DG:H5'	1.81	0.63
4:A:304:ALA:O	4:A:307:ARG:CG	2.44	0.63
4:A:437:ASN:ND2	4:A:440:THR:OG1	2.32	0.63
4:A:461:LYS:O	4:A:462:ILE:C	2.40	0.63
4:A:478:ARG:O	4:A:482:ILE:HG12	1.98	0.63
4:A:729:THR:N	4:A:733:PHE:O	2.31	0.63
4:B:27:HIS:HA	7:B:3169:HOH:O	1.98	0.63
4:B:278:TRP:CZ3	4:B:284:GLY:HA3	2.33	0.63
4:B:297:VAL:O	4:B:297:VAL:HG12	1.95	0.63
4:B:626:THR:O	4:B:628:SER:N	2.31	0.63
4:B:730:PRO:HD2	4:B:786:GLN:NE2	2.13	0.63
4:B:850:ALA:C	4:B:852:GLN:H	2.06	0.63
4:C:110:LYS:HE2	4:C:112:GLU:OE1	1.98	0.63
4:D:28:TYR:O	4:D:32:LEU:HD13	1.99	0.63
4:D:221:ILE:HG12	4:D:227:VAL:O	1.99	0.63
4:D:452:ILE:HG23	4:D:453:GLY:H	1.63	0.63
4:A:270:PRO:HD2	4:A:408:PHE:CE2	2.34	0.62
4:A:400:PHE:O	4:A:401:MET:C	2.42	0.62
4:A:459:TRP:O	4:A:460:LEU:O	2.16	0.62
4:A:570:ILE:O	4:A:573:ILE:HG23	1.99	0.62
4:B:539:SER:OG	4:B:560:ASN:ND2	2.32	0.62
4:C:163:LYS:HB3	4:C:164:LYS:NZ	2.13	0.62
4:C:313:MET:HA	7:C:3099:HOH:O	1.99	0.62
4:D:139:SER:HB2	4:D:210:ILE:HD13	1.81	0.62
2:L:1:G:H2'	2:L:2:C:C6	2.34	0.62
4:A:105:PHE:C	4:A:107:GLN:H	2.07	0.62
4:A:423:ARG:O	4:A:785:SER:HA	1.99	0.62
4:B:163:LYS:O	4:B:166:VAL:HG23	1.98	0.62
4:C:563:PRO:HD2	4:C:874:ASP:HB3	1.80	0.62
4:C:824:LEU:HD12	4:C:824:LEU:O	1.99	0.62
4:D:133:THR:HA	4:D:243:THR:HG22	1.79	0.62
4:D:590:THR:O	4:D:614:LYS:HB2	1.99	0.62
4:D:721:LYS:NZ	7:D:3061:HOH:O	2.29	0.62
4:A:4:ILE:CD1	4:A:256:THR:HA	2.29	0.62
4:A:630:THR:HA	7:A:3199:HOH:O	1.98	0.62
4:B:728:VAL:HG22	4:B:734:PRO:CA	2.29	0.62
4:B:828:VAL:HG11	4:B:883:ALA:HA	1.82	0.62
4:D:725:VAL:HB	4:D:737:GLN:HB3	1.81	0.62
4:A:457:TYR:CE2	4:A:461:LYS:CD	2.82	0.62
4:A:540:CYS:O	4:A:542:GLY:N	2.33	0.62
4:A:788:GLY:C	4:A:792:ARG:HH12	2.08	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:41:HIS:O	4:B:42:GLU:C	2.43	0.62
4:C:346:HIS:HA	4:C:395:ARG:NH1	2.14	0.62
4:C:423:ARG:HD2	4:C:781:ASN:HB3	1.81	0.62
4:C:474:PRO:HB2	4:C:476:PRO:CG	2.29	0.62
4:D:698:TRP:CE3	4:D:699:LEU:HD23	2.34	0.62
4:D:725:VAL:HG23	4:D:774:GLN:NE2	2.14	0.62
1:H:10:DT:OP2	4:B:641:SER:CB	2.48	0.62
4:A:106:LEU:HD21	4:A:212:VAL:HG13	1.81	0.62
4:A:544:GLN:OE1	4:A:559:VAL:HG23	1.99	0.62
4:B:158:GLU:HG2	4:B:195:LEU:HD22	1.81	0.62
4:B:403:GLU:OE1	4:B:404:GLN:N	2.32	0.62
4:B:571:TYR:CD2	4:B:631:LYS:HA	2.35	0.62
4:B:663:LYS:HE3	4:B:666:MET:HE1	1.81	0.62
4:B:668:THR:O	4:B:670:PRO:HD3	1.99	0.62
4:C:67:ASN:C	4:C:69:ALA:H	2.06	0.62
4:A:632:ARG:HB3	4:A:649:GLN:HE21	1.63	0.62
4:B:508:PRO:O	4:B:511:PHE:N	2.32	0.62
4:B:553:GLU:HG3	7:B:3114:HOH:O	2.00	0.62
4:B:610:LYS:O	4:B:611:LEU:O	2.17	0.62
4:C:137:VAL:O	4:C:140:ALA:HB3	1.99	0.62
4:C:787:ASP:C	4:C:787:ASP:OD1	2.42	0.62
4:D:169:GLN:HB3	4:D:182:PHE:CE2	2.34	0.62
4:A:11:PHE:HB3	4:A:41:HIS:CE1	2.34	0.62
4:B:261:LEU:C	4:B:263:GLY:H	2.07	0.62
4:B:578:VAL:HG13	4:B:680:LEU:HD23	1.80	0.62
4:D:323:ALA:C	4:D:325:ASN:H	2.07	0.62
4:D:327:ALA:HB2	4:D:415:TRP:HE1	1.61	0.62
4:D:471:ASP:CG	4:D:472:LYS:HD3	2.24	0.62
4:D:582:LEU:CD1	4:D:625:VAL:HG21	2.28	0.62
2:L:6:G:OP1	4:C:394:ARG:NH1	2.32	0.62
4:A:392:LYS:O	4:A:396:ILE:HG12	1.99	0.62
4:A:425:ARG:HD3	4:A:811:HIS:CD2	2.35	0.62
4:A:512:LEU:O	4:A:516:PHE:CE1	2.53	0.62
4:A:540:CYS:HB3	4:A:543:ILE:HG13	1.82	0.62
4:A:793:LYS:HA	4:A:796:VAL:HG23	1.82	0.62
4:B:281:ILE:HD11	4:B:308:TYR:C	2.24	0.62
4:B:823:ASN:O	4:B:824:LEU:C	2.40	0.62
4:C:303:LYS:NZ	4:C:303:LYS:CB	2.63	0.62
4:C:875:ILE:CG2	4:C:875:ILE:O	2.48	0.62
4:D:870:LEU:HD23	4:D:870:LEU:C	2.25	0.62
4:A:132:THR:O	4:A:132:THR:HG22	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:438:ASP:O	4:A:439:MET:C	2.42	0.62
4:A:588:ASN:HB3	7:A:3224:HOH:O	1.99	0.62
4:B:391:ARG:CG	7:B:3101:HOH:O	2.46	0.62
4:B:689:VAL:HG23	4:B:689:VAL:O	1.99	0.62
4:B:748:ASN:HD22	4:B:751:PHE:H	1.46	0.62
4:D:488:ASN:O	4:D:491:ALA:HB3	2.00	0.62
4:A:24:LEU:HD11	4:A:287:TRP:CG	2.35	0.62
4:A:514:PHE:CD1	4:A:514:PHE:C	2.76	0.62
4:A:578:VAL:HG13	4:A:680:LEU:HB3	1.82	0.62
4:A:632:ARG:HH21	6:A:2000:APC:C8	2.12	0.62
4:A:818:PRO:O	4:A:821:ALA:HB3	1.98	0.62
4:B:26:ASP:HB3	7:B:3098:HOH:O	2.00	0.62
4:B:475:PHE:O	4:B:478:ARG:N	2.32	0.62
4:B:792:ARG:O	4:B:796:VAL:HG23	2.00	0.62
4:D:324:GLN:HA	4:D:418:TYR:CD1	2.35	0.62
4:D:705:LEU:HD12	4:D:853:LEU:HD22	1.81	0.62
4:A:226:MET:HA	4:A:250:TYR:CD1	2.35	0.61
4:B:24:LEU:HD22	4:B:33:ALA:HA	1.80	0.61
4:B:464:GLY:HA3	4:B:514:PHE:CE2	2.35	0.61
4:C:557:ARG:HB3	4:C:557:ARG:HH11	1.64	0.61
1:H:6:DT:H5'	1:H:6:DT:H6	1.65	0.61
4:A:704:LYS:HE3	4:A:860:LYS:NZ	2.15	0.61
4:A:798:ALA:HB2	4:A:827:ALA:CB	2.30	0.61
4:A:825:PHE:CD1	4:A:829:ARG:NH1	2.63	0.61
4:B:549:MET:HE1	4:B:782:PHE:CE2	2.32	0.61
4:C:398:LEU:HD23	4:C:398:LEU:O	1.99	0.61
4:C:882:PHE:CD1	4:C:882:PHE:N	2.68	0.61
4:D:623:TYR:CA	4:D:666:MET:HE2	2.23	0.61
4:A:112:GLU:O	4:A:115:ALA:HB3	2.00	0.61
4:B:470:VAL:HG21	4:B:481:PHE:CD2	2.35	0.61
4:B:726:HIS:HD2	4:B:735:VAL:O	1.82	0.61
4:C:730:PRO:HD3	4:C:786:GLN:HE22	1.66	0.61
4:D:42:GLU:O	4:D:43:SER:C	2.43	0.61
4:D:304:ALA:HA	4:D:307:ARG:HD2	1.81	0.61
4:A:231:ARG:CG	4:A:234:ALA:HB2	2.30	0.61
4:A:347:CYS:O	4:A:349:VAL:N	2.33	0.61
4:A:786:GLN:OE1	4:A:841:VAL:HG21	2.00	0.61
4:B:42:GLU:O	4:B:43:SER:C	2.44	0.61
4:B:88:TRP:CZ2	4:B:215:ARG:HD3	2.35	0.61
4:B:823:ASN:N	4:B:823:ASN:HD22	1.98	0.61
4:C:14:ILE:CG2	4:C:288:ALA:HB1	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:19:ILE:HG12	4:C:20:PRO:CD	2.20	0.61
4:C:676:TYR:O	4:C:677:MET:C	2.43	0.61
4:C:728:VAL:HG22	4:C:734:PRO:CB	2.30	0.61
4:D:11:PHE:CE1	4:D:44:TYR:HB3	2.35	0.61
4:D:273:VAL:HA	4:D:415:TRP:HZ3	1.61	0.61
4:A:383:ALA:O	4:A:384:VAL:C	2.41	0.61
4:A:386:ARG:O	4:A:388:ASP:N	2.34	0.61
4:A:459:TRP:CZ3	4:A:475:PHE:HE1	2.18	0.61
4:A:563:PRO:HB3	4:A:878:SER:CA	2.29	0.61
4:B:538:GLY:HA2	4:B:882:PHE:O	2.00	0.61
4:B:574:VAL:CG2	4:B:685:VAL:HG12	2.30	0.61
4:B:783:VAL:O	4:B:786:GLN:N	2.31	0.61
4:D:139:SER:HB2	4:D:210:ILE:HD11	1.83	0.61
4:D:592:ASN:O	4:D:593:GLU:HB2	2.00	0.61
4:B:292:ARG:O	4:B:293:PRO:O	2.19	0.61
4:B:541:SER:O	4:B:542:GLY:C	2.43	0.61
4:C:291:ARG:HG2	7:C:3066:HOH:O	2.00	0.61
4:C:455:GLU:O	4:C:458:TYR:HB3	2.00	0.61
4:C:643:GLU:OE2	4:C:679:LYS:HD2	2.00	0.61
4:C:727:TRP:HB3	4:C:845:PHE:CD1	2.36	0.61
4:D:221:ILE:CG1	4:D:227:VAL:HG23	2.30	0.61
4:A:778:ILE:HG23	4:A:779:ALA:N	2.16	0.61
4:A:817:ILE:HB	4:A:818:PRO:CD	2.30	0.61
4:B:460:LEU:N	4:B:534:LEU:HD11	2.15	0.61
4:B:631:LYS:NZ	6:B:2001:APC:H3A2	2.16	0.61
4:B:676:TYR:CE1	4:B:680:LEU:HD11	2.36	0.61
4:C:495:SER:HB2	4:C:498:GLU:HB2	1.82	0.61
4:D:187:GLU:O	4:D:191:LEU:HG	2.00	0.61
4:D:226:MET:HE2	4:D:227:VAL:HG13	1.82	0.61
4:D:329:LYS:HD2	4:D:447:ALA:HA	1.82	0.61
4:A:43:SER:HA	4:A:46:MET:HE3	1.82	0.61
4:B:51:PHE:CD2	4:B:51:PHE:C	2.78	0.61
4:B:571:TYR:CD2	4:B:631:LYS:HG3	2.34	0.61
4:B:706:LEU:O	4:B:723:CYS:O	2.19	0.61
4:C:405:ALA:HB2	4:C:443:LEU:HD13	1.81	0.61
4:D:573:ILE:O	4:D:577:LYS:HG3	2.01	0.61
4:D:643:GLU:OE1	4:D:679:LYS:HD3	2.01	0.61
4:A:727:TRP:CD2	4:A:735:VAL:CG1	2.84	0.61
4:B:55:PHE:CE2	4:B:59:LEU:HD11	2.36	0.61
4:B:206:LYS:O	4:B:210:ILE:HG12	2.01	0.61
4:C:292:ARG:HG3	4:C:292:ARG:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:849:PHE:CD2	4:C:853:LEU:HD21	2.35	0.61
4:D:327:ALA:HA	4:D:415:TRP:CD1	2.35	0.61
4:D:631:LYS:CE	6:D:2003:APC:H3A2	2.31	0.61
4:A:77:LEU:CD2	4:A:119:ILE:HD12	2.31	0.61
4:A:390:ALA:O	4:A:393:SER:N	2.33	0.61
4:B:21:PHE:C	4:B:23:THR:N	2.58	0.61
4:B:281:ILE:HG22	4:B:282:THR:N	2.15	0.61
4:B:326:THR:O	4:B:415:TRP:CD1	2.54	0.61
4:B:437:ASN:C	4:B:437:ASN:ND2	2.54	0.61
4:B:582:LEU:HD13	4:B:621:LEU:HD12	1.82	0.61
4:B:827:ALA:O	4:B:828:VAL:C	2.44	0.61
4:C:303:LYS:HB2	4:C:303:LYS:HZ2	1.65	0.61
4:C:461:LYS:O	4:C:464:GLY:N	2.33	0.61
4:C:570:ILE:HA	4:C:573:ILE:HG22	1.81	0.61
4:C:828:VAL:HG23	4:C:829:ARG:N	2.12	0.61
4:D:330:ILE:HG21	4:D:409:ALA:HA	1.81	0.61
4:D:432:PHE:CE1	4:D:440:THR:HG23	2.36	0.61
4:D:859:ASP:HA	7:D:3136:HOH:O	2.00	0.61
1:H:10:DT:H5'	4:B:641:SER:N	2.15	0.60
1:N:11:DA:C6	4:D:639:TYR:CE2	2.89	0.60
4:A:373:ALA:HB2	7:A:3006:HOH:O	2.01	0.60
4:B:551:ARG:HG3	7:B:3047:HOH:O	2.01	0.60
4:B:795:VAL:O	4:B:796:VAL:C	2.39	0.60
4:C:84:ARG:NH1	4:C:84:ARG:HA	2.15	0.60
4:C:275:PRO:HB2	4:C:324:GLN:CD	2.25	0.60
4:C:386:ARG:HB3	7:C:3082:HOH:O	2.01	0.60
4:C:421:ASP:O	4:C:422:TRP:C	2.44	0.60
4:C:754:GLN:O	4:C:755:PHE:O	2.19	0.60
4:A:14:ILE:HA	7:A:3082:HOH:O	2.00	0.60
4:A:390:ALA:C	4:A:392:LYS:H	2.10	0.60
4:A:402:LEU:HG	4:A:439:MET:CE	2.31	0.60
4:A:457:TYR:OH	4:A:461:LYS:HD3	2.00	0.60
4:A:516:PHE:N	4:A:516:PHE:HD1	1.99	0.60
4:B:329:LYS:CG	4:B:329:LYS:O	2.49	0.60
4:B:626:THR:O	4:B:627:ARG:C	2.43	0.60
4:D:437:ASN:C	4:D:437:ASN:HD22	2.07	0.60
4:A:316:VAL:HG13	4:A:792:ARG:HE	1.66	0.60
4:A:348:PRO:C	4:A:349:VAL:CG2	2.74	0.60
4:A:488:ASN:O	4:A:491:ALA:HB3	2.01	0.60
4:A:682:TRP:O	4:A:682:TRP:CG	2.54	0.60
4:B:269:GLN:HG2	4:B:404:GLN:OE1	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:345:LYS:NZ	4:B:351:ASP:N	2.48	0.60
4:B:423:ARG:CD	4:B:781:ASN:ND2	2.64	0.60
4:B:427:TYR:CE1	4:B:811:HIS:NE2	2.69	0.60
4:B:439:MET:O	4:B:442:GLY:N	2.33	0.60
4:B:536:PHE:HE2	4:B:825:PHE:HB2	1.65	0.60
4:C:208:ASP:O	4:C:212:VAL:HG23	2.01	0.60
4:C:236:VAL:O	4:C:240:ASP:HB2	2.01	0.60
4:C:273:VAL:O	4:C:274:PRO:C	2.42	0.60
4:C:329:LYS:CD	4:C:447:ALA:HA	2.31	0.60
4:C:823:ASN:O	4:C:826:LYS:N	2.32	0.60
1:N:15:DC:C2'	1:N:16:DC:OP2	2.48	0.60
7:N:1048:HOH:O	4:D:772:HIS:HD2	1.83	0.60
4:A:25:ALA:O	4:A:29:GLY:N	2.32	0.60
4:A:496:PRO:HD2	7:A:3203:HOH:O	2.00	0.60
4:A:802:TYR:OH	4:A:830:GLU:OE2	2.20	0.60
4:B:677:MET:HG3	4:B:681:ILE:HD13	1.82	0.60
4:B:737:GLN:HE22	4:B:777:GLY:C	2.09	0.60
4:C:35:GLU:HG2	4:C:272:VAL:HG21	1.84	0.60
4:D:373:ALA:HB1	4:D:377:TRP:HE1	1.67	0.60
4:D:486:HIS:NE2	4:D:490:MET:HG3	2.16	0.60
1:H:3:DG:H2''	1:H:4:DA:C8	2.36	0.60
1:N:8:DG:H4'	7:N:1048:HOH:O	2.02	0.60
4:A:791:LEU:O	4:A:795:VAL:HG23	2.02	0.60
4:B:347:CYS:HB3	4:B:350:GLU:CG	2.32	0.60
4:B:433:ASN:CB	4:B:434:PRO:HD3	2.11	0.60
4:B:875:ILE:HG22	4:B:876:LEU:N	2.15	0.60
4:C:421:ASP:C	4:C:423:ARG:N	2.57	0.60
4:C:551:ARG:HE	4:C:872:LEU:CD2	2.14	0.60
4:D:207:GLU:HB3	4:D:211:HIS:NE2	2.15	0.60
4:D:292:ARG:H	4:D:293:PRO:HD3	1.65	0.60
4:A:459:TRP:HZ3	4:A:475:PHE:HE1	1.50	0.60
4:A:882:PHE:HD1	4:A:882:PHE:H	1.47	0.60
4:B:84:ARG:CD	4:B:219:MET:HG2	2.25	0.60
4:B:320:ILE:O	4:B:324:GLN:HB2	2.01	0.60
4:B:398:LEU:HD23	4:B:398:LEU:O	2.01	0.60
4:C:105:PHE:C	4:C:107:GLN:H	2.10	0.60
4:C:266:PRO:HG2	4:C:268:PHE:CZ	2.37	0.60
4:D:333:LYS:HZ2	4:D:516:PHE:HB3	1.63	0.60
1:H:9:DA:N6	3:J:1:DG:H21	2.00	0.60
4:A:47:GLY:O	4:A:50:ARG:HB3	2.01	0.60
4:A:159:ALA:O	4:A:163:LYS:HB2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:342:THR:HG22	4:A:348:PRO:HG3	1.83	0.60
4:A:546:PHE:CD2	4:A:692:ALA:HA	2.30	0.60
4:A:574:VAL:HG12	4:A:684:SER:HB3	1.82	0.60
4:B:59:LEU:HA	4:B:64:VAL:HG22	1.82	0.60
4:B:120:LYS:NZ	4:B:752:LEU:HD11	2.17	0.60
4:B:454:LYS:HG3	4:B:455:GLU:N	2.15	0.60
4:B:460:LEU:HA	4:B:534:LEU:HD21	1.82	0.60
4:B:525:GLY:C	4:B:527:SER:H	2.10	0.60
4:B:680:LEU:HD12	4:B:680:LEU:N	2.15	0.60
4:C:635:MET:CE	6:C:2002:APC:H8	2.30	0.60
4:D:729:THR:HB	4:D:789:SER:HB2	1.83	0.60
1:N:15:DC:H2''	1:N:16:DC:O5'	2.01	0.60
4:A:89:PHE:HA	4:A:103:PHE:HE1	1.64	0.60
4:A:329:LYS:HG2	4:A:447:ALA:HA	1.84	0.60
4:B:73:LEU:HD21	4:B:77:LEU:HD22	1.83	0.60
4:B:181:ALA:O	4:B:185:VAL:HG13	2.00	0.60
4:B:291:ARG:HG3	7:B:3037:HOH:O	2.00	0.60
4:C:21:PHE:C	4:C:23:THR:N	2.54	0.60
4:C:316:VAL:CG1	4:C:420:MET:HE1	2.32	0.60
4:C:333:LYS:CB	4:C:516:PHE:CD2	2.84	0.60
4:C:423:ARG:HD2	4:C:781:ASN:CG	2.26	0.60
4:D:833:VAL:HG22	4:D:875:ILE:HB	1.83	0.60
4:A:116:TYR:CE2	4:A:752:LEU:HD13	2.37	0.60
4:A:633:SER:OG	4:A:646:PHE:CG	2.44	0.60
4:C:492:CYS:SG	4:C:501:TRP:HE3	2.25	0.60
4:D:113:ALA:O	4:D:117:ILE:HG13	2.01	0.60
4:D:571:TYR:CD1	4:D:631:LYS:HA	2.37	0.60
4:A:82:ILE:HG21	4:A:112:GLU:OE2	2.01	0.60
4:A:536:PHE:HB3	4:A:882:PHE:HB3	1.84	0.60
4:A:842:LEU:O	4:A:845:PHE:HB3	2.02	0.60
4:B:292:ARG:N	4:B:293:PRO:HD3	2.16	0.60
4:B:300:HIS:NE2	4:B:422:TRP:HZ3	1.97	0.60
4:C:14:ILE:HG21	4:C:288:ALA:HB1	1.83	0.60
4:C:549:MET:HE1	4:C:786:GLN:HG2	1.83	0.60
4:D:54:MET:O	4:D:58:GLN:HG2	2.02	0.60
4:D:213:GLY:O	4:D:217:ILE:HG13	2.02	0.60
4:A:159:ALA:HB1	4:A:163:LYS:N	2.17	0.59
4:A:342:THR:CG2	4:A:398:LEU:HD21	2.33	0.59
4:A:778:ILE:CG2	4:A:779:ALA:N	2.65	0.59
4:B:401:MET:HE3	4:B:440:THR:HG21	1.82	0.59
4:B:571:TYR:CE1	7:B:3067:HOH:O	2.51	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:324:GLN:HG3	4:C:417:PRO:HA	1.84	0.59
4:D:646:PHE:O	4:D:647:ARG:O	2.19	0.59
2:F:3:G:O2'	4:A:389:LYS:NZ	2.35	0.59
4:A:380:ALA:O	4:A:383:ALA:HB3	2.02	0.59
4:A:428:ALA:N	4:A:435:GLN:HE22	2.00	0.59
4:A:669:GLN:CG	4:A:672:GLN:HE21	2.15	0.59
4:A:712:ASP:HA	7:A:3088:HOH:O	2.00	0.59
4:B:66:ASP:OD1	4:B:120:LYS:HE3	2.01	0.59
4:B:689:VAL:O	4:B:690:VAL:C	2.45	0.59
4:B:698:TRP:O	4:B:701:SER:N	2.35	0.59
4:C:496:PRO:HA	7:C:3071:HOH:O	2.02	0.59
4:C:525:GLY:O	4:C:527:SER:N	2.35	0.59
4:D:95:LYS:HD2	7:D:3092:HOH:O	2.02	0.59
4:D:846:TYR:HA	4:D:849:PHE:CE1	2.36	0.59
2:O:4:G:H2'	2:O:5:C:H6	1.67	0.59
4:A:741:LYS:HB2	4:A:770:ASP:HB2	1.84	0.59
4:B:163:LYS:HB3	4:B:164:LYS:NZ	2.17	0.59
4:B:215:ARG:HE	4:B:219:MET:HE2	1.65	0.59
4:B:345:LYS:O	4:B:346:HIS:C	2.45	0.59
4:B:418:TYR:CE2	4:B:428:ALA:CB	2.82	0.59
4:B:473:VAL:CG1	4:B:474:PRO:CD	2.79	0.59
4:C:299:THR:CG2	4:C:300:HIS:H	2.13	0.59
4:D:3:THR:HG23	7:D:3098:HOH:O	2.00	0.59
4:A:585:ASP:O	4:A:588:ASN:O	2.19	0.59
4:B:388:ASP:C	4:B:388:ASP:OD1	2.45	0.59
4:B:561:LEU:HD23	4:B:875:ILE:HD11	1.84	0.59
4:C:78:LEU:HD11	4:C:115:ALA:HB3	1.84	0.59
4:C:330:ILE:HG12	7:C:3016:HOH:O	2.02	0.59
4:C:695:ALA:O	4:C:699:LEU:HD12	2.03	0.59
4:C:875:ILE:O	4:C:875:ILE:HG22	2.01	0.59
4:D:322:ILE:HG22	4:D:323:ALA:N	2.17	0.59
4:A:205:HIS:HB3	4:A:207:GLU:HG2	1.84	0.59
4:A:849:PHE:CD2	4:A:853:LEU:HD21	2.37	0.59
4:B:662:GLY:C	4:B:663:LYS:O	2.45	0.59
4:C:14:ILE:HG21	4:C:288:ALA:CB	2.33	0.59
4:C:318:LYS:HE2	4:C:796:VAL:HG13	1.84	0.59
4:D:19:ILE:HG23	4:D:20:PRO:HD2	1.84	0.59
4:D:53:LYS:O	4:D:56:GLU:HB3	2.02	0.59
4:D:229:LEU:HA	4:D:244:ILE:HD13	1.84	0.59
3:M:5:DA:H2''	3:M:6:DT:H72	1.84	0.59
4:A:92:VAL:HG22	7:A:3011:HOH:O	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:294:LEU:CD1	4:A:429:VAL:HG21	2.29	0.59
4:B:398:LEU:CD2	4:B:398:LEU:C	2.75	0.59
4:B:545:HIS:O	4:B:546:PHE:C	2.42	0.59
4:B:663:LYS:CG	4:B:664:GLY:N	2.66	0.59
4:B:849:PHE:O	4:B:850:ALA:C	2.46	0.59
4:C:24:LEU:HD22	4:C:273:VAL:HG21	1.85	0.59
4:C:78:LEU:N	4:C:79:PRO:CD	2.65	0.59
4:C:306:MET:O	4:C:308:TYR:N	2.35	0.59
4:C:340:VAL:C	4:C:342:THR:N	2.60	0.59
4:C:433:ASN:OD1	4:C:433:ASN:C	2.46	0.59
4:C:706:LEU:O	4:C:723:CYS:O	2.20	0.59
4:C:726:HIS:HB2	4:C:736:TRP:CD1	2.37	0.59
4:D:100:PRO:HG2	4:D:103:PHE:HB2	1.83	0.59
4:D:725:VAL:HG23	4:D:774:GLN:HE21	1.66	0.59
4:A:15:GLU:HG2	4:A:18:ALA:O	2.03	0.59
4:A:96:ARG:NE	7:A:3009:HOH:O	2.33	0.59
4:A:143:ARG:HD3	7:A:3118:HOH:O	2.01	0.59
4:A:178:TYR:HD1	4:A:178:TYR:H	1.47	0.59
4:B:109:ILE:O	4:B:110:LYS:C	2.46	0.59
4:B:318:LYS:O	4:B:319:ALA:C	2.45	0.59
4:B:813:SER:C	4:B:814:PHE:CD1	2.81	0.59
4:C:88:TRP:NE1	4:C:215:ARG:HE	2.00	0.59
4:C:837:GLU:HG3	4:C:872:LEU:HD12	1.85	0.59
4:D:710:VAL:CG1	4:D:720:ARG:HB3	2.33	0.59
2:I:5:C:N3	2:I:6:G:N7	2.50	0.59
1:N:10:DT:H5'	4:D:641:SER:HA	1.83	0.59
4:A:35:GLU:O	4:A:36:GLN:C	2.46	0.59
4:A:80:LYS:CD	4:A:224:THR:HG22	2.32	0.59
4:A:629:VAL:HG12	4:A:629:VAL:O	2.02	0.59
4:A:640:GLY:O	4:A:641:SER:C	2.46	0.59
4:A:727:TRP:CH2	4:A:735:VAL:HG21	2.38	0.59
4:B:36:GLN:HA	4:B:36:GLN:OE1	2.03	0.59
4:B:770:ASP:OD1	4:B:772:HIS:N	2.36	0.59
4:B:784:HIS:O	4:B:785:SER:C	2.44	0.59
4:C:281:ILE:CG1	4:C:309:GLU:HA	2.33	0.59
4:C:452:ILE:HD11	4:C:457:TYR:N	2.18	0.59
4:A:649:GLN:O	4:A:650:VAL:C	2.46	0.59
4:A:660:ASP:HB3	7:A:3072:HOH:O	2.02	0.59
4:A:727:TRP:CE3	4:A:735:VAL:HG13	2.37	0.59
4:A:786:GLN:HA	4:A:786:GLN:NE2	2.03	0.59
4:A:793:LYS:O	4:A:794:THR:C	2.45	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:802:TYR:N	4:A:802:TYR:HD2	1.99	0.59
4:B:40:GLU:OE1	4:B:288:ALA:HB3	2.02	0.59
4:B:677:MET:O	4:B:678:ALA:C	2.44	0.59
4:B:803:GLY:O	4:B:804:ILE:C	2.46	0.59
4:C:308:TYR:HH	4:C:733:PHE:HE2	1.49	0.59
3:J:1:DG:H1'	3:J:2:DT:H71	1.83	0.59
4:A:154:ILE:CG2	4:A:190:MET:HE2	2.26	0.59
4:A:720:ARG:HH21	4:A:857:GLN:HE22	1.51	0.59
4:B:473:VAL:HG12	4:B:474:PRO:N	2.17	0.59
4:B:514:PHE:CG	4:B:514:PHE:O	2.56	0.59
4:B:576:LYS:O	4:B:579:ASN:N	2.36	0.59
4:B:742:PRO:HB3	4:B:744:GLN:CD	2.27	0.59
4:C:21:PHE:C	4:C:23:THR:H	2.11	0.59
4:C:724:ALA:HB2	4:C:738:GLU:HG3	1.85	0.59
4:D:726:HIS:CD2	4:D:736:TRP:CE2	2.90	0.59
1:H:13:DC:C4'	4:B:427:TYR:HE2	2.15	0.58
1:K:9:DA:H5'	7:K:731:HOH:O	2.01	0.58
4:A:76:THR:C	4:A:79:PRO:HD2	2.27	0.58
4:A:425:ARG:NH2	4:A:784:HIS:CE1	2.71	0.58
4:C:268:PHE:HB3	4:C:430:SER:HA	1.85	0.58
4:D:465:ALA:HB1	4:D:478:ARG:HB3	1.84	0.58
4:D:616:LEU:HD13	4:D:676:TYR:HB2	1.85	0.58
4:D:619:GLN:NE2	4:D:668:THR:H	2.01	0.58
4:D:668:THR:HG22	4:D:669:GLN:NE2	2.17	0.58
4:A:40:GLU:O	4:A:43:SER:HB2	2.04	0.58
4:A:810:ILE:O	4:A:812:ASP:N	2.36	0.58
4:B:728:VAL:HG13	4:B:733:PHE:C	2.28	0.58
4:C:252:GLU:HG2	7:C:3072:HOH:O	2.02	0.58
4:C:632:ARG:HA	4:C:635:MET:HG2	1.85	0.58
4:C:727:TRP:CZ2	4:C:735:VAL:HG11	2.38	0.58
4:D:472:LYS:HG3	4:D:567:VAL:HG11	1.84	0.58
4:A:13:ASP:CG	4:A:291:ARG:HH21	2.10	0.58
4:A:108:GLU:HG3	7:A:3115:HOH:O	2.02	0.58
4:A:404:GLN:HG2	4:A:432:PHE:CB	2.33	0.58
4:A:549:MET:HB3	4:A:836:TYR:HE1	1.67	0.58
4:A:570:ILE:O	4:A:574:VAL:HG23	2.02	0.58
4:A:619:GLN:O	4:A:622:ALA:HB3	2.03	0.58
4:B:144:ALA:O	4:B:145:ILE:C	2.46	0.58
4:B:236:VAL:CB	4:B:239:GLN:HB2	2.31	0.58
4:B:748:ASN:HD21	4:B:751:PHE:HB2	1.67	0.58
4:C:501:TRP:HB2	7:C:3116:HOH:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:21:PHE:C	4:D:23:THR:H	2.10	0.58
4:D:458:TYR:O	4:D:462:ILE:HG12	2.03	0.58
4:D:473:VAL:CG2	4:D:477:GLU:HG3	2.32	0.58
4:D:560:ASN:O	4:D:878:SER:OG	2.18	0.58
3:G:4:DG:H1'	3:G:5:DA:C8	2.38	0.58
4:B:585:ASP:OD2	4:B:613:THR:HB	2.03	0.58
4:B:610:LYS:O	4:B:611:LEU:C	2.46	0.58
4:B:814:PHE:CE2	4:B:828:VAL:HG13	2.39	0.58
4:C:50:ARG:CZ	4:C:267:MET:HE3	2.33	0.58
4:C:92:VAL:HG12	4:C:99:ARG:CG	2.27	0.58
4:C:161:HIS:O	4:C:163:LYS:N	2.36	0.58
4:C:329:LYS:HG3	4:C:445:THR:CG2	2.32	0.58
4:C:588:ASN:HD22	4:C:588:ASN:N	2.02	0.58
4:C:816:THR:HG22	4:C:817:ILE:HG13	1.86	0.58
4:C:830:GLU:O	4:C:831:THR:C	2.46	0.58
4:D:496:PRO:HD2	7:D:3035:HOH:O	2.02	0.58
4:A:516:PHE:N	4:A:516:PHE:CD1	2.70	0.58
4:A:551:ARG:HH21	4:A:872:LEU:HD11	1.67	0.58
4:A:727:TRP:CD2	4:A:735:VAL:HG13	2.39	0.58
4:B:46:MET:O	4:B:49:ALA:HB3	2.03	0.58
4:B:55:PHE:O	4:B:55:PHE:HD2	1.87	0.58
4:B:182:PHE:O	4:B:185:VAL:HG22	2.02	0.58
4:B:229:LEU:HD21	4:B:242:GLU:CD	2.29	0.58
4:C:299:THR:HG21	4:C:304:ALA:HB3	1.85	0.58
4:C:319:ALA:CB	4:C:792:ARG:HB3	2.34	0.58
4:C:322:ILE:HG21	4:C:795:VAL:HG12	1.85	0.58
4:C:398:LEU:HD23	4:C:398:LEU:C	2.29	0.58
4:C:477:GLU:HA	4:C:480:LYS:HB3	1.86	0.58
4:D:619:GLN:O	4:D:622:ALA:HB3	2.03	0.58
4:A:502:TRP:CD1	4:A:512:LEU:HD13	2.39	0.58
4:A:563:PRO:HB3	4:A:877:GLU:C	2.28	0.58
4:A:825:PHE:CD1	4:A:825:PHE:C	2.81	0.58
4:B:206:LYS:HB2	7:B:3155:HOH:O	2.02	0.58
4:B:389:LYS:O	4:B:392:LYS:HB3	2.03	0.58
4:B:645:GLY:C	4:B:647:ARG:N	2.60	0.58
4:C:423:ARG:NH1	4:C:423:ARG:CB	2.67	0.58
4:C:432:PHE:HZ	4:C:444:LEU:HD21	1.67	0.58
4:C:514:PHE:CD1	4:C:514:PHE:C	2.81	0.58
4:C:579:ASN:HA	4:C:582:LEU:HB2	1.86	0.58
4:D:40:GLU:OE1	4:D:288:ALA:N	2.34	0.58
4:D:830:GLU:HG2	4:D:876:LEU:CD2	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:374:LEU:C	4:A:376:ALA:H	2.12	0.58
4:A:392:LYS:O	4:A:392:LYS:HG2	2.03	0.58
4:A:582:LEU:HB2	4:A:621:LEU:HD21	1.86	0.58
4:A:635:MET:HE1	6:A:2000:APC:H3'	1.85	0.58
4:A:792:ARG:HG3	4:A:792:ARG:HH11	1.68	0.58
4:B:99:ARG:NH1	4:B:99:ARG:HG2	2.19	0.58
4:B:162:PHE:CD1	4:B:190:MET:SD	2.97	0.58
4:B:163:LYS:C	4:B:166:VAL:HG23	2.28	0.58
4:B:423:ARG:HD2	4:B:781:ASN:HD21	1.68	0.58
4:B:439:MET:O	4:B:440:THR:C	2.43	0.58
4:B:702:ALA:CB	4:B:849:PHE:CE2	2.84	0.58
4:B:751:PHE:CB	4:B:752:LEU:HD12	2.23	0.58
4:B:840:ASP:O	4:B:841:VAL:C	2.46	0.58
4:C:421:ASP:C	4:C:423:ARG:H	2.10	0.58
4:C:791:LEU:HD23	4:C:791:LEU:C	2.29	0.58
4:C:882:PHE:O	4:C:883:ALA:HB3	2.02	0.58
4:D:77:LEU:HD11	4:D:224:THR:OG1	2.03	0.58
4:D:230:HIS:NE2	4:D:245:GLU:HB2	2.19	0.58
4:D:308:TYR:CE2	4:D:734:PRO:O	2.56	0.58
4:D:619:GLN:NE2	4:D:666:MET:O	2.36	0.58
4:D:680:LEU:O	4:D:683:GLU:N	2.37	0.58
4:A:3:THR:HB	4:A:52:ARG:HH12	1.69	0.58
4:B:5:ASN:HD21	4:B:7:ALA:CA	2.17	0.58
4:B:54:MET:O	4:B:58:GLN:HG2	2.03	0.58
4:B:112:GLU:H	4:B:112:GLU:CD	2.11	0.58
4:B:423:ARG:HD2	4:B:781:ASN:ND2	2.18	0.58
4:C:19:ILE:CG1	4:C:20:PRO:HD2	2.20	0.58
4:C:452:ILE:HG22	4:C:528:TYR:O	2.04	0.58
4:C:553:GLU:HG2	4:C:554:VAL:N	2.19	0.58
4:C:849:PHE:HD2	4:C:853:LEU:HD21	1.68	0.58
4:A:50:ARG:HG2	4:A:50:ARG:HH11	1.68	0.58
4:A:270:PRO:HB3	4:A:416:PHE:CE1	2.39	0.58
4:A:511:PHE:CD2	4:A:511:PHE:O	2.57	0.58
4:B:753:GLY:O	4:B:754:GLN:HG2	2.04	0.58
4:B:843:ALA:HA	4:B:864:LEU:HD21	1.85	0.58
4:B:861:MET:O	4:B:862:PRO:O	2.21	0.58
4:C:433:ASN:HB2	4:C:434:PRO:HD2	1.85	0.58
4:C:701:SER:O	4:C:704:LYS:HB3	2.04	0.58
4:C:727:TRP:NE1	4:C:782:PHE:CD1	2.72	0.58
4:D:292:ARG:N	4:D:293:PRO:HD3	2.18	0.58
4:D:720:ARG:NH1	4:D:720:ARG:CG	2.52	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:463:HIS:O	4:A:466:ASN:N	2.36	0.58
4:A:796:VAL:O	4:A:797:TRP:C	2.45	0.58
4:A:809:LEU:C	4:A:810:ILE:HG13	2.28	0.58
4:A:881:ALA:C	4:A:882:PHE:O	2.45	0.58
4:B:439:MET:HG3	4:B:509:PHE:CG	2.38	0.58
4:C:401:MET:O	4:C:404:GLN:CB	2.52	0.58
4:C:476:PRO:HG2	4:C:477:GLU:H	1.69	0.58
4:C:737:GLN:OE1	4:C:778:ILE:HD13	2.04	0.58
4:D:748:ASN:HB2	4:D:753:GLY:CA	2.33	0.58
4:D:794:THR:OG1	4:D:831:THR:CG2	2.45	0.58
4:A:448:LYS:HG2	7:A:3094:HOH:O	2.04	0.57
4:A:623:TYR:HD1	4:A:663:LYS:HE3	1.69	0.57
4:A:629:VAL:CG1	4:A:677:MET:HE3	2.34	0.57
4:A:727:TRP:CZ2	4:A:735:VAL:HG11	2.39	0.57
4:B:582:LEU:HD13	4:B:621:LEU:CD1	2.33	0.57
4:B:631:LYS:O	4:B:632:ARG:C	2.47	0.57
4:C:308:TYR:O	4:C:310:ASP:N	2.37	0.57
4:C:553:GLU:O	4:C:554:VAL:C	2.47	0.57
1:E:14:DG:C2'	1:E:15:DC:C6	2.85	0.57
4:A:135:GLN:HB2	7:A:3052:HOH:O	2.02	0.57
4:A:416:PHE:CE2	4:A:434:PRO:HD3	2.40	0.57
4:A:471:ASP:OD1	4:A:472:LYS:CD	2.38	0.57
4:A:669:GLN:HB3	4:A:672:GLN:HG3	1.86	0.57
4:B:99:ARG:HG2	4:B:99:ARG:HH11	1.68	0.57
4:B:123:LEU:O	4:B:127:THR:HG23	2.04	0.57
4:B:436:GLY:HA3	7:B:3166:HOH:O	2.03	0.57
4:B:450:LYS:HB3	4:B:819:ALA:HB3	1.86	0.57
4:B:823:ASN:O	4:B:826:LYS:N	2.36	0.57
4:D:84:ARG:HB2	4:D:223:SER:HB3	1.87	0.57
4:B:737:GLN:HG2	4:B:774:GLN:NE2	2.18	0.57
4:C:275:PRO:CG	4:C:324:GLN:HG2	2.34	0.57
4:C:306:MET:C	4:C:308:TYR:N	2.61	0.57
4:C:308:TYR:CE2	4:C:734:PRO:HG2	2.38	0.57
4:C:326:THR:O	4:C:415:TRP:CD1	2.57	0.57
4:C:700:LYS:HA	4:C:778:ILE:HG21	1.86	0.57
4:D:100:PRO:O	4:D:104:GLN:HG2	2.04	0.57
4:D:155:ARG:HA	4:D:163:LYS:HE3	1.86	0.57
4:D:402:LEU:O	4:D:403:GLU:C	2.47	0.57
4:D:814:PHE:CE1	4:D:883:ALA:CB	2.87	0.57
3:M:2:DT:H2''	3:M:3:DC:O5'	2.02	0.57
4:A:462:ILE:CD1	4:A:478:ARG:HD2	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:657:PRO:O	4:A:661:SER:OG	2.13	0.57
4:A:828:VAL:O	4:A:831:THR:HG22	2.04	0.57
4:B:164:LYS:NZ	4:B:164:LYS:N	2.52	0.57
4:B:492:CYS:SG	4:B:502:TRP:HD1	2.25	0.57
4:B:642:LYS:HG2	4:B:682:TRP:CZ3	2.38	0.57
4:D:61:ALA:HB3	4:D:63:GLU:HG3	1.84	0.57
4:D:270:PRO:HD2	4:D:408:PHE:CE2	2.39	0.57
2:I:4:G:H5''	4:B:386:ARG:HD3	1.86	0.57
3:P:3:DC:H5'	7:D:3034:HOH:O	2.04	0.57
4:A:651:LEU:HD11	4:A:656:GLN:HE22	1.70	0.57
4:A:712:ASP:O	4:A:716:GLY:N	2.36	0.57
4:C:281:ILE:HG12	4:C:309:GLU:CA	2.34	0.57
4:C:281:ILE:CD1	4:C:309:GLU:HA	2.34	0.57
4:C:531:SER:OG	7:C:3088:HOH:O	2.17	0.57
4:C:583:GLN:O	4:C:587:ILE:HG12	2.05	0.57
4:C:704:LYS:NZ	4:C:775:GLU:OE2	2.32	0.57
4:D:486:HIS:NE2	4:D:490:MET:CG	2.67	0.57
4:A:646:PHE:O	4:A:647:ARG:C	2.48	0.57
4:A:849:PHE:O	4:A:852:GLN:N	2.38	0.57
4:A:882:PHE:N	4:A:882:PHE:CD1	2.71	0.57
4:B:146:GLU:O	4:B:147:ASP:C	2.46	0.57
4:C:727:TRP:CE2	4:C:735:VAL:HG11	2.39	0.57
4:D:545:HIS:O	4:D:546:PHE:C	2.47	0.57
4:D:711:LYS:C	4:D:719:LEU:HD13	2.29	0.57
4:D:870:LEU:CD2	4:D:872:LEU:HD23	2.34	0.57
4:A:461:LYS:HE3	4:A:479:ILE:HG23	1.84	0.57
4:A:468:ALA:HB2	4:A:511:PHE:CD1	2.38	0.57
4:A:626:THR:O	4:A:627:ARG:C	2.48	0.57
4:B:21:PHE:C	4:B:21:PHE:CD1	2.82	0.57
4:B:298:ARG:HE	4:B:419:ASN:CB	2.18	0.57
4:B:828:VAL:O	4:B:831:THR:HG22	2.05	0.57
4:C:10:ASP:OD1	7:C:3066:HOH:O	2.18	0.57
4:C:205:HIS:C	4:C:207:GLU:H	2.12	0.57
4:C:216:CYS:HA	4:C:219:MET:HE3	1.85	0.57
4:D:297:VAL:HG21	4:D:733:PHE:HZ	1.69	0.57
4:D:543:ILE:HG22	4:D:543:ILE:O	2.05	0.57
4:D:632:ARG:HH22	6:D:2003:APC:C5'	2.18	0.57
4:A:383:ALA:C	4:A:385:TYR:H	2.11	0.57
4:A:562:LEU:CD2	4:A:870:LEU:HD11	2.35	0.57
4:A:643:GLU:HG3	4:A:682:TRP:CG	2.39	0.57
4:B:571:TYR:HD2	4:B:631:LYS:HA	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:322:ILE:HG22	4:C:323:ALA:N	2.19	0.57
4:D:19:ILE:CG2	7:D:3014:HOH:O	2.51	0.57
4:D:323:ALA:C	4:D:325:ASN:N	2.61	0.57
4:D:458:TYR:C	4:D:458:TYR:CD2	2.82	0.57
4:D:720:ARG:NH1	4:D:721:LYS:O	2.38	0.57
4:A:374:LEU:H	4:A:374:LEU:HD12	1.68	0.57
4:A:404:GLN:HG2	4:A:432:PHE:HB2	1.86	0.57
4:B:422:TRP:CD1	4:B:422:TRP:C	2.83	0.57
4:B:557:ARG:HB2	4:B:562:LEU:HD12	1.86	0.57
4:B:677:MET:SD	4:B:681:ILE:CD1	2.93	0.57
4:B:780:PRO:HA	4:B:783:VAL:CG2	2.35	0.57
4:C:579:ASN:HA	4:C:582:LEU:CD1	2.33	0.57
4:D:88:TRP:O	4:D:92:VAL:HG23	2.04	0.57
4:D:236:VAL:HB	4:D:239:GLN:HB2	1.87	0.57
4:D:439:MET:HG3	4:D:509:PHE:CD2	2.40	0.57
4:A:137:VAL:HG12	4:A:217:ILE:HD11	1.86	0.57
4:A:429:VAL:HG12	4:A:430:SER:N	2.18	0.57
4:A:779:ALA:O	4:A:783:VAL:HG23	2.05	0.57
4:B:162:PHE:HD1	4:B:190:MET:SD	2.27	0.57
4:B:264:ILE:O	4:B:264:ILE:HG22	2.05	0.57
4:B:702:ALA:HB1	4:B:849:PHE:HE2	1.67	0.57
4:C:183:MET:HE3	4:C:186:VAL:HG21	1.87	0.57
4:C:711:LYS:HG2	4:C:718:ILE:HA	1.87	0.57
4:D:338:ALA:HB2	4:D:509:PHE:CE1	2.40	0.57
4:D:551:ARG:HB2	4:D:868:GLY:N	2.16	0.57
4:D:777:GLY:O	4:D:778:ILE:C	2.46	0.57
1:E:12:DT:C2'	1:E:13:DC:C5'	2.69	0.56
4:A:88:TRP:HE3	4:A:91:GLU:OE1	1.88	0.56
4:A:109:ILE:CD1	4:A:149:ALA:HB2	2.35	0.56
4:A:312:TYR:CZ	4:A:314:PRO:HG3	2.40	0.56
4:A:502:TRP:CG	4:A:512:LEU:CD1	2.88	0.56
4:A:583:GLN:CB	7:A:3056:HOH:O	2.46	0.56
4:A:685:VAL:O	4:A:687:VAL:N	2.37	0.56
4:A:777:GLY:O	4:A:781:ASN:OD1	2.23	0.56
4:A:828:VAL:CG2	4:A:829:ARG:H	2.14	0.56
4:B:457:TYR:CE1	4:B:521:VAL:HG11	2.40	0.56
4:B:536:PHE:CE2	4:B:825:PHE:HD2	2.23	0.56
4:B:734:PRO:O	4:B:734:PRO:CG	2.52	0.56
4:C:721:LYS:HG2	4:C:722:ARG:N	2.19	0.56
4:D:201:TRP:HA	4:D:204:TRP:HD1	1.69	0.56
4:A:423:ARG:HG2	4:A:781:ASN:HD22	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:807:PHE:CD1	4:A:807:PHE:N	2.73	0.56
4:A:830:GLU:O	4:A:831:THR:C	2.47	0.56
4:B:163:LYS:NZ	4:B:167:GLU:N	2.54	0.56
4:B:403:GLU:O	4:B:404:GLN:C	2.48	0.56
4:B:532:LEU:O	4:B:818:PRO:HD3	2.04	0.56
4:C:5:ASN:ND2	4:C:7:ALA:HB3	2.19	0.56
4:C:632:ARG:HH22	6:C:2002:APC:C5'	2.13	0.56
4:D:505:GLN:NE2	4:D:505:GLN:CA	2.66	0.56
4:D:745:THR:HB	4:D:756:ARG:NH1	2.21	0.56
1:H:17:DG:H3'	4:B:57:ARG:NH2	2.20	0.56
7:K:1088:HOH:O	4:C:641:SER:HA	2.06	0.56
4:A:155:ARG:CB	4:A:163:LYS:HE3	2.31	0.56
4:A:166:VAL:O	4:A:167:GLU:C	2.47	0.56
4:A:268:PHE:HB3	4:A:430:SER:HA	1.86	0.56
4:A:308:TYR:CE2	4:A:736:TRP:HZ3	2.23	0.56
4:A:379:ARG:HE	4:A:656:GLN:HG2	1.70	0.56
4:A:579:ASN:HA	4:A:582:LEU:CD1	2.35	0.56
4:A:820:ASP:O	4:A:823:ASN:HB2	2.06	0.56
4:B:66:ASP:OD1	4:B:752:LEU:HD21	2.05	0.56
4:B:173:ARG:NH1	4:B:182:PHE:CD1	2.74	0.56
4:B:261:LEU:C	4:B:263:GLY:N	2.63	0.56
4:B:471:ASP:C	4:B:472:LYS:HD2	2.31	0.56
4:B:616:LEU:O	4:B:618:GLY:N	2.38	0.56
4:B:632:ARG:CD	6:B:2001:APC:HN61	2.16	0.56
4:B:841:VAL:HG12	7:B:3081:HOH:O	2.05	0.56
4:C:334:VAL:HG21	4:C:513:ALA:CB	2.29	0.56
4:C:472:LYS:HE3	7:C:3049:HOH:O	2.05	0.56
4:C:534:LEU:HD12	4:C:821:ALA:HB2	1.86	0.56
4:C:831:THR:CG2	4:C:832:MET:N	2.69	0.56
4:D:420:MET:HA	4:D:425:ARG:O	2.04	0.56
4:D:512:LEU:O	4:D:515:CYS:HB2	2.05	0.56
4:A:436:GLY:HA3	4:A:440:THR:HB	1.87	0.56
4:A:508:PRO:HG2	4:A:509:PHE:H	1.69	0.56
4:A:734:PRO:HG2	4:A:734:PRO:O	2.05	0.56
4:A:816:THR:HG22	4:A:817:ILE:N	2.18	0.56
4:B:56:GLU:OE1	4:B:57:ARG:CA	2.53	0.56
4:B:233:ASN:CB	4:B:239:GLN:HB3	2.35	0.56
4:B:335:LEU:HD21	4:B:406:ASN:OD1	2.06	0.56
4:B:465:ALA:O	4:B:468:ALA:HB3	2.05	0.56
4:B:541:SER:O	4:B:544:GLN:HB3	2.04	0.56
4:B:634:VAL:HG22	4:B:634:VAL:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:695:ALA:O	4:B:699:LEU:CD1	2.50	0.56
4:B:846:TYR:CD2	4:B:864:LEU:HD11	2.40	0.56
4:C:50:ARG:NH1	4:C:267:MET:HE3	2.20	0.56
4:C:152:GLY:O	4:C:156:ASP:OD2	2.22	0.56
4:C:474:PRO:HB2	4:C:476:PRO:CD	2.36	0.56
4:C:551:ARG:CG	4:C:551:ARG:NH1	2.68	0.56
4:C:649:GLN:O	4:C:650:VAL:C	2.48	0.56
4:C:741:LYS:HB2	4:C:770:ASP:HB2	1.86	0.56
4:D:303:LYS:HG3	4:D:304:ALA:H	1.68	0.56
4:D:390:ALA:HB1	4:D:394:ARG:NH2	2.19	0.56
4:A:14:ILE:HG13	7:A:3082:HOH:O	2.05	0.56
4:A:109:ILE:HD13	4:A:145:ILE:CG2	2.20	0.56
4:A:792:ARG:O	4:A:796:VAL:HG22	2.06	0.56
4:A:798:ALA:HB2	4:A:827:ALA:HB1	1.86	0.56
4:B:19:ILE:CD1	4:B:20:PRO:HD2	2.35	0.56
4:B:105:PHE:C	4:B:107:GLN:H	2.13	0.56
4:B:210:ILE:O	4:B:214:VAL:HG22	2.06	0.56
4:B:446:LEU:HD13	4:B:806:SER:HB3	1.88	0.56
4:B:587:ILE:O	4:B:614:LYS:HE3	2.05	0.56
4:D:236:VAL:HG11	4:D:239:GLN:CD	2.31	0.56
4:D:501:TRP:HA	4:D:504:GLU:CD	2.30	0.56
4:A:81:MET:SD	4:A:85:ILE:HD11	2.45	0.56
4:A:143:ARG:HG2	7:A:3010:HOH:O	2.05	0.56
4:A:314:PRO:HD2	4:A:315:GLU:H	1.70	0.56
4:A:620:TRP:HA	4:A:620:TRP:CE3	2.40	0.56
4:B:5:ASN:HB3	4:B:8:LYS:HE3	1.88	0.56
4:B:89:PHE:HZ	4:B:106:LEU:O	1.89	0.56
4:B:302:LYS:HE3	4:B:306:MET:HE3	1.88	0.56
4:B:620:TRP:CD2	4:B:677:MET:HE2	2.40	0.56
4:B:783:VAL:O	4:B:784:HIS:O	2.24	0.56
4:C:335:LEU:HD21	4:C:406:ASN:OD1	2.06	0.56
4:C:685:VAL:C	4:C:687:VAL:H	2.13	0.56
4:D:669:GLN:HG3	4:D:672:GLN:NE2	2.21	0.56
4:D:712:ASP:HB2	4:D:719:LEU:HD11	1.88	0.56
4:D:828:VAL:HA	4:D:831:THR:CG2	2.35	0.56
4:A:347:CYS:SG	4:A:350:GLU:HG2	2.46	0.56
4:A:486:HIS:HE1	7:A:3212:HOH:O	1.89	0.56
4:A:854:HIS:HD2	4:A:856:SER:OG	1.89	0.56
4:B:109:ILE:HG13	4:B:149:ALA:HB2	1.88	0.56
4:B:199:GLU:HG2	4:B:201:TRP:HD1	1.70	0.56
4:B:381:ALA:C	4:B:383:ALA:H	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:550:LEU:HD11	4:B:695:ALA:HB2	1.88	0.56
4:B:804:ILE:HA	7:B:3072:HOH:O	2.04	0.56
4:C:161:HIS:C	4:C:163:LYS:N	2.62	0.56
4:C:452:ILE:HG13	4:C:456:GLY:HA3	1.86	0.56
4:C:485:ASN:O	4:C:489:ILE:HG13	2.06	0.56
4:C:711:LYS:HG2	4:C:717:GLU:O	2.06	0.56
4:D:199:GLU:OE2	4:D:202:SER:HB2	2.04	0.56
4:D:824:LEU:O	4:D:828:VAL:HG22	2.06	0.56
1:K:11:DA:H2'	1:K:12:DT:H73	1.88	0.56
4:A:316:VAL:HG13	4:A:792:ARG:NE	2.20	0.56
4:A:534:LEU:HD23	4:A:534:LEU:N	2.19	0.56
4:B:86:ASN:HB3	7:B:3090:HOH:O	2.04	0.56
4:B:112:GLU:CD	4:B:112:GLU:N	2.63	0.56
4:B:173:ARG:NH1	4:B:182:PHE:HD1	2.03	0.56
4:B:478:ARG:O	4:B:481:PHE:HB3	2.06	0.56
4:B:580:GLU:O	4:B:581:ILE:C	2.47	0.56
4:C:278:TRP:CZ3	4:C:284:GLY:HA3	2.41	0.56
4:C:423:ARG:CD	4:C:781:ASN:ND2	2.68	0.56
4:C:882:PHE:HD1	4:C:882:PHE:N	2.02	0.56
4:D:6:ILE:C	4:D:8:LYS:H	2.13	0.56
4:D:421:ASP:O	4:D:421:ASP:OD1	2.24	0.56
4:D:486:HIS:O	4:D:487:GLU:C	2.47	0.56
4:D:849:PHE:O	4:D:850:ALA:C	2.48	0.56
4:A:80:LYS:CE	4:A:224:THR:HG22	2.36	0.56
4:A:656:GLN:N	4:A:657:PRO:HD2	2.21	0.56
4:B:89:PHE:CZ	4:B:106:LEU:O	2.58	0.56
4:B:620:TRP:O	4:B:623:TYR:HB3	2.05	0.56
4:B:639:TYR:C	7:B:3018:HOH:O	2.48	0.56
4:B:730:PRO:HD2	4:B:786:GLN:HE21	1.69	0.56
4:B:746:ARG:NH2	4:B:753:GLY:HA2	2.21	0.56
4:B:779:ALA:O	4:B:783:VAL:HG22	2.06	0.56
4:B:846:TYR:CD1	4:B:850:ALA:HB2	2.41	0.56
4:C:281:ILE:HG22	4:C:282:THR:N	2.21	0.56
4:C:322:ILE:HG21	4:C:795:VAL:CG1	2.36	0.56
4:D:313:MET:O	4:D:317:TYR:HD2	1.89	0.56
4:D:432:PHE:CZ	4:D:444:LEU:HD11	2.40	0.56
4:D:812:ASP:OD1	4:D:812:ASP:N	2.38	0.56
1:E:9:DA:N6	3:G:1:DG:N2	2.54	0.56
4:A:281:ILE:HG13	4:A:309:GLU:HA	1.88	0.56
4:A:333:LYS:CB	4:A:516:PHE:CD2	2.89	0.56
4:B:157:LEU:O	4:B:158:GLU:C	2.48	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:329:LYS:HG2	4:B:445:THR:O	2.05	0.56
4:B:576:LYS:O	4:B:577:LYS:C	2.49	0.56
4:B:639:TYR:HA	7:B:3018:HOH:O	2.04	0.56
4:B:849:PHE:O	4:B:852:GLN:HB2	2.06	0.56
4:C:205:HIS:C	4:C:207:GLU:N	2.64	0.56
4:C:341:ILE:CD1	4:C:348:PRO:HB3	2.29	0.56
4:C:416:PHE:HB2	4:C:418:TYR:HE1	1.70	0.56
4:C:512:LEU:HD12	4:C:512:LEU:O	2.06	0.56
4:C:532:LEU:HD23	4:C:532:LEU:O	2.06	0.56
4:D:30:GLU:HB3	4:D:34:ARG:HH21	1.70	0.56
3:J:1:DG:H1'	3:J:2:DT:C7	2.36	0.55
4:A:433:ASN:HB2	4:A:434:PRO:HD2	1.88	0.55
4:A:545:HIS:HE1	4:A:787:ASP:HA	1.71	0.55
4:A:843:ALA:O	4:A:844:ASP:C	2.48	0.55
4:B:84:ARG:HD3	4:B:84:ARG:C	2.31	0.55
4:B:505:GLN:N	4:B:505:GLN:CD	2.58	0.55
4:C:116:TYR:OH	4:C:752:LEU:HD22	2.06	0.55
4:C:205:HIS:O	4:C:207:GLU:N	2.39	0.55
4:C:543:ILE:HD13	4:C:689:VAL:HG11	1.88	0.55
4:C:571:TYR:CE2	4:C:631:LYS:HE3	2.42	0.55
4:C:623:TYR:HA	4:C:666:MET:HE2	1.88	0.55
4:C:814:PHE:N	4:C:814:PHE:CD1	2.75	0.55
4:C:840:ASP:O	4:C:841:VAL:C	2.50	0.55
4:D:859:ASP:C	4:D:861:MET:H	2.14	0.55
1:N:12:DT:H5'	4:D:781:ASN:HD21	1.71	0.55
4:A:14:ILE:HD11	4:A:290:GLY:HA2	1.86	0.55
4:A:236:VAL:HB	4:A:239:GLN:HB2	1.88	0.55
4:A:342:THR:HG22	4:A:348:PRO:CG	2.35	0.55
4:A:563:PRO:CB	4:A:878:SER:HA	2.33	0.55
4:A:706:LEU:HD11	4:A:849:PHE:CD2	2.41	0.55
4:A:715:THR:CG2	4:A:717:GLU:HB2	2.36	0.55
4:A:824:LEU:O	4:A:827:ALA:N	2.39	0.55
4:B:407:LYS:CG	4:B:408:PHE:CE2	2.85	0.55
4:B:576:LYS:NZ	7:B:3102:HOH:O	2.39	0.55
4:B:783:VAL:O	4:B:784:HIS:C	2.48	0.55
4:C:16:LEU:HD21	4:C:41:HIS:ND1	2.20	0.55
4:C:50:ARG:NH1	4:C:50:ARG:CG	2.69	0.55
4:C:155:ARG:O	4:C:155:ARG:HG2	2.06	0.55
4:D:744:GLN:HB3	4:D:756:ARG:HB2	1.88	0.55
4:A:292:ARG:N	4:A:293:PRO:HD3	2.21	0.55
4:A:480:LYS:HE3	4:A:484:GLU:CD	2.31	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:514:PHE:O	4:A:515:CYS:C	2.45	0.55
4:A:526:LEU:HD12	4:A:526:LEU:H	1.66	0.55
4:B:71:LYS:N	4:B:72:PRO:CD	2.69	0.55
4:B:182:PHE:O	4:B:186:VAL:HG23	2.06	0.55
4:B:423:ARG:CG	4:B:423:ARG:HH11	2.19	0.55
4:B:473:VAL:HG11	4:B:477:GLU:CB	2.36	0.55
4:B:698:TRP:CZ2	4:B:864:LEU:HG	2.41	0.55
4:B:871:ASN:O	4:B:872:LEU:C	2.49	0.55
4:C:711:LYS:CG	4:C:718:ILE:HA	2.36	0.55
4:D:205:HIS:C	4:D:207:GLU:H	2.14	0.55
4:D:505:GLN:N	4:D:505:GLN:HE21	2.04	0.55
4:D:717:GLU:O	4:D:719:LEU:HD12	2.07	0.55
4:D:772:HIS:O	4:D:775:GLU:N	2.38	0.55
1:E:10:DT:OP2	4:A:645:GLY:HA3	2.05	0.55
1:N:9:DA:H2''	1:N:10:DT:OP1	2.05	0.55
4:A:59:LEU:HD23	4:A:64:VAL:HG22	1.88	0.55
4:A:578:VAL:CG1	4:A:680:LEU:HB3	2.36	0.55
4:A:650:VAL:O	4:A:654:THR:HG22	2.07	0.55
4:A:828:VAL:C	4:A:830:GLU:N	2.61	0.55
4:B:40:GLU:O	4:B:41:HIS:C	2.48	0.55
4:B:291:ARG:CB	7:B:3037:HOH:O	2.51	0.55
4:B:411:HIS:O	4:B:413:ALA:N	2.40	0.55
4:B:478:ARG:O	4:B:479:ILE:C	2.48	0.55
4:B:489:ILE:CG2	4:B:515:CYS:HB3	2.37	0.55
4:B:492:CYS:O	4:B:496:PRO:CD	2.50	0.55
4:D:400:PHE:CZ	4:D:431:MET:HE2	2.41	0.55
1:K:9:DA:N6	3:M:1:DG:N2	2.54	0.55
4:A:685:VAL:C	4:A:687:VAL:H	2.13	0.55
4:A:778:ILE:CG2	4:A:779:ALA:H	2.19	0.55
4:B:308:TYR:HE2	4:B:734:PRO:HG2	1.72	0.55
4:B:780:PRO:CD	4:B:781:ASN:H	2.19	0.55
4:D:817:ILE:HG12	4:D:820:ASP:OD2	2.05	0.55
3:J:1:DG:H4'	3:J:2:DT:H5'	1.87	0.55
4:A:402:LEU:CG	4:A:439:MET:HE1	2.36	0.55
4:A:474:PRO:HB2	4:A:476:PRO:HD2	1.88	0.55
4:A:632:ARG:HG2	7:A:3022:HOH:O	2.06	0.55
4:A:635:MET:HE2	6:A:2000:APC:C8	2.37	0.55
4:B:70:ALA:C	4:B:72:PRO:HD2	2.31	0.55
4:B:588:ASN:O	4:B:614:LYS:HD2	2.06	0.55
4:B:821:ALA:O	4:B:822:ALA:C	2.49	0.55
4:C:395:ARG:HE	4:C:399:GLU:CG	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:826:LYS:HD2	7:D:3041:HOH:O	2.05	0.55
4:A:308:TYR:O	4:A:311:VAL:N	2.35	0.55
4:A:350:GLU:O	7:A:3222:HOH:O	2.18	0.55
4:A:401:MET:N	4:A:401:MET:SD	2.79	0.55
4:A:669:GLN:HG2	4:A:672:GLN:NE2	2.20	0.55
4:A:797:TRP:CZ2	4:A:801:LYS:HG3	2.40	0.55
4:B:137:VAL:HG12	4:B:217:ILE:CD1	2.34	0.55
4:B:275:PRO:CD	7:B:3116:HOH:O	2.48	0.55
4:B:285:GLY:HA2	4:B:324:GLN:HE22	1.71	0.55
4:B:426:VAL:C	4:B:427:TYR:HD1	2.14	0.55
4:B:854:HIS:HD1	4:B:855:GLU:H	1.55	0.55
4:C:173:ARG:NH2	4:C:182:PHE:HB2	2.22	0.55
4:C:291:ARG:C	4:C:293:PRO:HD3	2.31	0.55
4:C:582:LEU:HD11	4:C:625:VAL:HG21	1.88	0.55
4:C:807:PHE:N	4:C:807:PHE:CD1	2.74	0.55
4:D:277:PRO:HA	7:D:3029:HOH:O	2.06	0.55
4:D:286:TYR:CZ	4:D:417:PRO:HG3	2.41	0.55
4:A:463:HIS:O	4:A:464:GLY:C	2.48	0.55
4:A:707:ALA:O	4:A:708:ALA:O	2.25	0.55
4:B:569:ASP:O	4:B:569:ASP:OD1	2.24	0.55
4:B:777:GLY:C	4:B:780:PRO:HD2	2.31	0.55
4:C:744:GLN:HA	4:C:756:ARG:HD3	1.89	0.55
4:D:21:PHE:C	4:D:23:THR:N	2.61	0.55
4:D:70:ALA:C	4:D:72:PRO:HD2	2.32	0.55
4:D:743:ILE:O	4:D:756:ARG:NH2	2.40	0.55
4:A:317:TYR:O	4:A:321:ASN:ND2	2.33	0.55
4:A:619:GLN:O	4:A:623:TYR:N	2.37	0.55
4:A:630:THR:O	4:A:631:LYS:O	2.25	0.55
4:A:779:ALA:HB3	4:A:780:PRO:CD	2.37	0.55
4:A:829:ARG:O	4:A:833:VAL:HG23	2.06	0.55
4:B:76:THR:CG2	7:B:3212:HOH:O	2.54	0.55
4:C:40:GLU:OE2	4:C:286:TYR:CD1	2.58	0.55
4:C:474:PRO:C	4:C:476:PRO:HD2	2.32	0.55
4:C:684:SER:O	4:C:687:VAL:HG22	2.07	0.55
4:C:770:ASP:OD1	4:C:770:ASP:O	2.25	0.55
4:D:448:LYS:CD	4:D:806:SER:HB3	2.36	0.55
4:D:652:GLU:O	4:D:657:PRO:HD3	2.06	0.55
4:D:857:GLN:C	4:D:859:ASP:H	2.15	0.55
4:A:14:ILE:N	4:A:14:ILE:CD1	2.69	0.55
4:A:42:GLU:O	4:A:43:SER:C	2.50	0.55
4:A:287:TRP:O	4:A:288:ALA:O	2.25	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:629:VAL:HG11	4:A:677:MET:HE3	1.89	0.55
4:B:479:ILE:O	4:B:480:LYS:C	2.49	0.55
4:B:803:GLY:O	4:B:804:ILE:O	2.25	0.55
4:C:46:MET:HE1	4:C:269:GLN:OE1	2.07	0.55
4:C:106:LEU:HG	4:C:212:VAL:HG13	1.89	0.55
4:C:579:ASN:OD1	4:C:582:LEU:HD12	2.07	0.55
4:C:737:GLN:HE22	4:C:777:GLY:C	2.14	0.55
4:D:311:VAL:CG1	4:D:312:TYR:N	2.70	0.55
4:D:816:THR:HG22	4:D:817:ILE:H	1.71	0.55
1:E:5:DA:H2	3:G:7:DT:O2	1.89	0.54
1:E:9:DA:C2	4:A:644:PHE:CD1	2.95	0.54
4:A:60:LYS:NZ	4:A:61:ALA:HB2	2.22	0.54
4:A:177:VAL:HB	7:A:3038:HOH:O	2.06	0.54
4:B:419:ASN:O	4:B:426:VAL:HA	2.07	0.54
4:B:587:ILE:HG22	4:B:588:ASN:HD22	1.71	0.54
4:C:278:TRP:CD2	4:C:284:GLY:HA3	2.42	0.54
4:C:306:MET:O	4:C:307:ARG:C	2.51	0.54
4:C:448:LYS:CE	4:C:806:SER:OG	2.54	0.54
4:D:241:SER:O	4:D:243:THR:HG23	2.06	0.54
4:D:794:THR:O	4:D:795:VAL:C	2.49	0.54
4:A:13:ASP:HB3	4:A:14:ILE:HD12	1.88	0.54
4:A:273:VAL:O	4:A:274:PRO:C	2.50	0.54
4:B:266:PRO:HG2	4:B:268:PHE:CE1	2.41	0.54
4:B:532:LEU:HG	4:B:533:PRO:HD2	1.90	0.54
4:C:45:GLU:O	4:C:48:GLU:HB3	2.07	0.54
4:C:728:VAL:HG22	4:C:734:PRO:HB3	1.89	0.54
4:C:777:GLY:O	4:C:781:ASN:OD1	2.25	0.54
4:C:814:PHE:CE1	4:C:883:ALA:CB	2.91	0.54
4:D:155:ARG:CA	4:D:163:LYS:HE3	2.37	0.54
4:D:508:PRO:O	4:D:509:PHE:C	2.48	0.54
4:D:558:ALA:HB1	4:D:570:ILE:HD13	1.88	0.54
1:K:12:DT:H5''	4:C:422:TRP:CH2	2.42	0.54
4:A:641:SER:HB2	4:A:646:PHE:HE1	1.73	0.54
4:B:27:HIS:HD2	7:B:3169:HOH:O	1.88	0.54
4:C:84:ARG:HB2	4:C:223:SER:HB3	1.89	0.54
4:C:278:TRP:CD1	4:C:320:ILE:HG22	2.43	0.54
4:C:334:VAL:CG2	4:C:513:ALA:HB2	2.29	0.54
4:C:710:VAL:HG13	4:C:710:VAL:O	2.07	0.54
4:D:538:GLY:O	4:D:539:SER:C	2.49	0.54
4:D:560:ASN:C	4:D:881:ALA:HB2	2.30	0.54
1:H:12:DT:C2'	1:H:13:DC:H6	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:DC:H2''	7:P:1110:HOH:O	2.06	0.54
4:A:6:ILE:HD11	4:A:259:GLY:C	2.33	0.54
4:A:401:MET:C	4:A:403:GLU:H	2.14	0.54
4:A:590:THR:OG1	4:A:613:THR:OG1	2.20	0.54
4:B:334:VAL:HG12	4:B:443:LEU:HD23	1.88	0.54
4:B:423:ARG:NH2	4:B:784:HIS:ND1	2.53	0.54
4:B:454:LYS:HG3	4:B:455:GLU:H	1.72	0.54
4:B:639:TYR:CA	7:B:3018:HOH:O	2.55	0.54
4:C:403:GLU:N	7:C:3123:HOH:O	2.39	0.54
4:C:508:PRO:HB2	4:C:509:PHE:HD2	1.71	0.54
4:C:509:PHE:HD2	4:C:509:PHE:H	1.54	0.54
4:C:576:LYS:O	4:C:580:GLU:HG3	2.07	0.54
4:D:577:LYS:O	4:D:581:ILE:HG13	2.07	0.54
4:D:632:ARG:HH22	6:D:2003:APC:H5'2	1.72	0.54
4:D:685:VAL:C	4:D:687:VAL:H	2.15	0.54
2:I:8:U:O3'	4:B:812:ASP:OD2	2.24	0.54
4:A:11:PHE:HB3	4:A:41:HIS:HE1	1.72	0.54
4:A:316:VAL:HG13	4:A:792:ARG:HD2	1.89	0.54
4:A:543:ILE:O	4:A:544:GLN:C	2.50	0.54
4:B:55:PHE:CD2	4:B:55:PHE:C	2.84	0.54
4:B:181:ALA:HA	4:B:184:GLN:NE2	2.22	0.54
4:B:469:GLY:C	4:B:471:ASP:H	2.15	0.54
4:B:472:LYS:NZ	6:B:2001:APC:O1G	2.31	0.54
4:B:573:ILE:HD13	7:B:3102:HOH:O	2.07	0.54
4:B:810:ILE:O	4:B:813:SER:HB2	2.07	0.54
4:C:793:LYS:NZ	4:C:835:THR:OG1	2.32	0.54
4:C:833:VAL:HG22	4:C:872:LEU:O	2.08	0.54
4:D:47:GLY:O	4:D:50:ARG:HB3	2.08	0.54
4:D:446:LEU:HG	4:D:533:PRO:HD3	1.90	0.54
4:A:204:TRP:HH2	4:A:212:VAL:HG21	1.67	0.54
4:A:555:GLY:O	4:A:558:ALA:HB3	2.08	0.54
4:A:620:TRP:CE2	4:A:677:MET:HB2	2.43	0.54
4:A:669:GLN:O	4:A:672:GLN:N	2.41	0.54
4:A:720:ARG:HH21	4:A:857:GLN:NE2	2.06	0.54
4:B:473:VAL:HG11	4:B:477:GLU:HB2	1.88	0.54
4:C:656:GLN:HA	4:C:656:GLN:HE21	1.72	0.54
4:D:50:ARG:NH1	4:D:267:MET:HG2	2.23	0.54
4:D:258:ALA:O	4:D:259:GLY:O	2.26	0.54
4:D:512:LEU:CA	4:D:515:CYS:SG	2.86	0.54
4:D:817:ILE:HB	4:D:818:PRO:CD	2.38	0.54
4:A:88:TRP:CE3	4:A:91:GLU:OE1	2.61	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:120:LYS:HG3	4:A:752:LEU:HD21	1.90	0.54
4:A:275:PRO:O	4:A:277:PRO:HD3	2.07	0.54
4:A:460:LEU:O	4:A:461:LYS:C	2.50	0.54
4:A:471:ASP:O	4:A:472:LYS:HG3	2.08	0.54
4:A:474:PRO:O	4:A:477:GLU:HB2	2.07	0.54
4:A:772:HIS:O	4:A:773:LYS:C	2.50	0.54
4:B:211:HIS:O	4:B:214:VAL:HG23	2.08	0.54
4:B:297:VAL:HG12	4:B:299:THR:HG22	1.88	0.54
4:B:512:LEU:C	4:B:514:PHE:N	2.64	0.54
4:B:790:HIS:HE1	4:B:831:THR:CG2	2.20	0.54
4:B:814:PHE:CD1	4:B:814:PHE:N	2.76	0.54
4:C:6:ILE:HD13	7:C:3031:HOH:O	2.06	0.54
4:C:273:VAL:HG23	4:C:274:PRO:O	2.08	0.54
4:C:726:HIS:CD2	4:C:736:TRP:CE2	2.96	0.54
4:D:19:ILE:CD1	4:D:20:PRO:HD2	2.36	0.54
4:D:744:GLN:HE21	4:D:756:ARG:H	1.56	0.54
4:A:216:CYS:O	4:A:219:MET:N	2.40	0.54
4:A:320:ILE:HD11	4:A:420:MET:HE2	1.90	0.54
4:A:395:ARG:O	4:A:399:GLU:HG3	2.08	0.54
4:A:401:MET:C	4:A:403:GLU:N	2.63	0.54
4:A:428:ALA:H	4:A:435:GLN:NE2	2.04	0.54
4:A:636:THR:HG21	6:A:2000:APC:N6	2.23	0.54
6:A:2000:APC:C4'	7:A:3238:HOH:O	2.41	0.54
4:B:823:ASN:O	4:B:825:PHE:N	2.40	0.54
4:B:882:PHE:HE2	7:B:3089:HOH:O	1.90	0.54
4:C:474:PRO:CB	4:C:476:PRO:HD2	2.37	0.54
4:D:275:PRO:HB2	4:D:324:GLN:CD	2.33	0.54
4:D:646:PHE:O	4:D:647:ARG:C	2.51	0.54
4:D:882:PHE:O	4:D:883:ALA:CB	2.56	0.54
1:H:15:DC:H2''	1:H:16:DC:H5'	1.89	0.54
4:A:44:TYR:CD2	4:A:266:PRO:HB3	2.43	0.54
4:A:485:ASN:HD22	4:A:488:ASN:ND2	2.06	0.54
4:A:654:THR:O	4:A:658:ALA:HB2	2.07	0.54
4:A:810:ILE:O	4:A:810:ILE:HG22	2.07	0.54
4:B:201:TRP:CD2	7:B:3009:HOH:O	2.61	0.54
4:B:388:ASP:O	4:B:389:LYS:C	2.51	0.54
4:B:754:GLN:O	4:B:755:PHE:O	2.25	0.54
4:B:850:ALA:C	4:B:852:GLN:N	2.64	0.54
4:C:120:LYS:HD2	4:C:751:PHE:HE2	1.72	0.54
4:C:199:GLU:HB2	7:C:3075:HOH:O	2.08	0.54
4:C:312:TYR:CE1	4:C:314:PRO:HG3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:457:TYR:CE1	4:C:521:VAL:CG1	2.87	0.54
4:D:201:TRP:O	4:D:204:TRP:HB2	2.07	0.54
4:D:259:GLY:O	4:D:260:ALA:C	2.50	0.54
4:D:507:SER:O	4:D:511:PHE:N	2.41	0.54
1:H:12:DT:H2''	1:H:13:DC:H5'	1.89	0.54
3:M:8:DC:H2''	3:M:9:DC:OP2	2.07	0.54
4:A:190:MET:HE3	7:A:3103:HOH:O	2.08	0.54
4:A:573:ILE:O	4:A:576:LYS:HB2	2.07	0.54
4:A:656:GLN:O	4:A:658:ALA:N	2.41	0.54
4:B:61:ALA:C	4:B:63:GLU:H	2.14	0.54
4:B:111:PRO:HG2	4:B:112:GLU:CD	2.33	0.54
4:B:333:LYS:O	4:B:337:VAL:CG2	2.54	0.54
4:B:703:ALA:O	4:B:704:LYS:C	2.50	0.54
4:C:89:PHE:HZ	4:C:106:LEU:O	1.91	0.54
4:C:490:MET:HA	4:C:490:MET:HE3	1.88	0.54
4:C:846:TYR:HA	4:C:849:PHE:CE1	2.42	0.54
4:D:530:CYS:HB3	4:D:818:PRO:HG2	1.90	0.54
4:D:551:ARG:HH11	4:D:551:ARG:HG3	1.73	0.54
4:D:594:VAL:HA	4:D:609:VAL:HA	1.90	0.54
4:D:829:ARG:O	4:D:833:VAL:HG23	2.08	0.54
4:D:840:ASP:C	4:D:842:LEU:N	2.65	0.54
2:F:6:G:O2'	2:F:7:A:H5'	2.07	0.53
4:A:36:GLN:HG3	4:A:273:VAL:HG22	1.91	0.53
4:A:459:TRP:HZ3	4:A:475:PHE:CE1	2.25	0.53
4:A:544:GLN:OE1	4:A:559:VAL:CG2	2.56	0.53
4:A:648:GLN:O	4:A:652:GLU:HG2	2.08	0.53
4:A:755:PHE:N	4:A:755:PHE:CD1	2.77	0.53
4:A:882:PHE:HD1	4:A:882:PHE:N	2.05	0.53
4:B:163:LYS:HZ2	4:B:166:VAL:HB	1.70	0.53
4:B:846:TYR:O	4:B:847:ASP:C	2.50	0.53
4:C:291:ARG:CG	7:C:3066:HOH:O	2.56	0.53
4:C:539:SER:HB2	4:C:544:GLN:OE1	2.08	0.53
4:C:706:LEU:HD22	4:C:725:VAL:CG2	2.36	0.53
4:D:264:ILE:HG22	4:D:292:ARG:HG2	1.89	0.53
4:D:508:PRO:O	4:D:510:CYS:N	2.41	0.53
1:N:11:DA:C5	4:D:639:TYR:CE2	2.96	0.53
4:A:78:LEU:O	4:A:82:ILE:HG13	2.08	0.53
4:A:292:ARG:HG3	4:A:292:ARG:O	2.09	0.53
4:A:316:VAL:HG13	4:A:792:ARG:CD	2.38	0.53
4:A:594:VAL:HA	4:A:609:VAL:HA	1.89	0.53
4:B:76:THR:HG22	7:B:3212:HOH:O	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:508:PRO:O	4:B:509:PHE:C	2.49	0.53
4:B:730:PRO:HD3	4:B:786:GLN:NE2	2.24	0.53
4:B:816:THR:HG21	4:B:820:ASP:CB	2.38	0.53
4:B:843:ALA:HA	4:B:864:LEU:CD2	2.38	0.53
4:C:705:LEU:HD21	4:C:860:LYS:HE3	1.90	0.53
4:D:19:ILE:HG21	7:D:3014:HOH:O	2.08	0.53
4:D:274:PRO:HB3	4:D:325:ASN:OD1	2.07	0.53
4:D:523:HIS:O	4:D:524:HIS:ND1	2.41	0.53
4:A:19:ILE:HG22	7:A:3120:HOH:O	2.04	0.53
4:A:105:PHE:O	4:A:107:GLN:N	2.41	0.53
4:A:236:VAL:HG11	4:A:239:GLN:HG3	1.89	0.53
4:B:201:TRP:CG	7:B:3009:HOH:O	2.60	0.53
4:B:263:GLY:C	7:B:3137:HOH:O	2.51	0.53
4:B:710:VAL:HG13	4:B:710:VAL:O	2.08	0.53
4:C:739:TYR:HD2	4:C:774:GLN:HA	1.73	0.53
4:D:14:ILE:HG21	4:D:288:ALA:HB1	1.89	0.53
4:D:448:LYS:HZ1	4:D:806:SER:HA	1.73	0.53
4:A:328:TRP:HA	4:A:446:LEU:HA	1.91	0.53
4:A:333:LYS:HB2	4:A:516:PHE:CD2	2.43	0.53
4:A:546:PHE:CZ	4:A:783:VAL:CG2	2.88	0.53
4:A:651:LEU:CD1	4:A:656:GLN:NE2	2.72	0.53
4:A:801:LYS:C	4:A:801:LYS:CD	2.80	0.53
4:A:861:MET:HE3	4:A:862:PRO:O	2.08	0.53
4:B:69:ALA:O	4:B:72:PRO:HD2	2.08	0.53
4:B:465:ALA:HB1	4:B:470:VAL:HB	1.89	0.53
4:B:633:SER:HB3	4:B:646:PHE:CD1	2.43	0.53
4:C:461:LYS:O	4:C:462:ILE:C	2.49	0.53
4:C:826:LYS:O	4:C:830:GLU:HG3	2.08	0.53
4:C:840:ASP:O	4:C:843:ALA:N	2.41	0.53
4:D:419:ASN:HD22	4:D:419:ASN:N	2.06	0.53
2:I:5:C:C2	2:I:6:G:C8	2.96	0.53
4:A:11:PHE:CZ	4:A:44:TYR:HB3	2.43	0.53
4:A:229:LEU:HD13	4:A:244:ILE:HD13	1.90	0.53
4:A:340:VAL:O	4:A:341:ILE:C	2.49	0.53
4:A:423:ARG:HH21	4:A:784:HIS:CB	2.22	0.53
4:A:643:GLU:HG3	4:A:682:TRP:CB	2.39	0.53
4:A:670:PRO:O	4:A:671:ASN:C	2.52	0.53
4:B:427:TYR:HE1	4:B:811:HIS:NE2	2.06	0.53
4:B:670:PRO:O	4:B:671:ASN:C	2.48	0.53
4:C:88:TRP:O	4:C:92:VAL:HG23	2.07	0.53
4:C:452:ILE:HG23	4:C:453:GLY:H	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:719:LEU:N	4:C:719:LEU:HD12	2.24	0.53
4:C:830:GLU:HG2	4:C:876:LEU:CD2	2.38	0.53
4:D:62:GLY:C	4:D:64:VAL:H	2.17	0.53
4:D:677:MET:O	4:D:680:LEU:HB2	2.08	0.53
4:D:810:ILE:HB	4:D:813:SER:CB	2.39	0.53
7:I:777:HOH:O	4:B:386:ARG:HD2	2.02	0.53
4:A:786:GLN:C	4:A:788:GLY:N	2.63	0.53
4:B:50:ARG:CG	4:B:50:ARG:HH11	2.22	0.53
4:B:99:ARG:NH2	7:B:3046:HOH:O	2.40	0.53
4:B:556:GLY:C	4:B:558:ALA:H	2.17	0.53
4:B:696:MET:O	4:B:700:LYS:HB2	2.08	0.53
4:B:795:VAL:O	4:B:796:VAL:O	2.27	0.53
4:D:161:HIS:C	4:D:163:LYS:H	2.17	0.53
4:D:338:ALA:C	4:D:340:VAL:H	2.16	0.53
4:D:537:ASP:O	4:D:882:PHE:HB2	2.08	0.53
4:D:619:GLN:HG2	4:D:666:MET:O	2.09	0.53
4:A:134:VAL:O	4:A:134:VAL:HG22	2.08	0.53
4:A:165:ASN:OD1	4:A:165:ASN:N	2.35	0.53
4:A:457:TYR:HE1	4:A:521:VAL:HG11	1.70	0.53
4:A:729:THR:OG1	4:A:733:PHE:HB3	2.08	0.53
4:B:278:TRP:N	4:B:321:ASN:OD1	2.27	0.53
4:C:14:ILE:HA	7:C:3014:HOH:O	2.09	0.53
4:C:118:THR:HG23	4:C:141:ILE:HD13	1.90	0.53
4:C:635:MET:HE1	6:C:2002:APC:H3A1	1.90	0.53
4:D:490:MET:C	4:D:493:ALA:HB3	2.33	0.53
4:D:631:LYS:O	4:D:632:ARG:C	2.51	0.53
4:D:754:GLN:O	4:D:755:PHE:O	2.27	0.53
1:H:10:DT:H4'	4:B:639:TYR:O	2.08	0.53
2:L:4:G:H1'	4:C:389:LYS:NZ	2.23	0.53
1:N:10:DT:H3	6:D:2003:APC:HN62	1.56	0.53
4:A:21:PHE:C	4:A:23:THR:N	2.64	0.53
4:A:30:GLU:HB2	7:A:3035:HOH:O	2.09	0.53
4:A:136:ALA:O	4:A:139:SER:HB3	2.08	0.53
4:A:617:ALA:O	4:A:618:GLY:C	2.52	0.53
4:A:680:LEU:O	4:A:681:ILE:C	2.50	0.53
4:B:21:PHE:O	4:B:21:PHE:HD1	1.91	0.53
4:B:68:ALA:HB3	4:B:261:LEU:HD21	1.91	0.53
4:C:80:LYS:HD2	4:C:224:THR:CG2	2.39	0.53
4:C:90:GLU:OE2	4:C:93:LYS:HD2	2.08	0.53
4:C:472:LYS:HA	4:C:567:VAL:HG11	1.89	0.53
4:C:592:ASN:O	4:C:593:GLU:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:849:PHE:O	4:C:852:GLN:N	2.42	0.53
4:D:230:HIS:O	4:D:230:HIS:ND1	2.41	0.53
4:D:261:LEU:C	4:D:263:GLY:N	2.66	0.53
1:H:13:DC:H4'	4:B:427:TYR:CE2	2.44	0.53
4:A:446:LEU:HB2	4:A:531:SER:O	2.09	0.53
4:B:407:LYS:HE2	4:B:408:PHE:CE2	2.44	0.53
4:B:616:LEU:C	4:B:618:GLY:N	2.66	0.53
4:B:737:GLN:NE2	4:B:739:TYR:HE2	1.99	0.53
4:C:96:ARG:HG2	4:C:96:ARG:HH11	1.74	0.53
4:C:689:VAL:O	4:C:690:VAL:C	2.52	0.53
4:C:711:LYS:HG2	4:C:717:GLU:C	2.34	0.53
4:C:737:GLN:OE1	4:C:778:ILE:HA	2.08	0.53
4:D:428:ALA:N	4:D:435:GLN:NE2	2.55	0.53
4:D:854:HIS:CG	4:D:855:GLU:N	2.76	0.53
3:M:5:DA:H2''	3:M:6:DT:C7	2.39	0.53
4:A:502:TRP:O	4:A:505:GLN:HB2	2.09	0.53
4:B:416:PHE:HE1	4:B:432:PHE:O	1.92	0.53
4:B:423:ARG:NH1	4:B:784:HIS:CB	2.71	0.53
4:B:793:LYS:HG3	7:B:3181:HOH:O	2.08	0.53
4:C:82:ILE:CD1	4:C:112:GLU:HA	2.39	0.53
4:C:97:GLY:O	4:C:98:LYS:C	2.52	0.53
4:C:316:VAL:HG13	4:C:420:MET:HE1	1.90	0.53
4:C:509:PHE:N	4:C:509:PHE:CD2	2.76	0.53
4:C:512:LEU:O	4:C:516:PHE:HD1	1.92	0.53
4:C:698:TRP:CZ2	4:C:864:LEU:HG	2.44	0.53
4:D:32:LEU:H	4:D:32:LEU:CD1	2.08	0.53
4:D:100:PRO:HG2	4:D:103:PHE:HB3	1.90	0.53
4:D:349:VAL:O	4:D:349:VAL:HG12	2.09	0.53
4:D:442:GLY:C	4:D:444:LEU:H	2.17	0.53
4:D:570:ILE:HA	4:D:573:ILE:HG22	1.91	0.53
4:D:571:TYR:HD1	4:D:631:LYS:HA	1.72	0.53
4:D:635:MET:HE1	6:D:2003:APC:H3A1	1.91	0.53
4:D:817:ILE:HB	4:D:818:PRO:HD2	1.90	0.53
4:D:849:PHE:O	4:D:852:GLN:N	2.34	0.53
3:J:4:DG:H1'	3:J:5:DA:C8	2.44	0.52
4:A:109:ILE:CG1	4:A:149:ALA:HB2	2.39	0.52
4:B:11:PHE:CE1	4:B:44:TYR:HB3	2.43	0.52
4:B:643:GLU:C	4:B:645:GLY:N	2.66	0.52
4:B:663:LYS:HG2	4:B:664:GLY:N	2.21	0.52
4:B:669:GLN:CB	4:B:672:GLN:HE21	2.22	0.52
4:C:158:GLU:OE1	4:C:195:LEU:HB3	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:871:ASN:ND2	4:C:873:ARG:HB2	2.24	0.52
4:D:233:ASN:HD22	4:D:239:GLN:HE21	1.56	0.52
4:D:543:ILE:HG21	4:D:689:VAL:HG11	1.91	0.52
4:D:744:GLN:CA	4:D:756:ARG:CZ	2.85	0.52
2:O:2:C:H5	7:O:443:HOH:O	1.92	0.52
4:A:569:ASP:O	4:A:573:ILE:HG22	2.08	0.52
4:A:647:ARG:O	4:A:648:GLN:C	2.53	0.52
4:A:664:GLY:HA2	4:A:667:PHE:CD2	2.39	0.52
4:A:727:TRP:CE2	4:A:735:VAL:CG1	2.88	0.52
4:B:5:ASN:HD21	4:B:7:ALA:C	2.17	0.52
4:B:307:ARG:HB3	4:B:736:TRP:CZ3	2.44	0.52
4:B:486:HIS:HE1	4:B:490:MET:HG3	1.73	0.52
4:B:525:GLY:C	4:B:527:SER:N	2.66	0.52
4:B:790:HIS:C	4:B:790:HIS:ND1	2.67	0.52
4:C:19:ILE:HG23	4:C:20:PRO:N	2.23	0.52
4:C:36:GLN:HG3	4:C:273:VAL:CG2	2.38	0.52
4:C:54:MET:SD	4:C:54:MET:C	2.93	0.52
4:C:320:ILE:O	4:C:324:GLN:HB2	2.09	0.52
4:C:515:CYS:O	4:C:516:PHE:C	2.51	0.52
4:C:845:PHE:O	4:C:848:GLN:N	2.41	0.52
4:D:114:VAL:HA	4:D:117:ILE:HD12	1.91	0.52
4:D:557:ARG:NH2	7:D:3021:HOH:O	2.43	0.52
4:D:739:TYR:HD2	4:D:774:GLN:HA	1.74	0.52
3:J:5:DA:H2''	3:J:6:DT:H72	1.91	0.52
1:N:6:DT:C6	1:N:6:DT:H5'	2.44	0.52
4:A:379:ARG:HD3	4:A:660:ASP:CG	2.34	0.52
4:A:755:PHE:N	4:A:755:PHE:HD1	2.07	0.52
4:B:122:THR:HG22	4:B:123:LEU:N	2.24	0.52
4:B:272:VAL:HG11	4:B:411:HIS:HD2	1.73	0.52
4:C:322:ILE:CG2	4:C:795:VAL:CG1	2.88	0.52
4:C:474:PRO:O	4:C:478:ARG:HG3	2.09	0.52
4:C:551:ARG:HD3	4:C:872:LEU:HD21	1.91	0.52
4:C:788:GLY:O	4:C:792:ARG:NH1	2.42	0.52
4:C:830:GLU:HG2	4:C:876:LEU:HD21	1.91	0.52
4:D:154:ILE:O	4:D:159:ALA:HB3	2.09	0.52
4:D:401:MET:HE3	4:D:440:THR:HG21	1.91	0.52
4:D:731:ASP:OD1	4:D:792:ARG:NH2	2.42	0.52
4:D:751:PHE:HB3	4:D:752:LEU:HD12	1.90	0.52
1:H:12:DT:C5'	4:B:423:ARG:HE	2.22	0.52
4:A:269:GLN:O	4:A:430:SER:HB2	2.10	0.52
4:A:518:TYR:CD1	4:A:518:TYR:C	2.87	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:544:GLN:HG2	4:A:559:VAL:CG2	2.30	0.52
4:A:551:ARG:O	4:A:868:GLY:HA3	2.08	0.52
4:B:19:ILE:HG23	4:B:20:PRO:CD	2.39	0.52
4:C:118:THR:O	4:C:122:THR:OG1	2.20	0.52
4:C:278:TRP:CD1	4:C:320:ILE:CG2	2.92	0.52
4:C:315:GLU:OE1	4:C:796:VAL:HG11	2.08	0.52
4:C:316:VAL:O	4:C:317:TYR:C	2.50	0.52
4:C:770:ASP:O	4:C:772:HIS:N	2.42	0.52
4:C:794:THR:OG1	4:C:831:THR:HG21	2.09	0.52
4:C:843:ALA:HA	4:C:864:LEU:HD21	1.92	0.52
4:D:207:GLU:O	4:D:211:HIS:CE1	2.63	0.52
4:D:384:VAL:HA	7:D:3158:HOH:O	2.10	0.52
4:D:631:LYS:HE2	4:D:635:MET:HE1	1.92	0.52
4:D:833:VAL:O	4:D:837:GLU:HG3	2.09	0.52
1:H:18:DC:H2''	4:B:63:GLU:OE1	2.10	0.52
2:O:6:G:O2'	2:O:7:A:H5'	2.09	0.52
4:A:403:GLU:O	4:A:404:GLN:C	2.52	0.52
4:A:437:ASN:O	4:A:438:ASP:C	2.46	0.52
4:A:476:PRO:HG2	4:A:477:GLU:H	1.74	0.52
4:A:546:PHE:HE2	4:A:696:MET:CG	2.22	0.52
4:A:694:GLU:OE1	4:A:865:PRO:HB3	2.10	0.52
4:B:231:ARG:HG2	4:B:234:ALA:CB	2.35	0.52
4:B:327:ALA:HB1	4:B:447:ALA:HB3	1.91	0.52
4:B:407:LYS:HG2	4:B:408:PHE:HE2	1.66	0.52
4:B:430:SER:O	4:B:432:PHE:N	2.43	0.52
4:B:569:ASP:O	4:B:572:GLY:N	2.41	0.52
4:B:810:ILE:N	4:B:813:SER:HB3	2.25	0.52
4:C:116:TYR:O	4:C:119:ILE:HG12	2.10	0.52
4:C:325:ASN:O	4:C:415:TRP:CD1	2.62	0.52
4:C:433:ASN:N	7:C:3164:HOH:O	2.41	0.52
4:D:116:TYR:CE2	4:D:752:LEU:HD22	2.44	0.52
4:D:564:SER:C	7:D:3040:HOH:O	2.51	0.52
3:G:5:DA:N6	7:G:73:HOH:O	2.43	0.52
1:K:14:DG:H3'	7:K:520:HOH:O	2.08	0.52
4:A:34:ARG:NH2	7:A:3166:HOH:O	2.43	0.52
4:A:42:GLU:O	4:A:45:GLU:N	2.42	0.52
4:A:422:TRP:CD1	4:A:423:ARG:HG3	2.45	0.52
4:A:433:ASN:OD1	4:A:435:GLN:N	2.41	0.52
4:A:545:HIS:O	4:A:546:PHE:C	2.52	0.52
4:B:58:GLN:NE2	7:B:3136:HOH:O	2.41	0.52
4:B:278:TRP:CD2	4:B:284:GLY:HA3	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:473:VAL:HG12	4:B:477:GLU:HB2	1.91	0.52
4:B:720:ARG:NH1	4:B:721:LYS:O	2.43	0.52
4:C:591:ASP:OD1	7:C:3122:HOH:O	2.19	0.52
4:C:777:GLY:C	4:C:780:PRO:HD2	2.35	0.52
4:C:794:THR:O	4:C:795:VAL:C	2.50	0.52
4:D:232:GLN:HB2	4:D:241:SER:O	2.09	0.52
4:D:322:ILE:HG21	4:D:795:VAL:HG12	1.92	0.52
4:D:506:ASP:O	4:D:508:PRO:HD2	2.09	0.52
4:A:16:LEU:HB3	4:A:37:LEU:HB3	1.92	0.52
4:A:134:VAL:HA	4:A:137:VAL:HB	1.92	0.52
4:A:299:THR:HG22	4:A:300:HIS:H	1.75	0.52
4:A:505:GLN:O	4:A:506:ASP:C	2.51	0.52
4:A:794:THR:O	4:A:795:VAL:C	2.51	0.52
4:B:330:ILE:HD11	4:B:405:ALA:HA	1.90	0.52
4:B:512:LEU:O	4:B:513:ALA:C	2.49	0.52
4:B:663:LYS:HE2	4:B:666:MET:HE1	1.91	0.52
4:B:699:LEU:HD11	4:B:842:LEU:HD11	1.90	0.52
4:B:872:LEU:O	4:B:874:ASP:N	2.43	0.52
4:B:882:PHE:O	4:B:883:ALA:HB3	2.09	0.52
4:D:95:LYS:HB2	4:D:95:LYS:HZ2	1.75	0.52
3:G:4:DG:H2''	3:G:5:DA:C8	2.45	0.52
1:N:11:DA:H2''	1:N:12:DT:O5'	2.10	0.52
4:A:141:ILE:CG2	4:A:145:ILE:HD11	2.39	0.52
4:A:596:THR:HG23	4:A:606:SER:O	2.09	0.52
4:A:627:ARG:NH2	6:A:2000:APC:O2G	2.43	0.52
4:B:276:LYS:HB2	4:B:287:TRP:CD2	2.45	0.52
4:B:422:TRP:NE1	4:B:781:ASN:ND2	2.57	0.52
4:B:705:LEU:C	4:B:707:ALA:H	2.17	0.52
4:C:846:TYR:HD2	4:C:864:LEU:HD11	1.74	0.52
4:D:337:VAL:HG12	4:D:341:ILE:HD11	1.92	0.52
4:D:809:LEU:O	4:D:810:ILE:HG13	2.10	0.52
4:D:848:GLN:OE1	4:D:848:GLN:HA	2.09	0.52
4:A:206:LYS:O	4:A:210:ILE:HG12	2.10	0.52
4:A:620:TRP:CZ2	4:A:677:MET:HB2	2.45	0.52
4:A:871:ASN:O	4:A:874:ASP:OD2	2.28	0.52
4:B:48:GLU:HG3	4:B:262:ALA:HB1	1.92	0.52
4:B:157:LEU:O	4:B:160:LYS:N	2.32	0.52
4:B:779:ALA:N	4:B:780:PRO:HD3	2.25	0.52
4:B:780:PRO:HB3	7:B:3018:HOH:O	2.10	0.52
4:B:849:PHE:HD1	4:B:849:PHE:H	1.56	0.52
4:C:4:ILE:CD1	4:C:256:THR:HG23	2.37	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:333:LYS:CD	4:C:516:PHE:HD2	2.15	0.52
4:D:316:VAL:O	4:D:317:TYR:C	2.52	0.52
4:D:404:GLN:HG2	4:D:432:PHE:CB	2.40	0.52
2:I:5:C:N3	2:I:6:G:C8	2.78	0.52
4:A:281:ILE:HG22	4:A:282:THR:N	2.23	0.52
4:A:281:ILE:HG13	4:A:309:GLU:CG	2.40	0.52
4:A:459:TRP:CH2	4:A:825:PHE:CE2	2.98	0.52
4:B:56:GLU:CD	4:B:57:ARG:N	2.68	0.52
4:B:450:LYS:N	4:B:529:ASN:HD21	2.07	0.52
4:B:722:ARG:NH1	4:B:768:GLU:OE2	2.42	0.52
4:C:101:THR:HA	4:C:104:GLN:CD	2.35	0.52
4:D:66:ASP:OD2	4:D:752:LEU:HD23	2.10	0.52
4:D:236:VAL:O	4:D:240:ASP:HB2	2.09	0.52
4:D:472:LYS:C	4:D:567:VAL:HG21	2.35	0.52
4:D:515:CYS:O	4:D:516:PHE:C	2.51	0.52
4:D:582:LEU:HD22	4:D:620:TRP:HB2	1.92	0.52
4:D:613:THR:HG22	4:D:676:TYR:HE1	1.75	0.52
1:H:9:DA:N6	3:J:1:DG:H22	2.05	0.51
4:A:270:PRO:HB3	4:A:416:PHE:CD1	2.45	0.51
4:A:457:TYR:CD1	4:A:521:VAL:HG21	2.40	0.51
4:A:521:VAL:HG12	4:A:522:GLN:N	2.24	0.51
4:A:810:ILE:CD1	7:A:3145:HOH:O	2.58	0.51
4:B:24:LEU:O	4:B:25:ALA:C	2.52	0.51
4:B:194:GLY:O	4:B:196:LEU:HD23	2.11	0.51
4:B:314:PRO:C	4:B:316:VAL:N	2.65	0.51
4:C:93:LYS:HA	4:C:99:ARG:NH2	2.25	0.51
4:C:338:ALA:O	4:C:339:ASN:C	2.43	0.51
4:C:404:GLN:HA	4:C:404:GLN:NE2	2.19	0.51
4:C:569:ASP:O	4:C:572:GLY:N	2.43	0.51
4:D:31:ARG:O	4:D:32:LEU:C	2.53	0.51
4:D:448:LYS:HZ2	4:D:806:SER:HB3	1.73	0.51
4:D:466:ASN:OD1	4:D:478:ARG:NH1	2.44	0.51
4:A:459:TRP:CZ3	4:A:475:PHE:CE1	2.99	0.51
4:A:631:LYS:O	4:A:632:ARG:C	2.53	0.51
4:B:49:ALA:O	4:B:50:ARG:C	2.52	0.51
4:B:166:VAL:O	4:B:167:GLU:C	2.53	0.51
4:B:516:PHE:O	4:B:519:ALA:HB3	2.10	0.51
4:B:648:GLN:O	4:B:649:GLN:C	2.53	0.51
4:C:215:ARG:O	4:C:218:GLU:HB2	2.10	0.51
4:C:405:ALA:CB	4:C:443:LEU:HD13	2.41	0.51
4:C:579:ASN:O	4:C:582:LEU:HB2	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:729:THR:OG1	4:C:733:PHE:N	2.40	0.51
4:D:647:ARG:O	4:D:648:GLN:C	2.53	0.51
4:D:745:THR:CG2	7:D:3056:HOH:O	2.59	0.51
1:E:3:DG:H2"	1:E:4:DA:C8	2.45	0.51
4:A:50:ARG:HH11	4:A:50:ARG:CG	2.23	0.51
4:A:379:ARG:HE	4:A:656:GLN:CG	2.23	0.51
4:A:679:LYS:O	4:A:680:LEU:C	2.51	0.51
4:A:812:ASP:N	4:A:812:ASP:OD1	2.38	0.51
4:B:194:GLY:O	4:B:196:LEU:CD2	2.59	0.51
4:B:704:LYS:HG3	4:B:775:GLU:OE1	2.10	0.51
4:B:875:ILE:O	4:B:877:GLU:N	2.43	0.51
4:C:15:GLU:CG	4:C:18:ALA:H	2.22	0.51
4:C:455:GLU:OE1	4:C:455:GLU:HA	2.09	0.51
4:C:668:THR:HB	4:C:669:GLN:NE2	2.25	0.51
4:C:870:LEU:HD23	4:C:871:ASN:C	2.35	0.51
4:D:84:ARG:CB	4:D:223:SER:HB3	2.41	0.51
4:D:814:PHE:CE1	4:D:883:ALA:HB1	2.45	0.51
1:H:17:DG:H2"	1:H:18:DC:C5	2.46	0.51
4:A:390:ALA:O	4:A:391:ARG:C	2.52	0.51
4:A:551:ARG:HB2	4:A:868:GLY:N	2.24	0.51
4:A:729:THR:HB	4:A:789:SER:HB2	1.92	0.51
4:B:116:TYR:C	4:B:116:TYR:CD2	2.89	0.51
4:B:254:ILE:O	4:B:255:ALA:C	2.52	0.51
4:B:339:ASN:O	4:B:343:LYS:CG	2.59	0.51
4:C:32:LEU:N	7:C:3157:HOH:O	2.29	0.51
4:C:36:GLN:OE1	4:C:36:GLN:HA	2.10	0.51
4:C:51:PHE:CZ	4:C:261:LEU:HD23	2.45	0.51
4:C:67:ASN:C	4:C:69:ALA:N	2.69	0.51
4:C:616:LEU:O	4:C:617:ALA:C	2.53	0.51
4:D:338:ALA:O	4:D:342:THR:HG23	2.10	0.51
4:D:472:LYS:CA	4:D:567:VAL:HG11	2.38	0.51
1:H:12:DT:H2"	1:H:13:DC:H6	1.76	0.51
1:H:15:DC:C2	1:H:16:DC:C5	2.99	0.51
1:K:11:DA:C8	4:C:639:TYR:CG	2.98	0.51
1:N:12:DT:H4'	4:D:423:ARG:HD2	1.93	0.51
4:A:292:ARG:N	4:A:293:PRO:CD	2.73	0.51
4:A:513:ALA:O	7:A:3098:HOH:O	2.19	0.51
4:A:689:VAL:O	4:A:691:ALA:N	2.44	0.51
4:A:754:GLN:O	4:A:755:PHE:O	2.28	0.51
4:A:828:VAL:C	4:A:830:GLU:H	2.19	0.51
4:B:136:ALA:O	4:B:139:SER:HB3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:322:ILE:HG22	4:B:323:ALA:N	2.24	0.51
4:B:432:PHE:CE2	4:B:444:LEU:HD11	2.44	0.51
4:C:120:LYS:HZ3	4:C:751:PHE:HD2	1.57	0.51
4:C:239:GLN:O	4:C:241:SER:N	2.43	0.51
4:C:540:CYS:O	4:C:541:SER:C	2.54	0.51
4:C:643:GLU:OE2	4:C:679:LYS:HA	2.11	0.51
4:D:475:PHE:HE2	4:D:879:ASP:CB	2.21	0.51
4:D:578:VAL:HG13	4:D:680:LEU:HB3	1.93	0.51
4:D:724:ALA:HB1	4:D:737:GLN:O	2.10	0.51
2:L:4:G:O2'	2:L:5:C:H5'	2.10	0.51
4:A:213:GLY:O	4:A:217:ILE:HG13	2.11	0.51
4:A:430:SER:OG	4:A:431:MET:N	2.41	0.51
4:A:439:MET:HG3	4:A:509:PHE:CD2	2.45	0.51
4:A:871:ASN:O	4:A:872:LEU:C	2.54	0.51
4:B:55:PHE:CD2	4:B:59:LEU:HD11	2.45	0.51
4:B:417:PRO:O	4:B:429:VAL:HG23	2.10	0.51
4:B:854:HIS:ND1	4:B:855:GLU:N	2.58	0.51
4:C:109:ILE:H	4:C:109:ILE:HD12	1.74	0.51
4:C:294:LEU:N	4:C:294:LEU:HD23	2.25	0.51
4:C:462:ILE:O	4:C:465:ALA:HB3	2.11	0.51
4:D:15:GLU:OE2	4:D:18:ALA:HB3	2.11	0.51
4:D:308:TYR:HE2	4:D:734:PRO:O	1.94	0.51
4:D:726:HIS:CD2	4:D:736:TRP:NE1	2.78	0.51
4:A:40:GLU:OE1	4:A:286:TYR:HB3	2.10	0.51
4:A:261:LEU:C	4:A:263:GLY:H	2.19	0.51
4:B:19:ILE:HG23	4:B:20:PRO:HD2	1.92	0.51
4:B:172:LYS:HB3	4:B:172:LYS:HZ3	1.76	0.51
4:C:59:LEU:HD22	4:C:64:VAL:CG1	2.39	0.51
4:D:76:THR:C	4:D:79:PRO:HD2	2.36	0.51
4:D:259:GLY:O	4:D:262:ALA:N	2.43	0.51
4:D:277:PRO:CA	7:D:3029:HOH:O	2.59	0.51
4:D:306:MET:O	4:D:309:GLU:N	2.42	0.51
4:D:324:GLN:HA	4:D:418:TYR:CE1	2.45	0.51
4:D:835:THR:HG22	4:D:836:TYR:CD2	2.46	0.51
1:N:11:DA:C4'	4:D:780:PRO:HG3	2.40	0.51
4:A:268:PHE:CB	4:A:430:SER:HA	2.40	0.51
4:A:303:LYS:NZ	7:A:3108:HOH:O	2.42	0.51
4:A:726:HIS:HB2	4:A:736:TRP:CD1	2.45	0.51
4:A:746:ARG:HH12	4:A:754:GLN:N	2.06	0.51
4:B:82:ILE:CD1	4:B:112:GLU:HG3	2.41	0.51
4:B:308:TYR:HA	4:B:311:VAL:HG21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:585:ASP:OD2	4:B:613:THR:CB	2.58	0.51
4:B:644:PHE:CD2	4:B:644:PHE:C	2.89	0.51
4:B:744:GLN:HB3	4:B:756:ARG:HB3	1.92	0.51
4:C:308:TYR:CZ	4:C:733:PHE:CE2	2.97	0.51
4:C:437:ASN:ND2	4:C:440:THR:OG1	2.44	0.51
4:C:777:GLY:O	4:C:781:ASN:CG	2.54	0.51
4:D:21:PHE:C	4:D:21:PHE:CD1	2.89	0.51
4:D:207:GLU:O	4:D:211:HIS:CG	2.64	0.51
4:D:221:ILE:HA	4:D:224:THR:O	2.11	0.51
4:D:541:SER:O	4:D:542:GLY:C	2.53	0.51
4:D:797:TRP:NE1	4:D:802:TYR:HE2	2.08	0.51
4:A:418:TYR:HD2	4:A:426:VAL:HG11	1.75	0.51
4:A:541:SER:O	4:A:542:GLY:C	2.52	0.51
4:A:676:TYR:O	4:A:677:MET:C	2.51	0.51
4:A:794:THR:HG1	4:A:831:THR:HG21	1.73	0.51
6:A:2000:APC:H5'2	7:A:3048:HOH:O	2.11	0.51
4:B:158:GLU:HG2	4:B:195:LEU:CB	2.41	0.51
4:B:329:LYS:O	4:B:330:ILE:C	2.52	0.51
4:B:432:PHE:C	4:B:432:PHE:CD2	2.89	0.51
4:B:571:TYR:HE2	4:B:631:LYS:HG3	1.68	0.51
4:B:729:THR:HG23	4:B:733:PHE:O	2.10	0.51
4:C:345:LYS:NZ	4:C:352:ILE:HG12	2.24	0.51
4:C:824:LEU:O	4:C:828:VAL:HG22	2.10	0.51
4:D:205:HIS:C	4:D:207:GLU:N	2.69	0.51
4:D:327:ALA:CB	4:D:415:TRP:NE1	2.73	0.51
4:D:455:GLU:O	4:D:458:TYR:HB3	2.11	0.51
4:D:843:ALA:O	4:D:846:TYR:N	2.42	0.51
1:N:15:DC:H2''	1:N:16:DC:OP2	2.09	0.51
4:A:115:ALA:O	4:A:119:ILE:HG12	2.11	0.51
4:A:721:LYS:CD	4:A:722:ARG:H	2.17	0.51
4:B:4:ILE:HD12	4:B:256:THR:HG23	1.92	0.51
4:B:535:ALA:HA	4:B:815:GLY:HA2	1.94	0.51
4:C:313:MET:O	4:C:317:TYR:HD2	1.94	0.51
4:D:7:ALA:HA	4:D:11:PHE:HD2	1.76	0.51
1:H:14:DG:C4	1:H:15:DC:C5	2.99	0.50
1:K:15:DC:H6	1:K:15:DC:H5'	1.75	0.50
4:A:644:PHE:C	4:A:644:PHE:CD2	2.88	0.50
4:C:307:ARG:HD3	4:C:736:TRP:CD2	2.45	0.50
4:C:329:LYS:HG3	4:C:445:THR:HG23	1.93	0.50
4:C:333:LYS:CD	4:C:516:PHE:CD2	2.93	0.50
4:C:442:GLY:O	4:C:444:LEU:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:550:LEU:C	4:C:867:LYS:HG3	2.36	0.50
4:C:852:GLN:NE2	7:C:3094:HOH:O	2.21	0.50
4:D:71:LYS:N	4:D:72:PRO:HD2	2.25	0.50
4:D:377:TRP:HA	7:D:3074:HOH:O	2.10	0.50
4:D:452:ILE:HD11	4:D:457:TYR:HA	1.94	0.50
1:H:9:DA:C2	4:B:644:PHE:CD1	2.98	0.50
1:H:9:DA:C5'	7:H:484:HOH:O	2.32	0.50
1:K:10:DT:H4'	4:C:639:TYR:O	2.12	0.50
4:A:43:SER:OG	4:A:267:MET:O	2.30	0.50
4:A:308:TYR:HE2	4:A:734:PRO:CG	2.12	0.50
4:A:338:ALA:C	4:A:340:VAL:N	2.66	0.50
4:A:475:PHE:O	4:A:476:PRO:C	2.50	0.50
4:A:651:LEU:HD11	4:A:656:GLN:NE2	2.25	0.50
4:B:30:GLU:O	4:B:31:ARG:C	2.53	0.50
4:B:780:PRO:CD	4:B:781:ASN:N	2.73	0.50
4:C:60:LYS:HG2	4:C:60:LYS:O	2.12	0.50
4:C:120:LYS:HD2	4:C:751:PHE:CE2	2.46	0.50
4:C:291:ARG:CB	7:C:3192:HOH:O	2.54	0.50
4:C:779:ALA:N	4:C:780:PRO:HD2	2.26	0.50
4:C:837:GLU:HG2	4:C:872:LEU:HD12	1.93	0.50
4:D:50:ARG:HD3	4:D:267:MET:HE3	1.92	0.50
4:D:166:VAL:O	4:D:167:GLU:C	2.53	0.50
4:D:676:TYR:CZ	4:D:680:LEU:HD11	2.46	0.50
4:A:223:SER:OG	4:A:224:THR:HG23	2.11	0.50
4:A:421:ASP:OD2	4:A:427:TYR:HE1	1.93	0.50
4:A:611:LEU:HD11	4:A:669:GLN:NE2	2.27	0.50
4:B:322:ILE:O	4:B:323:ALA:C	2.52	0.50
4:B:422:TRP:CE2	4:B:781:ASN:ND2	2.79	0.50
4:B:505:GLN:NE2	4:B:505:GLN:H	1.94	0.50
4:B:791:LEU:O	4:B:794:THR:N	2.42	0.50
4:B:824:LEU:O	4:B:824:LEU:HG	2.11	0.50
4:C:180:LYS:O	4:C:181:ALA:C	2.54	0.50
4:C:569:ASP:O	4:C:573:ILE:HG22	2.11	0.50
4:C:700:LYS:O	4:C:701:SER:C	2.54	0.50
4:D:158:GLU:HA	4:D:195:LEU:HD13	1.94	0.50
4:D:215:ARG:HA	4:D:218:GLU:OE1	2.10	0.50
4:D:275:PRO:HG2	4:D:324:GLN:CG	2.38	0.50
4:D:448:LYS:NZ	4:D:806:SER:CB	2.73	0.50
4:D:789:SER:HA	4:D:792:ARG:CZ	2.41	0.50
4:A:82:ILE:CG2	4:A:112:GLU:OE2	2.59	0.50
4:A:105:PHE:C	4:A:107:GLN:N	2.67	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:281:ILE:HD11	4:A:309:GLU:H	1.75	0.50
4:B:120:LYS:HG3	4:B:752:LEU:HD11	1.94	0.50
4:B:199:GLU:C	4:B:201:TRP:H	2.20	0.50
4:B:632:ARG:HH11	6:B:2001:APC:C8	2.24	0.50
4:B:676:TYR:O	4:B:677:MET:C	2.53	0.50
4:C:315:GLU:OE2	4:C:318:LYS:NZ	2.27	0.50
1:K:11:DA:C8	4:C:639:TYR:CB	2.93	0.50
1:K:11:DA:C2'	1:K:12:DT:C7	2.89	0.50
1:N:12:DT:O4'	4:D:423:ARG:CZ	2.58	0.50
4:B:67:ASN:O	4:B:68:ALA:C	2.54	0.50
4:B:159:ALA:HA	4:B:162:PHE:HB3	1.94	0.50
4:B:272:VAL:CG1	4:B:411:HIS:HD2	2.25	0.50
4:B:411:HIS:C	4:B:413:ALA:N	2.67	0.50
4:B:422:TRP:CD1	4:B:423:ARG:N	2.80	0.50
4:B:470:VAL:HG11	4:B:478:ARG:HA	1.93	0.50
4:B:770:ASP:OD1	4:B:770:ASP:O	2.29	0.50
4:C:43:SER:OG	4:C:269:GLN:HG3	2.12	0.50
4:C:548:ALA:C	4:C:550:LEU:H	2.19	0.50
4:C:672:GLN:HG3	7:C:3033:HOH:O	2.10	0.50
4:D:19:ILE:HG23	4:D:20:PRO:CD	2.41	0.50
4:D:665:LEU:HB2	7:D:3125:HOH:O	2.12	0.50
4:D:702:ALA:HB2	4:D:861:MET:CE	2.41	0.50
4:D:706:LEU:HD11	4:D:849:PHE:CG	2.46	0.50
4:D:828:VAL:HA	4:D:831:THR:HG22	1.93	0.50
4:A:113:ALA:O	4:A:114:VAL:C	2.54	0.50
4:A:158:GLU:CD	4:A:195:LEU:HB3	2.37	0.50
4:A:386:ARG:CD	7:A:3138:HOH:O	2.45	0.50
4:A:474:PRO:C	4:A:476:PRO:HD2	2.37	0.50
4:A:572:GLY:O	4:A:576:LYS:HG3	2.12	0.50
4:B:14:ILE:HG23	4:B:288:ALA:HB1	1.93	0.50
4:B:51:PHE:O	4:B:55:PHE:HB2	2.11	0.50
4:B:631:LYS:HZ1	6:B:2001:APC:H3A2	1.76	0.50
4:B:638:ALA:O	4:B:780:PRO:HB3	2.11	0.50
4:B:698:TRP:O	4:B:699:LEU:C	2.54	0.50
4:C:9:ASN:CA	4:C:12:SER:HB3	2.41	0.50
4:D:150:ARG:HG3	4:D:201:TRP:CD1	2.46	0.50
4:D:209:SER:HB2	7:D:3053:HOH:O	2.11	0.50
4:D:335:LEU:O	4:D:339:ASN:HB2	2.12	0.50
4:D:706:LEU:HD23	4:D:853:LEU:HD23	1.94	0.50
4:A:333:LYS:CB	4:A:516:PHE:HD2	2.23	0.50
4:A:579:ASN:HA	4:A:582:LEU:HG	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:158:GLU:OE2	4:B:190:MET:HE3	2.12	0.50
4:B:314:PRO:C	4:B:316:VAL:H	2.20	0.50
4:B:405:ALA:O	4:B:409:ALA:N	2.45	0.50
4:B:412:LYS:O	4:B:413:ALA:HB2	2.12	0.50
4:B:475:PHE:HB2	4:B:476:PRO:CD	2.42	0.50
4:B:690:VAL:C	4:B:693:VAL:HG23	2.36	0.50
4:C:446:LEU:H	4:C:533:PRO:HD3	1.76	0.50
4:C:446:LEU:HD12	4:C:817:ILE:HG23	1.93	0.50
4:C:623:TYR:CA	4:C:666:MET:HE2	2.42	0.50
4:C:849:PHE:O	4:C:850:ALA:C	2.54	0.50
4:D:92:VAL:CG1	4:D:99:ARG:HG3	2.41	0.50
4:D:304:ALA:HB1	7:D:3038:HOH:O	2.10	0.50
4:D:485:ASN:O	4:D:489:ILE:HG13	2.12	0.50
4:D:585:ASP:O	4:D:614:LYS:HA	2.12	0.50
4:D:706:LEU:HD21	4:D:849:PHE:HD2	1.76	0.50
3:J:5:DA:C2	3:J:6:DT:C2	2.99	0.50
1:K:11:DA:H8	4:C:639:TYR:HB3	1.74	0.50
1:K:16:DC:H2''	1:K:17:DG:H5'	1.93	0.50
4:A:19:ILE:HG23	4:A:20:PRO:CD	2.39	0.50
4:A:403:GLU:C	4:A:403:GLU:CD	2.80	0.50
4:B:159:ALA:HB1	4:B:163:LYS:N	2.27	0.50
4:B:162:PHE:HE1	4:B:190:MET:HG2	1.76	0.50
4:B:167:GLU:O	4:B:168:GLU:C	2.54	0.50
4:B:450:LYS:N	4:B:529:ASN:ND2	2.60	0.50
4:B:500:THR:O	4:B:503:ALA:HB3	2.11	0.50
4:B:623:TYR:HA	4:B:666:MET:CE	2.23	0.50
4:C:22:ASN:O	4:C:26:ASP:HB3	2.11	0.50
4:C:248:PRO:HB2	4:C:249:GLU:OE2	2.12	0.50
4:C:656:GLN:N	4:C:657:PRO:CD	2.75	0.50
4:D:402:LEU:CD2	4:D:443:LEU:CD1	2.88	0.50
1:H:10:DT:OP2	4:B:641:SER:HB3	2.12	0.50
1:K:10:DT:H5'	4:C:641:SER:CA	2.42	0.50
3:P:4:DG:H2''	3:P:5:DA:C8	2.47	0.50
4:A:112:GLU:CD	4:A:112:GLU:H	2.19	0.50
4:A:422:TRP:HD1	7:A:3029:HOH:O	1.95	0.50
4:A:719:LEU:HD22	4:A:854:HIS:CE1	2.47	0.50
4:A:829:ARG:NE	4:A:878:SER:O	2.42	0.50
4:A:846:TYR:CD1	4:A:850:ALA:HB2	2.47	0.50
4:B:6:ILE:C	4:B:8:LYS:H	2.19	0.50
4:B:268:PHE:HD2	4:B:429:VAL:HG12	1.77	0.50
4:C:140:ALA:O	4:C:141:ILE:C	2.55	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:433:ASN:C	7:C:3164:HOH:O	2.52	0.50
4:D:115:ALA:O	4:D:119:ILE:HG12	2.11	0.50
4:D:433:ASN:CB	4:D:434:PRO:CD	2.88	0.50
1:H:15:DC:OP2	7:H:411:HOH:O	2.19	0.49
1:K:16:DC:H2''	1:K:17:DG:C5'	2.42	0.49
1:N:10:DT:C5'	4:D:641:SER:N	2.75	0.49
4:A:385:TYR:CD2	4:A:385:TYR:C	2.90	0.49
4:A:778:ILE:O	4:A:779:ALA:C	2.54	0.49
4:A:849:PHE:O	4:A:850:ALA:C	2.55	0.49
4:B:92:VAL:HG11	4:B:100:PRO:HD2	1.94	0.49
4:C:14:ILE:HG12	4:C:288:ALA:HB1	1.94	0.49
4:C:221:ILE:HG23	4:C:227:VAL:O	2.12	0.49
4:C:232:GLN:NE2	7:C:3040:HOH:O	2.45	0.49
4:C:272:VAL:HG13	4:C:411:HIS:HD2	1.76	0.49
4:C:417:PRO:O	4:C:429:VAL:HG23	2.12	0.49
4:C:632:ARG:CZ	6:C:2002:APC:C8	2.90	0.49
4:C:668:THR:HB	4:C:669:GLN:HE22	1.75	0.49
4:D:72:PRO:HG3	4:D:257:ARG:HG3	1.94	0.49
4:D:404:GLN:HG2	4:D:432:PHE:HB2	1.94	0.49
4:D:489:ILE:HA	4:D:492:CYS:SG	2.52	0.49
4:D:797:TRP:CH2	4:D:801:LYS:HG3	2.47	0.49
1:H:13:DC:C4'	4:B:427:TYR:CE2	2.95	0.49
1:H:14:DG:H2''	1:H:15:DC:H6	1.77	0.49
1:H:18:DC:C2'	4:B:63:GLU:OE1	2.60	0.49
3:J:6:DT:H2''	3:J:7:DT:H71	1.94	0.49
1:K:5:DA:N6	3:M:5:DA:N6	2.60	0.49
4:A:71:LYS:N	4:A:72:PRO:HD2	2.27	0.49
4:A:154:ILE:HG23	4:A:190:MET:HE1	1.88	0.49
4:A:318:LYS:O	4:A:319:ALA:C	2.55	0.49
4:A:421:ASP:C	4:A:423:ARG:N	2.70	0.49
4:A:704:LYS:O	4:A:707:ALA:HB3	2.12	0.49
4:B:51:PHE:HE2	4:B:55:PHE:HD1	1.57	0.49
4:B:486:HIS:C	4:B:486:HIS:ND1	2.71	0.49
4:B:578:VAL:HG13	4:B:680:LEU:CD2	2.40	0.49
4:B:860:LYS:O	4:B:862:PRO:HD2	2.12	0.49
4:D:544:GLN:HG2	4:D:561:LEU:HD11	1.93	0.49
4:D:702:ALA:O	4:D:703:ALA:C	2.55	0.49
4:D:745:THR:H	4:D:756:ARG:HD3	1.76	0.49
3:G:6:DT:H2''	3:G:7:DT:OP2	2.12	0.49
1:N:15:DC:N3	1:N:16:DC:C4	2.80	0.49
4:A:84:ARG:HG3	4:A:222:GLU:HG2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:182:PHE:O	4:A:185:VAL:CG2	2.59	0.49
4:A:344:TRP:O	4:A:345:LYS:HG3	2.12	0.49
4:A:473:VAL:O	4:A:473:VAL:CG1	2.60	0.49
4:A:715:THR:HB	4:A:717:GLU:HB2	1.94	0.49
4:A:786:GLN:O	4:A:787:ASP:C	2.54	0.49
4:A:802:TYR:C	4:A:804:ILE:H	2.17	0.49
4:B:155:ARG:HH21	4:B:749:LEU:HB2	1.77	0.49
4:B:400:PHE:O	4:B:401:MET:C	2.50	0.49
4:B:647:ARG:HD3	7:B:3138:HOH:O	2.11	0.49
4:B:829:ARG:NH1	4:B:829:ARG:CG	2.68	0.49
4:C:161:HIS:C	4:C:163:LYS:H	2.20	0.49
4:C:458:TYR:CE1	4:C:479:ILE:HD11	2.47	0.49
4:C:474:PRO:HB2	4:C:476:PRO:HG2	1.94	0.49
4:C:711:LYS:HE2	4:C:716:GLY:O	2.12	0.49
4:C:870:LEU:HA	7:C:3053:HOH:O	2.11	0.49
4:A:60:LYS:HZ2	4:A:60:LYS:C	2.13	0.49
4:A:136:ALA:HA	7:A:3053:HOH:O	2.11	0.49
4:A:425:ARG:HD3	4:A:811:HIS:HD2	1.76	0.49
4:A:488:ASN:O	4:A:491:ALA:N	2.45	0.49
4:A:720:ARG:HE	4:A:854:HIS:H	1.60	0.49
4:B:193:LYS:HG3	4:B:194:GLY:H	1.77	0.49
4:B:203:SER:O	4:B:205:HIS:N	2.38	0.49
4:B:232:GLN:HG3	4:B:243:THR:CG2	2.43	0.49
4:B:826:LYS:HG2	4:B:830:GLU:HG3	1.94	0.49
4:C:250:TYR:O	4:C:254:ILE:HG13	2.12	0.49
4:C:323:ALA:O	4:C:324:GLN:C	2.55	0.49
4:C:669:GLN:NE2	4:C:669:GLN:N	2.60	0.49
4:C:854:HIS:O	4:C:857:GLN:HG2	2.13	0.49
4:D:379:ARG:HD2	7:D:3122:HOH:O	2.12	0.49
4:D:551:ARG:O	4:D:868:GLY:HA3	2.12	0.49
3:M:5:DA:C2'	3:M:6:DT:H72	2.42	0.49
4:A:60:LYS:O	4:A:60:LYS:CG	2.56	0.49
4:A:73:LEU:C	4:A:75:THR:H	2.20	0.49
4:A:267:MET:HE2	4:A:431:MET:HE1	1.93	0.49
4:B:194:GLY:O	4:B:195:LEU:C	2.56	0.49
4:B:272:VAL:HG11	4:B:411:HIS:CD2	2.48	0.49
4:B:421:ASP:O	4:B:424:GLY:N	2.45	0.49
4:B:459:TRP:CZ3	4:B:536:PHE:CZ	3.01	0.49
4:B:485:ASN:ND2	4:B:501:TRP:CZ2	2.80	0.49
4:C:324:GLN:CG	4:C:417:PRO:HA	2.42	0.49
4:C:824:LEU:HD12	4:C:824:LEU:C	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:ASP:O	4:D:13:ASP:CB	2.61	0.49
4:D:139:SER:CA	4:D:210:ILE:HD13	2.42	0.49
4:D:267:MET:HE2	4:D:431:MET:HE1	1.95	0.49
4:D:623:TYR:HA	4:D:666:MET:CE	2.32	0.49
4:D:830:GLU:HG2	4:D:876:LEU:HD21	1.94	0.49
1:E:15:DC:H2''	1:E:16:DC:C5'	2.41	0.49
2:F:1:G:C2	2:F:2:C:C2	3.01	0.49
4:A:42:GLU:CG	4:A:46:MET:HE2	2.39	0.49
4:A:264:ILE:HG22	4:A:292:ARG:HD3	1.95	0.49
4:A:308:TYR:C	4:A:311:VAL:HG23	2.37	0.49
4:A:465:ALA:CB	4:A:478:ARG:HB3	2.43	0.49
4:A:480:LYS:HG2	7:A:3046:HOH:O	2.13	0.49
4:A:524:HIS:O	4:A:525:GLY:O	2.30	0.49
4:A:629:VAL:HG11	4:A:677:MET:CE	2.43	0.49
4:A:643:GLU:OE2	4:A:679:LYS:HA	2.13	0.49
4:B:60:LYS:HE2	4:B:61:ALA:HB2	1.95	0.49
4:B:334:VAL:HG12	4:B:443:LEU:CD2	2.42	0.49
4:B:454:LYS:N	4:B:526:LEU:HD22	2.27	0.49
4:B:544:GLN:HA	4:B:559:VAL:HG21	1.94	0.49
4:B:560:ASN:OD1	4:B:568:GLN:HB2	2.12	0.49
4:B:784:HIS:C	4:B:786:GLN:N	2.69	0.49
4:C:84:ARG:HH11	4:C:84:ARG:CA	2.22	0.49
4:C:423:ARG:CD	4:C:781:ASN:HD22	2.25	0.49
4:C:651:LEU:C	4:C:651:LEU:CD1	2.86	0.49
4:D:306:MET:C	4:D:308:TYR:N	2.70	0.49
4:D:330:ILE:CG1	4:D:408:PHE:O	2.60	0.49
4:D:810:ILE:CB	4:D:813:SER:OG	2.53	0.49
4:D:814:PHE:CE1	4:D:883:ALA:HB2	2.47	0.49
4:D:840:ASP:O	4:D:841:VAL:C	2.54	0.49
4:A:169:GLN:O	4:A:173:ARG:CG	2.50	0.49
4:A:205:HIS:C	4:A:207:GLU:N	2.70	0.49
4:A:417:PRO:C	4:A:418:TYR:HD1	2.21	0.49
4:A:462:ILE:O	4:A:465:ALA:N	2.45	0.49
4:A:485:ASN:HA	7:A:3028:HOH:O	2.12	0.49
4:B:546:PHE:CE1	4:B:783:VAL:HG13	2.47	0.49
4:B:626:THR:C	4:B:628:SER:N	2.70	0.49
4:B:701:SER:O	4:B:702:ALA:C	2.55	0.49
4:B:726:HIS:CD2	4:B:736:TRP:CE2	3.01	0.49
4:C:24:LEU:CD2	4:C:273:VAL:HG21	2.42	0.49
4:D:326:THR:C	4:D:415:TRP:CD1	2.91	0.49
4:D:518:TYR:O	4:D:522:GLN:HG2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:810:ILE:N	4:D:813:SER:OG	2.46	0.49
1:K:7:DC:C6	1:K:8:DG:N7	2.80	0.49
4:A:505:GLN:C	4:A:507:SER:N	2.71	0.49
4:A:788:GLY:O	4:A:789:SER:C	2.56	0.49
4:B:281:ILE:HD11	4:B:309:GLU:N	2.28	0.49
4:B:404:GLN:HB3	4:B:432:PHE:CD1	2.48	0.49
4:B:804:ILE:CG2	4:B:807:PHE:CE2	2.96	0.49
4:B:826:LYS:O	4:B:830:GLU:HG3	2.13	0.49
4:C:305:LEU:C	4:C:305:LEU:CD2	2.86	0.49
4:C:340:VAL:HA	4:C:343:LYS:HD3	1.95	0.49
4:C:549:MET:HB3	4:C:836:TYR:CE1	2.48	0.49
4:C:734:PRO:O	4:C:734:PRO:HG2	2.13	0.49
4:C:786:GLN:O	4:C:789:SER:HB3	2.12	0.49
4:D:78:LEU:N	4:D:79:PRO:HD2	2.27	0.49
4:D:381:ALA:O	4:D:384:VAL:HB	2.12	0.49
1:H:3:DG:H1'	7:H:1116:HOH:O	2.12	0.49
1:H:15:DC:N3	1:H:16:DC:C4	2.80	0.49
4:A:548:ALA:C	4:A:550:LEU:N	2.63	0.49
4:A:617:ALA:O	4:A:620:TRP:N	2.46	0.49
4:A:697:ASN:O	4:A:698:TRP:C	2.55	0.49
4:B:105:PHE:HB3	4:B:204:TRP:CZ2	2.48	0.49
4:B:273:VAL:C	4:B:274:PRO:O	2.56	0.49
4:B:810:ILE:O	4:B:811:HIS:HB2	2.11	0.49
4:C:151:PHE:O	4:C:154:ILE:HG13	2.13	0.49
4:C:552:ASP:HB2	4:C:691:ALA:HB2	1.94	0.49
4:C:846:TYR:CD1	4:C:850:ALA:HB2	2.48	0.49
4:D:452:ILE:HG23	4:D:526:LEU:O	2.13	0.49
4:D:635:MET:HE1	6:D:2003:APC:C3A	2.43	0.49
1:H:17:DG:H2''	1:H:18:DC:C6	2.47	0.49
4:A:51:PHE:CZ	4:A:261:LEU:HB3	2.47	0.49
4:A:159:ALA:HA	4:A:162:PHE:HB3	1.94	0.49
4:A:178:TYR:CD1	4:A:178:TYR:N	2.77	0.49
4:A:721:LYS:HE2	7:A:3021:HOH:O	2.12	0.49
4:B:292:ARG:O	4:B:292:ARG:HG3	2.13	0.49
4:B:463:HIS:O	4:B:467:CYS:SG	2.71	0.49
4:B:737:GLN:C	4:B:774:GLN:HE22	2.21	0.49
4:C:36:GLN:CG	4:C:273:VAL:HG22	2.41	0.49
4:C:475:PHE:O	4:C:479:ILE:HG12	2.13	0.49
4:C:553:GLU:CG	4:C:554:VAL:H	2.25	0.49
4:C:730:PRO:HD3	4:C:786:GLN:NE2	2.27	0.49
4:D:84:ARG:CG	4:D:223:SER:HB3	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:116:TYR:HE2	4:D:752:LEU:HD13	1.77	0.49
4:D:338:ALA:C	4:D:340:VAL:N	2.70	0.49
4:D:345:LYS:O	4:D:346:HIS:C	2.51	0.49
1:E:16:DC:H2''	1:E:17:DG:C5'	2.42	0.48
1:H:9:DA:C5	4:B:644:PHE:CZ	3.01	0.48
1:K:9:DA:N6	3:M:1:DG:H22	2.11	0.48
4:A:89:PHE:HA	4:A:103:PHE:CZ	2.47	0.48
4:A:532:LEU:HA	4:A:533:PRO:HD2	1.64	0.48
4:A:619:GLN:NE2	4:A:666:MET:O	2.46	0.48
4:B:13:ASP:O	4:B:15:GLU:N	2.43	0.48
4:B:170:LEU:C	4:B:170:LEU:HD13	2.38	0.48
4:B:292:ARG:O	4:B:292:ARG:CG	2.61	0.48
4:B:301:SER:O	4:B:304:ALA:CB	2.59	0.48
4:B:698:TRP:O	4:B:701:SER:HB2	2.12	0.48
4:C:82:ILE:HD13	4:C:112:GLU:HA	1.95	0.48
4:C:786:GLN:NE2	4:C:841:VAL:HG11	2.28	0.48
4:C:871:ASN:HD21	4:C:873:ARG:HB2	1.78	0.48
4:D:347:CYS:O	4:D:349:VAL:N	2.46	0.48
4:D:523:HIS:C	4:D:524:HIS:HD1	2.21	0.48
4:D:646:PHE:O	4:D:650:VAL:HG23	2.13	0.48
1:H:16:DC:H2''	1:H:17:DG:OP2	2.13	0.48
1:K:13:DC:C2	1:K:14:DG:C8	3.00	0.48
1:N:14:DG:C4	1:N:15:DC:C5	3.02	0.48
4:A:347:CYS:C	4:A:349:VAL:N	2.68	0.48
4:A:462:ILE:O	4:A:463:HIS:C	2.55	0.48
4:A:559:VAL:HG23	4:A:559:VAL:O	2.12	0.48
4:A:634:VAL:O	4:A:637:LEU:HB3	2.13	0.48
4:A:720:ARG:HG2	4:A:720:ARG:O	2.13	0.48
4:A:797:TRP:CZ2	4:A:830:GLU:OE1	2.67	0.48
4:B:32:LEU:HD12	4:B:32:LEU:HA	1.67	0.48
4:B:418:TYR:HB3	4:B:426:VAL:CG1	2.44	0.48
4:B:549:MET:HG2	4:B:836:TYR:CE1	2.46	0.48
4:B:680:LEU:HD12	4:B:680:LEU:H	1.75	0.48
4:C:330:ILE:HG12	4:C:408:PHE:O	2.13	0.48
4:D:92:VAL:HG11	4:D:103:PHE:CG	2.48	0.48
4:D:158:GLU:CA	4:D:195:LEU:HD22	2.43	0.48
4:D:231:ARG:HG2	4:D:234:ALA:CB	2.36	0.48
1:K:11:DA:H2''	1:K:12:DT:O5'	2.12	0.48
4:A:39:LEU:O	4:A:42:GLU:N	2.46	0.48
4:A:85:ILE:O	4:A:85:ILE:HG22	2.13	0.48
4:A:89:PHE:CZ	4:A:106:LEU:O	2.65	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:333:LYS:HB3	4:A:516:PHE:CD2	2.48	0.48
4:A:463:HIS:O	4:A:465:ALA:N	2.46	0.48
4:A:512:LEU:O	4:A:516:PHE:CD1	2.66	0.48
4:A:633:SER:HB3	4:A:646:PHE:CE2	2.48	0.48
4:A:637:LEU:O	4:A:637:LEU:HG	2.11	0.48
4:A:668:THR:HG22	4:A:669:GLN:HE22	1.79	0.48
4:A:744:GLN:H	4:A:744:GLN:HG3	1.36	0.48
4:A:745:THR:HG22	4:A:746:ARG:N	2.28	0.48
4:A:777:GLY:O	4:A:781:ASN:HB2	2.12	0.48
4:B:109:ILE:N	4:B:109:ILE:CD1	2.75	0.48
4:B:109:ILE:HG22	4:B:110:LYS:O	2.13	0.48
4:B:347:CYS:HA	4:B:348:PRO:HD3	1.68	0.48
4:B:428:ALA:N	4:B:435:GLN:HE22	2.08	0.48
4:B:546:PHE:CE2	4:B:696:MET:HG3	2.48	0.48
4:B:794:THR:CG2	4:B:828:VAL:HA	2.43	0.48
4:B:860:LYS:O	4:B:862:PRO:CD	2.61	0.48
4:C:252:GLU:HA	7:C:3072:HOH:O	2.13	0.48
4:C:269:GLN:C	4:C:430:SER:HB3	2.38	0.48
4:C:297:VAL:HG21	4:C:733:PHE:HZ	1.78	0.48
4:C:317:TYR:C	4:C:321:ASN:HD21	2.21	0.48
4:C:832:MET:O	4:C:833:VAL:C	2.56	0.48
4:C:846:TYR:CD2	4:C:864:LEU:HD11	2.48	0.48
4:D:161:HIS:C	4:D:163:LYS:N	2.71	0.48
4:D:230:HIS:HB3	7:D:3168:HOH:O	2.13	0.48
4:D:269:GLN:NE2	4:D:407:LYS:HE2	2.25	0.48
4:D:485:ASN:OD1	4:D:485:ASN:N	2.46	0.48
4:D:745:THR:HG21	7:D:3056:HOH:O	2.13	0.48
4:A:348:PRO:C	4:A:349:VAL:HG23	2.37	0.48
4:A:401:MET:HG3	4:A:440:THR:HG23	1.96	0.48
4:A:477:GLU:O	4:A:480:LYS:N	2.46	0.48
4:A:619:GLN:O	4:A:622:ALA:N	2.47	0.48
4:A:826:LYS:O	4:A:827:ALA:C	2.56	0.48
4:B:84:ARG:HD3	4:B:84:ARG:O	2.13	0.48
4:B:264:ILE:O	4:B:292:ARG:NH1	2.45	0.48
4:B:421:ASP:O	4:B:422:TRP:C	2.55	0.48
4:B:616:LEU:O	4:B:617:ALA:C	2.56	0.48
4:C:78:LEU:HD21	4:C:82:ILE:HD11	1.96	0.48
4:C:303:LYS:NZ	4:C:303:LYS:HB2	2.28	0.48
4:C:306:MET:C	4:C:308:TYR:H	2.20	0.48
4:C:490:MET:O	4:C:493:ALA:HB3	2.14	0.48
4:C:502:TRP:CZ3	4:C:503:ALA:HB2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:512:LEU:HG	4:C:516:PHE:HE1	1.77	0.48
4:C:706:LEU:CD2	4:C:725:VAL:HG22	2.42	0.48
4:C:850:ALA:O	4:C:852:GLN:N	2.42	0.48
4:C:850:ALA:C	4:C:852:GLN:N	2.72	0.48
4:D:84:ARG:HG3	4:D:223:SER:HB3	1.95	0.48
4:D:273:VAL:CA	4:D:415:TRP:CE3	2.96	0.48
4:D:468:ALA:HA	4:D:505:GLN:HB3	1.96	0.48
4:D:779:ALA:O	4:D:783:VAL:CG2	2.61	0.48
3:J:2:DT:H2''	3:J:3:DC:O5'	2.14	0.48
2:L:8:U:O4	6:C:2002:APC:H1'	2.14	0.48
4:A:193:LYS:HA	7:A:3220:HOH:O	2.12	0.48
4:A:274:PRO:HD3	4:A:415:TRP:CZ3	2.48	0.48
4:A:276:LYS:O	4:A:277:PRO:C	2.57	0.48
4:A:304:ALA:HA	4:A:307:ARG:HD2	1.96	0.48
4:A:386:ARG:C	4:A:388:ASP:N	2.68	0.48
4:A:388:ASP:O	4:A:388:ASP:CG	2.56	0.48
4:A:639:TYR:HA	4:A:780:PRO:HB3	1.95	0.48
4:A:770:ASP:O	4:A:772:HIS:N	2.47	0.48
4:A:817:ILE:CB	4:A:818:PRO:CD	2.89	0.48
4:B:116:TYR:CE2	4:B:120:LYS:HB2	2.48	0.48
4:B:126:LEU:CD1	4:B:246:LEU:HB2	2.39	0.48
4:B:233:ASN:ND2	4:B:239:GLN:CD	2.70	0.48
4:B:450:LYS:HG2	4:B:451:PRO:HD2	1.94	0.48
4:B:685:VAL:C	4:B:687:VAL:N	2.70	0.48
4:B:787:ASP:OD1	4:B:788:GLY:N	2.46	0.48
4:C:464:GLY:HA3	4:C:514:PHE:CE2	2.48	0.48
4:C:489:ILE:O	4:C:492:CYS:HB2	2.13	0.48
4:C:755:PHE:N	4:C:755:PHE:CD1	2.80	0.48
4:D:323:ALA:O	4:D:324:GLN:C	2.55	0.48
4:D:544:GLN:HG2	4:D:561:LEU:CD1	2.43	0.48
4:D:546:PHE:HE2	4:D:696:MET:HE2	1.78	0.48
2:F:4:G:H2'	2:F:5:C:O4'	2.13	0.48
4:A:65:ALA:HB3	4:A:120:LYS:CE	2.42	0.48
4:A:105:PHE:CB	4:A:204:TRP:CZ2	2.89	0.48
4:A:278:TRP:CZ3	4:A:284:GLY:CA	2.93	0.48
4:A:546:PHE:HE2	4:A:696:MET:HG3	1.78	0.48
4:A:631:LYS:HG2	4:A:632:ARG:N	2.28	0.48
4:B:34:ARG:O	4:B:38:ALA:HB2	2.14	0.48
4:C:36:GLN:HE21	4:C:273:VAL:HG22	1.78	0.48
4:C:173:ARG:NH1	4:C:182:PHE:HB2	2.28	0.48
4:C:299:THR:HG21	4:C:304:ALA:CB	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:541:SER:O	4:C:542:GLY:C	2.56	0.48
4:D:88:TRP:CZ2	4:D:215:ARG:NH2	2.81	0.48
4:D:232:GLN:O	4:D:233:ASN:C	2.56	0.48
4:D:452:ILE:HG23	4:D:453:GLY:N	2.28	0.48
4:D:502:TRP:CD1	4:D:512:LEU:HD13	2.49	0.48
2:F:5:C:O2	2:F:5:C:H2'	2.14	0.48
1:K:5:DA:H2''	1:K:6:DT:OP2	2.13	0.48
1:K:11:DA:C4	1:K:12:DT:H72	2.48	0.48
4:A:81:MET:O	4:A:85:ILE:HG13	2.14	0.48
4:A:422:TRP:C	4:A:422:TRP:CD1	2.91	0.48
4:A:649:GLN:O	4:A:653:ASP:HB2	2.14	0.48
4:A:709:GLU:HB2	4:A:722:ARG:HE	1.79	0.48
4:B:304:ALA:O	4:B:307:ARG:HB2	2.13	0.48
4:B:422:TRP:CZ2	4:B:781:ASN:ND2	2.82	0.48
4:B:787:ASP:O	4:B:790:HIS:HB3	2.14	0.48
4:C:183:MET:HA	4:C:186:VAL:HB	1.96	0.48
4:C:269:GLN:C	4:C:430:SER:CB	2.87	0.48
4:C:404:GLN:CG	4:C:432:PHE:HB2	2.41	0.48
4:C:473:VAL:O	4:C:474:PRO:O	2.32	0.48
4:C:646:PHE:O	4:C:647:ARG:C	2.56	0.48
4:D:121:THR:O	4:D:124:ALA:HB3	2.14	0.48
4:D:387:LYS:HD3	7:D:3157:HOH:O	2.12	0.48
4:D:752:LEU:HD12	4:D:752:LEU:N	2.29	0.48
4:D:828:VAL:CA	4:D:831:THR:HG22	2.43	0.48
1:E:15:DC:H5''	4:A:431:MET:HE3	1.95	0.48
2:L:8:U:O4	6:C:2002:APC:N3	2.47	0.48
4:A:418:TYR:CD2	4:A:426:VAL:HG12	2.47	0.48
4:A:540:CYS:HB3	4:A:543:ILE:CG1	2.44	0.48
4:A:864:LEU:HD12	4:A:864:LEU:N	2.29	0.48
4:B:457:TYR:CD1	4:B:521:VAL:HG11	2.49	0.48
4:B:467:CYS:O	4:B:506:ASP:HB2	2.14	0.48
4:B:535:ALA:O	4:B:536:PHE:HD1	1.96	0.48
4:C:298:ARG:HA	7:C:3165:HOH:O	2.14	0.48
4:C:307:ARG:HD3	4:C:736:TRP:CE3	2.49	0.48
4:C:324:GLN:HE21	4:C:418:TYR:N	2.09	0.48
4:C:374:LEU:C	4:C:376:ALA:H	2.22	0.48
4:C:744:GLN:HB2	4:C:744:GLN:HE21	1.46	0.48
4:D:477:GLU:H	4:D:477:GLU:HG2	1.37	0.48
4:D:783:VAL:O	4:D:786:GLN:HB2	2.14	0.48
4:A:77:LEU:C	4:A:79:PRO:HD2	2.39	0.48
4:A:82:ILE:HG12	4:A:115:ALA:CB	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:138:ALA:HB1	4:A:214:VAL:HG23	1.96	0.48
4:A:656:GLN:C	4:A:658:ALA:N	2.68	0.48
4:A:786:GLN:CA	4:A:786:GLN:NE2	2.70	0.48
4:B:552:ASP:OD1	4:B:554:VAL:N	2.46	0.48
4:B:571:TYR:OH	4:B:635:MET:CE	2.52	0.48
6:B:2001:APC:O2B	6:B:2001:APC:O1A	2.32	0.48
4:C:199:GLU:HG2	4:C:201:TRP:HD1	1.78	0.48
4:C:392:LYS:O	4:C:396:ILE:HG12	2.14	0.48
4:C:397:SER:O	4:C:398:LEU:C	2.56	0.48
4:C:555:GLY:O	4:C:556:GLY:C	2.57	0.48
4:C:629:VAL:O	4:C:629:VAL:HG12	2.14	0.48
4:C:646:PHE:O	4:C:649:GLN:HB2	2.14	0.48
4:D:276:LYS:O	4:D:277:PRO:C	2.56	0.48
4:D:343:LYS:HA	7:D:3020:HOH:O	2.13	0.48
4:D:646:PHE:HE2	4:D:682:TRP:HE3	1.60	0.48
1:H:12:DT:H2'	1:H:13:DC:C6	2.49	0.48
4:A:19:ILE:HG21	7:A:3120:HOH:O	2.08	0.48
4:A:109:ILE:O	4:A:110:LYS:C	2.55	0.48
4:A:393:SER:O	4:A:396:ILE:N	2.45	0.48
4:B:400:PHE:CD1	4:B:400:PHE:C	2.91	0.48
4:B:642:LYS:HG2	4:B:682:TRP:HZ3	1.77	0.48
4:B:810:ILE:H	4:B:813:SER:HB3	1.79	0.48
4:C:101:THR:HA	4:C:104:GLN:NE2	2.28	0.48
4:C:333:LYS:NZ	7:C:3010:HOH:O	2.34	0.48
4:C:349:VAL:O	4:C:349:VAL:HG12	2.13	0.48
4:C:435:GLN:HA	4:C:810:ILE:HD11	1.96	0.48
4:D:134:VAL:HG12	4:D:242:GLU:O	2.13	0.48
4:D:322:ILE:HG13	7:D:3013:HOH:O	2.13	0.48
4:D:485:ASN:O	4:D:486:HIS:C	2.57	0.48
4:D:579:ASN:HD21	4:D:625:VAL:HG12	1.79	0.48
4:D:752:LEU:HB2	4:D:753:GLY:H	1.54	0.48
4:A:77:LEU:HD11	4:A:226:MET:SD	2.54	0.47
4:A:286:TYR:CE2	4:A:417:PRO:HG3	2.49	0.47
4:A:438:ASP:OD1	4:A:507:SER:HB3	2.14	0.47
4:A:502:TRP:CG	4:A:503:ALA:N	2.81	0.47
4:A:530:CYS:HB3	4:A:818:PRO:HG2	1.96	0.47
4:A:580:GLU:HG3	7:A:3111:HOH:O	2.13	0.47
4:B:21:PHE:CD1	4:B:21:PHE:O	2.67	0.47
4:B:46:MET:HE1	4:B:269:GLN:CD	2.39	0.47
4:B:220:LEU:C	4:B:222:GLU:N	2.70	0.47
4:B:687:VAL:HG23	4:B:687:VAL:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:840:ASP:O	4:B:843:ALA:N	2.47	0.47
4:C:36:GLN:HG2	4:C:273:VAL:HG13	1.96	0.47
4:C:105:PHE:C	4:C:107:GLN:N	2.70	0.47
4:C:292:ARG:O	4:C:292:ARG:CG	2.62	0.47
4:C:397:SER:OG	4:C:398:LEU:N	2.42	0.47
4:C:421:ASP:OD2	4:C:423:ARG:NH1	2.44	0.47
4:C:657:PRO:HG2	4:C:658:ALA:H	1.79	0.47
4:C:816:THR:HG22	4:C:817:ILE:N	2.29	0.47
4:C:846:TYR:O	4:C:847:ASP:C	2.57	0.47
4:D:546:PHE:CE2	4:D:696:MET:HE2	2.49	0.47
4:D:647:ARG:O	4:D:649:GLN:N	2.47	0.47
4:D:833:VAL:HG22	4:D:875:ILE:HD12	1.95	0.47
4:A:277:PRO:HA	4:A:321:ASN:OD1	2.14	0.47
4:A:525:GLY:O	4:A:526:LEU:C	2.57	0.47
4:A:630:THR:O	4:A:631:LYS:C	2.55	0.47
4:A:632:ARG:HA	4:A:635:MET:HG2	1.96	0.47
4:B:67:ASN:O	4:B:69:ALA:N	2.47	0.47
4:B:199:GLU:O	4:B:201:TRP:N	2.41	0.47
4:B:201:TRP:CB	7:B:3009:HOH:O	2.50	0.47
4:B:296:LEU:HD11	4:B:420:MET:HE2	1.95	0.47
4:B:423:ARG:HG3	4:B:781:ASN:ND2	2.14	0.47
4:B:439:MET:HG3	4:B:509:PHE:CD2	2.49	0.47
4:B:470:VAL:O	4:B:470:VAL:CG1	2.52	0.47
4:B:501:TRP:O	4:B:505:GLN:NE2	2.47	0.47
4:B:592:ASN:OD1	4:B:592:ASN:N	2.47	0.47
4:C:416:PHE:CZ	4:C:434:PRO:HD3	2.49	0.47
4:C:831:THR:HG22	4:C:832:MET:N	2.29	0.47
4:D:120:LYS:HG3	4:D:752:LEU:CD2	2.27	0.47
4:D:445:THR:OG1	4:D:533:PRO:HD2	2.15	0.47
4:D:569:ASP:OD2	4:D:572:GLY:N	2.45	0.47
1:K:8:DG:H2"	1:K:9:DA:C8	2.49	0.47
4:A:30:GLU:OE1	4:A:30:GLU:HA	2.13	0.47
4:A:274:PRO:HD3	4:A:415:TRP:CH2	2.48	0.47
4:A:318:LYS:HE3	4:A:800:GLU:OE2	2.14	0.47
4:A:416:PHE:CE2	4:A:434:PRO:CD	2.98	0.47
4:A:751:PHE:HB3	4:A:752:LEU:HD12	1.96	0.47
4:A:829:ARG:NH2	4:A:878:SER:O	2.47	0.47
4:A:840:ASP:O	4:A:841:VAL:C	2.56	0.47
4:B:61:ALA:C	4:B:63:GLU:N	2.71	0.47
4:B:106:LEU:HD11	4:B:212:VAL:HG13	1.95	0.47
4:B:155:ARG:NE	4:B:749:LEU:HD23	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:461:LYS:HG2	4:B:482:ILE:HG21	1.96	0.47
4:B:504:GLU:HB3	7:B:3140:HOH:O	2.13	0.47
4:C:308:TYR:O	4:C:309:GLU:C	2.56	0.47
4:C:345:LYS:HZ3	4:C:352:ILE:HG12	1.78	0.47
4:C:557:ARG:HD3	7:C:3150:HOH:O	2.15	0.47
4:C:575:ALA:O	4:C:578:VAL:HB	2.13	0.47
4:C:811:HIS:CD2	4:C:811:HIS:N	2.82	0.47
4:D:345:LYS:NZ	4:D:351:ASP:O	2.43	0.47
4:D:592:ASN:OD1	4:D:611:LEU:HA	2.15	0.47
4:A:60:LYS:HG3	7:A:3125:HOH:O	2.14	0.47
4:A:418:TYR:CD2	4:A:426:VAL:CG1	2.90	0.47
4:A:617:ALA:C	4:A:621:LEU:HD12	2.40	0.47
4:B:272:VAL:CG1	4:B:411:HIS:CD2	2.98	0.47
4:C:686:SER:HA	4:C:693:VAL:HG21	1.96	0.47
4:D:830:GLU:HA	4:D:876:LEU:HD21	1.95	0.47
4:A:24:LEU:O	4:A:25:ALA:C	2.56	0.47
4:A:59:LEU:CA	4:A:64:VAL:HG22	2.41	0.47
4:A:152:GLY:O	4:A:156:ASP:OD2	2.32	0.47
4:A:559:VAL:O	4:A:560:ASN:HB2	2.14	0.47
4:A:739:TYR:HB2	4:A:774:GLN:OE1	2.14	0.47
4:B:6:ILE:HG23	4:B:10:ASP:CG	2.39	0.47
4:B:51:PHE:HE2	4:B:55:PHE:CD1	2.33	0.47
4:B:142:GLY:O	4:B:143:ARG:C	2.57	0.47
4:B:669:GLN:HB3	4:B:672:GLN:HB2	1.97	0.47
4:B:696:MET:HG2	4:B:779:ALA:HB1	1.95	0.47
4:C:161:HIS:O	4:C:164:LYS:HG2	2.14	0.47
4:C:727:TRP:NE1	4:C:782:PHE:HD1	2.11	0.47
4:D:168:GLU:O	4:D:172:LYS:HG2	2.15	0.47
4:D:677:MET:O	4:D:678:ALA:C	2.55	0.47
4:D:720:ARG:HD2	4:D:852:GLN:O	2.14	0.47
1:K:2:DG:H1'	7:K:268:HOH:O	2.14	0.47
1:K:11:DA:C2	1:K:12:DT:N3	2.83	0.47
2:L:6:G:C2	2:L:7:A:C8	3.03	0.47
3:M:4:DG:H4'	3:M:5:DA:OP1	2.15	0.47
1:N:4:DA:C6	1:N:5:DA:C6	3.02	0.47
4:A:85:ILE:HG23	4:A:219:MET:SD	2.54	0.47
4:A:313:MET:HG3	4:A:313:MET:O	2.15	0.47
4:A:473:VAL:HG13	4:A:477:GLU:HB2	1.96	0.47
4:A:477:GLU:O	4:A:480:LYS:HB3	2.13	0.47
4:A:703:ALA:O	4:A:704:LYS:C	2.57	0.47
4:A:720:ARG:O	4:A:721:LYS:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:301:SER:O	4:B:302:LYS:C	2.56	0.47
4:B:308:TYR:CA	4:B:311:VAL:HG23	2.44	0.47
4:B:634:VAL:O	4:B:637:LEU:HB2	2.14	0.47
4:B:682:TRP:CD1	4:B:682:TRP:C	2.90	0.47
4:B:726:HIS:CD2	4:B:736:TRP:CD2	3.03	0.47
4:B:794:THR:HG21	4:B:828:VAL:HA	1.97	0.47
4:C:39:LEU:HD22	4:C:272:VAL:HG23	1.95	0.47
4:C:180:LYS:O	4:C:183:MET:N	2.41	0.47
4:C:183:MET:O	4:C:186:VAL:HB	2.15	0.47
4:C:559:VAL:CG2	4:C:561:LEU:HD13	2.37	0.47
4:D:387:LYS:HE2	7:D:3158:HOH:O	2.14	0.47
4:D:631:LYS:HE2	4:D:635:MET:SD	2.55	0.47
2:I:2:C:H2'	2:I:3:G:H8	1.80	0.47
3:J:7:DT:H2''	3:J:8:DC:C6	2.49	0.47
2:L:2:C:O5'	2:L:2:C:H6	1.98	0.47
1:N:2:DG:C2'	1:N:3:DG:C8	2.95	0.47
4:A:42:GLU:O	4:A:46:MET:N	2.44	0.47
4:A:80:LYS:HE2	4:A:224:THR:HG22	1.96	0.47
4:A:99:ARG:HD2	4:A:99:ARG:N	2.29	0.47
4:A:103:PHE:O	4:A:107:GLN:NE2	2.44	0.47
4:A:141:ILE:HB	4:A:213:GLY:HA2	1.97	0.47
4:A:190:MET:HB3	7:A:3103:HOH:O	2.14	0.47
4:A:347:CYS:C	4:A:349:VAL:H	2.22	0.47
4:A:632:ARG:HH22	6:A:2000:APC:H5'2	1.79	0.47
4:A:791:LEU:HA	4:A:814:PHE:HE2	1.80	0.47
4:A:828:VAL:CB	4:A:883:ALA:HA	2.44	0.47
4:A:869:ASN:N	4:A:869:ASN:HD22	2.13	0.47
4:B:44:TYR:HD1	4:B:44:TYR:H	1.63	0.47
4:B:150:ARG:C	4:B:152:GLY:N	2.70	0.47
4:B:159:ALA:O	4:B:161:HIS:N	2.47	0.47
4:B:279:THR:HG22	7:B:3148:HOH:O	2.14	0.47
4:B:652:GLU:O	4:B:657:PRO:HD3	2.13	0.47
4:C:41:HIS:C	4:C:41:HIS:CD2	2.92	0.47
4:C:71:LYS:N	4:C:72:PRO:HD2	2.30	0.47
4:C:109:ILE:HD12	4:C:109:ILE:N	2.29	0.47
4:C:616:LEU:HD13	4:C:676:TYR:HB2	1.95	0.47
4:D:14:ILE:HD12	4:D:14:ILE:N	2.23	0.47
4:D:133:THR:C	4:D:135:GLN:N	2.71	0.47
4:D:143:ARG:O	4:D:147:ASP:OD2	2.32	0.47
4:D:236:VAL:CG2	4:D:239:GLN:HB2	2.45	0.47
4:D:326:THR:C	4:D:415:TRP:HD1	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:435:GLN:HA	4:D:810:ILE:CD1	2.43	0.47
4:D:521:VAL:O	4:D:525:GLY:N	2.46	0.47
4:D:558:ALA:CB	4:D:570:ILE:HD13	2.45	0.47
4:D:629:VAL:HG22	4:D:654:THR:HG21	1.95	0.47
4:D:797:TRP:CZ2	4:D:801:LYS:HG3	2.50	0.47
4:D:836:TYR:CD2	4:D:836:TYR:N	2.81	0.47
4:D:857:GLN:C	4:D:859:ASP:N	2.70	0.47
3:P:5:DA:H2"	3:P:6:DT:H72	1.97	0.47
4:A:6:ILE:C	4:A:8:LYS:H	2.19	0.47
4:A:86:ASN:O	4:A:90:GLU:HG2	2.15	0.47
4:A:88:TRP:HA	4:A:91:GLU:CD	2.40	0.47
4:A:280:GLY:HA2	4:A:317:TYR:HE1	1.74	0.47
4:B:39:LEU:O	4:B:40:GLU:C	2.57	0.47
4:B:305:LEU:O	4:B:306:MET:C	2.57	0.47
4:B:428:ALA:H	4:B:435:GLN:NE2	2.11	0.47
4:B:647:ARG:O	4:B:650:VAL:N	2.48	0.47
4:B:656:GLN:N	4:B:657:PRO:HD2	2.29	0.47
4:B:690:VAL:O	4:B:691:ALA:C	2.58	0.47
4:B:806:SER:O	4:B:816:THR:HG23	2.14	0.47
4:C:117:ILE:HG21	4:C:145:ILE:HD13	1.97	0.47
4:C:162:PHE:CE1	4:C:190:MET:HE2	2.50	0.47
4:C:164:LYS:C	4:C:166:VAL:H	2.22	0.47
4:C:337:VAL:HG12	4:C:338:ALA:H	1.79	0.47
4:C:417:PRO:O	4:C:418:TYR:HD1	1.98	0.47
4:C:556:GLY:C	4:C:561:LEU:HB2	2.40	0.47
4:C:579:ASN:HA	4:C:582:LEU:CG	2.45	0.47
4:C:651:LEU:HB2	4:C:674:ALA:CB	2.45	0.47
4:C:830:GLU:HA	4:C:876:LEU:HD21	1.96	0.47
4:D:113:ALA:O	4:D:114:VAL:C	2.57	0.47
4:D:159:ALA:HB3	4:D:163:LYS:HD3	1.96	0.47
4:D:308:TYR:OH	4:D:734:PRO:O	2.26	0.47
4:D:631:LYS:HD3	4:D:635:MET:SD	2.54	0.47
4:A:77:LEU:CD1	4:A:226:MET:SD	3.03	0.47
4:A:311:VAL:HG12	4:A:312:TYR:H	1.77	0.47
4:A:457:TYR:C	4:A:457:TYR:CD2	2.93	0.47
4:A:471:ASP:OD1	4:A:471:ASP:C	2.55	0.47
4:A:481:PHE:O	4:A:482:ILE:C	2.54	0.47
4:A:656:GLN:C	4:A:658:ALA:H	2.22	0.47
4:A:706:LEU:HD11	4:A:849:PHE:CG	2.50	0.47
4:A:797:TRP:CH2	4:A:801:LYS:HG3	2.50	0.47
4:B:152:GLY:C	4:B:154:ILE:N	2.72	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:381:ALA:C	4:B:383:ALA:N	2.71	0.47
4:B:485:ASN:N	4:B:485:ASN:OD1	2.44	0.47
4:B:643:GLU:O	4:B:644:PHE:C	2.56	0.47
4:B:778:ILE:O	4:B:778:ILE:HG13	2.14	0.47
4:C:161:HIS:O	4:C:162:PHE:C	2.58	0.47
4:C:400:PHE:CZ	4:C:431:MET:CE	2.96	0.47
4:C:452:ILE:HG23	4:C:453:GLY:N	2.29	0.47
4:C:517:GLU:OE1	4:C:517:GLU:HA	2.14	0.47
4:D:374:LEU:O	4:D:378:LYS:HB2	2.14	0.47
4:D:416:PHE:O	4:D:418:TYR:CE1	2.68	0.47
4:B:205:HIS:C	4:B:207:GLU:N	2.72	0.47
4:B:492:CYS:SG	4:B:502:TRP:HB3	2.55	0.47
4:B:504:GLU:C	4:B:505:GLN:O	2.56	0.47
4:B:567:VAL:HG13	4:B:880:PHE:CD2	2.50	0.47
4:C:274:PRO:HA	4:C:275:PRO:HD3	1.77	0.47
4:C:314:PRO:HD3	7:C:3099:HOH:O	2.13	0.47
4:C:727:TRP:HB3	4:C:845:PHE:CE1	2.50	0.47
4:C:746:ARG:NH1	4:C:754:GLN:O	2.47	0.47
4:D:419:ASN:ND2	4:D:429:VAL:HG22	2.30	0.47
1:E:14:DG:C2'	1:E:15:DC:H6	2.28	0.46
3:G:4:DG:C1'	3:G:5:DA:C8	2.98	0.46
4:A:333:LYS:O	4:A:334:VAL:C	2.58	0.46
4:A:420:MET:HA	4:A:425:ARG:O	2.15	0.46
4:A:439:MET:HG3	4:A:509:PHE:CE2	2.49	0.46
4:A:647:ARG:CG	4:A:675:GLY:HA2	2.45	0.46
4:A:711:LYS:CB	4:A:711:LYS:NZ	2.78	0.46
4:B:36:GLN:OE1	4:B:36:GLN:CA	2.63	0.46
4:B:150:ARG:C	4:B:152:GLY:H	2.23	0.46
4:B:267:MET:HE3	4:B:431:MET:SD	2.55	0.46
4:B:403:GLU:O	4:B:405:ALA:N	2.48	0.46
4:B:570:ILE:O	4:B:570:ILE:HG13	2.14	0.46
4:B:675:GLY:O	4:B:678:ALA:HB3	2.15	0.46
4:B:729:THR:HB	4:B:789:SER:HB2	1.96	0.46
4:C:4:ILE:CD1	7:C:3146:HOH:O	2.62	0.46
4:C:9:ASN:C	4:C:12:SER:HB3	2.40	0.46
4:C:216:CYS:O	4:C:217:ILE:C	2.57	0.46
4:C:404:GLN:HE21	4:C:404:GLN:CA	2.15	0.46
4:C:553:GLU:CD	4:C:553:GLU:N	2.71	0.46
4:C:845:PHE:O	4:C:846:TYR:C	2.58	0.46
4:D:150:ARG:HH21	4:D:187:GLU:CD	2.22	0.46
4:D:631:LYS:HE2	6:D:2003:APC:H3A2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:706:LEU:CD2	4:D:853:LEU:HD23	2.44	0.46
4:D:782:PHE:CE2	4:D:786:GLN:OE1	2.68	0.46
4:D:823:ASN:O	4:D:826:LYS:N	2.48	0.46
1:H:12:DT:C2'	1:H:13:DC:C6	2.98	0.46
4:A:254:ILE:O	4:A:255:ALA:C	2.58	0.46
4:A:308:TYR:CE2	4:A:736:TRP:CZ3	3.03	0.46
4:A:311:VAL:CG1	4:A:312:TYR:N	2.77	0.46
4:A:410:ASN:HD22	4:A:410:ASN:N	2.12	0.46
4:B:247:ALA:CB	4:B:250:TYR:CD1	2.99	0.46
4:B:268:PHE:CD2	4:B:429:VAL:HG12	2.51	0.46
4:B:787:ASP:O	4:B:790:HIS:N	2.48	0.46
4:C:84:ARG:HD2	4:C:222:GLU:OE1	2.14	0.46
4:C:140:ALA:O	4:C:143:ARG:N	2.48	0.46
4:C:246:LEU:HG	4:C:247:ALA:N	2.29	0.46
4:C:260:ALA:O	4:C:261:LEU:C	2.59	0.46
4:C:391:ARG:O	4:C:391:ARG:HG2	2.14	0.46
4:C:598:THR:OG1	4:C:605:ILE:HD13	2.16	0.46
4:C:623:TYR:HD1	4:C:663:LYS:HE2	1.80	0.46
4:D:828:VAL:O	4:D:831:THR:HG22	2.16	0.46
2:F:7:A:H2'	2:F:8:U:C6	2.46	0.46
4:A:21:PHE:C	4:A:23:THR:H	2.23	0.46
4:A:347:CYS:HB3	4:A:350:GLU:CG	2.45	0.46
4:A:347:CYS:HB3	4:A:350:GLU:HB2	1.97	0.46
4:A:403:GLU:O	4:A:406:ASN:N	2.48	0.46
4:A:473:VAL:HA	4:A:474:PRO:HD2	1.62	0.46
4:A:489:ILE:O	4:A:490:MET:C	2.56	0.46
4:A:711:LYS:NZ	4:A:711:LYS:HB2	2.30	0.46
4:C:385:TYR:O	4:C:386:ARG:C	2.56	0.46
4:C:416:PHE:HB2	4:C:418:TYR:CE1	2.51	0.46
4:C:450:LYS:HD2	4:C:817:ILE:CD1	2.46	0.46
4:C:659:ILE:HG22	4:C:660:ASP:N	2.29	0.46
4:D:21:PHE:CD1	4:D:21:PHE:O	2.68	0.46
4:D:373:ALA:O	4:D:377:TRP:CD1	2.68	0.46
4:D:739:TYR:CD2	4:D:774:GLN:HA	2.50	0.46
4:D:784:HIS:O	4:D:787:ASP:N	2.49	0.46
4:A:59:LEU:HD23	4:A:64:VAL:CG1	2.46	0.46
4:A:281:ILE:HG22	4:A:282:THR:HG22	1.86	0.46
4:A:796:VAL:O	4:A:799:HIS:N	2.40	0.46
4:B:324:GLN:HG3	4:B:418:TYR:H	1.80	0.46
4:B:450:LYS:HB3	4:B:819:ALA:CB	2.45	0.46
4:B:472:LYS:C	4:B:567:VAL:HG21	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:520:GLY:HA3	4:B:528:TYR:CE1	2.50	0.46
4:B:823:ASN:C	4:B:825:PHE:N	2.70	0.46
4:C:92:VAL:HG12	4:C:92:VAL:O	2.15	0.46
4:C:729:THR:O	4:C:732:GLY:N	2.29	0.46
4:D:390:ALA:CB	4:D:394:ARG:HH21	2.28	0.46
4:D:684:SER:O	4:D:687:VAL:HG22	2.16	0.46
3:M:9:DC:H2''	7:M:350:HOH:O	2.15	0.46
1:N:12:DT:C2'	1:N:13:DC:H5'	2.22	0.46
4:A:89:PHE:HZ	4:A:106:LEU:O	1.99	0.46
4:A:261:LEU:C	4:A:263:GLY:N	2.72	0.46
4:A:274:PRO:HA	4:A:415:TRP:CG	2.50	0.46
4:A:646:PHE:O	4:A:647:ARG:O	2.33	0.46
4:A:726:HIS:CD2	4:A:736:TRP:CE2	3.03	0.46
4:B:158:GLU:HA	4:B:195:LEU:CD1	2.42	0.46
4:B:250:TYR:O	4:B:251:ALA:C	2.59	0.46
4:C:165:ASN:ND2	7:C:3138:HOH:O	2.48	0.46
4:C:475:PHE:N	4:C:476:PRO:CD	2.78	0.46
4:C:549:MET:CE	4:C:786:GLN:HG2	2.46	0.46
4:C:698:TRP:O	4:C:701:SER:HB2	2.16	0.46
4:C:727:TRP:CD1	4:C:782:PHE:HE1	2.33	0.46
4:D:328:TRP:CG	4:D:416:PHE:HE2	2.33	0.46
4:D:588:ASN:O	4:D:614:LYS:HG3	2.15	0.46
4:D:593:GLU:O	4:D:610:LYS:HB3	2.16	0.46
4:D:632:ARG:HG2	4:D:653:ASP:OD2	2.15	0.46
4:D:797:TRP:HD1	4:D:827:ALA:HB1	1.81	0.46
3:G:1:DG:H1'	3:G:2:DT:H72	1.98	0.46
1:H:3:DG:N2	3:J:9:DC:O2	2.48	0.46
4:A:109:ILE:HG12	4:A:148:GLU:HB3	1.97	0.46
4:A:520:GLY:HA3	4:A:528:TYR:CE2	2.50	0.46
4:A:727:TRP:CH2	4:A:735:VAL:CG2	2.99	0.46
4:B:60:LYS:O	4:B:60:LYS:HG2	2.15	0.46
4:B:459:TRP:CH2	4:B:825:PHE:CD2	3.04	0.46
4:B:556:GLY:C	4:B:558:ALA:N	2.72	0.46
4:C:82:ILE:HA	4:C:85:ILE:HD12	1.96	0.46
4:C:268:PHE:O	4:C:430:SER:HB2	2.15	0.46
4:C:329:LYS:HD3	4:C:447:ALA:HA	1.98	0.46
4:C:655:ILE:O	4:C:655:ILE:HG22	2.15	0.46
4:C:754:GLN:HB3	4:C:755:PHE:HD1	1.80	0.46
4:C:788:GLY:C	4:C:792:ARG:HH12	2.24	0.46
4:C:829:ARG:NH2	4:C:878:SER:O	2.47	0.46
4:D:81:MET:O	4:D:85:ILE:HG13	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:89:PHE:CZ	4:D:106:LEU:HB3	2.46	0.46
4:D:476:PRO:HG2	4:D:477:GLU:OE2	2.15	0.46
4:D:613:THR:HG22	4:D:676:TYR:CE1	2.51	0.46
4:A:139:SER:HB2	4:A:210:ILE:CD1	2.46	0.46
4:A:446:LEU:HD12	4:A:531:SER:O	2.15	0.46
4:A:502:TRP:CG	4:A:503:ALA:H	2.34	0.46
4:A:577:LYS:HB3	4:A:684:SER:OG	2.15	0.46
4:A:829:ARG:NH1	4:A:829:ARG:CG	2.57	0.46
4:B:11:PHE:C	4:B:13:ASP:N	2.73	0.46
4:B:172:LYS:NZ	4:B:172:LYS:CB	2.70	0.46
4:B:451:PRO:O	4:B:452:ILE:C	2.58	0.46
4:B:482:ILE:O	4:B:485:ASN:N	2.48	0.46
4:B:569:ASP:CG	4:B:569:ASP:O	2.58	0.46
4:B:680:LEU:H	4:B:680:LEU:CD1	2.29	0.46
4:B:748:ASN:ND2	4:B:751:PHE:N	2.60	0.46
4:C:349:VAL:HG13	4:C:503:ALA:O	2.16	0.46
4:C:551:ARG:HH12	4:C:867:LYS:HZ3	1.63	0.46
4:C:577:LYS:O	4:C:581:ILE:HG13	2.15	0.46
4:C:827:ALA:O	4:C:828:VAL:C	2.54	0.46
4:C:840:ASP:OD2	4:C:867:LYS:NZ	2.49	0.46
4:D:122:THR:O	4:D:125:CYS:N	2.48	0.46
4:D:422:TRP:CD1	4:D:422:TRP:O	2.69	0.46
4:A:112:GLU:CD	4:A:112:GLU:N	2.74	0.46
4:A:230:HIS:CE1	4:A:232:GLN:HE21	2.34	0.46
4:A:303:LYS:HE2	4:A:740:LYS:HZ1	1.81	0.46
4:A:404:GLN:NE2	4:A:404:GLN:CA	2.73	0.46
4:A:429:VAL:O	4:A:430:SER:O	2.33	0.46
4:A:517:GLU:OE1	4:A:517:GLU:HA	2.16	0.46
4:B:55:PHE:HE2	4:B:59:LEU:HD11	1.79	0.46
4:B:105:PHE:O	4:B:107:GLN:N	2.49	0.46
4:B:229:LEU:CD1	4:B:242:GLU:HG2	2.41	0.46
4:B:460:LEU:HD12	4:B:460:LEU:O	2.15	0.46
4:B:475:PHE:HB2	4:B:476:PRO:HD2	1.98	0.46
4:B:556:GLY:HA2	4:B:561:LEU:HD13	1.98	0.46
4:B:612:GLY:O	4:B:613:THR:C	2.58	0.46
4:B:615:ALA:O	4:B:616:LEU:C	2.58	0.46
4:B:727:TRP:CZ2	4:B:782:PHE:HA	2.51	0.46
4:C:43:SER:HA	4:C:46:MET:HE3	1.97	0.46
4:D:55:PHE:CZ	4:D:59:LEU:HD11	2.51	0.46
4:D:221:ILE:HG23	4:D:227:VAL:O	2.16	0.46
4:D:502:TRP:CG	4:D:512:LEU:HD13	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:825:PHE:O	4:D:828:VAL:HG23	2.16	0.46
4:A:689:VAL:C	4:A:691:ALA:N	2.72	0.46
4:B:164:LYS:N	4:B:164:LYS:HZ2	2.13	0.46
4:B:408:PHE:CD1	4:B:414:ILE:HG21	2.31	0.46
4:B:475:PHE:C	4:B:477:GLU:N	2.74	0.46
4:C:257:ARG:HG2	4:C:257:ARG:HH11	1.81	0.46
4:C:319:ALA:HB2	4:C:792:ARG:HB3	1.97	0.46
4:C:418:TYR:HD2	4:C:426:VAL:HG11	1.80	0.46
4:C:435:GLN:HG2	4:C:810:ILE:HG12	1.97	0.46
4:C:506:ASP:O	4:C:508:PRO:HD2	2.15	0.46
4:C:534:LEU:CD1	4:C:818:PRO:HA	2.46	0.46
4:C:786:GLN:O	4:C:788:GLY:N	2.49	0.46
4:C:848:GLN:OE1	4:C:848:GLN:HA	2.15	0.46
4:D:133:THR:C	4:D:135:GLN:H	2.22	0.46
4:D:261:LEU:C	4:D:263:GLY:H	2.23	0.46
4:D:281:ILE:HG12	4:D:309:GLU:HA	1.97	0.46
4:D:440:THR:C	4:D:442:GLY:N	2.74	0.46
4:D:470:VAL:CG1	4:D:473:VAL:HG11	2.40	0.46
4:D:543:ILE:HG21	4:D:689:VAL:CG1	2.45	0.46
4:D:744:GLN:HB3	4:D:756:ARG:CB	2.45	0.46
4:A:42:GLU:HG2	4:A:46:MET:CE	2.42	0.46
4:A:147:ASP:HB3	4:A:750:MET:CE	2.46	0.46
4:A:290:GLY:C	4:A:292:ARG:H	2.24	0.46
4:A:404:GLN:O	4:A:407:LYS:HB3	2.16	0.46
4:A:511:PHE:CD2	4:A:511:PHE:C	2.93	0.46
4:A:746:ARG:HB3	4:A:746:ARG:CZ	2.45	0.46
4:A:831:THR:CG2	4:A:832:MET:N	2.78	0.46
4:B:72:PRO:HG3	4:B:257:ARG:HG3	1.97	0.46
4:B:163:LYS:HA	4:B:163:LYS:HD2	1.71	0.46
4:B:433:ASN:HB2	4:B:434:PRO:HD2	1.88	0.46
4:B:459:TRP:O	4:B:460:LEU:C	2.56	0.46
4:C:14:ILE:CG2	4:C:288:ALA:CB	2.91	0.46
4:C:322:ILE:O	4:C:323:ALA:C	2.59	0.46
4:C:393:SER:C	4:C:395:ARG:H	2.24	0.46
4:C:462:ILE:CD1	4:C:479:ILE:HD11	2.45	0.46
4:C:646:PHE:HD1	4:C:649:GLN:OE1	1.99	0.46
4:C:809:LEU:HA	4:C:813:SER:O	2.17	0.46
4:D:135:GLN:HB3	7:D:3160:HOH:O	2.15	0.46
4:D:139:SER:CB	4:D:210:ILE:HD13	2.45	0.46
4:D:182:PHE:O	4:D:186:VAL:HG23	2.16	0.46
4:D:468:ALA:HB2	4:D:511:PHE:CE1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:699:LEU:HD11	4:D:782:PHE:CD2	2.50	0.46
1:K:15:DC:H6	1:K:15:DC:C5'	2.28	0.45
4:A:374:LEU:C	4:A:376:ALA:N	2.74	0.45
4:A:480:LYS:HG3	4:A:484:GLU:OE1	2.16	0.45
4:A:678:ALA:O	4:A:679:LYS:C	2.59	0.45
4:B:163:LYS:HB3	4:B:164:LYS:HZ2	1.79	0.45
4:B:164:LYS:HD3	4:B:164:LYS:HA	1.78	0.45
4:B:620:TRP:CD2	4:B:677:MET:CE	2.99	0.45
4:B:705:LEU:C	4:B:707:ALA:N	2.75	0.45
4:B:797:TRP:CZ2	4:B:801:LYS:HG3	2.51	0.45
4:C:89:PHE:CZ	4:C:106:LEU:O	2.68	0.45
4:C:148:GLU:OE1	4:C:749:LEU:HB2	2.15	0.45
4:C:490:MET:HE3	4:C:490:MET:CA	2.46	0.45
4:C:551:ARG:HE	4:C:872:LEU:HD11	1.80	0.45
4:C:617:ALA:O	4:C:618:GLY:C	2.58	0.45
4:D:236:VAL:O	4:D:240:ASP:CB	2.64	0.45
4:D:460:LEU:HD13	4:D:532:LEU:HD23	1.97	0.45
1:E:4:DA:H2''	1:E:5:DA:OP2	2.15	0.45
1:H:9:DA:H62	3:J:1:DG:H22	1.64	0.45
1:K:2:DG:H2''	1:K:3:DG:C8	2.52	0.45
2:L:1:G:C2	2:L:2:C:C2	3.04	0.45
4:A:92:VAL:CG1	4:A:99:ARG:HG3	2.45	0.45
4:A:386:ARG:C	4:A:388:ASP:H	2.25	0.45
4:A:701:SER:O	4:A:702:ALA:C	2.59	0.45
4:A:704:LYS:HE3	4:A:860:LYS:CE	2.46	0.45
4:A:798:ALA:HB1	4:A:804:ILE:HD12	1.98	0.45
4:A:801:LYS:HD3	4:A:801:LYS:O	2.13	0.45
4:B:257:ARG:HG2	4:B:257:ARG:NH1	2.30	0.45
4:B:279:THR:HG23	4:B:279:THR:O	2.15	0.45
4:B:373:ALA:O	4:B:377:TRP:CD1	2.70	0.45
4:B:384:VAL:O	4:B:384:VAL:HG12	2.16	0.45
4:B:636:THR:O	4:B:637:LEU:C	2.59	0.45
4:C:110:LYS:O	4:C:114:VAL:HG23	2.16	0.45
4:C:301:SER:O	4:C:302:LYS:C	2.59	0.45
4:C:334:VAL:O	4:C:337:VAL:HB	2.16	0.45
4:C:395:ARG:O	4:C:396:ILE:C	2.58	0.45
4:C:432:PHE:HE1	4:C:440:THR:HG23	1.81	0.45
4:C:437:ASN:ND2	4:C:440:THR:H	2.13	0.45
4:C:882:PHE:O	4:C:883:ALA:CB	2.64	0.45
4:D:12:SER:O	4:D:13:ASP:C	2.59	0.45
4:D:501:TRP:HA	4:D:504:GLU:OE2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:705:LEU:HB3	4:D:857:GLN:HE22	1.78	0.45
1:H:14:DG:H5'	1:H:14:DG:H8	1.82	0.45
4:A:153:ARG:HD2	7:A:3089:HOH:O	2.17	0.45
4:A:183:MET:HE2	4:A:183:MET:HA	1.98	0.45
4:A:261:LEU:O	4:A:263:GLY:N	2.50	0.45
4:A:416:PHE:HA	4:A:417:PRO:HD2	1.75	0.45
4:A:825:PHE:C	4:A:825:PHE:HD1	2.22	0.45
4:B:552:ASP:HB3	4:B:691:ALA:HB2	1.99	0.45
4:B:645:GLY:O	4:B:646:PHE:C	2.59	0.45
4:C:452:ILE:HG13	4:C:456:GLY:C	2.41	0.45
4:C:556:GLY:HA3	4:C:561:LEU:HD22	1.91	0.45
4:C:567:VAL:O	4:C:567:VAL:HG12	2.15	0.45
4:C:656:GLN:H	4:C:657:PRO:HD2	1.78	0.45
4:C:702:ALA:O	4:C:703:ALA:C	2.56	0.45
4:D:47:GLY:HA3	4:D:265:SER:O	2.16	0.45
4:D:126:LEU:HD11	4:D:227:VAL:HG12	1.97	0.45
4:D:342:THR:CG2	4:D:348:PRO:HG2	2.41	0.45
4:D:440:THR:O	4:D:444:LEU:HD12	2.16	0.45
4:D:656:GLN:N	4:D:657:PRO:CD	2.77	0.45
4:D:696:MET:O	4:D:700:LYS:HB2	2.16	0.45
4:D:704:LYS:HE3	4:D:860:LYS:NZ	2.32	0.45
4:D:709:GLU:O	4:D:711:LYS:HG3	2.16	0.45
4:D:827:ALA:O	4:D:828:VAL:C	2.59	0.45
4:D:840:ASP:C	4:D:842:LEU:H	2.23	0.45
1:E:2:DG:C2	7:E:42:HOH:O	2.56	0.45
4:A:145:ILE:HG12	4:A:145:ILE:H	1.55	0.45
4:A:281:ILE:HG13	4:A:309:GLU:HG2	1.98	0.45
4:A:304:ALA:C	4:A:307:ARG:HG3	2.36	0.45
4:A:341:ILE:O	4:A:342:THR:C	2.58	0.45
4:B:232:GLN:HG3	4:B:243:THR:HG23	1.98	0.45
4:B:577:LYS:O	4:B:580:GLU:HB2	2.16	0.45
4:B:633:SER:O	4:B:634:VAL:C	2.54	0.45
4:B:770:ASP:OD2	4:B:773:LYS:HD2	2.17	0.45
4:C:425:ARG:NH2	4:C:787:ASP:OD2	2.49	0.45
4:D:417:PRO:C	4:D:429:VAL:HG23	2.40	0.45
4:D:459:TRP:O	4:D:460:LEU:C	2.56	0.45
4:D:669:GLN:HG3	4:D:672:GLN:HE21	1.80	0.45
3:J:5:DA:C2'	3:J:6:DT:H72	2.47	0.45
2:L:4:G:H1'	4:C:389:LYS:HZ1	1.80	0.45
4:A:278:TRP:CD2	4:A:284:GLY:HA3	2.49	0.45
4:A:462:ILE:HG22	4:A:463:HIS:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:664:GLY:O	4:A:667:PHE:HB2	2.17	0.45
4:B:225:GLY:HA2	7:B:3035:HOH:O	2.16	0.45
4:B:685:VAL:O	4:B:687:VAL:N	2.49	0.45
4:C:164:LYS:NZ	4:C:164:LYS:N	2.64	0.45
4:C:814:PHE:CE1	4:C:883:ALA:HB1	2.52	0.45
4:D:42:GLU:O	4:D:45:GLU:N	2.50	0.45
4:D:322:ILE:HG21	7:D:3013:HOH:O	2.16	0.45
4:D:678:ALA:O	4:D:679:LYS:C	2.59	0.45
1:K:12:DT:N3	1:K:13:DC:C5	2.85	0.45
1:K:16:DC:H2''	1:K:17:DG:O5'	2.15	0.45
7:M:542:HOH:O	4:C:164:LYS:HB3	2.16	0.45
4:A:109:ILE:HG13	4:A:149:ALA:CB	2.46	0.45
4:A:148:GLU:OE2	4:A:749:LEU:HB2	2.15	0.45
4:A:208:ASP:OD2	4:A:208:ASP:N	2.50	0.45
4:A:330:ILE:HA	4:A:330:ILE:HD13	1.39	0.45
4:A:416:PHE:CZ	4:A:434:PRO:HD3	2.51	0.45
4:A:423:ARG:O	4:A:785:SER:HB2	2.16	0.45
4:A:518:TYR:O	4:A:518:TYR:HD1	1.98	0.45
4:A:746:ARG:NH1	4:A:754:GLN:H	2.11	0.45
4:B:404:GLN:HE21	4:B:404:GLN:HB2	1.35	0.45
4:B:436:GLY:O	4:B:441:LYS:HE2	2.15	0.45
4:B:552:ASP:CB	4:B:691:ALA:HB2	2.46	0.45
4:D:6:ILE:O	4:D:8:LYS:N	2.39	0.45
4:D:316:VAL:HG22	4:D:731:ASP:OD2	2.15	0.45
4:D:322:ILE:HD13	4:D:322:ILE:HA	1.79	0.45
4:D:437:ASN:ND2	4:D:437:ASN:C	2.75	0.45
1:H:9:DA:C6	4:B:644:PHE:CE1	3.04	0.45
4:A:39:LEU:O	4:A:40:GLU:C	2.60	0.45
4:B:36:GLN:HB3	4:B:37:LEU:HD12	1.97	0.45
4:B:105:PHE:C	4:B:107:GLN:N	2.75	0.45
4:B:252:GLU:O	4:B:253:ALA:C	2.58	0.45
4:B:334:VAL:CG1	4:B:443:LEU:HD23	2.46	0.45
4:B:402:LEU:HD23	4:B:402:LEU:HA	1.45	0.45
4:B:418:TYR:HE1	7:B:3028:HOH:O	1.99	0.45
4:B:455:GLU:O	4:B:458:TYR:HB3	2.16	0.45
4:B:459:TRP:HH2	4:B:825:PHE:CE2	2.34	0.45
4:B:726:HIS:HB2	4:B:736:TRP:CD1	2.52	0.45
4:B:790:HIS:C	4:B:790:HIS:HD1	2.24	0.45
4:B:804:ILE:HG22	4:B:807:PHE:CE2	2.52	0.45
4:C:279:THR:CG2	7:C:3038:HOH:O	2.59	0.45
4:D:84:ARG:HH11	4:D:84:ARG:HA	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:302:LYS:HE3	4:D:306:MET:CE	2.38	0.45
4:D:508:PRO:C	4:D:510:CYS:N	2.73	0.45
4:D:563:PRO:HB3	4:D:877:GLU:C	2.42	0.45
4:D:633:SER:HA	4:D:649:GLN:HE22	1.82	0.45
4:D:859:ASP:OD2	4:D:860:LYS:N	2.50	0.45
1:H:15:DC:H3'	7:H:334:HOH:O	2.16	0.45
4:A:473:VAL:O	4:A:473:VAL:HG13	2.17	0.45
4:A:868:GLY:C	4:A:869:ASN:HD22	2.25	0.45
4:B:19:ILE:O	4:B:21:PHE:N	2.42	0.45
4:C:269:GLN:HE21	4:C:269:GLN:HB3	1.56	0.45
4:C:525:GLY:C	4:C:527:SER:H	2.24	0.45
4:C:786:GLN:C	4:C:788:GLY:N	2.75	0.45
4:D:246:LEU:HD23	4:D:247:ALA:O	2.17	0.45
4:D:462:ILE:HD12	4:D:475:PHE:HD1	1.82	0.45
3:G:4:DG:H2''	3:G:5:DA:H8	1.81	0.45
1:H:10:DT:H5'	4:B:641:SER:H	1.79	0.45
1:N:10:DT:H5'	4:D:641:SER:CB	2.46	0.45
4:A:576:LYS:C	4:A:578:VAL:N	2.74	0.45
4:A:619:GLN:O	4:A:620:TRP:C	2.59	0.45
4:A:635:MET:HE2	6:A:2000:APC:H2'	1.98	0.45
4:B:205:HIS:O	4:B:207:GLU:N	2.50	0.45
4:B:419:ASN:O	4:B:420:MET:CG	2.65	0.45
4:B:702:ALA:O	4:B:703:ALA:C	2.60	0.45
4:B:864:LEU:O	4:B:865:PRO:C	2.59	0.45
4:C:287:TRP:O	4:C:288:ALA:O	2.35	0.45
4:C:502:TRP:C	4:C:504:GLU:H	2.24	0.45
4:C:507:SER:HA	4:C:508:PRO:HD2	1.62	0.45
4:C:849:PHE:O	4:C:852:GLN:HB2	2.17	0.45
4:D:5:ASN:HA	4:D:52:ARG:NH1	2.32	0.45
4:D:487:GLU:O	4:D:488:ASN:C	2.59	0.45
4:D:540:CYS:C	4:D:542:GLY:N	2.73	0.45
4:D:829:ARG:HH12	4:D:883:ALA:H	1.64	0.45
1:E:6:DT:H6	1:E:6:DT:H2'	1.55	0.45
1:H:15:DC:N3	1:H:16:DC:C5	2.85	0.45
1:H:18:DC:H2''	4:B:63:GLU:CD	2.41	0.45
4:A:8:LYS:O	4:A:12:SER:HB2	2.16	0.45
4:A:60:LYS:HG3	7:A:3023:HOH:O	2.16	0.45
4:A:401:MET:O	4:A:402:LEU:C	2.59	0.45
4:A:688:THR:CG2	4:A:689:VAL:HG13	2.30	0.45
4:B:50:ARG:HH11	4:B:50:ARG:HG2	1.82	0.45
4:B:114:VAL:O	4:B:115:ALA:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3:THR:HB	4:C:52:ARG:CZ	2.46	0.45
4:C:329:LYS:HG3	4:C:445:THR:HG22	1.99	0.45
4:C:432:PHE:CE1	4:C:440:THR:HG23	2.51	0.45
4:C:553:GLU:CG	4:C:554:VAL:N	2.80	0.45
4:D:331:ASN:ND2	4:D:334:VAL:HG23	2.32	0.45
4:D:502:TRP:CE3	4:D:503:ALA:N	2.85	0.45
4:D:816:THR:HG22	4:D:817:ILE:N	2.32	0.45
4:A:47:GLY:HA3	4:A:265:SER:O	2.18	0.44
4:A:554:VAL:O	4:A:557:ARG:HB3	2.17	0.44
4:B:138:ALA:O	4:B:213:GLY:HA3	2.17	0.44
4:B:164:LYS:N	4:B:164:LYS:HZ3	2.15	0.44
4:B:347:CYS:HB3	4:B:350:GLU:HG3	1.99	0.44
4:B:532:LEU:HG	4:B:533:PRO:CD	2.47	0.44
4:B:571:TYR:HD1	4:B:571:TYR:H	1.65	0.44
4:B:579:ASN:HA	4:B:582:LEU:HB2	1.98	0.44
4:B:643:GLU:HG3	4:B:682:TRP:HB3	1.99	0.44
4:B:875:ILE:C	4:B:877:GLU:H	2.25	0.44
4:C:488:ASN:O	4:C:491:ALA:HB3	2.16	0.44
4:C:845:PHE:O	4:C:848:GLN:CB	2.57	0.44
4:D:729:THR:HG23	4:D:733:PHE:O	2.17	0.44
4:A:19:ILE:HD13	4:A:19:ILE:HA	1.89	0.44
4:A:572:GLY:O	4:A:575:ALA:HB3	2.18	0.44
4:B:404:GLN:O	4:B:404:GLN:HG3	2.17	0.44
4:B:416:PHE:HD1	4:B:430:SER:OG	2.01	0.44
4:B:570:ILE:HA	4:B:573:ILE:HG22	1.98	0.44
4:B:640:GLY:O	4:B:641:SER:O	2.36	0.44
4:B:643:GLU:HG3	4:B:682:TRP:CB	2.47	0.44
4:C:71:LYS:N	4:C:72:PRO:CD	2.81	0.44
4:C:210:ILE:O	4:C:214:VAL:CG2	2.63	0.44
4:C:313:MET:O	4:C:317:TYR:CD2	2.70	0.44
4:C:323:ALA:O	4:C:325:ASN:N	2.49	0.44
4:C:460:LEU:O	4:C:514:PHE:CE2	2.70	0.44
4:D:340:VAL:O	4:D:343:LYS:HG2	2.17	0.44
4:D:511:PHE:O	4:D:514:PHE:HB3	2.16	0.44
4:D:620:TRP:O	4:D:621:LEU:C	2.57	0.44
4:D:631:LYS:HD2	4:D:632:ARG:NH1	2.32	0.44
4:A:56:GLU:HB2	7:A:3057:HOH:O	2.17	0.44
4:A:116:TYR:O	4:A:117:ILE:C	2.60	0.44
4:A:333:LYS:HB3	4:A:516:PHE:CE2	2.52	0.44
4:A:739:TYR:CD2	4:A:773:LYS:HB3	2.52	0.44
4:A:746:ARG:HB3	4:A:746:ARG:NH1	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:469:GLY:C	4:B:471:ASP:N	2.68	0.44
4:B:473:VAL:HG12	4:B:474:PRO:O	2.18	0.44
4:C:14:ILE:O	4:C:14:ILE:HG22	2.18	0.44
4:C:155:ARG:O	4:C:155:ARG:CG	2.65	0.44
4:C:617:ALA:O	4:C:621:LEU:HG	2.18	0.44
4:C:620:TRP:CZ3	4:C:667:PHE:HZ	2.35	0.44
4:C:647:ARG:O	4:C:648:GLN:C	2.60	0.44
4:D:64:VAL:C	4:D:66:ASP:H	2.25	0.44
4:D:327:ALA:CA	4:D:415:TRP:NE1	2.81	0.44
4:D:439:MET:CE	4:D:443:LEU:HD11	2.47	0.44
4:D:443:LEU:HD23	4:D:443:LEU:H	1.81	0.44
4:D:704:LYS:HE3	4:D:860:LYS:HZ1	1.82	0.44
4:D:706:LEU:HD21	4:D:849:PHE:CD2	2.53	0.44
2:F:4:G:H4'	4:A:389:LYS:HD3	1.99	0.44
1:K:6:DT:C6	1:K:6:DT:H5'	2.52	0.44
1:K:15:DC:H2''	1:K:16:DC:C5'	2.46	0.44
4:A:308:TYR:OH	4:A:733:PHE:CE2	2.70	0.44
4:A:846:TYR:HD1	4:A:850:ALA:HB2	1.82	0.44
4:B:19:ILE:HD13	4:B:20:PRO:HD2	1.98	0.44
4:B:169:GLN:HE21	4:B:169:GLN:HB3	1.51	0.44
4:B:460:LEU:CA	4:B:534:LEU:HD11	2.48	0.44
4:B:570:ILE:O	4:B:570:ILE:CG1	2.59	0.44
4:B:609:VAL:O	4:B:609:VAL:HG22	2.17	0.44
4:C:164:LYS:HZ3	4:C:164:LYS:N	2.16	0.44
4:C:403:GLU:C	4:C:403:GLU:CD	2.85	0.44
4:C:536:PHE:HB3	4:C:882:PHE:HB2	1.94	0.44
4:C:728:VAL:CG2	4:C:734:PRO:HB3	2.47	0.44
4:C:772:HIS:O	4:C:773:LYS:C	2.60	0.44
4:D:49:ALA:O	4:D:52:ARG:HB2	2.17	0.44
4:D:258:ALA:O	4:D:259:GLY:C	2.59	0.44
4:D:300:HIS:HA	7:D:3088:HOH:O	2.17	0.44
4:D:318:LYS:O	4:D:319:ALA:C	2.60	0.44
4:D:502:TRP:CZ3	4:D:503:ALA:HB2	2.52	0.44
4:D:795:VAL:HG12	7:D:3013:HOH:O	2.18	0.44
4:D:859:ASP:C	4:D:861:MET:N	2.75	0.44
1:H:15:DC:OP1	7:H:313:HOH:O	2.21	0.44
4:A:86:ASN:HD22	4:A:86:ASN:N	2.15	0.44
4:A:286:TYR:N	4:A:286:TYR:CD2	2.86	0.44
4:A:400:PHE:O	4:A:401:MET:O	2.36	0.44
4:A:463:HIS:C	4:A:465:ALA:N	2.76	0.44
4:A:631:LYS:NZ	6:A:2000:APC:O2A	2.39	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:340:VAL:O	4:B:343:LYS:HG3	2.17	0.44
4:B:421:ASP:OD2	4:B:425:ARG:HB2	2.17	0.44
4:B:640:GLY:O	4:B:641:SER:C	2.59	0.44
4:B:665:LEU:HA	4:B:665:LEU:HD23	1.82	0.44
4:D:482:ILE:HD12	4:D:514:PHE:HZ	1.83	0.44
4:D:646:PHE:HA	4:D:649:GLN:OE1	2.17	0.44
4:D:651:LEU:HD13	4:D:651:LEU:C	2.41	0.44
4:D:770:ASP:O	4:D:771:ALA:C	2.59	0.44
4:D:828:VAL:C	4:D:831:THR:HG22	2.43	0.44
1:K:13:DC:C2'	1:K:14:DG:H5'	2.45	0.44
4:A:16:LEU:HA	4:A:37:LEU:CD2	2.46	0.44
4:A:199:GLU:C	4:A:201:TRP:H	2.25	0.44
4:A:264:ILE:HG22	4:A:264:ILE:O	2.18	0.44
4:A:659:ILE:C	4:A:661:SER:H	2.24	0.44
4:A:699:LEU:O	4:A:702:ALA:HB3	2.18	0.44
4:A:710:VAL:O	4:A:710:VAL:HG13	2.18	0.44
4:A:794:THR:OG1	4:A:831:THR:CG2	2.48	0.44
4:A:797:TRP:CZ3	4:A:801:LYS:HB2	2.52	0.44
4:B:278:TRP:CZ3	4:B:284:GLY:CA	2.99	0.44
4:B:329:LYS:O	4:B:445:THR:HG23	2.17	0.44
4:B:460:LEU:HA	4:B:534:LEU:HD11	1.99	0.44
4:B:512:LEU:O	4:B:514:PHE:N	2.51	0.44
4:B:556:GLY:O	4:B:558:ALA:N	2.51	0.44
4:B:780:PRO:HD2	4:B:781:ASN:N	2.31	0.44
4:B:796:VAL:HG21	7:B:3141:HOH:O	2.18	0.44
4:C:69:ALA:HA	4:C:257:ARG:HD2	1.99	0.44
4:C:270:PRO:HD2	4:C:408:PHE:CE2	2.53	0.44
4:C:291:ARG:HD2	7:C:3077:HOH:O	2.17	0.44
4:C:307:ARG:HH11	4:C:307:ARG:HG3	1.82	0.44
4:C:308:TYR:CE2	4:C:734:PRO:O	2.71	0.44
4:C:571:TYR:HD1	4:C:634:VAL:HG11	1.83	0.44
4:D:14:ILE:HG21	4:D:288:ALA:CB	2.48	0.44
4:D:479:ILE:O	4:D:480:LYS:C	2.61	0.44
4:D:486:HIS:NE2	4:D:490:MET:HG2	2.33	0.44
4:D:611:LEU:HB2	4:D:616:LEU:HD21	2.00	0.44
4:D:870:LEU:HD23	4:D:871:ASN:N	2.33	0.44
4:A:133:THR:O	4:A:137:VAL:HG23	2.17	0.44
4:A:320:ILE:HG23	4:A:418:TYR:O	2.18	0.44
4:A:338:ALA:C	4:A:340:VAL:H	2.26	0.44
4:A:556:GLY:O	4:A:557:ARG:C	2.61	0.44
4:B:40:GLU:O	4:B:43:SER:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:50:ARG:HG2	4:B:50:ARG:NH1	2.33	0.44
4:B:199:GLU:HG2	4:B:201:TRP:CD1	2.51	0.44
4:B:220:LEU:O	4:B:223:SER:N	2.46	0.44
4:B:290:GLY:C	4:B:292:ARG:H	2.25	0.44
4:B:430:SER:OG	4:B:432:PHE:O	2.34	0.44
4:B:645:GLY:C	4:B:647:ARG:H	2.26	0.44
4:B:651:LEU:HA	4:B:655:ILE:HD12	1.99	0.44
4:B:699:LEU:HD12	4:B:699:LEU:H	1.82	0.44
4:B:823:ASN:N	4:B:823:ASN:ND2	2.60	0.44
4:C:685:VAL:O	4:C:687:VAL:N	2.51	0.44
4:D:14:ILE:CG2	4:D:288:ALA:CB	2.91	0.44
4:D:743:ILE:HD12	4:D:766:ASP:HB3	2.00	0.44
4:D:804:ILE:H	4:D:804:ILE:HG13	1.47	0.44
4:A:306:MET:C	4:A:308:TYR:H	2.25	0.44
4:A:436:GLY:HA3	4:A:440:THR:CB	2.48	0.44
4:A:446:LEU:HD13	4:A:817:ILE:HG23	1.99	0.44
4:A:578:VAL:O	4:A:581:ILE:N	2.50	0.44
4:A:802:TYR:HD2	4:A:802:TYR:H	1.63	0.44
4:B:26:ASP:CG	4:B:26:ASP:O	2.61	0.44
4:B:164:LYS:HZ3	4:B:164:LYS:H	1.65	0.44
4:B:340:VAL:O	4:B:341:ILE:C	2.52	0.44
4:B:505:GLN:HG3	4:B:511:PHE:CD2	2.53	0.44
4:C:103:PHE:CD2	4:C:103:PHE:C	2.96	0.44
4:C:236:VAL:CG1	4:C:239:GLN:HB2	2.48	0.44
4:C:295:ALA:C	4:C:297:VAL:N	2.75	0.44
4:C:440:THR:O	4:C:441:LYS:C	2.60	0.44
4:C:450:LYS:O	4:C:529:ASN:HA	2.18	0.44
4:C:550:LEU:O	4:C:867:LYS:HG3	2.18	0.44
4:C:840:ASP:C	4:C:842:LEU:N	2.75	0.44
4:D:151:PHE:CD2	4:D:750:MET:HE1	2.52	0.44
4:D:233:ASN:O	4:D:236:VAL:HG23	2.17	0.44
1:E:12:DT:C2	1:E:13:DC:C6	3.06	0.44
1:K:3:DG:H5'	7:K:268:HOH:O	2.17	0.44
1:K:10:DT:H5'	4:C:641:SER:HA	1.99	0.44
1:N:10:DT:H4'	4:D:639:TYR:O	2.17	0.44
4:A:282:THR:OG1	4:A:283:GLY:N	2.45	0.44
4:A:676:TYR:O	4:A:678:ALA:N	2.50	0.44
4:B:227:VAL:HB	4:B:245:GLU:O	2.17	0.44
4:B:322:ILE:HD13	4:B:322:ILE:HA	1.73	0.44
4:B:495:SER:N	4:B:496:PRO:CD	2.80	0.44
4:B:570:ILE:HG23	4:B:571:TYR:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:752:LEU:HB2	4:B:753:GLY:H	1.69	0.44
4:C:296:LEU:HA	4:C:296:LEU:HD12	1.85	0.44
4:C:390:ALA:C	4:C:392:LYS:H	2.26	0.44
4:C:543:ILE:O	4:C:544:GLN:C	2.60	0.44
4:C:632:ARG:O	4:C:633:SER:C	2.59	0.44
4:C:857:GLN:C	4:C:859:ASP:H	2.26	0.44
4:D:459:TRP:O	4:D:462:ILE:N	2.51	0.44
4:D:778:ILE:O	4:D:782:PHE:HB2	2.18	0.44
4:D:809:LEU:C	4:D:810:ILE:HG13	2.42	0.44
1:E:13:DC:H5'	1:E:13:DC:H6	1.82	0.43
1:E:15:DC:H2'	1:E:16:DC:C6	2.53	0.43
4:A:78:LEU:CD1	4:A:119:ILE:HG13	2.48	0.43
4:A:215:ARG:NH1	4:A:218:GLU:OE2	2.47	0.43
4:A:226:MET:O	4:A:247:ALA:CB	2.66	0.43
4:A:286:TYR:H	4:A:286:TYR:HD2	1.66	0.43
4:A:620:TRP:NE1	4:A:677:MET:HB2	2.33	0.43
4:A:713:LYS:O	4:A:714:LYS:HD3	2.18	0.43
4:B:84:ARG:O	4:B:84:ARG:NH1	2.51	0.43
4:B:556:GLY:O	4:B:559:VAL:N	2.51	0.43
4:B:718:ILE:C	4:B:719:LEU:HD12	2.43	0.43
4:C:402:LEU:HD23	4:C:402:LEU:HA	1.79	0.43
4:D:268:PHE:CD2	4:D:429:VAL:CG1	3.00	0.43
4:D:471:ASP:CG	4:D:472:LYS:CD	2.91	0.43
1:K:2:DG:N2	7:K:239:HOH:O	2.50	0.43
1:K:7:DC:H6	1:K:7:DC:H2'	1.47	0.43
4:A:56:GLU:C	4:A:56:GLU:OE1	2.61	0.43
4:A:110:LYS:O	4:A:113:ALA:HB3	2.18	0.43
4:A:320:ILE:CG2	4:A:418:TYR:O	2.67	0.43
4:A:804:ILE:HG23	4:A:816:THR:HG21	2.00	0.43
4:B:233:ASN:HB3	4:B:239:GLN:HB3	2.00	0.43
4:B:791:LEU:O	4:B:792:ARG:C	2.61	0.43
4:C:136:ALA:HA	7:C:3021:HOH:O	2.17	0.43
4:C:462:ILE:CD1	4:C:479:ILE:CD1	2.96	0.43
4:C:462:ILE:HG23	4:C:478:ARG:HD2	2.00	0.43
4:C:698:TRP:NE1	4:C:864:LEU:HA	2.33	0.43
4:C:706:LEU:HD11	4:C:849:PHE:CG	2.54	0.43
4:C:721:LYS:HG2	4:C:722:ARG:H	1.81	0.43
4:C:818:PRO:O	4:C:821:ALA:HB3	2.18	0.43
4:D:422:TRP:O	4:D:422:TRP:HD1	2.00	0.43
4:D:532:LEU:HA	4:D:533:PRO:HD2	1.58	0.43
4:D:843:ALA:C	4:D:845:PHE:N	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:125:CYS:O	4:A:128:SER:HB3	2.18	0.43
4:A:320:ILE:HG23	4:A:320:ILE:HD12	1.74	0.43
4:A:521:VAL:O	4:A:525:GLY:N	2.51	0.43
4:A:647:ARG:HD2	4:A:675:GLY:CA	2.25	0.43
4:A:780:PRO:O	4:A:784:HIS:HB2	2.18	0.43
4:B:220:LEU:O	4:B:221:ILE:C	2.61	0.43
4:B:267:MET:HE3	4:B:267:MET:HB3	1.62	0.43
4:B:514:PHE:CD1	4:B:514:PHE:C	2.91	0.43
4:B:582:LEU:HD23	4:B:582:LEU:HA	1.86	0.43
4:B:685:VAL:C	4:B:687:VAL:H	2.26	0.43
4:B:810:ILE:C	4:B:813:SER:HB2	2.43	0.43
4:C:66:ASP:OD2	4:C:66:ASP:N	2.51	0.43
4:C:231:ARG:CG	4:C:234:ALA:HB2	2.42	0.43
4:C:532:LEU:HA	4:C:533:PRO:HD2	1.77	0.43
4:C:570:ILE:O	4:C:573:ILE:HG23	2.18	0.43
4:C:592:ASN:ND2	4:C:611:LEU:CD2	2.81	0.43
4:C:727:TRP:CD2	4:C:735:VAL:CG1	3.01	0.43
4:C:737:GLN:O	4:C:774:GLN:NE2	2.51	0.43
4:C:808:ALA:HB3	4:C:815:GLY:HA3	2.00	0.43
4:D:122:THR:HG21	4:D:226:MET:CE	2.48	0.43
4:D:379:ARG:HD3	4:D:660:ASP:OD2	2.18	0.43
4:D:545:HIS:ND1	4:D:832:MET:HE1	2.33	0.43
4:D:784:HIS:C	4:D:786:GLN:N	2.76	0.43
4:D:794:THR:HA	4:D:797:TRP:HB3	1.99	0.43
1:K:11:DA:N1	1:K:12:DT:C4	2.86	0.43
4:A:65:ALA:CB	4:A:120:LYS:HG2	2.48	0.43
4:A:234:ALA:HA	4:A:240:ASP:OD2	2.18	0.43
4:A:276:LYS:O	4:A:277:PRO:O	2.36	0.43
4:A:651:LEU:HA	4:A:655:ILE:HB	1.99	0.43
4:A:748:ASN:CG	4:A:749:LEU:N	2.76	0.43
4:A:820:ASP:N	4:A:820:ASP:OD1	2.51	0.43
4:B:86:ASN:ND2	7:B:3033:HOH:O	2.37	0.43
4:B:577:LYS:CB	4:B:684:SER:HB3	2.47	0.43
4:C:68:ALA:O	4:C:257:ARG:HD2	2.17	0.43
4:C:298:ARG:HG3	4:C:420:MET:O	2.17	0.43
4:C:308:TYR:HA	4:C:311:VAL:CG2	2.48	0.43
4:D:169:GLN:HB3	4:D:182:PHE:CZ	2.53	0.43
4:D:545:HIS:O	4:D:549:MET:HG2	2.18	0.43
4:D:744:GLN:HA	4:D:756:ARG:NH2	2.33	0.43
4:D:825:PHE:O	4:D:828:VAL:CG2	2.67	0.43
4:D:829:ARG:HB3	4:D:876:LEU:HD23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:51:PHE:HZ	4:A:261:LEU:HD23	1.83	0.43
4:A:204:TRP:CZ3	4:A:212:VAL:HG21	2.50	0.43
4:A:476:PRO:O	4:A:477:GLU:C	2.62	0.43
4:A:643:GLU:OE2	4:A:679:LYS:CA	2.67	0.43
4:B:252:GLU:C	4:B:254:ILE:N	2.76	0.43
4:B:307:ARG:HD3	4:B:736:TRP:CD2	2.52	0.43
4:B:324:GLN:HE21	4:B:417:PRO:HA	1.84	0.43
4:B:394:ARG:HE	4:B:394:ARG:HB2	1.49	0.43
4:B:401:MET:HE3	4:B:440:THR:CG2	2.46	0.43
4:C:47:GLY:CA	4:C:265:SER:O	2.59	0.43
4:C:452:ILE:CG1	4:C:457:TYR:N	2.81	0.43
4:C:696:MET:O	4:C:700:LYS:HB2	2.18	0.43
4:C:755:PHE:N	4:C:755:PHE:HD1	2.16	0.43
4:C:778:ILE:HA	4:C:778:ILE:HD12	1.65	0.43
4:D:147:ASP:HB3	4:D:750:MET:HE1	2.01	0.43
4:D:401:MET:HG3	4:D:440:THR:OG1	2.19	0.43
4:D:461:LYS:HE3	4:D:479:ILE:HG23	2.00	0.43
4:D:554:VAL:O	4:D:557:ARG:HB3	2.19	0.43
4:D:743:ILE:O	4:D:743:ILE:HG22	2.19	0.43
4:D:830:GLU:HG2	4:D:876:LEU:HD22	2.00	0.43
1:H:9:DA:H2"	1:H:10:DT:OP1	2.18	0.43
4:A:73:LEU:HD11	4:A:254:ILE:HG13	2.00	0.43
4:A:477:GLU:O	4:A:478:ARG:C	2.61	0.43
4:A:540:CYS:C	4:A:542:GLY:N	2.74	0.43
4:B:306:MET:O	4:B:308:TYR:N	2.52	0.43
4:B:341:ILE:O	4:B:343:LYS:N	2.51	0.43
4:B:569:ASP:O	4:B:570:ILE:C	2.60	0.43
4:B:809:LEU:C	4:B:810:ILE:CG1	2.92	0.43
4:B:831:THR:HG23	4:B:832:MET:N	2.33	0.43
4:B:875:ILE:C	4:B:877:GLU:N	2.75	0.43
4:C:248:PRO:HD2	4:C:249:GLU:OE2	2.19	0.43
4:C:485:ASN:OD1	4:C:485:ASN:N	2.51	0.43
4:C:563:PRO:HD3	4:C:874:ASP:O	2.19	0.43
4:C:823:ASN:O	4:C:824:LEU:C	2.61	0.43
4:D:305:LEU:O	4:D:306:MET:C	2.60	0.43
4:D:472:LYS:CG	4:D:567:VAL:HG11	2.49	0.43
4:D:489:ILE:HG13	4:D:489:ILE:H	1.40	0.43
4:D:837:GLU:HG2	4:D:872:LEU:HD12	2.01	0.43
3:J:5:DA:H2"	3:J:6:DT:C7	2.48	0.43
2:L:5:C:H5"	4:C:390:ALA:HB1	2.01	0.43
4:A:8:LYS:HB3	4:A:9:ASN:H	1.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:122:THR:O	4:A:126:LEU:HG	2.19	0.43
4:A:178:TYR:O	4:A:181:ALA:HB3	2.18	0.43
4:A:274:PRO:HA	4:A:275:PRO:HD3	1.89	0.43
4:A:308:TYR:HA	4:A:311:VAL:HG23	1.99	0.43
4:A:344:TRP:O	4:A:345:LYS:CB	2.66	0.43
4:A:459:TRP:NE1	4:A:822:ALA:HA	2.29	0.43
4:A:461:LYS:HE3	4:A:479:ILE:CG2	2.48	0.43
4:A:465:ALA:HB2	4:A:482:ILE:HD11	2.00	0.43
4:A:502:TRP:CE2	4:A:512:LEU:CD1	2.97	0.43
4:A:545:HIS:H	4:A:545:HIS:CD2	2.36	0.43
4:A:546:PHE:O	4:A:547:SER:C	2.60	0.43
4:A:549:MET:HB3	4:A:836:TYR:CE1	2.51	0.43
4:B:78:LEU:N	4:B:79:PRO:HD2	2.34	0.43
4:B:395:ARG:O	4:B:396:ILE:C	2.60	0.43
4:B:407:LYS:CG	4:B:408:PHE:HE2	2.27	0.43
4:B:411:HIS:O	4:B:412:LYS:C	2.62	0.43
4:B:416:PHE:CD1	4:B:430:SER:OG	2.71	0.43
4:B:435:GLN:HG2	4:B:810:ILE:HG12	2.00	0.43
4:B:635:MET:C	4:B:637:LEU:H	2.27	0.43
4:C:502:TRP:O	4:C:504:GLU:N	2.51	0.43
4:D:21:PHE:CE1	4:D:25:ALA:HB2	2.54	0.43
4:D:78:LEU:O	4:D:82:ILE:HG13	2.18	0.43
4:D:95:LYS:HE3	7:D:3065:HOH:O	2.17	0.43
4:D:452:ILE:HG22	4:D:528:TYR:O	2.18	0.43
4:D:583:GLN:HB3	7:D:3135:HOH:O	2.19	0.43
4:A:396:ILE:HG23	4:A:396:ILE:HD12	1.65	0.43
4:A:793:LYS:CA	4:A:796:VAL:HG23	2.48	0.43
4:B:13:ASP:OD1	4:B:14:ILE:N	2.51	0.43
4:B:163:LYS:HA	4:B:166:VAL:HG23	2.00	0.43
4:B:865:PRO:HA	7:B:3135:HOH:O	2.19	0.43
4:C:70:ALA:O	4:C:73:LEU:HB2	2.18	0.43
4:C:162:PHE:CD1	4:C:190:MET:HE2	2.54	0.43
4:C:246:LEU:HD12	4:C:247:ALA:H	1.83	0.43
4:C:412:LYS:O	4:C:413:ALA:HB2	2.19	0.43
4:C:881:ALA:O	4:C:883:ALA:OXT	2.37	0.43
4:D:159:ALA:CB	4:D:163:LYS:HD3	2.49	0.43
4:D:395:ARG:O	4:D:396:ILE:C	2.60	0.43
4:D:419:ASN:HB3	4:D:420:MET:H	1.53	0.43
4:D:741:LYS:HA	4:D:742:PRO:HD3	1.79	0.43
4:D:744:GLN:NE2	4:D:756:ARG:H	2.16	0.43
3:G:8:DC:H2"	3:G:9:DC:OP2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:57:ARG:HA	4:A:60:LYS:HB3	2.01	0.43
4:A:78:LEU:HD13	4:A:119:ILE:HG13	2.00	0.43
4:A:201:TRP:O	4:A:204:TRP:HB2	2.19	0.43
4:A:219:MET:O	4:A:222:GLU:HB3	2.19	0.43
4:A:615:ALA:O	4:A:618:GLY:N	2.51	0.43
4:A:646:PHE:C	4:A:650:VAL:HG23	2.43	0.43
4:A:846:TYR:O	4:A:847:ASP:C	2.62	0.43
4:B:109:ILE:HD12	4:B:109:ILE:H	1.78	0.43
4:B:261:LEU:HD12	4:B:261:LEU:HA	1.81	0.43
4:B:421:ASP:OD1	4:B:424:GLY:N	2.50	0.43
4:B:437:ASN:O	4:B:441:LYS:HG2	2.19	0.43
4:B:455:GLU:HG2	4:B:822:ALA:HB2	2.00	0.43
4:B:724:ALA:HB2	4:B:738:GLU:HG3	2.00	0.43
4:C:120:LYS:HG3	4:C:752:LEU:CD1	2.46	0.43
4:C:267:MET:HE2	4:C:431:MET:CE	2.49	0.43
4:C:289:ASN:HB2	7:C:3014:HOH:O	2.17	0.43
4:C:373:ALA:O	4:C:377:TRP:CD1	2.71	0.43
4:C:531:SER:O	4:C:817:ILE:HG22	2.18	0.43
4:C:548:ALA:O	4:C:550:LEU:N	2.52	0.43
4:D:126:LEU:HD13	4:D:246:LEU:HB2	2.00	0.43
4:D:306:MET:C	4:D:308:TYR:H	2.26	0.43
4:A:14:ILE:CD1	4:A:14:ILE:H	2.32	0.43
4:A:159:ALA:HB3	4:A:163:LYS:HD3	2.01	0.43
4:A:223:SER:HA	7:A:3147:HOH:O	2.19	0.43
4:A:338:ALA:O	4:A:339:ASN:C	2.59	0.43
4:A:517:GLU:O	4:A:520:GLY:N	2.42	0.43
4:A:546:PHE:HA	4:A:549:MET:HG2	2.01	0.43
4:A:619:GLN:HA	4:A:622:ALA:HB3	2.01	0.43
4:B:14:ILE:O	4:B:14:ILE:HG22	2.19	0.43
4:B:56:GLU:OE1	4:B:57:ARG:N	2.52	0.43
4:B:141:ILE:O	4:B:145:ILE:HG12	2.19	0.43
4:B:158:GLU:HG2	4:B:195:LEU:CD2	2.47	0.43
4:B:520:GLY:HA3	4:B:528:TYR:CZ	2.54	0.43
4:B:596:THR:CG2	4:B:605:ILE:HG23	2.49	0.43
4:B:643:GLU:HB2	7:B:3053:HOH:O	2.19	0.43
4:B:726:HIS:CD2	4:B:736:TRP:CD1	3.06	0.43
4:C:9:ASN:HA	4:C:12:SER:CB	2.47	0.43
4:C:214:VAL:O	4:C:215:ARG:C	2.61	0.43
4:C:710:VAL:HG21	4:C:856:SER:OG	2.18	0.43
4:C:727:TRP:CD1	4:C:782:PHE:CE1	3.06	0.43
4:D:158:GLU:CD	4:D:195:LEU:HB3	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:303:LYS:HE2	4:D:307:ARG:HH12	1.84	0.43
4:D:306:MET:O	4:D:309:GLU:HB2	2.19	0.43
4:D:451:PRO:O	4:D:452:ILE:C	2.62	0.43
4:A:631:LYS:HZ2	6:A:2000:APC:PA	2.41	0.42
4:A:742:PRO:HB3	4:A:744:GLN:OE1	2.19	0.42
4:B:17:ALA:O	4:B:21:PHE:HE2	2.02	0.42
4:B:80:LYS:HD3	4:B:224:THR:HG23	1.99	0.42
4:B:110:LYS:CD	4:B:111:PRO:HD2	2.39	0.42
4:B:744:GLN:HA	4:B:756:ARG:HD3	2.01	0.42
4:C:8:LYS:HB2	7:C:3187:HOH:O	2.18	0.42
4:C:340:VAL:C	4:C:342:THR:H	2.27	0.42
4:C:786:GLN:O	4:C:789:SER:N	2.51	0.42
4:D:134:VAL:HB	4:D:244:ILE:HG12	2.01	0.42
4:D:340:VAL:HG11	4:D:497:LEU:HD11	2.01	0.42
4:D:352:ILE:HA	4:D:353:PRO:HD2	1.54	0.42
4:D:478:ARG:O	4:D:481:PHE:HB3	2.19	0.42
4:D:520:GLY:O	4:D:524:HIS:HB2	2.18	0.42
4:D:535:ALA:HA	4:D:814:PHE:O	2.19	0.42
4:A:89:PHE:O	4:A:93:LYS:HG3	2.19	0.42
4:A:246:LEU:HD23	4:A:251:ALA:HB2	2.01	0.42
4:A:266:PRO:HD2	4:A:292:ARG:NH1	2.34	0.42
4:A:610:LYS:O	4:A:611:LEU:O	2.37	0.42
4:A:640:GLY:O	4:A:641:SER:O	2.37	0.42
4:A:770:ASP:O	4:A:770:ASP:CG	2.62	0.42
4:B:31:ARG:HB3	4:B:31:ARG:NH1	2.32	0.42
4:B:259:GLY:O	4:B:262:ALA:N	2.52	0.42
4:B:504:GLU:O	4:B:505:GLN:O	2.37	0.42
4:B:714:LYS:HD3	4:B:714:LYS:HA	1.77	0.42
4:B:798:ALA:O	4:B:802:TYR:O	2.38	0.42
4:B:864:LEU:O	4:B:865:PRO:O	2.36	0.42
4:C:342:THR:HG21	4:C:439:MET:HE1	2.01	0.42
4:C:632:ARG:NH1	6:C:2002:APC:C8	2.83	0.42
4:C:680:LEU:O	4:C:681:ILE:C	2.62	0.42
4:D:106:LEU:HD11	4:D:215:ARG:HG2	2.01	0.42
4:D:231:ARG:NH1	4:D:242:GLU:HB2	2.34	0.42
4:D:337:VAL:HG12	4:D:341:ILE:CD1	2.48	0.42
4:D:442:GLY:O	4:D:444:LEU:N	2.52	0.42
4:D:861:MET:HA	4:D:862:PRO:HD2	1.84	0.42
3:M:4:DG:C2	3:M:5:DA:C2	3.07	0.42
4:A:84:ARG:NH1	4:A:91:GLU:OE2	2.52	0.42
4:A:205:HIS:O	4:A:208:ASP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:331:ASN:O	4:A:333:LYS:N	2.53	0.42
4:A:810:ILE:N	4:A:813:SER:O	2.46	0.42
4:B:259:GLY:O	4:B:260:ALA:C	2.62	0.42
4:B:305:LEU:O	4:B:307:ARG:N	2.53	0.42
4:B:341:ILE:C	4:B:343:LYS:N	2.77	0.42
4:B:533:PRO:HA	4:B:816:THR:O	2.18	0.42
4:B:613:THR:HG21	7:B:3104:HOH:O	2.19	0.42
4:C:305:LEU:O	4:C:305:LEU:HD23	2.19	0.42
4:C:318:LYS:HE2	4:C:796:VAL:CG1	2.48	0.42
4:C:326:THR:O	4:C:415:TRP:HD1	1.99	0.42
4:C:428:ALA:H	4:C:435:GLN:HE22	1.66	0.42
4:C:487:GLU:O	4:C:488:ASN:C	2.62	0.42
4:C:699:LEU:O	4:C:778:ILE:HG12	2.19	0.42
4:C:701:SER:O	4:C:702:ALA:C	2.61	0.42
4:D:68:ALA:HB3	4:D:261:LEU:HD21	2.01	0.42
4:D:125:CYS:O	4:D:128:SER:CB	2.62	0.42
4:D:334:VAL:HG12	4:D:443:LEU:HD22	2.01	0.42
4:D:433:ASN:OD1	4:D:433:ASN:C	2.62	0.42
4:D:474:PRO:HA	4:D:880:PHE:CE1	2.54	0.42
4:D:669:GLN:O	4:D:670:PRO:C	2.62	0.42
4:A:308:TYR:OH	4:A:733:PHE:HE2	2.02	0.42
4:A:675:GLY:O	4:A:678:ALA:HB3	2.18	0.42
4:A:720:ARG:C	4:A:721:LYS:O	2.62	0.42
4:A:793:LYS:HB3	4:A:831:THR:OG1	2.19	0.42
4:A:801:LYS:HD3	4:A:802:TYR:CD2	2.54	0.42
4:B:19:ILE:HG23	4:B:20:PRO:N	2.34	0.42
4:B:36:GLN:O	4:B:39:LEU:N	2.45	0.42
4:B:51:PHE:CE2	4:B:55:PHE:CD1	3.03	0.42
4:B:144:ALA:O	4:B:147:ASP:N	2.53	0.42
4:B:511:PHE:O	4:B:514:PHE:HB3	2.19	0.42
4:B:571:TYR:HH	4:B:635:MET:HE3	1.76	0.42
4:B:662:GLY:O	4:B:663:LYS:C	2.61	0.42
4:B:678:ALA:O	4:B:679:LYS:C	2.61	0.42
4:B:749:LEU:HD12	4:B:750:MET:HG3	2.01	0.42
4:C:36:GLN:NE2	4:C:273:VAL:HG22	2.34	0.42
4:C:162:PHE:CE2	4:C:165:ASN:HB2	2.54	0.42
4:C:462:ILE:HG12	4:C:479:ILE:HD11	2.02	0.42
4:C:512:LEU:O	4:C:516:PHE:CD1	2.71	0.42
4:C:693:VAL:HG12	4:C:694:GLU:N	2.34	0.42
4:D:89:PHE:CD2	4:D:107:GLN:OE1	2.73	0.42
4:D:207:GLU:O	4:D:211:HIS:CD2	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:247:ALA:HA	4:D:248:PRO:HD3	1.80	0.42
4:D:486:HIS:HA	4:D:489:ILE:CD1	2.40	0.42
4:D:579:ASN:ND2	4:D:625:VAL:HG12	2.35	0.42
3:G:3:DC:C4	3:G:4:DG:N7	2.88	0.42
1:H:14:DG:H2'	1:H:15:DC:C5	2.55	0.42
4:A:73:LEU:C	4:A:75:THR:N	2.77	0.42
4:A:205:HIS:C	4:A:207:GLU:H	2.27	0.42
4:A:226:MET:HG3	4:A:250:TYR:HD1	1.83	0.42
4:A:236:VAL:HG11	4:A:239:GLN:OE1	2.19	0.42
4:A:276:LYS:HB2	4:A:287:TRP:CD2	2.54	0.42
4:A:395:ARG:O	4:A:399:GLU:CG	2.68	0.42
4:A:704:LYS:O	4:A:707:ALA:N	2.47	0.42
4:A:830:GLU:O	4:A:832:MET:N	2.51	0.42
4:B:19:ILE:C	4:B:21:PHE:H	2.26	0.42
4:B:163:LYS:HZ1	4:B:167:GLU:HG2	1.85	0.42
4:B:669:GLN:O	4:B:670:PRO:C	2.62	0.42
4:C:205:HIS:HB3	4:C:208:ASP:OD2	2.18	0.42
4:C:607:GLU:C	4:C:608:LYS:HG2	2.44	0.42
4:C:650:VAL:HG11	4:C:674:ALA:HA	2.00	0.42
4:C:698:TRP:O	4:C:701:SER:N	2.53	0.42
4:C:714:LYS:HD3	4:C:714:LYS:HA	1.74	0.42
4:C:733:PHE:C	4:C:733:PHE:CD2	2.97	0.42
4:C:799:HIS:HA	4:C:804:ILE:O	2.20	0.42
4:D:64:VAL:HG21	4:D:127:THR:HG21	2.01	0.42
4:D:116:TYR:CZ	4:D:752:LEU:HD22	2.54	0.42
4:D:122:THR:O	4:D:125:CYS:HB2	2.19	0.42
4:D:303:LYS:HE2	4:D:307:ARG:NH1	2.34	0.42
4:D:727:TRP:CE2	4:D:735:VAL:CG1	3.03	0.42
4:A:163:LYS:HD2	4:A:163:LYS:HA	1.93	0.42
4:A:166:VAL:HG12	4:A:170:LEU:HD12	2.01	0.42
4:A:333:LYS:CB	4:A:516:PHE:CE2	3.03	0.42
4:A:333:LYS:HE3	4:A:516:PHE:HB3	2.01	0.42
4:A:556:GLY:CA	4:A:561:LEU:HB2	2.49	0.42
4:A:722:ARG:CB	4:A:769:ILE:HD13	2.19	0.42
4:A:817:ILE:O	4:A:818:PRO:C	2.63	0.42
4:A:832:MET:O	4:A:834:ASP:N	2.53	0.42
4:B:264:ILE:CG2	4:B:292:ARG:HB2	2.39	0.42
4:B:518:TYR:CE1	4:B:522:GLN:NE2	2.88	0.42
4:C:286:TYR:CE2	4:C:417:PRO:HG3	2.54	0.42
4:C:322:ILE:HA	4:C:322:ILE:HD13	1.74	0.42
4:C:329:LYS:HD2	4:C:447:ALA:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:833:VAL:HG11	4:C:873:ARG:HD3	2.01	0.42
4:C:834:ASP:O	4:C:837:GLU:N	2.44	0.42
4:D:257:ARG:NH1	4:D:261:LEU:HD13	2.34	0.42
4:D:384:VAL:O	4:D:384:VAL:HG12	2.19	0.42
4:D:425:ARG:HB3	4:D:427:TYR:CE1	2.49	0.42
4:D:579:ASN:OD1	4:D:625:VAL:HB	2.18	0.42
4:D:631:LYS:CD	4:D:635:MET:SD	3.08	0.42
4:D:684:SER:C	4:D:687:VAL:HG22	2.45	0.42
4:D:794:THR:CB	4:D:831:THR:HG21	2.47	0.42
4:D:836:TYR:N	4:D:836:TYR:HD2	2.16	0.42
4:A:116:TYR:HH	4:A:752:LEU:HD22	1.85	0.42
4:A:121:THR:OG1	4:A:751:PHE:HE1	2.02	0.42
4:A:215:ARG:O	4:A:219:MET:HG3	2.20	0.42
4:A:216:CYS:O	4:A:217:ILE:C	2.61	0.42
4:A:407:LYS:HB2	4:A:407:LYS:HE3	1.85	0.42
4:A:488:ASN:O	4:A:491:ALA:CB	2.67	0.42
4:A:510:CYS:O	4:A:512:LEU:N	2.53	0.42
4:A:543:ILE:O	4:A:544:GLN:O	2.37	0.42
4:A:779:ALA:HB3	4:A:780:PRO:HD3	2.02	0.42
4:B:432:PHE:O	4:B:432:PHE:HD2	2.01	0.42
4:B:458:TYR:CD2	4:B:458:TYR:C	2.97	0.42
4:B:545:HIS:HE1	4:B:787:ASP:HA	1.84	0.42
4:B:567:VAL:CG1	4:B:880:PHE:CG	3.01	0.42
4:B:581:ILE:O	4:B:584:ALA:HB3	2.20	0.42
4:B:793:LYS:CG	7:B:3181:HOH:O	2.66	0.42
4:B:804:ILE:HG21	4:B:807:PHE:CE2	2.54	0.42
4:B:840:ASP:HB3	4:B:843:ALA:HB3	2.02	0.42
4:C:132:THR:HG21	4:C:244:ILE:O	2.20	0.42
4:C:247:ALA:HA	4:C:248:PRO:HD3	1.89	0.42
4:C:257:ARG:HG2	4:C:257:ARG:NH1	2.34	0.42
4:C:631:LYS:NZ	6:C:2002:APC:C3A	2.47	0.42
4:C:756:ARG:HG3	7:C:3143:HOH:O	2.20	0.42
4:D:6:ILE:C	4:D:8:LYS:N	2.78	0.42
4:D:166:VAL:HG11	4:D:183:MET:CE	2.50	0.42
4:D:239:GLN:O	4:D:241:SER:N	2.52	0.42
4:D:396:ILE:HD13	4:D:396:ILE:HA	1.84	0.42
4:D:473:VAL:N	4:D:567:VAL:CG2	2.79	0.42
4:D:537:ASP:C	4:D:882:PHE:HB2	2.44	0.42
4:D:631:LYS:HE2	4:D:635:MET:CE	2.50	0.42
4:D:643:GLU:HB2	4:D:682:TRP:CD1	2.54	0.42
4:D:712:ASP:O	4:D:716:GLY:N	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:728:VAL:HG22	4:D:734:PRO:HA	2.01	0.42
4:D:745:THR:O	4:D:746:ARG:HG3	2.20	0.42
4:D:787:ASP:OD1	4:D:787:ASP:C	2.62	0.42
2:L:3:G:H5''	4:C:172:LYS:CD	2.50	0.42
1:N:12:DT:H5'	4:D:781:ASN:ND2	2.34	0.42
4:A:13:ASP:OD2	4:A:291:ARG:NH2	2.50	0.42
4:A:19:ILE:O	4:A:21:PHE:N	2.49	0.42
4:A:65:ALA:HB3	4:A:120:LYS:CD	2.49	0.42
4:A:172:LYS:NZ	7:A:3192:HOH:O	2.44	0.42
4:A:281:ILE:HG23	4:A:305:LEU:HD11	2.01	0.42
4:A:402:LEU:CD1	4:A:439:MET:HE1	2.49	0.42
4:A:668:THR:CG2	4:A:669:GLN:HE22	2.32	0.42
4:A:686:SER:HA	4:A:693:VAL:HG21	2.01	0.42
4:B:19:ILE:CG2	4:B:20:PRO:N	2.83	0.42
4:B:308:TYR:CD2	4:B:313:MET:HE1	2.54	0.42
4:B:430:SER:O	4:B:430:SER:OG	2.21	0.42
4:B:530:CYS:SG	4:B:818:PRO:HG2	2.60	0.42
4:B:661:SER:CB	7:B:3192:HOH:O	2.68	0.42
4:B:709:GLU:O	4:B:709:GLU:HG2	2.20	0.42
4:B:726:HIS:CD2	4:B:736:TRP:CG	3.08	0.42
4:C:109:ILE:HD13	4:C:145:ILE:HG22	2.01	0.42
4:C:191:LEU:O	4:C:196:LEU:HD22	2.20	0.42
4:C:322:ILE:CG1	7:C:3131:HOH:O	2.59	0.42
4:C:330:ILE:HA	4:C:330:ILE:HD13	1.74	0.42
4:C:461:LYS:C	4:C:463:HIS:N	2.76	0.42
4:D:36:GLN:CA	4:D:36:GLN:HE21	2.28	0.42
4:D:133:THR:HA	4:D:243:THR:CG2	2.48	0.42
4:D:161:HIS:CE1	7:D:3114:HOH:O	2.64	0.42
4:D:339:ASN:O	4:D:343:LYS:HD3	2.20	0.42
4:D:632:ARG:HH22	6:D:2003:APC:H5'1	1.85	0.42
1:H:11:DA:N3	4:B:784:HIS:HE1	2.17	0.42
4:A:40:GLU:CD	4:A:286:TYR:HB3	2.45	0.42
4:A:254:ILE:HG22	4:A:255:ALA:N	2.34	0.42
4:A:505:GLN:O	4:A:508:PRO:HD3	2.19	0.42
4:B:19:ILE:HG22	4:B:21:PHE:HB3	2.01	0.42
4:B:19:ILE:HD12	4:B:20:PRO:HD2	2.00	0.42
4:B:276:LYS:O	4:B:277:PRO:C	2.61	0.42
4:B:280:GLY:HA2	4:B:317:TYR:OH	2.20	0.42
4:B:308:TYR:CE2	4:B:734:PRO:O	2.73	0.42
4:B:347:CYS:HB3	4:B:350:GLU:HG2	2.00	0.42
4:C:63:GLU:O	4:C:66:ASP:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:101:THR:HG23	4:C:104:GLN:HE22	1.84	0.42
4:C:164:LYS:C	4:C:166:VAL:N	2.78	0.42
4:C:303:LYS:NZ	4:C:303:LYS:HB3	2.35	0.42
4:C:571:TYR:HD1	4:C:634:VAL:CG1	2.33	0.42
4:C:713:LYS:HD2	4:C:713:LYS:HA	1.83	0.42
4:C:789:SER:O	4:C:793:LYS:HG3	2.19	0.42
4:D:423:ARG:NH2	4:D:784:HIS:ND1	2.67	0.42
4:D:809:LEU:HA	4:D:813:SER:O	2.19	0.42
4:D:854:HIS:HD2	4:D:856:SER:H	1.55	0.42
4:A:71:LYS:N	4:A:72:PRO:CD	2.82	0.42
4:A:100:PRO:HG2	4:A:103:PHE:CB	2.46	0.42
4:A:287:TRP:C	4:A:288:ALA:O	2.63	0.42
4:A:292:ARG:O	4:A:292:ARG:CG	2.63	0.42
4:A:553:GLU:OE1	4:A:553:GLU:N	2.53	0.42
4:A:629:VAL:HG12	4:A:677:MET:HE3	2.01	0.42
4:A:782:PHE:O	4:A:783:VAL:C	2.62	0.42
4:A:801:LYS:CD	4:A:802:TYR:CD2	3.02	0.42
4:A:830:GLU:C	4:A:832:MET:N	2.73	0.42
4:B:6:ILE:O	4:B:8:LYS:N	2.44	0.42
4:B:56:GLU:CD	4:B:56:GLU:C	2.87	0.42
4:B:158:GLU:HA	4:B:195:LEU:HD22	2.01	0.42
4:B:170:LEU:HD22	4:B:179:LYS:HG2	2.01	0.42
4:B:247:ALA:HB3	4:B:250:TYR:CD1	2.55	0.42
4:B:339:ASN:O	4:B:343:LYS:HD3	2.15	0.42
4:B:352:ILE:HA	4:B:353:PRO:HD2	1.69	0.42
4:B:419:ASN:C	4:B:420:MET:HG3	2.45	0.42
4:B:561:LEU:N	4:B:561:LEU:HD12	2.35	0.42
4:B:817:ILE:O	4:B:818:PRO:C	2.61	0.42
4:C:329:LYS:HD3	4:C:446:LEU:O	2.20	0.42
4:C:459:TRP:C	4:C:461:LYS:N	2.75	0.42
4:D:281:ILE:HG22	4:D:282:THR:CG2	2.42	0.42
1:N:11:DA:H4'	4:D:780:PRO:HG3	2.00	0.41
3:P:7:DT:H2''	3:P:8:DC:OP2	2.21	0.41
4:A:108:GLU:CG	7:A:3115:HOH:O	2.63	0.41
4:A:291:ARG:CB	7:A:3193:HOH:O	2.56	0.41
4:A:291:ARG:CG	7:A:3193:HOH:O	2.67	0.41
4:A:330:ILE:HG21	4:A:409:ALA:HA	2.02	0.41
4:A:659:ILE:HG22	4:A:660:ASP:N	2.35	0.41
4:A:737:GLN:C	4:A:774:GLN:HE22	2.27	0.41
4:A:864:LEU:HD12	4:A:864:LEU:H	1.84	0.41
4:B:179:LYS:O	4:B:750:MET:SD	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:247:ALA:CB	4:B:250:TYR:HD1	2.33	0.41
4:B:416:PHE:CD2	4:B:416:PHE:N	2.88	0.41
4:B:450:LYS:C	4:B:529:ASN:OD1	2.63	0.41
4:B:578:VAL:HG21	4:B:681:ILE:HD12	2.01	0.41
4:C:292:ARG:N	4:C:293:PRO:CD	2.82	0.41
4:C:390:ALA:C	4:C:392:LYS:N	2.78	0.41
4:C:473:VAL:HA	4:C:474:PRO:HD2	1.90	0.41
4:C:610:LYS:HD2	7:C:3085:HOH:O	2.19	0.41
4:C:619:GLN:O	4:C:666:MET:HG3	2.20	0.41
4:C:870:LEU:HD23	4:C:871:ASN:N	2.35	0.41
4:D:32:LEU:HD12	4:D:32:LEU:N	2.12	0.41
4:D:161:HIS:O	4:D:163:LYS:N	2.53	0.41
4:D:264:ILE:HG22	4:D:264:ILE:O	2.19	0.41
4:D:545:HIS:C	4:D:549:MET:HE3	2.45	0.41
4:D:702:ALA:HB2	4:D:861:MET:HE1	2.02	0.41
1:K:14:DG:C4	1:K:15:DC:C5	3.08	0.41
4:A:6:ILE:C	4:A:8:LYS:N	2.76	0.41
4:A:244:ILE:HG22	4:A:245:GLU:N	2.34	0.41
4:A:348:PRO:HB2	4:A:349:VAL:HG23	2.03	0.41
4:A:401:MET:O	4:A:404:GLN:N	2.53	0.41
4:A:421:ASP:OD2	4:A:427:TYR:CE1	2.71	0.41
4:B:6:ILE:O	4:B:10:ASP:HB3	2.19	0.41
4:B:116:TYR:O	4:B:117:ILE:C	2.63	0.41
4:B:122:THR:HG22	4:B:226:MET:HE1	1.96	0.41
4:B:155:ARG:NH2	4:B:749:LEU:HB2	2.34	0.41
4:B:537:ASP:N	4:B:882:PHE:CD2	2.73	0.41
4:B:650:VAL:O	4:B:654:THR:HG23	2.20	0.41
4:B:773:LYS:HE3	7:B:3124:HOH:O	2.19	0.41
4:B:864:LEU:HA	4:B:865:PRO:HD2	1.72	0.41
4:C:261:LEU:O	4:C:263:GLY:N	2.52	0.41
4:C:420:MET:SD	4:C:733:PHE:CE1	3.13	0.41
4:C:437:ASN:ND2	4:C:440:THR:CB	2.83	0.41
4:C:635:MET:HG3	6:C:2002:APC:N7	2.36	0.41
4:D:291:ARG:O	4:D:292:ARG:HB2	2.20	0.41
4:D:572:GLY:O	4:D:573:ILE:C	2.62	0.41
1:H:13:DC:O4'	4:B:427:TYR:CE2	2.53	0.41
1:K:3:DG:C2	1:K:4:DA:C2	3.08	0.41
4:A:40:GLU:HG2	4:A:286:TYR:CD1	2.49	0.41
4:A:142:GLY:O	4:A:143:ARG:C	2.62	0.41
4:A:454:LYS:H	4:A:526:LEU:HD23	1.81	0.41
4:A:482:ILE:O	4:A:482:ILE:HG22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:706:LEU:HD11	4:A:849:PHE:HB2	2.02	0.41
4:B:115:ALA:O	4:B:119:ILE:HG12	2.21	0.41
4:B:205:HIS:C	4:B:207:GLU:H	2.29	0.41
4:B:345:LYS:HB3	4:B:345:LYS:HE2	1.68	0.41
4:B:381:ALA:O	4:B:383:ALA:N	2.53	0.41
4:B:537:ASP:O	4:B:882:PHE:CD2	2.72	0.41
4:B:587:ILE:HD13	4:B:587:ILE:HA	1.83	0.41
4:B:655:ILE:HG12	4:B:667:PHE:CE1	2.55	0.41
4:B:677:MET:HE2	4:B:677:MET:HB2	1.62	0.41
4:B:738:GLU:HG2	4:B:738:GLU:O	2.20	0.41
4:B:770:ASP:O	4:B:770:ASP:CG	2.63	0.41
4:C:55:PHE:CE2	4:C:59:LEU:HD21	2.55	0.41
4:C:58:GLN:HA	4:C:58:GLN:NE2	2.35	0.41
4:C:423:ARG:HD2	4:C:781:ASN:HD22	1.81	0.41
4:C:448:LYS:CG	4:C:806:SER:OG	2.69	0.41
4:C:461:LYS:O	4:C:463:HIS:N	2.53	0.41
4:C:517:GLU:C	4:C:519:ALA:N	2.77	0.41
4:C:727:TRP:CD2	4:C:735:VAL:HG13	2.55	0.41
4:C:738:GLU:CA	4:C:774:GLN:HE22	2.28	0.41
4:D:116:TYR:HE2	4:D:752:LEU:HD22	1.86	0.41
4:D:345:LYS:C	4:D:347:CYS:N	2.74	0.41
4:D:440:THR:C	4:D:442:GLY:H	2.28	0.41
4:D:570:ILE:HG23	4:D:571:TYR:N	2.35	0.41
4:D:680:LEU:O	4:D:681:ILE:C	2.63	0.41
4:D:733:PHE:HA	4:D:734:PRO:HD2	1.93	0.41
1:K:14:DG:H2''	1:K:15:DC:C6	2.56	0.41
2:L:7:A:H2'	2:L:8:U:H6	1.85	0.41
4:A:314:PRO:CD	4:A:315:GLU:H	2.33	0.41
4:A:462:ILE:CD1	4:A:475:PHE:CD1	3.03	0.41
4:A:475:PHE:HD2	4:A:475:PHE:H	1.68	0.41
4:A:668:THR:O	4:A:670:PRO:HD3	2.20	0.41
4:B:308:TYR:HD2	4:B:313:MET:HE1	1.85	0.41
4:B:314:PRO:O	4:B:315:GLU:C	2.61	0.41
4:B:464:GLY:HA3	4:B:514:PHE:CZ	2.55	0.41
4:B:592:ASN:O	4:B:593:GLU:HB2	2.20	0.41
4:B:617:ALA:O	4:B:621:LEU:HD12	2.19	0.41
4:B:745:THR:O	4:B:746:ARG:HB2	2.20	0.41
4:B:793:LYS:HE2	4:B:835:THR:OG1	2.20	0.41
4:C:278:TRP:HB2	4:C:321:ASN:OD1	2.20	0.41
4:C:330:ILE:HG13	4:C:409:ALA:HA	2.00	0.41
4:C:424:GLY:O	4:C:425:ARG:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:ILE:CG2	4:D:20:PRO:N	2.84	0.41
4:D:19:ILE:HD13	4:D:19:ILE:HA	1.95	0.41
4:D:51:PHE:C	4:D:51:PHE:CD2	2.98	0.41
4:D:146:GLU:HG3	4:D:204:TRP:CE2	2.55	0.41
4:D:191:LEU:HD23	4:D:195:LEU:O	2.21	0.41
4:D:717:GLU:HA	7:D:3025:HOH:O	2.20	0.41
4:D:735:VAL:HG23	4:D:736:TRP:N	2.35	0.41
4:D:870:LEU:C	4:D:870:LEU:CD2	2.92	0.41
4:A:31:ARG:NH2	4:A:32:LEU:HD11	2.34	0.41
4:A:59:LEU:HD23	4:A:64:VAL:HG21	1.99	0.41
4:A:743:ILE:HA	7:A:3130:HOH:O	2.19	0.41
4:A:873:ARG:O	4:A:876:LEU:HD12	2.20	0.41
4:B:111:PRO:HG2	4:B:112:GLU:H	1.86	0.41
4:B:144:ALA:C	4:B:146:GLU:N	2.77	0.41
4:B:589:GLY:O	4:B:614:LYS:HD2	2.20	0.41
4:B:682:TRP:O	4:B:686:SER:OG	2.16	0.41
4:C:138:ALA:O	4:C:139:SER:C	2.63	0.41
4:C:329:LYS:CG	4:C:445:THR:HG23	2.50	0.41
4:C:335:LEU:O	4:C:336:ALA:C	2.63	0.41
4:C:452:ILE:HG13	4:C:456:GLY:CA	2.50	0.41
4:C:620:TRP:NE1	4:C:677:MET:HB2	2.36	0.41
4:D:455:GLU:OE1	4:D:455:GLU:HA	2.19	0.41
4:D:642:LYS:HB3	4:D:682:TRP:CH2	2.56	0.41
4:D:724:ALA:HA	4:D:774:GLN:NE2	2.35	0.41
4:D:778:ILE:CG2	4:D:779:ALA:H	2.30	0.41
4:A:454:LYS:HA	4:A:526:LEU:HD21	2.01	0.41
4:A:505:GLN:C	4:A:507:SER:H	2.29	0.41
4:A:588:ASN:N	4:A:588:ASN:HD22	2.19	0.41
4:A:632:ARG:O	4:A:636:THR:HG23	2.20	0.41
4:B:62:GLY:C	4:B:64:VAL:H	2.28	0.41
4:B:329:LYS:O	4:B:329:LYS:HG3	2.20	0.41
4:B:845:PHE:CD1	4:B:845:PHE:O	2.73	0.41
4:C:135:GLN:OE1	4:C:210:ILE:HG21	2.21	0.41
4:C:137:VAL:O	4:C:141:ILE:HG13	2.20	0.41
4:C:158:GLU:HA	4:C:195:LEU:CD1	2.43	0.41
4:C:176:HIS:O	4:C:179:LYS:HB2	2.20	0.41
4:C:336:ALA:O	4:C:337:VAL:O	2.38	0.41
4:C:337:VAL:HG21	4:C:512:LEU:CD2	2.45	0.41
4:C:416:PHE:HA	4:C:417:PRO:HD2	1.99	0.41
4:C:486:HIS:O	4:C:489:ILE:HB	2.20	0.41
4:C:534:LEU:HD12	4:C:818:PRO:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:543:ILE:O	4:C:544:GLN:O	2.39	0.41
4:C:557:ARG:HB3	4:C:557:ARG:NH1	2.33	0.41
4:C:559:VAL:O	4:C:560:ASN:HB2	2.21	0.41
4:C:786:GLN:C	4:C:788:GLY:H	2.28	0.41
4:D:125:CYS:HB3	4:D:137:VAL:HG22	2.02	0.41
4:D:306:MET:O	4:D:307:ARG:C	2.63	0.41
4:D:349:VAL:C	4:D:352:ILE:HD11	2.45	0.41
4:D:420:MET:HG2	4:D:425:ARG:O	2.20	0.41
4:D:646:PHE:HD1	4:D:649:GLN:OE1	2.03	0.41
4:D:829:ARG:HH11	4:D:829:ARG:CG	2.25	0.41
1:K:6:DT:H2''	1:K:7:DC:OP2	2.20	0.41
1:N:9:DA:N6	3:P:1:DG:N2	2.68	0.41
4:A:14:ILE:HG23	4:A:288:ALA:HB1	2.02	0.41
4:A:78:LEU:HD12	4:A:78:LEU:HA	1.83	0.41
4:A:384:VAL:HG12	4:A:384:VAL:O	2.20	0.41
4:A:544:GLN:O	4:A:547:SER:N	2.54	0.41
4:A:825:PHE:HE1	4:A:829:ARG:CZ	2.26	0.41
4:A:857:GLN:C	4:A:859:ASP:N	2.77	0.41
4:B:114:VAL:HG13	4:B:145:ILE:HD12	2.03	0.41
4:B:233:ASN:HB2	4:B:239:GLN:O	2.21	0.41
4:B:269:GLN:NE2	4:B:407:LYS:HZ3	2.19	0.41
4:B:474:PRO:HA	4:B:880:PHE:CE1	2.56	0.41
4:B:477:GLU:O	4:B:480:LYS:HB3	2.20	0.41
4:B:515:CYS:O	4:B:516:PHE:C	2.60	0.41
4:B:698:TRP:CE2	4:B:861:MET:HE2	2.55	0.41
4:B:771:ALA:O	4:B:772:HIS:C	2.57	0.41
4:B:817:ILE:HG13	4:B:820:ASP:HB2	2.02	0.41
4:C:6:ILE:C	4:C:8:LYS:H	2.28	0.41
4:C:261:LEU:O	4:C:262:ALA:C	2.63	0.41
4:C:295:ALA:O	4:C:296:LEU:C	2.63	0.41
4:C:330:ILE:HG13	4:C:408:PHE:C	2.45	0.41
4:C:446:LEU:CD1	4:C:817:ILE:HG23	2.50	0.41
4:C:556:GLY:O	4:C:561:LEU:HB2	2.21	0.41
4:C:557:ARG:O	4:C:557:ARG:HG2	2.19	0.41
4:C:733:PHE:C	4:C:733:PHE:HD2	2.29	0.41
4:D:21:PHE:O	4:D:21:PHE:HD1	2.03	0.41
4:D:92:VAL:HG11	4:D:103:PHE:CD1	2.54	0.41
4:D:254:ILE:HG13	4:D:254:ILE:H	1.70	0.41
4:D:304:ALA:HA	4:D:307:ARG:HG3	2.03	0.41
4:D:416:PHE:HA	4:D:417:PRO:HD2	1.80	0.41
4:D:732:GLY:O	4:D:734:PRO:HD3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:744:GLN:CG	4:D:756:ARG:HB3	2.46	0.41
4:D:828:VAL:CB	4:D:883:ALA:HA	2.40	0.41
1:N:17:DG:P	4:D:57:ARG:HH12	2.44	0.41
4:A:257:ARG:CD	4:A:261:LEU:HD13	2.49	0.41
4:A:306:MET:C	4:A:308:TYR:N	2.77	0.41
4:A:424:GLY:O	4:A:425:ARG:C	2.63	0.41
4:A:457:TYR:CD1	4:A:521:VAL:HG11	2.55	0.41
4:A:459:TRP:C	4:A:534:LEU:HD13	2.46	0.41
4:A:635:MET:CE	6:A:2000:APC:H2'	2.51	0.41
4:A:709:GLU:HB2	4:A:722:ARG:NE	2.35	0.41
4:A:792:ARG:HH11	4:A:792:ARG:CG	2.30	0.41
4:B:57:ARG:O	4:B:60:LYS:HB3	2.21	0.41
4:B:268:PHE:CD1	4:B:286:TYR:CE2	3.09	0.41
4:B:323:ALA:HB1	4:B:809:LEU:HD11	2.02	0.41
4:B:419:ASN:C	4:B:420:MET:CG	2.94	0.41
4:B:461:LYS:HD3	4:B:483:GLU:OE2	2.21	0.41
4:B:490:MET:HE3	4:B:490:MET:HB3	1.94	0.41
4:B:676:TYR:CD1	4:B:680:LEU:HD11	2.56	0.41
4:B:730:PRO:HD3	7:B:3081:HOH:O	2.21	0.41
4:C:186:VAL:HG13	4:C:190:MET:HE3	2.02	0.41
4:C:215:ARG:HG3	4:C:219:MET:HE2	2.03	0.41
4:C:217:ILE:O	4:C:218:GLU:C	2.61	0.41
4:C:272:VAL:HG13	4:C:411:HIS:CD2	2.55	0.41
4:C:297:VAL:CG2	4:C:733:PHE:HZ	2.34	0.41
4:C:619:GLN:NE2	4:C:668:THR:H	2.19	0.41
4:C:711:LYS:HG3	4:C:718:ILE:HA	2.03	0.41
4:D:24:LEU:O	4:D:25:ALA:C	2.64	0.41
4:D:51:PHE:O	4:D:52:ARG:C	2.63	0.41
4:D:282:THR:OG1	4:D:283:GLY:N	2.52	0.41
4:D:702:ALA:O	4:D:704:LYS:N	2.54	0.41
1:K:12:DT:O4'	4:C:423:ARG:NH2	2.54	0.41
4:A:110:LYS:O	4:A:114:VAL:HG23	2.21	0.41
4:A:308:TYR:HH	4:A:733:PHE:HE2	1.68	0.41
4:A:437:ASN:O	4:A:438:ASP:O	2.39	0.41
4:A:477:GLU:C	4:A:479:ILE:N	2.78	0.41
4:A:514:PHE:O	4:A:517:GLU:N	2.45	0.41
4:A:559:VAL:CG1	7:A:3104:HOH:O	2.68	0.41
4:A:630:THR:CA	7:A:3199:HOH:O	2.62	0.41
4:A:715:THR:HG21	4:A:717:GLU:OE2	2.21	0.41
4:A:780:PRO:O	4:A:781:ASN:C	2.64	0.41
4:A:794:THR:HG21	4:A:828:VAL:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:36:GLN:O	4:B:37:LEU:C	2.63	0.41
4:B:67:ASN:C	4:B:69:ALA:N	2.78	0.41
4:B:105:PHE:CE1	4:B:208:ASP:HB3	2.55	0.41
4:B:335:LEU:HG	4:B:339:ASN:ND2	2.36	0.41
4:B:541:SER:O	4:B:542:GLY:O	2.38	0.41
4:B:569:ASP:OD1	4:B:572:GLY:N	2.50	0.41
4:B:570:ILE:O	4:B:571:TYR:C	2.59	0.41
4:B:581:ILE:O	4:B:584:ALA:N	2.50	0.41
4:B:619:GLN:HE22	4:B:668:THR:H	1.68	0.41
4:B:673:ALA:O	4:B:676:TYR:HB3	2.20	0.41
4:B:700:LYS:HE3	4:B:775:GLU:HG2	2.03	0.41
4:B:805:GLU:HB2	7:B:3030:HOH:O	2.21	0.41
4:C:36:GLN:NE2	4:C:271:CYS:HB3	2.35	0.41
4:C:78:LEU:HD11	4:C:115:ALA:CB	2.51	0.41
4:C:199:GLU:HG2	4:C:201:TRP:CD1	2.55	0.41
4:C:269:GLN:O	4:C:430:SER:CB	2.65	0.41
4:C:308:TYR:CE2	4:C:736:TRP:HZ3	2.38	0.41
4:C:385:TYR:O	4:C:388:ASP:N	2.54	0.41
4:C:393:SER:C	4:C:395:ARG:N	2.78	0.41
4:C:445:THR:OG1	4:C:532:LEU:HA	2.21	0.41
4:C:576:LYS:HB3	7:C:3018:HOH:O	2.19	0.41
4:C:632:ARG:CZ	6:C:2002:APC:N7	2.84	0.41
4:C:685:VAL:C	4:C:687:VAL:N	2.78	0.41
4:C:696:MET:HG2	4:C:779:ALA:HB1	2.02	0.41
4:C:698:TRP:HE3	4:C:699:LEU:HG	1.85	0.41
4:C:699:LEU:HD22	4:C:782:PHE:CG	2.56	0.41
4:C:729:THR:OG1	4:C:733:PHE:HB3	2.21	0.41
4:D:6:ILE:HB	4:D:11:PHE:CE2	2.55	0.41
4:D:183:MET:HE1	4:D:186:VAL:HG11	2.02	0.41
4:D:400:PHE:O	4:D:404:GLN:HB2	2.21	0.41
4:D:442:GLY:C	4:D:444:LEU:N	2.79	0.41
4:D:570:ILE:O	4:D:573:ILE:HG22	2.20	0.41
4:D:582:LEU:CD2	4:D:620:TRP:HB2	2.49	0.41
4:D:843:ALA:HB2	4:D:864:LEU:HD21	2.03	0.41
1:E:12:DT:C2'	1:E:13:DC:H6	2.33	0.41
4:A:103:PHE:CE2	7:A:3227:HOH:O	2.57	0.41
4:A:199:GLU:O	4:A:201:TRP:N	2.44	0.41
4:A:247:ALA:O	4:A:248:PRO:C	2.64	0.41
4:A:432:PHE:CD1	4:A:432:PHE:C	2.98	0.41
4:A:569:ASP:O	4:A:570:ILE:C	2.65	0.41
4:A:705:LEU:O	4:A:708:ALA:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:727:TRP:O	4:A:734:PRO:HA	2.21	0.41
4:A:734:PRO:O	4:A:734:PRO:CG	2.68	0.41
4:B:78:LEU:O	4:B:79:PRO:C	2.64	0.41
4:B:555:GLY:O	4:B:556:GLY:C	2.64	0.41
4:B:634:VAL:O	4:B:634:VAL:CG2	2.69	0.41
4:B:678:ALA:O	4:B:681:ILE:N	2.54	0.41
4:C:3:THR:HG23	4:C:258:ALA:HB3	2.02	0.41
4:C:11:PHE:CE1	4:C:44:TYR:HB3	2.56	0.41
4:C:106:LEU:HG	4:C:212:VAL:CG1	2.51	0.41
4:C:397:SER:O	4:C:400:PHE:N	2.44	0.41
4:C:421:ASP:O	4:C:424:GLY:N	2.48	0.41
4:C:733:PHE:HB2	4:C:792:ARG:HH21	1.86	0.41
4:D:36:GLN:HG2	4:D:272:VAL:HB	2.02	0.41
4:D:77:LEU:HD21	4:D:226:MET:HB2	2.03	0.41
4:D:133:THR:HG22	4:D:243:THR:HG22	2.03	0.41
4:D:201:TRP:HA	4:D:204:TRP:CD1	2.51	0.41
4:D:402:LEU:HD23	4:D:402:LEU:HA	1.59	0.41
4:D:421:ASP:O	4:D:422:TRP:C	2.63	0.41
4:D:448:LYS:HD2	4:D:806:SER:HB3	2.03	0.41
4:D:482:ILE:HD12	4:D:514:PHE:CZ	2.55	0.41
4:D:489:ILE:C	4:D:492:CYS:SG	3.04	0.41
4:D:619:GLN:CG	4:D:666:MET:O	2.68	0.41
4:D:698:TRP:CZ3	4:D:699:LEU:HD23	2.56	0.41
2:I:4:G:H4'	4:B:389:LYS:HE3	2.03	0.40
1:K:12:DT:H4'	4:C:423:ARG:NH1	2.36	0.40
1:N:15:DC:N3	1:N:16:DC:C5	2.89	0.40
4:A:19:ILE:CG2	4:A:20:PRO:N	2.84	0.40
4:A:42:GLU:C	4:A:46:MET:HE2	2.46	0.40
4:A:144:ALA:O	4:A:145:ILE:C	2.64	0.40
4:A:479:ILE:O	4:A:480:LYS:C	2.64	0.40
4:A:544:GLN:O	4:A:545:HIS:C	2.64	0.40
4:A:646:PHE:N	4:A:646:PHE:CD1	2.88	0.40
4:A:658:ALA:O	4:A:661:SER:HB2	2.21	0.40
4:A:741:LYS:HE2	4:A:741:LYS:HB3	1.82	0.40
4:B:341:ILE:N	4:B:341:ILE:HD12	2.36	0.40
4:B:502:TRP:CE3	4:B:512:LEU:HD22	2.56	0.40
4:B:646:PHE:O	4:B:647:ARG:O	2.39	0.40
4:B:797:TRP:CH2	4:B:801:LYS:HG3	2.56	0.40
4:C:677:MET:O	4:C:678:ALA:C	2.63	0.40
4:C:834:ASP:O	4:C:837:GLU:HB2	2.21	0.40
4:D:347:CYS:HB3	4:D:350:GLU:CG	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:349:VAL:HG13	4:D:503:ALA:HB1	2.03	0.40
4:D:588:ASN:HB3	4:D:589:GLY:H	1.65	0.40
4:D:642:LYS:O	4:D:646:PHE:CD2	2.74	0.40
1:H:15:DC:C5'	7:H:642:HOH:O	2.69	0.40
4:A:74:ILE:O	4:A:74:ILE:HG22	2.21	0.40
4:A:103:PHE:CD2	4:A:107:GLN:NE2	2.89	0.40
4:A:126:LEU:HD23	4:A:132:THR:HG23	2.03	0.40
4:A:331:ASN:O	4:A:332:LYS:C	2.64	0.40
4:A:433:ASN:CB	4:A:434:PRO:HD2	2.50	0.40
4:A:620:TRP:HZ3	4:A:623:TYR:HD2	1.69	0.40
4:A:816:THR:HG21	4:A:820:ASP:HB2	2.03	0.40
4:A:867:LYS:N	4:A:867:LYS:HD2	2.36	0.40
4:B:210:ILE:O	4:B:211:HIS:C	2.63	0.40
4:B:230:HIS:CE1	4:B:232:GLN:HE21	2.39	0.40
4:B:329:LYS:CD	4:B:447:ALA:HA	2.45	0.40
4:B:418:TYR:CD2	4:B:427:TYR:O	2.67	0.40
4:B:680:LEU:N	4:B:680:LEU:CD1	2.80	0.40
4:B:768:GLU:O	4:B:769:ILE:C	2.63	0.40
4:C:13:ASP:CB	7:C:3077:HOH:O	2.69	0.40
4:C:21:PHE:C	4:C:21:PHE:CD1	2.99	0.40
4:C:281:ILE:HA	4:C:281:ILE:HD12	1.83	0.40
4:C:425:ARG:HB2	4:C:427:TYR:HE1	1.86	0.40
4:C:563:PRO:CD	4:C:874:ASP:HB3	2.48	0.40
4:C:720:ARG:HG2	4:C:720:ARG:HH11	1.85	0.40
4:D:296:LEU:O	4:D:296:LEU:HG	2.21	0.40
4:D:327:ALA:HB2	4:D:415:TRP:CE2	2.56	0.40
4:D:439:MET:HG3	4:D:509:PHE:CE2	2.56	0.40
4:D:539:SER:HB3	4:D:559:VAL:HG12	2.02	0.40
4:D:649:GLN:O	4:D:650:VAL:C	2.62	0.40
4:D:733:PHE:HB2	4:D:792:ARG:NH2	2.37	0.40
4:D:735:VAL:CG2	4:D:736:TRP:N	2.85	0.40
4:D:827:ALA:O	4:D:831:THR:HG22	2.21	0.40
1:K:5:DA:H1'	7:K:712:HOH:O	2.20	0.40
2:L:6:G:C6	2:L:7:A:N7	2.89	0.40
3:M:7:DT:H2''	3:M:8:DC:C6	2.56	0.40
4:A:51:PHE:CD2	4:A:262:ALA:HB2	2.56	0.40
4:A:58:GLN:HG3	4:A:67:ASN:ND2	2.36	0.40
4:A:386:ARG:HE	4:A:386:ARG:HB2	1.20	0.40
4:A:832:MET:O	4:A:833:VAL:C	2.64	0.40
4:B:306:MET:C	4:B:308:TYR:N	2.79	0.40
4:B:523:HIS:C	4:B:524:HIS:ND1	2.79	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:779:ALA:O	4:B:783:VAL:CG2	2.69	0.40
4:C:64:VAL:C	4:C:66:ASP:H	2.29	0.40
4:C:473:VAL:O	4:C:474:PRO:C	2.63	0.40
4:C:491:ALA:O	4:C:494:LYS:N	2.55	0.40
4:C:548:ALA:C	4:C:550:LEU:N	2.79	0.40
4:C:576:LYS:HD3	7:C:3018:HOH:O	2.21	0.40
4:C:712:ASP:O	4:C:716:GLY:N	2.55	0.40
4:C:729:THR:HA	4:C:730:PRO:HD3	1.88	0.40
4:C:730:PRO:CD	4:C:786:GLN:NE2	2.84	0.40
4:D:236:VAL:CB	4:D:239:GLN:HB2	2.51	0.40
4:D:274:PRO:HA	4:D:275:PRO:HD3	1.93	0.40
4:D:571:TYR:CD1	4:D:634:VAL:CG1	3.04	0.40
4:D:737:GLN:HG2	4:D:774:GLN:OE1	2.20	0.40
4:D:744:GLN:HE21	4:D:756:ARG:N	2.18	0.40
3:J:6:DT:C2'	3:J:7:DT:H71	2.50	0.40
3:M:4:DG:H2''	3:M:5:DA:C8	2.57	0.40
2:O:6:G:H3'	7:O:144:HOH:O	2.20	0.40
4:A:56:GLU:HG3	7:A:3057:HOH:O	2.20	0.40
4:A:404:GLN:HG2	4:A:432:PHE:CD2	2.55	0.40
4:A:550:LEU:HD21	4:A:865:PRO:HG2	2.04	0.40
4:A:664:GLY:O	4:A:665:LEU:C	2.64	0.40
4:A:704:LYS:HE3	4:A:860:LYS:HZ3	1.83	0.40
4:A:793:LYS:C	4:A:796:VAL:HG23	2.45	0.40
4:B:88:TRP:O	4:B:92:VAL:HG23	2.22	0.40
4:B:109:ILE:CD1	4:B:109:ILE:H	2.33	0.40
4:B:116:TYR:CE2	4:B:752:LEU:HD13	2.56	0.40
4:B:154:ILE:O	4:B:155:ARG:C	2.64	0.40
4:B:220:LEU:O	4:B:222:GLU:N	2.54	0.40
4:B:572:GLY:O	4:B:575:ALA:HB3	2.21	0.40
4:B:577:LYS:O	4:B:578:VAL:C	2.63	0.40
4:B:577:LYS:HB3	4:B:684:SER:HB3	2.03	0.40
4:B:643:GLU:C	4:B:645:GLY:H	2.30	0.40
4:B:643:GLU:O	4:B:645:GLY:N	2.54	0.40
4:B:810:ILE:HB	4:B:813:SER:HB2	2.03	0.40
4:C:59:LEU:HA	4:C:64:VAL:HG22	2.03	0.40
4:C:84:ARG:CB	4:C:223:SER:HB3	2.49	0.40
4:C:120:LYS:HD3	4:C:120:LYS:C	2.46	0.40
4:C:463:HIS:HE1	4:C:532:LEU:HD11	1.86	0.40
4:C:540:CYS:HB2	4:C:559:VAL:HG12	2.04	0.40
4:D:141:ILE:O	4:D:145:ILE:CG1	2.66	0.40
4:D:157:LEU:O	4:D:158:GLU:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:294:LEU:HD13	4:D:419:ASN:HD21	1.86	0.40
4:D:726:HIS:CD2	4:D:735:VAL:O	2.74	0.40
4:D:788:GLY:C	4:D:792:ARG:NH1	2.79	0.40
4:A:24:LEU:HD21	4:A:287:TRP:CD2	2.56	0.40
4:A:120:LYS:C	4:A:122:THR:N	2.79	0.40
4:A:287:TRP:O	4:A:288:ALA:C	2.64	0.40
4:A:485:ASN:O	4:A:486:HIS:C	2.62	0.40
4:A:868:GLY:N	7:A:3164:HOH:O	2.54	0.40
4:B:185:VAL:O	4:B:188:ALA:HB3	2.22	0.40
4:B:229:LEU:HD11	4:B:242:GLU:CG	2.42	0.40
4:B:306:MET:O	4:B:309:GLU:N	2.51	0.40
4:B:831:THR:O	4:B:832:MET:C	2.63	0.40
4:C:261:LEU:HD12	4:C:261:LEU:HA	1.82	0.40
4:C:414:ILE:C	4:C:415:TRP:CE3	3.00	0.40
4:C:483:GLU:O	4:C:486:HIS:N	2.52	0.40
4:C:523:HIS:CD2	4:C:523:HIS:N	2.90	0.40
4:C:551:ARG:HE	4:C:872:LEU:CG	2.34	0.40
4:C:698:TRP:C	4:C:700:LYS:N	2.78	0.40
4:C:749:LEU:CD1	4:C:750:MET:HG2	2.46	0.40
4:C:756:ARG:CG	7:C:3143:HOH:O	2.70	0.40
4:C:770:ASP:OD1	4:C:770:ASP:C	2.64	0.40
4:C:817:ILE:HD12	4:C:819:ALA:HB3	2.04	0.40
4:D:22:ASN:HA	4:D:25:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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
4	A	851/883 (96%)	570 (67%)	198 (23%)	83 (10%)	0 2
4	B	851/883 (96%)	578 (68%)	188 (22%)	85 (10%)	0 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	851/883 (96%)	608 (71%)	178 (21%)	65 (8%)	1	5
4	D	851/883 (96%)	623 (73%)	174 (20%)	54 (6%)	1	8
All	All	3404/3532 (96%)	2379 (70%)	738 (22%)	287 (8%)	0	4

All (287) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	7	ALA
4	A	194	GLY
4	A	199	GLU
4	A	281	ILE
4	A	288	ALA
4	A	309	GLU
4	A	353	PRO
4	A	387	LYS
4	A	391	ARG
4	A	402	LEU
4	A	430	SER
4	A	506	ASP
4	A	508	PRO
4	A	526	LEU
4	A	549	MET
4	A	592	ASN
4	A	631	LYS
4	A	686	SER
4	A	708	ALA
4	A	721	LYS
4	A	744	GLN
4	A	745	THR
4	A	746	ARG
4	A	755	PHE
4	A	803	GLY
4	A	850	ALA
4	B	262	ALA
4	B	274	PRO
4	B	293	PRO
4	B	391	ARG
4	B	452	ILE
4	B	539	SER
4	B	610	LYS
4	B	611	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	646	PHE
4	B	647	ARG
4	B	663	LYS
4	B	690	VAL
4	B	706	LEU
4	B	755	PHE
4	B	784	HIS
4	B	785	SER
4	B	796	VAL
4	B	804	ILE
4	B	841	VAL
4	B	851	ASP
4	C	68	ALA
4	C	106	LEU
4	C	240	ASP
4	C	288	ALA
4	C	309	GLU
4	C	337	VAL
4	C	422	TRP
4	C	503	ALA
4	C	508	PRO
4	C	526	LEU
4	C	539	SER
4	C	631	LYS
4	C	744	GLN
4	C	745	THR
4	C	755	PHE
4	C	771	ALA
4	C	841	VAL
4	D	307	ARG
4	D	324	GLN
4	D	353	PRO
4	D	508	PRO
4	D	539	SER
4	D	541	SER
4	D	592	ASN
4	D	647	ARG
4	D	663	LYS
4	D	755	PHE
4	D	841	VAL
4	A	60	LYS
4	A	106	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	177	VAL
4	A	200	ALA
4	A	332	LYS
4	A	375	THR
4	A	384	VAL
4	A	401	MET
4	A	422	TRP
4	A	438	ASP
4	A	474	PRO
4	A	544	GLN
4	A	632	ARG
4	A	641	SER
4	A	678	ALA
4	A	771	ALA
4	A	811	HIS
4	A	882	PHE
4	B	14	ILE
4	B	36	GLN
4	B	106	LEU
4	B	167	GLU
4	B	176	HIS
4	B	194	GLY
4	B	298	ARG
4	B	307	ARG
4	B	314	PRO
4	B	315	GLU
4	B	412	LYS
4	B	430	SER
4	B	431	MET
4	B	470	VAL
4	B	526	LEU
4	B	542	GLY
4	B	589	GLY
4	B	592	ASN
4	B	641	SER
4	B	721	LYS
4	B	746	ARG
4	B	865	PRO
4	B	873	ARG
4	B	876	LEU
4	C	7	ALA
4	C	162	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	307	ARG
4	C	314	PRO
4	C	339	ASN
4	C	443	LEU
4	C	474	PRO
4	C	544	GLN
4	C	686	SER
4	C	690	VAL
4	C	796	VAL
4	C	811	HIS
4	C	882	PHE
4	D	7	ALA
4	D	119	ILE
4	D	167	GLU
4	D	259	GLY
4	D	292	ARG
4	D	422	TRP
4	D	443	LEU
4	D	452	ILE
4	D	593	GLU
4	D	648	GLN
4	D	745	THR
4	D	882	PHE
4	A	100	PRO
4	A	262	ALA
4	A	277	PRO
4	A	460	LEU
4	A	511	PHE
4	A	525	GLY
4	A	541	SER
4	A	542	GLY
4	A	647	ARG
4	A	660	ASP
4	A	734	PRO
4	A	797	TRP
4	A	825	PHE
4	A	872	LEU
4	B	7	ALA
4	B	68	ALA
4	B	150	ARG
4	B	199	GLU
4	B	200	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	260	ALA
4	B	348	PRO
4	B	382	ALA
4	B	505	GLN
4	B	508	PRO
4	B	551	ARG
4	B	593	GLU
4	B	617	ALA
4	B	627	ARG
4	B	628	SER
4	B	678	ALA
4	B	810	ILE
4	B	862	PRO
4	C	98	LYS
4	C	140	ALA
4	C	199	GLU
4	C	206	LYS
4	C	262	ALA
4	C	549	MET
4	C	647	ARG
4	C	850	ALA
4	C	851	ASP
4	D	240	ASP
4	D	288	ALA
4	D	309	GLU
4	D	314	PRO
4	D	348	PRO
4	D	405	ALA
4	D	544	GLN
4	D	589	GLY
4	A	160	LYS
4	A	204	TRP
4	A	274	PRO
4	A	345	LYS
4	A	425	ARG
4	A	464	GLY
4	A	611	LEU
4	A	670	PRO
4	A	677	MET
4	A	796	VAL
4	B	50	ARG
4	B	160	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	277	PRO
4	B	395	ARG
4	B	396	ILE
4	B	476	PRO
4	B	580	GLU
4	B	631	LYS
4	B	648	GLN
4	B	705	LEU
4	B	752	LEU
4	B	811	HIS
4	B	824	LEU
4	B	850	ALA
4	C	200	ALA
4	C	353	PRO
4	C	476	PRO
4	C	592	ASN
4	C	787	ASP
4	D	65	ALA
4	D	260	ALA
4	D	631	LYS
4	D	722	ARG
4	A	4	ILE
4	A	313	MET
4	A	348	PRO
4	A	383	ALA
4	A	560	ASN
4	A	690	VAL
4	B	115	ALA
4	B	265	SER
4	B	342	THR
4	B	557	ARG
4	B	780	PRO
4	C	102	ALA
4	C	348	PRO
4	C	541	SER
4	C	542	GLY
4	C	632	ARG
4	C	663	LYS
4	C	701	SER
4	C	832	MET
4	D	63	GLU
4	D	162	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	467	CYS
4	D	474	PRO
4	D	691	ALA
4	D	704	LYS
4	D	744	GLN
4	A	292	ARG
4	A	593	GLU
4	B	254	ILE
4	C	4	ILE
4	C	211	HIS
4	C	235	GLY
4	C	341	ILE
4	C	648	GLN
4	C	872	LEU
4	D	275	PRO
4	D	336	ALA
4	D	715	THR
4	D	811	HIS
4	D	850	ALA
4	D	860	LYS
4	A	710	VAL
4	B	270	PRO
4	B	479	ILE
4	C	804	ILE
4	D	114	VAL
4	D	194	GLY
4	D	693	VAL
4	A	533	PRO
4	A	650	VAL
4	C	19	ILE
4	C	141	ILE
4	C	322	ILE
4	C	567	VAL
4	A	841	VAL
4	B	353	PRO
4	C	194	GLY
4	C	833	VAL
4	D	337	VAL
4	A	270	PRO
4	A	567	VAL
4	A	669	GLN
4	D	97	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	4	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	
4	A	703/729 (96%)	556 (79%)	147 (21%)	1	6
4	B	703/729 (96%)	562 (80%)	141 (20%)	1	7
4	C	703/729 (96%)	579 (82%)	124 (18%)	2	10
4	D	703/729 (96%)	590 (84%)	113 (16%)	2	13
All	All	2812/2916 (96%)	2287 (81%)	525 (19%)	1	9

All (525) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	14	ILE
4	A	16	LEU
4	A	19	ILE
4	A	23	THR
4	A	27	HIS
4	A	36	GLN
4	A	50	ARG
4	A	53	LYS
4	A	56	GLU
4	A	57	ARG
4	A	60	LYS
4	A	77	LEU
4	A	84	ARG
4	A	96	ARG
4	A	101	THR
4	A	104	GLN
4	A	120	LYS
4	A	121	THR
4	A	130	ASP
4	A	143	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	145	ILE
4	A	155	ARG
4	A	157	LEU
4	A	160	LYS
4	A	165	ASN
4	A	170	LEU
4	A	183	MET
4	A	190	MET
4	A	206	LYS
4	A	207	GLU
4	A	221	ILE
4	A	248	PRO
4	A	257	ARG
4	A	261	LEU
4	A	273	VAL
4	A	274	PRO
4	A	282	THR
4	A	293	PRO
4	A	299	THR
4	A	301	SER
4	A	305	LEU
4	A	307	ARG
4	A	309	GLU
4	A	322	ILE
4	A	330	ILE
4	A	333	LYS
4	A	343	LYS
4	A	345	LYS
4	A	384	VAL
4	A	388	ASP
4	A	393	SER
4	A	401	MET
4	A	402	LEU
4	A	404	GLN
4	A	422	TRP
4	A	423	ARG
4	A	429	VAL
4	A	430	SER
4	A	433	ASN
4	A	440	THR
4	A	444	LEU
4	A	448	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	451	PRO
4	A	452	ILE
4	A	454	LYS
4	A	457	TYR
4	A	462	ILE
4	A	470	VAL
4	A	472	LYS
4	A	473	VAL
4	A	475	PHE
4	A	489	ILE
4	A	495	SER
4	A	510	CYS
4	A	514	PHE
4	A	516	PHE
4	A	517	GLU
4	A	521	VAL
4	A	531	SER
4	A	540	CYS
4	A	543	ILE
4	A	550	LEU
4	A	554	VAL
4	A	559	VAL
4	A	561	LEU
4	A	565	GLU
4	A	573	ILE
4	A	574	VAL
4	A	594	VAL
4	A	613	THR
4	A	620	TRP
4	A	625	VAL
4	A	626	THR
4	A	630	THR
4	A	632	ARG
4	A	634	VAL
4	A	641	SER
4	A	643	GLU
4	A	647	ARG
4	A	651	LEU
4	A	656	GLN
4	A	665	LEU
4	A	669	GLN
4	A	670	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	671	ASN
4	A	688	THR
4	A	690	VAL
4	A	693	VAL
4	A	706	LEU
4	A	711	LYS
4	A	730	PRO
4	A	734	PRO
4	A	735	VAL
4	A	743	ILE
4	A	744	GLN
4	A	746	ARG
4	A	749	LEU
4	A	752	LEU
4	A	755	PHE
4	A	766	ASP
4	A	776	SER
4	A	778	ILE
4	A	783	VAL
4	A	786	GLN
4	A	787	ASP
4	A	791	LEU
4	A	796	VAL
4	A	801	LYS
4	A	802	TYR
4	A	806	SER
4	A	814	PHE
4	A	816	THR
4	A	817	ILE
4	A	820	ASP
4	A	828	VAL
4	A	829	ARG
4	A	831	THR
4	A	832	MET
4	A	833	VAL
4	A	839	CYS
4	A	841	VAL
4	A	842	LEU
4	A	851	ASP
4	A	860	LYS
4	A	869	ASN
4	A	879	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	882	PHE
4	B	13	ASP
4	B	15	GLU
4	B	16	LEU
4	B	19	ILE
4	B	21	PHE
4	B	22	ASN
4	B	24	LEU
4	B	27	HIS
4	B	31	ARG
4	B	32	LEU
4	B	36	GLN
4	B	39	LEU
4	B	50	ARG
4	B	56	GLU
4	B	71	LYS
4	B	84	ARG
4	B	101	THR
4	B	109	ILE
4	B	120	LYS
4	B	123	LEU
4	B	132	THR
4	B	164	LYS
4	B	166	VAL
4	B	168	GLU
4	B	172	LYS
4	B	184	GLN
4	B	195	LEU
4	B	206	LYS
4	B	207	GLU
4	B	209	SER
4	B	214	VAL
4	B	224	THR
4	B	243	THR
4	B	252	GLU
4	B	254	ILE
4	B	256	THR
4	B	261	LEU
4	B	264	ILE
4	B	267	MET
4	B	272	VAL
4	B	273	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	277	PRO
4	B	279	THR
4	B	281	ILE
4	B	299	THR
4	B	305	LEU
4	B	314	PRO
4	B	322	ILE
4	B	324	GLN
4	B	330	ILE
4	B	332	LYS
4	B	334	VAL
4	B	337	VAL
4	B	343	LYS
4	B	349	VAL
4	B	351	ASP
4	B	378	LYS
4	B	388	ASP
4	B	394	ARG
4	B	397	SER
4	B	398	LEU
4	B	402	LEU
4	B	408	PHE
4	B	419	ASN
4	B	422	TRP
4	B	423	ARG
4	B	429	VAL
4	B	437	ASN
4	B	441	LYS
4	B	452	ILE
4	B	455	GLU
4	B	461	LYS
4	B	467	CYS
4	B	472	LYS
4	B	483	GLU
4	B	492	CYS
4	B	494	LYS
4	B	495	SER
4	B	497	LEU
4	B	500	THR
4	B	512	LEU
4	B	527	SER
4	B	540	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	552	ASP
4	B	554	VAL
4	B	560	ASN
4	B	567	VAL
4	B	569	ASP
4	B	582	LEU
4	B	587	ILE
4	B	592	ASN
4	B	621	LEU
4	B	626	THR
4	B	633	SER
4	B	643	GLU
4	B	651	LEU
4	B	654	THR
4	B	656	GLN
4	B	666	MET
4	B	668	THR
4	B	681	ILE
4	B	683	GLU
4	B	685	VAL
4	B	687	VAL
4	B	690	VAL
4	B	693	VAL
4	B	700	LYS
4	B	704	LYS
4	B	713	LYS
4	B	715	THR
4	B	722	ARG
4	B	725	VAL
4	B	731	ASP
4	B	734	PRO
4	B	735	VAL
4	B	744	GLN
4	B	745	THR
4	B	749	LEU
4	B	752	LEU
4	B	769	ILE
4	B	770	ASP
4	B	776	SER
4	B	780	PRO
4	B	783	VAL
4	B	785	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	786	GLN
4	B	801	LYS
4	B	809	LEU
4	B	813	SER
4	B	823	ASN
4	B	828	VAL
4	B	832	MET
4	B	841	VAL
4	B	842	LEU
4	B	849	PHE
4	B	855	GLU
4	B	859	ASP
4	B	860	LYS
4	B	869	ASN
4	B	870	LEU
4	B	877	GLU
4	C	2	ASN
4	C	3	THR
4	C	9	ASN
4	C	16	LEU
4	C	26	ASP
4	C	30	GLU
4	C	32	LEU
4	C	36	GLN
4	C	37	LEU
4	C	40	GLU
4	C	50	ARG
4	C	59	LEU
4	C	64	VAL
4	C	84	ARG
4	C	95	LYS
4	C	96	ARG
4	C	107	GLN
4	C	119	ILE
4	C	120	LYS
4	C	121	THR
4	C	143	ARG
4	C	145	ILE
4	C	164	LYS
4	C	170	LEU
4	C	183	MET
4	C	186	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	195	LEU
4	C	210	ILE
4	C	214	VAL
4	C	227	VAL
4	C	237	VAL
4	C	244	ILE
4	C	249	GLU
4	C	256	THR
4	C	267	MET
4	C	272	VAL
4	C	281	ILE
4	C	282	THR
4	C	294	LEU
4	C	301	SER
4	C	303	LYS
4	C	305	LEU
4	C	313	MET
4	C	322	ILE
4	C	325	ASN
4	C	335	LEU
4	C	343	LYS
4	C	347	CYS
4	C	350	GLU
4	C	355	ILE
4	C	377	TRP
4	C	378	LYS
4	C	379	ARG
4	C	387	LYS
4	C	397	SER
4	C	403	GLU
4	C	404	GLN
4	C	415	TRP
4	C	422	TRP
4	C	423	ARG
4	C	434	PRO
4	C	437	ASN
4	C	441	LYS
4	C	467	CYS
4	C	470	VAL
4	C	473	VAL
4	C	483	GLU
4	C	509	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	510	CYS
4	C	514	PHE
4	C	517	GLU
4	C	531	SER
4	C	532	LEU
4	C	541	SER
4	C	544	GLN
4	C	551	ARG
4	C	559	VAL
4	C	565	GLU
4	C	573	ILE
4	C	588	ASN
4	C	601	ASN
4	C	614	LYS
4	C	636	THR
4	C	651	LEU
4	C	659	ILE
4	C	661	SER
4	C	663	LYS
4	C	671	ASN
4	C	690	VAL
4	C	694	GLU
4	C	700	LYS
4	C	706	LEU
4	C	711	LYS
4	C	722	ARG
4	C	729	THR
4	C	734	PRO
4	C	735	VAL
4	C	744	GLN
4	C	749	LEU
4	C	750	MET
4	C	751	PHE
4	C	754	GLN
4	C	755	PHE
4	C	768	GLU
4	C	783	VAL
4	C	786	GLN
4	C	787	ASP
4	C	789	SER
4	C	801	LYS
4	C	814	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	817	ILE
4	C	824	LEU
4	C	828	VAL
4	C	831	THR
4	C	832	MET
4	C	838	SER
4	C	841	VAL
4	C	842	LEU
4	C	860	LYS
4	C	867	LYS
4	C	869	ASN
4	C	872	LEU
4	C	880	PHE
4	C	882	PHE
4	D	13	ASP
4	D	16	LEU
4	D	19	ILE
4	D	22	ASN
4	D	27	HIS
4	D	36	GLN
4	D	39	LEU
4	D	40	GLU
4	D	48	GLU
4	D	50	ARG
4	D	54	MET
4	D	56	GLU
4	D	59	LEU
4	D	84	ARG
4	D	95	LYS
4	D	101	THR
4	D	109	ILE
4	D	131	ASN
4	D	143	ARG
4	D	145	ILE
4	D	171	ASN
4	D	174	VAL
4	D	176	HIS
4	D	183	MET
4	D	190	MET
4	D	206	LYS
4	D	215	ARG
4	D	219	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	232	GLN
4	D	236	VAL
4	D	269	GLN
4	D	271	CYS
4	D	281	ILE
4	D	282	THR
4	D	296	LEU
4	D	297	VAL
4	D	299	THR
4	D	305	LEU
4	D	335	LEU
4	D	341	ILE
4	D	348	PRO
4	D	351	ASP
4	D	375	THR
4	D	391	ARG
4	D	394	ARG
4	D	398	LEU
4	D	412	LYS
4	D	420	MET
4	D	422	TRP
4	D	423	ARG
4	D	425	ARG
4	D	431	MET
4	D	435	GLN
4	D	437	ASN
4	D	441	LYS
4	D	443	LEU
4	D	448	LYS
4	D	450	LYS
4	D	452	ILE
4	D	467	CYS
4	D	470	VAL
4	D	477	GLU
4	D	492	CYS
4	D	495	SER
4	D	497	LEU
4	D	499	ASN
4	D	510	CYS
4	D	530	CYS
4	D	532	LEU
4	D	540	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	554	VAL
4	D	559	VAL
4	D	601	ASN
4	D	606	SER
4	D	630	THR
4	D	631	LYS
4	D	632	ARG
4	D	652	GLU
4	D	661	SER
4	D	666	MET
4	D	700	LYS
4	D	705	LEU
4	D	710	VAL
4	D	713	LYS
4	D	718	ILE
4	D	720	ARG
4	D	721	LYS
4	D	722	ARG
4	D	723	CYS
4	D	730	PRO
4	D	734	PRO
4	D	735	VAL
4	D	749	LEU
4	D	750	MET
4	D	752	LEU
4	D	776	SER
4	D	783	VAL
4	D	786	GLN
4	D	787	ASP
4	D	791	LEU
4	D	800	GLU
4	D	801	LYS
4	D	806	SER
4	D	812	ASP
4	D	813	SER
4	D	820	ASP
4	D	828	VAL
4	D	842	LEU
4	D	851	ASP
4	D	857	GLN
4	D	860	LYS
4	D	864	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	882	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	ASN
4	A	41	HIS
4	A	86	ASN
4	A	135	GLN
4	A	171	ASN
4	A	184	GLN
4	A	205	HIS
4	A	211	HIS
4	A	230	HIS
4	A	232	GLN
4	A	239	GLN
4	A	269	GLN
4	A	289	ASN
4	A	404	GLN
4	A	410	ASN
4	A	419	ASN
4	A	435	GLN
4	A	437	ASN
4	A	466	ASN
4	A	485	ASN
4	A	486	HIS
4	A	488	ASN
4	A	545	HIS
4	A	588	ASN
4	A	592	ASN
4	A	649	GLN
4	A	656	GLN
4	A	669	GLN
4	A	672	GLN
4	A	748	ASN
4	A	754	GLN
4	A	781	ASN
4	A	823	ASN
4	A	848	GLN
4	A	854	HIS
4	A	857	GLN
4	A	869	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	871	ASN
4	B	5	ASN
4	B	107	GLN
4	B	135	GLN
4	B	161	HIS
4	B	169	GLN
4	B	171	ASN
4	B	232	GLN
4	B	233	ASN
4	B	239	GLN
4	B	269	GLN
4	B	324	GLN
4	B	404	GLN
4	B	419	ASN
4	B	435	GLN
4	B	437	ASN
4	B	486	HIS
4	B	488	ASN
4	B	499	ASN
4	B	505	GLN
4	B	529	ASN
4	B	544	GLN
4	B	545	HIS
4	B	588	ASN
4	B	619	GLN
4	B	656	GLN
4	B	672	GLN
4	B	726	HIS
4	B	748	ASN
4	B	772	HIS
4	B	781	ASN
4	B	786	GLN
4	B	823	ASN
4	B	848	GLN
4	B	852	GLN
4	B	869	ASN
4	C	5	ASN
4	C	58	GLN
4	C	86	ASN
4	C	104	GLN
4	C	107	GLN
4	C	169	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	171	ASN
4	C	269	GLN
4	C	289	ASN
4	C	324	GLN
4	C	339	ASN
4	C	410	ASN
4	C	435	GLN
4	C	437	ASN
4	C	463	HIS
4	C	499	ASN
4	C	560	ASN
4	C	588	ASN
4	C	656	GLN
4	C	669	GLN
4	C	726	HIS
4	C	737	GLN
4	C	744	GLN
4	C	781	ASN
4	C	786	GLN
4	D	22	ASN
4	D	27	HIS
4	D	41	HIS
4	D	86	ASN
4	D	107	GLN
4	D	161	HIS
4	D	169	GLN
4	D	184	GLN
4	D	239	GLN
4	D	269	GLN
4	D	289	ASN
4	D	324	GLN
4	D	331	ASN
4	D	410	ASN
4	D	419	ASN
4	D	435	GLN
4	D	437	ASN
4	D	463	HIS
4	D	499	ASN
4	D	544	GLN
4	D	619	GLN
4	D	669	GLN
4	D	726	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	737	GLN
4	D	744	GLN
4	D	748	ASN
4	D	754	GLN
4	D	790	HIS
4	D	823	ASN
4	D	854	HIS
4	D	857	GLN
4	D	871	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	7/12 (58%)	0	0
2	I	7/12 (58%)	1 (14%)	0
2	L	7/12 (58%)	0	0
2	O	7/12 (58%)	0	0
All	All	28/48 (58%)	1 (3%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	8	U

There are no RNA pucker outliers to report.

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	APC	A	2000	5	29,33,33	1.61	3 (10%)	44,52,52	1.41	7 (15%)
6	APC	D	2003	5	29,33,33	1.80	5 (17%)	44,52,52	1.38	6 (13%)
6	APC	B	2001	5	29,33,33	1.52	6 (20%)	44,52,52	1.58	7 (15%)
6	APC	C	2002	5	29,33,33	1.62	6 (20%)	44,52,52	1.14	4 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	APC	A	2000	5	-	6/19/38/38	0/3/3/3
6	APC	D	2003	5	-	8/19/38/38	0/3/3/3
6	APC	B	2001	5	-	8/19/38/38	0/3/3/3
6	APC	C	2002	5	-	5/19/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2003	APC	PB-O3B	7.26	1.66	1.58
6	A	2000	APC	PB-O3B	6.65	1.65	1.58
6	C	2002	APC	PB-O3B	5.59	1.64	1.58
6	B	2001	APC	PB-O3B	4.57	1.63	1.58
6	B	2001	APC	PB-O2B	-2.77	1.49	1.56
6	B	2001	APC	PA-O2A	-2.51	1.50	1.56
6	C	2002	APC	C5-C6	2.50	1.48	1.41
6	C	2002	APC	PA-O2A	-2.49	1.50	1.56
6	B	2001	APC	C5'-C4'	2.45	1.58	1.51
6	C	2002	APC	C2-N1	2.38	1.38	1.33
6	D	2003	APC	C2-N3	2.33	1.38	1.33
6	B	2001	APC	C2-N3	2.28	1.38	1.33
6	A	2000	APC	PB-O2B	-2.25	1.50	1.56
6	C	2002	APC	C2-N3	2.12	1.37	1.33
6	C	2002	APC	PB-O2B	-2.10	1.51	1.56
6	D	2003	APC	PA-O2A	-2.06	1.51	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2001	APC	C1'-N9	2.03	1.51	1.46
6	D	2003	APC	PB-O2B	-2.01	1.51	1.56
6	A	2000	APC	C2-N1	2.01	1.37	1.33
6	D	2003	APC	C2-N1	2.01	1.37	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2001	APC	C2'-C1'-N9	4.72	125.03	113.30
6	D	2003	APC	C2'-C1'-N9	4.51	124.50	113.30
6	B	2001	APC	O1A-PA-C3A	-4.49	97.24	109.05
6	A	2000	APC	O1A-PA-C3A	3.54	118.37	109.05
6	B	2001	APC	C2'-C3'-C4'	3.43	109.23	102.61
6	B	2001	APC	PB-O3B-PG	-3.37	120.37	132.45
6	D	2003	APC	O2B-PB-O1B	3.35	120.85	109.95
6	C	2002	APC	O2B-PB-O1B	3.18	120.31	109.95
6	D	2003	APC	O2A-PA-O1A	3.16	120.24	109.95
6	A	2000	APC	O2A-PA-O1A	3.03	119.80	109.95
6	C	2002	APC	O2A-PA-O1A	3.03	119.80	109.95
6	B	2001	APC	O2B-PB-O1B	3.02	119.77	109.95
6	C	2002	APC	C2'-C3'-C4'	2.99	108.40	102.61
6	A	2000	APC	O3G-PG-O3B	2.94	114.49	104.64
6	A	2000	APC	O2B-PB-O1B	2.93	119.50	109.95
6	A	2000	APC	PB-O3B-PG	-2.63	123.02	132.45
6	B	2001	APC	O2A-PA-O1A	2.63	118.51	109.95
6	D	2003	APC	O2'-C2'-C3'	2.55	119.99	111.82
6	D	2003	APC	C2'-C3'-C4'	2.26	106.97	102.61
6	C	2002	APC	PB-O3B-PG	-2.22	124.51	132.45
6	A	2000	APC	O4'-C4'-C3'	2.20	109.53	105.15
6	A	2000	APC	C2'-C3'-C4'	2.16	106.78	102.61
6	B	2001	APC	O2A-PA-C3A	2.07	115.32	106.73
6	D	2003	APC	O2B-PB-C3A	2.07	115.31	106.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2000	APC	PB-C3A-PA-O1A
6	A	2000	APC	PB-C3A-PA-O2A
6	A	2000	APC	PB-C3A-PA-O5'
6	B	2001	APC	PA-C3A-PB-O1B
6	B	2001	APC	PA-C3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	2001	APC	PA-C3A-PB-O3B
6	B	2001	APC	C5'-O5'-PA-O1A
6	C	2002	APC	PA-C3A-PB-O1B
6	C	2002	APC	PA-C3A-PB-O2B
6	C	2002	APC	PA-C3A-PB-O3B
6	C	2002	APC	PB-C3A-PA-O1A
6	C	2002	APC	PB-C3A-PA-O2A
6	D	2003	APC	PB-O3B-PG-O2G
6	D	2003	APC	PB-O3B-PG-O3G
6	D	2003	APC	PA-C3A-PB-O1B
6	D	2003	APC	PA-C3A-PB-O2B
6	D	2003	APC	PA-C3A-PB-O3B
6	D	2003	APC	PB-C3A-PA-O1A
6	D	2003	APC	PB-C3A-PA-O2A
6	D	2003	APC	PB-C3A-PA-O5'
6	A	2000	APC	O4'-C4'-C5'-O5'
6	B	2001	APC	O4'-C4'-C5'-O5'
6	A	2000	APC	C3'-C4'-C5'-O5'
6	A	2000	APC	PA-C3A-PB-O2B
6	B	2001	APC	PB-C3A-PA-O2A
6	B	2001	APC	PB-C3A-PA-O1A
6	B	2001	APC	C5'-O5'-PA-O2A

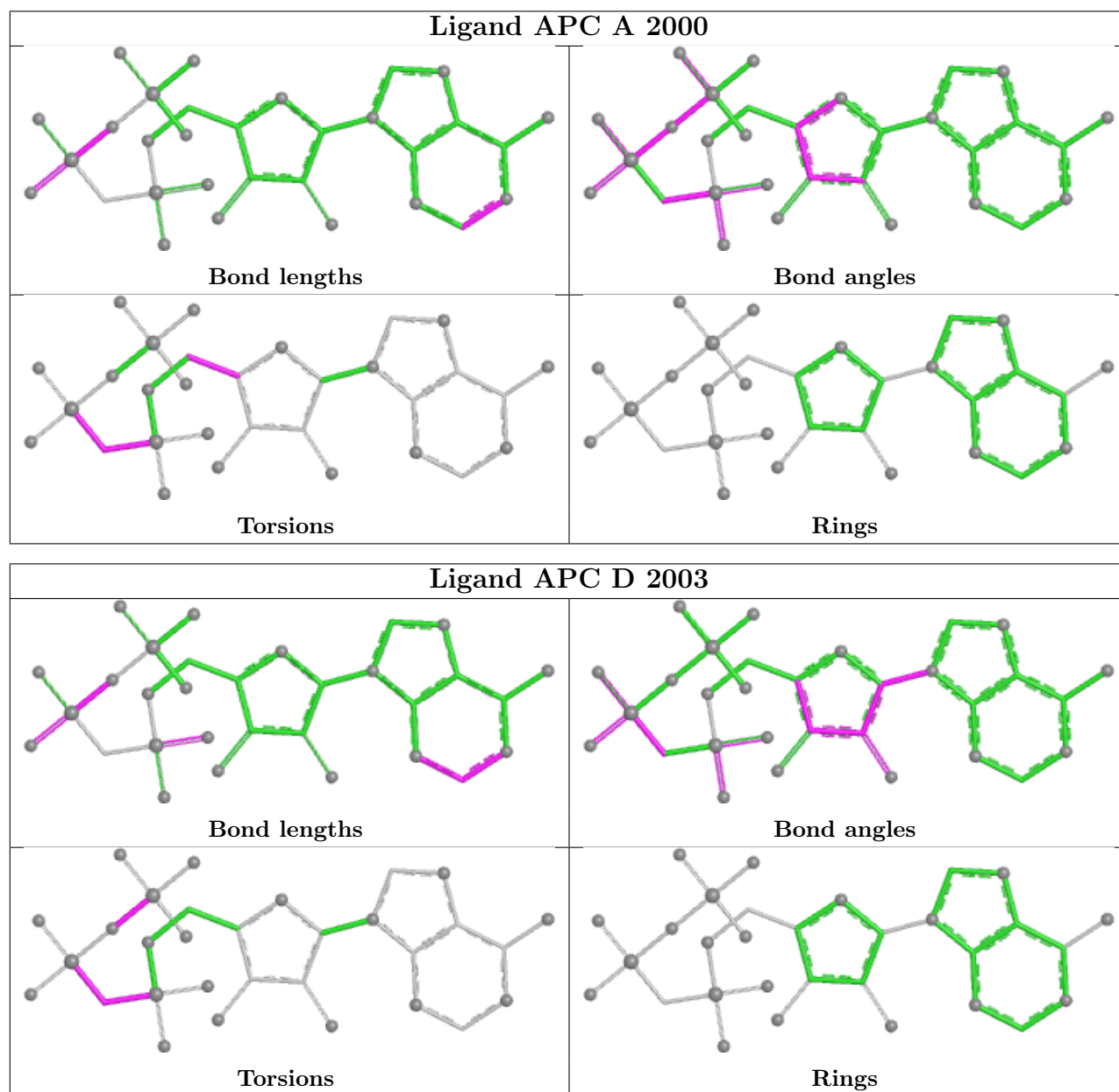
There are no ring outliers.

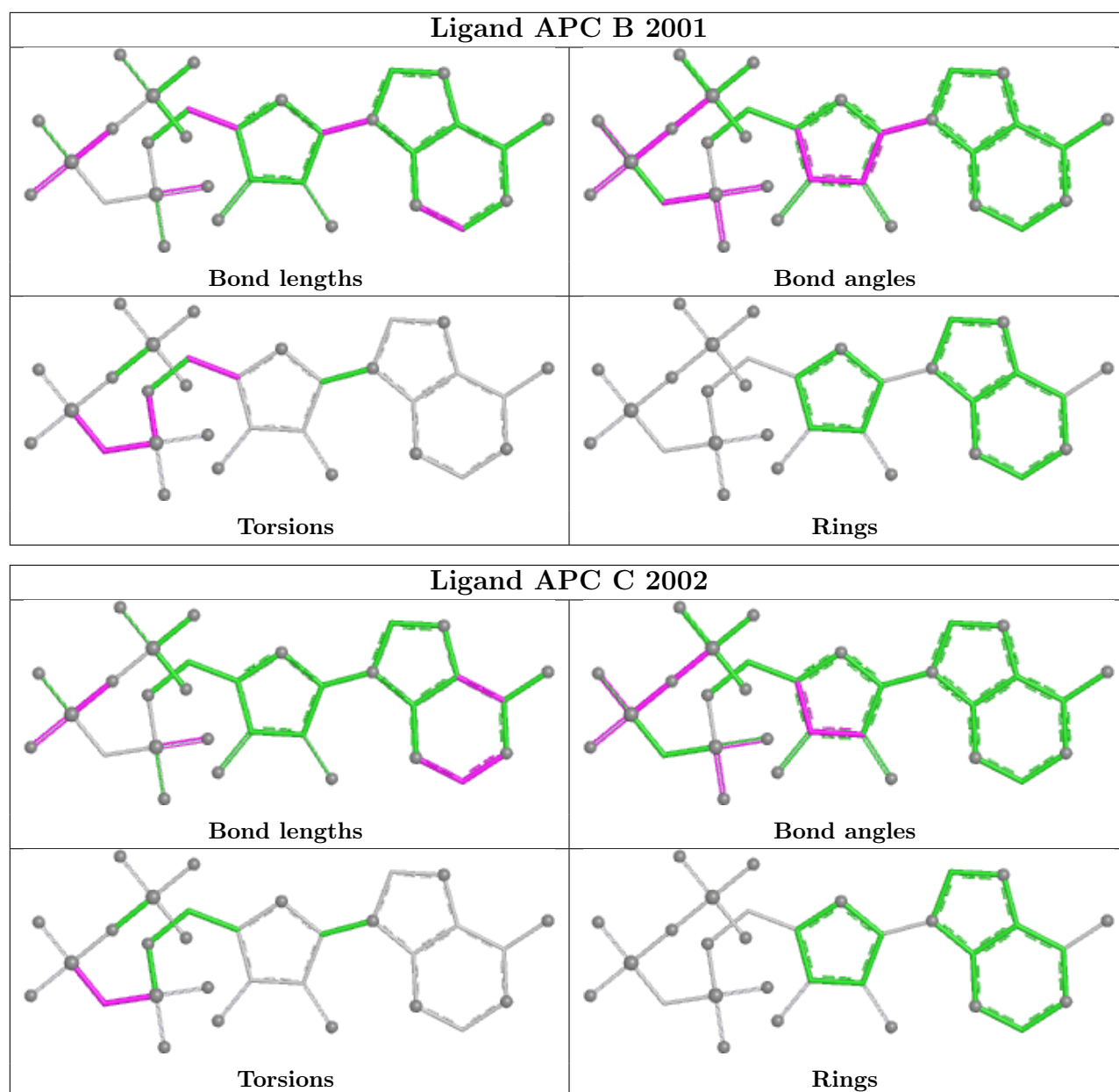
4 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2000	APC	16	0
6	D	2003	APC	8	0
6	B	2001	APC	10	0
6	C	2002	APC	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	17/18 (94%)	0.08	0 100 100	19, 58, 179, 181	0
1	H	17/18 (94%)	-0.17	0 100 100	21, 75, 158, 171	0
1	K	17/18 (94%)	0.05	0 100 100	48, 94, 157, 159	0
1	N	17/18 (94%)	0.08	0 100 100	51, 102, 172, 173	0
2	F	8/12 (66%)	-0.83	0 100 100	17, 23, 82, 93	0
2	I	8/12 (66%)	-0.73	0 100 100	17, 38, 82, 92	0
2	L	8/12 (66%)	-0.11	0 100 100	47, 52, 113, 118	0
2	O	8/12 (66%)	-0.10	0 100 100	51, 80, 132, 144	0
3	G	9/10 (90%)	0.91	2 (22%) 2 2	146, 153, 176, 183	0
3	J	9/10 (90%)	0.62	1 (11%) 10 7	130, 138, 162, 163	0
3	M	9/10 (90%)	0.34	1 (11%) 10 7	134, 146, 155, 158	0
3	P	9/10 (90%)	0.97	1 (11%) 10 7	157, 167, 172, 172	0
4	A	857/883 (97%)	-0.05	17 (1%) 65 45	15, 76, 141, 153	0
4	B	857/883 (97%)	-0.20	7 (0%) 82 67	10, 69, 131, 150	0
4	C	857/883 (97%)	0.08	10 (1%) 76 58	47, 93, 134, 160	0
4	D	857/883 (97%)	0.22	17 (1%) 65 45	41, 102, 144, 156	0
All	All	3564/3692 (96%)	0.02	56 (1%) 70 51	10, 89, 142, 183	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	116	TYR	5.4
4	B	16	LEU	4.9
3	P	1	DG	4.1
4	B	129	ALA	4.1
4	A	753	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	C	226	MET	3.8
4	D	65	ALA	3.7
4	A	752	LEU	3.7
4	C	541	SER	3.7
4	D	226	MET	3.6
4	D	216	CYS	3.3
4	A	70	ALA	3.2
4	A	148	GLU	3.2
4	C	434	PRO	3.2
3	G	1	DG	3.0
4	D	113	ALA	3.0
4	C	375	THR	2.9
4	D	110	LYS	2.8
4	A	244	ILE	2.8
4	D	686	SER	2.8
4	A	226	MET	2.8
4	A	606	SER	2.8
4	C	16	LEU	2.7
4	D	212	VAL	2.7
4	B	754	GLN	2.7
4	B	130	ASP	2.6
4	A	120	LYS	2.6
4	D	24	LEU	2.5
3	G	9	DC	2.5
4	B	234	ALA	2.5
4	A	667	PHE	2.5
4	D	816	THR	2.4
4	B	883	ALA	2.4
4	A	601	ASN	2.4
4	A	113	ALA	2.4
4	D	281	ILE	2.3
4	C	354	ALA	2.3
4	B	94	ALA	2.3
4	C	402	LEU	2.3
4	D	435	GLN	2.3
4	A	749	LEU	2.2
4	C	692	ALA	2.2
4	D	751	PHE	2.2
4	C	883	ALA	2.1
3	J	1	DG	2.1
4	A	751	PHE	2.1
4	A	754	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	A	168	GLU	2.1
3	M	1	DG	2.1
4	D	172	LYS	2.1
4	D	229	LEU	2.1
4	D	747	LEU	2.1
4	C	418	TYR	2.1
4	D	595	VAL	2.0
4	A	746	ARG	2.0
4	D	748	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

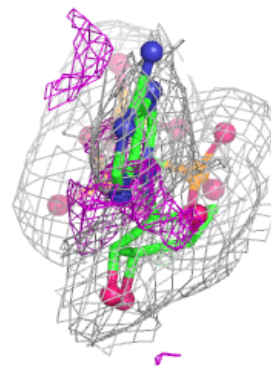
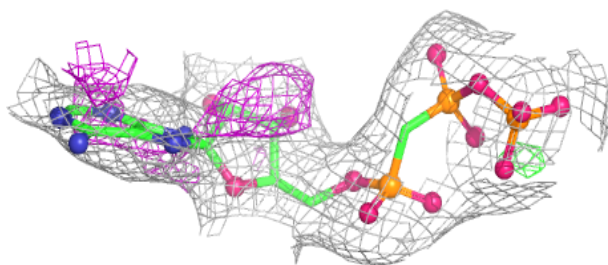
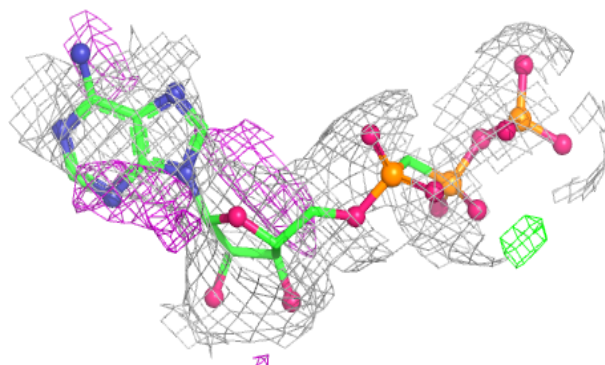
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	D	3004	1/1	0.57	0.16	79,79,79,79	0
5	MG	B	3002	1/1	0.84	0.21	65,65,65,65	0
5	MG	C	3007	1/1	0.91	0.13	46,46,46,46	0
5	MG	D	3008	1/1	0.91	0.08	16,16,16,16	0
6	APC	B	2001	31/31	0.92	0.10	28,47,63,68	0
6	APC	C	2002	31/31	0.93	0.10	65,70,77,78	0
6	APC	D	2003	31/31	0.93	0.08	48,57,61,63	0
6	APC	A	2000	31/31	0.95	0.09	34,58,80,82	0
5	MG	C	3003	1/1	0.97	0.06	41,41,41,41	0
5	MG	F	3005	1/1	0.97	0.06	18,18,18,18	0
5	MG	A	3001	1/1	0.98	0.04	22,22,22,22	0
5	MG	B	3006	1/1	0.98	0.07	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

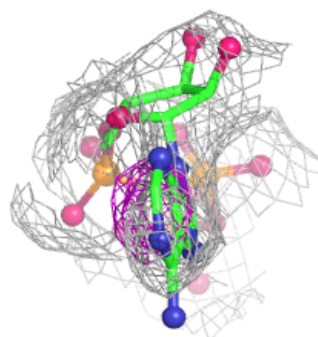
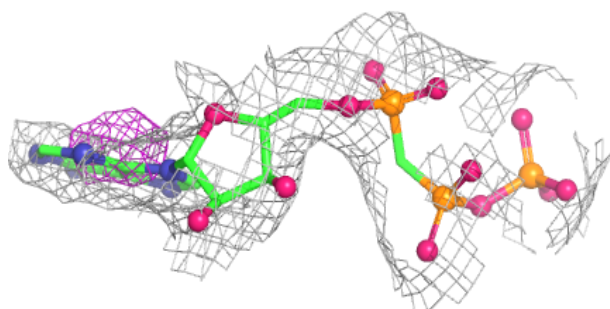
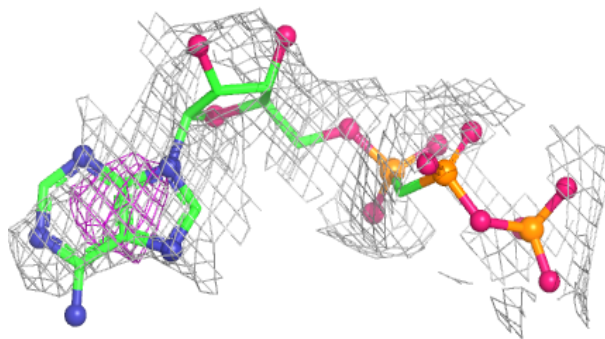
Electron density around APC B 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

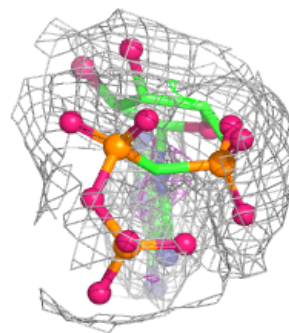
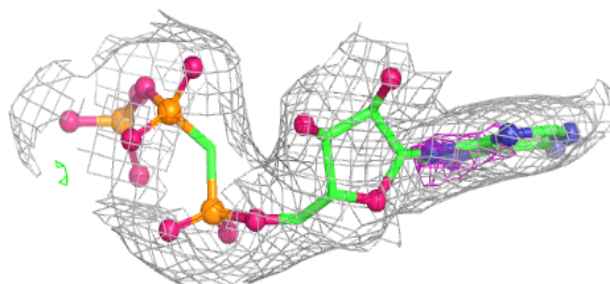
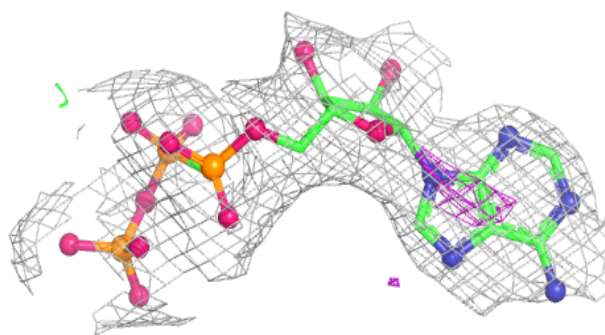


Electron density around APC C 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

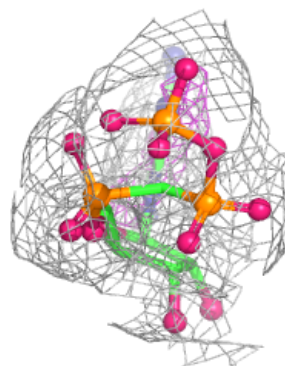
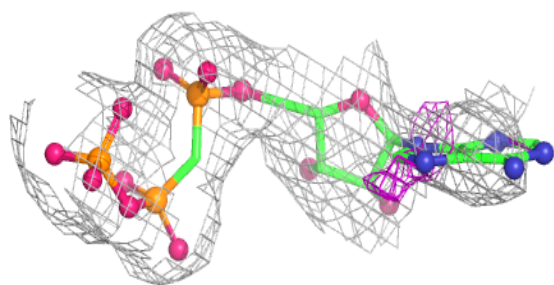
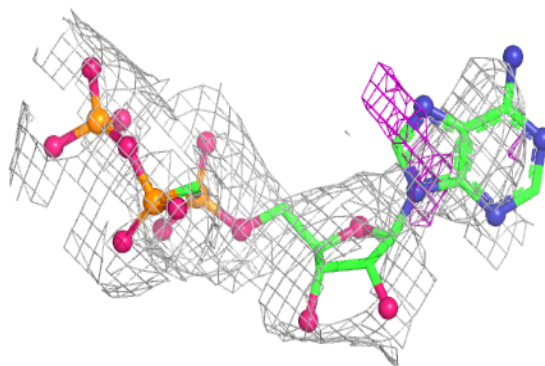
**Electron density around APC D 2003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around APC A 2000:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.