



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:10 AM GMT

PDB ID : 3O8O
Title : Structure of phosphofructokinase from *Saccharomyces cerevisiae*
Authors : Banaszak, K.; Mechin, I.; Kopperschlager, G.; Rypniewski, W.
Deposited on : 2010-08-03
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

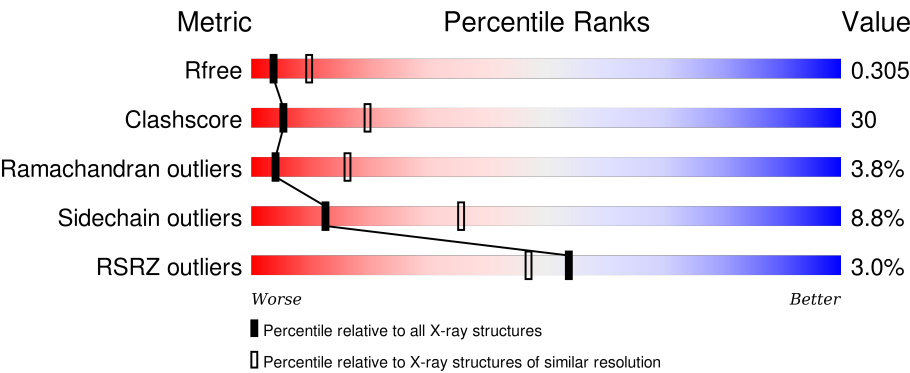
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	787	<div><div>3%</div><div>52%37%6% • 5%</div></div>
1	C	787	<div><div>4%</div><div>51%38%5% • 5%</div></div>
1	E	787	<div><div>3%</div><div>53%35%6% • •</div></div>
1	G	787	<div><div>4%</div><div>53%34%6% • 5%</div></div>
2	B	766	<div><div>3%</div><div>53%39%7% •</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	766	
2	F	766	
2	H	766	

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
4	FDP	C	3	-	-	-	X
4	FDP	H	8	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46645 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.

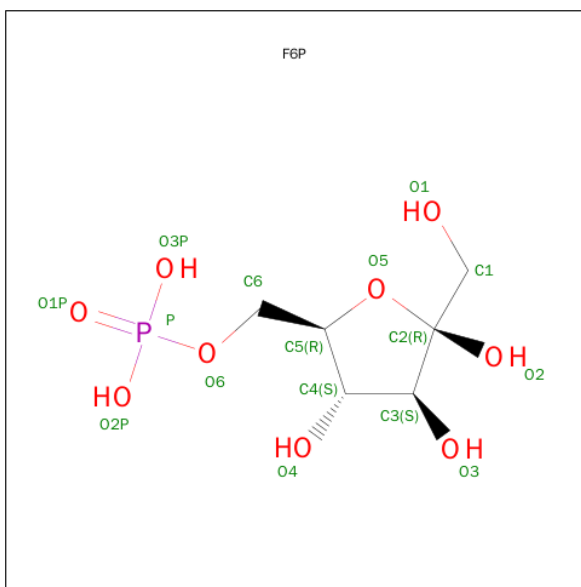
- Molecule 1 is a protein called 6-phosphofructokinase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	273	0	0
			5759	3620	1019	1098	22			
1	C	750	Total	C	N	O	S	196	0	0
			5759	3620	1019	1098	22			
1	E	752	Total	C	N	O	S	260	0	0
			5777	3631	1023	1101	22			
1	G	746	Total	C	N	O	S	289	0	0
			5733	3604	1015	1092	22			

- Molecule 2 is a protein called 6-phosphofructokinase subunit beta.

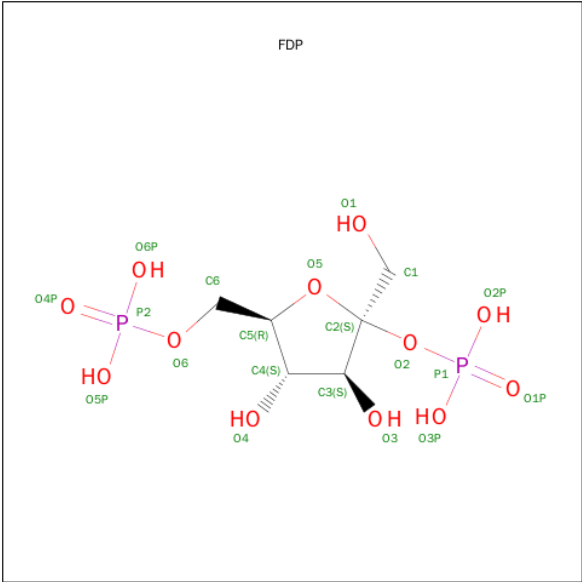
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	763	Total	C	N	O	S	364	0	0
			5834	3652	1034	1118	30			
2	D	763	Total	C	N	O	S	266	0	0
			5834	3652	1034	1118	30			
2	F	762	Total	C	N	O	S	279	0	0
			5827	3647	1033	1117	30			
2	H	763	Total	C	N	O	S	173	0	0
			5834	3652	1034	1118	30			

- Molecule 3 is SUGAR (FRUCTOSE-6-PHOSPHATE) (three-letter code: F6P) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		
3	E	1	Total	C	O	P	0	0
			16	6	9	1		
3	F	1	Total	C	O	P	0	0
			16	6	9	1		
3	G	1	Total	C	O	P	0	0
			16	6	9	1		
3	H	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is SUGAR (FRUCTOSE-2,6-DIPHOSPHATE) (three-letter code: FDP) (formula: C₆H₁₄O₁₂P₂).

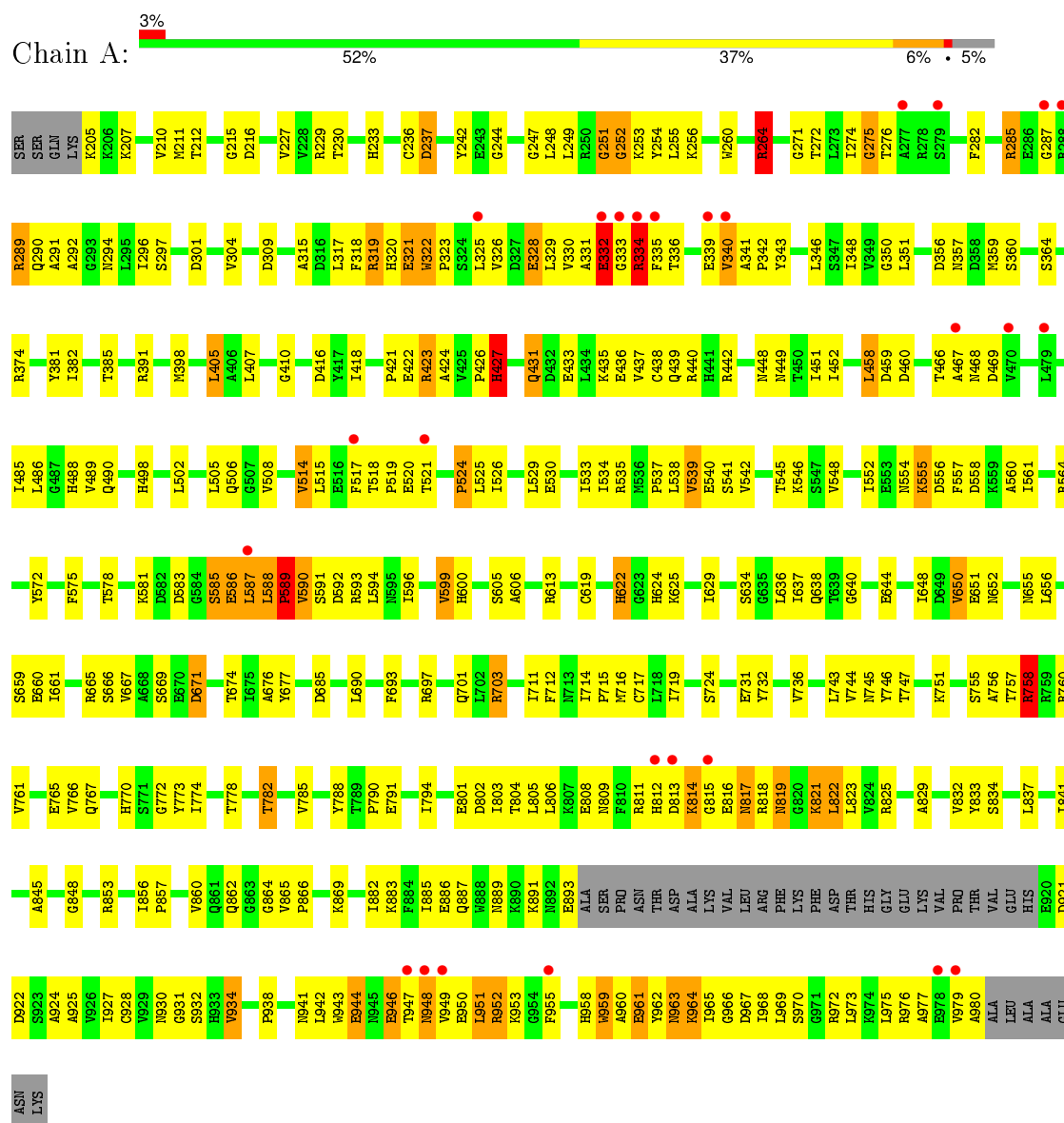


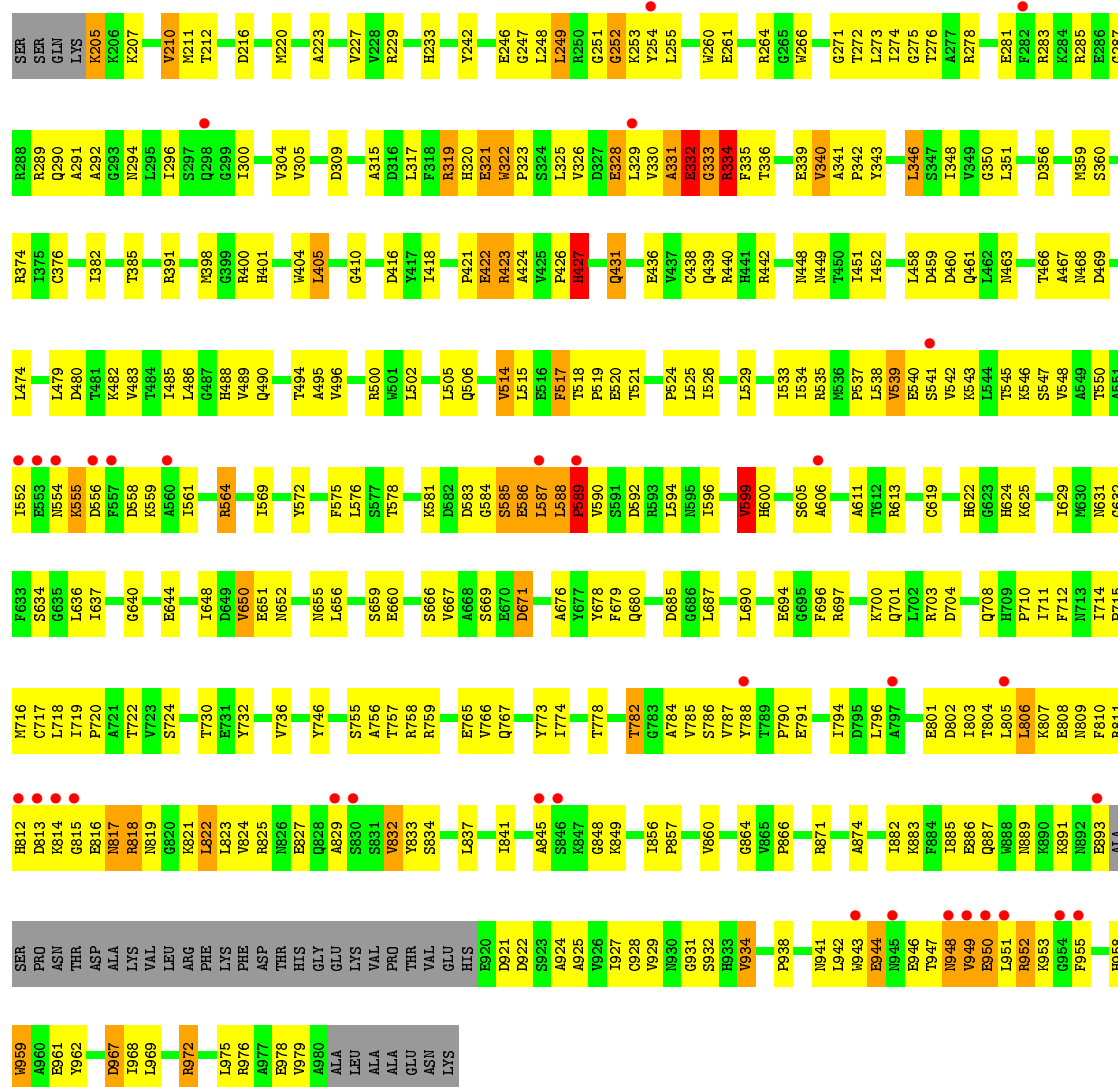
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		
4	E	1	Total	C	O	P	0	0
			20	6	12	2		
4	F	1	Total	C	O	P	0	0
			20	6	12	2		
4	G	1	Total	C	O	P	0	0
			20	6	12	2		
4	H	1	Total	C	O	P	0	0
			20	6	12	2		

3 Residue-property plots

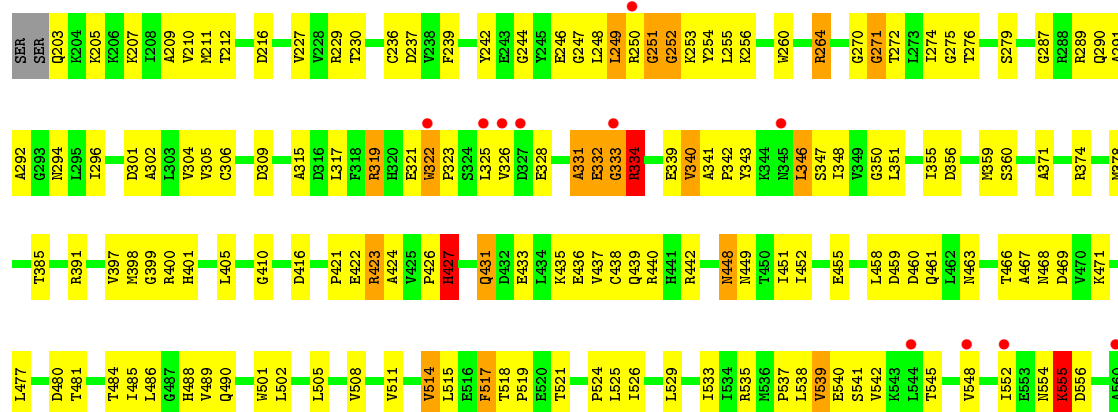
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

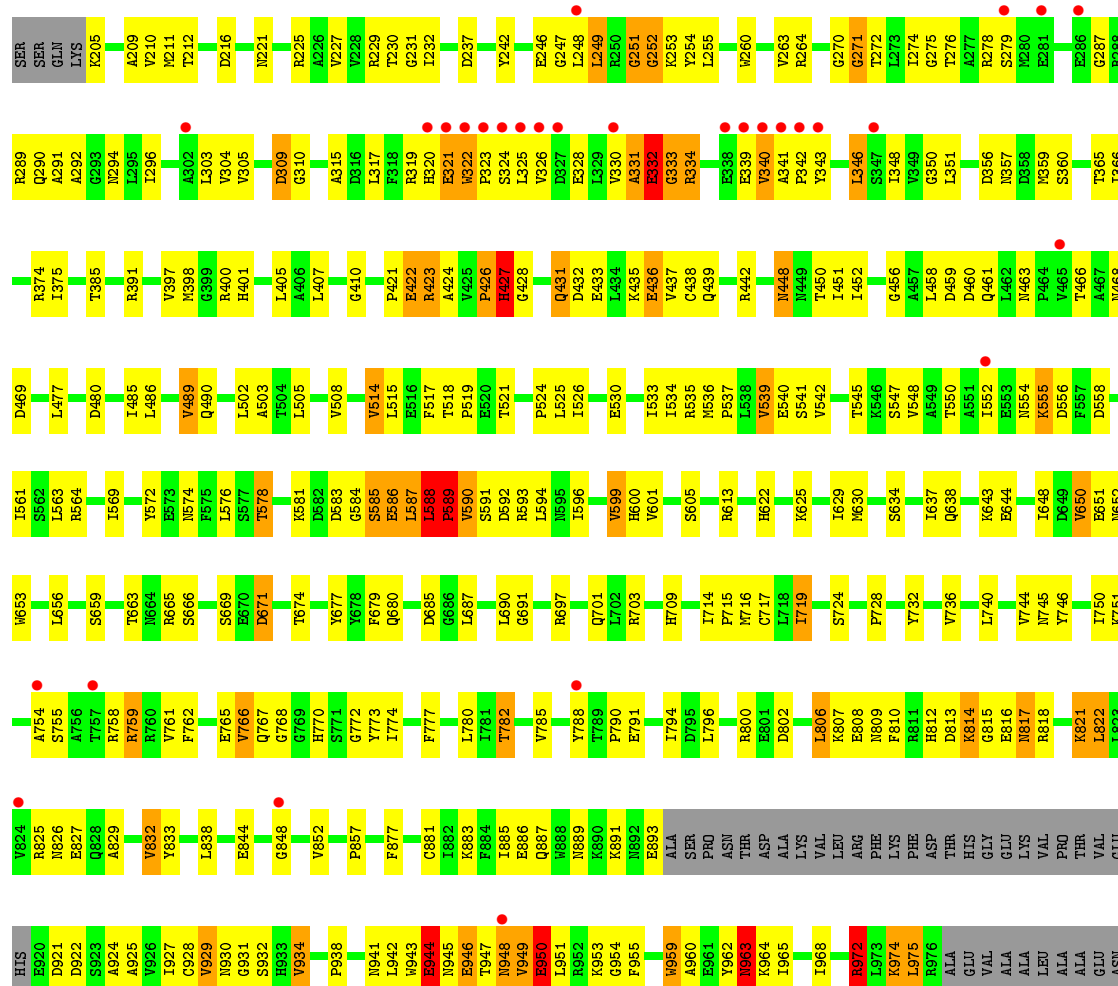
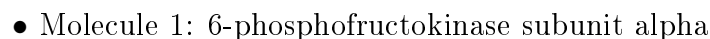
• Molecule 1: 6-phosphofructokinase subunit alpha





• Molecule 1: 6-phosphofructokinase subunit alpha



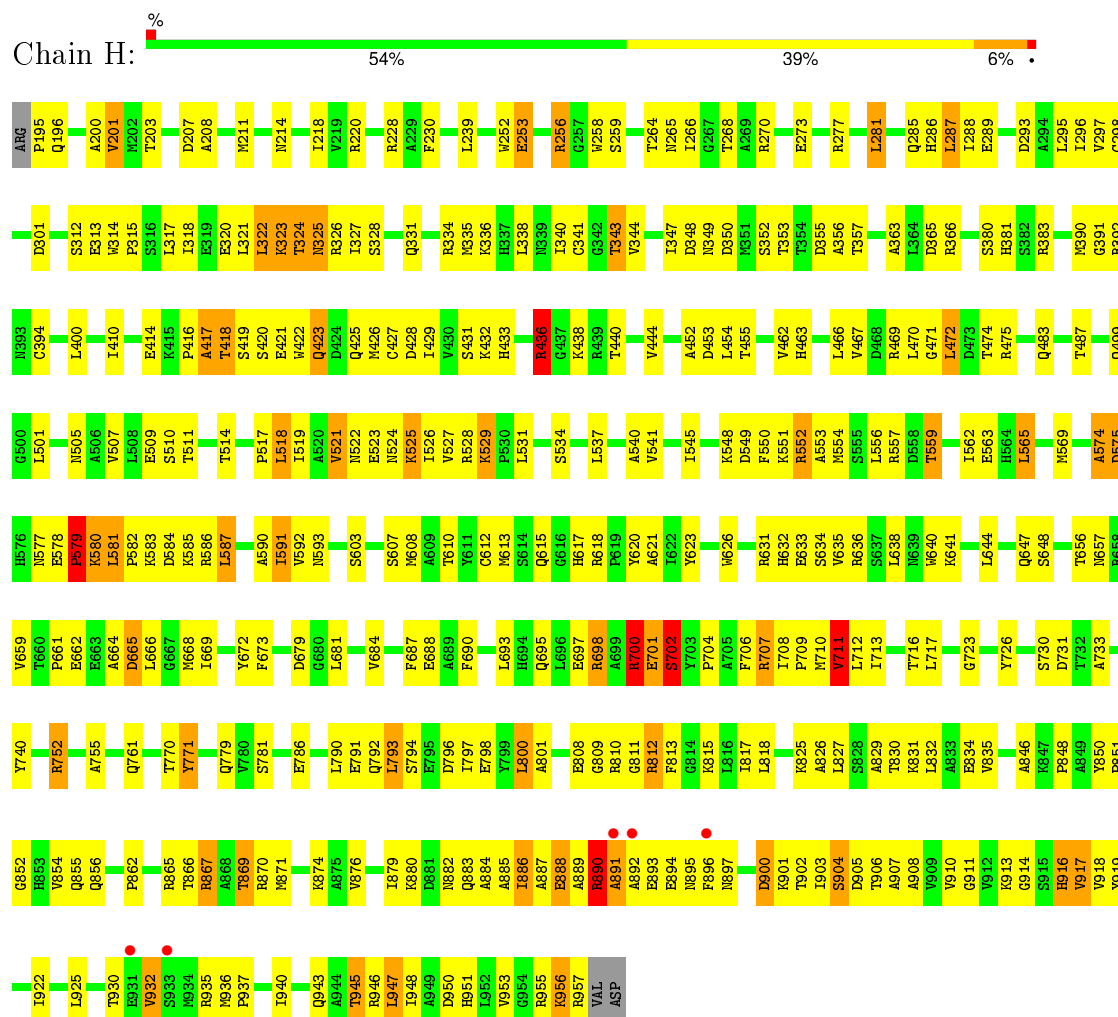


A378	D283	A379	D284	A380	D285	A381	D286	A382	D287	A383	D288	A384	D289	A385	D290	A386	D291	A387	D292	A388	D293	A389	D294	A390	D295	A391	D296	A392	D297	A393	D298	A394	D299	A395	D300	A396	D301	A397	D302	A398	D303	A399	D304	A400	D305	A401	D306	A402	D307	A403	D308	A404	D309	A405	D310	A406	D311	A407	D312	A408	D313	A409	D314	A410	D315	A411	D316	A412	D317	A413	D318	A414	D319	A415	D320	A416	D321	A417	D322	A418	D323	A419	D324	A420	D325	A421	D326	A422	D327	A423	D328	A424	D329	A425	D330	A426	D331	A427	D332	A428	D333	A429	D334	A430	D335	A431	D336	A432	D337	A433	D338	A434	D339	A435	D340	A436	D341	A437	D342	A438	D343	A439	D344	A440	D345	A441	D346	A442	D347	A443	D348	A444	D349	A445	D350	A446	D351	A447	D352	A448	D353	A449	D354	A450	D355	A451	D356	A452	D357	A453	D358	A454	D359	A455	D360	A456	D361	A457	D362	A458	D363	A459	D364	A460	D365	A461	D366	A462	D367	A463	D368	A464	D369	A465	D370	A466	D371	A467	D372	A468	D373	A469	D374	A470	D375	A471	D376	A472	D377	A473	D378	A474	D379	A475	D380	A476	D381	A477	D382	A478	D383	A479	D384	A480	D385	A481	D386	A482	D387	A483	D388	A484	D389	A485	D390	A486	D391	A487	D392	A488	D393	A489	D394	A490	D395	A491	D396	A492	D397	A493	D398	A494	D399	A495	D400	A496	D401	A497	D402	A498	D403	A499	D404	A500	D405	A501	D406	A502	D407	A503	D408	A504	D409	A505	D410	A506	D411	A507	D412	A508	D413	A509	D414	A510	D415	A511	D416	A512	D417	A513	D418	A514	D419	A515	D420	A516	D421	A517	D422	A518	D423	A519	D424	A520	D425	A521	D426	A522	D427	A523	D428	A524	D429	A525	D430	A526	D431	A527	D432	A528	D433	A529	D434	A530	D435	A531	D436	A532	D437	A533	D438	A534	D439	A535	D440	A536	D441	A537	D442	A538	D443	A539	D444	A540	D445	A541	D446	A542	D447	A543	D448	A544	D449	A545	D450	A546	D451	A547	D452	A548	D453	A549	D454	A550	D455	A551	D456	A552	D457	A553	D458	A554	D459	A555	D460	A556	D461	A557	D462	A558	D463	A559	D464	A560	D465	A561	D466	A562	D467	A563	D468	A564	D469	A565	D470	A566	D471	A567	D472	A568	D473	A569	D474	A570	D475	A571	D476	A572	D477	A573	D478	A574	D479	A575	D480	A576	D481	A577	D482	A578	D483	A579	D484	A580	D485	A581	D486	A582	D487	A583	D488	A584	D489	A585	D490	A586	D491	A587	D492	A588	D493	A589	D494	A590	D495	A591	D496	A592	D497	A593	D498	A594	D499	A595	D500	A596	D501	A597	D502	A598	D503	A599	D504	A600	D505	A601	D506	A602	D507	A603	D508	A604	D509	A605	D510	A606	D511	A607	D512	A608	D513	A609	D514	A610	D515	A611	D516	A612	D517	A613	D518	A614	D519	A615	D520	A616	D521	A617	D522	A618	D523	A619	D524	A620	D525	A621	D526	A622	D527	A623	D528	A624	D529	A625	D530	A626	D531	A627	D532	A628	D533	A629	D534	A630	D535	A631	D536	A632	D537	A633	D53
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----





● Molecule 2: 6-phosphofructokinase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	180.05Å 186.21Å 236.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.90 34.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.90) 98.4 (34.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.309 0.257 , 0.305	Depositor DCC
R_{free} test set	3446 reflections (1.99%)	DCC
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.3	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 172763 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	46645	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FDP, F6P

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	A	0.53	0/5860	0.80	13/7925 (0.2%)
1	C	0.58	1/5860 (0.0%)	0.83	11/7925 (0.1%)
1	E	0.57	0/5878	0.82	17/7948 (0.2%)
1	G	0.59	1/5834 (0.0%)	0.80	9/7889 (0.1%)
2	B	0.52	1/5940 (0.0%)	0.79	14/8038 (0.2%)
2	D	0.55	1/5940 (0.0%)	0.83	20/8038 (0.2%)
2	F	0.51	0/5932	0.80	17/8027 (0.2%)
2	H	0.59	0/5940	0.84	19/8038 (0.2%)
All	All	0.56	4/47184 (0.0%)	0.81	120/63828 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	376	CYS	CB-SG	-7.40	1.69	1.82
2	B	741	CYS	CB-SG	-5.75	1.72	1.81
2	D	760	CYS	CB-SG	-5.12	1.73	1.81
1	G	881	CYS	CB-SG	-5.10	1.73	1.81

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	759	ARG	NE-CZ-NH1	-9.97	115.32	120.30
1	C	283	ARG	NE-CZ-NH2	9.78	125.19	120.30
2	H	436	ARG	NE-CZ-NH1	-9.71	115.44	120.30
1	A	289	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	C	283	ARG	NE-CZ-NH1	-9.64	115.48	120.30
1	E	759	ARG	NE-CZ-NH2	9.21	124.91	120.30
1	A	289	ARG	NE-CZ-NH2	9.11	124.86	120.30
2	D	334	ARG	NE-CZ-NH1	-8.87	115.87	120.30
1	G	264	ARG	NE-CZ-NH2	-8.32	116.14	120.30
2	H	631	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	F	636	ARG	NE-CZ-NH2	8.13	124.36	120.30
1	C	818	ARG	NE-CZ-NH1	-8.10	116.25	120.30
2	D	334	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	A	264	ARG	NE-CZ-NH2	7.96	124.28	120.30
2	F	636	ARG	NE-CZ-NH1	-7.86	116.37	120.30
2	D	326	ARG	NE-CZ-NH1	-7.72	116.44	120.30
2	H	631	ARG	NE-CZ-NH2	7.71	124.15	120.30
1	C	264	ARG	NE-CZ-NH2	-7.69	116.45	120.30
2	D	923	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	C	818	ARG	NE-CZ-NH2	7.66	124.13	120.30
2	D	923	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	E	758	ARG	NE-CZ-NH1	-7.58	116.51	120.30
2	H	436	ARG	NE-CZ-NH2	7.55	124.07	120.30
2	B	698	ARG	NE-CZ-NH2	7.55	124.07	120.30
2	F	698	ARG	NE-CZ-NH2	-7.50	116.55	120.30
2	D	812	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	D	326	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	G	264	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	H	270	ARG	NE-CZ-NH2	-7.32	116.64	120.30
2	B	698	ARG	NE-CZ-NH1	-7.32	116.64	120.30
2	F	812	ARG	NE-CZ-NH2	-7.30	116.65	120.30
2	F	698	ARG	NE-CZ-NH1	7.29	123.94	120.30
2	H	812	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	A	319	ARG	NE-CZ-NH2	7.07	123.83	120.30
2	H	270	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	D	698	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	E	264	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	E	319	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	C	592	ASP	N-CA-C	-6.84	92.53	111.00
2	B	812	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	E	758	ARG	NE-CZ-NH2	6.82	123.71	120.30
2	H	698	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	H	812	ARG	NE-CZ-NH2	6.77	123.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	E	264	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	A	264	ARG	NE-CZ-NH1	-6.70	116.95	120.30
2	F	270	ARG	NE-CZ-NH1	-6.67	116.96	120.30
2	D	270	ARG	NE-CZ-NH2	-6.67	116.97	120.30
2	D	698	ARG	NE-CZ-NH2	6.63	123.61	120.30
2	D	812	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	334	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	C	334	ARG	NE-CZ-NH2	-6.58	117.01	120.30
2	B	812	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	G	334	ARG	NE-CZ-NH2	-6.56	117.02	120.30
2	D	277	ARG	NE-CZ-NH2	6.55	123.58	120.30
2	B	270	ARG	NE-CZ-NH1	-6.51	117.04	120.30
2	H	277	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	264	ARG	NE-CZ-NH1	6.49	123.55	120.30
2	B	277	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	E	334	ARG	NE-CZ-NH1	-6.48	117.06	120.30
2	B	277	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	H	698	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	E	592	ASP	N-CA-C	-6.38	93.76	111.00
2	D	270	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	285	ARG	NE-CZ-NH2	6.35	123.48	120.30
2	H	277	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	F	812	ARG	NE-CZ-NH1	6.33	123.47	120.30
2	D	277	ARG	NE-CZ-NH1	-6.33	117.14	120.30
2	F	618	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	285	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	G	592	ASP	N-CA-C	-6.28	94.04	111.00
2	D	436	ARG	NE-CZ-NH2	-6.27	117.16	120.30
2	H	811	GLY	N-CA-C	6.21	128.62	113.10
1	E	334	ARG	NE-CZ-NH2	6.20	123.40	120.30
2	D	618	ARG	NE-CZ-NH1	-6.17	117.22	120.30
2	B	436	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	D	811	GLY	N-CA-C	6.13	128.42	113.10
1	C	599	VAL	CB-CA-C	-6.13	99.76	111.40
2	B	811	GLY	N-CA-C	6.11	128.38	113.10
2	F	270	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	A	334	ARG	NE-CZ-NH2	6.07	123.33	120.30
2	B	270	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	592	ASP	N-CA-C	-6.06	94.65	111.00
2	D	618	ARG	NE-CZ-NH2	6.04	123.32	120.30
2	B	618	ARG	NE-CZ-NH1	-6.03	117.29	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	618	ARG	NE-CZ-NH2	6.01	123.30	120.30
1	E	811	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	H	618	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	D	436	ARG	NE-CZ-NH1	5.89	123.24	120.30
2	F	436	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	F	890	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	G	334	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	H	890	ARG	NE-CZ-NH2	5.74	123.17	120.30
2	F	811	GLY	N-CA-C	5.72	127.41	113.10
1	E	319	ARG	NE-CZ-NH2	-5.71	117.45	120.30
2	F	277	ARG	NE-CZ-NH1	-5.67	117.47	120.30
2	F	277	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	811	ARG	NE-CZ-NH2	5.58	123.09	120.30
2	F	618	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	H	890	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	G	319	ARG	NE-CZ-NH1	-5.54	117.53	120.30
2	H	618	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	H	731	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	972	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	B	890	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	B	585	LYS	N-CA-C	-5.30	96.68	111.00
2	H	352	SER	N-CA-C	5.29	125.28	111.00
1	E	719	ILE	N-CA-C	-5.22	96.89	111.00
1	G	945	ASN	N-CA-C	-5.21	96.92	111.00
1	G	588	LEU	N-CA-C	-5.20	96.97	111.00
1	A	811	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	E	811	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	E	588	LEU	N-CA-C	-5.15	97.09	111.00
1	C	811	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	E	205	LYS	N-CA-C	5.08	124.73	111.00
2	F	352	SER	N-CA-C	5.07	124.69	111.00
2	D	585	LYS	N-CA-C	-5.07	97.32	111.00
1	E	593	ARG	N-CA-C	-5.07	97.32	111.00
1	G	719	ILE	N-CA-C	-5.05	97.36	111.00
2	F	436	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	771	TYR	Sidechain
2	D	771	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	F	771	TYR	Sidechain
2	H	771	TYR	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	A	5759	0	5758	334	0
1	C	5759	0	5758	326	0
1	E	5777	0	5779	323	0
1	G	5733	0	5733	306	0
2	B	5834	0	5799	366	0
2	D	5834	0	5799	349	0
2	F	5827	0	5791	327	1
2	H	5834	0	5799	373	1
3	A	16	0	11	4	0
3	B	16	0	11	4	0
3	C	16	0	11	1	0
3	D	16	0	11	3	0
3	E	16	0	11	2	0
3	F	16	0	11	4	0
3	G	16	0	11	2	0
3	H	16	0	11	5	0
4	A	20	0	10	6	0
4	B	20	0	10	3	0
4	C	20	0	10	1	0
4	D	20	0	10	2	0
4	E	20	0	10	0	0
4	F	20	0	10	3	0
4	G	20	0	10	0	0
4	H	20	0	10	2	0
All	All	46645	0	46384	2612	1

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 30.

All (2612) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:HIS:HB3	1:C:460:ASP:HB2	1.33	1.10
1:A:665:ARG:HH21	4:A:1:FDP:H62	1.12	1.07
1:A:427:HIS:HB3	1:A:460:ASP:HB2	1.35	1.06
2:H:874:LYS:HD3	2:H:917:VAL:HG11	1.34	1.06
1:G:427:HIS:HB3	1:G:460:ASP:HB2	1.40	1.03
1:E:427:HIS:HB3	1:E:460:ASP:HB2	1.40	1.02
2:B:416:PRO:O	2:B:418:THR:HG22	1.60	1.02
2:H:416:PRO:O	2:H:418:THR:HG22	1.61	0.99
2:H:578:GLU:O	2:H:580:LYS:N	1.95	0.99
2:D:416:PRO:O	2:D:418:THR:HG22	1.60	0.98
2:H:214:ASN:ND2	2:H:343:THR:HG21	1.78	0.98
2:B:418:THR:HA	2:B:421:GLU:HB2	1.44	0.98
2:D:874:LYS:HD3	2:D:917:VAL:HG11	1.43	0.98
1:C:518:THR:OG1	1:C:521:THR:HG23	1.64	0.97
1:E:599:VAL:HG13	1:E:629:ILE:HB	1.46	0.97
2:B:418:THR:HG23	2:B:419:SER:H	1.28	0.97
2:D:418:THR:HG23	2:D:419:SER:H	1.26	0.97
1:C:804:THR:CG2	1:C:979:VAL:HG21	1.95	0.97
2:B:635:VAL:O	2:B:636:ARG:HD2	1.64	0.97
1:A:665:ARG:NH2	4:A:1:FDP:H62	1.79	0.96
1:A:599:VAL:HG13	1:A:629:ILE:HB	1.48	0.96
1:G:599:VAL:HG13	1:G:629:ILE:HB	1.44	0.96
2:F:416:PRO:O	2:F:418:THR:HG22	1.65	0.96
2:B:711:VAL:HA	2:B:908:ALA:O	1.66	0.95
1:E:821:LYS:HZ2	1:E:821:LYS:HB2	1.31	0.95
1:A:319:ARG:HB2	1:A:348:ILE:HD12	1.48	0.95
2:H:578:GLU:O	2:H:580:LYS:HG3	1.66	0.95
2:B:578:GLU:O	2:B:580:LYS:HG3	1.66	0.94
2:F:418:THR:HG23	2:F:419:SER:H	1.31	0.94
1:C:669:SER:H	1:C:701:GLN:HE22	1.14	0.94
2:F:701:GLU:O	2:F:702:SER:HB2	1.68	0.94
2:H:577:ASN:HB3	2:H:579:PRO:HG2	1.46	0.94
1:G:581:LYS:HB3	1:G:586:GLU:HB3	1.49	0.94
2:D:578:GLU:O	2:D:580:LYS:N	2.01	0.94
2:F:578:GLU:O	2:F:580:LYS:N	2.01	0.93
2:D:577:ASN:HB3	2:D:579:PRO:HG2	1.51	0.93
1:C:466:THR:HG22	1:C:468:ASN:H	1.33	0.93
2:B:577:ASN:HB3	2:B:579:PRO:HG2	1.51	0.93
2:D:882:ASN:HD22	2:D:906:THR:HG22	1.34	0.93
2:H:418:THR:HG23	2:H:419:SER:H	1.32	0.93
2:B:701:GLU:O	2:B:702:SER:HB2	1.69	0.93
1:A:466:THR:HG22	1:A:468:ASN:H	1.32	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:THR:HG22	1:E:468:ASN:H	1.29	0.93
2:B:882:ASN:HD22	2:B:906:THR:HG22	1.34	0.93
1:E:581:LYS:HB3	1:E:586:GLU:HB3	1.51	0.92
1:A:669:SER:H	1:A:701:GLN:HE22	1.13	0.92
2:B:913:LYS:O	2:B:916:HIS:HB2	1.70	0.92
2:B:578:GLU:O	2:B:580:LYS:N	2.03	0.92
1:E:431:GLN:HE21	1:E:431:GLN:H	1.15	0.91
1:E:431:GLN:NE2	1:E:431:GLN:H	1.66	0.91
2:B:790:LEU:HD11	1:C:841:ILE:CG2	2.00	0.91
1:G:212:THR:HG21	1:G:272:THR:OG1	1.70	0.90
2:D:635:VAL:O	2:D:636:ARG:HD2	1.71	0.90
1:C:431:GLN:H	1:C:431:GLN:NE2	1.68	0.90
2:F:607:SER:OG	2:F:869:THR:HB	1.69	0.90
2:H:701:GLU:O	2:H:702:SER:HB2	1.71	0.90
2:B:214:ASN:ND2	2:B:343:THR:HG21	1.86	0.90
2:F:214:ASN:ND2	2:F:343:THR:HG21	1.86	0.90
2:D:711:VAL:HA	2:D:908:ALA:O	1.72	0.90
1:G:669:SER:H	1:G:701:GLN:HE22	1.13	0.90
2:H:792:GLN:HE22	2:H:957:ARG:CB	1.85	0.89
1:G:825:ARG:NH1	1:G:829:ALA:HB3	1.87	0.89
2:F:711:VAL:HA	2:F:908:ALA:O	1.70	0.89
2:F:882:ASN:HD22	2:F:906:THR:HG22	1.37	0.89
2:D:701:GLU:O	2:D:702:SER:HB2	1.71	0.89
2:F:577:ASN:C	2:F:579:PRO:HD2	1.93	0.89
1:E:212:THR:HG21	1:E:272:THR:OG1	1.73	0.88
2:B:577:ASN:C	2:B:579:PRO:HD2	1.93	0.88
1:A:356:ASP:OD2	3:A:988:F6P:H11	1.73	0.88
2:H:214:ASN:HD21	2:H:343:THR:HG21	1.37	0.87
1:G:466:THR:HB	1:G:469:ASP:OD1	1.74	0.87
2:D:913:LYS:O	2:D:916:HIS:HB2	1.75	0.87
1:A:328:GLU:O	1:A:332:GLU:HG3	1.75	0.87
1:E:947:THR:HG22	1:E:953:LYS:H	1.38	0.87
2:F:578:GLU:O	2:F:580:LYS:HG3	1.74	0.87
2:H:711:VAL:HA	2:H:908:ALA:O	1.74	0.86
1:A:809:ASN:HB2	1:A:975:LEU:HD11	1.57	0.86
2:B:793:LEU:O	2:B:797:ILE:HG13	1.76	0.86
1:G:466:THR:HG22	1:G:468:ASN:H	1.37	0.86
1:A:431:GLN:NE2	1:A:431:GLN:H	1.73	0.86
2:D:582:PRO:HD2	2:D:615:GLN:O	1.75	0.86
1:G:974:LYS:HG2	1:G:975:LEU:HD13	1.58	0.86
1:E:319:ARG:HB2	1:E:348:ILE:HD12	1.56	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:348:ASP:OD2	3:H:986:F6P:H11	1.74	0.86
2:H:577:ASN:C	2:H:579:PRO:HD2	1.96	0.85
2:F:348:ASP:OD2	3:F:984:F6P:H11	1.77	0.85
2:F:577:ASN:HB3	2:F:579:PRO:HG2	1.58	0.85
1:G:505:LEU:HB3	1:G:533:ILE:HD11	1.58	0.85
2:D:577:ASN:C	2:D:579:PRO:HD2	1.96	0.85
2:B:790:LEU:HD11	1:C:841:ILE:HG21	1.57	0.85
2:F:582:PRO:HD2	2:F:615:GLN:O	1.77	0.84
1:E:949:VAL:O	1:E:951:LEU:N	2.10	0.84
2:B:936:MET:HB2	2:B:937:PRO:HD2	1.59	0.84
1:G:975:LEU:H	1:G:975:LEU:HD22	1.40	0.84
1:G:505:LEU:HB3	1:G:533:ILE:CD1	2.08	0.84
2:D:381:HIS:HB2	2:D:383:ARG:HG3	1.60	0.84
2:D:578:GLU:N	2:D:579:PRO:HD2	1.93	0.83
2:D:214:ASN:ND2	2:D:343:THR:HG21	1.93	0.83
1:E:669:SER:H	1:E:701:GLN:HE22	1.22	0.83
2:F:554:MET:HG2	2:F:562:ILE:HG12	1.58	0.83
2:B:427:CYS:SG	2:B:470:LEU:HD23	2.19	0.83
1:A:336:THR:OG1	1:A:339:GLU:HG3	1.78	0.83
1:C:431:GLN:H	1:C:431:GLN:HE21	1.23	0.83
2:B:582:PRO:HD2	2:B:615:GLN:O	1.79	0.83
2:D:575:ASP:HB3	2:D:613:MET:HB3	1.60	0.83
1:E:583:ASP:HB3	1:E:585:SER:OG	1.78	0.83
1:E:588:LEU:HD13	1:E:593:ARG:HH12	1.43	0.83
1:C:587:LEU:O	1:C:622:HIS:HA	1.79	0.83
1:E:844:GLU:OE2	2:H:826:ALA:N	2.12	0.83
2:D:607:SER:OG	2:D:869:THR:HB	1.79	0.82
1:A:505:LEU:HB3	1:A:533:ILE:HD11	1.60	0.82
2:H:936:MET:HB2	2:H:937:PRO:HD2	1.59	0.82
2:H:792:GLN:HE22	2:H:957:ARG:HB2	1.43	0.82
1:G:583:ASP:HB3	1:G:585:SER:OG	1.78	0.82
1:G:782:THR:HG21	1:G:822:LEU:HD11	1.60	0.82
2:F:381:HIS:HB2	2:F:383:ARG:HG3	1.60	0.82
2:F:936:MET:HB2	2:F:937:PRO:HD2	1.62	0.82
1:E:466:THR:HB	1:E:469:ASP:OD1	1.79	0.81
1:E:822:LEU:O	1:E:822:LEU:HD12	1.80	0.81
2:H:578:GLU:N	2:H:579:PRO:HD2	1.95	0.81
1:A:466:THR:HB	1:A:469:ASP:OD1	1.80	0.81
1:A:212:THR:HG21	1:A:272:THR:OG1	1.80	0.81
1:C:212:THR:HG21	1:C:272:THR:OG1	1.80	0.81
1:G:963:ASN:ND2	1:G:963:ASN:H	1.76	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:214:ASN:HD21	2:F:343:THR:HG21	1.44	0.81
1:A:505:LEU:HB3	1:A:533:ILE:CD1	2.09	0.81
1:G:703:ARG:HD3	1:G:921:ASP:OD1	1.79	0.81
1:C:466:THR:HG22	1:C:468:ASN:N	1.95	0.81
2:H:882:ASN:HD22	2:H:906:THR:HG22	1.46	0.81
2:H:587:LEU:H	2:H:617:HIS:HD1	1.28	0.81
1:A:947:THR:HG22	1:A:953:LYS:H	1.45	0.81
1:A:669:SER:H	1:A:701:GLN:NE2	1.78	0.81
1:G:770:HIS:O	1:G:953:LYS:HD2	1.80	0.81
1:G:431:GLN:NE2	1:G:431:GLN:H	1.80	0.80
1:A:289:ARG:HB2	1:A:325:LEU:HD22	1.63	0.80
2:H:664:ALA:O	2:H:665:ASP:HB3	1.81	0.80
1:A:518:THR:OG1	1:A:521:THR:HG23	1.82	0.80
2:H:418:THR:HA	2:H:421:GLU:HB2	1.63	0.80
2:B:710:MET:O	2:B:711:VAL:HG12	1.82	0.80
1:G:518:THR:OG1	1:G:521:THR:HG23	1.82	0.80
2:F:664:ALA:O	2:F:665:ASP:HB3	1.82	0.79
2:D:554:MET:HG2	2:D:562:ILE:HG12	1.65	0.79
2:F:418:THR:HA	2:F:421:GLU:HB2	1.63	0.79
1:E:466:THR:HG22	1:E:468:ASN:N	1.97	0.79
1:E:796:LEU:HD22	2:H:790:LEU:HD22	1.63	0.79
2:D:467:VAL:O	2:D:471:GLY:HA2	1.81	0.79
2:H:575:ASP:HB3	2:H:613:MET:HB3	1.65	0.79
2:H:195:PRO:HG2	2:H:334:ARG:HH11	1.45	0.79
1:C:427:HIS:CB	1:C:460:ASP:HB2	2.12	0.79
1:G:588:LEU:HD13	1:G:593:ARG:HH12	1.46	0.79
2:F:826:ALA:N	1:G:844:GLU:OE2	2.16	0.79
1:G:669:SER:H	1:G:701:GLN:NE2	1.80	0.79
2:H:582:PRO:HD2	2:H:615:GLN:O	1.82	0.78
1:E:813:ASP:CG	1:E:814:LYS:H	1.84	0.78
2:B:900:ASP:H	2:B:903:ILE:HD11	1.48	0.78
2:B:467:VAL:O	2:B:471:GLY:HA2	1.82	0.78
2:H:581:LEU:HB2	2:H:582:PRO:HD3	1.65	0.78
2:H:381:HIS:HB2	2:H:383:ARG:HG3	1.65	0.78
2:D:587:LEU:N	2:D:587:LEU:HD12	1.98	0.78
1:C:505:LEU:HB3	1:C:533:ILE:CD1	2.14	0.78
1:G:782:THR:CG2	1:G:822:LEU:HD11	2.13	0.78
2:B:578:GLU:N	2:B:579:PRO:HD2	1.99	0.78
2:B:886:ILE:O	2:B:890:ARG:HB2	1.83	0.78
2:H:390:MET:HG3	2:H:483:GLN:NE2	1.99	0.78
1:A:427:HIS:CB	1:A:460:ASP:HB2	2.14	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:ARG:HD2	1:E:346:LEU:O	1.84	0.77
2:H:913:LYS:O	2:H:916:HIS:HB2	1.84	0.77
2:B:587:LEU:H	2:B:617:HIS:HD1	1.32	0.77
1:G:466:THR:HG22	1:G:468:ASN:N	1.98	0.77
1:E:950:GLU:O	1:E:951:LEU:HB2	1.85	0.77
1:E:541:SER:O	1:E:545:THR:HG23	1.83	0.77
1:A:770:HIS:CD2	1:A:951:LEU:HA	2.20	0.77
2:D:664:ALA:O	2:D:665:ASP:HB3	1.83	0.77
2:B:575:ASP:HB3	2:B:613:MET:HB3	1.65	0.77
2:F:436:ARG:NH2	2:F:575:ASP:OD1	2.16	0.77
1:C:328:GLU:O	1:C:332:GLU:HG3	1.84	0.77
2:F:946:ARG:HG3	2:F:946:ARG:HH21	1.49	0.77
2:D:348:ASP:OD2	3:D:982:F6P:H11	1.84	0.77
1:C:947:THR:HG22	1:C:953:LYS:H	1.50	0.77
1:A:466:THR:HG22	1:A:468:ASN:N	1.99	0.77
1:A:431:GLN:HE21	1:A:431:GLN:H	1.28	0.77
1:C:289:ARG:HG2	1:C:329:LEU:HD21	1.66	0.77
2:B:390:MET:HG3	2:B:483:GLN:NE2	1.99	0.77
1:A:947:THR:HG21	1:A:951:LEU:HB2	1.64	0.77
2:F:467:VAL:O	2:F:471:GLY:HA2	1.85	0.77
2:H:418:THR:HG23	2:H:419:SER:N	1.99	0.76
2:B:935:ARG:HH12	4:B:2:FDP:P1	2.07	0.76
1:C:669:SER:H	1:C:701:GLN:NE2	1.82	0.76
1:E:590:VAL:HG23	1:E:591:SER:H	1.50	0.76
1:G:974:LYS:HG2	1:G:975:LEU:N	1.99	0.76
1:A:782:THR:HG21	1:A:822:LEU:HD11	1.66	0.76
1:A:587:LEU:O	1:A:622:HIS:HA	1.85	0.76
1:C:466:THR:HB	1:C:469:ASP:OD1	1.85	0.76
2:B:581:LEU:HB2	2:B:582:PRO:HD3	1.67	0.76
2:F:578:GLU:N	2:F:579:PRO:HD2	2.01	0.76
1:E:587:LEU:O	1:E:622:HIS:HA	1.86	0.76
2:D:900:ASP:H	2:D:903:ILE:HD11	1.51	0.76
1:C:319:ARG:HD3	1:C:346:LEU:O	1.86	0.76
1:G:422:GLU:O	1:G:423:ARG:HD2	1.85	0.76
2:B:505:ASN:O	2:B:509:GLU:HG2	1.86	0.76
1:C:356:ASP:OD2	3:C:988:F6P:H11	1.85	0.76
1:C:825:ARG:NH1	1:C:829:ALA:HB3	2.00	0.76
2:D:418:THR:HG23	2:D:419:SER:N	2.00	0.76
1:A:583:ASP:HB3	1:A:585:SER:OG	1.86	0.76
2:B:418:THR:HG23	2:B:419:SER:N	2.00	0.76
2:F:913:LYS:O	2:F:916:HIS:HB2	1.86	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:ASP:CG	1:A:814:LYS:H	1.89	0.76
2:H:903:ILE:HD12	2:H:904:SER:N	2.01	0.76
1:G:326:VAL:HG13	1:G:340:VAL:HG21	1.66	0.75
2:D:793:LEU:O	2:D:797:ILE:HG13	1.87	0.75
1:A:326:VAL:O	1:A:330:VAL:HG23	1.85	0.75
2:H:710:MET:O	2:H:711:VAL:HG12	1.85	0.75
1:E:782:THR:HG21	1:E:822:LEU:HD11	1.66	0.75
2:F:427:CYS:SG	2:F:470:LEU:HD23	2.26	0.75
1:C:276:THR:HG23	1:C:276:THR:O	1.86	0.75
1:C:287:GLY:O	1:C:290:GLN:HB3	1.85	0.75
1:C:613:ARG:HA	1:C:650:VAL:HG21	1.69	0.75
2:H:583:LYS:O	2:H:585:LYS:N	2.19	0.75
1:C:505:LEU:HB3	1:C:533:ILE:HD11	1.69	0.75
1:G:431:GLN:HE21	1:G:431:GLN:H	1.35	0.75
2:H:418:THR:CG2	2:H:419:SER:H	1.91	0.74
1:G:822:LEU:HD12	1:G:822:LEU:O	1.86	0.74
1:E:800:ARG:HD2	2:H:790:LEU:HB3	1.68	0.74
2:H:607:SER:OG	2:H:869:THR:HB	1.87	0.74
2:B:381:HIS:HB2	2:B:383:ARG:HG3	1.68	0.74
2:H:946:ARG:HH21	2:H:946:ARG:HG3	1.53	0.74
2:D:946:ARG:HH21	2:D:946:ARG:HG3	1.52	0.74
1:A:348:ILE:O	1:A:524:PRO:HD2	1.86	0.74
2:B:607:SER:OG	2:B:869:THR:HB	1.88	0.74
2:B:214:ASN:HD21	2:B:343:THR:HG21	1.50	0.74
1:E:669:SER:H	1:E:701:GLN:NE2	1.86	0.74
2:B:903:ILE:HD12	2:B:904:SER:N	2.03	0.74
1:G:360:SER:N	1:G:545:THR:HG22	2.03	0.74
1:G:589:PRO:HD2	1:G:622:HIS:O	1.87	0.74
2:D:587:LEU:H	2:D:617:HIS:HD1	1.35	0.74
2:B:414:GLU:OE1	2:B:557:ARG:NH1	2.20	0.74
2:F:903:ILE:HD12	2:F:904:SER:N	2.02	0.74
2:F:505:ASN:O	2:F:509:GLU:HG2	1.87	0.74
2:F:418:THR:HG23	2:F:419:SER:N	2.03	0.73
1:A:330:VAL:HA	1:A:335:PHE:O	1.87	0.73
1:E:505:LEU:HB3	1:E:533:ILE:CD1	2.17	0.73
1:C:205:LYS:O	1:C:207:LYS:HD2	1.88	0.73
2:B:946:ARG:HG3	2:B:946:ARG:HH21	1.51	0.73
1:C:804:THR:HG23	1:C:979:VAL:HG21	1.69	0.73
1:G:587:LEU:O	1:G:622:HIS:HA	1.88	0.73
1:G:770:HIS:CB	1:G:951:LEU:HB3	2.19	0.73
1:C:334:ARG:HG3	1:C:335:PHE:CD1	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:THR:CG2	1:A:822:LEU:HD11	2.18	0.73
2:F:203:THR:OG1	2:F:264:THR:HG21	1.88	0.73
2:D:892:ALA:HB3	2:D:894:GLU:HG2	1.71	0.73
1:C:599:VAL:HG13	1:C:629:ILE:HB	1.68	0.73
1:E:613:ARG:HD2	1:E:650:VAL:O	1.89	0.73
2:B:633:GLU:HB2	2:B:672:TYR:CZ	2.24	0.73
1:C:326:VAL:O	1:C:330:VAL:HG23	1.86	0.73
2:F:285:GLN:O	2:F:289:GLU:HG3	1.88	0.73
1:G:590:VAL:HG23	1:G:591:SER:H	1.53	0.73
2:B:392:ARG:HH21	3:B:980:F6P:H12	1.52	0.73
2:F:889:ALA:C	2:F:891:ALA:H	1.92	0.73
1:G:486:LEU:O	1:G:489:VAL:HG22	1.89	0.73
1:E:703:ARG:HD3	1:E:921:ASP:OD1	1.87	0.72
1:E:832:VAL:O	2:H:831:LYS:NZ	2.20	0.72
2:F:900:ASP:H	2:F:903:ILE:HD11	1.53	0.72
2:H:554:MET:HG2	2:H:562:ILE:HG12	1.70	0.72
2:D:327:ILE:HA	2:D:331:GLN:HE22	1.52	0.72
2:F:392:ARG:HH21	3:F:984:F6P:H12	1.54	0.72
1:A:336:THR:HG1	1:A:339:GLU:HG3	1.52	0.72
1:A:825:ARG:NH1	1:A:829:ALA:HB3	2.04	0.72
1:C:594:LEU:HD21	1:C:889:ASN:ND2	2.04	0.72
2:B:956:LYS:NZ	2:B:956:LYS:HA	2.03	0.72
1:A:289:ARG:HD2	1:A:328:GLU:HB3	1.72	0.72
2:B:285:GLN:O	2:B:289:GLU:HG3	1.88	0.72
2:D:936:MET:HB2	2:D:937:PRO:HD2	1.72	0.72
2:H:323:LYS:O	2:H:324:THR:HB	1.88	0.72
2:D:264:THR:HG22	2:D:266:ILE:H	1.54	0.72
1:G:292:ALA:O	1:G:296:ILE:HG13	1.90	0.72
2:H:889:ALA:C	2:H:891:ALA:H	1.92	0.72
2:H:467:VAL:O	2:H:471:GLY:HA2	1.89	0.72
2:H:701:GLU:HB3	2:H:897:ASN:HD22	1.53	0.72
1:A:685:ASP:O	1:A:714:ILE:HB	1.89	0.72
1:G:448:ASN:HD22	1:G:448:ASN:H	1.35	0.71
1:E:287:GLY:O	1:E:290:GLN:HB3	1.89	0.71
2:B:900:ASP:N	2:B:903:ILE:HD11	2.04	0.71
1:E:782:THR:CG2	1:E:822:LEU:HD11	2.19	0.71
2:H:414:GLU:OE1	2:H:557:ARG:NH1	2.22	0.71
2:D:583:LYS:O	2:D:585:LYS:N	2.23	0.71
1:G:613:ARG:HA	1:G:650:VAL:HG21	1.71	0.71
2:B:587:LEU:N	2:B:587:LEU:HD12	2.05	0.71
1:E:385:THR:HA	2:F:207:ASP:OD2	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:418:THR:CG2	2:D:419:SER:H	1.91	0.71
1:G:360:SER:H	1:G:545:THR:HG22	1.54	0.71
2:H:285:GLN:O	2:H:289:GLU:HG3	1.90	0.71
1:C:782:THR:HG21	1:C:822:LEU:HD11	1.72	0.71
1:C:537:PRO:HG2	1:C:540:GLU:HB2	1.71	0.71
1:E:518:THR:OG1	1:E:521:THR:HG23	1.90	0.71
1:C:422:GLU:HG2	1:C:564:ARG:HD2	1.71	0.71
1:G:505:LEU:CB	1:G:533:ILE:HD11	2.20	0.71
2:H:428:ASP:OD1	2:H:432:LYS:NZ	2.23	0.71
1:A:287:GLY:O	1:A:290:GLN:HB3	1.91	0.71
2:B:348:ASP:OD2	3:B:980:F6P:H11	1.90	0.71
2:D:587:LEU:HD23	2:D:883:GLN:NE2	2.05	0.71
1:C:285:ARG:NH2	1:C:328:GLU:OE2	2.24	0.71
1:A:946:GLU:O	1:A:955:PHE:CZ	2.44	0.71
1:A:336:THR:HG23	1:A:339:GLU:CD	2.10	0.70
2:F:201:VAL:HG11	2:F:218:ILE:HD13	1.72	0.70
2:B:956:LYS:HZ3	2:B:956:LYS:HA	1.56	0.70
1:A:613:ARG:HA	1:A:650:VAL:HG21	1.73	0.70
1:G:427:HIS:CB	1:G:460:ASP:HB2	2.16	0.70
1:A:216:ASP:OD2	2:B:377:THR:HA	1.90	0.70
1:E:844:GLU:OE2	2:H:825:LYS:N	2.24	0.70
1:A:822:LEU:O	1:A:822:LEU:HD12	1.91	0.70
1:E:832:VAL:HG22	2:H:834:GLU:HB3	1.72	0.70
1:C:541:SER:O	1:C:545:THR:HG23	1.91	0.70
1:G:326:VAL:HG13	1:G:340:VAL:CG2	2.21	0.70
2:F:522:ASN:ND2	2:F:527:VAL:HG21	2.05	0.70
1:A:703:ARG:HD3	1:A:921:ASP:OD1	1.91	0.70
2:H:203:THR:OG1	2:H:264:THR:HG21	1.92	0.70
1:A:767:GLN:NE2	4:A:1:FDP:H3	2.06	0.70
2:D:710:MET:O	2:D:711:VAL:HG12	1.91	0.70
1:G:326:VAL:O	1:G:330:VAL:HG23	1.91	0.70
2:F:418:THR:HG1	2:F:422:TRP:HD1	1.31	0.70
1:C:587:LEU:HB3	1:C:622:HIS:CE1	2.27	0.70
2:F:900:ASP:N	2:F:903:ILE:HD11	2.06	0.70
1:E:427:HIS:CB	1:E:460:ASP:HB2	2.20	0.70
1:G:947:THR:HG22	1:G:953:LYS:H	1.56	0.70
1:E:356:ASP:OD2	3:E:988:F6P:H11	1.91	0.70
2:F:827:LEU:HB3	2:F:832:LEU:HD13	1.72	0.70
1:A:588:LEU:HD13	1:A:593:ARG:HH12	1.55	0.70
1:G:541:SER:O	1:G:545:THR:HG23	1.92	0.70
2:D:704:PRO:HA	2:D:707:ARG:HG2	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:822:LEU:C	1:E:822:LEU:HD12	2.12	0.69
2:F:288:ILE:HA	2:F:335:MET:HE1	1.72	0.69
2:H:281:LEU:HD23	2:H:326:ARG:NH2	2.07	0.69
2:F:621:ALA:HB2	2:F:638:LEU:HD11	1.74	0.69
2:H:704:PRO:HA	2:H:707:ARG:HG2	1.74	0.69
2:H:792:GLN:HE22	2:H:957:ARG:HB3	1.55	0.69
2:F:575:ASP:HB3	2:F:613:MET:HB3	1.72	0.69
1:A:594:LEU:HD21	1:A:889:ASN:ND2	2.07	0.69
2:D:505:ASN:O	2:D:509:GLU:HG2	1.92	0.69
1:E:796:LEU:HD11	2:H:793:LEU:HD13	1.73	0.69
1:C:249:LEU:HD21	1:C:281:GLU:HB3	1.73	0.69
2:F:327:ILE:HA	2:F:331:GLN:HE22	1.58	0.69
2:D:328:SER:H	2:D:331:GLN:NE2	1.89	0.69
1:G:594:LEU:HD21	1:G:889:ASN:ND2	2.07	0.69
1:E:947:THR:HG23	1:E:947:THR:O	1.91	0.69
2:B:930:THR:HG22	2:B:932:VAL:N	2.08	0.69
1:A:505:LEU:CB	1:A:533:ILE:HD11	2.21	0.69
2:F:581:LEU:HB2	2:F:582:PRO:HD3	1.73	0.69
2:B:664:ALA:O	2:B:665:ASP:HB3	1.91	0.69
1:G:637:ILE:HD13	1:G:671:ASP:HB3	1.73	0.69
1:C:212:THR:O	1:C:212:THR:HG23	1.91	0.69
1:C:613:ARG:HD2	1:C:650:VAL:O	1.93	0.69
2:D:323:LYS:O	2:D:324:THR:HB	1.93	0.69
2:B:889:ALA:C	2:B:891:ALA:H	1.95	0.69
1:C:600:HIS:HD2	1:C:659:SER:OG	1.75	0.69
2:B:418:THR:CG2	2:B:419:SER:H	1.93	0.69
2:D:903:ILE:HD12	2:D:904:SER:N	2.07	0.69
1:G:422:GLU:HG2	1:G:564:ARG:HD2	1.74	0.69
1:E:589:PRO:HD2	1:E:622:HIS:O	1.94	0.68
1:C:931:GLY:O	1:C:932:SER:HB3	1.92	0.68
1:G:287:GLY:O	1:G:290:GLN:HB3	1.93	0.68
1:C:703:ARG:HD3	1:C:921:ASP:OD1	1.94	0.68
2:F:834:GLU:HB3	1:G:832:VAL:HG22	1.75	0.68
2:F:583:LYS:O	2:F:585:LYS:N	2.26	0.68
1:G:814:LYS:NZ	1:G:814:LYS:HA	2.08	0.68
2:D:889:ALA:C	2:D:891:ALA:H	1.97	0.68
2:B:288:ILE:HA	2:B:335:MET:HE1	1.75	0.68
2:B:583:LYS:O	2:B:585:LYS:N	2.27	0.68
1:A:422:GLU:O	1:A:423:ARG:HD2	1.93	0.68
1:C:319:ARG:HG2	1:C:346:LEU:HB3	1.75	0.68
2:H:418:THR:HG1	2:H:422:TRP:HD1	1.39	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:579:PRO:O	2:H:580:LYS:C	2.31	0.68
2:F:323:LYS:O	2:F:324:THR:HB	1.94	0.68
2:B:201:VAL:HG11	2:B:218:ILE:HD13	1.74	0.68
2:D:907:ALA:O	2:D:922:ILE:HG22	1.94	0.68
2:D:930:THR:HG22	2:D:932:VAL:N	2.07	0.68
2:B:327:ILE:HA	2:B:331:GLN:HE22	1.59	0.68
2:D:589:ILE:HD13	2:D:879:ILE:HG21	1.74	0.68
2:H:681:LEU:O	2:H:710:MET:O	2.10	0.68
1:C:637:ILE:HD13	1:C:671:ASP:HB3	1.75	0.68
2:B:436:ARG:NH2	2:B:575:ASP:OD1	2.22	0.68
2:B:323:LYS:O	2:B:324:THR:HB	1.92	0.68
2:D:591:ILE:HD13	2:D:592:VAL:H	1.59	0.68
1:E:210:VAL:CG1	1:E:227:VAL:HG11	2.24	0.68
1:G:947:THR:O	1:G:947:THR:HG23	1.94	0.67
1:C:505:LEU:CB	1:C:533:ILE:HD11	2.24	0.67
2:F:201:VAL:CG1	2:F:218:ILE:HD13	2.24	0.67
2:F:633:GLU:HB2	2:F:672:TYR:CZ	2.27	0.67
1:G:770:HIS:HB2	1:G:951:LEU:HB3	1.74	0.67
1:C:326:VAL:HG13	1:C:340:VAL:HG21	1.76	0.67
2:D:317:LEU:O	2:D:321:LEU:HD23	1.94	0.67
2:D:930:THR:HG22	2:D:932:VAL:H	1.57	0.67
2:B:595:GLY:O	2:B:656:THR:OG1	2.12	0.67
2:F:341:CYS:HB2	2:F:507:VAL:HG13	1.75	0.67
1:E:637:ILE:HD13	1:E:671:ASP:HB3	1.77	0.67
1:A:746:TYR:CD1	2:B:854:VAL:HG11	2.29	0.67
2:B:462:VAL:O	2:B:466:LEU:HD23	1.95	0.67
2:H:525:LYS:NZ	2:H:525:LYS:HB2	2.09	0.67
1:E:947:THR:O	1:E:948:ASN:C	2.32	0.67
1:E:814:LYS:O	1:E:816:GLU:HG3	1.93	0.67
2:H:591:ILE:HD13	2:H:592:VAL:H	1.60	0.67
1:A:732:TYR:CE1	1:A:736:VAL:HB	2.30	0.67
2:B:950:ASP:OD1	2:B:955:ARG:HD3	1.94	0.67
1:E:825:ARG:NH1	1:E:829:ALA:HB3	2.09	0.67
1:E:776:SER:HB3	1:E:963:ASN:HD21	1.59	0.67
2:D:827:LEU:HB3	2:D:832:LEU:HD13	1.76	0.67
2:H:196:GLN:NE2	2:H:228:ARG:HD3	2.10	0.67
2:F:950:ASP:OD1	2:F:955:ARG:HD3	1.94	0.67
1:E:587:LEU:C	1:E:589:PRO:HD3	2.14	0.67
2:H:264:THR:CG2	2:H:266:ILE:HG12	2.25	0.67
1:E:600:HIS:HD2	1:E:659:SER:OG	1.77	0.67
1:C:249:LEU:CD1	1:C:290:GLN:HG2	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:ASN:O	2:F:327:ILE:N	2.23	0.67
1:C:326:VAL:HG13	1:C:340:VAL:CG2	2.25	0.67
2:H:317:LEU:O	2:H:321:LEU:HD23	1.94	0.67
2:B:240:VAL:HG21	2:B:273:GLU:HB2	1.77	0.67
2:H:579:PRO:O	2:H:581:LEU:N	2.28	0.67
2:D:400:LEU:HD12	2:D:866:THR:HG21	1.77	0.67
1:A:724:SER:OG	4:A:1:FDP:H12	1.95	0.66
2:D:203:THR:OG1	2:D:264:THR:HG21	1.95	0.66
2:F:244:PRO:O	2:F:245:GLU:HB3	1.95	0.66
1:C:697:ARG:HH22	1:C:949:VAL:HG22	1.60	0.66
2:F:710:MET:O	2:F:711:VAL:HG12	1.94	0.66
2:H:264:THR:HG22	2:H:266:ILE:H	1.59	0.66
1:C:746:TYR:CD1	2:D:854:VAL:HG11	2.29	0.66
2:H:894:GLU:C	2:H:896:PHE:H	1.98	0.66
1:A:599:VAL:CG1	1:A:629:ILE:HB	2.25	0.66
2:D:587:LEU:HD12	2:D:587:LEU:H	1.60	0.66
1:E:505:LEU:HB3	1:E:533:ILE:HD11	1.77	0.66
1:A:961:GLU:O	1:A:964:LYS:HG2	1.95	0.66
1:E:755:SER:HB3	1:E:817:ASN:O	1.96	0.66
1:G:581:LYS:HD2	1:G:586:GLU:HB2	1.75	0.66
2:F:579:PRO:O	2:F:580:LYS:C	2.33	0.66
2:F:256:ARG:HD2	2:F:812:ARG:O	1.95	0.66
1:C:319:ARG:HB2	1:C:348:ILE:HD12	1.76	0.66
1:G:356:ASP:OD2	3:G:988:F6P:H11	1.96	0.66
2:H:635:VAL:O	2:H:636:ARG:HD2	1.96	0.66
2:D:575:ASP:CB	2:D:613:MET:HB3	2.25	0.66
1:C:212:THR:HG22	1:C:274:ILE:HG13	1.77	0.66
2:D:240:VAL:HG21	2:D:273:GLU:HB2	1.77	0.66
1:G:400:ARG:HH11	1:G:400:ARG:HG2	1.60	0.66
1:A:427:HIS:HA	1:A:459:ASP:HB2	1.77	0.66
1:A:693:PHE:CD2	1:A:952:ARG:HB3	2.31	0.66
2:H:325:ASN:O	2:H:327:ILE:N	2.27	0.66
1:E:212:THR:HG23	1:E:212:THR:O	1.95	0.66
1:E:800:ARG:NH2	2:H:791:GLU:HG3	2.11	0.66
1:E:505:LEU:CB	1:E:533:ILE:HD11	2.26	0.66
2:D:201:VAL:HG11	2:D:218:ILE:HD13	1.76	0.66
1:C:400:ARG:HG2	1:C:400:ARG:HH11	1.59	0.66
1:A:816:GLU:O	1:A:818:ARG:N	2.28	0.66
2:H:827:LEU:HB3	2:H:832:LEU:HD13	1.77	0.66
1:C:816:GLU:O	1:C:818:ARG:N	2.29	0.66
2:D:256:ARG:HD2	2:D:812:ARG:O	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:ALA:O	2:D:211:MET:HG3	1.96	0.65
1:C:427:HIS:HA	1:C:459:ASP:HB2	1.77	0.65
2:B:579:PRO:O	2:B:580:LYS:C	2.34	0.65
1:C:587:LEU:C	1:C:589:PRO:HD3	2.15	0.65
1:A:212:THR:HG22	1:A:274:ILE:HG13	1.77	0.65
2:D:552:ARG:C	2:D:552:ARG:HD3	2.16	0.65
2:D:214:ASN:HD21	2:D:343:THR:HG21	1.60	0.65
1:C:778:THR:O	1:C:782:THR:HB	1.96	0.65
1:E:253:LYS:C	1:E:255:LEU:H	1.98	0.65
2:B:681:LEU:O	2:B:710:MET:O	2.15	0.65
2:F:681:LEU:O	2:F:710:MET:O	2.15	0.65
1:C:360:SER:N	1:C:545:THR:HG22	2.11	0.65
2:B:579:PRO:O	2:B:581:LEU:N	2.30	0.65
1:E:360:SER:N	1:E:545:THR:HG22	2.11	0.65
1:A:587:LEU:C	1:A:589:PRO:HD3	2.17	0.65
2:B:201:VAL:CG1	2:B:218:ILE:HD13	2.27	0.65
2:D:201:VAL:CG1	2:D:218:ILE:HD13	2.26	0.65
2:H:522:ASN:ND2	2:H:527:VAL:HG21	2.11	0.65
1:C:253:LYS:C	1:C:255:LEU:H	2.00	0.65
2:F:579:PRO:O	2:F:581:LEU:N	2.30	0.65
2:D:701:GLU:HB2	2:D:897:ASN:HD22	1.62	0.65
1:C:360:SER:H	1:C:545:THR:HG22	1.62	0.65
2:H:793:LEU:O	2:H:797:ILE:HG13	1.96	0.65
2:D:549:ASP:OD2	2:D:552:ARG:HB2	1.97	0.65
1:G:773:TYR:HA	1:G:959:TRP:CD2	2.32	0.65
2:B:453:ASP:CG	2:B:455:THR:HG23	2.17	0.65
1:C:330:VAL:HA	1:C:335:PHE:O	1.97	0.65
2:B:827:LEU:HB3	2:B:832:LEU:HD13	1.78	0.65
2:F:591:ILE:HD13	2:F:592:VAL:H	1.62	0.64
1:A:360:SER:N	1:A:545:THR:HG22	2.12	0.64
1:A:251:GLY:O	1:A:252:GLY:O	2.15	0.64
2:B:693:LEU:CD2	2:B:922:ILE:HB	2.27	0.64
2:D:418:THR:HG1	2:D:422:TRP:HD1	1.36	0.64
2:D:390:MET:HG3	2:D:483:GLN:NE2	2.13	0.64
1:G:802:ASP:OD1	1:G:972:ARG:NH2	2.28	0.64
2:D:950:ASP:OD1	2:D:955:ARG:HD3	1.97	0.64
2:D:681:LEU:O	2:D:710:MET:O	2.16	0.64
1:A:947:THR:CG2	1:A:951:LEU:HB2	2.26	0.64
2:D:462:VAL:O	2:D:466:LEU:HD23	1.98	0.64
2:F:264:THR:HG22	2:F:266:ILE:H	1.62	0.64
1:E:289:ARG:HB2	1:E:325:LEU:HD22	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:CG1	1:A:227:VAL:HG11	2.28	0.64
1:E:581:LYS:HD2	1:E:586:GLU:HB2	1.80	0.64
2:H:935:ARG:HH12	4:H:8:FDP:P1	2.19	0.64
1:A:212:THR:HG23	1:A:212:THR:O	1.97	0.64
2:H:876:VAL:HG12	2:H:880:LYS:HE3	1.79	0.64
2:F:436:ARG:HG3	2:F:436:ARG:O	1.97	0.64
2:D:900:ASP:N	2:D:903:ILE:HD11	2.12	0.64
2:F:930:THR:HG22	2:F:932:VAL:N	2.12	0.64
2:B:392:ARG:NH2	3:B:980:F6P:H12	2.11	0.64
2:H:321:LEU:O	2:H:325:ASN:O	2.16	0.64
2:F:320:GLU:O	2:F:324:THR:HG22	1.97	0.64
2:B:203:THR:OG1	2:B:264:THR:HG21	1.96	0.64
2:B:575:ASP:CB	2:B:613:MET:HB3	2.28	0.64
1:E:292:ALA:O	1:E:296:ILE:HG13	1.98	0.64
1:G:581:LYS:HB3	1:G:586:GLU:CB	2.27	0.64
1:G:587:LEU:C	1:G:589:PRO:HD3	2.17	0.64
2:F:522:ASN:HD22	2:F:527:VAL:HG21	1.61	0.64
1:G:685:ASP:O	1:G:714:ILE:HB	1.97	0.64
2:F:907:ALA:O	2:F:922:ILE:HG22	1.97	0.64
1:C:289:ARG:HB2	1:C:325:LEU:HD22	1.79	0.64
1:A:541:SER:O	1:A:545:THR:HG23	1.97	0.64
1:A:537:PRO:HG2	1:A:540:GLU:HB2	1.79	0.64
1:A:809:ASN:HB2	1:A:975:LEU:CD1	2.27	0.63
1:A:253:LYS:C	1:A:255:LEU:H	2.00	0.63
2:D:801:ALA:O	2:D:805:GLU:HG3	1.97	0.63
2:B:591:ILE:HD13	2:B:592:VAL:H	1.62	0.63
2:F:220:ARG:HD2	2:F:252:TRP:CE2	2.33	0.63
1:E:931:GLY:O	1:E:932:SER:HB3	1.98	0.63
1:A:947:THR:HG23	1:A:947:THR:O	1.98	0.63
2:H:327:ILE:HA	2:H:331:GLN:HE22	1.63	0.63
2:B:511:THR:OG1	2:B:514:THR:HG23	1.99	0.63
2:B:752:ARG:HD2	2:B:809:GLY:O	1.98	0.63
1:E:427:HIS:HA	1:E:459:ASP:HB2	1.80	0.63
2:F:793:LEU:O	2:F:797:ILE:HG13	1.97	0.63
1:E:950:GLU:HG2	1:E:950:GLU:O	1.98	0.63
1:C:216:ASP:OD2	2:D:377:THR:HA	1.99	0.63
1:A:947:THR:O	1:A:948:ASN:C	2.36	0.63
1:C:329:LEU:HD22	1:C:334:ARG:HG2	1.81	0.63
2:D:433:HIS:ND1	2:D:640:TRP:CZ2	2.67	0.63
1:C:941:ASN:O	1:C:944:GLU:HG3	1.99	0.63
2:B:298:CYS:SG	2:B:343:THR:HG22	2.38	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ARG:HH11	1:A:921:ASP:CG	2.01	0.63
1:C:336:THR:OG1	1:C:339:GLU:HG3	1.98	0.63
2:D:633:GLU:HB2	2:D:672:TYR:CZ	2.33	0.63
1:C:422:GLU:CG	1:C:564:ARG:HD2	2.28	0.63
2:B:436:ARG:HG3	2:B:436:ARG:O	1.97	0.63
1:G:613:ARG:HD2	1:G:650:VAL:O	1.98	0.63
1:C:805:LEU:HD21	1:C:976:ARG:HG2	1.80	0.63
1:A:398:MET:HE3	1:A:488:HIS:HA	1.80	0.63
1:A:341:ALA:HB3	1:A:342:PRO:CD	2.28	0.63
2:F:281:LEU:HD23	2:F:326:ARG:NH2	2.14	0.63
2:B:201:VAL:HG11	2:B:218:ILE:CD1	2.28	0.63
1:A:757:THR:HG23	2:B:597:PRO:HD3	1.81	0.63
1:C:622:HIS:HD2	1:C:886:GLU:OE1	1.82	0.63
2:H:436:ARG:HH12	2:H:575:ASP:CG	2.02	0.63
2:D:463:HIS:HD2	2:D:474:THR:HG22	1.64	0.63
2:H:950:ASP:OD1	2:H:955:ARG:HD3	1.97	0.63
1:G:746:TYR:CE1	2:H:854:VAL:CG1	2.82	0.63
2:H:466:LEU:HD12	2:H:472:LEU:HD11	1.81	0.63
1:G:276:THR:O	1:G:276:THR:HG23	1.98	0.63
2:F:701:GLU:HB3	2:F:897:ASN:HD22	1.62	0.62
1:A:341:ALA:HB3	1:A:342:PRO:HD3	1.81	0.62
2:D:641:LYS:O	2:D:644:LEU:HD12	1.99	0.62
2:F:494:ILE:HG23	2:F:774:LEU:HD23	1.80	0.62
2:B:577:ASN:C	2:B:579:PRO:CD	2.67	0.62
1:E:360:SER:H	1:E:545:THR:HG22	1.64	0.62
1:C:348:ILE:O	1:C:524:PRO:HD2	2.00	0.62
1:G:410:GLY:HA2	1:G:452:ILE:HD12	1.80	0.62
2:H:930:THR:HG22	2:H:932:VAL:N	2.14	0.62
1:E:249:LEU:CD1	1:E:290:GLN:HG2	2.29	0.62
2:F:433:HIS:ND1	2:F:640:TRP:CZ2	2.67	0.62
1:G:348:ILE:O	1:G:524:PRO:HD2	1.99	0.62
1:G:212:THR:HG23	1:G:212:THR:O	1.98	0.62
1:A:613:ARG:HD2	1:A:650:VAL:O	1.98	0.62
2:H:892:ALA:O	2:H:894:GLU:N	2.30	0.62
2:B:704:PRO:HA	2:B:707:ARG:HG2	1.79	0.62
1:A:542:VAL:O	1:A:546:LYS:HB2	1.99	0.62
1:C:710:PRO:HG2	1:G:674:THR:HA	1.81	0.62
2:H:577:ASN:C	2:H:579:PRO:CD	2.68	0.62
1:G:788:TYR:HB3	1:G:794:ILE:HD11	1.81	0.62
2:H:505:ASN:O	2:H:509:GLU:HG2	1.98	0.62
1:E:485:ILE:N	1:E:485:ILE:HD12	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:552:ARG:HD3	2:H:552:ARG:C	2.19	0.62
1:E:508:VAL:HG11	1:E:965:ILE:HD12	1.82	0.62
2:D:704:PRO:HA	2:D:707:ARG:HH11	1.64	0.62
1:C:216:ASP:H	2:D:381:HIS:HE1	1.48	0.62
1:C:251:GLY:O	1:C:252:GLY:O	2.17	0.62
2:F:641:LYS:O	2:F:644:LEU:HD12	1.99	0.62
2:D:779:GLN:HA	2:D:953:VAL:HG21	1.80	0.62
1:C:422:GLU:O	1:C:423:ARG:HD2	2.00	0.62
1:E:594:LEU:HD21	1:E:889:ASN:ND2	2.14	0.62
1:G:451:ILE:HD12	1:G:451:ILE:N	2.15	0.62
2:B:341:CYS:HB2	2:B:507:VAL:HG13	1.82	0.62
2:D:436:ARG:O	2:D:436:ARG:HG3	1.99	0.62
2:F:201:VAL:HG11	2:F:218:ILE:CD1	2.28	0.62
2:B:264:THR:CG2	2:B:266:ILE:HG12	2.29	0.62
2:F:786:GLU:OE2	2:F:946:ARG:NH2	2.24	0.62
1:C:613:ARG:HA	1:C:650:VAL:CG2	2.30	0.62
2:D:591:ILE:HD13	2:D:592:VAL:N	2.15	0.62
1:E:711:ILE:O	1:E:714:ILE:HG23	2.00	0.62
1:E:801:GLU:OE1	1:E:976:ARG:HD3	1.99	0.62
2:D:717:LEU:HB2	2:D:733:ALA:CB	2.29	0.62
1:E:276:THR:HG23	1:E:276:THR:O	2.00	0.62
2:F:418:THR:CG2	2:F:419:SER:H	1.95	0.62
1:E:348:ILE:O	1:E:524:PRO:HD2	2.00	0.62
1:A:590:VAL:HG23	1:A:591:SER:H	1.63	0.62
1:A:422:GLU:HG2	1:A:564:ARG:HD2	1.81	0.61
1:G:427:HIS:HA	1:G:459:ASP:HB2	1.81	0.61
1:G:822:LEU:HD12	1:G:822:LEU:C	2.19	0.61
2:D:665:ASP:O	2:D:669:ILE:HG12	2.00	0.61
2:D:392:ARG:HH21	3:D:982:F6P:H12	1.65	0.61
1:A:822:LEU:C	1:A:822:LEU:HD12	2.20	0.61
1:C:461:GLN:HB2	1:C:463:ASN:ND2	2.14	0.61
2:H:341:CYS:HB2	2:H:507:VAL:HG13	1.82	0.61
2:H:256:ARG:HD2	2:H:812:ARG:O	1.99	0.61
2:H:239:LEU:O	2:H:286:HIS:HD2	1.82	0.61
2:F:892:ALA:O	2:F:894:GLU:N	2.30	0.61
2:F:587:LEU:H	2:F:617:HIS:HD1	1.47	0.61
1:A:596:ILE:HD12	1:A:885:ILE:HG21	1.82	0.61
2:D:579:PRO:O	2:D:581:LEU:N	2.33	0.61
1:E:400:ARG:HG3	1:E:401:HIS:H	1.64	0.61
1:E:400:ARG:HG3	1:E:401:HIS:N	2.15	0.61
2:F:577:ASN:C	2:F:579:PRO:CD	2.68	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:PRO:HD2	1:C:622:HIS:O	2.01	0.61
2:B:704:PRO:HA	2:B:707:ARG:HH11	1.64	0.61
1:C:391:ARG:O	1:C:448:ASN:HA	2.00	0.61
2:H:940:ILE:HD12	2:H:943:GLN:NE2	2.15	0.61
2:D:298:CYS:HA	2:D:343:THR:O	2.00	0.61
1:C:822:LEU:O	1:C:822:LEU:HD12	2.00	0.61
2:H:892:ALA:C	2:H:894:GLU:H	2.03	0.61
2:H:889:ALA:O	2:H:891:ALA:N	2.33	0.61
1:E:816:GLU:O	1:E:818:ARG:N	2.33	0.61
2:D:786:GLU:OE2	2:D:946:ARG:NH2	2.23	0.61
2:D:322:LEU:O	2:D:324:THR:N	2.32	0.61
1:C:832:VAL:HG12	1:C:833:TYR:CD1	2.36	0.61
2:F:781:SER:HA	2:F:818:LEU:O	2.01	0.61
1:C:669:SER:N	1:C:701:GLN:NE2	2.49	0.61
2:H:701:GLU:HB3	2:H:897:ASN:ND2	2.16	0.61
2:H:256:ARG:NH1	2:H:813:PHE:CE1	2.68	0.61
2:H:587:LEU:HD23	2:H:883:GLN:NE2	2.16	0.61
2:H:647:GLN:HE22	2:H:869:THR:CG2	2.14	0.61
1:A:242:TYR:O	1:A:247:GLY:HA3	2.01	0.61
1:A:600:HIS:HD2	1:A:659:SER:OG	1.83	0.61
1:E:588:LEU:HD13	1:E:593:ARG:NH1	2.14	0.61
1:A:801:GLU:OE1	1:A:976:ARG:NE	2.34	0.61
2:H:400:LEU:HD12	2:H:866:THR:HG21	1.81	0.61
1:G:247:GLY:HA2	1:G:254:TYR:HD2	1.66	0.61
2:B:463:HIS:HD2	2:B:474:THR:HG22	1.66	0.61
2:D:578:GLU:N	2:D:579:PRO:CD	2.64	0.60
1:C:805:LEU:HD11	1:C:972:ARG:HG3	1.83	0.60
2:H:591:ILE:HD13	2:H:592:VAL:N	2.16	0.60
1:A:276:THR:O	1:A:276:THR:HG23	2.00	0.60
2:B:587:LEU:HD21	2:B:883:GLN:CG	2.31	0.60
2:D:436:ARG:NH2	2:D:575:ASP:OD1	2.32	0.60
2:D:577:ASN:HB3	2:D:579:PRO:CG	2.30	0.60
2:D:321:LEU:O	2:D:325:ASN:O	2.20	0.60
1:G:448:ASN:H	1:G:448:ASN:ND2	1.99	0.60
2:D:414:GLU:OE1	2:D:557:ARG:NH1	2.34	0.60
1:C:619:CYS:SG	1:C:882:ILE:HD12	2.41	0.60
1:E:422:GLU:HG2	1:E:564:ARG:HD2	1.82	0.60
2:B:935:ARG:NH1	4:B:2:FDP:O3P	2.34	0.60
2:B:633:GLU:HB2	2:B:672:TYR:OH	2.01	0.60
1:C:822:LEU:C	1:C:822:LEU:HD12	2.22	0.60
2:D:792:GLN:HE22	2:D:957:ARG:C	2.04	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:599:VAL:CG1	1:G:629:ILE:HB	2.25	0.60
1:E:813:ASP:CG	1:E:814:LYS:N	2.55	0.60
1:A:959:TRP:O	1:A:960:ALA:C	2.39	0.60
1:C:400:ARG:HG3	1:C:401:HIS:H	1.65	0.60
1:C:791:GLU:OE1	1:C:791:GLU:N	2.28	0.60
2:D:314:TRP:HB3	2:D:315:PRO:HD3	1.83	0.60
1:E:788:TYR:HB3	1:E:794:ILE:HD11	1.84	0.60
1:G:622:HIS:HD2	1:G:886:GLU:OE1	1.85	0.60
2:F:521:VAL:HG13	2:F:526:ILE:HD13	1.82	0.60
1:C:794:ILE:O	1:C:794:ILE:HG22	2.02	0.60
2:H:770:THR:CG2	2:H:946:ARG:HD2	2.32	0.60
2:H:324:THR:HG23	2:H:326:ARG:HG3	1.82	0.60
2:B:591:ILE:HD13	2:B:592:VAL:N	2.16	0.60
1:G:599:VAL:HG13	1:G:629:ILE:CB	2.26	0.60
1:G:669:SER:N	1:G:701:GLN:NE2	2.50	0.60
2:F:288:ILE:HA	2:F:335:MET:CE	2.32	0.60
1:E:210:VAL:HG12	1:E:304:VAL:HB	1.83	0.60
1:E:422:GLU:O	1:E:423:ARG:HD2	2.01	0.60
2:D:587:LEU:HD21	2:D:883:GLN:CG	2.32	0.60
2:B:930:THR:HG22	2:B:932:VAL:H	1.65	0.60
2:D:220:ARG:HD2	2:D:252:TRP:CZ2	2.37	0.60
1:A:947:THR:CG2	1:A:953:LYS:H	2.14	0.59
1:G:613:ARG:HA	1:G:650:VAL:CG2	2.32	0.59
1:E:341:ALA:HB3	1:E:342:PRO:CD	2.32	0.59
4:A:1:FDP:O4P	2:B:847:LYS:NZ	2.34	0.59
1:G:590:VAL:HG23	1:G:591:SER:N	2.18	0.59
1:G:974:LYS:CG	1:G:975:LEU:HD13	2.30	0.59
2:H:900:ASP:H	2:H:903:ILE:HD11	1.66	0.59
1:G:400:ARG:HG3	1:G:401:HIS:H	1.66	0.59
2:F:591:ILE:HD13	2:F:592:VAL:N	2.17	0.59
2:H:195:PRO:HG2	2:H:334:ARG:NH1	2.15	0.59
2:B:288:ILE:HA	2:B:335:MET:CE	2.32	0.59
1:A:690:LEU:HD23	1:A:719:ILE:HB	1.83	0.59
1:G:341:ALA:HB3	1:G:342:PRO:CD	2.32	0.59
2:H:798:GLU:O	2:H:801:ALA:HB3	2.03	0.59
1:E:821:LYS:CB	1:E:821:LYS:HZ2	2.08	0.59
2:F:414:GLU:OE1	2:F:557:ARG:NH1	2.35	0.59
2:B:256:ARG:HD2	2:B:812:ARG:O	2.03	0.59
1:A:439:GLN:HA	1:A:439:GLN:OE1	2.02	0.59
1:C:427:HIS:C	1:C:427:HIS:ND1	2.56	0.59
2:B:577:ASN:HB3	2:B:579:PRO:CG	2.30	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:LEU:O	2:B:325:ASN:O	2.20	0.59
1:A:841:ILE:CG2	2:D:790:LEU:HD11	2.32	0.59
1:E:594:LEU:N	1:E:624:HIS:ND1	2.48	0.59
2:D:704:PRO:HA	2:D:707:ARG:NH1	2.18	0.59
2:F:554:MET:HG2	2:F:562:ILE:CG1	2.29	0.59
2:H:587:LEU:HD12	2:H:587:LEU:N	2.18	0.59
2:D:320:GLU:O	2:D:324:THR:HG22	2.03	0.59
2:B:892:ALA:O	2:B:894:GLU:N	2.32	0.59
1:A:634:SER:HB3	1:A:666:SER:CB	2.32	0.59
1:G:679:PHE:CE2	1:G:687:LEU:HD22	2.38	0.59
1:A:613:ARG:HA	1:A:650:VAL:CG2	2.33	0.59
2:F:328:SER:H	2:F:331:GLN:NE2	2.00	0.59
1:G:537:PRO:HG2	1:G:540:GLU:HB2	1.84	0.59
2:H:621:ALA:HB2	2:H:638:LEU:HD11	1.83	0.59
2:D:577:ASN:C	2:D:579:PRO:CD	2.70	0.59
1:C:782:THR:CG2	1:C:822:LEU:HD11	2.32	0.59
2:B:661:PRO:HD2	2:B:695:GLN:NE2	2.17	0.59
1:C:972:ARG:HD3	1:C:976:ARG:HH21	1.67	0.59
2:F:417:ALA:O	2:F:418:THR:HB	2.02	0.59
1:G:697:ARG:NH1	1:G:943:TRP:HH2	2.01	0.59
2:H:436:ARG:NH1	2:H:575:ASP:OD2	2.34	0.59
1:G:773:TYR:HD1	1:G:959:TRP:CD1	2.21	0.59
1:A:756:ALA:HB1	2:B:597:PRO:HB3	1.85	0.59
1:E:319:ARG:NH1	1:E:517:PHE:HE2	2.00	0.58
1:G:949:VAL:O	1:G:950:GLU:O	2.21	0.58
2:B:264:THR:HG22	2:B:266:ILE:H	1.67	0.58
1:A:968:ILE:HD13	1:A:973:LEU:HD12	1.84	0.58
2:D:615:GLN:OE1	2:D:880:LYS:NZ	2.36	0.58
2:H:900:ASP:N	2:H:903:ILE:HD11	2.18	0.58
2:F:344:VAL:HG22	2:F:357:THR:HG22	1.85	0.58
1:E:636:LEU:HD12	1:E:640:GLY:HA2	1.84	0.58
1:C:438:CYS:O	1:C:442:ARG:HG3	2.02	0.58
2:F:264:THR:CG2	2:F:266:ILE:HG12	2.33	0.58
1:C:685:ASP:O	1:C:714:ILE:HB	2.04	0.58
2:D:200:ALA:HA	2:D:230:PHE:O	2.02	0.58
2:H:907:ALA:O	2:H:922:ILE:HG22	2.02	0.58
1:C:809:ASN:HB2	1:C:975:LEU:CD1	2.33	0.58
1:C:466:THR:CG2	1:C:468:ASN:H	2.12	0.58
1:A:518:THR:HB	1:A:519:PRO:HD2	1.85	0.58
2:B:647:GLN:HE22	2:B:869:THR:CG2	2.16	0.58
2:F:903:ILE:HD12	2:F:904:SER:H	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:VAL:HG13	1:A:629:ILE:CB	2.28	0.58
2:B:587:LEU:HD23	2:B:883:GLN:NE2	2.19	0.58
2:D:579:PRO:O	2:D:580:LYS:C	2.41	0.58
2:F:575:ASP:CB	2:F:613:MET:HB3	2.33	0.58
2:F:317:LEU:O	2:F:321:LEU:HD23	2.03	0.58
1:C:336:THR:HG23	1:C:339:GLU:CD	2.24	0.58
1:E:539:VAL:O	1:E:542:VAL:HG22	2.03	0.58
1:C:766:VAL:HG11	1:C:774:ILE:HG22	1.84	0.58
1:G:539:VAL:O	1:G:542:VAL:HG22	2.04	0.58
1:C:439:GLN:HA	1:C:439:GLN:OE1	2.04	0.58
2:H:578:GLU:N	2:H:579:PRO:CD	2.64	0.58
1:A:976:ARG:O	1:A:979:VAL:HB	2.03	0.58
2:H:575:ASP:CB	2:H:613:MET:HB3	2.33	0.58
1:C:947:THR:HG22	1:C:953:LYS:N	2.17	0.58
1:E:703:ARG:HH11	1:E:921:ASP:CG	2.06	0.58
1:C:703:ARG:HH11	1:C:921:ASP:CG	2.06	0.58
1:G:253:LYS:C	1:G:255:LEU:H	2.06	0.58
1:G:583:ASP:C	1:G:585:SER:H	2.07	0.58
2:B:298:CYS:HA	2:B:343:THR:O	2.04	0.58
1:A:766:VAL:HG11	1:A:774:ILE:HG22	1.84	0.58
1:C:424:ALA:HB1	1:C:459:ASP:C	2.24	0.58
1:A:216:ASP:H	2:B:381:HIS:HE1	1.52	0.58
1:E:947:THR:CG2	1:E:953:LYS:H	2.14	0.58
2:D:661:PRO:HD2	2:D:695:GLN:NE2	2.18	0.58
1:G:928:CYS:O	1:G:934:VAL:HA	2.04	0.58
1:A:651:GLU:HG3	1:A:652:ASN:ND2	2.18	0.58
2:F:418:THR:CG2	2:F:419:SER:N	2.66	0.58
2:B:903:ILE:HD12	2:B:904:SER:H	1.67	0.58
1:A:669:SER:N	1:A:701:GLN:NE2	2.48	0.58
2:D:325:ASN:O	2:D:327:ILE:N	2.31	0.58
1:G:400:ARG:HG3	1:G:401:HIS:N	2.19	0.58
1:A:291:ALA:O	1:A:294:ASN:N	2.37	0.58
2:H:709:PRO:HB2	2:H:879:ILE:HD13	1.86	0.58
2:B:679:ASP:O	2:B:708:ILE:HB	2.04	0.58
1:G:963:ASN:ND2	1:G:963:ASN:N	2.51	0.57
2:D:327:ILE:HA	2:D:331:GLN:NE2	2.19	0.57
2:H:320:GLU:O	2:H:324:THR:HG22	2.03	0.57
1:G:448:ASN:HD22	1:G:448:ASN:N	1.99	0.57
2:B:327:ILE:HB	2:B:331:GLN:HE21	1.69	0.57
1:E:438:CYS:O	1:E:442:ARG:HG3	2.04	0.57
2:D:285:GLN:O	2:D:289:GLU:HG3	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:522:ASN:ND2	2:D:527:VAL:HG21	2.19	0.57
1:G:941:ASN:O	1:G:944:GLU:HG3	2.04	0.57
2:F:327:ILE:HA	2:F:331:GLN:NE2	2.18	0.57
2:H:288:ILE:HA	2:H:335:MET:CE	2.34	0.57
1:C:967:ASP:OD2	1:C:972:ARG:HD2	2.05	0.57
2:F:793:LEU:HD13	1:G:796:LEU:HD11	1.84	0.57
2:D:632:HIS:O	2:D:633:GLU:C	2.42	0.57
2:D:752:ARG:HD2	2:D:809:GLY:O	2.04	0.57
1:G:427:HIS:ND1	1:G:427:HIS:C	2.57	0.57
2:H:786:GLU:OE2	2:H:946:ARG:NH2	2.23	0.57
2:B:324:THR:HG23	2:B:326:ARG:HG3	1.86	0.57
2:D:264:THR:HG22	2:D:266:ILE:N	2.18	0.57
1:A:360:SER:H	1:A:545:THR:HG22	1.67	0.57
2:F:792:GLN:HE22	2:F:957:ARG:HB3	1.68	0.57
1:E:211:MET:HE3	1:E:305:VAL:HG22	1.86	0.57
1:E:251:GLY:O	1:E:252:GLY:O	2.22	0.57
1:A:485:ILE:N	1:A:485:ILE:HD12	2.18	0.57
2:H:418:THR:OG1	2:H:419:SER:N	2.35	0.57
2:F:414:GLU:OE2	2:F:414:GLU:N	2.35	0.57
2:D:587:LEU:CD2	2:D:883:GLN:NE2	2.68	0.57
1:A:589:PRO:HD2	1:A:622:HIS:O	2.04	0.57
1:C:400:ARG:HG3	1:C:401:HIS:N	2.19	0.57
2:D:244:PRO:O	2:D:245:GLU:HB3	2.04	0.57
1:E:427:HIS:ND1	1:E:427:HIS:C	2.58	0.57
2:B:422:TRP:CH2	2:B:465:VAL:HG21	2.39	0.57
1:E:590:VAL:HG23	1:E:591:SER:N	2.17	0.57
2:D:892:ALA:C	2:D:894:GLU:H	2.08	0.57
2:B:693:LEU:HD23	2:B:922:ILE:HB	1.86	0.57
1:E:350:GLY:O	1:E:351:LEU:HD23	2.05	0.57
1:E:949:VAL:O	1:E:952:ARG:N	2.38	0.57
2:B:892:ALA:C	2:B:894:GLU:H	2.06	0.57
1:C:320:HIS:O	1:C:321:GLU:HB2	2.05	0.57
1:A:424:ALA:HB1	1:A:459:ASP:C	2.25	0.57
2:H:874:LYS:HD2	2:H:917:VAL:HG21	1.87	0.57
2:H:416:PRO:HG2	2:H:550:PHE:CZ	2.40	0.57
2:B:890:ARG:HG2	2:B:890:ARG:O	2.05	0.57
2:F:889:ALA:O	2:F:891:ALA:N	2.35	0.57
2:F:790:LEU:HD22	1:G:796:LEU:HD22	1.87	0.57
1:G:251:GLY:O	1:G:252:GLY:O	2.22	0.57
1:C:341:ALA:HB3	1:C:342:PRO:CD	2.34	0.57
1:C:832:VAL:HG12	1:C:833:TYR:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:GLU:C	2:B:896:PHE:H	2.07	0.57
2:F:511:THR:OG1	2:F:514:THR:HG23	2.05	0.57
1:G:317:LEU:HD12	1:G:317:LEU:N	2.20	0.57
2:H:501:LEU:HD12	2:H:501:LEU:O	2.04	0.57
1:G:270:GLY:O	1:G:271:GLY:O	2.22	0.57
1:E:431:GLN:O	1:E:435:LYS:HG3	2.05	0.57
1:E:486:LEU:O	1:E:489:VAL:HG22	2.05	0.57
2:H:752:ARG:HD2	2:H:809:GLY:O	2.05	0.57
1:C:421:PRO:C	1:C:423:ARG:H	2.08	0.56
2:B:417:ALA:O	2:B:418:THR:HB	2.04	0.56
2:F:701:GLU:HB3	2:F:897:ASN:ND2	2.20	0.56
2:F:577:ASN:HB3	2:F:579:PRO:CG	2.33	0.56
1:E:212:THR:HG22	1:E:274:ILE:HG13	1.87	0.56
1:G:703:ARG:HH11	1:G:921:ASP:CG	2.08	0.56
2:D:709:PRO:HB2	2:D:879:ILE:HD13	1.87	0.56
1:A:210:VAL:HG12	1:A:304:VAL:HB	1.86	0.56
2:F:220:ARG:HD2	2:F:252:TRP:CZ2	2.40	0.56
2:F:894:GLU:C	2:F:896:PHE:H	2.08	0.56
1:A:329:LEU:O	1:A:334:ARG:HB3	2.05	0.56
2:F:537:LEU:O	2:F:540:ALA:HB3	2.05	0.56
2:F:779:GLN:HA	2:F:953:VAL:HG21	1.87	0.56
2:H:298:CYS:HA	2:H:343:THR:O	2.05	0.56
1:G:422:GLU:CG	1:G:564:ARG:HD2	2.35	0.56
1:A:794:ILE:HD11	1:A:829:ALA:HB1	1.87	0.56
1:A:860:VAL:HG11	2:B:740:TYR:CD1	2.39	0.56
1:A:841:ILE:HG21	2:D:790:LEU:HD11	1.87	0.56
2:F:940:ILE:HD12	2:F:943:GLN:NE2	2.19	0.56
2:H:201:VAL:HG13	2:H:218:ILE:HG21	1.87	0.56
2:H:554:MET:HG2	2:H:562:ILE:CG1	2.34	0.56
2:B:322:LEU:O	2:B:324:THR:N	2.34	0.56
2:F:281:LEU:HD12	2:F:317:LEU:CD2	2.36	0.56
1:A:964:LYS:H	1:A:964:LYS:HD2	1.69	0.56
2:B:704:PRO:HA	2:B:707:ARG:NH1	2.21	0.56
1:E:977:ALA:C	1:E:979:VAL:H	2.07	0.56
2:H:633:GLU:HB2	2:H:672:TYR:CZ	2.40	0.56
2:F:347:ILE:HB	2:F:363:ALA:HB2	1.87	0.56
1:A:385:THR:HA	2:B:207:ASP:OD2	2.05	0.56
1:G:249:LEU:CD1	1:G:290:GLN:HG2	2.35	0.56
1:E:928:CYS:O	1:E:934:VAL:HA	2.05	0.56
1:E:451:ILE:HD12	1:E:451:ILE:N	2.20	0.56
2:B:418:THR:HG1	2:B:422:TRP:HD1	1.43	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:THR:HG22	1:C:979:VAL:HG21	1.83	0.56
1:C:331:ALA:O	1:C:332:GLU:C	2.43	0.56
1:A:778:THR:O	1:A:782:THR:HB	2.05	0.56
2:D:770:THR:CG2	2:D:946:ARG:HD2	2.35	0.56
2:H:704:PRO:HA	2:H:707:ARG:HH11	1.70	0.56
2:H:522:ASN:HD22	2:H:527:VAL:HG21	1.70	0.56
2:D:565:LEU:O	2:D:569:MET:HG2	2.05	0.56
2:H:521:VAL:HG13	2:H:526:ILE:HD13	1.87	0.56
2:D:874:LYS:CD	2:D:917:VAL:HG11	2.28	0.56
1:C:802:ASP:OD1	1:C:972:ARG:NH2	2.23	0.56
1:C:249:LEU:HD21	1:C:281:GLU:CB	2.36	0.56
1:A:941:ASN:O	1:A:944:GLU:HG3	2.06	0.56
2:D:657:ASN:OD1	2:D:659:VAL:HG23	2.06	0.56
1:C:634:SER:HB3	1:C:666:SER:CB	2.36	0.56
2:H:657:ASN:OD1	2:H:659:VAL:HG23	2.05	0.56
2:F:578:GLU:N	2:F:579:PRO:CD	2.68	0.56
1:G:814:LYS:HZ2	1:G:814:LYS:HA	1.69	0.56
1:G:385:THR:HA	2:H:207:ASP:OD2	2.06	0.56
1:E:583:ASP:C	1:E:585:SER:H	2.08	0.56
1:C:948:ASN:O	1:C:950:GLU:N	2.33	0.56
2:F:752:ARG:HD2	2:F:809:GLY:O	2.05	0.56
1:C:539:VAL:O	1:C:542:VAL:HG22	2.06	0.56
2:B:420:SER:HA	2:B:423:GLN:NE2	2.21	0.56
2:D:704:PRO:HA	2:D:707:ARG:CG	2.35	0.56
1:C:746:TYR:CE1	2:D:854:VAL:CG1	2.88	0.56
1:G:883:LYS:O	1:G:887:GLN:HG3	2.06	0.56
2:F:208:ALA:O	2:F:211:MET:HG3	2.04	0.56
1:C:801:GLU:OE1	1:C:976:ARG:HD3	2.06	0.56
1:E:949:VAL:O	1:E:950:GLU:C	2.41	0.56
1:E:537:PRO:HG2	1:E:540:GLU:HB2	1.86	0.56
1:G:211:MET:HE3	1:G:305:VAL:HG22	1.88	0.56
1:G:331:ALA:O	1:G:332:GLU:C	2.43	0.56
2:B:350:ASP:HB3	2:B:394:CYS:HB2	1.87	0.56
2:H:577:ASN:HB3	2:H:579:PRO:CG	2.28	0.55
2:B:886:ILE:HD12	2:B:887:ALA:N	2.20	0.55
2:F:770:THR:CG2	2:F:946:ARG:HD2	2.36	0.55
2:D:892:ALA:O	2:D:894:GLU:N	2.33	0.55
2:H:549:ASP:OD2	2:H:552:ARG:HB2	2.07	0.55
1:G:210:VAL:CG1	1:G:227:VAL:HG11	2.36	0.55
1:G:350:GLY:O	1:G:351:LEU:HD23	2.05	0.55
2:H:537:LEU:O	2:H:540:ALA:HB3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:968:ILE:HG12	1:E:973:LEU:HD12	1.88	0.55
2:D:347:ILE:HB	2:D:363:ALA:HB2	1.87	0.55
1:A:431:GLN:O	1:A:435:LYS:HG3	2.06	0.55
1:C:331:ALA:O	1:C:333:GLY:N	2.39	0.55
2:D:328:SER:N	2:D:331:GLN:NE2	2.54	0.55
1:E:341:ALA:HB3	1:E:342:PRO:HD3	1.88	0.55
1:G:690:LEU:HD23	1:G:719:ILE:HB	1.87	0.55
2:H:392:ARG:HH21	3:H:986:F6P:H12	1.72	0.55
1:G:963:ASN:H	1:G:963:ASN:HD22	1.52	0.55
2:D:679:ASP:O	2:D:708:ILE:HB	2.05	0.55
2:F:324:THR:HG23	2:F:326:ARG:HG3	1.87	0.55
2:B:665:ASP:O	2:B:669:ILE:HG12	2.05	0.55
1:E:572:TYR:CE2	1:E:576:LEU:HD11	2.41	0.55
1:E:679:PHE:CE2	1:E:687:LEU:HD22	2.41	0.55
1:A:391:ARG:O	1:A:448:ASN:HA	2.06	0.55
1:G:893:GLU:HA	1:G:893:GLU:OE2	2.06	0.55
1:C:812:HIS:CD2	1:C:812:HIS:N	2.74	0.55
1:A:422:GLU:CG	1:A:564:ARG:HD2	2.36	0.55
2:F:876:VAL:HG12	2:F:880:LYS:HE3	1.89	0.55
1:E:589:PRO:O	1:E:593:ARG:NH1	2.39	0.55
2:F:589:ILE:HD13	2:F:879:ILE:HG21	1.89	0.55
1:C:421:PRO:O	1:C:423:ARG:N	2.40	0.55
1:E:822:LEU:C	1:E:822:LEU:CD1	2.74	0.55
2:F:886:ILE:HD12	2:F:887:ALA:N	2.21	0.55
2:H:704:PRO:HA	2:H:707:ARG:CG	2.37	0.55
2:B:578:GLU:N	2:B:579:PRO:CD	2.68	0.55
1:A:809:ASN:CA	1:A:975:LEU:HD21	2.37	0.55
2:D:587:LEU:N	2:D:587:LEU:CD1	2.68	0.55
1:A:322:TRP:HB3	1:A:323:PRO:HD3	1.89	0.55
2:H:264:THR:HG22	2:H:266:ILE:HG12	1.88	0.55
1:G:755:SER:HB3	1:G:817:ASN:O	2.06	0.55
2:B:418:THR:HA	2:B:421:GLU:CB	2.28	0.55
1:C:320:HIS:O	1:C:321:GLU:CB	2.54	0.55
1:C:210:VAL:CG1	1:C:227:VAL:HG11	2.37	0.55
1:C:893:GLU:OE2	1:C:893:GLU:HA	2.07	0.55
2:B:701:GLU:O	2:B:701:GLU:CD	2.45	0.55
2:D:647:GLN:HE22	2:D:869:THR:CG2	2.20	0.55
2:D:554:MET:HG2	2:D:562:ILE:CG1	2.37	0.55
1:A:813:ASP:CG	1:A:814:LYS:N	2.60	0.55
2:B:632:HIS:O	2:B:633:GLU:C	2.45	0.55
1:G:391:ARG:HG2	1:G:480:ASP:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:556:ASP:OD2	1:C:559:LYS:HB2	2.07	0.55
2:F:239:LEU:HD22	2:F:287:LEU:HD22	1.88	0.55
1:G:548:VAL:O	1:G:552:ILE:HG12	2.07	0.55
1:G:424:ALA:HB1	1:G:459:ASP:C	2.27	0.55
2:B:578:GLU:C	2:B:580:LYS:H	2.10	0.55
2:B:587:LEU:HD21	2:B:883:GLN:HG3	1.88	0.55
1:E:669:SER:N	1:E:701:GLN:NE2	2.54	0.55
2:H:587:LEU:HD21	2:H:883:GLN:CG	2.37	0.55
1:A:946:GLU:CD	1:A:946:GLU:O	2.45	0.55
2:D:851:PRO:O	2:D:854:VAL:HG22	2.07	0.55
1:C:583:ASP:C	1:C:585:SER:H	2.09	0.55
1:E:717:CYS:HA	1:E:925:ALA:O	2.07	0.55
2:F:662:GLU:H	2:F:695:GLN:HE22	1.53	0.55
1:G:922:ASP:HA	1:G:938:PRO:HG3	1.88	0.55
1:E:893:GLU:OE2	1:E:893:GLU:HA	2.06	0.55
2:B:900:ASP:O	2:B:903:ILE:HG13	2.08	0.55
1:G:825:ARG:HH11	1:G:829:ALA:HB3	1.69	0.55
1:C:599:VAL:CG1	1:C:629:ILE:HB	2.37	0.55
1:E:613:ARG:HA	1:E:650:VAL:HG21	1.87	0.55
1:A:946:GLU:CD	1:A:946:GLU:C	2.65	0.55
2:B:314:TRP:HB3	2:B:315:PRO:HD3	1.88	0.55
1:A:637:ILE:HD13	1:A:671:ASP:HB3	1.89	0.55
1:A:922:ASP:HA	1:A:938:PRO:HG3	1.89	0.55
2:B:239:LEU:O	2:B:286:HIS:HD2	1.89	0.55
1:E:697:ARG:NH1	1:E:943:TRP:HH2	2.04	0.54
1:A:519:PRO:HG2	1:A:520:GLU:H	1.72	0.54
2:D:770:THR:HG23	2:D:946:ARG:HD2	1.90	0.54
1:G:581:LYS:C	1:G:583:ASP:H	2.10	0.54
1:G:423:ARG:CD	1:G:561:ILE:HD12	2.37	0.54
2:F:889:ALA:C	2:F:891:ALA:N	2.61	0.54
1:E:837:LEU:HD22	2:H:831:LYS:HD2	1.88	0.54
1:C:594:LEU:N	1:C:624:HIS:ND1	2.52	0.54
2:H:220:ARG:HD2	2:H:252:TRP:CZ2	2.42	0.54
1:G:816:GLU:O	1:G:818:ARG:N	2.40	0.54
1:C:291:ALA:O	1:C:294:ASN:N	2.40	0.54
1:C:229:ARG:HD3	1:C:260:TRP:CZ2	2.42	0.54
1:E:424:ALA:HB1	1:E:459:ASP:C	2.28	0.54
2:F:416:PRO:O	2:F:417:ALA:C	2.45	0.54
2:B:582:PRO:O	2:B:586:ARG:NH1	2.37	0.54
1:G:586:GLU:O	1:G:587:LEU:C	2.46	0.54
2:D:578:GLU:C	2:D:580:LYS:H	2.09	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:MET:HB3	3:A:988:F6P:O3	2.07	0.54
2:B:320:GLU:O	2:B:324:THR:HG22	2.07	0.54
2:F:780:VAL:HG12	2:F:781:SER:N	2.23	0.54
1:C:790:PRO:HD2	1:C:791:GLU:OE1	2.07	0.54
1:A:438:CYS:O	1:A:442:ARG:HG3	2.06	0.54
2:H:417:ALA:O	2:H:418:THR:HB	2.08	0.54
2:F:582:PRO:O	2:F:586:ARG:NH1	2.37	0.54
2:F:575:ASP:OD1	2:F:575:ASP:C	2.45	0.54
2:D:680:GLY:HA3	2:D:879:ILE:HD12	1.88	0.54
1:G:438:CYS:O	1:G:442:ARG:HG3	2.08	0.54
2:B:278:GLU:HA	2:B:278:GLU:OE1	2.07	0.54
1:G:697:ARG:O	1:G:701:GLN:HG3	2.08	0.54
2:B:325:ASN:O	2:B:327:ILE:N	2.31	0.54
1:A:360:SER:HB3	1:A:545:THR:HG22	1.90	0.54
1:E:806:LEU:O	1:E:807:LYS:C	2.45	0.54
2:H:541:VAL:O	2:H:545:ILE:HG12	2.08	0.54
2:H:704:PRO:HA	2:H:707:ARG:NH1	2.23	0.54
2:H:894:GLU:O	2:H:896:PHE:N	2.41	0.54
2:H:431:SER:OG	2:H:470:LEU:HD11	2.07	0.54
1:G:554:ASN:O	1:G:556:ASP:N	2.41	0.54
1:E:813:ASP:OD1	1:E:814:LYS:N	2.17	0.54
2:F:946:ARG:CG	2:F:946:ARG:HH21	2.21	0.54
2:B:889:ALA:O	2:B:891:ALA:N	2.41	0.54
2:D:220:ARG:HD2	2:D:252:TRP:CE2	2.42	0.54
1:A:931:GLY:O	1:A:932:SER:HB3	2.07	0.54
1:E:378:MET:HE3	2:F:482:VAL:HG21	1.88	0.54
2:H:416:PRO:HD2	2:H:550:PHE:CD1	2.42	0.54
1:E:315:ALA:O	1:E:348:ILE:HD13	2.08	0.54
2:H:348:ASP:OD2	3:H:986:F6P:C1	2.52	0.54
1:C:599:VAL:HG13	1:C:629:ILE:CB	2.38	0.54
2:D:201:VAL:HG11	2:D:218:ILE:CD1	2.36	0.54
1:G:341:ALA:HB3	1:G:342:PRO:HD3	1.89	0.54
1:G:634:SER:HB3	1:G:666:SER:CB	2.38	0.54
1:C:801:GLU:O	1:C:805:LEU:HG	2.08	0.54
2:F:418:THR:OG1	2:F:419:SER:N	2.41	0.54
1:E:466:THR:CG2	1:E:468:ASN:H	2.11	0.54
1:G:518:THR:HB	1:G:519:PRO:HD2	1.90	0.54
2:B:740:TYR:CE1	2:B:851:PRO:HB3	2.43	0.54
2:H:341:CYS:SG	2:H:519:ILE:CD1	2.96	0.54
1:A:596:ILE:CD1	1:A:885:ILE:HG21	2.38	0.54
2:D:522:ASN:HD21	2:D:529:LYS:CE	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:320:HIS:O	1:G:321:GLU:HB2	2.07	0.54
2:B:709:PRO:HB2	2:B:879:ILE:HD13	1.90	0.54
2:F:350:ASP:HB3	2:F:394:CYS:HB2	1.90	0.54
1:G:248:LEU:HG	1:G:291:ALA:HB1	1.89	0.54
2:B:418:THR:CA	2:B:421:GLU:HB2	2.29	0.54
1:E:319:ARG:HB2	1:E:348:ILE:CD1	2.34	0.54
2:D:381:HIS:CD2	2:D:383:ARG:HH21	2.26	0.54
1:E:946:GLU:C	1:E:946:GLU:CD	2.66	0.54
1:C:329:LEU:O	1:C:334:ARG:HB3	2.08	0.54
1:G:398:MET:HB3	3:G:988:F6P:O3	2.08	0.54
1:E:685:ASP:O	1:E:715:PRO:HD2	2.07	0.54
1:G:210:VAL:HG12	1:G:304:VAL:HB	1.90	0.54
2:B:798:GLU:O	2:B:801:ALA:HB3	2.08	0.54
1:E:596:ILE:HD12	1:E:885:ILE:HG21	1.90	0.54
2:D:239:LEU:O	2:D:286:HIS:HD2	1.90	0.54
1:G:931:GLY:O	1:G:932:SER:HB3	2.08	0.54
1:E:948:ASN:O	1:E:950:GLU:N	2.40	0.53
2:D:889:ALA:O	2:D:891:ALA:N	2.41	0.53
2:H:324:THR:O	2:H:325:ASN:HB2	2.08	0.53
2:B:453:ASP:OD2	2:B:455:THR:HG23	2.07	0.53
1:E:289:ARG:HA	1:E:325:LEU:HD13	1.89	0.53
2:F:752:ARG:CZ	2:F:811:GLY:HA2	2.38	0.53
2:F:829:ALA:HB3	2:F:850:TYR:CZ	2.43	0.53
2:F:466:LEU:HD12	2:F:472:LEU:HD11	1.89	0.53
1:G:767:GLN:HG2	1:G:827:GLU:OE2	2.08	0.53
2:F:518:LEU:HD23	2:F:518:LEU:C	2.28	0.53
1:E:809:ASN:OD1	1:E:809:ASN:C	2.46	0.53
1:A:289:ARG:CD	1:A:328:GLU:HB3	2.38	0.53
2:H:886:ILE:HD12	2:H:887:ALA:N	2.23	0.53
2:D:466:LEU:HD12	2:D:472:LEU:HD11	1.89	0.53
2:D:522:ASN:HD21	2:D:529:LYS:NZ	2.06	0.53
2:B:779:GLN:HA	2:B:953:VAL:HG21	1.91	0.53
1:E:958:HIS:CD2	1:E:958:HIS:H	2.26	0.53
1:C:596:ILE:HD12	1:C:885:ILE:HG21	1.90	0.53
1:A:636:LEU:HD12	1:A:640:GLY:HA2	1.90	0.53
2:B:541:VAL:O	2:B:545:ILE:HG12	2.08	0.53
1:A:947:THR:HG22	1:A:953:LYS:O	2.07	0.53
2:D:931:GLU:HG3	2:D:931:GLU:O	2.08	0.53
2:D:591:ILE:HB	2:D:608:MET:CE	2.39	0.53
2:H:208:ALA:O	2:H:211:MET:HG3	2.08	0.53
1:E:554:ASN:O	1:E:556:ASP:N	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:463:HIS:HD2	2:F:474:THR:HG22	1.73	0.53
1:G:216:ASP:H	2:H:381:HIS:HE1	1.54	0.53
2:H:281:LEU:HD12	2:H:317:LEU:CD2	2.39	0.53
2:H:327:ILE:HA	2:H:331:GLN:NE2	2.23	0.53
2:F:341:CYS:CB	2:F:507:VAL:HG13	2.38	0.53
2:B:680:GLY:HA3	2:B:879:ILE:HD12	1.89	0.53
1:A:350:GLY:O	1:A:351:LEU:HD23	2.08	0.53
2:H:883:GLN:O	2:H:887:ALA:HB2	2.09	0.53
1:A:685:ASP:O	1:A:715:PRO:HD2	2.09	0.53
1:A:802:ASP:OD1	1:A:972:ARG:NH2	2.36	0.53
2:B:589:ILE:HD13	2:B:879:ILE:HG21	1.91	0.53
2:B:366:ARG:HG2	2:B:482:VAL:O	2.09	0.53
2:D:541:VAL:O	2:D:545:ILE:HG12	2.08	0.53
2:H:641:LYS:O	2:H:644:LEU:HD12	2.08	0.53
1:C:276:THR:HG21	2:D:381:HIS:CE1	2.43	0.53
1:A:212:THR:HG23	1:A:275:GLY:O	2.08	0.53
2:H:903:ILE:HD12	2:H:904:SER:H	1.70	0.53
1:A:248:LEU:HG	1:A:291:ALA:HB1	1.91	0.53
2:B:907:ALA:O	2:B:922:ILE:HG22	2.08	0.53
2:H:314:TRP:HB3	2:H:315:PRO:HD3	1.91	0.53
2:F:353:THR:CG2	2:F:534:SER:HA	2.38	0.53
1:C:422:GLU:OE1	1:C:564:ARG:NH1	2.34	0.53
1:E:599:VAL:CG1	1:E:629:ILE:HB	2.29	0.53
1:A:285:ARG:NH2	1:A:328:GLU:OE2	2.42	0.53
2:H:889:ALA:C	2:H:891:ALA:N	2.61	0.53
1:G:770:HIS:CG	1:G:951:LEU:HB3	2.43	0.53
1:C:685:ASP:O	1:C:715:PRO:HD2	2.09	0.53
2:D:528:ARG:O	2:D:529:LYS:HD2	2.09	0.53
2:H:201:VAL:CG1	2:H:218:ILE:HD13	2.39	0.53
2:B:208:ALA:O	2:B:211:MET:HG3	2.09	0.53
1:E:525:LEU:HD23	1:E:525:LEU:C	2.28	0.53
2:D:264:THR:CG2	2:D:266:ILE:HG12	2.39	0.53
2:H:426:MET:CE	2:H:466:LEU:HD22	2.39	0.53
2:B:794:SER:OG	1:C:796:LEU:HD12	2.08	0.53
1:E:778:THR:O	1:E:782:THR:HB	2.09	0.53
2:F:770:THR:HG23	2:F:946:ARG:HD2	1.89	0.53
2:D:779:GLN:OE1	2:D:953:VAL:HG22	2.09	0.53
1:E:977:ALA:C	1:E:979:VAL:N	2.62	0.53
2:D:522:ASN:HD22	2:D:527:VAL:HG21	1.74	0.53
1:A:619:CYS:SG	1:A:882:ILE:HD12	2.49	0.53
1:C:767:GLN:HG2	1:C:827:GLU:OE2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:350:ASP:HB3	2:H:394:CYS:HB2	1.91	0.53
2:D:350:ASP:HB3	2:D:394:CYS:HB2	1.90	0.53
2:F:648:SER:HA	2:F:865:ARG:HD3	1.89	0.53
2:B:753:GLY:HA2	2:B:804:PHE:CD2	2.44	0.53
2:B:353:THR:CG2	2:B:534:SER:HA	2.38	0.53
2:B:353:THR:HG21	2:B:534:SER:HA	1.90	0.53
2:D:353:THR:CG2	2:D:534:SER:HA	2.39	0.53
2:D:353:THR:HG21	2:D:534:SER:HA	1.91	0.53
2:H:717:LEU:C	2:H:717:LEU:HD12	2.29	0.52
1:G:317:LEU:CD1	1:G:317:LEU:H	2.22	0.52
2:B:779:GLN:OE1	2:B:953:VAL:HG22	2.08	0.52
1:C:803:ILE:HD13	1:C:845:ALA:CB	2.39	0.52
1:A:230:THR:OG1	1:A:508:VAL:HG22	2.09	0.52
2:B:717:LEU:HB2	2:B:733:ALA:CB	2.39	0.52
2:B:381:HIS:CD2	2:B:383:ARG:HH21	2.28	0.52
1:E:770:HIS:CD2	1:E:951:LEU:HA	2.44	0.52
1:E:944:GLU:HA	1:E:946:GLU:OE1	2.09	0.52
2:H:322:LEU:O	2:H:324:THR:N	2.37	0.52
2:H:327:ILE:HB	2:H:331:GLN:HE21	1.73	0.52
2:B:327:ILE:HA	2:B:331:GLN:NE2	2.23	0.52
2:F:892:ALA:C	2:F:894:GLU:H	2.09	0.52
2:D:626:TRP:NE1	2:D:661:PRO:HG3	2.24	0.52
2:D:522:ASN:HD21	2:D:529:LYS:HE3	1.74	0.52
2:B:801:ALA:O	2:B:805:GLU:HG3	2.09	0.52
1:E:461:GLN:HB2	1:E:463:ASN:ND2	2.24	0.52
2:D:697:GLU:O	2:D:700:ARG:HB2	2.08	0.52
2:H:664:ALA:O	2:H:665:ASP:CB	2.57	0.52
2:D:886:ILE:HD12	2:D:887:ALA:N	2.24	0.52
2:B:704:PRO:HA	2:B:707:ARG:CG	2.38	0.52
1:A:236:CYS:SG	1:A:515:LEU:HD21	2.49	0.52
1:A:374:ARG:HD2	2:B:373:TYR:CZ	2.45	0.52
2:F:697:GLU:O	2:F:700:ARG:HB2	2.08	0.52
1:A:301:ASP:OD1	1:A:301:ASP:N	2.43	0.52
2:H:665:ASP:O	2:H:669:ILE:HG12	2.09	0.52
1:G:331:ALA:O	1:G:333:GLY:N	2.42	0.52
1:C:958:HIS:C	1:C:959:TRP:CD1	2.82	0.52
2:B:697:GLU:O	2:B:700:ARG:HB2	2.09	0.52
2:B:547:ALA:O	2:B:549:ASP:N	2.43	0.52
1:C:717:CYS:HA	1:C:925:ALA:O	2.09	0.52
1:C:813:ASP:O	1:C:815:GLY:N	2.40	0.52
1:A:205:LYS:HE3	1:A:237:ASP:CG	2.29	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:972:ARG:HH11	1:C:976:ARG:HH21	1.58	0.52
1:G:951:LEU:HD22	1:G:951:LEU:N	2.25	0.52
2:B:662:GLU:H	2:B:695:GLN:HE22	1.56	0.52
1:A:233:HIS:CD2	1:A:968:ILE:HD12	2.44	0.52
2:F:462:VAL:O	2:F:466:LEU:HD23	2.09	0.52
1:A:320:HIS:O	1:A:321:GLU:HB2	2.10	0.52
2:F:701:GLU:CD	2:F:701:GLU:O	2.48	0.52
2:H:701:GLU:O	2:H:702:SER:CB	2.53	0.52
1:A:323:PRO:O	1:A:326:VAL:HB	2.09	0.52
2:B:328:SER:H	2:B:331:GLN:NE2	2.06	0.52
2:B:365:ASP:HA	2:B:862:PRO:HG2	1.92	0.52
2:D:537:LEU:O	2:D:540:ALA:HB3	2.08	0.52
2:B:771:TYR:OH	2:B:945:THR:HG21	2.10	0.52
1:C:805:LEU:O	1:C:975:LEU:HD13	2.10	0.52
1:A:289:ARG:HA	1:A:325:LEU:HD13	1.92	0.52
1:A:292:ALA:O	1:A:296:ILE:HG13	2.09	0.52
1:G:317:LEU:HD12	1:G:317:LEU:H	1.74	0.52
2:B:312:SER:O	2:B:315:PRO:HD2	2.10	0.52
1:A:865:VAL:HG13	1:A:866:PRO:HD2	1.92	0.52
2:D:343:THR:HG22	2:D:343:THR:O	2.09	0.52
1:C:947:THR:HG23	1:C:952:ARG:N	2.25	0.52
2:D:293:ASP:HB3	2:D:335:MET:HE3	1.92	0.52
2:H:298:CYS:SG	2:H:343:THR:HG22	2.50	0.52
2:F:578:GLU:C	2:F:580:LYS:H	2.13	0.52
1:E:581:LYS:HB3	1:E:586:GLU:CB	2.30	0.52
2:F:883:GLN:O	2:F:887:ALA:HB2	2.09	0.52
2:H:522:ASN:HD21	2:H:529:LYS:CE	2.23	0.52
1:E:812:HIS:CD2	1:E:812:HIS:N	2.78	0.52
1:G:466:THR:CG2	1:G:468:ASN:H	2.15	0.52
1:E:319:ARG:HG3	1:E:346:LEU:HB3	1.91	0.52
1:E:946:GLU:CD	1:E:946:GLU:O	2.49	0.52
2:D:587:LEU:HD21	2:D:883:GLN:HG3	1.92	0.52
1:C:322:TRP:CZ3	1:C:343:TYR:O	2.63	0.52
2:F:945:THR:HA	2:F:948:ILE:HG12	1.92	0.52
1:G:525:LEU:HD23	1:G:525:LEU:C	2.30	0.52
1:C:825:ARG:HH11	1:C:829:ALA:HB3	1.75	0.51
1:C:809:ASN:HB2	1:C:975:LEU:HD11	1.91	0.51
2:F:665:ASP:O	2:F:669:ILE:HG12	2.10	0.51
2:F:264:THR:HG22	2:F:266:ILE:HG12	1.93	0.51
1:C:782:THR:HG22	1:C:784:ALA:H	1.75	0.51
2:F:717:LEU:HD12	2:F:717:LEU:C	2.30	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:716:MET:O	1:G:924:ALA:HA	2.10	0.51
1:C:518:THR:HB	1:C:519:PRO:HD2	1.92	0.51
1:E:800:ARG:HG3	2:H:790:LEU:HD13	1.93	0.51
2:D:903:ILE:HD12	2:D:904:SER:H	1.74	0.51
2:F:341:CYS:HB2	2:F:507:VAL:CG1	2.40	0.51
1:E:841:ILE:HD11	2:H:827:LEU:HD21	1.92	0.51
2:H:522:ASN:HD21	2:H:529:LYS:NZ	2.08	0.51
1:A:320:HIS:O	1:A:321:GLU:CB	2.57	0.51
1:A:823:LEU:N	1:A:823:LEU:HD12	2.25	0.51
1:G:439:GLN:HA	1:G:439:GLN:OE1	2.10	0.51
2:D:416:PRO:HD2	2:D:550:PHE:CD1	2.45	0.51
1:C:805:LEU:HD13	1:C:972:ARG:HA	1.91	0.51
2:B:673:PHE:HZ	2:B:681:LEU:HD22	1.74	0.51
2:F:615:GLN:OE1	2:F:880:LYS:NZ	2.43	0.51
1:A:289:ARG:NH2	1:A:328:GLU:HG2	2.25	0.51
1:C:276:THR:CG2	1:C:276:THR:O	2.57	0.51
1:G:421:PRO:C	1:G:423:ARG:H	2.12	0.51
1:G:322:TRP:HB3	1:G:323:PRO:HD3	1.91	0.51
2:F:327:ILE:HB	2:F:331:GLN:HE21	1.74	0.51
1:C:746:TYR:CE1	2:D:854:VAL:HG13	2.45	0.51
2:D:288:ILE:HA	2:D:335:MET:HE1	1.91	0.51
2:D:771:TYR:OH	2:D:945:THR:HG21	2.10	0.51
1:G:572:TYR:CE2	1:G:576:LEU:HD11	2.45	0.51
1:A:928:CYS:O	1:A:934:VAL:HA	2.10	0.51
1:C:558:ASP:O	1:C:561:ILE:HG22	2.11	0.51
2:H:911:GLY:O	2:H:917:VAL:HA	2.09	0.51
2:F:392:ARG:NH2	3:F:984:F6P:H12	2.23	0.51
1:E:518:THR:HB	1:E:519:PRO:HD2	1.92	0.51
2:F:239:LEU:HD22	2:F:287:LEU:CD2	2.40	0.51
1:A:381:TYR:CE2	2:B:366:ARG:HD2	2.46	0.51
1:A:963:ASN:O	1:A:967:ASP:N	2.41	0.51
1:A:966:GLY:O	1:A:970:SER:HB3	2.10	0.51
2:D:754:ARG:NH2	2:D:847:LYS:HE3	2.25	0.51
1:G:596:ILE:HD12	1:G:885:ILE:HG21	1.93	0.51
2:B:657:ASN:OD1	2:B:659:VAL:HG23	2.10	0.51
2:B:715:ALA:HB2	2:B:728:LEU:HB2	1.90	0.51
2:B:433:HIS:ND1	2:B:640:TRP:CZ2	2.78	0.51
1:C:697:ARG:NH2	1:C:949:VAL:HG22	2.25	0.51
1:G:583:ASP:O	1:G:583:ASP:OD2	2.29	0.51
2:B:916:HIS:O	2:B:917:VAL:HG23	2.11	0.51
2:B:797:ILE:HD13	2:B:836:ILE:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:852:GLY:O	2:H:855:GLN:HG3	2.10	0.51
1:G:947:THR:HG22	1:G:953:LYS:O	2.11	0.51
1:E:776:SER:CB	1:E:963:ASN:HD21	2.23	0.51
1:G:291:ALA:O	1:G:294:ASN:N	2.44	0.51
2:B:683:ILE:O	2:B:712:LEU:HD12	2.11	0.51
2:H:578:GLU:C	2:H:580:LYS:H	2.09	0.51
2:B:587:LEU:N	2:B:587:LEU:CD1	2.74	0.51
1:E:431:GLN:N	1:E:431:GLN:HE21	1.98	0.51
1:E:391:ARG:HG2	1:E:480:ASP:HB3	1.93	0.51
1:A:860:VAL:HG11	2:B:740:TYR:CE1	2.46	0.51
1:E:400:ARG:HG2	1:E:400:ARG:HH11	1.76	0.51
1:A:600:HIS:CE1	1:A:661:ILE:HD11	2.45	0.51
1:C:398:MET:HG3	1:C:490:GLN:NE2	2.25	0.51
2:B:349:ASN:OD1	2:B:356:ALA:HA	2.11	0.51
2:H:418:THR:O	2:H:419:SER:HB2	2.10	0.51
2:F:298:CYS:CB	2:F:343:THR:HG22	2.40	0.51
1:A:951:LEU:N	1:A:951:LEU:HD23	2.25	0.51
2:D:935:ARG:O	2:D:936:MET:HB3	2.10	0.51
1:A:229:ARG:HD3	1:A:260:TRP:CZ2	2.45	0.51
2:D:563:GLU:OE2	2:D:870:ARG:NE	2.32	0.51
1:C:676:ALA:HB2	1:C:712:PHE:CZ	2.46	0.51
1:E:767:GLN:HG2	1:E:827:GLU:OE2	2.11	0.51
2:H:438:LYS:HG2	2:H:440:THR:O	2.10	0.51
1:G:732:TYR:CE1	1:G:736:VAL:HB	2.46	0.51
1:G:588:LEU:HD13	1:G:593:ARG:NH1	2.21	0.51
1:G:212:THR:HG22	1:G:274:ILE:HG13	1.93	0.51
2:D:797:ILE:HD13	2:D:836:ILE:HA	1.93	0.51
2:F:344:VAL:CG2	2:F:357:THR:HG22	2.40	0.51
1:C:542:VAL:O	1:C:546:LYS:HB2	2.10	0.51
2:F:541:VAL:O	2:F:545:ILE:HG12	2.11	0.51
1:E:883:LYS:O	1:E:887:GLN:HG3	2.09	0.51
2:H:603:SER:HB3	2:H:647:GLN:OE1	2.11	0.51
2:B:201:VAL:HG13	2:B:218:ILE:HG21	1.93	0.51
2:F:347:ILE:HB	2:F:363:ALA:CB	2.40	0.51
1:E:790:PRO:HD2	1:E:791:GLU:OE1	2.11	0.51
2:H:453:ASP:O	2:H:454:LEU:HB2	2.10	0.51
1:E:229:ARG:HD3	1:E:260:TRP:CZ2	2.46	0.51
1:A:758:ARG:NH1	2:B:655:GLY:CA	2.73	0.51
1:A:812:HIS:N	1:A:812:HIS:CD2	2.77	0.51
1:C:809:ASN:HB2	1:C:975:LEU:CD2	2.40	0.51
1:A:809:ASN:HA	1:A:975:LEU:HD21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:679:ASP:O	2:H:708:ILE:HB	2.10	0.51
2:H:436:ARG:HG3	2:H:436:ARG:O	2.10	0.51
2:D:798:GLU:O	2:D:801:ALA:HB3	2.11	0.51
1:E:791:GLU:CD	1:E:959:TRP:HH2	2.15	0.51
1:C:495:ALA:HB3	1:C:500:ARG:HG2	1.92	0.51
1:E:391:ARG:O	1:E:448:ASN:HA	2.10	0.50
1:G:330:VAL:HG22	1:G:340:VAL:HG11	1.93	0.50
1:C:249:LEU:HD13	1:C:290:GLN:HG2	1.93	0.50
1:G:246:GLU:O	1:G:249:LEU:HB3	2.11	0.50
1:C:252:GLY:O	1:C:253:LYS:HB3	2.10	0.50
2:D:633:GLU:HB2	2:D:672:TYR:OH	2.12	0.50
2:F:494:ILE:HD13	2:F:771:TYR:HD2	1.76	0.50
1:E:423:ARG:CD	1:E:561:ILE:HD12	2.41	0.50
2:H:662:GLU:H	2:H:695:GLN:HE22	1.59	0.50
2:H:697:GLU:O	2:H:700:ARG:HB2	2.12	0.50
2:F:565:LEU:O	2:F:569:MET:HG2	2.11	0.50
2:D:416:PRO:HG2	2:D:550:PHE:CZ	2.46	0.50
2:F:381:HIS:CB	2:F:383:ARG:HG3	2.36	0.50
1:A:590:VAL:HG23	1:A:591:SER:N	2.27	0.50
1:G:242:TYR:O	1:G:247:GLY:HA3	2.10	0.50
1:E:322:TRP:CZ3	1:E:343:TYR:O	2.65	0.50
2:F:239:LEU:O	2:F:286:HIS:HD2	1.95	0.50
1:A:381:TYR:HD2	2:B:486:GLY:CA	2.24	0.50
1:G:600:HIS:HD2	1:G:659:SER:OG	1.93	0.50
1:E:538:LEU:C	1:E:538:LEU:HD23	2.31	0.50
1:C:276:THR:CG2	2:D:381:HIS:CE1	2.95	0.50
2:D:587:LEU:CD1	2:D:587:LEU:H	2.23	0.50
2:D:256:ARG:NH1	2:D:813:PHE:CE1	2.79	0.50
2:H:528:ARG:O	2:H:529:LYS:HD2	2.12	0.50
2:H:201:VAL:CG1	2:H:218:ILE:HG21	2.42	0.50
2:F:726:TYR:OH	2:F:864:ASP:OD2	2.23	0.50
1:G:754:ALA:HB2	1:G:762:PHE:CE1	2.45	0.50
1:C:538:LEU:HD23	1:C:538:LEU:C	2.31	0.50
1:A:427:HIS:ND1	1:A:427:HIS:C	2.65	0.50
2:H:717:LEU:HB2	2:H:733:ALA:CB	2.41	0.50
2:H:328:SER:H	2:H:331:GLN:NE2	2.09	0.50
1:C:860:VAL:HG11	2:D:740:TYR:CD1	2.46	0.50
1:G:320:HIS:O	1:G:321:GLU:CB	2.59	0.50
1:A:962:TYR:O	1:A:965:ILE:N	2.44	0.50
1:C:233:HIS:CE1	1:C:968:ILE:HD13	2.47	0.50
2:F:390:MET:HG3	2:F:483:GLN:NE2	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:CYS:HB2	2:D:507:VAL:HG13	1.93	0.50
2:H:463:HIS:HD2	2:H:474:THR:HG22	1.76	0.50
1:G:638:GLN:O	1:G:638:GLN:HG3	2.10	0.50
1:C:525:LEU:C	1:C:525:LEU:HD23	2.31	0.50
1:C:431:GLN:N	1:C:431:GLN:NE2	2.50	0.50
2:F:298:CYS:HA	2:F:343:THR:O	2.12	0.50
2:D:889:ALA:C	2:D:891:ALA:N	2.64	0.50
2:F:522:ASN:HD21	2:F:529:LYS:CE	2.24	0.50
2:H:201:VAL:HG11	2:H:218:ILE:HD13	1.93	0.50
2:B:545:ILE:HD11	2:B:553:ALA:CB	2.41	0.50
2:D:744:VAL:O	2:D:747:SER:HB3	2.12	0.50
1:G:717:CYS:HA	1:G:925:ALA:O	2.12	0.50
2:H:416:PRO:O	2:H:417:ALA:C	2.49	0.50
1:C:342:PRO:HG2	1:C:343:TYR:CD1	2.46	0.50
1:A:622:HIS:HD2	1:A:886:GLU:OE1	1.95	0.50
2:H:253:GLU:O	2:H:256:ARG:HB3	2.12	0.50
2:B:626:TRP:NE1	2:B:661:PRO:HG3	2.26	0.50
1:E:410:GLY:HA2	1:E:452:ILE:HD12	1.94	0.50
1:C:708:GLN:O	1:G:709:HIS:HE1	1.94	0.50
2:H:565:LEU:O	2:H:569:MET:HG2	2.12	0.50
2:D:420:SER:HA	2:D:423:GLN:NE2	2.26	0.50
2:D:582:PRO:O	2:D:586:ARG:NH1	2.41	0.50
2:F:428:ASP:OD2	2:F:432:LYS:NZ	2.45	0.50
2:F:930:THR:HG22	2:F:932:VAL:H	1.76	0.50
2:H:427:CYS:SG	2:H:470:LEU:HD23	2.52	0.50
1:A:790:PRO:HD2	1:A:791:GLU:OE1	2.11	0.50
2:D:761:GLN:HG3	2:D:855:GLN:NE2	2.27	0.50
2:H:781:SER:HA	2:H:818:LEU:O	2.11	0.50
2:F:947:LEU:HD22	2:F:951:HIS:CE1	2.46	0.50
2:D:422:TRP:CH2	2:D:465:VAL:HG21	2.46	0.50
1:C:667:VAL:HG11	1:C:697:ARG:HD3	1.93	0.50
2:H:711:VAL:CG2	2:H:910:VAL:HG22	2.41	0.50
2:H:525:LYS:HB2	2:H:525:LYS:HZ3	1.74	0.50
1:C:942:LEU:C	1:C:944:GLU:H	2.16	0.50
2:H:347:ILE:HB	2:H:363:ALA:HB2	1.93	0.50
1:G:485:ILE:HD12	1:G:485:ILE:N	2.26	0.50
2:D:298:CYS:SG	2:D:343:THR:HG22	2.51	0.50
2:D:883:GLN:O	2:D:887:ALA:HB2	2.11	0.50
2:D:327:ILE:CA	2:D:331:GLN:NE2	2.75	0.50
2:D:935:ARG:NH1	4:D:4:FDP:O3P	2.45	0.50
2:B:201:VAL:CG1	2:B:218:ILE:HG21	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:VAL:O	1:A:542:VAL:HG22	2.11	0.50
2:B:253:GLU:O	2:B:256:ARG:HB3	2.12	0.50
2:D:662:GLU:H	2:D:695:GLN:HE22	1.59	0.50
1:C:660:GLU:C	2:D:752:ARG:HH22	2.14	0.50
2:H:453:ASP:CG	2:H:455:THR:HG23	2.32	0.50
2:F:726:TYR:CE1	2:F:730:SER:HB3	2.46	0.50
1:E:248:LEU:HG	1:E:291:ALA:HB1	1.94	0.50
2:D:416:PRO:O	2:D:417:ALA:C	2.50	0.49
2:B:580:LYS:HD2	2:B:586:ARG:NH2	2.27	0.49
1:C:212:THR:O	1:C:212:THR:CG2	2.59	0.49
1:A:594:LEU:N	1:A:624:HIS:ND1	2.55	0.49
2:B:851:PRO:O	2:B:854:VAL:HG22	2.12	0.49
2:H:894:GLU:C	2:H:896:PHE:N	2.65	0.49
1:G:291:ALA:HA	1:G:294:ASN:ND2	2.27	0.49
2:B:574:ALA:CB	2:B:610:THR:HB	2.41	0.49
2:D:354:THR:CB	2:D:520:ALA:HB1	2.42	0.49
2:B:418:THR:HG21	2:B:422:TRP:HD1	1.77	0.49
1:A:339:GLU:C	1:A:341:ALA:H	2.15	0.49
1:E:398:MET:HE1	1:E:488:HIS:HA	1.94	0.49
2:B:426:MET:CE	2:B:466:LEU:HD22	2.41	0.49
2:B:264:THR:HG22	2:B:266:ILE:N	2.26	0.49
2:H:626:TRP:CE2	2:H:661:PRO:HG3	2.47	0.49
1:E:634:SER:HB3	1:E:666:SER:CB	2.42	0.49
1:A:883:LYS:O	1:A:887:GLN:HG3	2.11	0.49
2:B:400:LEU:HD12	2:B:866:THR:HG21	1.94	0.49
2:H:410:ILE:HA	2:H:444:VAL:O	2.11	0.49
1:E:242:TYR:O	1:E:247:GLY:HA3	2.12	0.49
1:C:636:LEU:HD12	1:C:640:GLY:HA2	1.95	0.49
2:F:400:LEU:CD1	2:F:866:THR:HG21	2.42	0.49
2:B:518:LEU:HD23	2:B:518:LEU:C	2.32	0.49
2:F:298:CYS:SG	2:F:343:THR:HG22	2.53	0.49
1:E:941:ASN:O	1:E:944:GLU:HG3	2.12	0.49
1:E:800:ARG:HG3	2:H:790:LEU:CD1	2.42	0.49
1:E:977:ALA:O	1:E:979:VAL:N	2.44	0.49
2:D:830:THR:HA	2:D:848:PRO:HB3	1.94	0.49
2:B:521:VAL:HG13	2:B:526:ILE:HD13	1.94	0.49
2:F:851:PRO:O	2:F:854:VAL:HG22	2.12	0.49
2:D:683:ILE:O	2:D:712:LEU:HD12	2.13	0.49
2:B:711:VAL:CG2	2:B:910:VAL:HG22	2.42	0.49
2:F:522:ASN:HD21	2:F:529:LYS:NZ	2.09	0.49
2:F:253:GLU:O	2:F:256:ARG:HB3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLY:CA	1:A:294:ASN:ND2	2.75	0.49
2:H:201:VAL:HG11	2:H:218:ILE:CD1	2.42	0.49
2:F:400:LEU:HD12	2:F:866:THR:HG21	1.92	0.49
1:C:786:SER:HB3	1:C:823:LEU:HG	1.93	0.49
2:H:590:ALA:HA	2:H:620:TYR:O	2.13	0.49
1:A:893:GLU:HA	1:A:893:GLU:OE2	2.12	0.49
2:H:268:THR:O	2:H:268:THR:HG23	2.12	0.49
1:E:599:VAL:HG13	1:E:629:ILE:CB	2.30	0.49
2:B:587:LEU:HD12	2:B:587:LEU:H	1.75	0.49
2:D:381:HIS:CB	2:D:383:ARG:HG3	2.38	0.49
2:D:679:ASP:HB3	2:D:883:GLN:HE22	1.76	0.49
2:B:770:THR:CG2	2:B:946:ARG:HD2	2.42	0.49
2:F:528:ARG:O	2:F:529:LYS:HD2	2.12	0.49
2:F:800:LEU:HD21	2:F:817:ILE:HD11	1.95	0.49
2:D:753:GLY:HA2	2:D:804:PHE:CD2	2.47	0.49
1:A:538:LEU:C	1:A:538:LEU:HD23	2.32	0.49
1:C:746:TYR:CE1	2:D:854:VAL:HG11	2.47	0.49
1:E:253:LYS:C	1:E:255:LEU:N	2.64	0.49
1:C:833:TYR:HA	1:C:837:LEU:HD23	1.94	0.49
1:E:342:PRO:HG2	1:E:343:TYR:CD1	2.47	0.49
2:D:523:GLU:O	2:D:524:ASN:C	2.50	0.49
1:G:309:ASP:OD1	1:G:310:GLY:N	2.46	0.49
2:B:220:ARG:HD2	2:B:252:TRP:CE2	2.48	0.49
2:H:353:THR:CG2	2:H:534:SER:HA	2.43	0.49
1:E:805:LEU:HD23	1:E:805:LEU:N	2.28	0.49
2:D:916:HIS:O	2:D:917:VAL:HG23	2.12	0.49
2:B:904:SER:O	2:B:906:THR:N	2.44	0.49
1:G:765:GLU:HA	1:G:825:ARG:O	2.13	0.49
1:A:975:LEU:O	1:A:979:VAL:HG23	2.13	0.49
1:G:974:LYS:CG	1:G:975:LEU:N	2.68	0.49
1:C:782:THR:HG22	1:C:784:ALA:N	2.28	0.49
2:F:281:LEU:HD12	2:F:317:LEU:HD23	1.94	0.49
2:B:327:ILE:HB	2:B:331:GLN:NE2	2.27	0.49
2:F:256:ARG:NH1	2:F:813:PHE:CE1	2.80	0.49
1:G:746:TYR:CE1	2:H:854:VAL:HG11	2.47	0.49
1:A:242:TYR:N	1:A:242:TYR:CD1	2.81	0.49
2:B:662:GLU:HG3	2:B:695:GLN:NE2	2.28	0.49
1:C:374:ARG:NH2	1:C:494:THR:O	2.45	0.49
2:B:382:SER:HA	2:B:439:ARG:O	2.12	0.49
2:D:453:ASP:CG	2:D:455:THR:HG23	2.33	0.49
2:D:946:ARG:HH21	2:D:946:ARG:CG	2.21	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:626:TRP:CE2	2:B:661:PRO:HG3	2.47	0.49
2:D:626:TRP:CE2	2:D:661:PRO:HG3	2.48	0.49
1:A:508:VAL:HG21	1:A:969:LEU:HD11	1.94	0.49
1:E:651:GLU:HG3	1:E:652:ASN:ND2	2.28	0.49
2:D:726:TYR:CE1	2:D:730:SER:HB3	2.48	0.49
1:C:242:TYR:O	1:C:247:GLY:HA3	2.13	0.49
2:H:587:LEU:CD2	2:H:883:GLN:NE2	2.75	0.49
2:H:381:HIS:CB	2:H:383:ARG:HG3	2.40	0.49
1:A:247:GLY:HA2	1:A:254:TYR:HD2	1.77	0.49
1:C:210:VAL:HG12	1:C:304:VAL:HB	1.95	0.49
1:E:242:TYR:CD1	1:E:242:TYR:N	2.81	0.49
2:F:453:ASP:O	2:F:454:LEU:HB2	2.12	0.49
2:H:593:ASN:HA	2:H:684:VAL:O	2.13	0.49
1:G:375:ILE:HD13	1:G:397:VAL:HG11	1.94	0.49
1:C:928:CYS:O	1:C:934:VAL:HA	2.12	0.49
2:D:438:LYS:HG2	2:D:440:THR:O	2.13	0.49
1:C:975:LEU:O	1:C:979:VAL:HG23	2.12	0.49
2:H:665:ASP:OD1	2:H:668:MET:HG2	2.13	0.49
1:E:398:MET:HG3	1:E:490:GLN:NE2	2.28	0.49
1:C:703:ARG:C	1:C:703:ARG:HD2	2.33	0.49
1:A:772:GLY:C	1:A:959:TRP:CZ3	2.86	0.49
1:G:959:TRP:CD1	1:G:959:TRP:N	2.81	0.49
1:E:422:GLU:CG	1:E:564:ARG:HD2	2.41	0.49
2:B:549:ASP:OD2	2:B:552:ARG:HB2	2.12	0.49
1:E:746:TYR:CE1	2:F:854:VAL:CG1	2.96	0.49
1:E:716:MET:O	1:E:924:ALA:HA	2.13	0.49
2:F:798:GLU:O	2:F:801:ALA:HB3	2.13	0.49
1:C:651:GLU:HG3	1:C:652:ASN:ND2	2.27	0.49
2:D:874:LYS:HD2	2:D:917:VAL:HG21	1.95	0.48
1:E:581:LYS:C	1:E:583:ASP:H	2.15	0.48
1:C:947:THR:O	1:C:947:THR:HG23	2.13	0.48
1:C:315:ALA:O	1:C:348:ILE:HD13	2.13	0.48
2:B:786:GLU:OE2	2:B:946:ARG:NH2	2.31	0.48
2:H:281:LEU:CD2	2:H:326:ARG:NH2	2.75	0.48
2:F:322:LEU:O	2:F:324:THR:N	2.42	0.48
2:D:608:MET:SD	2:D:608:MET:C	2.91	0.48
1:G:342:PRO:HG2	1:G:343:TYR:CD1	2.48	0.48
1:A:317:LEU:N	1:A:317:LEU:HD12	2.28	0.48
2:F:740:TYR:CE1	2:F:851:PRO:HB3	2.48	0.48
2:H:779:GLN:HA	2:H:953:VAL:HG21	1.94	0.48
2:D:304:LEU:HD13	2:D:518:LEU:HD12	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:518:LEU:C	2:D:518:LEU:HD23	2.34	0.48
1:G:744:VAL:HG12	1:G:745:ASN:N	2.27	0.48
2:F:421:GLU:O	2:F:425:GLN:HB2	2.13	0.48
2:D:707:ARG:HE	2:D:897:ASN:CG	2.15	0.48
1:E:943:TRP:HA	1:E:946:GLU:HG3	1.94	0.48
2:B:956:LYS:NZ	2:B:956:LYS:CA	2.73	0.48
2:B:781:SER:HA	2:B:818:LEU:O	2.13	0.48
1:C:788:TYR:HB3	1:C:794:ILE:HD11	1.93	0.48
1:E:466:THR:HB	1:E:469:ASP:CG	2.31	0.48
1:E:583:ASP:O	1:E:583:ASP:OD2	2.31	0.48
1:E:360:SER:HB3	1:E:545:THR:HG22	1.94	0.48
2:F:723:GLY:O	2:F:911:GLY:HA3	2.13	0.48
2:F:327:ILE:CA	2:F:331:GLN:NE2	2.76	0.48
1:E:930:ASN:O	1:E:931:GLY:C	2.51	0.48
2:B:690:PHE:HA	2:B:712:LEU:HD22	1.94	0.48
1:C:548:VAL:O	1:C:552:ILE:HG12	2.13	0.48
1:A:864:GLY:CA	2:B:743:VAL:HG22	2.44	0.48
1:A:466:THR:CG2	1:A:468:ASN:H	2.15	0.48
2:F:647:GLN:HE22	2:F:869:THR:CG2	2.27	0.48
1:A:398:MET:HG3	1:A:490:GLN:NE2	2.28	0.48
1:A:822:LEU:C	1:A:822:LEU:CD1	2.81	0.48
1:G:421:PRO:HB3	1:G:456:GLY:O	2.12	0.48
2:D:692:SER:O	2:D:693:LEU:C	2.51	0.48
1:A:964:LYS:H	1:A:964:LYS:CD	2.23	0.48
2:D:288:ILE:HA	2:D:335:MET:CE	2.43	0.48
2:B:499:GLN:HG2	2:B:526:ILE:HD12	1.95	0.48
2:D:378:ALA:HB2	2:D:385:PHE:CE1	2.48	0.48
2:B:648:SER:HA	2:B:865:ARG:HD3	1.94	0.48
1:E:586:GLU:O	1:E:587:LEU:C	2.52	0.48
2:F:321:LEU:O	2:F:325:ASN:O	2.31	0.48
1:A:746:TYR:CE1	2:B:854:VAL:CG1	2.97	0.48
1:G:942:LEU:C	1:G:944:GLU:H	2.16	0.48
1:C:773:TYR:N	1:C:959:TRP:CH2	2.80	0.48
2:F:453:ASP:CG	2:F:455:THR:HG23	2.32	0.48
1:C:292:ALA:O	1:C:296:ILE:HG13	2.14	0.48
1:E:501:TRP:HZ2	1:E:962:TYR:HH	1.59	0.48
1:C:410:GLY:HA2	1:C:452:ILE:HD12	1.94	0.48
1:G:822:LEU:CD1	1:G:822:LEU:C	2.80	0.48
1:A:586:GLU:O	1:A:587:LEU:C	2.50	0.48
1:A:581:LYS:C	1:A:583:ASP:H	2.17	0.48
1:G:360:SER:HB3	1:G:545:THR:HG22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:608:MET:SD	2:B:608:MET:C	2.92	0.48
1:C:631:ASN:OD1	2:D:752:ARG:HG3	2.13	0.48
1:G:772:GLY:HA2	1:G:826:ASN:HD22	1.78	0.48
2:F:658:ARG:HH21	4:F:6:FDP:H62	1.78	0.48
1:E:601:VAL:O	1:E:691:GLY:HA3	2.14	0.48
2:F:418:THR:HA	2:F:421:GLU:CB	2.39	0.48
1:E:319:ARG:NH1	1:E:517:PHE:CE2	2.80	0.48
1:E:942:LEU:C	1:E:944:GLU:H	2.17	0.48
1:C:341:ALA:HB3	1:C:342:PRO:HD3	1.96	0.48
2:B:201:VAL:HA	2:B:296:ILE:O	2.14	0.48
1:A:968:ILE:CD1	1:A:973:LEU:HD12	2.44	0.48
2:D:522:ASN:O	2:D:523:GLU:C	2.52	0.48
2:H:220:ARG:HD2	2:H:252:TRP:CE2	2.48	0.48
1:A:508:VAL:CG2	1:A:969:LEU:HD11	2.44	0.48
2:H:662:GLU:H	2:H:695:GLN:NE2	2.12	0.48
2:B:594:VAL:HB	2:B:689:ALA:HB2	1.95	0.48
1:E:548:VAL:O	1:E:552:ILE:HG12	2.14	0.48
2:B:354:THR:CB	2:B:520:ALA:HB1	2.44	0.48
1:A:410:GLY:HA2	1:A:452:ILE:HD12	1.96	0.48
1:G:740:LEU:HD13	1:G:777:PHE:CE2	2.48	0.48
1:E:250:ARG:HG3	1:E:250:ARG:NH1	2.29	0.48
2:D:701:GLU:CD	2:D:701:GLU:O	2.52	0.48
1:A:804:THR:CG2	1:A:979:VAL:HG21	2.44	0.48
2:B:466:LEU:HD12	2:B:472:LEU:HD11	1.95	0.48
2:F:353:THR:HG21	2:F:534:SER:HA	1.95	0.48
1:A:966:GLY:O	1:A:970:SER:CB	2.62	0.48
1:E:247:GLY:HA2	1:E:254:TYR:HD2	1.78	0.48
2:D:521:VAL:HG13	2:D:526:ILE:HD13	1.95	0.48
1:A:558:ASP:O	1:A:561:ILE:HG22	2.13	0.48
2:F:418:THR:HG21	2:F:422:TRP:HD1	1.78	0.48
1:A:466:THR:CG2	1:A:467:ALA:N	2.77	0.48
1:A:977:ALA:C	1:A:979:VAL:N	2.67	0.48
2:B:467:VAL:O	2:B:471:GLY:CA	2.58	0.48
1:C:947:THR:O	1:C:948:ASN:O	2.32	0.48
2:B:946:ARG:CG	2:B:946:ARG:HH21	2.21	0.48
1:A:253:LYS:C	1:A:255:LEU:N	2.66	0.48
1:G:315:ALA:O	1:G:348:ILE:HD13	2.13	0.48
2:D:354:THR:HB	2:D:520:ALA:HB1	1.95	0.48
2:H:874:LYS:CD	2:H:917:VAL:HG21	2.43	0.48
1:A:289:ARG:NH2	1:A:328:GLU:OE2	2.45	0.48
1:A:212:THR:CG2	1:A:275:GLY:O	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LYS:C	1:C:255:LEU:N	2.66	0.48
2:F:709:PRO:HB2	2:F:879:ILE:HD13	1.96	0.48
2:H:626:TRP:NE1	2:H:661:PRO:HG3	2.29	0.48
1:G:790:PRO:HD2	1:G:791:GLU:OE1	2.14	0.48
1:A:676:ALA:HB2	1:A:712:PHE:CZ	2.49	0.48
1:C:421:PRO:C	1:C:423:ARG:N	2.67	0.47
1:A:805:LEU:HD23	1:A:805:LEU:N	2.29	0.47
2:H:390:MET:HB3	3:H:986:F6P:O3	2.13	0.47
2:H:887:ALA:C	2:H:889:ALA:H	2.17	0.47
2:F:770:THR:OG1	2:F:946:ARG:HD3	2.14	0.47
2:F:522:ASN:HD21	2:F:529:LYS:HE3	1.79	0.47
2:H:522:ASN:HD21	2:H:529:LYS:HE3	1.78	0.47
1:A:755:SER:HB3	1:A:817:ASN:O	2.14	0.47
2:D:518:LEU:O	2:D:518:LEU:HD23	2.14	0.47
2:B:853:HIS:C	2:B:855:GLN:N	2.66	0.47
1:E:690:LEU:HD23	1:E:719:ILE:HB	1.96	0.47
2:F:312:SER:O	2:F:315:PRO:HD2	2.14	0.47
1:C:423:ARG:CD	1:C:561:ILE:HD12	2.44	0.47
1:A:289:ARG:N	1:A:325:LEU:HD13	2.29	0.47
2:H:383:ARG:NH1	2:H:475:ARG:CZ	2.77	0.47
2:F:946:ARG:NH2	2:F:946:ARG:HG3	2.25	0.47
2:H:770:THR:HG23	2:H:946:ARG:HD2	1.96	0.47
2:B:607:SER:OG	2:B:869:THR:CB	2.61	0.47
1:G:242:TYR:N	1:G:242:TYR:CD1	2.81	0.47
2:H:829:ALA:HB3	2:H:850:TYR:CZ	2.49	0.47
2:D:344:VAL:HG22	2:D:357:THR:HG22	1.96	0.47
2:H:830:THR:HA	2:H:848:PRO:HB3	1.97	0.47
2:H:298:CYS:CB	2:H:343:THR:HG22	2.44	0.47
2:D:911:GLY:O	2:D:917:VAL:HA	2.13	0.47
1:C:825:ARG:NH2	1:C:834:SER:HA	2.30	0.47
1:E:216:ASP:OD2	2:F:377:THR:HA	2.14	0.47
2:H:587:LEU:HD23	2:H:679:ASP:HB3	1.96	0.47
1:C:746:TYR:CD1	2:D:854:VAL:CG1	2.97	0.47
1:C:766:VAL:CG1	1:C:774:ILE:HG22	2.44	0.47
2:B:494:ILE:HD13	2:B:771:TYR:HD2	1.79	0.47
1:C:350:GLY:O	1:C:351:LEU:HD23	2.14	0.47
1:E:529:LEU:HA	1:E:529:LEU:HD23	1.70	0.47
1:C:804:THR:O	1:C:805:LEU:C	2.53	0.47
1:C:586:GLU:O	1:C:587:LEU:C	2.51	0.47
1:A:583:ASP:C	1:A:585:SER:H	2.16	0.47
2:F:706:PHE:C	2:F:708:ILE:H	2.17	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201:VAL:HG13	2:F:218:ILE:HG21	1.96	0.47
2:D:717:LEU:C	2:D:717:LEU:HD12	2.34	0.47
1:C:391:ARG:NH1	1:C:482:LYS:HE3	2.30	0.47
2:F:662:GLU:H	2:F:695:GLN:NE2	2.13	0.47
2:F:426:MET:CE	2:F:466:LEU:HD22	2.44	0.47
1:C:755:SER:HB3	1:C:817:ASN:O	2.13	0.47
2:B:684:VAL:HG22	2:B:713:ILE:HB	1.95	0.47
1:G:808:GLU:O	1:G:809:ASN:C	2.53	0.47
2:B:295:LEU:O	2:B:340:ILE:HA	2.14	0.47
2:H:418:THR:HA	2:H:421:GLU:CB	2.40	0.47
1:A:518:THR:CB	1:A:519:PRO:HD2	2.44	0.47
2:B:285:GLN:OE1	2:B:326:ARG:HD2	2.14	0.47
2:D:935:ARG:HH12	4:D:4:FDP:P1	2.38	0.47
1:A:958:HIS:ND1	1:A:959:TRP:HD1	2.12	0.47
1:E:685:ASP:O	1:E:714:ILE:HB	2.14	0.47
1:C:317:LEU:N	1:C:317:LEU:HD12	2.29	0.47
2:D:347:ILE:HB	2:D:363:ALA:CB	2.45	0.47
1:C:696:PHE:HA	1:C:718:LEU:HD22	1.96	0.47
2:F:202:MET:HE3	2:F:295:LEU:HD21	1.97	0.47
1:C:322:TRP:O	1:C:326:VAL:HG23	2.15	0.47
2:H:285:GLN:OE1	2:H:326:ARG:HD2	2.15	0.47
1:A:667:VAL:HG11	1:A:697:ARG:HD3	1.97	0.47
2:B:327:ILE:CA	2:B:331:GLN:NE2	2.78	0.47
2:H:591:ILE:HB	2:H:608:MET:CE	2.44	0.47
2:H:832:LEU:HA	2:H:832:LEU:HD12	1.80	0.47
2:F:718:SER:HB3	2:F:762:GLY:HA2	1.97	0.47
1:E:732:TYR:CE1	1:E:736:VAL:HB	2.50	0.47
1:A:211:MET:HG3	1:A:244:GLY:HA2	1.96	0.47
2:D:481:HIS:O	2:D:482:VAL:C	2.52	0.47
2:H:420:SER:O	2:H:423:GLN:HG2	2.15	0.47
2:B:940:ILE:HD12	2:B:943:GLN:NE2	2.29	0.47
1:A:421:PRO:C	1:A:423:ARG:H	2.16	0.47
2:B:416:PRO:HD2	2:B:550:PHE:CD1	2.49	0.47
2:D:418:THR:OG1	2:D:419:SER:N	2.44	0.47
2:D:418:THR:HG21	2:D:422:TRP:HD1	1.79	0.47
1:A:315:ALA:O	1:A:348:ILE:HD13	2.14	0.47
1:E:622:HIS:HD2	1:E:886:GLU:OE1	1.98	0.47
1:E:586:GLU:CG	1:E:587:LEU:N	2.78	0.47
1:C:328:GLU:O	1:C:332:GLU:CG	2.59	0.47
2:F:431:SER:OG	2:F:470:LEU:HD11	2.14	0.47
2:B:392:ARG:HH21	3:B:980:F6P:C1	2.23	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:327:ILE:HG13	2:D:327:ILE:O	2.14	0.47
1:G:391:ARG:O	1:G:448:ASN:HA	2.15	0.47
1:C:822:LEU:CD1	1:C:822:LEU:C	2.83	0.47
2:H:428:ASP:CG	2:H:432:LYS:NZ	2.67	0.47
2:H:264:THR:HG22	2:H:266:ILE:N	2.27	0.47
1:A:252:GLY:O	1:A:253:LYS:HB3	2.14	0.47
1:G:972:ARG:HG3	1:G:972:ARG:HH11	1.80	0.47
1:G:746:TYR:CE1	2:H:854:VAL:HG13	2.49	0.47
1:C:391:ARG:HG2	1:C:480:ASP:HB3	1.96	0.47
2:H:288:ILE:HA	2:H:335:MET:HE1	1.96	0.47
1:C:581:LYS:C	1:C:583:ASP:H	2.18	0.47
1:A:514:VAL:HG12	1:A:515:LEU:N	2.29	0.47
1:E:746:TYR:CE2	1:E:857:PRO:HG3	2.50	0.47
1:G:433:GLU:O	1:G:437:VAL:HG23	2.14	0.47
2:H:740:TYR:CE1	2:H:851:PRO:HB3	2.50	0.47
1:A:674:THR:O	1:A:677:TYR:HB3	2.15	0.47
2:B:475:ARG:HG2	2:B:475:ARG:HH11	1.80	0.47
2:F:657:ASN:OD1	2:F:659:VAL:HG23	2.15	0.47
1:A:548:VAL:O	1:A:552:ILE:HG12	2.15	0.47
1:E:439:GLN:OE1	1:E:439:GLN:HA	2.15	0.47
2:F:365:ASP:HA	2:F:862:PRO:HG2	1.97	0.47
1:A:336:THR:HG23	1:A:339:GLU:OE1	2.15	0.47
1:C:212:THR:CG2	1:C:274:ILE:HG13	2.44	0.47
2:H:647:GLN:HE22	2:H:869:THR:HG22	1.79	0.47
2:D:324:THR:O	2:D:325:ASN:HB2	2.15	0.47
2:F:327:ILE:HB	2:F:331:GLN:NE2	2.30	0.47
1:A:758:ARG:NH1	2:B:655:GLY:HA3	2.30	0.47
2:H:344:VAL:HG22	2:H:357:THR:HG22	1.97	0.47
2:F:593:ASN:HA	2:F:684:VAL:O	2.14	0.47
1:G:812:HIS:N	1:G:812:HIS:CD2	2.82	0.47
2:F:770:THR:OG1	2:F:946:ARG:CD	2.63	0.47
2:B:946:ARG:HG3	2:B:946:ARG:NH2	2.26	0.47
2:B:827:LEU:HD21	1:C:837:LEU:HD11	1.96	0.47
2:F:680:GLY:HA3	2:F:879:ILE:HD12	1.97	0.47
2:F:518:LEU:HD23	2:F:518:LEU:O	2.15	0.47
1:C:416:ASP:OD2	1:C:449:ASN:HA	2.15	0.47
2:F:416:PRO:HG2	2:F:550:PHE:CZ	2.50	0.47
1:G:949:VAL:O	1:G:950:GLU:C	2.52	0.47
2:H:946:ARG:CG	2:H:946:ARG:HH21	2.21	0.47
1:E:398:MET:HB3	3:E:988:F6P:O3	2.15	0.47
2:F:631:ARG:O	2:F:632:HIS:ND1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:ALA:O	1:G:348:ILE:CD1	2.63	0.47
2:D:662:GLU:H	2:D:695:GLN:NE2	2.13	0.47
2:B:706:PHE:C	2:B:708:ILE:H	2.18	0.47
2:D:522:ASN:ND2	2:D:529:LYS:HE3	2.30	0.47
2:D:453:ASP:OD2	2:D:455:THR:HG23	2.15	0.47
2:D:304:LEU:O	2:D:307:ALA:HB3	2.14	0.47
2:H:867:ARG:O	2:H:871:MET:HG2	2.15	0.47
2:D:421:GLU:O	2:D:425:GLN:HB2	2.15	0.47
1:A:418:ILE:HG12	1:A:575:PHE:CE2	2.49	0.47
1:E:821:LYS:NZ	1:E:821:LYS:HB2	2.17	0.46
1:C:697:ARG:O	1:C:701:GLN:HG3	2.15	0.46
1:A:588:LEU:O	1:A:589:PRO:O	2.32	0.46
1:G:773:TYR:HA	1:G:959:TRP:CE3	2.50	0.46
2:D:690:PHE:HA	2:D:712:LEU:HD22	1.97	0.46
1:E:803:ILE:HD13	1:E:845:ALA:CB	2.45	0.46
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.72	0.46
1:G:630:MET:SD	1:G:643:LYS:HD3	2.55	0.46
2:H:623:TYR:HB2	2:H:634:SER:HB2	1.97	0.46
2:D:416:PRO:HB2	2:D:452:ALA:HA	1.98	0.46
2:D:701:GLU:HB2	2:D:897:ASN:ND2	2.30	0.46
1:C:216:ASP:HA	1:C:220:MET:SD	2.56	0.46
2:F:935:ARG:O	2:F:936:MET:HB3	2.15	0.46
1:A:952:ARG:HH11	1:A:952:ARG:HG3	1.81	0.46
2:F:825:LYS:N	1:G:844:GLU:OE2	2.48	0.46
2:F:632:HIS:O	2:F:633:GLU:C	2.54	0.46
1:A:773:TYR:N	1:A:959:TRP:CH2	2.83	0.46
1:E:754:ALA:HB2	1:E:762:PHE:CE1	2.50	0.46
1:E:676:ALA:HB2	1:E:712:PHE:CZ	2.50	0.46
1:C:514:VAL:O	1:C:517:PHE:HB2	2.15	0.46
2:D:417:ALA:O	2:D:418:THR:HB	2.14	0.46
2:D:420:SER:O	2:D:423:GLN:HG2	2.16	0.46
1:E:586:GLU:CD	1:E:587:LEU:H	2.17	0.46
2:D:711:VAL:CG2	2:D:910:VAL:HG22	2.44	0.46
2:H:587:LEU:HD21	2:H:883:GLN:HG3	1.98	0.46
1:A:951:LEU:H	1:A:951:LEU:HD23	1.80	0.46
1:G:650:VAL:HG23	1:G:653:TRP:CE3	2.49	0.46
2:B:889:ALA:C	2:B:891:ALA:N	2.64	0.46
2:H:341:CYS:HB2	2:H:507:VAL:CG1	2.45	0.46
2:H:293:ASP:HB3	2:H:335:MET:HE3	1.97	0.46
1:E:596:ILE:CD1	1:E:885:ILE:HG21	2.46	0.46
2:D:560:GLU:OE1	2:D:870:ARG:NH1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:347:ILE:HB	2:H:363:ALA:CB	2.45	0.46
1:C:640:GLY:HA3	1:C:678:TYR:CE2	2.50	0.46
1:C:486:LEU:O	1:C:489:VAL:HG22	2.15	0.46
1:A:832:VAL:HG12	1:A:833:TYR:N	2.30	0.46
2:B:587:LEU:N	2:B:617:HIS:HD1	2.09	0.46
2:F:432:LYS:HE2	2:F:577:ASN:ND2	2.30	0.46
1:E:212:THR:CG2	1:E:212:THR:O	2.62	0.46
1:G:216:ASP:H	2:H:381:HIS:CE1	2.33	0.46
2:H:325:ASN:C	2:H:327:ILE:H	2.17	0.46
2:D:400:LEU:CD1	2:D:866:THR:HG21	2.45	0.46
2:F:244:PRO:O	2:F:245:GLU:CB	2.60	0.46
1:A:294:ASN:O	1:A:297:SER:HB3	2.14	0.46
1:E:976:ARG:O	1:E:979:VAL:N	2.47	0.46
1:E:856:ILE:O	1:E:857:PRO:C	2.53	0.46
2:B:623:TYR:HB2	2:B:634:SER:HB2	1.98	0.46
1:C:716:MET:O	1:C:924:ALA:HA	2.15	0.46
2:B:420:SER:C	2:B:423:GLN:HE21	2.19	0.46
1:G:584:GLY:O	1:G:588:LEU:HB2	2.16	0.46
1:G:585:SER:O	1:G:586:GLU:O	2.32	0.46
2:F:523:GLU:O	2:F:524:ASN:C	2.53	0.46
1:C:703:ARG:O	1:C:703:ARG:HD2	2.15	0.46
2:D:740:TYR:CE1	2:D:851:PRO:HB3	2.50	0.46
2:H:662:GLU:HG3	2:H:695:GLN:NE2	2.31	0.46
1:G:766:VAL:HG11	1:G:774:ILE:HG22	1.98	0.46
1:E:611:ALA:HB2	1:E:874:ALA:HB1	1.96	0.46
2:B:420:SER:O	2:B:423:GLN:HG2	2.16	0.46
2:B:740:TYR:CD1	2:B:851:PRO:HB3	2.51	0.46
2:B:591:ILE:HD13	2:B:682:ILE:O	2.16	0.46
1:E:323:PRO:O	1:E:326:VAL:HB	2.16	0.46
2:B:876:VAL:HG12	2:B:880:LYS:HE3	1.97	0.46
2:F:679:ASP:O	2:F:708:ILE:HB	2.15	0.46
2:B:583:LYS:O	2:B:585:LYS:HB2	2.15	0.46
2:F:626:TRP:CE2	2:F:661:PRO:HG3	2.50	0.46
1:A:864:GLY:HA3	2:B:743:VAL:HG22	1.96	0.46
1:C:526:ILE:HD13	1:C:535:ARG:HG2	1.98	0.46
2:H:581:LEU:HB2	2:H:615:GLN:NE2	2.31	0.46
2:F:577:ASN:CA	2:F:579:PRO:HD2	2.46	0.46
2:B:911:GLY:O	2:B:917:VAL:HA	2.16	0.46
2:D:704:PRO:CA	2:D:707:ARG:NH1	2.79	0.46
2:H:717:LEU:HG	4:H:8:FDP:O3	2.16	0.46
2:D:552:ARG:O	2:D:552:ARG:HD3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLN:HG2	1:A:526:ILE:HG22	1.98	0.46
1:G:547:SER:O	1:G:550:THR:HB	2.15	0.46
1:G:759:ARG:HA	1:G:810:PHE:CE2	2.50	0.46
1:E:853:ARG:HG2	1:E:853:ARG:HH11	1.80	0.46
2:F:416:PRO:HD2	2:F:550:PHE:CD1	2.50	0.46
1:A:289:ARG:CA	1:A:325:LEU:HD13	2.46	0.46
2:D:706:PHE:C	2:D:708:ILE:H	2.19	0.46
1:A:589:PRO:O	1:A:590:VAL:O	2.34	0.46
1:E:613:ARG:HA	1:E:650:VAL:CG2	2.46	0.46
1:A:650:VAL:HG13	1:A:650:VAL:O	2.16	0.46
2:B:704:PRO:CA	2:B:707:ARG:NH1	2.79	0.46
2:F:314:TRP:HB3	2:F:315:PRO:HD3	1.98	0.46
1:C:514:VAL:HG12	1:C:515:LEU:N	2.31	0.46
1:G:601:VAL:O	1:G:691:GLY:HA3	2.16	0.46
1:G:230:THR:OG1	1:G:508:VAL:HG22	2.16	0.46
2:F:547:ALA:O	2:F:549:ASP:N	2.49	0.46
1:C:883:LYS:O	1:C:887:GLN:HG3	2.16	0.46
1:E:331:ALA:O	1:E:333:GLY:N	2.49	0.46
1:G:960:ALA:C	1:G:962:TYR:N	2.66	0.46
1:A:765:GLU:HA	1:A:825:ARG:O	2.16	0.46
2:H:256:ARG:CZ	2:H:813:PHE:CE1	2.98	0.46
2:F:947:LEU:HD22	2:F:951:HIS:NE2	2.30	0.46
1:G:366:ILE:HD13	1:G:503:ALA:CB	2.46	0.46
2:H:755:ALA:HA	2:H:815:LYS:O	2.15	0.46
1:A:717:CYS:HA	1:A:925:ALA:O	2.16	0.46
2:B:200:ALA:HA	2:B:230:PHE:O	2.15	0.46
1:C:207:LYS:HB3	1:C:300:ILE:HG12	1.98	0.45
2:F:832:LEU:HA	2:F:832:LEU:HD12	1.78	0.45
2:H:892:ALA:C	2:H:894:GLU:N	2.70	0.45
2:B:341:CYS:SG	2:B:519:ILE:CD1	3.04	0.45
2:H:288:ILE:HG12	2:H:335:MET:HE2	1.98	0.45
1:A:655:ASN:O	1:A:865:VAL:HG22	2.16	0.45
1:E:773:TYR:HA	1:E:959:TRP:CD2	2.50	0.45
1:A:526:ILE:HD13	1:A:535:ARG:HG2	1.98	0.45
2:F:420:SER:HA	2:F:423:GLN:NE2	2.30	0.45
2:H:200:ALA:HB2	2:H:230:PHE:HB2	1.98	0.45
2:H:796:ASP:O	2:H:800:LEU:HB2	2.15	0.45
1:A:525:LEU:C	1:A:525:LEU:HD23	2.36	0.45
2:B:420:SER:CA	2:B:423:GLN:NE2	2.80	0.45
2:H:581:LEU:CB	2:H:582:PRO:HD3	2.42	0.45
2:B:615:GLN:HB2	2:B:617:HIS:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:THR:CG2	1:C:467:ALA:N	2.79	0.45
2:B:701:GLU:OE2	2:B:701:GLU:O	2.34	0.45
2:F:607:SER:OG	2:F:869:THR:CB	2.52	0.45
1:E:315:ALA:O	1:E:348:ILE:CD1	2.64	0.45
2:B:414:GLU:N	2:B:414:GLU:OE2	2.45	0.45
1:E:488:HIS:C	1:E:490:GLN:N	2.67	0.45
2:D:547:ALA:O	2:D:549:ASP:N	2.49	0.45
2:H:420:SER:HA	2:H:423:GLN:NE2	2.30	0.45
1:E:710:PRO:HA	1:E:713:ASN:ND2	2.31	0.45
1:E:696:PHE:HA	1:E:718:LEU:HD22	1.98	0.45
2:D:511:THR:OG1	2:D:514:THR:HG23	2.15	0.45
1:C:732:TYR:CE1	1:C:736:VAL:HB	2.51	0.45
1:C:519:PRO:HG2	1:C:520:GLU:H	1.79	0.45
1:C:809:ASN:N	1:C:975:LEU:HD22	2.31	0.45
1:A:356:ASP:OD2	3:A:988:F6P:C1	2.56	0.45
2:H:348:ASP:CG	3:H:986:F6P:H11	2.36	0.45
2:H:883:GLN:O	2:H:887:ALA:CB	2.64	0.45
2:D:587:LEU:N	2:D:617:HIS:HD1	2.07	0.45
1:C:952:ARG:HH11	1:C:952:ARG:HG3	1.78	0.45
1:E:613:ARG:NH1	1:E:613:ARG:HG2	2.30	0.45
2:H:414:GLU:HB3	2:H:554:MET:HE2	1.98	0.45
1:A:613:ARG:NH1	1:A:613:ARG:HG2	2.31	0.45
1:A:255:LEU:C	1:A:255:LEU:HD23	2.36	0.45
1:A:291:ALA:O	1:A:292:ALA:C	2.54	0.45
1:G:746:TYR:CE2	1:G:857:PRO:HG3	2.51	0.45
1:C:496:VAL:O	1:C:500:ARG:HG3	2.16	0.45
1:A:486:LEU:O	1:A:489:VAL:HG22	2.16	0.45
2:B:298:CYS:SG	2:B:343:THR:CG2	3.04	0.45
2:D:693:LEU:CD2	2:D:922:ILE:HB	2.46	0.45
2:H:633:GLU:O	2:H:633:GLU:HG2	2.16	0.45
2:F:717:LEU:HB2	2:F:733:ALA:CB	2.45	0.45
2:B:354:THR:HB	2:B:520:ALA:HB1	1.98	0.45
1:C:759:ARG:HD2	1:C:849:LYS:O	2.17	0.45
1:E:922:ASP:HA	1:E:938:PRO:HG3	1.97	0.45
1:A:747:THR:O	1:A:751:LYS:HB2	2.17	0.45
2:B:424:ASP:OD1	2:B:469:ARG:NH2	2.49	0.45
2:D:382:SER:HA	2:D:439:ARG:O	2.17	0.45
2:B:418:THR:O	2:B:419:SER:HB2	2.17	0.45
2:B:418:THR:OG1	2:B:419:SER:N	2.49	0.45
1:C:809:ASN:HB2	1:C:975:LEU:HD21	1.99	0.45
1:G:466:THR:HB	1:G:469:ASP:CG	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:THR:O	1:A:805:LEU:C	2.55	0.45
1:E:796:LEU:HD21	2:H:835:VAL:HG11	1.98	0.45
1:A:813:ASP:O	1:A:815:GLY:N	2.46	0.45
2:B:770:THR:HG23	2:B:946:ARG:HD2	1.97	0.45
2:F:264:THR:HG22	2:F:266:ILE:N	2.29	0.45
2:H:323:LYS:O	2:H:324:THR:CB	2.63	0.45
2:F:633:GLU:HB2	2:F:672:TYR:OH	2.16	0.45
2:H:522:ASN:ND2	2:H:529:LYS:HE3	2.32	0.45
2:B:220:ARG:HD2	2:B:252:TRP:CZ2	2.51	0.45
2:F:684:VAL:HG22	2:F:713:ILE:HB	1.99	0.45
2:B:523:GLU:O	2:B:524:ASN:C	2.55	0.45
2:D:781:SER:HA	2:D:818:LEU:O	2.16	0.45
2:H:698:ARG:HD2	2:H:698:ARG:O	2.16	0.45
2:F:484:ARG:NH1	2:F:484:ARG:HG3	2.31	0.45
2:D:578:GLU:C	2:D:580:LYS:N	2.69	0.45
1:A:322:TRP:CZ3	1:A:343:TYR:O	2.70	0.45
1:E:832:VAL:CG2	2:H:834:GLU:HB3	2.45	0.45
1:C:856:ILE:O	1:C:857:PRO:C	2.53	0.45
1:E:289:ARG:CA	1:E:325:LEU:HD13	2.46	0.45
1:G:221:ASN:ND2	1:G:270:GLY:O	2.49	0.45
1:A:716:MET:O	1:A:924:ALA:HA	2.17	0.45
2:H:518:LEU:C	2:H:518:LEU:HD23	2.36	0.45
1:A:451:ILE:HD12	1:A:451:ILE:N	2.32	0.45
2:B:416:PRO:O	2:B:417:ALA:C	2.54	0.45
2:H:761:GLN:HG3	2:H:855:GLN:NE2	2.30	0.45
1:C:334:ARG:HG3	1:C:335:PHE:CE1	2.51	0.45
1:E:832:VAL:HG12	1:E:833:TYR:N	2.32	0.45
1:A:766:VAL:CG1	1:A:774:ILE:HG22	2.47	0.45
2:H:499:GLN:HG2	2:H:526:ILE:HD12	1.99	0.45
1:E:439:GLN:NE2	1:E:477:LEU:HD11	2.32	0.45
2:F:484:ARG:HH11	2:F:484:ARG:HG3	1.82	0.45
1:G:209:ALA:O	1:G:303:LEU:HD12	2.16	0.45
2:B:347:ILE:HB	2:B:363:ALA:HB2	1.98	0.45
1:G:435:LYS:HD3	1:G:477:LEU:HB2	1.99	0.45
2:B:422:TRP:CZ3	2:B:465:VAL:HG21	2.51	0.45
1:G:586:GLU:CD	1:G:587:LEU:H	2.20	0.45
2:D:900:ASP:O	2:D:901:LYS:C	2.56	0.45
2:D:946:ARG:HG3	2:D:946:ARG:NH2	2.27	0.45
2:F:900:ASP:O	2:F:901:LYS:C	2.54	0.45
1:E:505:LEU:HB2	1:E:533:ILE:HD11	1.97	0.45
2:H:281:LEU:HD12	2:H:317:LEU:HD22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:ARG:NH1	1:C:400:ARG:HG2	2.30	0.45
2:D:426:MET:CE	2:D:466:LEU:HD22	2.46	0.45
2:F:931:GLU:HG3	2:F:931:GLU:O	2.16	0.45
2:H:462:VAL:O	2:H:466:LEU:HD23	2.17	0.45
2:F:771:TYR:OH	2:F:945:THR:HG21	2.17	0.45
2:B:662:GLU:H	2:B:695:GLN:NE2	2.14	0.45
1:C:584:GLY:O	1:C:585:SER:O	2.35	0.45
2:H:684:VAL:HG22	2:H:713:ILE:HB	1.98	0.45
2:F:354:THR:CB	2:F:520:ALA:HB1	2.47	0.45
2:F:791:GLU:HG3	1:G:800:ARG:NH2	2.31	0.45
1:E:236:CYS:SG	1:E:515:LEU:HD21	2.57	0.45
1:E:440:ARG:HH11	1:E:440:ARG:HB2	1.81	0.45
1:E:448:ASN:H	1:E:448:ASN:ND2	2.15	0.45
1:A:589:PRO:HD2	1:A:622:HIS:HB3	1.99	0.45
2:D:900:ASP:O	2:D:903:ILE:HG13	2.17	0.45
1:G:249:LEU:HD13	1:G:290:GLN:HG2	1.98	0.45
2:B:463:HIS:CD2	2:B:474:THR:HG22	2.49	0.45
2:B:518:LEU:HD23	2:B:518:LEU:O	2.16	0.45
2:H:755:ALA:O	2:H:846:ALA:HA	2.16	0.45
1:C:211:MET:CE	1:C:305:VAL:HG22	2.47	0.45
2:H:511:THR:OG1	2:H:514:THR:HG23	2.16	0.45
2:B:609:ALA:O	2:B:612:CYS:HB2	2.16	0.45
2:F:744:VAL:O	2:F:747:SER:HB3	2.17	0.45
1:A:557:PHE:O	1:A:560:ALA:HB3	2.17	0.45
1:A:761:VAL:HA	1:A:821:LYS:O	2.16	0.45
1:G:927:ILE:O	1:G:927:ILE:HG23	2.17	0.45
2:H:578:GLU:C	2:H:580:LYS:N	2.67	0.45
1:G:323:PRO:O	1:G:326:VAL:HB	2.17	0.45
2:D:892:ALA:CB	2:D:894:GLU:HG2	2.43	0.45
2:F:887:ALA:C	2:F:889:ALA:H	2.21	0.45
1:A:942:LEU:C	1:A:944:GLU:H	2.19	0.45
1:E:255:LEU:HD23	1:E:256:LYS:N	2.32	0.45
2:D:312:SER:O	2:D:315:PRO:HD2	2.17	0.45
1:C:248:LEU:HG	1:C:291:ALA:HB1	1.98	0.45
2:B:717:LEU:HB2	2:B:733:ALA:HB2	1.98	0.45
1:A:407:LEU:HD11	1:A:572:TYR:HA	1.97	0.45
1:C:485:ILE:N	1:C:485:ILE:HD12	2.32	0.45
2:B:590:ALA:HA	2:B:620:TYR:O	2.17	0.45
2:F:595:GLY:O	2:F:656:THR:OG1	2.30	0.45
2:H:679:ASP:HB3	2:H:883:GLN:HE22	1.81	0.44
2:H:831:LYS:HA	2:H:831:LYS:HD3	1.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:ALA:O	1:A:961:GLU:C	2.56	0.44
1:G:960:ALA:O	1:G:962:TYR:N	2.50	0.44
1:G:514:VAL:HG12	1:G:515:LEU:N	2.33	0.44
2:H:726:TYR:CE1	2:H:730:SER:HB3	2.52	0.44
1:C:451:ILE:N	1:C:451:ILE:HD12	2.32	0.44
1:A:215:GLY:HA2	2:B:381:HIS:HE2	1.82	0.44
1:E:796:LEU:CD1	2:H:793:LEU:HD13	2.43	0.44
1:C:385:THR:HA	2:D:207:ASP:OD2	2.17	0.44
1:E:230:THR:OG1	1:E:508:VAL:HG22	2.16	0.44
2:F:830:THR:HA	2:F:848:PRO:HB3	1.99	0.44
1:G:585:SER:O	1:G:586:GLU:C	2.53	0.44
2:F:711:VAL:CG2	2:F:910:VAL:HG22	2.47	0.44
1:G:963:ASN:N	1:G:963:ASN:HD22	2.12	0.44
1:G:421:PRO:C	1:G:423:ARG:N	2.71	0.44
1:C:594:LEU:CD2	1:C:889:ASN:ND2	2.78	0.44
1:G:249:LEU:HD12	1:G:249:LEU:C	2.37	0.44
2:D:717:LEU:HB2	2:D:733:ALA:HB2	1.98	0.44
1:A:442:ARG:NH1	1:A:449:ASN:OD1	2.39	0.44
1:G:960:ALA:C	1:G:962:TYR:H	2.20	0.44
2:D:196:GLN:CD	2:D:228:ARG:HG2	2.36	0.44
1:A:264:ARG:HD2	1:A:819:ASN:HD22	1.81	0.44
2:B:537:LEU:O	2:B:540:ALA:HB3	2.18	0.44
1:G:780:LEU:C	1:G:780:LEU:HD13	2.37	0.44
1:E:697:ARG:O	1:E:701:GLN:HG3	2.18	0.44
1:G:947:THR:O	1:G:950:GLU:N	2.50	0.44
1:G:421:PRO:HG2	1:G:422:GLU:OE2	2.17	0.44
1:E:650:VAL:O	1:E:650:VAL:HG13	2.16	0.44
2:D:327:ILE:HB	2:D:331:GLN:HE21	1.83	0.44
1:A:794:ILE:HG22	1:A:794:ILE:O	2.17	0.44
1:E:255:LEU:C	1:E:255:LEU:HD23	2.37	0.44
2:B:239:LEU:HD22	2:B:287:LEU:HD22	1.99	0.44
2:F:697:GLU:HA	2:F:700:ARG:HD3	1.99	0.44
2:D:918:VAL:HG12	2:D:919:TYR:H	1.83	0.44
1:G:946:GLU:O	1:G:955:PHE:CZ	2.71	0.44
2:H:348:ASP:OD1	2:H:391:GLY:HA2	2.17	0.44
2:B:886:ILE:O	2:B:890:ARG:CB	2.59	0.44
2:F:522:ASN:ND2	2:F:529:LYS:HE3	2.32	0.44
2:D:589:ILE:CD1	2:D:879:ILE:HG21	2.46	0.44
1:A:746:TYR:CD1	2:B:854:VAL:CG1	3.00	0.44
1:A:746:TYR:CE1	2:B:854:VAL:HG13	2.52	0.44
1:C:746:TYR:CE2	1:C:857:PRO:HG3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:ILE:HB	2:B:608:MET:CE	2.46	0.44
1:E:416:ASP:OD2	1:E:449:ASN:HA	2.16	0.44
1:C:554:ASN:O	1:C:556:ASP:N	2.50	0.44
2:B:867:ARG:O	2:B:871:MET:HG2	2.17	0.44
1:E:739:CYS:SG	1:E:861:GLN:HB3	2.57	0.44
2:D:648:SER:HA	2:D:865:ARG:HD3	1.98	0.44
2:F:690:PHE:HA	2:F:712:LEU:HD22	1.99	0.44
1:E:301:ASP:OD1	1:E:301:ASP:N	2.51	0.44
1:C:423:ARG:O	1:C:424:ALA:C	2.56	0.44
1:A:423:ARG:O	1:A:424:ALA:C	2.56	0.44
2:F:578:GLU:C	2:F:580:LYS:N	2.70	0.44
2:B:481:HIS:C	2:B:483:GLN:N	2.68	0.44
1:E:210:VAL:HG23	1:E:210:VAL:O	2.17	0.44
2:H:608:MET:C	2:H:608:MET:SD	2.95	0.44
2:F:591:ILE:HB	2:F:608:MET:CE	2.48	0.44
1:C:291:ALA:HA	1:C:294:ASN:ND2	2.33	0.44
2:D:541:VAL:HG22	2:D:556:LEU:HB2	1.99	0.44
2:H:453:ASP:OD2	2:H:455:THR:HG23	2.18	0.44
1:G:809:ASN:C	1:G:809:ASN:OD1	2.55	0.44
1:C:418:ILE:HG12	1:C:575:PHE:CE2	2.53	0.44
2:H:574:ALA:CB	2:H:610:THR:HB	2.47	0.44
2:F:755:ALA:HA	2:F:815:LYS:O	2.16	0.44
2:B:416:PRO:HG2	2:B:550:PHE:CZ	2.53	0.44
2:B:935:ARG:O	2:B:936:MET:HB3	2.18	0.44
1:A:589:PRO:O	1:A:593:ARG:NH1	2.50	0.44
2:F:883:GLN:O	2:F:887:ALA:CB	2.66	0.44
1:G:255:LEU:HD23	1:G:255:LEU:C	2.38	0.44
2:F:354:THR:HB	2:F:520:ALA:HB1	2.00	0.44
1:C:572:TYR:CE2	1:C:576:LEU:HD11	2.53	0.44
1:C:690:LEU:HD23	1:C:719:ILE:HB	2.00	0.44
2:H:771:TYR:OH	2:H:945:THR:HG21	2.17	0.44
1:C:927:ILE:O	1:C:927:ILE:HG23	2.18	0.44
1:E:578:THR:HG23	1:E:578:THR:O	2.16	0.44
2:D:501:LEU:HD12	2:D:501:LEU:O	2.18	0.44
1:E:785:VAL:O	1:E:785:VAL:CG2	2.65	0.44
1:A:767:GLN:HB3	4:A:1:FDP:O1	2.18	0.44
1:G:212:THR:CG2	1:G:212:THR:O	2.63	0.44
2:F:554:MET:CG	2:F:562:ILE:HG12	2.39	0.44
2:H:717:LEU:HD23	2:H:856:GLN:HG2	1.99	0.44
1:C:249:LEU:C	1:C:249:LEU:HD12	2.37	0.44
2:H:327:ILE:HB	2:H:331:GLN:NE2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:692:SER:O	2:B:693:LEU:C	2.56	0.44
1:E:485:ILE:CD1	1:E:485:ILE:N	2.80	0.44
2:F:349:ASN:OD1	2:F:356:ALA:HA	2.17	0.44
1:C:596:ILE:CD1	1:C:885:ILE:HG21	2.48	0.44
2:H:349:ASN:OD1	2:H:356:ALA:HA	2.17	0.44
2:B:344:VAL:HG22	2:B:357:THR:HG22	1.99	0.44
2:D:389:VAL:O	2:D:447:GLU:HB3	2.18	0.44
1:C:547:SER:O	1:C:550:THR:HB	2.18	0.44
2:H:414:GLU:N	2:H:414:GLU:OE2	2.51	0.44
2:F:740:TYR:CD1	2:F:851:PRO:HB3	2.52	0.44
1:C:823:LEU:HD12	1:C:823:LEU:N	2.33	0.44
1:G:366:ILE:HD13	1:G:503:ALA:HB2	1.99	0.44
2:F:238:GLY:O	2:F:241:ARG:O	2.35	0.44
1:C:405:LEU:HD12	1:C:405:LEU:HA	1.88	0.44
2:B:561:PHE:CD2	2:B:561:PHE:C	2.91	0.44
1:A:423:ARG:CD	1:A:561:ILE:HD12	2.48	0.43
2:H:416:PRO:HB2	2:H:452:ALA:HA	2.00	0.43
2:B:900:ASP:CG	2:B:903:ILE:HG13	2.38	0.43
2:B:298:CYS:CB	2:B:343:THR:HG22	2.48	0.43
1:C:587:LEU:CB	1:C:622:HIS:CE1	2.99	0.43
2:D:892:ALA:HB3	2:D:894:GLU:CG	2.46	0.43
1:E:837:LEU:HD13	2:H:831:LYS:HG3	1.98	0.43
1:G:685:ASP:O	1:G:715:PRO:HD2	2.17	0.43
1:A:247:GLY:HA2	1:A:254:TYR:CD2	2.53	0.43
1:E:339:GLU:C	1:E:341:ALA:H	2.21	0.43
1:G:679:PHE:HE2	1:G:687:LEU:HD22	1.82	0.43
1:E:374:ARG:HG2	1:E:489:VAL:O	2.17	0.43
1:C:211:MET:HE3	1:C:305:VAL:HG22	2.00	0.43
1:C:724:SER:OG	4:C:3:FDP:H12	2.18	0.43
1:G:426:PRO:O	1:G:428:GLY:N	2.51	0.43
2:B:711:VAL:HG22	2:B:910:VAL:CG2	2.48	0.43
2:H:701:GLU:O	2:H:701:GLU:OE2	2.36	0.43
1:E:947:THR:HG22	1:E:953:LYS:O	2.18	0.43
1:E:800:ARG:HH22	2:H:791:GLU:HG3	1.81	0.43
1:C:330:VAL:HG22	1:C:340:VAL:HG11	1.99	0.43
2:H:946:ARG:CG	2:H:946:ARG:NH2	2.80	0.43
2:H:704:PRO:CA	2:H:707:ARG:NH1	2.81	0.43
1:G:398:MET:HG3	1:G:490:GLN:NE2	2.34	0.43
1:C:382:ILE:O	1:C:385:THR:HG22	2.17	0.43
2:F:608:MET:C	2:F:608:MET:SD	2.97	0.43
2:H:239:LEU:O	2:H:286:HIS:CD2	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:494:ILE:HD13	2:D:771:TYR:HD2	1.83	0.43
4:F:6:FDP:O2P	4:F:6:FDP:O5	2.35	0.43
1:C:961:GLU:O	1:C:962:TYR:C	2.57	0.43
2:B:567:ASN:O	2:B:571:ILE:HG12	2.17	0.43
2:B:438:LYS:HG2	2:B:440:THR:O	2.17	0.43
2:F:692:SER:O	2:F:693:LEU:C	2.56	0.43
1:G:591:SER:HA	1:G:593:ARG:HG3	2.00	0.43
2:F:580:LYS:O	2:F:581:LEU:C	2.55	0.43
1:C:315:ALA:O	1:C:348:ILE:CD1	2.67	0.43
2:H:313:GLU:O	2:H:317:LEU:HG	2.18	0.43
2:H:327:ILE:CA	2:H:331:GLN:NE2	2.81	0.43
2:H:428:ASP:OD2	2:H:432:LYS:NZ	2.51	0.43
1:G:246:GLU:HA	1:G:279:SER:HB2	2.00	0.43
2:F:894:GLU:O	2:F:896:PHE:N	2.50	0.43
2:F:661:PRO:HD2	2:F:695:GLN:NE2	2.33	0.43
1:C:757:THR:HG23	2:D:597:PRO:HD3	2.01	0.43
1:C:680:GLN:HB3	1:G:680:GLN:HE22	1.82	0.43
1:G:806:LEU:O	1:G:807:LYS:C	2.56	0.43
1:G:813:ASP:O	1:G:815:GLY:N	2.46	0.43
1:G:665:ARG:HG2	1:G:665:ARG:HH11	1.83	0.43
1:C:421:PRO:HG2	1:C:422:GLU:OE2	2.19	0.43
2:H:723:GLY:O	2:H:911:GLY:HA3	2.18	0.43
2:D:418:THR:HG23	2:D:451:ALA:HB1	2.00	0.43
2:D:418:THR:O	2:D:419:SER:HB2	2.19	0.43
2:B:587:LEU:CD2	2:B:883:GLN:NE2	2.81	0.43
1:E:589:PRO:O	1:E:590:VAL:O	2.35	0.43
1:A:979:VAL:O	1:A:980:ALA:HB2	2.18	0.43
1:E:703:ARG:HD2	1:E:703:ARG:O	2.18	0.43
2:H:467:VAL:O	2:H:471:GLY:CA	2.61	0.43
1:G:448:ASN:ND2	1:G:448:ASN:N	2.61	0.43
1:E:246:GLU:O	1:E:249:LEU:HB3	2.18	0.43
1:A:944:GLU:HA	1:A:946:GLU:OE1	2.18	0.43
2:F:201:VAL:CG1	2:F:218:ILE:HG21	2.48	0.43
2:B:740:TYR:CZ	2:B:851:PRO:HB3	2.53	0.43
1:A:731:GLU:HG2	1:A:958:HIS:CD2	2.53	0.43
2:D:201:VAL:HA	2:D:296:ILE:O	2.18	0.43
1:E:421:PRO:C	1:E:423:ARG:H	2.20	0.43
2:H:693:LEU:CD2	2:H:922:ILE:HB	2.49	0.43
2:F:792:GLN:HE22	2:F:957:ARG:CB	2.31	0.43
1:G:271:GLY:HA3	2:H:380:SER:OG	2.19	0.43
2:F:239:LEU:HA	2:F:239:LEU:HD23	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ALA:O	1:A:866:PRO:HB3	2.19	0.43
1:G:407:LEU:HD11	1:G:572:TYR:HA	2.00	0.43
2:H:344:VAL:CG2	2:H:357:THR:HG22	2.49	0.43
2:B:763:GLY:O	2:B:822:ASN:HB2	2.19	0.43
1:E:433:GLU:O	1:E:437:VAL:HG23	2.18	0.43
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.83	0.43
2:H:421:GLU:O	2:H:425:GLN:HB2	2.18	0.43
1:C:801:GLU:OE1	1:C:976:ARG:CZ	2.67	0.43
2:D:580:LYS:O	2:D:582:PRO:N	2.52	0.43
2:B:723:GLY:O	2:B:911:GLY:HA3	2.17	0.43
1:A:285:ARG:NH1	1:A:325:LEU:HD23	2.33	0.43
1:C:950:GLU:HG3	1:C:951:LEU:HG	2.00	0.43
2:B:631:ARG:O	2:B:632:HIS:ND1	2.51	0.43
2:B:633:GLU:CG	2:B:672:TYR:CE1	3.02	0.43
2:B:633:GLU:HG3	2:B:672:TYR:CE1	2.54	0.43
1:A:251:GLY:HA3	1:A:294:ASN:ND2	2.33	0.43
2:B:264:THR:HG22	2:B:266:ILE:HG12	1.98	0.43
1:E:322:TRP:HB3	1:E:323:PRO:HD3	2.00	0.43
1:A:973:LEU:HA	1:A:973:LEU:HD23	1.71	0.43
2:B:236:TYR:O	2:B:239:LEU:N	2.45	0.43
2:D:499:GLN:HG2	2:D:526:ILE:HD12	2.01	0.43
1:E:592:ASP:C	1:E:592:ASP:OD1	2.57	0.43
2:D:420:SER:C	2:D:423:GLN:HE21	2.22	0.43
2:D:707:ARG:NE	2:D:897:ASN:CG	2.72	0.43
2:D:883:GLN:O	2:D:887:ALA:CB	2.66	0.43
2:H:647:GLN:HE22	2:H:869:THR:HG21	1.80	0.43
1:A:959:TRP:CD1	1:A:959:TRP:N	2.87	0.43
2:H:552:ARG:HD3	2:H:552:ARG:O	2.17	0.43
1:G:548:VAL:HG22	1:G:563:LEU:HD13	1.99	0.43
1:E:959:TRP:N	1:E:959:TRP:CD1	2.83	0.43
2:H:420:SER:C	2:H:423:GLN:HE21	2.22	0.43
2:B:947:LEU:HD22	2:B:951:HIS:CE1	2.54	0.43
2:D:295:LEU:O	2:D:340:ILE:HA	2.18	0.43
1:C:625:LYS:HG2	1:C:644:GLU:OE2	2.18	0.43
2:B:744:VAL:O	2:B:747:SER:HB3	2.19	0.43
1:A:853:ARG:HG2	1:A:853:ARG:HH11	1.83	0.43
1:C:979:VAL:HG12	1:C:979:VAL:O	2.19	0.43
1:A:319:ARG:HB2	1:A:348:ILE:CD1	2.34	0.43
2:B:580:LYS:O	2:B:581:LEU:C	2.57	0.43
1:A:703:ARG:C	1:A:703:ARG:HD2	2.39	0.43
2:B:273:GLU:H	2:B:273:GLU:CD	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:755:SER:O	1:E:758:ARG:NH2	2.34	0.43
1:G:247:GLY:HA2	1:G:254:TYR:CD2	2.49	0.43
1:G:270:GLY:O	1:G:271:GLY:C	2.56	0.43
2:H:632:HIS:O	2:H:633:GLU:C	2.57	0.43
2:H:312:SER:O	2:H:315:PRO:HD2	2.19	0.43
2:B:639:ASN:O	2:B:640:TRP:C	2.57	0.43
2:F:545:ILE:HD11	2:F:553:ALA:CB	2.49	0.43
2:D:341:CYS:HB2	2:D:507:VAL:CG1	2.49	0.43
2:F:295:LEU:O	2:F:340:ILE:HA	2.18	0.43
2:D:784:PRO:HA	2:D:823:ALA:HA	1.99	0.43
1:G:357:ASN:HA	1:G:365:THR:CG2	2.49	0.43
2:H:918:VAL:HG12	2:H:919:TYR:H	1.83	0.43
2:D:519:ILE:HD12	2:D:519:ILE:N	2.33	0.43
1:C:805:LEU:HA	1:C:975:LEU:HB3	2.01	0.43
2:F:581:LEU:HB2	2:F:615:GLN:NE2	2.34	0.43
1:E:585:SER:O	1:E:586:GLU:C	2.57	0.43
2:H:575:ASP:OD1	2:H:575:ASP:C	2.56	0.43
2:F:633:GLU:O	2:F:633:GLU:HG2	2.19	0.43
1:E:765:GLU:HA	1:E:825:ARG:O	2.19	0.43
1:G:674:THR:O	1:G:677:TYR:HB3	2.18	0.43
1:G:342:PRO:HG2	1:G:343:TYR:CE1	2.54	0.43
2:B:894:GLU:O	2:B:896:PHE:N	2.51	0.43
2:B:494:ILE:HG23	2:B:774:LEU:HD23	1.99	0.43
2:B:627:SER:HB3	2:B:659:VAL:HG21	2.01	0.43
1:C:806:LEU:O	1:C:807:LYS:C	2.57	0.43
1:G:724:SER:OG	1:G:768:GLY:HA2	2.18	0.43
1:E:743:LEU:HD23	1:E:743:LEU:HA	1.81	0.43
1:E:391:ARG:NH2	3:F:984:F6P:O2P	2.51	0.43
2:D:647:GLN:HE22	2:D:869:THR:HG22	1.84	0.43
2:B:575:ASP:OD1	2:B:575:ASP:C	2.56	0.43
2:D:231:VAL:HG13	2:D:266:ILE:HG21	1.99	0.43
1:A:860:VAL:CG1	2:B:740:TYR:CE1	3.02	0.43
2:H:523:GLU:O	2:H:524:ASN:C	2.56	0.43
1:A:756:ALA:HB2	2:B:651:GLY:HA2	2.00	0.43
2:B:239:LEU:HD23	2:B:239:LEU:HA	1.77	0.43
2:B:715:ALA:CB	2:B:728:LEU:HB2	2.49	0.43
2:D:726:TYR:OH	2:D:864:ASP:OD2	2.29	0.43
2:D:202:MET:CE	2:D:295:LEU:HD21	2.49	0.43
1:G:526:ILE:HD13	1:G:535:ARG:HG2	2.00	0.43
2:B:830:THR:HA	2:B:848:PRO:HB3	2.01	0.43
2:B:800:LEU:HD21	2:B:817:ILE:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:ALA:HB2	1:C:874:ALA:HB1	2.01	0.43
2:B:420:SER:CA	2:B:423:GLN:HE21	2.31	0.43
1:C:794:ILE:HD11	1:C:829:ALA:HB1	2.00	0.43
2:H:587:LEU:HB3	2:H:679:ASP:HB2	2.01	0.43
2:D:253:GLU:O	2:D:256:ARG:HB3	2.19	0.43
2:B:278:GLU:CA	2:B:278:GLU:OE1	2.67	0.43
1:A:530:GLU:HA	1:A:932:SER:HB3	2.01	0.43
2:H:314:TRP:CD2	2:H:338:LEU:HB2	2.54	0.43
2:D:288:ILE:HD11	2:D:318:ILE:HG22	2.00	0.43
2:H:661:PRO:HD2	2:H:695:GLN:NE2	2.34	0.43
2:H:353:THR:HG21	2:H:534:SER:HA	2.01	0.43
2:B:238:GLY:O	2:B:241:ARG:O	2.37	0.43
1:E:674:THR:O	1:E:677:TYR:HB3	2.19	0.43
2:B:558:ASP:O	2:B:560:GLU:N	2.51	0.43
1:C:543:LYS:NZ	1:C:543:LYS:HB2	2.34	0.43
1:C:587:LEU:O	1:C:589:PRO:HD3	2.18	0.42
2:F:765:SER:HB2	2:F:936:MET:CE	2.48	0.42
1:A:703:ARG:NH1	1:A:921:ASP:OD2	2.52	0.42
1:G:271:GLY:HA3	2:H:380:SER:HG	1.84	0.42
1:A:317:LEU:H	1:A:317:LEU:CD1	2.31	0.42
1:E:962:TYR:CD2	1:E:962:TYR:N	2.85	0.42
1:G:229:ARG:HD3	1:G:260:TRP:CZ2	2.53	0.42
2:H:947:LEU:HD22	2:H:951:HIS:NE2	2.34	0.42
1:A:744:VAL:HG12	1:A:745:ASN:N	2.33	0.42
2:B:580:LYS:CD	2:B:586:ARG:NH2	2.82	0.42
2:D:880:LYS:HE2	2:D:880:LYS:HB3	1.76	0.42
2:F:665:ASP:OD1	2:F:668:MET:HG2	2.19	0.42
2:D:679:ASP:HB3	2:D:883:GLN:NE2	2.34	0.42
1:A:942:LEU:O	1:A:944:GLU:N	2.45	0.42
1:A:943:TRP:HA	1:A:946:GLU:HG3	2.01	0.42
1:A:634:SER:HB3	1:A:666:SER:OG	2.18	0.42
2:B:947:LEU:HD22	2:B:951:HIS:NE2	2.33	0.42
1:E:270:GLY:O	1:E:271:GLY:O	2.37	0.42
1:E:397:VAL:O	1:E:455:GLU:HG3	2.19	0.42
1:C:569:ILE:H	1:C:569:ILE:HD12	1.84	0.42
2:F:418:THR:HA	2:F:421:GLU:HG3	2.01	0.42
2:D:607:SER:OG	2:D:869:THR:CB	2.60	0.42
2:H:717:LEU:HB2	2:H:733:ALA:HB2	2.00	0.42
1:C:323:PRO:O	1:C:326:VAL:HB	2.19	0.42
2:D:892:ALA:HB1	2:D:894:GLU:OE1	2.19	0.42
1:E:246:GLU:OE1	1:E:246:GLU:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:GLU:C	1:G:341:ALA:H	2.22	0.42
2:H:355:ASP:OD1	2:H:559:THR:HG22	2.19	0.42
1:G:877:PHE:CZ	1:G:929:VAL:HG22	2.54	0.42
1:A:856:ILE:O	1:A:857:PRO:C	2.58	0.42
1:C:655:ASN:HB3	1:C:871:ARG:NH1	2.34	0.42
1:G:663:THR:O	1:G:663:THR:HG23	2.18	0.42
1:A:421:PRO:C	1:A:423:ARG:N	2.72	0.42
1:A:212:THR:O	1:A:212:THR:CG2	2.66	0.42
1:G:421:PRO:O	1:G:423:ARG:N	2.52	0.42
1:E:703:ARG:HD2	1:E:703:ARG:C	2.39	0.42
1:A:837:LEU:HD11	2:D:827:LEU:HD21	2.00	0.42
1:G:746:TYR:CD1	2:H:854:VAL:HG11	2.54	0.42
1:C:223:ALA:O	1:C:227:VAL:HG23	2.19	0.42
2:F:314:TRP:O	2:F:315:PRO:C	2.56	0.42
2:B:593:ASN:HA	2:B:684:VAL:O	2.19	0.42
1:A:529:LEU:HD12	1:A:534:ILE:HD13	2.00	0.42
2:B:880:LYS:HE2	2:B:880:LYS:HB3	1.69	0.42
1:G:534:ILE:HD11	1:G:536:MET:HE2	2.01	0.42
1:E:526:ILE:HD13	1:E:535:ARG:HG2	2.02	0.42
2:D:410:ILE:HA	2:D:444:VAL:O	2.20	0.42
1:E:865:VAL:CG1	1:E:871:ARG:HH21	2.32	0.42
2:B:931:GLU:O	2:B:931:GLU:HG3	2.19	0.42
1:A:440:ARG:HH11	1:A:440:ARG:HB2	1.84	0.42
1:C:261:GLU:CD	1:C:261:GLU:H	2.23	0.42
1:C:278:ARG:NH1	1:C:278:ARG:HG3	2.33	0.42
2:F:422:TRP:CH2	2:F:465:VAL:HG21	2.53	0.42
1:G:212:THR:CG2	1:G:275:GLY:O	2.68	0.42
2:H:706:PHE:C	2:H:708:ILE:H	2.22	0.42
1:E:833:TYR:HA	1:E:837:LEU:HD23	2.02	0.42
2:B:665:ASP:OD1	2:B:668:MET:HG2	2.19	0.42
1:G:972:ARG:CG	1:G:972:ARG:HH11	2.31	0.42
2:F:892:ALA:C	2:F:894:GLU:N	2.73	0.42
1:G:211:MET:CE	1:G:305:VAL:HG22	2.48	0.42
2:B:379:ASN:HA	2:B:440:THR:HG23	2.01	0.42
2:F:590:ALA:HA	2:F:620:TYR:O	2.19	0.42
1:G:461:GLN:HB2	1:G:463:ASN:ND2	2.35	0.42
2:H:701:GLU:O	2:H:701:GLU:CD	2.58	0.42
2:B:936:MET:CB	2:B:937:PRO:HD2	2.36	0.42
1:C:246:GLU:O	1:C:249:LEU:HB3	2.20	0.42
1:A:711:ILE:O	1:A:714:ILE:HG23	2.19	0.42
2:F:288:ILE:HD11	2:F:318:ILE:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:THR:HG22	1:E:511:VAL:HG11	2.01	0.42
1:A:317:LEU:O	1:A:321:GLU:HB3	2.20	0.42
1:G:962:TYR:O	1:G:965:ILE:N	2.52	0.42
1:G:964:LYS:HG2	1:G:964:LYS:H	1.57	0.42
2:B:796:ASP:O	2:B:800:LEU:HB2	2.20	0.42
2:B:755:ALA:O	2:B:846:ALA:HA	2.20	0.42
2:B:666:LEU:HD12	2:B:666:LEU:HA	1.81	0.42
1:G:838:LEU:HD12	1:G:838:LEU:HA	1.86	0.42
2:H:580:LYS:O	2:H:581:LEU:C	2.58	0.42
1:E:944:GLU:C	1:E:945:ASN:HD22	2.22	0.42
2:H:687:PHE:CE2	2:H:935:ARG:HA	2.55	0.42
1:E:216:ASP:H	2:F:381:HIS:HE1	1.67	0.42
2:D:587:LEU:HB3	2:D:679:ASP:OD2	2.19	0.42
2:D:887:ALA:C	2:D:889:ALA:H	2.22	0.42
1:C:694:GLU:CD	1:C:952:ARG:HH21	2.23	0.42
1:C:326:VAL:HG13	1:C:340:VAL:HG22	1.99	0.42
1:A:613:ARG:HG2	1:A:613:ARG:HH11	1.85	0.42
2:F:328:SER:N	2:F:331:GLN:NE2	2.66	0.42
2:F:835:VAL:HG13	1:G:833:TYR:OH	2.19	0.42
1:E:442:ARG:NH1	1:E:449:ASN:OD1	2.43	0.42
1:C:278:ARG:HG3	1:C:278:ARG:HH11	1.84	0.42
1:C:529:LEU:HB2	1:C:534:ILE:HD13	2.01	0.42
1:G:761:VAL:O	1:G:852:VAL:HA	2.19	0.42
1:E:663:THR:HG23	1:E:663:THR:O	2.19	0.42
1:E:317:LEU:HD12	1:E:317:LEU:N	2.34	0.42
2:B:831:LYS:HA	2:B:831:LYS:HD3	1.79	0.42
2:H:578:GLU:O	2:H:580:LYS:CG	2.54	0.42
1:A:808:GLU:O	1:A:809:ASN:C	2.57	0.42
2:D:607:SER:CB	2:D:869:THR:HB	2.49	0.42
2:H:617:HIS:NE2	2:H:880:LYS:NZ	2.62	0.42
2:D:946:ARG:NH2	2:D:946:ARG:CG	2.80	0.42
1:E:249:LEU:C	1:E:249:LEU:HD12	2.40	0.42
1:E:518:THR:CB	1:E:519:PRO:HD2	2.49	0.42
2:H:591:ILE:HB	2:H:608:MET:HE1	2.02	0.42
1:E:291:ALA:O	1:E:294:ASN:N	2.53	0.42
2:F:715:ALA:HB2	2:F:728:LEU:HB2	2.02	0.42
1:G:574:ASN:O	1:G:578:THR:HB	2.19	0.42
1:G:569:ILE:H	1:G:569:ILE:HD12	1.84	0.42
1:E:586:GLU:HG3	1:E:587:LEU:N	2.34	0.42
1:A:587:LEU:HB3	1:A:622:HIS:CE1	2.55	0.42
1:G:246:GLU:CA	1:G:279:SER:HB2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:ILE:HD13	1:A:968:ILE:HA	1.81	0.42
2:H:201:VAL:HA	2:H:296:ILE:O	2.20	0.42
1:G:930:ASN:O	1:G:931:GLY:C	2.57	0.42
1:E:731:GLU:HG2	1:E:958:HIS:CG	2.55	0.42
2:B:717:LEU:HD12	2:B:717:LEU:C	2.40	0.42
2:H:420:SER:CA	2:H:423:GLN:HE21	2.33	0.42
2:D:202:MET:HE3	2:D:295:LEU:HD21	2.01	0.42
1:C:679:PHE:CE2	1:C:687:LEU:HD22	2.54	0.42
2:F:623:TYR:HB2	2:F:634:SER:HB2	2.02	0.42
2:H:433:HIS:ND1	2:H:640:TRP:CZ2	2.88	0.42
1:E:302:ALA:HA	1:E:347:SER:HB2	2.02	0.42
1:C:808:GLU:OE2	1:C:978:GLU:OE1	2.38	0.42
2:B:578:GLU:O	2:B:580:LYS:CG	2.53	0.42
2:D:876:VAL:HG12	2:D:880:LYS:HE3	2.01	0.42
2:F:428:ASP:CG	2:F:432:LYS:HZ3	2.23	0.42
2:H:935:ARG:O	2:H:936:MET:HB3	2.18	0.42
2:D:392:ARG:NH2	3:D:982:F6P:H12	2.33	0.42
2:D:900:ASP:CG	2:D:903:ILE:HG13	2.40	0.42
2:F:911:GLY:O	2:F:917:VAL:HA	2.19	0.42
2:H:522:ASN:O	2:H:523:GLU:C	2.58	0.42
2:H:400:LEU:CD1	2:H:866:THR:HG21	2.48	0.42
1:E:322:TRP:O	1:E:326:VAL:HG23	2.20	0.42
1:A:416:ASP:OD2	1:A:449:ASN:HA	2.20	0.42
2:H:545:ILE:HD11	2:H:553:ALA:CB	2.49	0.42
1:G:578:THR:O	1:G:578:THR:HG23	2.20	0.42
2:D:219:VAL:O	2:D:223:ILE:HG13	2.20	0.42
2:D:666:LEU:HA	2:D:666:LEU:HD12	1.90	0.42
2:B:419:SER:O	2:B:423:GLN:NE2	2.52	0.41
2:B:416:PRO:HB2	2:B:452:ALA:HA	2.03	0.41
2:B:882:ASN:ND2	2:B:906:THR:HG22	2.17	0.41
1:G:974:LYS:CD	1:G:975:LEU:HD13	2.50	0.41
2:H:886:ILE:O	2:H:890:ARG:N	2.52	0.41
2:B:231:VAL:HG13	2:B:266:ILE:HG21	2.02	0.41
2:B:892:ALA:C	2:B:894:GLU:N	2.71	0.41
2:D:662:GLU:HG3	2:D:695:GLN:NE2	2.34	0.41
1:G:317:LEU:CD1	1:G:317:LEU:N	2.81	0.41
1:A:862:GLN:NE2	2:B:747:SER:OG	2.53	0.41
2:H:918:VAL:HG12	2:H:919:TYR:N	2.35	0.41
1:C:756:ALA:HB2	2:D:651:GLY:HA2	2.01	0.41
1:G:728:PRO:HG3	1:G:954:GLY:CA	2.50	0.41
2:H:258:TRP:CH2	2:H:265:ASN:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:594:VAL:O	2:F:685:GLY:HA3	2.19	0.41
1:C:440:ARG:HB2	1:C:440:ARG:HH11	1.86	0.41
1:A:424:ALA:HA	1:A:458:LEU:O	2.20	0.41
2:F:418:THR:CG2	2:F:422:TRP:HD1	2.31	0.41
1:A:801:GLU:O	1:A:805:LEU:HG	2.20	0.41
2:D:575:ASP:C	2:D:575:ASP:OD1	2.57	0.41
2:B:288:ILE:HG12	2:B:335:MET:HE2	2.01	0.41
1:G:972:ARG:NH1	1:G:972:ARG:CG	2.83	0.41
1:G:346:LEU:HD13	1:G:348:ILE:HD11	2.02	0.41
1:A:233:HIS:NE2	1:A:968:ILE:HD12	2.35	0.41
1:E:211:MET:HG3	1:E:244:GLY:HA2	2.02	0.41
2:B:239:LEU:O	2:B:286:HIS:CD2	2.72	0.41
1:C:229:ARG:NH1	1:C:969:LEU:O	2.52	0.41
1:G:877:PHE:HZ	1:G:929:VAL:HG22	1.85	0.41
1:A:282:PHE:HZ	1:A:318:PHE:CD1	2.38	0.41
1:E:471:LYS:HG3	1:E:481:THR:HG22	2.02	0.41
2:F:573:SER:O	2:F:574:ALA:O	2.39	0.41
2:F:415:LYS:N	2:F:416:PRO:HD3	2.35	0.41
2:D:298:CYS:CB	2:D:343:THR:HG22	2.50	0.41
2:H:886:ILE:O	2:H:890:ARG:HB2	2.20	0.41
2:H:887:ALA:C	2:H:889:ALA:N	2.74	0.41
2:D:587:LEU:HB3	2:D:679:ASP:HB2	2.02	0.41
2:B:327:ILE:HG13	2:B:327:ILE:O	2.20	0.41
1:E:963:ASN:HD22	1:E:963:ASN:N	2.17	0.41
2:B:341:CYS:HB2	2:B:507:VAL:CG1	2.48	0.41
2:F:236:TYR:O	2:F:239:LEU:HB2	2.21	0.41
2:F:626:TRP:NE1	2:F:661:PRO:HG3	2.35	0.41
1:C:242:TYR:N	1:C:242:TYR:CD1	2.88	0.41
1:G:724:SER:CB	1:G:768:GLY:HA2	2.50	0.41
2:F:516:SER:O	2:F:531:LEU:HB2	2.20	0.41
1:E:787:VAL:HA	1:E:824:VAL:O	2.20	0.41
1:E:355:ILE:HB	1:E:371:ALA:HB2	2.02	0.41
2:D:420:SER:CA	2:D:423:GLN:NE2	2.83	0.41
2:F:417:ALA:O	2:F:418:THR:CB	2.69	0.41
1:G:586:GLU:CG	1:G:587:LEU:N	2.83	0.41
2:B:904:SER:C	2:B:906:THR:H	2.23	0.41
2:H:792:GLN:NE2	2:H:957:ARG:HB3	2.29	0.41
2:H:717:LEU:HD11	2:H:761:GLN:HE21	1.86	0.41
2:D:587:LEU:HD23	2:D:679:ASP:HB3	2.02	0.41
2:B:647:GLN:HE22	2:B:869:THR:HG21	1.83	0.41
2:F:694:HIS:HA	2:F:922:ILE:HG12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:GLU:C	2:B:896:PHE:N	2.74	0.41
1:C:488:HIS:C	1:C:490:GLN:N	2.71	0.41
1:C:506:GLN:HG2	1:C:526:ILE:HG22	2.03	0.41
1:G:780:LEU:O	1:G:780:LEU:HD13	2.20	0.41
1:G:728:PRO:HG3	1:G:954:GLY:HA2	2.02	0.41
1:G:289:ARG:HA	1:G:325:LEU:HD13	2.02	0.41
1:E:209:ALA:HA	1:E:239:PHE:O	2.21	0.41
1:G:651:GLU:HG3	1:G:652:ASN:ND2	2.35	0.41
2:D:800:LEU:HD21	2:D:817:ILE:HD11	2.02	0.41
1:A:927:ILE:HG23	1:A:927:ILE:O	2.19	0.41
1:C:474:LEU:HD22	1:C:479:LEU:HD12	2.03	0.41
2:H:298:CYS:HB2	2:H:343:THR:CG2	2.50	0.41
2:B:343:THR:O	2:B:343:THR:HG22	2.21	0.41
2:H:711:VAL:CG1	2:H:711:VAL:O	2.67	0.41
2:F:916:HIS:O	2:F:917:VAL:HB	2.21	0.41
2:H:428:ASP:O	2:H:432:LYS:HG3	2.20	0.41
2:F:293:ASP:HB3	2:F:335:MET:HE3	2.01	0.41
2:D:591:ILE:HB	2:D:608:MET:HE3	2.02	0.41
1:A:746:TYR:CE1	2:B:854:VAL:HG11	2.55	0.41
2:F:797:ILE:HD13	2:F:836:ILE:HA	2.03	0.41
2:D:672:TYR:O	2:D:676:TYR:HD1	2.03	0.41
1:E:788:TYR:HE1	1:E:823:LEU:HD23	1.85	0.41
2:H:288:ILE:HD11	2:H:318:ILE:HG22	2.02	0.41
1:A:823:LEU:N	1:A:823:LEU:CD1	2.83	0.41
2:F:796:ASP:O	2:F:800:LEU:HB2	2.19	0.41
2:B:475:ARG:HG2	2:B:475:ARG:NH1	2.36	0.41
1:G:962:TYR:O	1:G:964:LYS:N	2.54	0.41
2:F:755:ALA:O	2:F:846:ALA:HA	2.20	0.41
2:F:413:PRO:HB3	2:F:448:GLY:O	2.20	0.41
2:D:573:SER:O	2:D:574:ALA:C	2.59	0.41
1:C:787:VAL:HA	1:C:824:VAL:O	2.21	0.41
1:E:606:ALA:O	1:E:866:PRO:HB3	2.20	0.41
2:H:295:LEU:O	2:H:340:ILE:HA	2.20	0.41
2:B:418:THR:CG2	2:B:422:TRP:HD1	2.33	0.41
2:F:414:GLU:C	2:F:416:PRO:HD3	2.41	0.41
1:E:782:THR:HG22	1:E:784:ALA:N	2.36	0.41
1:A:947:THR:O	1:A:950:GLU:O	2.37	0.41
1:A:950:GLU:O	1:A:952:ARG:N	2.47	0.41
2:D:467:VAL:O	2:D:471:GLY:CA	2.61	0.41
2:B:946:ARG:CG	2:B:946:ARG:NH2	2.80	0.41
1:E:246:GLU:CA	1:E:279:SER:HB2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:GLU:OE1	1:G:246:GLU:HA	2.20	0.41
2:B:453:ASP:O	2:B:454:LEU:HB2	2.20	0.41
2:H:462:VAL:HG12	2:H:466:LEU:HD23	2.02	0.41
2:H:930:THR:HG22	2:H:932:VAL:H	1.83	0.41
1:G:450:THR:C	1:G:451:ILE:HD12	2.40	0.41
1:E:421:PRO:HG2	1:E:422:GLU:OE2	2.20	0.41
2:D:747:SER:O	2:D:750:SER:HB2	2.20	0.41
2:H:347:ILE:CG2	2:H:363:ALA:HB2	2.50	0.41
2:F:365:ASP:OD2	2:F:369:LYS:NZ	2.46	0.41
1:C:759:ARG:HG2	1:C:810:PHE:CD2	2.56	0.41
2:H:429:ILE:HG13	2:H:433:HIS:CD2	2.55	0.41
2:H:365:ASP:HA	2:H:862:PRO:HG2	2.02	0.41
2:B:622:ILE:HG23	2:B:629:LEU:HD13	2.02	0.41
1:E:734:LEU:HD21	1:E:873:THR:HG22	2.02	0.41
2:B:418:THR:OG1	2:B:422:TRP:N	2.35	0.41
1:C:805:LEU:HD23	1:C:805:LEU:N	2.35	0.41
2:H:390:MET:HG3	2:H:483:GLN:HE22	1.82	0.41
2:H:888:GLU:OE1	2:H:889:ALA:HB2	2.20	0.41
1:A:697:ARG:NH1	1:A:943:TRP:HH2	2.19	0.41
2:D:207:ASP:HA	2:D:211:MET:SD	2.61	0.41
2:F:694:HIS:CA	2:F:922:ILE:HG12	2.51	0.41
1:E:341:ALA:CB	1:E:342:PRO:CD	2.98	0.41
1:E:968:ILE:CG1	1:E:973:LEU:HD12	2.51	0.41
2:F:236:TYR:O	2:F:239:LEU:N	2.52	0.41
2:F:717:LEU:HD12	2:F:718:SER:N	2.36	0.41
1:E:746:TYR:CE1	2:F:854:VAL:HG13	2.55	0.41
2:F:761:GLN:HB3	4:F:6:FDP:O1	2.21	0.41
2:B:524:ASN:HB2	2:B:914:GLY:HA2	2.02	0.41
2:D:574:ALA:CB	2:D:610:THR:O	2.68	0.41
2:H:690:PHE:HA	2:H:712:LEU:HD22	2.03	0.41
1:C:922:ASP:HA	1:C:938:PRO:HG3	2.02	0.41
2:F:407:ALA:HB1	2:F:442:ILE:O	2.21	0.41
2:D:831:LYS:HA	2:D:831:LYS:HD3	1.82	0.41
1:E:819:ASN:O	1:E:821:LYS:HE3	2.20	0.41
2:B:577:ASN:CA	2:B:579:PRO:HD2	2.51	0.41
1:C:697:ARG:NH1	1:C:943:TRP:HH2	2.18	0.41
2:B:900:ASP:O	2:B:901:LYS:C	2.59	0.41
1:E:591:SER:HA	1:E:593:ARG:HG3	2.02	0.41
1:C:216:ASP:H	2:D:381:HIS:CE1	2.33	0.41
2:F:765:SER:HB2	2:F:936:MET:HE3	2.03	0.41
2:H:612:CYS:HB3	2:H:617:HIS:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:522:ASN:O	2:F:523:GLU:C	2.59	0.41
2:D:930:THR:HG22	2:D:931:GLU:N	2.35	0.41
1:C:317:LEU:CD1	1:C:317:LEU:H	2.34	0.41
1:G:317:LEU:O	1:G:321:GLU:HB3	2.21	0.41
1:A:758:ARG:NH2	1:A:817:ASN:HA	2.36	0.41
2:H:648:SER:HA	2:H:865:ARG:HD3	2.03	0.41
2:F:438:LYS:HG2	2:F:440:THR:O	2.21	0.41
1:A:357:ASN:OD1	1:A:364:SER:HA	2.21	0.41
1:C:266:TRP:CD2	1:C:273:LEU:HD12	2.55	0.41
1:C:424:ALA:HB1	1:C:459:ASP:O	2.21	0.41
1:A:421:PRO:O	1:A:423:ARG:N	2.54	0.41
2:D:723:GLY:O	2:D:911:GLY:HA3	2.21	0.41
1:C:765:GLU:HA	1:C:825:ARG:O	2.20	0.41
1:G:590:VAL:CG2	1:G:591:SER:H	2.22	0.41
2:B:903:ILE:HG13	2:B:903:ILE:H	1.68	0.41
1:E:431:GLN:N	1:E:431:GLN:NE2	2.50	0.41
2:D:673:PHE:HZ	2:D:681:LEU:HD22	1.86	0.41
2:H:381:HIS:CD2	2:H:383:ARG:HH21	2.39	0.41
1:C:613:ARG:HG2	1:C:613:ARG:NH1	2.36	0.41
2:H:325:ASN:O	2:H:326:ARG:HB2	2.20	0.41
1:E:249:LEU:HD13	1:E:290:GLN:HG2	2.01	0.41
1:E:289:ARG:N	1:E:325:LEU:HD13	2.35	0.41
1:A:660:GLU:C	2:B:752:ARG:HH22	2.24	0.41
2:B:341:CYS:CB	2:B:507:VAL:HG13	2.47	0.41
1:E:399:GLY:O	1:E:400:ARG:HB3	2.21	0.41
2:D:314:TRP:O	2:D:315:PRO:C	2.59	0.41
2:F:349:ASN:HA	2:F:357:THR:OG1	2.21	0.41
1:C:774:ILE:HD13	1:C:774:ILE:HA	1.98	0.41
2:D:752:ARG:CZ	2:D:811:GLY:HA2	2.50	0.41
2:F:662:GLU:HG3	2:F:695:GLN:NE2	2.36	0.41
2:D:239:LEU:HA	2:D:239:LEU:HD23	1.87	0.41
1:E:554:ASN:O	1:E:555:LYS:C	2.59	0.41
2:H:314:TRP:O	2:H:315:PRO:C	2.55	0.41
1:A:788:TYR:HE1	1:A:823:LEU:HD23	1.85	0.41
2:D:494:ILE:HG23	2:D:774:LEU:HD23	2.03	0.41
1:E:247:GLY:HA2	1:E:254:TYR:CD2	2.55	0.41
2:D:379:ASN:HA	2:D:440:THR:HG23	2.02	0.41
2:B:219:VAL:O	2:B:223:ILE:HG13	2.21	0.41
2:B:611:TYR:CG	2:B:873:ILE:HG12	2.56	0.41
2:B:410:ILE:HA	2:B:444:VAL:O	2.21	0.41
1:C:606:ALA:O	1:C:866:PRO:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:788:TYR:OH	1:C:802:ASP:OD2	2.37	0.41
1:G:589:PRO:O	1:G:593:ARG:NH1	2.54	0.41
1:A:825:ARG:NH2	1:A:834:SER:HA	2.36	0.41
2:D:879:ILE:HA	2:D:879:ILE:HD13	1.92	0.41
2:F:591:ILE:HG12	2:F:682:ILE:CG2	2.51	0.41
2:D:523:GLU:OE1	2:D:915:SER:HB3	2.21	0.41
1:C:317:LEU:O	1:C:321:GLU:HB3	2.21	0.41
1:A:930:ASN:O	1:A:931:GLY:C	2.58	0.41
1:E:710:PRO:HA	1:E:713:ASN:HD22	1.86	0.41
2:B:755:ALA:HA	2:B:815:LYS:O	2.21	0.41
2:B:726:TYR:CE1	2:B:730:SER:HB3	2.55	0.41
1:C:518:THR:OG1	1:C:521:THR:CG2	2.53	0.40
2:H:587:LEU:CD1	2:H:587:LEU:N	2.84	0.40
2:B:390:MET:HG3	2:B:483:GLN:HE22	1.82	0.40
1:G:558:ASP:O	1:G:561:ILE:HG22	2.20	0.40
2:H:322:LEU:HA	2:H:322:LEU:HD23	1.86	0.40
1:A:837:LEU:HD11	1:A:841:ILE:HD11	2.02	0.40
2:H:239:LEU:HD22	2:H:287:LEU:HD22	2.02	0.40
2:F:587:LEU:N	2:F:617:HIS:HD1	2.16	0.40
1:C:711:ILE:O	1:C:714:ILE:HG23	2.20	0.40
1:E:539:VAL:O	1:E:542:VAL:CG2	2.68	0.40
1:E:211:MET:CE	1:E:305:VAL:HG22	2.49	0.40
2:F:347:ILE:CG2	2:F:363:ALA:HB2	2.51	0.40
2:H:541:VAL:HG22	2:H:556:LEU:HB2	2.03	0.40
1:G:530:GLU:HA	1:G:932:SER:HB3	2.02	0.40
1:G:754:ALA:HB2	1:G:762:PHE:HE1	1.86	0.40
2:D:853:HIS:C	2:D:855:GLN:N	2.74	0.40
2:H:726:TYR:O	2:H:726:TYR:CD2	2.74	0.40
1:A:433:GLU:O	1:A:437:VAL:HG23	2.20	0.40
1:G:625:LYS:HG2	1:G:644:GLU:OE2	2.21	0.40
1:A:498:HIS:HD2	1:A:869:LYS:NZ	2.19	0.40
1:G:750:ILE:HG13	1:G:751:LYS:N	2.35	0.40
2:D:365:ASP:HA	2:D:862:PRO:HG2	2.03	0.40
2:D:590:ALA:HA	2:D:620:TYR:O	2.21	0.40
1:A:638:GLN:HG3	1:A:638:GLN:O	2.20	0.40
1:E:466:THR:CG2	1:E:467:ALA:N	2.84	0.40
3:A:988:F6P:O2P	2:B:383:ARG:NH2	2.48	0.40
2:F:916:HIS:O	2:F:917:VAL:CB	2.69	0.40
1:G:832:VAL:HG12	1:G:833:TYR:N	2.36	0.40
2:F:341:CYS:SG	2:F:519:ILE:CD1	3.09	0.40
2:F:930:THR:HG22	2:F:931:GLU:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:752:ARG:CZ	2:B:811:GLY:HA2	2.51	0.40
2:H:341:CYS:CB	2:H:507:VAL:HG13	2.49	0.40
1:C:247:GLY:HA2	1:C:254:TYR:HD2	1.85	0.40
2:D:344:VAL:CG2	2:D:357:THR:HG22	2.52	0.40
1:G:231:GLY:O	1:G:232:ILE:C	2.59	0.40
1:C:864:GLY:HA3	2:D:743:VAL:HG22	2.04	0.40
1:A:554:ASN:O	1:A:556:ASP:N	2.55	0.40
1:E:975:LEU:O	1:E:978:GLU:HB2	2.21	0.40
2:H:563:GLU:OE2	2:H:870:ARG:NE	2.34	0.40
2:D:580:LYS:O	2:D:581:LEU:C	2.59	0.40
1:E:584:GLY:O	1:E:588:LEU:HB2	2.20	0.40
2:D:711:VAL:HG22	2:D:910:VAL:CG2	2.51	0.40
1:G:975:LEU:HD22	1:G:975:LEU:N	2.20	0.40
1:A:947:THR:HG21	1:A:951:LEU:CB	2.43	0.40
2:H:666:LEU:O	2:H:669:ILE:HB	2.21	0.40
2:D:884:ALA:O	2:D:887:ALA:HB3	2.20	0.40
2:H:900:ASP:O	2:H:901:LYS:C	2.60	0.40
2:F:679:ASP:HB3	2:F:883:GLN:HE22	1.86	0.40
2:F:288:ILE:HG12	2:F:335:MET:HE2	2.03	0.40
2:H:239:LEU:HD23	2:H:239:LEU:HA	1.87	0.40
2:D:244:PRO:O	2:D:245:GLU:CB	2.68	0.40
2:D:545:ILE:HD11	2:D:553:ALA:CB	2.51	0.40
2:H:800:LEU:HD21	2:H:817:ILE:HD11	2.03	0.40
1:C:483:VAL:HG12	1:C:485:ILE:CD1	2.51	0.40
2:D:408:ASP:OD1	2:D:441:THR:HA	2.22	0.40
1:A:625:LYS:HG2	1:A:644:GLU:OE2	2.20	0.40
2:F:366:ARG:NH2	2:F:487:THR:O	2.53	0.40
1:C:700:LYS:NZ	1:C:704:ASP:OD2	2.54	0.40
1:A:743:LEU:HD23	1:A:743:LEU:HA	1.93	0.40
2:D:419:SER:O	2:D:423:GLN:NE2	2.55	0.40
2:D:701:GLU:OE2	2:D:701:GLU:O	2.39	0.40
1:E:448:ASN:HD22	1:E:448:ASN:H	1.67	0.40
2:F:936:MET:CB	2:F:937:PRO:HD2	2.37	0.40
1:A:770:HIS:CG	1:A:951:LEU:HA	2.55	0.40
2:H:946:ARG:HG3	2:H:946:ARG:NH2	2.27	0.40
2:F:888:GLU:OE1	2:F:889:ALA:HB2	2.20	0.40
1:E:837:LEU:HD22	2:H:831:LYS:CD	2.51	0.40
2:H:325:ASN:C	2:H:327:ILE:N	2.74	0.40
2:D:201:VAL:HG13	2:D:218:ILE:HG21	2.03	0.40
2:B:519:ILE:HD12	2:B:519:ILE:N	2.37	0.40
1:C:584:GLY:O	1:C:588:LEU:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:754:ALA:HB2	1:G:762:PHE:CD1	2.56	0.40
2:H:420:SER:CA	2:H:423:GLN:NE2	2.85	0.40
1:E:514:VAL:HG12	1:E:515:LEU:N	2.36	0.40
1:C:404:TRP:HE3	1:C:405:LEU:HD13	1.86	0.40
1:C:720:PRO:HG2	1:C:730:THR:HG21	2.04	0.40
1:E:648:ILE:HD13	1:E:648:ILE:O	2.22	0.40
1:E:780:LEU:HD13	1:E:780:LEU:C	2.42	0.40
1:G:225:ARG:HA	1:G:263:VAL:HG11	2.03	0.40
1:C:518:THR:HG23	1:C:521:THR:HG21	2.03	0.40
2:F:647:GLN:HE22	2:F:869:THR:HG22	1.86	0.40
1:A:760:ARG:NH1	4:B:2:FDP:O6P	2.53	0.40
1:E:669:SER:HB3	1:E:701:GLN:CD	2.42	0.40
1:C:589:PRO:HD2	1:C:622:HIS:HB3	2.03	0.40
2:D:587:LEU:HB3	2:D:679:ASP:CB	2.52	0.40
1:A:837:LEU:HD11	2:D:827:LEU:CD2	2.51	0.40
2:B:832:LEU:HD12	2:B:832:LEU:HA	1.77	0.40
1:A:255:LEU:HD23	1:A:256:LYS:N	2.37	0.40
1:E:484:THR:C	1:E:485:ILE:HD12	2.41	0.40
1:A:382:ILE:O	1:A:385:THR:HG22	2.22	0.40
2:B:949:ALA:O	2:B:953:VAL:HG12	2.21	0.40
1:E:746:TYR:CE1	2:F:854:VAL:HG11	2.57	0.40
2:H:740:TYR:CD1	2:H:851:PRO:HB3	2.56	0.40
2:H:945:THR:HA	2:H:948:ILE:HG12	2.03	0.40
1:G:761:VAL:HA	1:G:821:LYS:O	2.21	0.40
1:G:432:ASP:O	1:G:436:GLU:HB2	2.21	0.40
1:A:803:ILE:HD13	1:A:845:ALA:CB	2.52	0.40
2:D:475:ARG:HG2	2:D:475:ARG:HH11	1.87	0.40
1:G:278:ARG:HG3	1:G:278:ARG:NH1	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:333:GLU:OE2	2:H:578:GLU:OE1[4_446]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	A	746/787 (95%)	630 (84%)	87 (12%)	29 (4%)	4	15
1	C	746/787 (95%)	634 (85%)	85 (11%)	27 (4%)	4	18
1	E	748/787 (95%)	643 (86%)	74 (10%)	31 (4%)	3	14
1	G	742/787 (94%)	632 (85%)	79 (11%)	31 (4%)	3	13
2	B	761/766 (99%)	675 (89%)	61 (8%)	25 (3%)	5	20
2	D	761/766 (99%)	672 (88%)	59 (8%)	30 (4%)	4	15
2	F	760/766 (99%)	674 (89%)	58 (8%)	28 (4%)	4	17
2	H	761/766 (99%)	680 (89%)	53 (7%)	28 (4%)	4	17
All	All	6025/6212 (97%)	5240 (87%)	556 (9%)	229 (4%)	4	16

All (229) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLY
1	A	321	GLU
1	A	331	ALA
1	A	585	SER
1	A	587	LEU
1	A	589	PRO
1	A	590	VAL
1	A	817	ASN
1	A	948	ASN
2	B	324	THR
2	B	418	THR
2	B	548	LYS
2	B	559	THR
2	B	574	ALA
2	B	579	PRO
2	B	580	LYS
2	B	584	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	884	ALA
2	B	885	ALA
2	B	891	ALA
2	B	905	ASP
2	B	917	VAL
1	C	252	GLY
1	C	321	GLU
1	C	331	ALA
1	C	555	LYS
1	C	585	SER
1	C	586	GLU
1	C	587	LEU
1	C	590	VAL
1	C	671	ASP
1	C	817	ASN
1	C	948	ASN
1	C	949	VAL
2	D	324	THR
2	D	418	THR
2	D	548	LYS
2	D	574	ALA
2	D	579	PRO
2	D	580	LYS
2	D	584	ASP
2	D	884	ALA
2	D	885	ALA
2	D	891	ALA
1	E	252	GLY
1	E	271	GLY
1	E	321	GLU
1	E	331	ALA
1	E	555	LYS
1	E	585	SER
1	E	590	VAL
1	E	817	ASN
1	E	950	GLU
1	E	976	ARG
2	F	324	THR
2	F	418	THR
2	F	548	LYS
2	F	574	ALA
2	F	579	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	580	LYS
2	F	584	ASP
2	F	884	ALA
2	F	885	ALA
2	F	891	ALA
1	G	252	GLY
1	G	271	GLY
1	G	321	GLU
1	G	331	ALA
1	G	427	HIS
1	G	555	LYS
1	G	585	SER
1	G	586	GLU
1	G	590	VAL
1	G	817	ASN
1	G	948	ASN
1	G	950	GLU
2	H	324	THR
2	H	418	THR
2	H	548	LYS
2	H	574	ALA
2	H	579	PRO
2	H	580	LYS
2	H	584	ASP
2	H	885	ALA
2	H	891	ALA
1	A	271	GLY
1	A	275	GLY
1	A	332	GLU
1	A	334	ARG
1	A	555	LYS
1	A	586	GLU
1	A	671	ASP
1	A	848	GLY
1	A	951	LEU
1	A	961	GLU
2	B	417	ALA
2	B	625	GLY
2	B	700	ARG
2	B	702	SER
2	B	711	VAL
2	B	890	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	893	GLU
2	B	895	ASN
2	B	932	VAL
1	C	271	GLY
1	C	332	GLU
1	C	333	GLY
1	C	334	ARG
1	C	422	GLU
1	C	427	HIS
1	C	589	PRO
1	C	848	GLY
2	D	323	LYS
2	D	417	ALA
2	D	559	THR
2	D	702	SER
2	D	711	VAL
2	D	810	ARG
2	D	890	ARG
2	D	893	GLU
2	D	895	ASN
2	D	905	ASP
2	D	917	VAL
2	D	932	VAL
1	E	332	GLU
1	E	334	ARG
1	E	586	GLU
1	E	587	LEU
1	E	589	PRO
1	E	671	ASP
1	E	848	GLY
1	E	949	VAL
2	F	417	ALA
2	F	702	SER
2	F	711	VAL
2	F	890	ARG
2	F	893	GLU
2	F	895	ASN
2	F	905	ASP
2	F	917	VAL
1	G	332	GLU
1	G	334	ARG
1	G	587	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	848	GLY
1	G	972	ARG
2	H	417	ALA
2	H	559	THR
2	H	700	ARG
2	H	702	SER
2	H	711	VAL
2	H	890	ARG
2	H	893	GLU
2	H	895	ASN
2	H	917	VAL
1	A	427	HIS
1	A	944	GLU
2	B	323	LYS
1	C	806	LEU
1	C	952	ARG
2	D	625	GLY
2	D	700	ARG
1	E	333	GLY
1	E	427	HIS
1	E	632	GLY
1	E	806	LEU
1	E	948	ASN
1	E	951	LEU
1	E	978	GLU
2	F	559	THR
2	F	700	ARG
1	G	251	GLY
1	G	333	GLY
1	G	589	PRO
1	G	671	ASP
1	G	963	ASN
2	H	323	LYS
2	H	665	ASP
2	H	884	ALA
2	H	905	ASP
1	A	806	LEU
1	A	963	ASN
1	C	632	GLY
1	C	944	GLU
2	D	557	ARG
2	D	956	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	665	ASP
2	F	752	ARG
1	G	422	GLU
1	G	426	PRO
1	G	806	LEU
1	G	944	GLU
1	G	949	VAL
1	G	974	LYS
2	H	752	ARG
1	A	251	GLY
1	A	758	ARG
1	C	426	PRO
2	D	581	LEU
2	D	752	ARG
1	E	275	GLY
1	E	426	PRO
1	E	974	LYS
2	F	325	ASN
2	F	932	VAL
1	G	758	ARG
2	H	956	LYS
1	A	949	VAL
2	B	581	LEU
2	B	914	GLY
1	C	950	GLU
2	D	665	ASP
1	E	758	ARG
2	F	581	LEU
1	G	759	ARG
2	H	325	ASN
2	H	914	GLY
1	A	340	VAL
2	F	886	ILE
2	H	581	LEU
1	E	251	GLY
2	F	914	GLY
1	A	333	GLY
1	A	426	PRO
2	D	243	GLY
1	E	340	VAL
1	G	968	ILE
1	C	275	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	243	GLY
2	H	886	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	
1	A	614/645 (95%)	567 (92%)	47 (8%)	16	42
1	C	614/645 (95%)	567 (92%)	47 (8%)	16	42
1	E	616/645 (96%)	565 (92%)	51 (8%)	14	38
1	G	612/645 (95%)	561 (92%)	51 (8%)	14	38
2	B	612/615 (100%)	552 (90%)	60 (10%)	10	30
2	D	612/615 (100%)	552 (90%)	60 (10%)	10	30
2	F	611/615 (99%)	554 (91%)	57 (9%)	11	32
2	H	612/615 (100%)	553 (90%)	59 (10%)	10	31
All	All	4903/5040 (97%)	4471 (91%)	432 (9%)	12	35

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	LYS
1	A	237	ASP
1	A	249	LEU
1	A	264	ARG
1	A	309	ASP
1	A	322	TRP
1	A	328	GLU
1	A	332	GLU
1	A	334	ARG
1	A	340	VAL
1	A	346	LEU
1	A	359	MET
1	A	405	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	423	ARG
1	A	427	HIS
1	A	431	GLN
1	A	436	GLU
1	A	458	LEU
1	A	502	LEU
1	A	514	VAL
1	A	517	PHE
1	A	524	PRO
1	A	539	VAL
1	A	555	LYS
1	A	578	THR
1	A	588	LEU
1	A	589	PRO
1	A	599	VAL
1	A	605	SER
1	A	622	HIS
1	A	648	ILE
1	A	650	VAL
1	A	656	LEU
1	A	703	ARG
1	A	758	ARG
1	A	782	THR
1	A	785	VAL
1	A	814	LYS
1	A	819	ASN
1	A	821	LYS
1	A	822	LEU
1	A	891	LYS
1	A	934	VAL
1	A	946	GLU
1	A	952	ARG
1	A	959	TRP
1	A	964	LYS
2	B	201	VAL
2	B	253	GLU
2	B	256	ARG
2	B	259	SER
2	B	273	GLU
2	B	281	LEU
2	B	287	LEU
2	B	297	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	301	ASP
2	B	322	LEU
2	B	336	LYS
2	B	343	THR
2	B	366	ARG
2	B	389	VAL
2	B	423	GLN
2	B	436	ARG
2	B	469	ARG
2	B	472	LEU
2	B	487	THR
2	B	510	SER
2	B	518	LEU
2	B	521	VAL
2	B	525	LYS
2	B	531	LEU
2	B	551	LYS
2	B	552	ARG
2	B	565	LEU
2	B	575	ASP
2	B	579	PRO
2	B	583	LYS
2	B	584	ASP
2	B	586	ARG
2	B	587	LEU
2	B	591	ILE
2	B	608	MET
2	B	619	PRO
2	B	673	PHE
2	B	688	GLU
2	B	698	ARG
2	B	700	ARG
2	B	701	GLU
2	B	702	SER
2	B	707	ARG
2	B	711	VAL
2	B	716	THR
2	B	793	LEU
2	B	794	SER
2	B	800	LEU
2	B	808	GLU
2	B	810	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	867	ARG
2	B	869	THR
2	B	888	GLU
2	B	893	GLU
2	B	902	THR
2	B	916	HIS
2	B	925	LEU
2	B	945	THR
2	B	947	LEU
2	B	956	LYS
1	C	205	LYS
1	C	210	VAL
1	C	249	LEU
1	C	309	ASP
1	C	319	ARG
1	C	322	TRP
1	C	328	GLU
1	C	332	GLU
1	C	340	VAL
1	C	346	LEU
1	C	359	MET
1	C	405	LEU
1	C	423	ARG
1	C	427	HIS
1	C	431	GLN
1	C	436	GLU
1	C	458	LEU
1	C	502	LEU
1	C	514	VAL
1	C	517	PHE
1	C	539	VAL
1	C	555	LYS
1	C	564	ARG
1	C	578	THR
1	C	588	LEU
1	C	589	PRO
1	C	599	VAL
1	C	605	SER
1	C	648	ILE
1	C	650	VAL
1	C	656	LEU
1	C	722	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	758	ARG
1	C	782	THR
1	C	785	VAL
1	C	814	LYS
1	C	819	ASN
1	C	821	LYS
1	C	822	LEU
1	C	832	VAL
1	C	891	LYS
1	C	929	VAL
1	C	934	VAL
1	C	946	GLU
1	C	955	PHE
1	C	959	TRP
1	C	967	ASP
2	D	201	VAL
2	D	250	PHE
2	D	253	GLU
2	D	256	ARG
2	D	259	SER
2	D	273	GLU
2	D	281	LEU
2	D	287	LEU
2	D	297	VAL
2	D	301	ASP
2	D	322	LEU
2	D	336	LYS
2	D	343	THR
2	D	344	VAL
2	D	366	ARG
2	D	389	VAL
2	D	423	GLN
2	D	436	ARG
2	D	469	ARG
2	D	472	LEU
2	D	487	THR
2	D	510	SER
2	D	517	PRO
2	D	518	LEU
2	D	521	VAL
2	D	525	LYS
2	D	531	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	551	LYS
2	D	552	ARG
2	D	565	LEU
2	D	575	ASP
2	D	579	PRO
2	D	584	ASP
2	D	586	ARG
2	D	587	LEU
2	D	591	ILE
2	D	608	MET
2	D	673	PHE
2	D	688	GLU
2	D	698	ARG
2	D	700	ARG
2	D	701	GLU
2	D	702	SER
2	D	707	ARG
2	D	711	VAL
2	D	716	THR
2	D	793	LEU
2	D	794	SER
2	D	800	LEU
2	D	808	GLU
2	D	810	ARG
2	D	867	ARG
2	D	869	THR
2	D	888	GLU
2	D	916	HIS
2	D	932	VAL
2	D	945	THR
2	D	947	LEU
2	D	956	LYS
2	D	957	ARG
1	E	203	GLN
1	E	207	LYS
1	E	237	ASP
1	E	249	LEU
1	E	264	ARG
1	E	306	CYS
1	E	309	ASP
1	E	322	TRP
1	E	328	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	332	GLU
1	E	334	ARG
1	E	340	VAL
1	E	346	LEU
1	E	359	MET
1	E	405	LEU
1	E	423	ARG
1	E	427	HIS
1	E	431	GLN
1	E	436	GLU
1	E	448	ASN
1	E	458	LEU
1	E	502	LEU
1	E	514	VAL
1	E	517	PHE
1	E	539	VAL
1	E	555	LYS
1	E	564	ARG
1	E	578	THR
1	E	588	LEU
1	E	589	PRO
1	E	599	VAL
1	E	605	SER
1	E	622	HIS
1	E	648	ILE
1	E	650	VAL
1	E	656	LEU
1	E	758	ARG
1	E	766	VAL
1	E	782	THR
1	E	785	VAL
1	E	814	LYS
1	E	819	ASN
1	E	821	LYS
1	E	822	LEU
1	E	891	LYS
1	E	929	VAL
1	E	934	VAL
1	E	944	GLU
1	E	946	GLU
1	E	959	TRP
1	E	976	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	201	VAL
2	F	253	GLU
2	F	256	ARG
2	F	259	SER
2	F	273	GLU
2	F	277	ARG
2	F	281	LEU
2	F	287	LEU
2	F	301	ASP
2	F	322	LEU
2	F	336	LYS
2	F	343	THR
2	F	344	VAL
2	F	366	ARG
2	F	389	VAL
2	F	423	GLN
2	F	469	ARG
2	F	472	LEU
2	F	487	THR
2	F	510	SER
2	F	518	LEU
2	F	521	VAL
2	F	525	LYS
2	F	531	LEU
2	F	551	LYS
2	F	552	ARG
2	F	565	LEU
2	F	575	ASP
2	F	579	PRO
2	F	583	LYS
2	F	586	ARG
2	F	587	LEU
2	F	591	ILE
2	F	608	MET
2	F	636	ARG
2	F	673	PHE
2	F	688	GLU
2	F	700	ARG
2	F	701	GLU
2	F	702	SER
2	F	707	ARG
2	F	711	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	716	THR
2	F	793	LEU
2	F	794	SER
2	F	800	LEU
2	F	808	GLU
2	F	810	ARG
2	F	867	ARG
2	F	869	THR
2	F	888	GLU
2	F	893	GLU
2	F	916	HIS
2	F	925	LEU
2	F	945	THR
2	F	947	LEU
2	F	956	LYS
1	G	205	LYS
1	G	237	ASP
1	G	249	LEU
1	G	309	ASP
1	G	322	TRP
1	G	324	SER
1	G	328	GLU
1	G	332	GLU
1	G	340	VAL
1	G	346	LEU
1	G	359	MET
1	G	374	ARG
1	G	405	LEU
1	G	423	ARG
1	G	427	HIS
1	G	431	GLN
1	G	436	GLU
1	G	448	ASN
1	G	458	LEU
1	G	489	VAL
1	G	502	LEU
1	G	514	VAL
1	G	517	PHE
1	G	539	VAL
1	G	555	LYS
1	G	578	THR
1	G	588	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	589	PRO
1	G	599	VAL
1	G	605	SER
1	G	648	ILE
1	G	650	VAL
1	G	656	LEU
1	G	766	VAL
1	G	782	THR
1	G	785	VAL
1	G	814	LYS
1	G	821	LYS
1	G	822	LEU
1	G	832	VAL
1	G	891	LYS
1	G	929	VAL
1	G	934	VAL
1	G	944	GLU
1	G	946	GLU
1	G	948	ASN
1	G	950	GLU
1	G	959	TRP
1	G	963	ASN
1	G	972	ARG
1	G	975	LEU
2	H	201	VAL
2	H	253	GLU
2	H	256	ARG
2	H	259	SER
2	H	273	GLU
2	H	281	LEU
2	H	287	LEU
2	H	297	VAL
2	H	301	ASP
2	H	322	LEU
2	H	336	LYS
2	H	343	THR
2	H	366	ARG
2	H	423	GLN
2	H	436	ARG
2	H	469	ARG
2	H	472	LEU
2	H	487	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	510	SER
2	H	517	PRO
2	H	518	LEU
2	H	521	VAL
2	H	525	LYS
2	H	529	LYS
2	H	531	LEU
2	H	551	LYS
2	H	552	ARG
2	H	565	LEU
2	H	575	ASP
2	H	579	PRO
2	H	586	ARG
2	H	587	LEU
2	H	591	ILE
2	H	656	THR
2	H	673	PHE
2	H	688	GLU
2	H	700	ARG
2	H	701	GLU
2	H	702	SER
2	H	707	ARG
2	H	711	VAL
2	H	716	THR
2	H	793	LEU
2	H	794	SER
2	H	800	LEU
2	H	808	GLU
2	H	810	ARG
2	H	867	ARG
2	H	869	THR
2	H	888	GLU
2	H	900	ASP
2	H	902	THR
2	H	904	SER
2	H	916	HIS
2	H	925	LEU
2	H	932	VAL
2	H	945	THR
2	H	947	LEU
2	H	956	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
1	A	431	GLN
1	A	448	ASN
1	A	498	HIS
1	A	506	GLN
1	A	600	HIS
1	A	652	ASN
1	A	701	GLN
1	A	767	GLN
1	A	770	HIS
1	A	812	HIS
1	A	819	ASN
1	A	828	GLN
1	A	836	GLN
1	A	862	GLN
1	A	889	ASN
1	A	930	ASN
1	A	945	ASN
2	B	196	GLN
2	B	214	ASN
2	B	286	HIS
2	B	331	GLN
2	B	381	HIS
2	B	423	GLN
2	B	463	HIS
2	B	572	ASN
2	B	577	ASN
2	B	674	GLN
2	B	695	GLN
2	B	761	GLN
2	B	882	ASN
2	B	943	GLN
1	C	431	GLN
1	C	448	ASN
1	C	463	ASN
1	C	498	HIS
1	C	506	GLN
1	C	574	ASN
1	C	600	HIS
1	C	622	HIS
1	C	652	ASN
1	C	701	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	708	GLN
1	C	709	HIS
1	C	767	GLN
1	C	812	HIS
1	C	819	ASN
1	C	828	GLN
1	C	836	GLN
1	C	862	GLN
1	C	889	ASN
2	D	196	GLN
2	D	214	ASN
2	D	286	HIS
2	D	331	GLN
2	D	381	HIS
2	D	423	GLN
2	D	463	HIS
2	D	522	ASN
2	D	572	ASN
2	D	577	ASN
2	D	674	GLN
2	D	695	GLN
2	D	746	GLN
2	D	761	GLN
2	D	792	GLN
2	D	882	ASN
2	D	897	ASN
2	D	941	HIS
2	D	943	GLN
1	E	294	ASN
1	E	431	GLN
1	E	448	ASN
1	E	463	ASN
1	E	498	HIS
1	E	506	GLN
1	E	600	HIS
1	E	622	HIS
1	E	652	ASN
1	E	701	GLN
1	E	767	GLN
1	E	770	HIS
1	E	812	HIS
1	E	828	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	836	GLN
1	E	862	GLN
1	E	889	ASN
1	E	930	ASN
1	E	945	ASN
1	E	958	HIS
1	E	963	ASN
2	F	196	GLN
2	F	214	ASN
2	F	286	HIS
2	F	331	GLN
2	F	381	HIS
2	F	423	GLN
2	F	463	HIS
2	F	522	ASN
2	F	572	ASN
2	F	577	ASN
2	F	695	GLN
2	F	746	GLN
2	F	792	GLN
2	F	882	ASN
2	F	897	ASN
2	F	943	GLN
1	G	431	GLN
1	G	448	ASN
1	G	463	ASN
1	G	498	HIS
1	G	506	GLN
1	G	600	HIS
1	G	652	ASN
1	G	680	GLN
1	G	701	GLN
1	G	709	HIS
1	G	767	GLN
1	G	812	HIS
1	G	819	ASN
1	G	828	GLN
1	G	836	GLN
1	G	862	GLN
1	G	889	ASN
1	G	930	ASN
1	G	945	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	963	ASN
2	H	196	GLN
2	H	214	ASN
2	H	286	HIS
2	H	331	GLN
2	H	381	HIS
2	H	423	GLN
2	H	463	HIS
2	H	522	ASN
2	H	572	ASN
2	H	577	ASN
2	H	674	GLN
2	H	695	GLN
2	H	761	GLN
2	H	792	GLN
2	H	882	ASN
2	H	897	ASN
2	H	943	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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	$\# Z > 2$
4	FDP	A	1	-	20,20,20	0.98	0	27,32,32	0.85	1 (3%)
3	F6P	A	988	-	15,16,16	0.94	0	16,25,25	3.85	5 (31%)
4	FDP	B	2	-	20,20,20	0.98	0	27,32,32	0.90	1 (3%)
3	F6P	B	980	-	15,16,16	1.05	1 (6%)	16,25,25	1.01	1 (6%)
4	FDP	C	3	-	20,20,20	1.00	0	27,32,32	0.88	1 (3%)
3	F6P	C	988	-	15,16,16	0.92	0	16,25,25	0.86	0
4	FDP	D	4	-	20,20,20	0.97	0	27,32,32	0.91	2 (7%)
3	F6P	D	982	-	15,16,16	0.90	0	16,25,25	0.75	0
4	FDP	E	5	-	20,20,20	0.98	0	27,32,32	0.99	2 (7%)
3	F6P	E	988	-	15,16,16	0.84	0	16,25,25	0.76	0
4	FDP	F	6	-	20,20,20	0.99	0	27,32,32	1.02	3 (11%)
3	F6P	F	984	-	15,16,16	0.90	0	16,25,25	0.88	0
4	FDP	G	7	-	20,20,20	0.98	0	27,32,32	0.93	2 (7%)
3	F6P	G	988	-	15,16,16	1.10	2 (13%)	16,25,25	3.76	6 (37%)
4	FDP	H	8	-	20,20,20	1.00	0	27,32,32	1.03	1 (3%)
3	F6P	H	986	-	15,16,16	0.85	0	16,25,25	0.75	0

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
4	FDP	A	1	-	-	0/12/34/34	0/1/1/1
3	F6P	A	988	-	-	0/9/28/28	0/1/1/1
4	FDP	B	2	-	-	0/12/34/34	0/1/1/1
3	F6P	B	980	-	-	0/9/28/28	0/1/1/1
4	FDP	C	3	-	-	0/12/34/34	0/1/1/1
3	F6P	C	988	-	-	0/9/28/28	0/1/1/1
4	FDP	D	4	-	-	0/12/34/34	0/1/1/1
3	F6P	D	982	-	-	0/9/28/28	0/1/1/1
4	FDP	E	5	-	-	0/12/34/34	0/1/1/1
3	F6P	E	988	-	-	0/9/28/28	0/1/1/1
4	FDP	F	6	-	-	0/12/34/34	0/1/1/1
3	F6P	F	984	-	-	0/9/28/28	0/1/1/1
4	FDP	G	7	-	-	0/12/34/34	0/1/1/1
3	F6P	G	988	-	-	0/9/28/28	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FDP	H	8	-	-	0/12/34/34	0/1/1/1
3	F6P	H	986	-	-	0/9/28/28	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	988	F6P	O5-C2	-2.20	1.39	1.43
3	G	988	F6P	P-O2P	2.05	1.62	1.54
3	B	980	F6P	P-O3P	2.35	1.63	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	988	F6P	O3P-P-O1P	-8.22	84.12	110.58
3	A	988	F6P	O3P-P-O6	-8.07	83.32	106.56
3	G	988	F6P	O3P-P-O6	-8.00	83.52	106.56
3	G	988	F6P	O3P-P-O1P	-7.72	85.74	110.58
3	A	988	F6P	O3P-P-O2P	-6.35	83.21	107.38
3	G	988	F6P	O3P-P-O2P	-5.92	84.83	107.38
3	B	980	F6P	O5-C5-C6	-2.27	104.31	109.49
4	F	6	FDP	C2-O5-C5	-2.13	102.27	108.44
4	G	7	FDP	O6-P2-O4P	2.01	112.25	107.14
4	D	4	FDP	O6-P2-O4P	2.15	112.61	107.14
4	C	3	FDP	O2-P1-O1P	2.32	112.90	107.11
4	D	4	FDP	O2-P1-O1P	2.32	112.90	107.11
4	B	2	FDP	O2-P1-O1P	2.34	112.94	107.11
3	G	988	F6P	O2P-P-O1P	2.34	118.12	110.58
4	E	5	FDP	O6-P2-O4P	2.35	113.13	107.14
4	F	6	FDP	O6-P2-O4P	2.40	113.26	107.14
4	A	1	FDP	O2-P1-O1P	2.40	113.11	107.11
4	F	6	FDP	O2-P1-O1P	2.61	113.64	107.11
4	H	8	FDP	O2-P1-O1P	2.67	113.77	107.11
3	G	988	F6P	O2P-P-O6	2.77	114.54	106.56
4	E	5	FDP	O2-P1-O1P	2.78	114.05	107.11
4	G	7	FDP	O2-P1-O1P	2.88	114.30	107.11
3	A	988	F6P	O2P-P-O6	3.19	115.76	106.56
3	G	988	F6P	O6-P-O1P	6.94	124.80	107.14
3	A	988	F6P	O6-P-O1P	7.01	124.98	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	FDP	6	0
3	A	988	F6P	4	0
4	B	2	FDP	3	0
3	B	980	F6P	4	0
4	C	3	FDP	1	0
3	C	988	F6P	1	0
4	D	4	FDP	2	0
3	D	982	F6P	3	0
3	E	988	F6P	2	0
4	F	6	FDP	3	0
3	F	984	F6P	4	0
3	G	988	F6P	2	0
4	H	8	FDP	2	0
3	H	986	F6P	5	0

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	A	750/787 (95%)	0.02	26 (3%)	48	40	22, 61, 81, 81	67 (8%)
1	C	750/787 (95%)	0.06	34 (4%)	37	31	16, 56, 81, 81	49 (6%)
1	E	752/787 (95%)	-0.06	22 (2%)	55	49	22, 53, 81, 81	58 (7%)
1	G	744/787 (94%)	-0.10	29 (3%)	43	36	19, 52, 81, 81	60 (8%)
2	B	763/766 (99%)	0.06	25 (3%)	50	42	27, 70, 81, 81	88 (11%)
2	D	761/766 (99%)	-0.14	16 (2%)	67	62	20, 60, 81, 81	54 (7%)
2	F	762/766 (99%)	-0.07	22 (2%)	55	49	25, 61, 81, 81	61 (8%)
2	H	763/766 (99%)	-0.30	5 (0%)	89	88	21, 47, 79, 81	37 (4%)
All	All	6045/6212 (97%)	-0.07	179 (2%)	54	47	16, 57, 81, 81	474 (7%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	812	HIS	7.1
1	C	815	GLY	7.0
1	G	327	ASP	6.6
1	G	326	VAL	6.2
1	C	949	VAL	6.0
1	C	813	ASP	5.9
2	F	895	ASN	5.9
1	G	342	PRO	5.4
1	G	325	LEU	5.1
1	G	338	GLU	4.9
2	F	893	GLU	4.8
2	F	896	PHE	4.7
1	C	805	LEU	4.6
1	C	587	LEU	4.6
2	D	941	HIS	4.6
1	A	949	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	812	HIS	4.4
2	F	582	PRO	4.2
1	E	325	LEU	4.1
1	C	955	PHE	4.1
1	G	341	ALA	4.0
2	F	271	CYS	4.0
2	D	895	ASN	4.0
1	C	829	ALA	3.8
2	F	581	LEU	3.8
1	C	954	GLY	3.8
1	G	322	TRP	3.7
1	A	340	VAL	3.7
2	F	892	ALA	3.6
1	C	556	ASP	3.6
1	G	323	PRO	3.6
2	D	666	LEU	3.5
2	F	553	ALA	3.5
1	E	326	VAL	3.5
2	F	325	ASN	3.5
1	E	811	ARG	3.5
1	C	552	ILE	3.5
2	B	472	LEU	3.5
2	D	417	ALA	3.4
2	B	417	ALA	3.4
2	F	545	ILE	3.4
1	A	813	ASP	3.4
1	A	279	SER	3.4
1	C	845	ALA	3.4
1	E	552	ILE	3.3
1	A	587	LEU	3.3
2	B	896	PHE	3.3
1	C	554	ASN	3.2
1	C	948	ASN	3.2
1	G	320	HIS	3.2
1	E	980	ALA	3.1
1	E	819	ASN	3.1
1	G	330	VAL	3.1
1	C	589	PRO	3.1
1	A	467	ALA	3.1
1	E	544	LEU	3.1
1	C	814	LYS	3.1
2	H	891	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	978	GLU	3.1
1	A	335	PHE	3.0
1	G	339	GLU	3.0
1	G	347	SER	3.0
1	A	334	ARG	3.0
1	A	277	ALA	3.0
1	E	948	ASN	3.0
2	D	926	TYR	3.0
1	G	788	TYR	2.9
1	A	517	PHE	2.9
1	G	757	THR	2.9
1	A	470	VAL	2.9
1	C	788	TYR	2.9
2	F	899	ASP	2.9
1	G	754	ALA	2.9
1	C	797	ALA	2.8
2	B	538	THR	2.8
1	C	560	ALA	2.8
2	D	897	ASN	2.8
1	A	333	GLY	2.8
2	D	665	ASP	2.7
2	F	938	LYS	2.7
1	E	345	ASN	2.7
1	C	846	SER	2.7
2	B	466	LEU	2.7
2	D	603	SER	2.7
2	B	666	LEU	2.7
2	H	933	SER	2.6
1	G	324	SER	2.6
1	G	948	ASN	2.6
1	A	521	THR	2.6
1	G	321	GLU	2.5
1	E	250	ARG	2.5
1	E	548	VAL	2.5
1	G	824	VAL	2.5
2	B	811	GLY	2.5
2	B	887	ALA	2.5
2	B	273	GLU	2.5
2	D	892	ALA	2.5
2	F	542	ALA	2.5
2	H	892	ALA	2.5
1	A	339	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	557	PHE	2.5
2	F	702	SER	2.5
1	G	302	ALA	2.5
1	A	979	VAL	2.5
2	B	545	ILE	2.5
1	C	282	PHE	2.5
1	A	815	GLY	2.5
1	E	327	ASP	2.4
1	C	541	SER	2.4
1	C	298	GLN	2.4
2	D	545	ILE	2.4
1	A	947	THR	2.4
1	E	808	GLU	2.4
1	A	479	LEU	2.4
2	B	541	VAL	2.4
1	C	830	SER	2.4
1	G	343	TYR	2.4
2	B	455	THR	2.4
2	H	896	PHE	2.3
2	B	895	ASN	2.3
2	F	329	ASN	2.3
1	C	951	LEU	2.3
1	E	560	ALA	2.3
2	B	886	ILE	2.3
1	A	287	GLY	2.3
1	E	821	LYS	2.3
1	C	329	LEU	2.3
2	F	703	TYR	2.3
1	C	893	GLU	2.3
2	D	664	ALA	2.3
1	G	286	GLU	2.3
2	B	888	GLU	2.3
2	B	582	PRO	2.3
2	F	933	SER	2.3
1	C	950	GLU	2.3
2	D	807	ALA	2.3
1	G	279	SER	2.3
2	F	808	GLU	2.3
1	C	943	TRP	2.3
2	B	956	LYS	2.3
1	C	606	ALA	2.2
2	B	279	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	733	SER	2.2
1	E	803	ILE	2.2
2	B	702	SER	2.2
1	G	340	VAL	2.2
2	F	243	GLY	2.2
1	G	848	GLY	2.2
1	A	332	GLU	2.2
1	C	553	GLU	2.2
2	H	931	GLU	2.2
1	C	945	ASN	2.2
1	A	288	ARG	2.2
1	G	552	ILE	2.2
1	A	325	LEU	2.2
2	B	915	SER	2.2
2	F	664	ALA	2.2
2	D	418	THR	2.2
2	F	931	GLU	2.2
2	B	576	HIS	2.2
2	B	703	TYR	2.2
2	D	452	ALA	2.2
1	E	722	THR	2.2
1	A	955	PHE	2.1
1	E	333	GLY	2.1
1	A	948	ASN	2.1
2	D	537	LEU	2.1
1	E	807	LYS	2.1
2	B	468	ASP	2.1
1	G	465	VAL	2.1
1	C	254	TYR	2.1
1	E	949	VAL	2.1
1	E	322	TRP	2.1
2	D	582	PRO	2.0
2	B	911	GLY	2.0
1	G	248	LEU	2.0
2	B	437	GLY	2.0
1	G	281	GLU	2.0
2	F	888	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	FDP	C	3	20/20	0.85	0.34	3.73	79,82,82,82	0
4	FDP	H	8	20/20	0.85	0.33	2.73	81,82,82,82	0
4	FDP	F	6	20/20	0.89	0.27	1.96	81,82,82,82	0
3	F6P	D	982	16/16	0.94	0.22	1.63	65,67,70,71	0
3	F6P	G	988	16/16	0.96	0.20	1.48	61,62,64,68	0
4	FDP	A	1	20/20	0.91	0.21	1.09	77,82,82,82	0
4	FDP	B	2	20/20	0.95	0.17	0.89	65,68,70,71	0
3	F6P	E	988	16/16	0.94	0.19	0.56	62,66,66,68	0
3	F6P	C	988	16/16	0.92	0.19	0.50	75,78,80,80	0
3	F6P	H	986	16/16	0.97	0.16	0.45	41,47,47,49	0
3	F6P	F	984	16/16	0.95	0.18	0.35	56,57,63,64	0
3	F6P	A	988	16/16	0.91	0.17	0.14	79,82,82,82	0
4	FDP	G	7	20/20	0.91	0.18	0.14	80,82,82,82	0
4	FDP	D	4	20/20	0.96	0.14	-0.44	52,54,56,57	0
3	F6P	B	980	16/16	0.93	0.16	-0.80	77,80,82,82	0
4	FDP	E	5	20/20	0.95	0.15	-0.85	66,70,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.