



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:14 AM UTC

PDB ID : 6WOX / pdb_00006wox
Title : Thermus thermophilus RNA polymerase initially transcribing complex with 2'dCTP
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2020-04-26
Resolution : 3.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

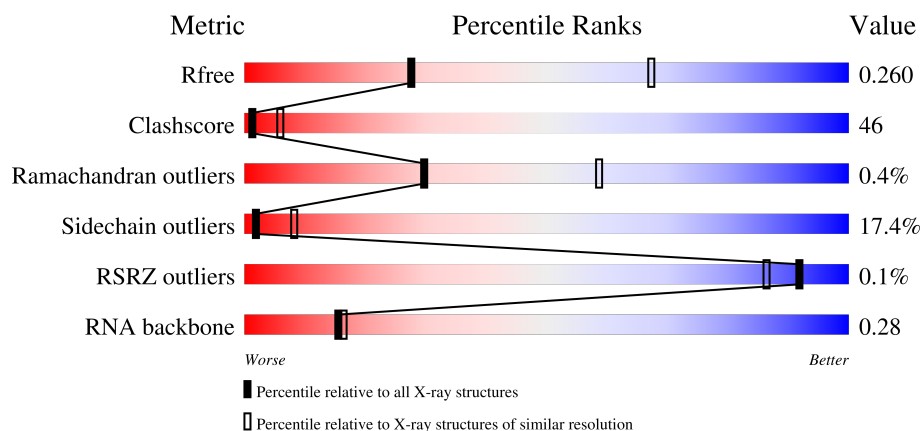
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 Å.

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



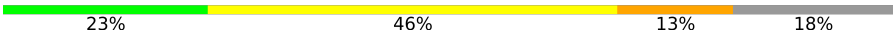
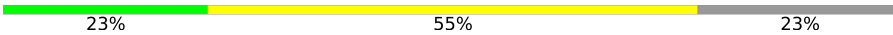
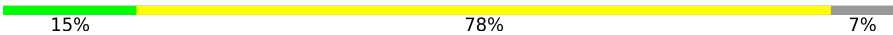
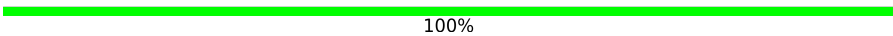
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)
RNA backbone	3983	1040 (3.38-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	315	15% 46% 10% 28%
1	B	315	21% 41% 9% 29%
2	C	1119	34% 55% 10% .
3	D	1505	37% 52% 10% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	99	 32% 56% 7% 5%
5	F	423	 23% 46% 13% 18%
6	G	22	 23% 55% 23%
7	H	27	 15% 78% 7%
8	I	3	 100%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 28581 atoms, of which 12 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1485	Total	C	N	O	S	0	0	0
			11721	7431	2063	2192	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	86	LYS	ARG	conflict	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			351	166	65	103	17			

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

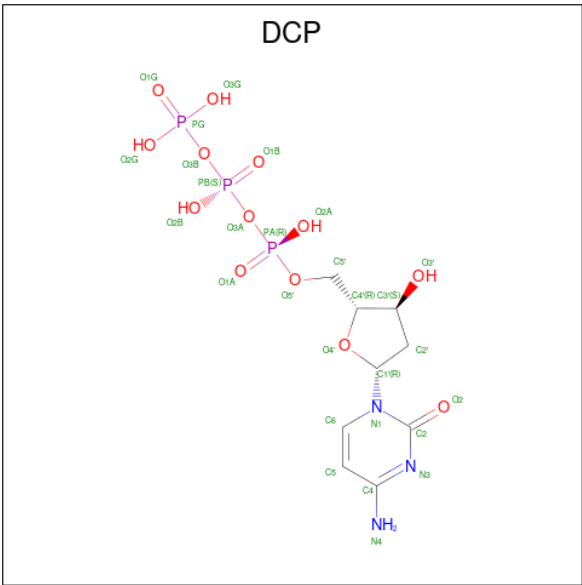
- Molecule 8 is a RNA chain called RNA (5'-R(*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			62	29	13	18	2			

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Na	0	0
			1	1		

- Molecule 10 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
10	D	1	Total	C	H	N	O	P	0	0
			40	9	12	3	13	3		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Mg	0	0
			1	1		

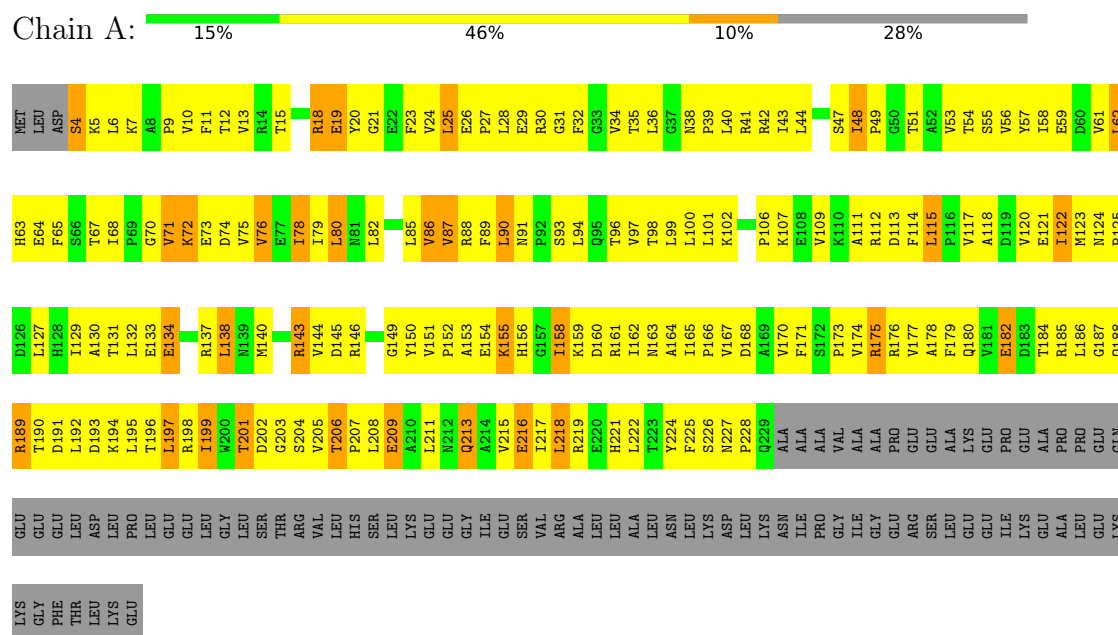
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	2	Total	Zn	0	0
			2	2		

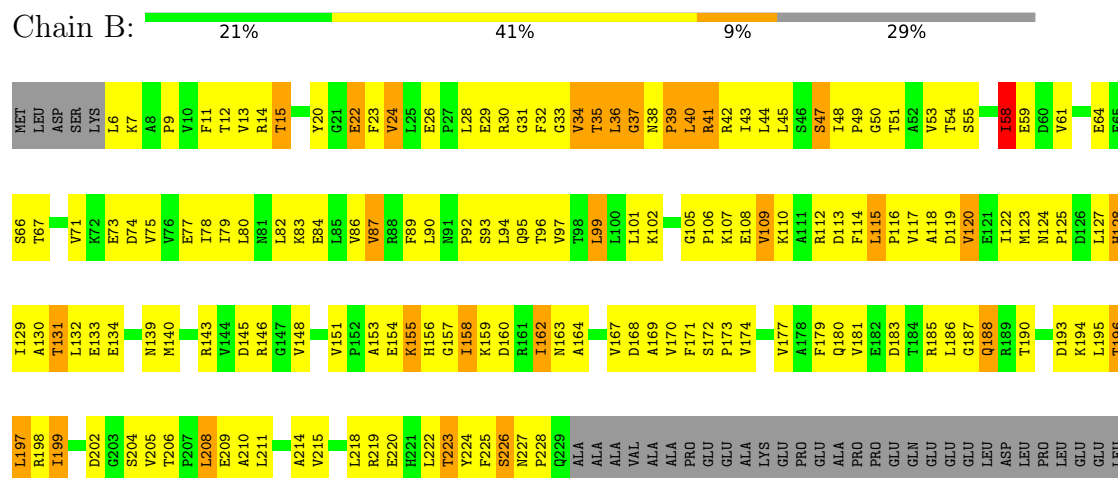
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



GLY	LEU	SER	THR	ARG	VAL	LEU	HIS	SER	LYS	GLU	GLY	ILE	SER	VAL	ARG	ALA	LEU	LEU	ALA	LEU	LEU	LEU	ASN	ILE	PRO	GLY	ILE	R39	GLY	GLY	ARG	SER	LEU	GLU	GLY	LYS	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 2: DNA-directed RNA polymerase subunit beta

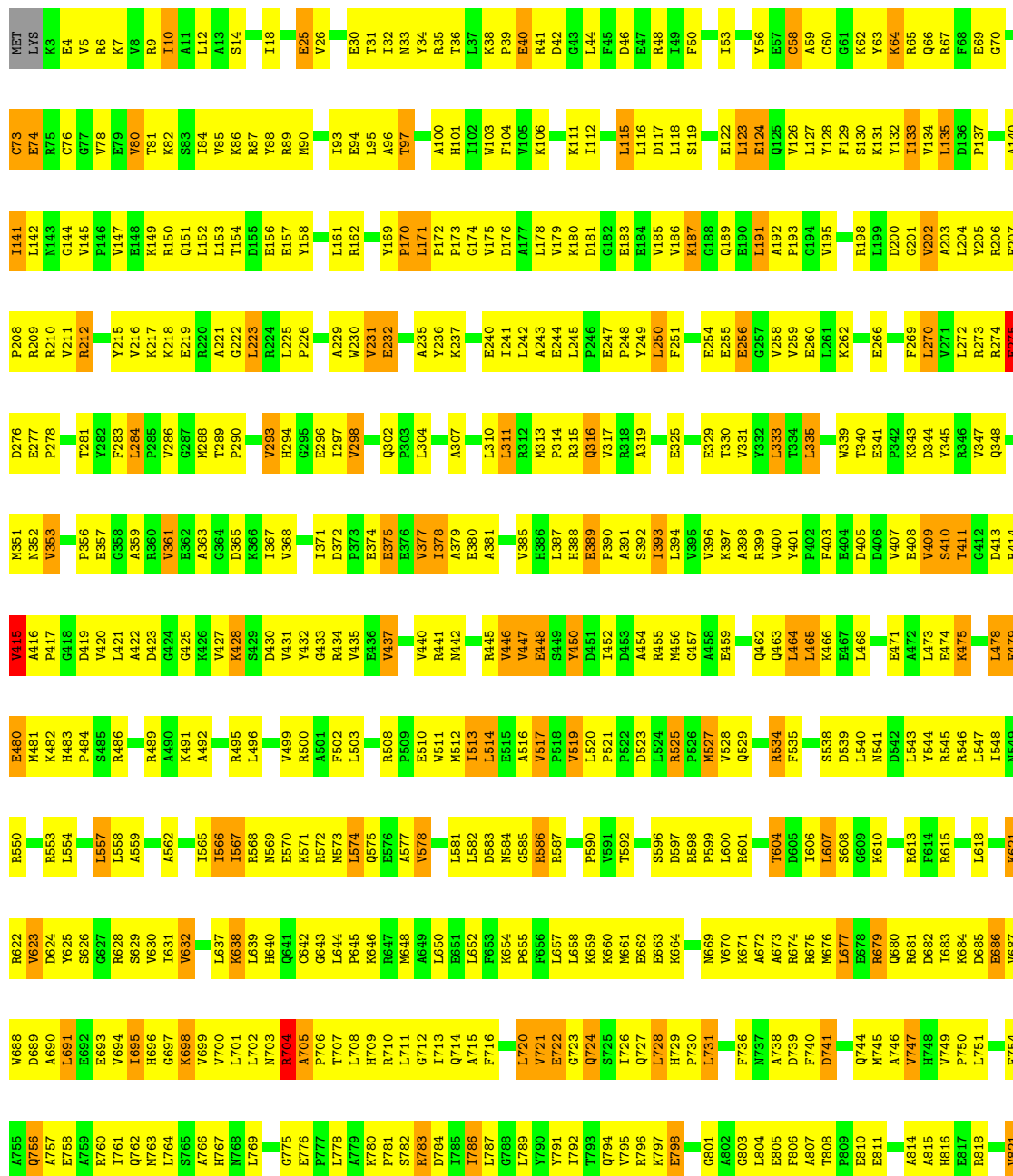
Chain C:  34% 55% 10%

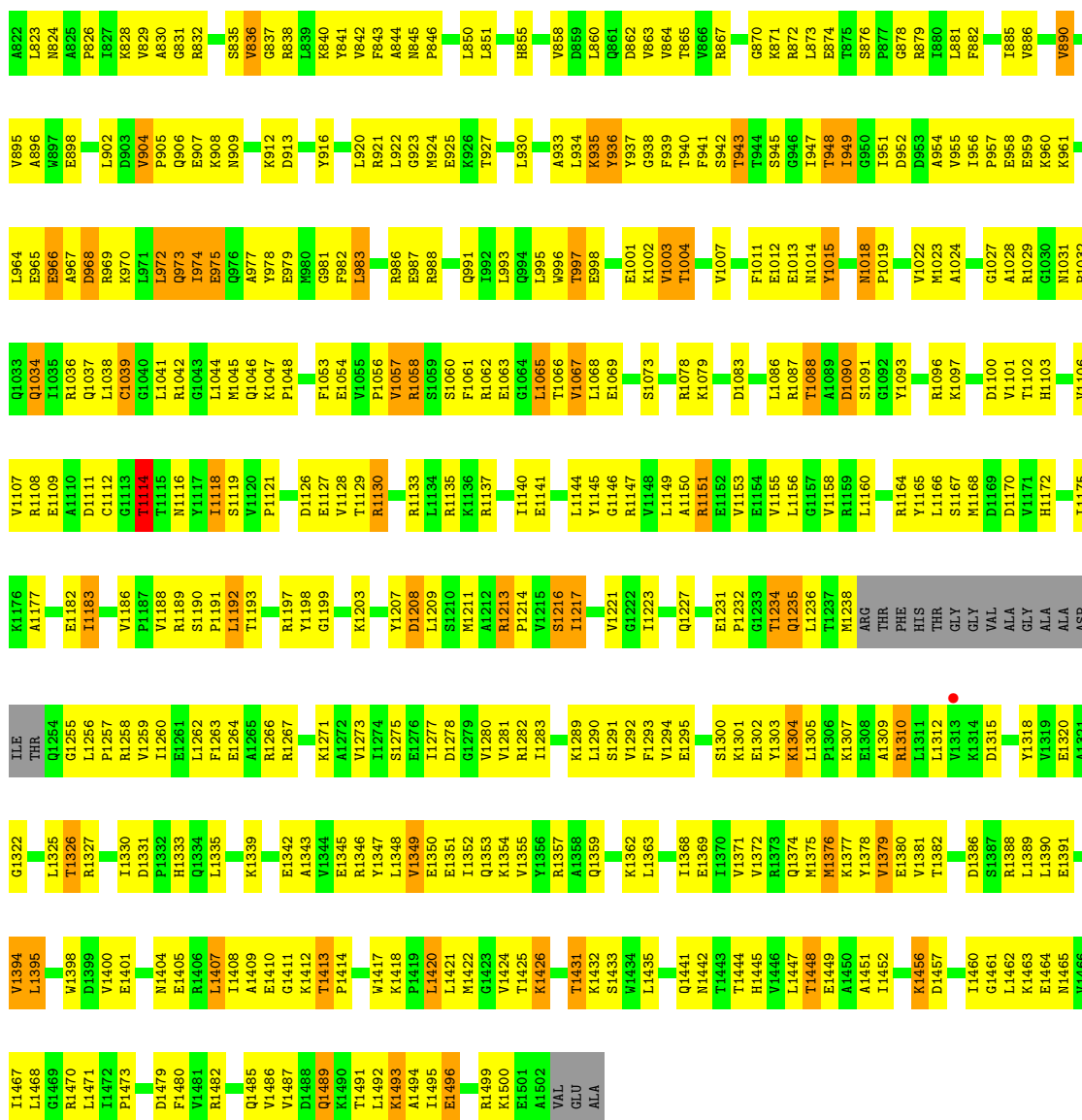
P904	D837	R772	E706		Q567	A497	G424	M359	I283	G215	I140	D67	M1
R906	K839	L773	R707	Q639	A568	Q498	F425	M359	R284	E216	I140	D67	E2
F906	L839	L774	T708	R640	A499	A499	D426	M361	L285	L217	S143	Y71	I3
G908	N841	D975	E709	R641	P570	N500	V427	M361	L290	Q219	F148	L73	F6
A909	R842	S776	T710	R642	L571	T501	R428	M362	L291	G220	T149	G74	G7
K910	H843	I777	E711	V643	L572	P502	D429	S363	R292	L221	P150	E75	R8
E911		E780	A712	V644		L503		S364	E364	M222		P76	
P912	V848	K781	T715	V645	P577	E504	R432	D385	F293	L222	R154		R10
E913	V849	A782	K716	V649	V578	I508	T433	S366	E297	D223		R84	E11
I914	A850	R783	L717	R650	N580	A509	H434	L367	F298	E224	R157	E85	V12
K915	R851	D784	R718	K651	T581	A510	V435	T368	K299	S225		K86	
E916	L852	V785	P719	K651	G582	E511	R437	P369	D300	F227	A160	D87	L15
	R853	K786	E720	L655	L583	R512	I438	A370	E301	A228	S161	L88	
Q920	P854	D787	E721	A656	E584	V513	C439	K371	L372	M229	I162		L18
A921	V855	T788	R723	D657	S585	V514		V373	P305	R230	I163		T19
F922		S789	T724	D657	R586		E442	N374		E233	P164		E20
		R790	D725	S661	V587	B517	T443	S375	Y309	E334		P93	I21
F926	R858	L791	D726	E662	V588	K518	P444	R376	L310	A234	K167	L94	Q22
G927	H860	V792	T727	N663	V589	Q519	E445	P377	F311	L235	R168	Y95	V23
K928	L861	P793	H728	G664	D590	E510	G446	L378	A312	I236	G169	A96	E24
R929	P862		E729	F665	S591	V524	A447	E379	L313	R237	P170	R97	
G930	D863	E796	S730	L666	L592		R448		T314	L238	W171	Y26	
K931	R864	K797		A667	A593	E528	I449	R383		F239	I172	L100	R27
E932	T865	G798	L734	L668	A594	V529	G450	E384	V317	T240	D173	L101	R28
G933	P866	V799	R735	G669	L595	E530	L451	F385	G319	L241	L174	H102	A29
F934	R867	V800	D736	Q670	Y596	F531	L452	F386	P318	R242	E175	K103	L30
G935	R868	R801	L737	N671	A597	N532	T453	R387	G320	R243	V176	D104	Q31
V936	R869	R802	D738	V672	E598	D533	S454	R388	E321	E177	M105	T105	A32
D937	T870	T803	E739	L673	E599	V634		S389	V322	D246	P178	G106	D33
K938	L871	V804	E740	V674	S535		A459	Q390	D323	P247	H179	L107	
R939	N872	R805	G741	A675	P536	E602	R460	L391		R248	G180	I108	P36
E940	L873		V742	L676	A603	K537	V461	S392	D326	K249	V181	E109	E37
V941	R874	R808	V743	M677	E604	Q538	D462		G327	R250	V182	K109	
	G875		R744	P678	K605	V539	E463		L328		S183	D111	R39
V943	R876		I745	F679	V606	F540	L464	K395		A253	M184	E112	E40
L944	P877	G812		D680	D607	S541		D396	R331	V254	K185	V113	M41
R945	R878	V813	E748	G681	G608	V542	T467	T398	R332			F114	
E946	R879	E814	V749	E682	N609	N543	R468	N399	R333	V257	K190	L115	T44
A947	N880	R815	P751	V682	R610	T544		P400	R334	G258		Y258	Q45
K948	R881	K816	G752	F684	T611	N545	R472	L401	T335	G259	L193	I118	A46
	L882		D753	E685	V612	L546	R473	S402	V336	L260	L194	P119	
R949	G883	V819	I754		R613	L647	V475	S403	G337	I261	L195	M121	R49
Q951	K884	R820	L755	V689	V614	P548	V476	L404	E338	A262	L196	G204	E50
L952	L885	E821	T756	L690	Y615	R614	V477	R405	L339	R405	V194	P119	
V953	L886	V822	G757	S691	E616	L550	G477	H406	P264	P264	L197	M121	F51
	R887	V823	R758	E692	D617	E551	V478	K407	T341	R265		D124	P53
T954	R888	R824	T759	E693	G618			R408	D342	R266	L200	F127	I54
	R889	V825	T760	L694	R619	D554	E482	R409	Q343	R267		I128	E55
K957	V890	R826	F761	L695	L620			I410	F344	Y267	D203	I128	E56
P959	G891	V827	K762	K696	V621	R557	Y485	S411	R345	D268	Q204	I129	
E960	L892		G763	R697	A568	M486	T487	A412	L269	G270	T206	G131	ASP
		Q828	E764	D698	R626	L559	L413	L413	E271	L207	A208	A132	LYS
E961	R897	V830	S765	F699	R627	V560	A488	G414	L348	A272		D133	GLY
Q962	Q898	R831	T766	Y700	F628	G661			L351		R209	I134	LYS
L963	R899	V832	P767	T701	V629	S562	D492	L418	A352	E278	E210	V135	GLY
	R900	N901	T768	S702	R630	M663	R493	T419	R353	E279	G212	I136	GLY
F967	Y901	Q834	P769	I703	S631	M564	Y494		G354	K280	G212	V137	L64
L968	L902	V835	E770	H704	N632	O565	T495	R422	V355	L261	A213	L281	V65
V969	R903	G926	E771	T705	E623	T566	L486	A423	R356	G292		O149	



• Molecule 3: DNA-directed RNA polymerase subunit beta'

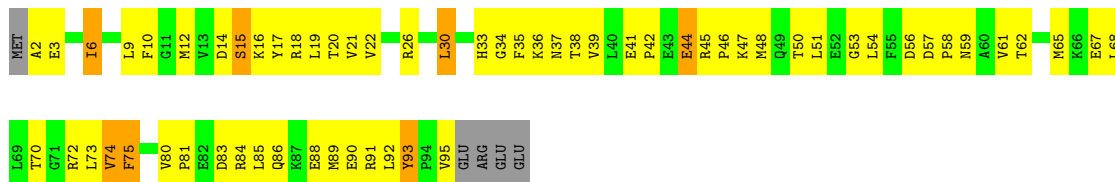
Chain D: 37% 52% 10% .





• Molecule 4: DNA-directed RNA polymerase subunit omega

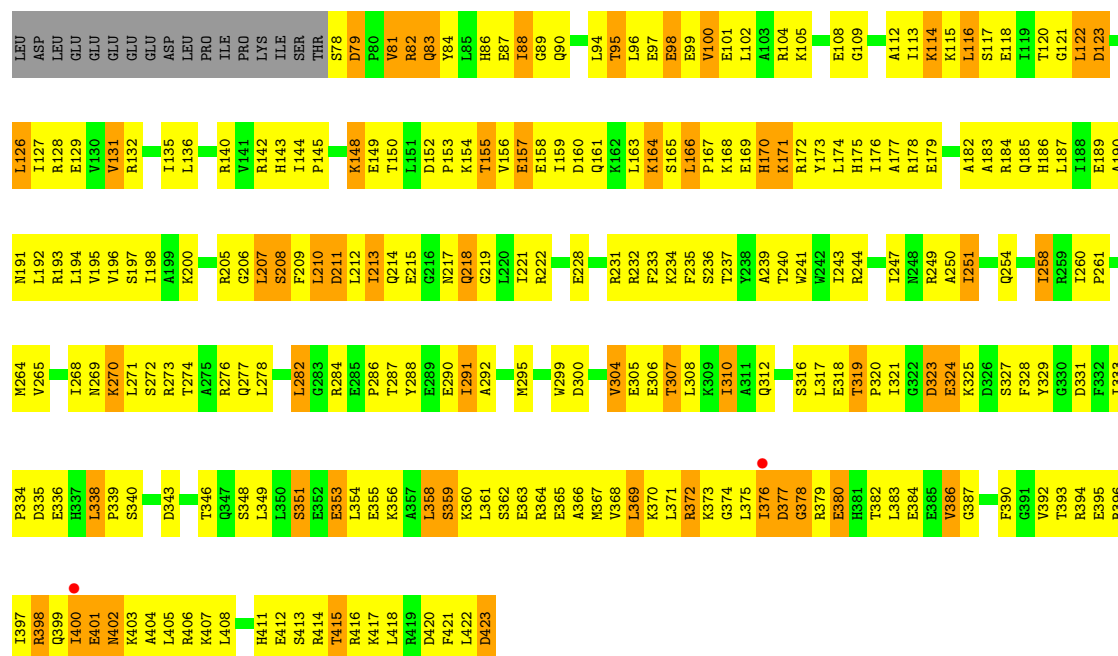
Chain E: 32% 56% 7% 5%



• Molecule 5: RNA polymerase sigma factor SigA

Chain F: 23% 46% 13% 18%





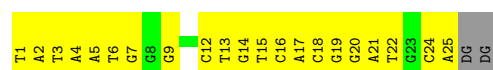
- Molecule 6: DNA (5'-D(P*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*A P*G)-3')

Chain G: 23% 55% 23%



- Molecule 7: DNA (25-MER)

Chain H: 15% 78% 7%



- Molecule 8: RNA (5'-R(*GP*CP*A)-3')

Chain I: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.44Å 102.65Å 295.38Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	29.93 – 3.14 29.93 – 3.14	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.93-3.14) 93.5 (29.93-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.196 , 0.261 0.197 , 0.260	Depositor DCC
R_{free} test set	2004 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28581	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	0/1814	0.68	0/2466
1	B	0.47	0/1799	0.68	0/2447
2	C	0.47	1/8937 (0.0%)	0.69	1/12087 (0.0%)
3	D	0.48	2/11927 (0.0%)	0.72	8/16127 (0.0%)
4	E	0.44	0/775	0.63	0/1045
5	F	0.44	0/2852	0.66	0/3837
6	G	0.57	0/393	0.64	0/605
7	H	0.52	0/580	0.65	0/895
8	I	0.42	0/69	0.74	0/106
All	All	0.47	3/29146 (0.0%)	0.70	9/39615 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
3	D	0	5
5	F	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	135	LEU	C-N	5.89	1.38	1.33
3	D	1114	THR	CB-CG2	5.33	1.70	1.52
2	C	682	TYR	CA-C	5.18	1.59	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	135	LEU	CA-C-N	6.78	129.32	122.00
3	D	135	LEU	C-N-CA	6.78	129.32	122.00
2	C	682	TYR	O-C-N	-6.77	113.59	122.59
3	D	170	PRO	CA-C-N	-5.82	105.08	122.71
3	D	170	PRO	C-N-CA	-5.82	105.08	122.71
3	D	1234	THR	CA-C-N	5.71	131.99	121.70
3	D	1234	THR	C-N-CA	5.71	131.99	121.70
3	D	415	VAL	CA-C-N	5.52	135.26	121.80
3	D	415	VAL	C-N-CA	5.52	135.26	121.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	ILE	Peptide
2	C	362	GLY	Peptide
3	D	275	GLU	Peptide
3	D	64	LYS	Peptide
3	D	704	ARG	Peptide
3	D	782	SER	Peptide
3	D	983	LEU	Peptide
5	F	323	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	226	0
1	B	1767	0	1816	222	0
2	C	8770	0	8874	850	0
3	D	11721	0	11941	1167	0
4	E	761	0	778	89	0
5	F	2807	0	2882	300	0
6	G	351	0	192	17	0
7	H	516	0	283	41	0
8	I	62	0	34	0	0
9	C	1	0	0	0	0
10	D	28	12	12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	1	0	0	0	0
12	D	2	0	0	0	0
All	All	28569	12	28646	2656	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (2656) 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)
3:D:203:ALA:HB1	3:D:393:ILE:HD11	1.17	1.15
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.21	1.14
3:D:1234:THR:HB	3:D:1235:GLN:HB2	1.31	1.13
3:D:767:HIS:HA	3:D:924:MET:HE3	1.28	1.12
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	1.21	1.12
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.21	1.11
2:C:805:ARG:HG3	2:C:823:VAL:HG23	1.31	1.10
3:D:367:ILE:HD11	3:D:379:ALA:HB2	1.35	1.09
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.17	1.08
2:C:766:GLU:HG2	2:C:767:PRO:HD2	1.34	1.08
5:F:362:SER:HB3	5:F:365:GLU:HG2	1.30	1.07
3:D:657:LEU:HG	3:D:661:MET:HE2	1.34	1.06
2:C:690:ILE:HG13	2:C:852:ILE:HG23	1.37	1.06
3:D:65:ARG:HB3	5:F:377:ASP:HA	1.37	1.06
3:D:1060:SER:HB3	3:D:1063:GLU:HG3	1.32	1.06
1:B:53:VAL:HG12	1:B:167:VAL:HG11	1.33	1.05
2:C:690:ILE:HD11	2:C:852:ILE:HD13	1.38	1.05
2:C:474:VAL:HG11	2:C:529:VAL:HG12	1.38	1.05
3:D:683:ILE:HG23	3:D:687:VAL:HG11	1.39	1.05
3:D:70:GLY:H	3:D:80:VAL:HG23	1.19	1.04
1:A:88:ARG:HB3	1:A:123:MET:HE3	1.36	1.04
5:F:412:GLU:HG3	5:F:418:LEU:HD13	1.40	1.03
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.41	1.02
3:D:791:TYR:CE1	3:D:945:SER:HB2	1.95	1.02
4:E:9:LEU:HD23	4:E:12:MET:HE3	1.40	1.01
2:C:878:SER:HA	3:D:1034:GLN:HE22	1.22	1.01
1:A:25:LEU:HB3	1:A:28:LEU:HD11	1.39	1.00
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.42	1.00
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.41	1.00
2:C:734:LEU:HD23	2:C:737:LEU:HD12	1.44	1.00
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.43	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:O	1:A:155:LYS:NZ	1.95	0.99
2:C:944:LEU:HD11	2:C:963:LEU:HD21	1.46	0.98
3:D:582:LEU:O	3:D:604:THR:HG23	1.65	0.97
2:C:1012:PRO:HB2	2:C:1021:LEU:HD13	1.46	0.97
2:C:890:LEU:HB2	2:C:914:ILE:HD12	1.46	0.96
3:D:689:ASP:HB3	4:E:51:LEU:HD13	1.44	0.96
5:F:361:LEU:HD11	5:F:411:HIS:HB2	1.48	0.96
2:C:495:THR:HG23	2:C:517:ARG:HG3	1.45	0.95
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.31	0.95
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.48	0.95
1:A:88:ARG:CB	1:A:123:MET:HE3	1.97	0.95
3:D:1273:VAL:H	3:D:1326:THR:HG23	1.30	0.95
3:D:259:VAL:HG13	3:D:270:LEU:HD21	1.49	0.94
3:D:1234:THR:CB	3:D:1235:GLN:HB2	1.98	0.93
5:F:95:THR:H	5:F:98:GLU:HG3	1.31	0.93
5:F:386:VAL:HA	5:F:390:PHE:CE1	2.02	0.93
2:C:775:ARG:HH11	5:F:422:LEU:HD23	1.30	0.93
3:D:709:HIS:HA	3:D:1227:GLN:HG2	1.48	0.92
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.02	0.92
3:D:65:ARG:CB	5:F:377:ASP:HA	2.00	0.92
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.51	0.92
2:C:182:VAL:HG22	2:C:221:LEU:HD23	1.50	0.91
2:C:674:VAL:HG23	2:C:869:VAL:HB	1.48	0.91
3:D:1042:ARG:HB3	3:D:1057:VAL:HG13	1.52	0.91
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.02	0.91
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.52	0.91
2:C:958:THR:HG23	2:C:961:GLU:HG3	1.53	0.91
3:D:520:LEU:O	3:D:525:ARG:NH1	2.03	0.91
2:C:878:SER:HA	3:D:1034:GLN:NE2	1.85	0.91
2:C:180:GLY:O	2:C:217:LEU:HD22	1.70	0.90
3:D:67:ARG:NH2	5:F:377:ASP:OD2	2.04	0.90
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.54	0.90
2:C:751:PRO:HA	2:C:792:VAL:HG22	1.52	0.89
2:C:627:ARG:HH21	2:C:641:PRO:HD3	1.35	0.89
2:C:715:THR:HG22	2:C:717:LEU:H	1.37	0.89
3:D:407:VAL:HG13	3:D:422:ALA:HB2	1.53	0.89
3:D:1342:GLU:N	3:D:1342:GLU:OE1	2.03	0.89
2:C:690:ILE:CG1	2:C:852:ILE:HG23	2.03	0.89
2:C:815:LEU:HD12	2:C:819:VAL:HG23	1.53	0.89
1:A:62:LEU:HA	1:A:163:ASN:HB3	1.55	0.88
2:C:569:VAL:HG21	2:C:1000:MET:CE	2.03	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1479:ASP:OD1	3:D:1482:ARG:NH1	2.05	0.88
2:C:1093:GLN:HB3	3:D:90:MET:HE2	1.55	0.88
3:D:843:PHE:HE2	3:D:864:VAL:HG11	1.38	0.88
4:E:50:THR:HG22	4:E:53:GLY:O	1.71	0.88
5:F:166:LEU:HB2	5:F:171:LYS:HB2	1.56	0.88
5:F:367:MET:HE3	5:F:368:VAL:HG13	1.54	0.88
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.06	0.88
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.09	0.88
3:D:181:ASP:HB2	3:D:205:TYR:HD1	1.40	0.87
3:D:216:VAL:HA	3:D:340:THR:HG22	1.54	0.87
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.04	0.87
3:D:1410:GLU:HB3	3:D:1412:LYS:HE3	1.57	0.87
5:F:109:GLY:O	5:F:113:ILE:HG13	1.75	0.87
7:H:21:DA:H1'	7:H:22:DT:H5'	1.58	0.86
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.10	0.86
5:F:361:LEU:CD1	5:F:411:HIS:HB2	2.06	0.86
2:C:929:ARG:NH2	2:C:940:GLU:OE2	2.07	0.86
2:C:1012:PRO:CB	2:C:1021:LEU:HD13	2.05	0.86
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.55	0.86
3:D:1232:PRO:O	3:D:1235:GLN:HB3	1.75	0.86
5:F:338:LEU:HD23	5:F:339:PRO:CD	2.05	0.86
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.41	0.86
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.57	0.86
1:A:198:ARG:O	1:A:199:ILE:HG12	1.75	0.86
2:C:816:LYS:O	2:C:819:VAL:HG22	1.76	0.86
3:D:1213:ARG:HG3	3:D:1214:PRO:HD2	1.58	0.86
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.58	0.85
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.09	0.85
3:D:335:LEU:H	3:D:335:LEU:HD12	1.40	0.85
3:D:828:LYS:HE2	3:D:831:GLY:H	1.38	0.85
1:B:36:LEU:O	1:B:38:ASN:N	2.08	0.85
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.58	0.85
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.58	0.85
5:F:95:THR:HG22	5:F:98:GLU:CG	2.06	0.85
3:D:371:ILE:HD13	5:F:232:ARG:HD3	1.58	0.84
3:D:798:GLU:CG	3:D:824:ASN:HB2	2.07	0.84
2:C:841:ASN:HD22	2:C:992:MET:HE2	1.40	0.84
2:C:853:LEU:HB2	2:C:858:MET:CE	2.07	0.84
2:C:204:GLN:HG2	2:C:227:PHE:CZ	2.12	0.84
3:D:798:GLU:HG3	3:D:824:ASN:HB2	1.56	0.84
1:A:18:ARG:HH21	1:A:88:ARG:CZ	1.89	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:369:LEU:HD23	5:F:372:ARG:HB2	1.60	0.84
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.59	0.84
5:F:95:THR:HG22	5:F:98:GLU:HG2	1.57	0.84
3:D:474:GLU:OE2	3:D:1388:ARG:NH2	2.11	0.84
3:D:65:ARG:HD3	5:F:377:ASP:HA	1.57	0.83
2:C:888:THR:HG22	2:C:990:GLY:HA3	1.60	0.83
2:C:1008:ARG:HD2	2:C:1028:GLY:O	1.78	0.83
1:A:121:GLU:HB3	1:A:123:MET:HE2	1.59	0.83
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.13	0.83
2:C:260:LEU:C	2:C:261:ILE:HD12	2.04	0.83
3:D:41:ARG:HE	3:D:48:ARG:HD3	1.42	0.83
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.08	0.83
3:D:795:VAL:O	3:D:797:LYS:NZ	2.12	0.83
1:B:86:VAL:HG12	1:B:124:ASN:OD1	1.79	0.83
2:C:756:VAL:HG21	2:C:823:VAL:HG11	1.60	0.82
2:C:938:LYS:O	2:C:941:VAL:HG22	1.78	0.82
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.61	0.82
3:D:810:GLU:N	3:D:810:GLU:OE2	2.12	0.82
3:D:671:LYS:HZ2	5:F:423:ASP:HA	1.44	0.82
5:F:390:PHE:CD2	5:F:397:ILE:HG12	2.15	0.82
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	1.59	0.81
5:F:362:SER:HB3	5:F:365:GLU:CG	2.10	0.81
5:F:112:ALA:O	5:F:116:LEU:HB2	1.80	0.81
2:C:569:VAL:HG21	2:C:1000:MET:HE1	1.62	0.81
3:D:1236:LEU:HD22	3:D:1359:GLN:HG3	1.61	0.81
5:F:364:ARG:HA	5:F:367:MET:HG2	1.61	0.81
1:B:117:VAL:HG12	1:B:118:ALA:H	1.43	0.81
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.61	0.81
2:C:1055:LEU:CD2	2:C:1079:PRO:HB3	2.10	0.81
2:C:808:ARG:NH2	2:C:808:ARG:HB3	1.96	0.81
2:C:715:THR:HG22	2:C:717:LEU:N	1.96	0.80
3:D:838:ARG:HD3	3:D:874:GLU:HG2	1.63	0.80
3:D:1192:LEU:HD23	3:D:1369:GLU:HB3	1.62	0.80
1:B:107:LYS:NZ	1:B:113:ASP:OD2	2.13	0.80
1:A:55:SER:CB	1:A:158:ILE:HG22	2.09	0.80
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.63	0.80
1:A:115:LEU:O	1:A:115:LEU:HD23	1.81	0.80
3:D:137:PRO:HB3	3:D:147:VAL:HG23	1.64	0.80
1:A:222:LEU:CD2	1:B:218:LEU:HD23	2.07	0.80
7:H:20:DG:H2''	7:H:21:DA:H5'	1.63	0.80
2:C:102:HIS:HB2	2:C:107:LEU:HB2	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1376:MET:HE1	3:D:1421:LEU:HD13	1.63	0.79
2:C:109:LYS:HD2	2:C:110:GLU:H	1.47	0.79
2:C:495:THR:HG23	2:C:517:ARG:CG	2.11	0.79
3:D:401:TYR:OH	3:D:430:ASP:HB2	1.82	0.79
1:A:89:PHE:HB2	1:A:146:ARG:HH22	1.45	0.79
1:A:218:LEU:O	1:A:222:LEU:HD12	1.82	0.79
2:C:460:ARG:HD2	2:C:485:TYR:CE1	2.17	0.79
2:C:833:LEU:HD12	2:C:834:GLN:N	1.97	0.79
3:D:683:ILE:CG2	3:D:687:VAL:HG11	2.12	0.79
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.64	0.79
5:F:123:ASP:OD1	5:F:126:LEU:N	2.14	0.79
2:C:25:SER:OG	2:C:335:THR:OG1	2.01	0.79
2:C:627:ARG:NH2	2:C:640:ARG:HA	1.97	0.79
2:C:1055:LEU:HD21	2:C:1079:PRO:HB3	1.63	0.79
5:F:120:THR:HG23	5:F:122:LEU:H	1.46	0.79
2:C:109:LYS:CG	2:C:368:THR:HG22	2.08	0.79
3:D:175:VAL:CG1	3:D:193:PRO:HG2	2.13	0.79
3:D:1493:LYS:NZ	3:D:1496:GLU:OE2	2.16	0.79
2:C:140:ILE:HD13	2:C:331:ARG:HH11	1.48	0.78
3:D:421:LEU:HD13	3:D:428:LYS:HA	1.64	0.78
3:D:885:ILE:HD13	3:D:937:TYR:CD1	2.19	0.78
2:C:710:ILE:HG22	2:C:823:VAL:HG12	1.63	0.78
3:D:65:ARG:HD3	5:F:377:ASP:CA	2.13	0.78
1:A:164:ALA:O	1:A:166:PRO:HD3	1.84	0.78
2:C:149:THR:HA	2:C:322:VAL:HG13	1.66	0.78
3:D:776:GLU:OE2	3:D:1362:LYS:HD3	1.82	0.78
3:D:410:SER:O	3:D:435:VAL:HG11	1.84	0.78
1:A:40:LEU:HD23	1:A:218:LEU:HD12	1.66	0.78
1:A:20:TYR:O	1:A:207:PRO:HG2	1.84	0.78
1:B:185:ARG:NH1	1:B:187:GLY:O	2.16	0.78
2:C:859:PRO:O	2:C:867:VAL:HG22	1.84	0.78
2:C:967:PHE:O	2:C:970:GLY:N	2.15	0.78
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.19	0.78
2:C:260:LEU:HB3	2:C:261:ILE:CD1	2.13	0.77
3:D:298:VAL:HG12	3:D:302:GLN:CD	2.09	0.77
2:C:366:SER:O	2:C:371:LYS:NZ	2.17	0.77
2:C:424:GLY:O	2:C:428:ARG:HD2	1.83	0.77
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.12	0.77
2:C:474:VAL:HG11	2:C:529:VAL:CG1	2.13	0.77
1:B:115:LEU:HD22	1:B:116:PRO:HD2	1.64	0.77
1:B:128:HIS:HE1	1:B:131:THR:HG22	1.50	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:65:VAL:HG22	2:C:101:ILE:HG23	1.67	0.77
2:C:1115:LEU:HD23	3:D:85:VAL:CG1	2.15	0.77
3:D:721:VAL:HG23	3:D:722:GLU:O	1.83	0.77
3:D:254:GLU:O	3:D:255:GLU:HG2	1.85	0.77
3:D:315:ARG:H	3:D:315:ARG:HD2	1.48	0.77
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.18	0.76
1:B:115:LEU:HD22	1:B:116:PRO:CD	2.15	0.76
5:F:392:VAL:HG21	5:F:396:ARG:HG2	1.65	0.76
2:C:808:ARG:HB3	2:C:808:ARG:HH21	1.47	0.76
2:C:196:LEU:O	2:C:196:LEU:HD22	1.86	0.76
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.68	0.76
3:D:241:ILE:HD12	3:D:310:LEU:HD23	1.65	0.76
3:D:650:LEU:HD12	3:D:657:LEU:HD22	1.67	0.76
6:G:3:DT:H2"	6:G:4:DG:C8	2.21	0.76
1:A:101:LEU:HD23	1:A:102:LYS:N	2.00	0.76
5:F:287:THR:HG23	5:F:290:GLU:OE2	1.86	0.76
3:D:275:GLU:O	3:D:277:GLU:N	2.18	0.76
3:D:558:LEU:HD23	3:D:567:ILE:CD1	2.16	0.76
3:D:1489:GLN:HE22	3:D:1492:LEU:HD12	1.48	0.76
5:F:274:THR:O	5:F:278:LEU:HG	1.86	0.76
1:A:18:ARG:HH11	1:A:18:ARG:HG3	1.49	0.76
1:A:79:ILE:HD12	1:A:167:VAL:CG2	2.16	0.76
3:D:1496:GLU:O	3:D:1500:LYS:HG2	1.86	0.76
5:F:96:LEU:O	5:F:100:VAL:HG23	1.86	0.76
3:D:284:LEU:HD23	3:D:290:PRO:HG3	1.68	0.75
3:D:407:VAL:HA	3:D:422:ALA:HB1	1.68	0.75
5:F:131:VAL:HG11	5:F:177:ALA:HB1	1.68	0.75
5:F:354:LEU:HD12	5:F:355:GLU:N	2.01	0.75
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.68	0.75
3:D:473:LEU:HD21	3:D:495:ARG:NH2	2.01	0.75
2:C:317:VAL:HB	2:C:320:HIS:CD2	2.21	0.75
5:F:361:LEU:HG	5:F:411:HIS:HD2	1.50	0.75
2:C:124:ASP:HA	2:C:592:LEU:HD13	1.67	0.75
2:C:513:VAL:HG22	2:C:524:VAL:O	1.84	0.75
2:C:905:ILE:HG23	2:C:906:PHE:HD1	1.52	0.75
3:D:764:LEU:HB3	3:D:767:HIS:CD2	2.22	0.75
1:A:18:ARG:HH11	1:A:18:ARG:CG	2.00	0.75
1:A:150:TYR:CE1	2:C:696:LYS:HG2	2.22	0.75
2:C:211:LEU:HD23	2:C:218:VAL:HG22	1.68	0.75
3:D:259:VAL:HG13	3:D:270:LEU:CD2	2.17	0.75
2:C:886:LEU:HD11	3:D:951:ILE:HD13	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1236:LEU:CD2	3:D:1359:GLN:HG3	2.16	0.74
2:C:56:GLU:OE2	2:C:103:LYS:HE2	1.86	0.74
3:D:1283:ILE:HG13	3:D:1315:ASP:OD2	1.88	0.74
3:D:1375:MET:HE2	3:D:1424:VAL:HG13	1.69	0.74
3:D:671:LYS:NZ	5:F:423:ASP:HA	2.03	0.74
3:D:1422:MET:HE3	3:D:1426:LYS:HG2	1.68	0.74
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.69	0.74
3:D:1042:ARG:HB3	3:D:1057:VAL:CG1	2.17	0.74
1:A:35:THR:OG1	1:B:42:ARG:HD3	1.88	0.74
2:C:988:VAL:HG23	3:D:948:THR:CG2	2.18	0.74
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.51	0.74
3:D:864:VAL:HG12	3:D:865:THR:N	2.03	0.74
3:D:1028:ALA:O	3:D:1029:ARG:HG2	1.86	0.74
2:C:805:ARG:HG3	2:C:823:VAL:CG2	2.15	0.73
3:D:864:VAL:HG12	3:D:865:THR:H	1.51	0.73
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.70	0.73
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.53	0.73
3:D:62:LYS:HD2	3:D:63:TYR:CE2	2.23	0.73
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.68	0.73
1:A:206:THR:HG22	1:A:209:GLU:CG	2.18	0.73
2:C:143:SER:HB2	2:C:332:ARG:HD2	1.68	0.73
2:C:690:ILE:CD1	2:C:852:ILE:HG23	2.18	0.73
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.19	0.73
3:D:1494:ALA:CB	4:E:92:LEU:HD11	2.17	0.73
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.02	0.73
2:C:49:ARG:NH1	2:C:52:PHE:O	2.21	0.73
2:C:718:GLY:HA3	2:C:761:PHE:CE1	2.24	0.73
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.69	0.73
5:F:362:SER:CB	5:F:365:GLU:HG2	2.14	0.73
2:C:564:MET:HG2	2:C:997:LEU:HD11	1.70	0.73
3:D:236:TYR:H	3:D:319:ALA:HB3	1.53	0.73
3:D:930:LEU:HD11	3:D:934:LEU:HD11	1.69	0.73
1:A:11:PHE:CD2	1:B:225:PHE:HA	2.24	0.73
1:B:71:VAL:HG22	1:B:132:LEU:CD1	2.19	0.73
2:C:927:GLY:HA2	2:C:930:LYS:HE3	1.70	0.73
2:C:958:THR:HG23	2:C:961:GLU:CG	2.18	0.73
3:D:82:LYS:HB2	3:D:84:ILE:HG22	1.69	0.73
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.70	0.73
2:C:418:LEU:HD21	2:C:427:VAL:HG11	1.71	0.73
1:B:86:VAL:CG1	1:B:123:MET:HB2	2.19	0.73
3:D:1057:VAL:HG23	3:D:1069:GLU:CD	2.13	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.71	0.73
5:F:228:GLU:OE2	5:F:231:ARG:NE	2.20	0.73
3:D:348:GLN:HB2	3:D:351:MET:HG3	1.69	0.72
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.71	0.72
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.54	0.72
1:B:77:GLU:HG2	3:D:872:ARG:HH11	1.54	0.72
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.71	0.72
2:C:1005:MET:SD	3:D:648:MET:HG3	2.29	0.72
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.24	0.72
3:D:973:GLN:HG3	3:D:973:GLN:O	1.89	0.72
1:A:20:TYR:OH	1:A:198:ARG:NE	2.22	0.72
7:H:24:DC:H2''	7:H:25:DA:OP2	1.90	0.72
1:A:226:SER:O	1:A:228:PRO:HD3	1.90	0.72
1:B:84:GLU:OE2	3:D:867:ARG:NH1	2.22	0.72
1:B:220:GLU:O	1:B:223:THR:OG1	2.06	0.72
2:C:937:ASP:OD1	2:C:939:ARG:HG2	1.90	0.72
3:D:122:GLU:HG2	3:D:152:LEU:HD11	1.71	0.72
3:D:185:VAL:HG13	3:D:189:GLN:OE1	1.90	0.72
2:C:906:PHE:CE2	3:D:1067:VAL:HA	2.25	0.72
1:B:106:PRO:HD3	1:B:134:GLU:HG2	1.71	0.72
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.19	0.72
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.25	0.72
4:E:30:LEU:HD22	4:E:35:PHE:HD1	1.55	0.72
3:D:693:GLU:HA	4:E:48:MET:HE1	1.69	0.72
3:D:475:LYS:HA	3:D:478:LEU:HD11	1.72	0.71
3:D:486:ARG:HG3	3:D:489:ARG:NH2	2.04	0.71
2:C:767:PRO:HG3	2:C:782:ALA:HB1	1.72	0.71
2:C:879:ARG:NH2	10:D:1601:DCP:O1G	2.22	0.71
3:D:767:HIS:HA	3:D:924:MET:CE	2.16	0.71
3:D:475:LYS:O	3:D:478:LEU:HD12	1.91	0.71
1:B:73:GLU:OE1	1:B:73:GLU:N	2.22	0.71
1:B:109:VAL:C	1:B:110:LYS:HD2	2.16	0.71
2:C:835:VAL:HA	2:C:849:VAL:HG12	1.72	0.71
2:C:503:LEU:HD22	2:C:508:ILE:HA	1.71	0.71
3:D:1045:MET:HE3	3:D:1046:GLN:H	1.55	0.71
1:B:127:LEU:HD23	1:B:128:HIS:N	2.05	0.71
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.26	0.71
3:D:684:LYS:O	3:D:687:VAL:HG12	1.90	0.71
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	1.90	0.71
6:G:6:DA:H2''	6:G:7:DT:O5'	1.91	0.71
3:D:1431:THR:HG23	3:D:1433:SER:N	2.06	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:VAL:HG11	2:C:217:LEU:HD13	1.71	0.71
2:C:317:VAL:HG13	2:C:318:PRO:HD2	1.73	0.71
3:D:1213:ARG:HG3	3:D:1214:PRO:CD	2.21	0.71
3:D:1499:ARG:NH1	4:E:84:ARG:HG2	2.06	0.71
1:A:101:LEU:O	1:A:102:LYS:HG2	1.90	0.71
3:D:30:GLU:OE1	3:D:40:GLU:HG2	1.90	0.71
3:D:500:ARG:NH1	3:D:1390:LEU:HD21	2.05	0.71
3:D:1078:ARG:HG2	3:D:1078:ARG:HH11	1.54	0.71
3:D:658:LEU:HD23	3:D:661:MET:CE	2.21	0.70
1:A:73:GLU:OE2	1:A:130:ALA:HA	1.90	0.70
1:B:96:THR:HG22	1:B:97:VAL:H	1.56	0.70
2:C:1066:ALA:O	2:C:1069:ALA:N	2.24	0.70
3:D:975:GLU:O	3:D:979:GLU:HB2	1.90	0.70
3:D:1208:ASP:OD2	3:D:1211:MET:HE2	1.90	0.70
3:D:1422:MET:HE3	3:D:1426:LYS:CG	2.21	0.70
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.73	0.70
1:A:55:SER:HB3	1:A:158:ILE:HG22	1.72	0.70
1:B:124:ASN:ND2	1:B:127:LEU:HD12	2.06	0.70
3:D:704:ARG:CB	3:D:745:MET:HE2	2.19	0.70
2:C:143:SER:HB2	2:C:332:ARG:CD	2.20	0.70
2:C:775:ARG:NH1	5:F:422:LEU:HD23	2.05	0.70
2:C:833:LEU:HD12	2:C:834:GLN:H	1.56	0.70
3:D:1389:LEU:O	3:D:1390:LEU:HD23	1.90	0.70
3:D:1342:GLU:H	3:D:1342:GLU:CD	1.99	0.70
5:F:364:ARG:HA	5:F:367:MET:CG	2.22	0.70
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.74	0.70
3:D:982:PHE:O	3:D:983:LEU:HG	1.91	0.70
3:D:1156:LEU:HD23	3:D:1182:GLU:OE1	1.91	0.70
5:F:353:GLU:OE2	5:F:417:LYS:HG3	1.90	0.70
1:A:30:ARG:HB2	1:A:191:ASP:O	1.91	0.70
2:C:102:HIS:HB2	2:C:107:LEU:CB	2.22	0.70
2:C:878:SER:CA	3:D:1034:GLN:HE22	2.00	0.70
2:C:988:VAL:HG21	3:D:949:ILE:O	1.91	0.70
2:C:223:ASP:O	2:C:226:VAL:HG23	1.92	0.70
2:C:811:PRO:O	2:C:813:VAL:HG12	1.91	0.70
3:D:697:GLY:O	3:D:760:ARG:NH1	2.23	0.70
5:F:234:LYS:HD3	7:H:5:DA:OP2	1.92	0.70
5:F:328:PHE:HB2	5:F:331:ASP:OD2	1.92	0.70
1:A:39:PRO:HG3	1:B:39:PRO:HG2	1.72	0.70
1:B:197:LEU:HD12	1:B:198:ARG:N	2.07	0.70
2:C:352:ALA:O	2:C:356:ARG:HD2	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:910:LYS:O	2:C:914:ILE:HG22	1.92	0.69
1:A:211:LEU:O	1:A:215:VAL:HG23	1.92	0.69
3:D:65:ARG:HD3	5:F:377:ASP:H	1.58	0.69
3:D:615:ARG:HD2	3:D:1096:ARG:NH2	2.07	0.69
3:D:885:ILE:HG23	3:D:937:TYR:CE1	2.27	0.69
1:A:72:LYS:NZ	2:C:643:VAL:O	2.23	0.69
1:B:106:PRO:CD	1:B:134:GLU:HG2	2.22	0.69
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.74	0.69
2:C:756:VAL:HG21	2:C:823:VAL:CG1	2.22	0.69
3:D:116:LEU:HB2	3:D:118:LEU:HD12	1.74	0.69
3:D:371:ILE:HG13	3:D:372:ASP:N	2.07	0.69
3:D:816:HIS:HB2	3:D:836:VAL:HG11	1.75	0.69
3:D:1137:ARG:O	3:D:1141:GLU:HG3	1.92	0.69
3:D:1271:LYS:HD2	3:D:1331:ASP:HB2	1.73	0.69
5:F:369:LEU:O	5:F:369:LEU:HD22	1.93	0.69
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.74	0.69
1:B:226:SER:O	1:B:228:PRO:HD3	1.93	0.69
2:C:585:GLU:O	2:C:588:VAL:HG12	1.90	0.69
2:C:263:ASP:O	2:C:265:ARG:N	2.24	0.69
3:D:645:PRO:HG2	3:D:724:GLN:O	1.91	0.69
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.72	0.69
1:B:38:ASN:HB3	1:B:39:PRO:CD	2.22	0.69
2:C:719:PRO:HD2	2:C:761:PHE:HE1	1.56	0.69
3:D:573:MET:SD	5:F:210:LEU:HB3	2.33	0.69
2:C:874:LEU:HD12	3:D:784:ASP:OD1	1.93	0.69
3:D:7:LYS:HD3	3:D:1456:LYS:NZ	2.06	0.69
3:D:116:LEU:HB2	3:D:118:LEU:CD1	2.23	0.69
2:C:195:LEU:CD1	2:C:234:ALA:HB1	2.23	0.69
2:C:587:VAL:O	2:C:591:SER:HB3	1.93	0.69
5:F:286:PRO:HB2	5:F:291:ILE:HD12	1.73	0.69
6:G:6:DA:H5"	6:G:6:DA:C8	2.28	0.69
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.23	0.69
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.74	0.69
4:E:50:THR:CG2	4:E:53:GLY:H	2.05	0.69
5:F:157:GLU:O	5:F:161:GLN:HG2	1.93	0.69
3:D:65:ARG:HB3	5:F:377:ASP:CA	2.20	0.68
3:D:284:LEU:HD12	3:D:288:MET:HE1	1.75	0.68
3:D:431:VAL:HG21	3:D:448:GLU:OE1	1.93	0.68
3:D:62:LYS:HB3	3:D:63:TYR:CD2	2.28	0.68
3:D:169:TYR:O	3:D:392:SER:OG	2.06	0.68
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:644:VAL:HG22	2:C:645:VAL:H	1.59	0.68
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.75	0.68
3:D:739:ASP:OD1	3:D:741:ASP:OD1	2.11	0.68
3:D:1024:ALA:HA	3:D:1029:ARG:O	1.94	0.68
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.74	0.68
2:C:234:ALA:HA	2:C:237:ARG:HB2	1.75	0.68
2:C:260:LEU:CB	2:C:261:ILE:HD12	2.22	0.68
3:D:226:PRO:HD3	3:D:249:TYR:CD2	2.28	0.68
3:D:262:LYS:HE2	3:D:341:GLU:OE2	1.94	0.68
1:B:102:LYS:HG3	1:B:139:ASN:OD1	1.93	0.68
2:C:1009:SER:O	3:D:624:ASP:HB3	1.94	0.68
3:D:93:ILE:HD13	3:D:548:ILE:HG12	1.75	0.68
3:D:1234:THR:CA	3:D:1235:GLN:HB2	2.24	0.68
3:D:1496:GLU:O	3:D:1496:GLU:HG3	1.93	0.68
4:E:39:VAL:HG21	4:E:72:ARG:HB3	1.75	0.68
5:F:361:LEU:HD11	5:F:411:HIS:CB	2.21	0.68
1:A:206:THR:HB	1:A:209:GLU:OE1	1.93	0.68
2:C:861:LEU:HD12	2:C:865:THR:HB	1.75	0.68
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.42	0.68
3:D:41:ARG:NE	3:D:48:ARG:HD3	2.09	0.68
2:C:681:GLY:HA2	3:D:939:PHE:CE1	2.28	0.68
2:C:719:PRO:HD2	2:C:761:PHE:CE1	2.28	0.68
3:D:103:TRP:HE1	3:D:604:THR:HG21	1.57	0.68
3:D:208:PRO:CG	3:D:353:VAL:HG11	2.24	0.68
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.28	0.68
3:D:1003:VAL:O	3:D:1007:VAL:HG23	1.94	0.68
2:C:54:ILE:HG21	2:C:355:VAL:CG2	2.24	0.68
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.27	0.68
2:C:880:MET:HE1	3:D:1037:GLN:CD	2.19	0.68
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.29	0.68
1:A:106:PRO:HD3	1:A:134:GLU:OE1	1.94	0.68
2:C:716:LYS:C	2:C:717:LEU:HD12	2.17	0.68
2:C:1001:VAL:CG1	3:D:724:GLN:HB2	2.24	0.67
3:D:132:TYR:OH	3:D:568:ARG:NH2	2.27	0.67
3:D:156:GLU:N	3:D:156:GLU:OE2	2.24	0.67
4:E:80:VAL:HG12	4:E:81:PRO:O	1.93	0.67
2:C:513:VAL:HG21	2:C:529:VAL:HG21	1.76	0.67
3:D:650:LEU:HD12	3:D:657:LEU:CD2	2.25	0.67
3:D:814:ALA:O	3:D:818:ARG:HG3	1.94	0.67
1:A:55:SER:HB2	1:A:158:ILE:HG22	1.76	0.67
1:B:185:ARG:HB2	1:B:190:THR:OG1	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:VAL:HG22	2:C:182:VAL:HG12	1.76	0.67
2:C:715:THR:HB	2:C:718:GLY:O	1.94	0.67
3:D:1486:VAL:HA	4:E:74:VAL:O	1.93	0.67
5:F:104:ARG:HG2	5:F:108:GLU:OE2	1.95	0.67
1:A:107:LYS:NZ	1:A:113:ASP:OD2	2.20	0.67
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.30	0.67
2:C:1056:LYS:HD3	3:D:751:LEU:HD11	1.76	0.67
5:F:371:LEU:CD1	5:F:379:ARG:HG3	2.24	0.67
1:B:24:VAL:HG13	1:B:196:THR:OG1	1.93	0.67
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.77	0.67
2:C:560:MET:O	2:C:564:MET:HB2	1.94	0.67
2:C:588:VAL:HG11	2:C:664:GLY:O	1.93	0.67
3:D:93:ILE:CD1	3:D:548:ILE:HG12	2.25	0.67
2:C:547:ILE:O	2:C:905:ILE:HD11	1.95	0.67
3:D:250:LEU:N	3:D:250:LEU:HD23	2.09	0.67
3:D:411:THR:HG22	5:F:178:ARG:HB3	1.77	0.67
3:D:1047:LYS:HG2	3:D:1048:PRO:HD2	1.77	0.67
5:F:375:LEU:HD23	5:F:375:LEU:O	1.95	0.67
6:G:6:DA:H5"	6:G:6:DA:H8	1.59	0.67
2:C:337:GLY:O	2:C:341:THR:HG23	1.95	0.67
2:C:751:PRO:HA	2:C:792:VAL:CG2	2.24	0.67
2:C:22:GLN:O	2:C:121:MET:HE1	1.95	0.67
3:D:129:PHE:CD2	3:D:456:MET:HB3	2.29	0.67
4:E:9:LEU:CD2	4:E:12:MET:HE3	2.20	0.67
2:C:182:VAL:HG22	2:C:221:LEU:CD2	2.22	0.67
2:C:359:MET:O	2:C:360:LEU:HD13	1.95	0.67
3:D:916:TYR:CE2	3:D:920:LEU:HD11	2.30	0.67
3:D:1310:ARG:HB2	3:D:1327:ARG:HD2	1.76	0.67
2:C:221:LEU:O	2:C:221:LEU:HD22	1.95	0.67
2:C:928:LYS:O	2:C:932:GLU:HG3	1.95	0.67
3:D:226:PRO:HD3	3:D:249:TYR:CE2	2.30	0.67
5:F:222:ARG:NE	5:F:222:ARG:HA	2.10	0.67
1:A:86:VAL:HG21	1:A:202:ASP:HB2	1.76	0.66
1:A:213:GLN:O	1:A:217:ILE:HG13	1.94	0.66
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.30	0.66
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.78	0.66
2:C:888:THR:HG22	2:C:990:GLY:CA	2.24	0.66
3:D:154:THR:OG1	3:D:157:GLU:HG3	1.95	0.66
1:A:153:ALA:C	1:A:155:LYS:H	2.03	0.66
3:D:394:LEU:HG	3:D:396:VAL:HG23	1.76	0.66
5:F:129:GLU:HG2	5:F:144:ILE:HG13	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:370:LYS:O	5:F:371:LEU:HD22	1.95	0.66
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.77	0.66
3:D:348:GLN:N	3:D:351:MET:HE2	2.10	0.66
3:D:791:TYR:CD1	3:D:945:SER:HB2	2.31	0.66
3:D:948:THR:HG23	3:D:949:ILE:N	2.10	0.66
3:D:65:ARG:CD	5:F:377:ASP:HA	2.26	0.66
3:D:66:GLN:OE1	5:F:376:ILE:HG12	1.95	0.66
3:D:1290:LEU:HB2	3:D:1307:LYS:HG2	1.77	0.66
3:D:1413:THR:HG22	3:D:1414:PRO:HD2	1.77	0.66
5:F:355:GLU:OE2	5:F:370:LYS:NZ	2.22	0.66
7:H:21:DA:H1'	7:H:22:DT:C5'	2.26	0.66
1:A:67:THR:HG21	2:C:609:ASN:OD1	1.96	0.66
1:A:213:GLN:NE2	1:A:213:GLN:HA	2.09	0.66
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.76	0.66
1:B:94:LEU:HD23	1:B:95:GLN:N	2.10	0.66
2:C:54:ILE:HG21	2:C:355:VAL:HG23	1.78	0.66
2:C:503:LEU:CD2	2:C:508:ILE:HA	2.25	0.66
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.77	0.66
3:D:479:GLU:OE2	3:D:482:LYS:NZ	2.25	0.66
3:D:645:PRO:HB3	3:D:723:GLY:O	1.96	0.66
3:D:940:THR:O	3:D:943:THR:HG23	1.95	0.66
5:F:365:GLU:OE2	5:F:407:LYS:HD2	1.96	0.66
1:A:9:PRO:HB3	1:A:27:PRO:O	1.96	0.66
3:D:175:VAL:HG11	3:D:193:PRO:HG2	1.76	0.66
3:D:241:ILE:CD1	3:D:310:LEU:HD23	2.24	0.66
3:D:367:ILE:HB	3:D:377:VAL:CG2	2.26	0.66
3:D:882:PHE:CE2	3:D:906:GLN:HG3	2.31	0.66
3:D:519:VAL:HG22	3:D:544:TYR:CE1	2.31	0.66
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.77	0.66
1:A:19:GLU:O	1:A:207:PRO:HG3	1.94	0.66
2:C:206:THR:HA	2:C:209:ARG:HB3	1.77	0.66
2:C:853:LEU:HD12	2:C:858:MET:HE1	1.77	0.66
2:C:946:ARG:HH21	2:C:946:ARG:HG3	1.60	0.66
5:F:386:VAL:HA	5:F:390:PHE:HE1	1.56	0.66
2:C:317:VAL:CG1	2:C:318:PRO:HD2	2.25	0.66
2:C:1060:ILE:HD11	2:C:1083:GLU:HB2	1.76	0.66
3:D:258:VAL:HG12	3:D:273:ARG:O	1.95	0.66
5:F:260:ILE:HG13	5:F:265:VAL:HG23	1.78	0.66
5:F:392:VAL:HG22	5:F:393:THR:H	1.60	0.66
2:C:564:MET:HG2	2:C:997:LEU:CD1	2.25	0.66
3:D:664:LYS:HE3	3:D:693:GLU:OE2	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:13:DT:H3'	7:H:14:DG:H5'	1.78	0.65
3:D:1126:ASP:O	3:D:1130:ARG:HA	1.96	0.65
1:A:88:ARG:HB3	1:A:123:MET:CE	2.20	0.65
2:C:177:GLU:CG	2:C:178:PRO:HD2	2.23	0.65
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.79	0.65
3:D:529:GLN:HG3	3:D:535:PHE:CE2	2.30	0.65
5:F:291:ILE:HG21	5:F:304:VAL:HG21	1.78	0.65
1:A:10:VAL:N	1:A:26:GLU:O	2.24	0.65
2:C:926:PHE:O	2:C:929:ARG:HB3	1.96	0.65
2:C:266:ARG:O	2:C:266:ARG:HG3	1.95	0.65
2:C:540:PHE:HB3	2:C:544:THR:CG2	2.26	0.65
2:C:1054:THR:OG1	2:C:1055:LEU:HD23	1.96	0.65
3:D:116:LEU:HD21	3:D:465:LEU:HD12	1.77	0.65
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.79	0.65
1:B:101:LEU:HD11	1:B:109:VAL:CG1	2.27	0.65
3:D:478:LEU:O	3:D:481:MET:N	2.30	0.65
3:D:1065:LEU:HD23	3:D:1069:GLU:CB	2.14	0.65
4:E:50:THR:HG23	4:E:53:GLY:H	1.60	0.65
1:B:112:ARG:HG3	1:B:113:ASP:OD1	1.96	0.65
2:C:312:ALA:HB1	2:C:317:VAL:HG21	1.78	0.65
3:D:256:GLU:HG2	3:D:274:ARG:NH1	2.12	0.65
3:D:823:LEU:HD11	3:D:837:GLY:HA2	1.78	0.65
2:C:890:LEU:HB2	2:C:914:ILE:CD1	2.24	0.65
3:D:103:TRP:HE1	3:D:604:THR:CG2	2.10	0.65
3:D:111:LYS:HD2	3:D:1452:ILE:CD1	2.27	0.65
3:D:658:LEU:HA	3:D:661:MET:HE3	1.78	0.65
5:F:101:GLU:O	5:F:105:LYS:HG3	1.97	0.65
1:B:96:THR:HG22	1:B:97:VAL:N	2.12	0.65
2:C:250:ARG:HD2	2:C:250:ARG:O	1.97	0.65
2:C:446:GLY:O	2:C:449:ILE:HG22	1.96	0.65
2:C:605:LYS:O	2:C:606:VAL:HG23	1.97	0.65
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.79	0.65
3:D:65:ARG:HD3	5:F:377:ASP:N	2.11	0.65
3:D:1380:GLU:N	3:D:1420:LEU:HD22	2.11	0.65
7:H:13:DT:H3'	7:H:14:DG:C5'	2.26	0.65
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.11	0.65
2:C:64:LEU:HD23	2:C:102:HIS:HA	1.78	0.65
3:D:904:VAL:HG22	3:D:905:PRO:CD	2.27	0.65
2:C:356:ARG:HA	2:C:359:MET:HB2	1.79	0.64
2:C:474:VAL:CG1	2:C:529:VAL:HG12	2.23	0.64
2:C:889:HIS:CD2	3:D:951:ILE:HG22	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:764:LEU:HB3	3:D:767:HIS:HD2	1.62	0.64
3:D:801:GLY:HA3	3:D:821:VAL:HG22	1.78	0.64
5:F:364:ARG:HD2	5:F:364:ARG:C	2.22	0.64
2:C:193:LEU:HG	2:C:197:LEU:CD1	2.28	0.64
2:C:605:LYS:HB2	2:C:612:VAL:HG12	1.80	0.64
5:F:153:PRO:HA	5:F:156:VAL:HG12	1.78	0.64
5:F:412:GLU:CG	5:F:418:LEU:HD13	2.21	0.64
2:C:605:LYS:HB2	2:C:612:VAL:CG1	2.28	0.64
2:C:689:VAL:HG11	2:C:853:LEU:HD11	1.79	0.64
3:D:236:TYR:CE1	3:D:242:LEU:HB2	2.33	0.64
3:D:791:TYR:CZ	3:D:945:SER:HB2	2.32	0.64
5:F:171:LYS:HD3	5:F:175:HIS:CE1	2.32	0.64
1:A:4:SER:O	1:A:189:ARG:NH2	2.29	0.64
2:C:1110:ASP:OD1	2:C:1112:PHE:N	2.28	0.64
3:D:256:GLU:HG2	3:D:274:ARG:HH11	1.62	0.64
3:D:1045:MET:HE3	3:D:1045:MET:HA	1.79	0.64
3:D:1405:GLU:HA	3:D:1408:ILE:CG1	2.28	0.64
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.06	0.64
2:C:238:LEU:HD12	2:C:241:LEU:HB2	1.80	0.64
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.79	0.64
3:D:972:LEU:HA	3:D:975:GLU:HB3	1.78	0.64
4:E:75:PHE:H	4:E:75:PHE:HD2	1.44	0.64
5:F:402:ASN:O	5:F:406:ARG:HB2	1.97	0.64
1:A:219:ARG:HG3	1:B:219:ARG:HG3	1.79	0.64
1:B:26:GLU:CD	1:B:194:LYS:HG3	2.22	0.64
3:D:1405:GLU:HA	3:D:1408:ILE:HG13	1.79	0.64
5:F:393:THR:HG22	5:F:394:ARG:H	1.60	0.64
1:A:9:PRO:HB2	1:A:26:GLU:O	1.98	0.64
5:F:260:ILE:HG13	5:F:265:VAL:CG2	2.28	0.64
1:A:44:LEU:O	1:A:174:VAL:HG21	1.98	0.64
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.80	0.64
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.78	0.64
3:D:1097:LYS:HD3	3:D:1425:THR:OG1	1.98	0.64
4:E:30:LEU:HD22	4:E:35:PHE:CD1	2.32	0.64
5:F:392:VAL:CG2	5:F:396:ARG:HG2	2.26	0.64
2:C:692:GLU:HG2	2:C:696:LYS:HE3	1.80	0.64
5:F:271:LEU:HD21	5:F:307:THR:HG21	1.80	0.64
1:B:64:GLU:HG3	1:B:79:ILE:CD1	2.28	0.64
1:B:117:VAL:HG12	1:B:118:ALA:N	2.13	0.64
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.11	0.64
2:C:477:GLY:O	2:C:508:ILE:HG13	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:884:GLN:HB2	2:C:992:MET:CE	2.28	0.64
3:D:554:LEU:CD1	3:D:570:GLU:HB3	2.28	0.64
2:C:808:ARG:HD3	2:C:814:GLU:HG3	1.79	0.63
3:D:1273:VAL:H	3:D:1326:THR:CG2	2.08	0.63
5:F:373:LYS:HD3	5:F:380:GLU:OE1	1.96	0.63
2:C:23:VAL:HG23	2:C:24:GLU:H	1.63	0.63
3:D:407:VAL:O	5:F:171:LYS:HE2	1.99	0.63
2:C:211:LEU:HB3	2:C:218:VAL:CG2	2.28	0.63
3:D:63:TYR:OH	3:D:74:GLU:OE1	2.14	0.63
3:D:203:ALA:CB	3:D:393:ILE:HD11	2.11	0.63
1:A:222:LEU:HD21	1:B:218:LEU:CD2	2.11	0.63
2:C:339:LEU:HD11	2:C:391:LEU:HD12	1.79	0.63
5:F:368:VAL:CB	5:F:397:ILE:HD11	2.28	0.63
2:C:403:SER:O	2:C:407:LYS:HG3	1.99	0.63
2:C:748:GLU:HG3	2:C:799:ILE:HD11	1.80	0.63
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.34	0.63
3:D:1130:ARG:HB3	3:D:1130:ARG:NH1	2.13	0.63
5:F:116:LEU:O	5:F:116:LEU:HD23	1.98	0.63
1:B:32:PHE:HA	1:B:35:THR:HB	1.79	0.63
1:B:107:LYS:HG2	1:B:108:GLU:H	1.63	0.63
2:C:683:ASN:CB	2:C:872:ASN:HB2	2.27	0.63
5:F:157:GLU:HA	5:F:157:GLU:OE1	1.98	0.63
3:D:1065:LEU:CD2	3:D:1069:GLU:HB3	2.12	0.63
5:F:372:ARG:HA	5:F:372:ARG:HE	1.62	0.63
2:C:762:LYS:HG2	2:C:786:LYS:HG3	1.79	0.63
2:C:1060:ILE:CD1	2:C:1083:GLU:HB2	2.29	0.63
3:D:63:TYR:CE2	3:D:73:CYS:HB2	2.33	0.63
3:D:1494:ALA:HB1	4:E:92:LEU:HD11	1.80	0.63
2:C:875:GLY:O	2:C:879:ARG:HB2	1.99	0.63
2:C:963:LEU:N	2:C:963:LEU:HD23	2.12	0.63
3:D:242:LEU:HD21	3:D:311:LEU:CD1	2.29	0.63
5:F:408:LEU:HA	5:F:411:HIS:HB3	1.80	0.63
2:C:237:ARG:O	2:C:240:THR:OG1	2.16	0.62
3:D:38:LYS:HB3	3:D:39:PRO:HD2	1.80	0.62
3:D:986:ARG:NH1	3:D:986:ARG:HB2	2.14	0.62
2:C:718:GLY:HA3	2:C:761:PHE:CD1	2.34	0.62
2:C:944:LEU:HD11	2:C:963:LEU:CD2	2.27	0.62
5:F:376:ILE:O	5:F:377:ASP:HB3	1.98	0.62
1:A:47:SER:O	1:A:49:PRO:HD3	2.00	0.62
2:C:257:VAL:HG23	2:C:258:TYR:H	1.63	0.62
1:B:53:VAL:HG12	1:B:167:VAL:CG1	2.22	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:409:ARG:NH1	2:C:442:GLU:OE2	2.32	0.62
2:C:726:ILE:HG21	2:C:729:LEU:HD22	1.80	0.62
2:C:880:MET:HE1	3:D:1037:GLN:NE2	2.14	0.62
2:C:880:MET:HE2	3:D:1061:PHE:HE2	1.64	0.62
3:D:204:LEU:O	3:D:393:ILE:HG13	1.98	0.62
3:D:502:PHE:CZ	3:D:512:MET:HE2	2.35	0.62
3:D:601:ARG:HD2	5:F:318:GLU:HG2	1.82	0.62
3:D:955:VAL:O	3:D:957:PRO:HD3	1.99	0.62
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.80	0.62
3:D:130:SER:O	3:D:131:LYS:HG3	2.00	0.62
3:D:761:ILE:HD13	4:E:19:LEU:CD2	2.29	0.62
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.81	0.62
5:F:358:LEU:HD12	5:F:370:LYS:HD2	1.81	0.62
3:D:82:LYS:O	3:D:85:VAL:HG22	2.00	0.62
3:D:408:GLU:OE1	3:D:408:GLU:HA	1.98	0.62
3:D:597:ASP:O	3:D:599:PRO:HD3	1.99	0.62
3:D:1353:GLN:O	3:D:1357:ARG:HG3	1.98	0.62
2:C:73:LEU:HD22	2:C:92:ALA:HB3	1.81	0.62
4:E:30:LEU:HD23	4:E:35:PHE:HA	1.81	0.62
2:C:683:ASN:CB	2:C:872:ASN:HD22	2.13	0.62
2:C:755:LEU:CD1	2:C:792:VAL:HG12	2.30	0.62
2:C:1067:TYR:CE1	2:C:1071:ILE:HD13	2.34	0.62
3:D:368:VAL:HB	3:D:377:VAL:HG13	1.81	0.62
5:F:206:GLY:O	5:F:207:LEU:HD23	1.99	0.62
1:A:122:ILE:O	1:A:122:ILE:HG22	2.00	0.62
1:A:224:TYR:CG	1:B:9:PRO:HG2	2.34	0.62
2:C:339:LEU:CD1	2:C:391:LEU:HD12	2.29	0.62
3:D:236:TYR:N	3:D:319:ALA:HB3	2.14	0.62
3:D:835:SER:H	3:D:838:ARG:HG3	1.63	0.62
1:B:118:ALA:O	1:B:119:ASP:HB2	1.99	0.62
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.80	0.62
3:D:221:ALA:O	3:D:335:LEU:HD12	1.99	0.62
3:D:407:VAL:HA	3:D:422:ALA:CB	2.29	0.62
2:C:193:LEU:HG	2:C:197:LEU:HD11	1.82	0.61
2:C:897:LEU:N	2:C:897:LEU:HD23	2.15	0.61
3:D:407:VAL:HG13	3:D:422:ALA:CB	2.28	0.61
3:D:407:VAL:CG1	3:D:422:ALA:HB2	2.27	0.61
3:D:661:MET:HE1	3:D:677:LEU:HD11	1.82	0.61
1:B:33:GLY:C	1:B:181:VAL:HG21	2.25	0.61
3:D:231:VAL:HG13	3:D:242:LEU:O	2.01	0.61
3:D:558:LEU:HD23	3:D:567:ILE:HD11	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:689:ASP:HB3	4:E:51:LEU:CD1	2.27	0.61
2:C:755:LEU:HD11	2:C:792:VAL:HG12	1.81	0.61
3:D:208:PRO:HG3	3:D:353:VAL:HG11	1.82	0.61
3:D:572:ARG:NH1	5:F:83:GLN:HG2	2.14	0.61
3:D:703:ASN:HB3	3:D:746:ALA:HB3	1.82	0.61
3:D:1090:ASP:N	3:D:1090:ASP:OD1	2.28	0.61
5:F:364:ARG:O	5:F:367:MET:HG3	1.99	0.61
1:A:79:ILE:HD12	1:A:167:VAL:HG22	1.81	0.61
1:A:133:GLU:OE2	2:C:605:LYS:HD3	2.01	0.61
2:C:53:PRO:HB3	2:C:67:ASP:OD2	2.00	0.61
5:F:367:MET:HA	5:F:370:LYS:HB3	1.83	0.61
7:H:17:DA:H2''	7:H:18:DC:H5'	1.83	0.61
1:B:53:VAL:CG1	1:B:167:VAL:HG11	2.21	0.61
2:C:1092:LEU:CD1	2:C:1099:VAL:HG21	2.30	0.61
3:D:1410:GLU:CB	3:D:1412:LYS:HE3	2.29	0.61
5:F:196:VAL:HG11	7:H:7:DG:H4'	1.83	0.61
1:A:215:VAL:HG13	1:B:222:LEU:CD2	2.25	0.61
3:D:141:ILE:HD12	3:D:145:VAL:C	2.26	0.61
3:D:417:PRO:HG3	3:D:430:ASP:O	2.01	0.61
3:D:704:ARG:HG2	3:D:705:ALA:H	1.65	0.61
2:C:23:VAL:HG23	2:C:24:GLU:N	2.16	0.61
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.36	0.61
5:F:368:VAL:HB	5:F:397:ILE:HD11	1.82	0.61
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.83	0.61
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.82	0.61
2:C:257:VAL:HG23	2:C:258:TYR:N	2.16	0.61
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.36	0.61
1:B:30:ARG:NE	2:C:854:PRO:HG3	2.15	0.61
1:B:94:LEU:HD21	1:B:96:THR:O	2.01	0.61
2:C:598:GLU:O	2:C:651:LYS:HE3	2.00	0.61
3:D:36:THR:O	3:D:38:LYS:HG3	2.01	0.61
3:D:705:ALA:CB	3:D:706:PRO:CD	2.77	0.61
1:A:180:GLN:HG3	2:C:934:PHE:CD1	2.35	0.60
2:C:1058:ASP:OD2	2:C:1084:SER:HB2	2.01	0.60
3:D:700:VAL:O	3:D:701:LEU:HD23	2.00	0.60
3:D:930:LEU:CD1	3:D:934:LEU:HD11	2.31	0.60
3:D:1045:MET:HA	3:D:1045:MET:CE	2.30	0.60
3:D:298:VAL:HA	3:D:302:GLN:OE1	2.01	0.60
3:D:314:PRO:HD2	3:D:317:VAL:CG1	2.30	0.60
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.02	0.60
3:D:1078:ARG:HG2	3:D:1078:ARG:NH1	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:95:THR:N	5:F:98:GLU:HG3	2.10	0.60
2:C:944:LEU:CD1	2:C:963:LEU:HD21	2.29	0.60
3:D:7:LYS:HD3	3:D:1456:LYS:HZ3	1.66	0.60
3:D:781:PRO:HB2	3:D:786:ILE:HG22	1.83	0.60
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.82	0.60
1:B:211:LEU:O	1:B:215:VAL:HG23	2.00	0.60
2:C:355:VAL:HG23	2:C:356:ARG:N	2.17	0.60
2:C:462:ASP:HB3	2:C:468:ARG:CD	2.31	0.60
2:C:723:THR:OG1	2:C:725:ASP:N	2.33	0.60
1:A:39:PRO:O	1:A:43:ILE:HG13	2.00	0.60
1:B:202:ASP:OD1	1:B:204:SER:HB3	2.01	0.60
2:C:627:ARG:NH2	2:C:641:PRO:HD3	2.13	0.60
2:C:1047:HIS:CE1	3:D:1471:LEU:HD21	2.37	0.60
3:D:801:GLY:CA	3:D:821:VAL:HG22	2.31	0.60
1:A:38:ASN:HB3	1:A:39:PRO:CD	2.31	0.60
2:C:999:HIS:HB3	2:C:1004:LYS:HZ1	1.65	0.60
3:D:180:LYS:O	3:D:183:GLU:HB2	2.01	0.60
3:D:750:PRO:HB2	3:D:756:GLN:HE22	1.65	0.60
3:D:970:LYS:HA	3:D:973:GLN:HB3	1.83	0.60
3:D:1126:ASP:OD2	3:D:1133:ARG:HG3	2.01	0.60
5:F:153:PRO:O	5:F:156:VAL:HG12	2.02	0.60
2:C:492:ASP:HB3	2:C:518:LYS:HG2	1.84	0.60
5:F:316:SER:O	5:F:319:THR:OG1	2.19	0.60
2:C:167:LYS:HE3	7:H:12:DC:C5	2.37	0.60
2:C:1055:LEU:HD23	2:C:1055:LEU:N	2.17	0.60
3:D:767:HIS:CA	3:D:924:MET:HE3	2.19	0.60
3:D:1442:ASN:HD21	6:G:11:DT:H4'	1.66	0.60
5:F:236:SER:OG	7:H:5:DA:OP2	2.15	0.60
1:A:9:PRO:CD	1:B:224:TYR:CD2	2.85	0.60
1:A:222:LEU:HD23	1:B:215:VAL:HG13	1.84	0.60
3:D:415:VAL:HG22	3:D:419:ASP:OD2	2.01	0.60
3:D:1290:LEU:CB	3:D:1307:LYS:HG2	2.32	0.60
1:A:55:SER:HB2	1:A:158:ILE:O	2.01	0.60
2:C:65:VAL:CG2	2:C:101:ILE:HG23	2.31	0.60
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.17	0.60
3:D:348:GLN:H	3:D:351:MET:HE2	1.67	0.60
3:D:711:LEU:HD22	3:D:714:GLN:NE2	2.17	0.60
5:F:401:GLU:O	5:F:405:LEU:HD13	2.01	0.60
1:A:182:GLU:HG3	1:A:194:LYS:HE2	1.83	0.59
3:D:411:THR:HG22	5:F:178:ARG:CB	2.32	0.59
3:D:687:VAL:O	3:D:690:ALA:HB3	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.28	0.59
3:D:1267:ARG:NH2	3:D:1331:ASP:OD2	2.34	0.59
3:D:1394:VAL:HG22	3:D:1420:LEU:HD23	1.83	0.59
5:F:89:GLY:HA3	7:H:7:DG:C6	2.37	0.59
1:B:97:VAL:HG12	1:B:99:LEU:HD12	1.83	0.59
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.38	0.59
3:D:547:LEU:HD12	3:D:577:ALA:CB	2.32	0.59
3:D:823:LEU:HD11	3:D:837:GLY:CA	2.33	0.59
3:D:1057:VAL:HG21	3:D:1065:LEU:HD21	1.83	0.59
1:A:18:ARG:HH21	1:A:88:ARG:NH1	2.00	0.59
1:B:106:PRO:CG	1:B:134:GLU:HG2	2.32	0.59
2:C:666:LEU:HD11	2:C:668:LEU:HD21	1.84	0.59
3:D:242:LEU:CD2	3:D:311:LEU:HD12	2.31	0.59
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.37	0.59
3:D:411:THR:HA	3:D:435:VAL:HG13	1.83	0.59
3:D:547:LEU:HD12	3:D:577:ALA:HB3	1.84	0.59
3:D:760:ARG:HH22	4:E:62:THR:HG22	1.67	0.59
3:D:1160:LEU:HD23	3:D:1164:ARG:NH1	2.17	0.59
7:H:15:DT:H2''	7:H:16:DC:H5'	1.85	0.59
1:A:48:ILE:O	1:A:173:PRO:HD3	2.03	0.59
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.84	0.59
3:D:314:PRO:HB2	3:D:317:VAL:CG1	2.32	0.59
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.85	0.59
3:D:1371:VAL:O	3:D:1374:GLN:N	2.33	0.59
2:C:361:MET:HG3	2:C:361:MET:O	2.01	0.59
2:C:1099:VAL:CG2	3:D:10:ILE:HG13	2.33	0.59
3:D:652:LEU:HB3	3:D:749:VAL:CG2	2.32	0.59
3:D:1118:ILE:HD13	3:D:1190:SER:CB	2.32	0.59
2:C:425:PHE:HE2	3:D:1086:LEU:HD12	1.67	0.59
2:C:759:THR:HA	2:C:786:LYS:O	2.02	0.59
3:D:483:HIS:ND1	3:D:484:PRO:O	2.33	0.59
4:E:83:ASP:HA	4:E:86:GLN:HG2	1.83	0.59
5:F:360:LYS:O	5:F:361:LEU:HD23	2.03	0.59
5:F:371:LEU:HD12	5:F:379:ARG:HG3	1.84	0.59
1:A:185:ARG:NH2	1:A:187:GLY:O	2.35	0.59
2:C:559:LEU:C	2:C:559:LEU:HD23	2.28	0.59
2:C:598:GLU:C	2:C:599:GLU:HG2	2.28	0.59
3:D:807:ALA:O	3:D:830:ALA:HB2	2.03	0.59
3:D:885:ILE:HG23	3:D:937:TYR:CD1	2.38	0.59
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.68	0.59
1:B:128:HIS:C	1:B:128:HIS:CD2	2.81	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1019:PRO:O	3:D:1023:MET:HE2	2.03	0.59
3:D:1156:LEU:O	3:D:1158:VAL:HG23	2.03	0.59
1:A:150:TYR:HE1	2:C:696:LYS:HA	1.67	0.59
2:C:91:GLN:HA	2:C:119:PRO:HA	1.85	0.59
2:C:644:VAL:HG22	2:C:645:VAL:N	2.17	0.59
2:C:705:ILE:HG23	2:C:827:VAL:O	2.02	0.59
2:C:727:PRO:HB2	2:C:728:HIS:CD2	2.36	0.59
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.84	0.59
3:D:566:ILE:HD11	5:F:192:LEU:CD2	2.33	0.59
3:D:1234:THR:H	3:D:1235:GLN:CB	2.16	0.59
3:D:1422:MET:CE	3:D:1426:LYS:HG2	2.31	0.59
5:F:153:PRO:C	5:F:156:VAL:HG12	2.28	0.59
1:A:196:THR:HG21	2:C:934:PHE:CE1	2.38	0.58
1:B:38:ASN:OD1	2:C:979:THR:HG22	2.03	0.58
2:C:139:GLN:HB2	2:C:391:LEU:HD11	1.84	0.58
2:C:217:LEU:O	2:C:220:GLY:N	2.36	0.58
2:C:626:ARG:H	2:C:639:GLN:HE21	1.50	0.58
3:D:1130:ARG:HB3	3:D:1130:ARG:HH11	1.68	0.58
4:E:95:VAL:O	4:E:95:VAL:HG12	2.03	0.58
5:F:208:SER:OG	5:F:211:ASP:HB2	2.03	0.58
1:A:188:GLN:OE1	1:A:188:GLN:HA	2.03	0.58
2:C:838:LYS:HD3	2:C:997:LEU:HD12	1.85	0.58
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.68	0.58
2:C:952:LEU:HD12	2:C:969:GLN:OE1	2.03	0.58
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.84	0.58
3:D:403:PHE:HB2	3:D:423:ASP:OD2	2.03	0.58
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.85	0.58
2:C:150:PRO:HG3	2:C:322:VAL:HG21	1.85	0.58
2:C:1031:ARG:HB2	3:D:622:ARG:NH1	2.18	0.58
3:D:95:LEU:HD22	3:D:574:LEU:HD21	1.85	0.58
3:D:140:ALA:HA	3:D:450:TYR:CD1	2.39	0.58
3:D:882:PHE:CZ	3:D:906:GLN:HG3	2.38	0.58
3:D:936:TYR:C	3:D:936:TYR:HD2	2.11	0.58
3:D:1060:SER:HB3	3:D:1063:GLU:CG	2.22	0.58
2:C:21:ILE:HD11	2:C:461:VAL:HG11	1.85	0.58
2:C:422:ARG:HH22	7:H:13:DT:C3'	2.17	0.58
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.85	0.58
2:C:988:VAL:HG21	3:D:949:ILE:C	2.29	0.58
3:D:696:HIS:CE1	4:E:48:MET:HB3	2.38	0.58
3:D:750:PRO:HB2	3:D:756:GLN:NE2	2.18	0.58
1:B:162:ILE:HD12	1:B:163:ASN:H	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:VAL:HG21	2:C:472:ARG:NE	2.19	0.58
2:C:127:PHE:O	2:C:133:ASP:HA	2.03	0.58
2:C:502:PRO:O	2:C:503:LEU:HD23	2.04	0.58
3:D:529:GLN:HA	3:D:534:ARG:O	2.03	0.58
1:A:57:TYR:HE2	1:A:59:GLU:HA	1.69	0.58
1:B:64:GLU:O	1:B:75:VAL:HB	2.04	0.58
3:D:103:TRP:CZ2	3:D:1444:THR:HG22	2.39	0.58
3:D:202:VAL:O	3:D:202:VAL:HG22	2.02	0.58
3:D:230:TRP:CZ3	3:D:333:LEU:HD21	2.39	0.58
3:D:646:LYS:CB	3:D:720:LEU:HD23	2.33	0.58
3:D:983:LEU:HB3	3:D:987:GLU:OE2	2.03	0.58
5:F:166:LEU:CB	5:F:171:LYS:HB2	2.32	0.58
2:C:128:ILE:C	2:C:129:ILE:HD12	2.28	0.58
2:C:578:VAL:HG13	2:C:671:ASN:CG	2.29	0.58
2:C:853:LEU:HD12	2:C:858:MET:CE	2.33	0.58
3:D:728:LEU:HD12	3:D:729:HIS:H	1.67	0.58
3:D:806:PHE:O	3:D:829:VAL:HA	2.04	0.58
2:C:56:GLU:CD	2:C:103:LYS:HE2	2.28	0.58
2:C:167:LYS:HE3	7:H:12:DC:H5	1.68	0.58
3:D:185:VAL:CG1	3:D:186:VAL:N	2.67	0.58
3:D:628:ARG:HD3	6:G:17:DC:H4'	1.85	0.58
3:D:851:LEU:HD11	3:D:855:HIS:HE1	1.69	0.58
3:D:936:TYR:C	3:D:936:TYR:CD2	2.82	0.58
2:C:501:THR:CG2	2:C:514:VAL:HG23	2.34	0.58
2:C:657:ASP:OD2	2:C:663:ASN:N	2.33	0.58
3:D:398:ALA:HB1	3:D:446:VAL:O	2.04	0.58
3:D:700:VAL:C	3:D:701:LEU:HD23	2.29	0.58
3:D:993:LEU:O	3:D:997:THR:OG1	2.21	0.58
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.37	0.58
5:F:163:LEU:HB3	5:F:174:LEU:HD13	1.85	0.58
1:A:31:GLY:N	1:A:193:ASP:OD2	2.36	0.57
2:C:367:LEU:HA	2:C:371:LYS:HZ2	1.68	0.57
2:C:974:LEU:HD11	2:C:989:VAL:HG21	1.86	0.57
2:C:1093:GLN:CB	3:D:90:MET:HE2	2.33	0.57
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.39	0.57
3:D:293:VAL:HG23	3:D:294:HIS:O	2.04	0.57
7:H:16:DC:H2''	7:H:17:DA:C8	2.39	0.57
3:D:93:ILE:HD11	3:D:548:ILE:HD11	1.85	0.57
3:D:137:PRO:CB	3:D:147:VAL:HG23	2.32	0.57
3:D:221:ALA:CB	3:D:281:THR:HG22	2.34	0.57
3:D:557:LEU:HD13	3:D:566:ILE:CG2	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:216:VAL:HA	3:D:340:THR:CG2	2.30	0.57
3:D:1004:THR:OG1	3:D:1036:ARG:HD3	2.04	0.57
5:F:404:ALA:O	5:F:408:LEU:HG	2.04	0.57
2:C:767:PRO:CG	2:C:782:ALA:HB1	2.35	0.57
3:D:378:ILE:HD12	3:D:378:ILE:N	2.19	0.57
5:F:219:GLY:O	5:F:222:ARG:N	2.38	0.57
2:C:128:ILE:O	2:C:129:ILE:HD12	2.04	0.57
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.35	0.57
3:D:706:PRO:CB	3:D:708:LEU:HD21	2.35	0.57
3:D:117:ASP:HB2	3:D:495:ARG:NH1	2.19	0.57
3:D:223:LEU:HD11	3:D:288:MET:SD	2.44	0.57
1:B:170:VAL:O	1:B:170:VAL:HG12	2.05	0.57
3:D:1305:LEU:HD13	3:D:1309:ALA:CB	2.35	0.57
5:F:369:LEU:CD2	5:F:372:ARG:HB2	2.35	0.57
1:A:25:LEU:HD23	1:A:28:LEU:HD21	1.86	0.57
1:A:34:VAL:HG21	1:B:42:ARG:CZ	2.33	0.57
1:A:156:HIS:NE2	1:A:167:VAL:O	2.31	0.57
1:B:208:LEU:HD12	1:B:208:LEU:O	2.05	0.57
2:C:388:ARG:HG3	2:C:388:ARG:HH11	1.70	0.57
3:D:371:ILE:HG13	3:D:372:ASP:H	1.68	0.57
3:D:930:LEU:O	3:D:934:LEU:HD12	2.04	0.57
3:D:1101:VAL:HG22	3:D:1101:VAL:O	2.05	0.57
5:F:271:LEU:CD2	5:F:307:THR:HG21	2.35	0.57
5:F:338:LEU:CD2	5:F:339:PRO:HD2	2.14	0.57
3:D:97:THR:HG22	3:D:554:LEU:HD21	1.86	0.57
3:D:574:LEU:O	3:D:578:VAL:HG12	2.05	0.57
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.40	0.57
2:C:798:GLY:HA3	2:C:828:ALA:O	2.05	0.57
2:C:1019:GLN:HE21	3:D:621:LYS:HE3	1.70	0.57
3:D:135:LEU:O	3:D:149:LYS:HE3	2.05	0.57
3:D:140:ALA:HA	3:D:450:TYR:CE1	2.39	0.57
3:D:235:ALA:HB1	3:D:319:ALA:O	2.05	0.57
3:D:885:ILE:HD13	3:D:937:TYR:HD1	1.70	0.57
5:F:207:LEU:HB2	5:F:212:LEU:HD21	1.87	0.57
2:C:196:LEU:HD22	2:C:196:LEU:C	2.30	0.56
4:E:41:GLU:N	4:E:44:GLU:OE2	2.34	0.56
1:A:26:GLU:OE2	1:A:194:LYS:HD3	2.05	0.56
1:B:66:SER:O	1:B:75:VAL:HG23	2.05	0.56
1:B:107:LYS:HG2	1:B:108:GLU:N	2.20	0.56
2:C:214:TYR:HD2	2:C:218:VAL:CG2	2.17	0.56
2:C:596:TYR:C	2:C:655:LEU:HD13	2.29	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:670:GLN:HG2	2:C:699:PHE:CE2	2.40	0.56
1:A:62:LEU:HD12	1:A:62:LEU:N	2.21	0.56
2:C:74:GLY:O	2:C:92:ALA:HB1	2.05	0.56
2:C:405:ARG:NE	2:C:566:THR:HG21	2.21	0.56
2:C:1009:SER:HA	3:D:625:TYR:HD1	1.70	0.56
3:D:171:LEU:HD21	3:D:390:PRO:HD2	1.88	0.56
3:D:180:LYS:HA	3:D:205:TYR:OH	2.05	0.56
3:D:242:LEU:HD23	3:D:311:LEU:HD12	1.87	0.56
3:D:691:LEU:O	3:D:694:VAL:HB	2.05	0.56
3:D:709:HIS:C	3:D:711:LEU:H	2.13	0.56
3:D:864:VAL:CG1	3:D:865:THR:H	2.15	0.56
3:D:955:VAL:O	3:D:955:VAL:HG23	2.04	0.56
3:D:1057:VAL:HG23	3:D:1069:GLU:OE2	2.03	0.56
5:F:131:VAL:HG11	5:F:177:ALA:CB	2.33	0.56
5:F:234:LYS:HD3	7:H:5:DA:P	2.46	0.56
2:C:376:ARG:HD3	5:F:276:ARG:HD2	1.87	0.56
2:C:640:ARG:O	2:C:656:ALA:HB1	2.05	0.56
3:D:646:LYS:HB3	3:D:720:LEU:HD23	1.87	0.56
3:D:761:ILE:HD13	4:E:19:LEU:HD21	1.87	0.56
3:D:1217:ILE:HG21	3:D:1480:PHE:CG	2.41	0.56
3:D:1295:GLU:HA	3:D:1300:SER:CB	2.36	0.56
2:C:428:ARG:NH2	2:C:447:ALA:O	2.39	0.56
3:D:171:LEU:HD11	3:D:390:PRO:O	2.05	0.56
3:D:284:LEU:HD12	3:D:288:MET:CE	2.34	0.56
4:E:61:VAL:O	4:E:65:MET:HG3	2.06	0.56
2:C:262:ALA:O	2:C:264:PRO:HD3	2.06	0.56
2:C:727:PRO:HB3	2:C:783:ARG:NH1	2.21	0.56
3:D:40:GLU:OE1	3:D:40:GLU:HA	2.04	0.56
3:D:711:LEU:HD22	3:D:714:GLN:HE21	1.71	0.56
3:D:821:VAL:CG1	3:D:836:VAL:HG21	2.36	0.56
3:D:951:ILE:HD11	3:D:1062:ARG:HG3	1.85	0.56
3:D:968:ASP:O	3:D:972:LEU:HG	2.05	0.56
3:D:1258:ARG:NH2	3:D:1262:LEU:HD21	2.20	0.56
1:A:32:PHE:HA	1:A:35:THR:HB	1.88	0.56
1:A:201:THR:HG23	1:A:203:GLY:H	1.69	0.56
2:C:95:TYR:CE2	2:C:114:PHE:HD1	2.24	0.56
2:C:326:ASP:OD2	2:C:426:ASP:HB3	2.06	0.56
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.17	0.56
2:C:614:ARG:NH2	2:C:618:GLY:O	2.39	0.56
2:C:971:LYS:HA	2:C:987:ILE:O	2.06	0.56
3:D:662:GLU:OE2	3:D:669:ASN:HA	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.87	0.56
3:D:885:ILE:HG21	3:D:937:TYR:HD1	1.70	0.56
3:D:1031:ASN:HB2	3:D:1032:PRO:CD	2.36	0.56
5:F:171:LYS:HD3	5:F:175:HIS:HE1	1.69	0.56
2:C:150:PRO:CD	2:C:322:VAL:HG11	2.35	0.56
2:C:836:GLY:HA3	2:C:1001:VAL:CG2	2.36	0.56
2:C:1015:LEU:HD11	5:F:333:ILE:HG21	1.86	0.56
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.06	0.56
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.87	0.56
3:D:1190:SER:OG	3:D:1191:PRO:HD2	2.06	0.56
4:E:36:LYS:HB2	4:E:93:TYR:HB3	1.88	0.56
1:A:65:PHE:CE2	2:C:703:ILE:CG2	2.89	0.56
2:C:278:GLU:HG2	2:C:283:ILE:O	2.05	0.56
2:C:878:SER:OG	3:D:1029:ARG:HD2	2.06	0.56
3:D:126:VAL:O	3:D:457:GLY:N	2.38	0.56
3:D:1197:ARG:HD3	3:D:1198:TYR:CE2	2.41	0.56
1:A:9:PRO:HB2	1:A:26:GLU:C	2.31	0.56
1:A:64:GLU:HA	1:A:165:ILE:HD13	1.86	0.56
2:C:258:TYR:CD1	2:C:263:ASP:HB2	2.41	0.56
2:C:879:ARG:HH22	10:D:1601:DCP:PG	2.29	0.56
2:C:1019:GLN:NE2	3:D:621:LYS:HE3	2.21	0.56
3:D:18:ILE:HD13	3:D:516:ALA:O	2.06	0.56
3:D:879:ARG:HB3	3:D:902:LEU:CD1	2.35	0.56
5:F:367:MET:HE3	5:F:368:VAL:CG1	2.32	0.56
2:C:586:ARG:O	2:C:589:ARG:HB2	2.06	0.55
2:C:617:ASP:N	2:C:617:ASP:OD1	2.39	0.55
2:C:742:VAL:CG1	2:C:803:THR:HG21	2.36	0.55
3:D:348:GLN:H	3:D:351:MET:CE	2.19	0.55
2:C:150:PRO:HD3	2:C:322:VAL:HG21	1.88	0.55
2:C:551:GLU:OE2	2:C:551:GLU:N	2.30	0.55
2:C:1018:GLN:NE2	5:F:335:ASP:OD2	2.35	0.55
2:C:1048:THR:O	2:C:1052:MET:HE2	2.06	0.55
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.25	0.55
3:D:41:ARG:HH21	3:D:48:ARG:HH11	1.54	0.55
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.42	0.55
5:F:260:ILE:HD11	5:F:265:VAL:HG22	1.87	0.55
1:B:59:GLU:HB2	1:B:139:ASN:HB3	1.89	0.55
1:B:99:LEU:HD23	1:B:114:PHE:HB3	1.88	0.55
1:B:197:LEU:HD12	1:B:198:ARG:H	1.70	0.55
2:C:139:GLN:HB2	2:C:391:LEU:CD1	2.36	0.55
2:C:726:ILE:CG2	2:C:729:LEU:HD22	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:948:GLU:HG3	2:C:953:VAL:HG23	1.86	0.55
3:D:961:LYS:HA	3:D:964:LEU:HB2	1.88	0.55
5:F:390:PHE:CE2	5:F:397:ILE:HG12	2.42	0.55
2:C:577:PRO:HB3	2:C:993:PHE:CD1	2.41	0.55
2:C:581:THR:HB	2:C:905:ILE:HD13	1.89	0.55
3:D:70:GLY:N	3:D:80:VAL:HG23	2.04	0.55
3:D:554:LEU:HB2	3:D:570:GLU:HG3	1.87	0.55
3:D:706:PRO:HB2	3:D:708:LEU:HD21	1.89	0.55
3:D:885:ILE:CG2	3:D:937:TYR:HD1	2.19	0.55
3:D:1155:VAL:HG11	3:D:1183:ILE:HD12	1.88	0.55
3:D:1234:THR:N	3:D:1235:GLN:CB	2.69	0.55
4:E:45:ARG:O	4:E:47:LYS:HG2	2.06	0.55
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.87	0.55
1:A:131:THR:C	1:A:132:LEU:HD12	2.30	0.55
3:D:528:VAL:O	3:D:535:PHE:HA	2.06	0.55
3:D:1047:LYS:HG3	3:D:1053:PHE:CZ	2.40	0.55
7:H:21:DA:H2''	7:H:22:DT:OP2	2.05	0.55
1:A:68:ILE:HG22	1:A:71:VAL:HG13	1.89	0.55
2:C:598:GLU:O	2:C:599:GLU:HG2	2.05	0.55
3:D:185:VAL:HG13	3:D:189:GLN:CD	2.32	0.55
3:D:187:LYS:HD2	3:D:200:ASP:OD2	2.07	0.55
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.89	0.55
3:D:231:VAL:HG13	3:D:242:LEU:C	2.32	0.55
3:D:709:HIS:O	3:D:711:LEU:N	2.39	0.55
3:D:864:VAL:CG1	3:D:865:THR:N	2.70	0.55
3:D:1047:LYS:HG3	3:D:1053:PHE:CE2	2.41	0.55
3:D:1495:ILE:HG23	4:E:88:GLU:OE2	2.07	0.55
5:F:135:ILE:HD11	5:F:182:ALA:HB2	1.87	0.55
5:F:372:ARG:HA	5:F:372:ARG:NE	2.21	0.55
1:A:206:THR:HG22	1:A:209:GLU:HG2	1.89	0.55
2:C:820:ARG:NH1	2:C:820:ARG:HB3	2.21	0.55
3:D:1198:TYR:CE2	3:D:1460:ILE:HD13	2.42	0.55
4:E:85:LEU:HD21	4:E:89:MET:HE2	1.89	0.55
5:F:237:THR:HG21	7:H:3:DT:H5''	1.88	0.55
1:A:18:ARG:NH2	1:A:88:ARG:CZ	2.66	0.55
1:A:23:PHE:CD2	1:A:211:LEU:HD23	2.42	0.55
1:B:162:ILE:HD12	1:B:163:ASN:N	2.22	0.55
2:C:181:VAL:HG23	2:C:221:LEU:HA	1.89	0.55
2:C:375:SER:OG	2:C:379:GLU:OE1	2.24	0.55
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.06	0.55
2:C:1019:GLN:HG2	2:C:1057:SER:OG	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:421:LEU:HD13	3:D:428:LYS:CA	2.35	0.55
3:D:977:ALA:O	3:D:982:PHE:HB3	2.06	0.55
1:A:6:LEU:HD23	1:A:7:LYS:N	2.21	0.55
1:A:65:PHE:CE2	2:C:703:ILE:HG21	2.42	0.55
1:B:12:THR:HB	1:B:24:VAL:HG23	1.89	0.55
1:B:44:LEU:HD21	1:B:211:LEU:HA	1.88	0.55
2:C:36:PRO:HA	2:C:39:ARG:HG3	1.88	0.55
2:C:111:ASP:OD2	2:C:370:ALA:HB2	2.07	0.55
2:C:693:GLU:CD	2:C:696:LYS:HD2	2.32	0.55
2:C:882:LEU:HD11	3:D:1038:LEU:HD22	1.87	0.55
3:D:183:GLU:HG3	3:D:185:VAL:HG23	1.88	0.55
3:D:371:ILE:HD11	5:F:232:ARG:NH1	2.21	0.55
3:D:650:LEU:CD1	3:D:657:LEU:CD2	2.84	0.55
3:D:767:HIS:CE1	4:E:3:GLU:HB2	2.42	0.55
3:D:885:ILE:CG2	3:D:937:TYR:CD1	2.90	0.55
2:C:150:PRO:CG	2:C:322:VAL:HG21	2.36	0.55
2:C:422:ARG:HH22	7:H:13:DT:H3'	1.72	0.55
2:C:459:ALA:C	2:C:460:ARG:HG3	2.32	0.55
3:D:982:PHE:C	3:D:983:LEU:HG	2.32	0.55
1:A:153:ALA:O	1:A:155:LYS:N	2.39	0.54
2:C:736:ASP:O	2:C:744:ARG:HG2	2.07	0.54
2:C:915:LYS:HE3	2:C:968:LEU:O	2.07	0.54
3:D:59:ALA:CB	3:D:78:VAL:HG21	2.32	0.54
3:D:409:VAL:HG23	3:D:435:VAL:HG21	1.88	0.54
5:F:129:GLU:CG	5:F:144:ILE:HG13	2.36	0.54
5:F:153:PRO:HA	5:F:156:VAL:CG1	2.37	0.54
1:B:101:LEU:HD12	1:B:113:ASP:O	2.06	0.54
1:B:117:VAL:CG1	1:B:118:ALA:H	2.16	0.54
1:B:224:TYR:N	1:B:224:TYR:CD1	2.75	0.54
2:C:293:PHE:HD1	2:C:298:PHE:CE1	2.25	0.54
2:C:367:LEU:HA	2:C:371:LYS:NZ	2.22	0.54
2:C:502:PRO:C	2:C:503:LEU:HD23	2.32	0.54
2:C:1101:THR:HG21	2:C:1111:ILE:HG21	1.89	0.54
3:D:258:VAL:HA	3:D:296:GLU:O	2.07	0.54
3:D:270:LEU:HD13	3:D:304:LEU:HD13	1.89	0.54
3:D:315:ARG:H	3:D:315:ARG:CD	2.19	0.54
1:A:34:VAL:CG2	1:B:42:ARG:CZ	2.85	0.54
1:B:173:PRO:CB	1:B:205:VAL:HG12	2.38	0.54
2:C:281:LEU:HD23	2:C:309:TYR:HD1	1.72	0.54
2:C:362:GLY:O	2:C:363:SER:HB3	2.06	0.54
2:C:708:TYR:OH	2:C:796:GLU:HG2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:272:SER:O	5:F:276:ARG:HG3	2.07	0.54
5:F:387:GLY:CA	5:F:394:ARG:HG2	2.38	0.54
1:B:219:ARG:HA	1:B:222:LEU:HD12	1.89	0.54
2:C:540:PHE:HB3	2:C:544:THR:HG21	1.88	0.54
2:C:719:PRO:CD	2:C:761:PHE:HE1	2.21	0.54
2:C:911:GLU:N	2:C:912:PRO:HD2	2.23	0.54
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.90	0.54
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.88	0.54
3:D:1376:MET:HE1	3:D:1421:LEU:CD1	2.36	0.54
5:F:265:VAL:O	5:F:269:ASN:ND2	2.40	0.54
1:B:89:PHE:HB2	1:B:146:ARG:HH21	1.72	0.54
3:D:361:VAL:HG21	3:D:379:ALA:HB1	1.89	0.54
3:D:697:GLY:HA3	4:E:59:ASN:HD22	1.72	0.54
3:D:1492:LEU:O	3:D:1492:LEU:HD13	2.08	0.54
1:A:175:ARG:HH12	1:A:176:ARG:NH1	2.06	0.54
1:B:64:GLU:OE2	1:B:79:ILE:HD13	2.08	0.54
2:C:136:ILE:HG21	2:C:336:VAL:HG23	1.90	0.54
2:C:742:VAL:HG12	2:C:743:VAL:O	2.08	0.54
2:C:1001:VAL:HG11	3:D:724:GLN:HB2	1.89	0.54
1:A:9:PRO:HD3	1:B:224:TYR:CD2	2.42	0.54
1:B:26:GLU:CB	1:B:194:LYS:HG3	2.36	0.54
3:D:648:MET:HE1	3:D:747:VAL:HG21	1.88	0.54
3:D:1264:GLU:OE1	3:D:1264:GLU:HA	2.06	0.54
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.08	0.54
3:D:1492:LEU:O	3:D:1492:LEU:HD22	2.07	0.54
1:A:42:ARG:NH2	1:B:34:VAL:HG22	2.22	0.54
2:C:1004:LYS:HD3	3:D:744:GLN:HE22	1.73	0.54
3:D:529:GLN:HG3	3:D:535:PHE:CZ	2.43	0.54
5:F:295:MET:HE3	5:F:299:TRP:CE2	2.41	0.54
7:H:19:DG:H2"	7:H:20:DG:C8	2.42	0.54
1:A:111:ALA:HB2	1:A:127:LEU:HB3	1.89	0.54
1:B:33:GLY:O	1:B:181:VAL:HG21	2.07	0.54
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.38	0.54
2:C:626:ARG:H	2:C:639:GLN:NE2	2.05	0.54
2:C:748:GLU:HA	2:C:799:ILE:HD13	1.89	0.54
3:D:93:ILE:HD11	3:D:548:ILE:CG1	2.38	0.54
3:D:124:GLU:OE2	3:D:587:ARG:NH1	2.40	0.54
3:D:378:ILE:HD12	3:D:378:ILE:H	1.73	0.54
3:D:749:VAL:HG12	3:D:750:PRO:O	2.08	0.54
3:D:1045:MET:HG3	3:D:1073:SER:HA	1.90	0.54
3:D:1192:LEU:CD2	3:D:1369:GLU:HB3	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:164:LYS:HD2	5:F:164:LYS:O	2.06	0.54
5:F:240:THR:O	5:F:240:THR:HG22	2.07	0.54
5:F:319:THR:HG22	5:F:320:PRO:HD2	1.90	0.54
1:A:40:LEU:CD2	1:A:218:LEU:HD12	2.37	0.54
1:A:94:LEU:O	1:A:146:ARG:NH1	2.41	0.54
1:B:44:LEU:HB2	1:B:177:VAL:HG21	1.89	0.54
1:B:54:THR:CG2	1:B:143:ARG:HG2	2.38	0.54
1:B:173:PRO:HB2	1:B:205:VAL:HG12	1.90	0.54
2:C:84:ARG:HD3	2:C:629:TYR:OH	2.08	0.54
3:D:141:ILE:HD12	3:D:145:VAL:N	2.23	0.54
3:D:207:PHE:HB2	3:D:391:ALA:HB2	1.90	0.54
3:D:446:VAL:O	3:D:446:VAL:HG12	2.08	0.54
3:D:850:LEU:HD11	3:D:881:LEU:HD13	1.89	0.54
3:D:996:TRP:HH2	3:D:1058:ARG:HH22	1.56	0.54
3:D:1289:LYS:NZ	3:D:1304:LYS:HB2	2.23	0.54
2:C:418:LEU:CD2	2:C:427:VAL:HG11	2.38	0.53
2:C:569:VAL:HG21	2:C:1000:MET:HE2	1.88	0.53
2:C:596:TYR:O	2:C:655:LEU:HD13	2.08	0.53
3:D:180:LYS:O	3:D:183:GLU:CB	2.57	0.53
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.89	0.53
3:D:209:ARG:NH2	3:D:391:ALA:HA	2.23	0.53
3:D:766:ALA:HB3	4:E:2:ALA:HA	1.89	0.53
3:D:966:GLU:HG2	3:D:969:ARG:NH1	2.22	0.53
3:D:1444:THR:O	3:D:1445:HIS:C	2.51	0.53
5:F:397:ILE:O	5:F:401:GLU:HB2	2.07	0.53
1:A:82:LEU:HD23	1:A:129:ILE:HD12	1.89	0.53
2:C:12:VAL:HG21	2:C:472:ARG:CD	2.38	0.53
2:C:211:LEU:HB3	2:C:218:VAL:HG22	1.88	0.53
3:D:116:LEU:HD11	3:D:465:LEU:CD1	2.38	0.53
3:D:135:LEU:HD11	3:D:463:GLN:CG	2.38	0.53
3:D:157:GLU:O	3:D:161:LEU:HG	2.08	0.53
3:D:1263:PHE:O	3:D:1375:MET:HE2	2.09	0.53
1:A:6:LEU:HD23	1:A:7:LYS:H	1.73	0.53
1:A:11:PHE:CE2	1:B:225:PHE:HA	2.43	0.53
1:A:34:VAL:HG23	1:A:35:THR:N	2.24	0.53
2:C:55:GLU:O	2:C:359:MET:HE1	2.08	0.53
2:C:988:VAL:HG23	3:D:948:THR:HG23	1.90	0.53
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.41	0.53
3:D:758:GLU:HA	3:D:762:GLN:OE1	2.08	0.53
5:F:161:GLN:O	5:F:165:SER:OG	2.20	0.53
5:F:372:ARG:O	5:F:373:LYS:HG2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:ILE:HG23	2:C:171:TRP:CE2	2.43	0.53
2:C:670:GLN:HB2	2:C:700:TYR:CE1	2.43	0.53
2:C:729:LEU:HD21	2:C:754:ILE:HD11	1.90	0.53
3:D:26:VAL:HG12	3:D:548:ILE:HD13	1.90	0.53
3:D:767:HIS:CE1	4:E:6:ILE:HD13	2.43	0.53
3:D:1291:SER:OG	3:D:1302:GLU:HG3	2.08	0.53
3:D:1300:SER:OG	3:D:1301:LYS:N	2.40	0.53
5:F:264:MET:O	5:F:268:ILE:HG13	2.08	0.53
6:G:8:DC:H42	7:H:20:DG:H1	1.55	0.53
1:B:74:ASP:O	1:B:78:ILE:HG13	2.08	0.53
2:C:112:GLU:HG3	2:C:112:GLU:O	2.07	0.53
2:C:805:ARG:CG	2:C:823:VAL:HG23	2.22	0.53
2:C:950:LEU:HB2	2:C:952:LEU:CD2	2.38	0.53
3:D:978:TYR:O	3:D:981:GLY:N	2.40	0.53
3:D:1487:VAL:HG12	4:E:85:LEU:HD11	1.91	0.53
2:C:292:ARG:HD3	2:C:299:LYS:HB2	1.89	0.53
2:C:974:LEU:HD22	2:C:987:ILE:CB	2.38	0.53
2:C:1099:VAL:HG22	3:D:10:ILE:HG13	1.90	0.53
3:D:64:LYS:O	3:D:65:ARG:HG3	2.08	0.53
3:D:116:LEU:HD12	3:D:118:LEU:HD12	1.89	0.53
3:D:347:VAL:HA	3:D:351:MET:HE3	1.89	0.53
3:D:409:VAL:CG2	3:D:435:VAL:HG21	2.39	0.53
3:D:1422:MET:HE3	3:D:1426:LYS:CD	2.39	0.53
5:F:127:ILE:O	5:F:131:VAL:HG23	2.09	0.53
1:A:152:PRO:O	1:A:155:LYS:HB3	2.09	0.53
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.43	0.53
2:C:542:VAL:HG12	2:C:543:ASN:N	2.24	0.53
2:C:682:TYR:CE1	2:C:851:LYS:HD3	2.44	0.53
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.44	0.53
3:D:33:ASN:N	3:D:38:LYS:O	2.32	0.53
5:F:155:THR:HA	5:F:158:GLU:HB2	1.90	0.53
1:A:41:ARG:HG3	1:A:177:VAL:CG1	2.37	0.53
1:A:122:ILE:O	1:A:125:PRO:HD3	2.09	0.53
1:A:227:ASN:HD22	1:A:227:ASN:C	2.16	0.53
1:B:101:LEU:HD11	1:B:109:VAL:HG11	1.90	0.53
1:B:205:VAL:HG22	1:B:206:THR:N	2.23	0.53
2:C:683:ASN:HB3	2:C:872:ASN:CB	2.33	0.53
2:C:683:ASN:CG	2:C:872:ASN:HB2	2.34	0.53
3:D:274:ARG:O	3:D:275:GLU:C	2.52	0.53
3:D:313:MET:HE2	3:D:319:ALA:HB2	1.89	0.53
3:D:565:ILE:HD11	5:F:189:GLU:OE1	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:789:LEU:HD23	3:D:938:GLY:HA2	1.91	0.53
3:D:957:PRO:HG3	3:D:1007:VAL:HG22	1.91	0.53
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.91	0.53
2:C:129:ILE:HG22	2:C:129:ILE:O	2.09	0.53
2:C:150:PRO:HD3	2:C:322:VAL:CG2	2.39	0.53
2:C:831:ARG:NE	2:C:1002:GLU:OE1	2.42	0.53
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.39	0.53
3:D:44:LEU:O	3:D:525:ARG:NH2	2.42	0.53
3:D:851:LEU:HD11	3:D:855:HIS:CE1	2.44	0.53
3:D:1495:ILE:HA	4:E:88:GLU:OE2	2.09	0.53
1:B:58:ILE:HG22	1:B:61:VAL:CG2	2.39	0.53
2:C:29:ALA:O	2:C:44:ILE:HB	2.09	0.53
2:C:486:MET:HE1	2:C:494:TYR:CD2	2.44	0.53
2:C:524:VAL:HG22	2:C:528:GLU:HB2	1.91	0.53
2:C:808:ARG:HG3	2:C:814:GLU:HA	1.91	0.53
3:D:686:GLU:H	3:D:686:GLU:CD	2.16	0.53
3:D:1109:GLU:C	3:D:1217:ILE:HD11	2.34	0.53
4:E:37:ASN:HA	4:E:93:TYR:CE2	2.44	0.53
5:F:374:GLY:N	5:F:378:GLY:HA2	2.24	0.53
1:A:149:GLY:O	1:A:171:PHE:HB2	2.09	0.52
1:B:120:VAL:O	1:B:120:VAL:HG12	2.08	0.52
2:C:102:HIS:ND1	2:C:105:THR:HG23	2.25	0.52
3:D:135:LEU:HD11	3:D:463:GLN:HG2	1.89	0.52
3:D:698:LYS:HB2	3:D:756:GLN:OE1	2.09	0.52
3:D:1431:THR:HG23	3:D:1433:SER:H	1.73	0.52
1:A:6:LEU:HD21	1:A:27:PRO:HG2	1.91	0.52
2:C:841:ASN:ND2	2:C:992:MET:HE2	2.18	0.52
3:D:116:LEU:HD12	3:D:118:LEU:CD1	2.40	0.52
3:D:204:LEU:HD11	3:D:445:ARG:HE	1.74	0.52
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.42	0.52
3:D:699:VAL:HB	3:D:716:PHE:O	2.10	0.52
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.90	0.52
4:E:42:PRO:HA	4:E:45:ARG:HG3	1.90	0.52
5:F:81:VAL:HG12	5:F:82:ARG:N	2.23	0.52
2:C:974:LEU:HD22	2:C:987:ILE:HB	1.92	0.52
3:D:955:VAL:HG22	3:D:1011:PHE:CE1	2.44	0.52
5:F:113:ILE:CD1	5:F:128:ARG:HG3	2.38	0.52
5:F:210:LEU:O	5:F:213:ILE:N	2.42	0.52
2:C:841:ASN:HD22	2:C:992:MET:CE	2.17	0.52
3:D:728:LEU:HD12	3:D:729:HIS:N	2.24	0.52
3:D:1013:GLU:C	3:D:1014:ASN:OD1	2.53	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:94:LEU:HD11	5:F:187:LEU:HD12	1.92	0.52
1:A:42:ARG:NH2	1:B:31:GLY:O	2.35	0.52
2:C:74:GLY:O	2:C:93:PRO:HD2	2.10	0.52
2:C:140:ILE:CD1	2:C:331:ARG:HH11	2.20	0.52
2:C:200:LEU:HD13	2:C:300:ASP:CB	2.29	0.52
2:C:239:PHE:HE2	2:C:246:ASP:HB3	1.74	0.52
2:C:540:PHE:CD1	2:C:544:THR:HG21	2.45	0.52
2:C:880:MET:CE	3:D:1061:PHE:HE2	2.23	0.52
2:C:1047:HIS:O	2:C:1051:GLU:HG3	2.10	0.52
3:D:204:LEU:HD22	3:D:441:ARG:CZ	2.40	0.52
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.25	0.52
3:D:806:PHE:O	3:D:829:VAL:HG13	2.10	0.52
3:D:879:ARG:HB3	3:D:902:LEU:HD12	1.91	0.52
1:A:216:GLU:OE1	1:A:219:ARG:NH2	2.42	0.52
1:A:226:SER:C	1:A:228:PRO:HD3	2.34	0.52
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.45	0.52
3:D:798:GLU:HG2	3:D:824:ASN:HB2	1.89	0.52
3:D:1277:ILE:HD13	3:D:1278:ASP:O	2.09	0.52
5:F:413:SER:HA	5:F:416:ARG:NH2	2.25	0.52
1:B:7:LYS:HE3	1:B:186:LEU:CD2	2.39	0.52
1:B:58:ILE:HD11	1:B:140:MET:SD	2.50	0.52
1:B:97:VAL:CG1	1:B:99:LEU:HD12	2.39	0.52
2:C:182:VAL:HG23	2:C:193:LEU:HB3	1.90	0.52
2:C:280:LYS:HE3	2:C:309:TYR:CE1	2.45	0.52
2:C:328:LEU:HD11	2:C:438:ILE:HD13	1.91	0.52
3:D:405:ASP:N	3:D:423:ASP:OD1	2.39	0.52
3:D:626:SER:HA	3:D:747:VAL:O	2.10	0.52
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.09	0.52
3:D:1038:LEU:O	3:D:1060:SER:OG	2.27	0.52
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.91	0.52
5:F:88:ILE:HD11	5:F:192:LEU:CD1	2.39	0.52
5:F:239:ALA:C	5:F:241:TRP:H	2.16	0.52
1:A:97:VAL:HG12	1:A:98:THR:N	2.24	0.52
1:B:96:THR:O	1:B:97:VAL:HG23	2.10	0.52
1:B:188:GLN:HG2	3:D:685:ASP:OD2	2.09	0.52
3:D:171:LEU:HD12	3:D:171:LEU:O	2.10	0.52
3:D:181:ASP:N	3:D:205:TYR:CE1	2.78	0.52
3:D:367:ILE:HB	3:D:377:VAL:HG22	1.90	0.52
3:D:546:ARG:O	3:D:550:ARG:HG3	2.09	0.52
3:D:566:ILE:HG22	3:D:567:ILE:N	2.24	0.52
3:D:798:GLU:HG3	3:D:824:ASN:CB	2.36	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:HIS:ND1	1:A:224:TYR:HE2	2.07	0.52
2:C:253:ALA:O	2:C:257:VAL:HG22	2.09	0.52
2:C:422:ARG:NH2	7:H:13:DT:H5'	2.24	0.52
2:C:550:LEU:HD23	2:C:906:PHE:HE1	1.75	0.52
2:C:587:VAL:HG11	2:C:666:LEU:HD22	1.92	0.52
2:C:1037:VAL:HG13	2:C:1049:LEU:CD1	2.38	0.52
3:D:314:PRO:HD2	3:D:317:VAL:HG11	1.92	0.52
3:D:916:TYR:CZ	3:D:920:LEU:HD11	2.44	0.52
1:A:58:ILE:O	1:A:61:VAL:HB	2.10	0.52
2:C:281:LEU:O	2:C:283:ILE:HG23	2.10	0.52
2:C:498:GLN:NE2	3:D:1068:LEU:HD12	2.25	0.52
3:D:42:ASP:N	3:D:46:ASP:OD2	2.38	0.52
3:D:767:HIS:HE1	4:E:3:GLU:HB2	1.73	0.52
3:D:968:ASP:N	3:D:968:ASP:OD1	2.37	0.52
4:E:47:LYS:NZ	4:E:56:ASP:OD1	2.32	0.52
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.91	0.51
1:B:14:ARG:HB3	1:B:14:ARG:NH1	2.25	0.51
3:D:41:ARG:HH21	3:D:48:ARG:NH1	2.09	0.51
3:D:86:LYS:HB2	3:D:523:ASP:OD2	2.11	0.51
3:D:343:LYS:NZ	3:D:380:GLU:OE2	2.42	0.51
3:D:462:GLN:O	3:D:466:LYS:HB2	2.10	0.51
3:D:729:HIS:CE1	3:D:730:PRO:HD2	2.45	0.51
3:D:1263:PHE:CE1	3:D:1352:ILE:HD13	2.44	0.51
5:F:366:ALA:O	5:F:370:LYS:HB2	2.10	0.51
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.92	0.51
1:B:20:TYR:CZ	1:B:22:GLU:HG2	2.46	0.51
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.92	0.51
3:D:658:LEU:HD23	3:D:661:MET:HE3	1.92	0.51
3:D:1140:ILE:HG22	3:D:1144:LEU:HD12	1.92	0.51
3:D:1431:THR:HG23	3:D:1432:LYS:N	2.25	0.51
3:D:1445:HIS:O	3:D:1449:GLU:HG3	2.10	0.51
5:F:193:ARG:HG2	7:H:7:DG:H5'	1.92	0.51
2:C:236:ILE:CG2	2:C:248:PRO:HB2	2.40	0.51
2:C:690:ILE:HG13	2:C:852:ILE:CG2	2.25	0.51
2:C:704:HIS:HD2	2:C:831:ARG:HD2	1.69	0.51
2:C:915:LYS:HD3	2:C:968:LEU:HB3	1.90	0.51
3:D:499:VAL:HG12	3:D:503:LEU:CD1	2.40	0.51
3:D:1207:TYR:HA	3:D:1213:ARG:O	2.09	0.51
3:D:1394:VAL:HG22	3:D:1420:LEU:CD2	2.40	0.51
3:D:1487:VAL:O	4:E:74:VAL:HG23	2.10	0.51
2:C:224:GLU:C	2:C:226:VAL:N	2.68	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:498:GLN:HE21	3:D:1068:LEU:HD12	1.76	0.51
3:D:122:GLU:HG2	3:D:152:LEU:CD1	2.38	0.51
3:D:832:ARG:H	3:D:832:ARG:NE	2.08	0.51
1:A:44:LEU:HB3	1:A:177:VAL:HG21	1.93	0.51
2:C:693:GLU:HG2	2:C:855:VAL:HB	1.91	0.51
2:C:974:LEU:CD2	2:C:987:ILE:HG21	2.41	0.51
3:D:236:TYR:HB3	3:D:313:MET:HG3	1.91	0.51
3:D:811:GLU:O	3:D:814:ALA:HB3	2.10	0.51
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.46	0.51
3:D:1192:LEU:CD1	3:D:1345:GLU:HB3	2.40	0.51
3:D:1489:GLN:NE2	3:D:1492:LEU:HB3	2.25	0.51
4:E:39:VAL:CG2	4:E:72:ARG:HB3	2.39	0.51
5:F:186:HIS:ND1	5:F:186:HIS:O	2.44	0.51
1:B:54:THR:HG23	1:B:143:ARG:HG2	1.93	0.51
2:C:340:MET:SD	2:C:340:MET:C	2.93	0.51
2:C:709:GLU:OE2	2:C:824:ARG:HD3	2.11	0.51
3:D:74:GLU:CD	3:D:74:GLU:H	2.18	0.51
3:D:343:LYS:CD	3:D:345:TYR:HE2	2.24	0.51
3:D:422:ALA:O	3:D:427:VAL:HG12	2.10	0.51
3:D:554:LEU:HD12	3:D:570:GLU:HB3	1.90	0.51
3:D:803:GLY:HA2	3:D:826:PRO:O	2.10	0.51
2:C:6:PHE:CG	2:C:909:ALA:HB2	2.46	0.51
2:C:461:VAL:HG23	2:C:461:VAL:O	2.10	0.51
2:C:613:VAL:HG23	2:C:613:VAL:O	2.09	0.51
3:D:62:LYS:HB3	3:D:63:TYR:HD2	1.71	0.51
3:D:661:MET:SD	3:D:677:LEU:HD21	2.50	0.51
3:D:1045:MET:HE3	3:D:1045:MET:CA	2.41	0.51
1:B:54:THR:HG21	1:B:145:ASP:OD1	2.11	0.51
2:C:340:MET:HB2	2:C:385:PHE:CE2	2.45	0.51
3:D:1216:SER:HB3	4:E:15:SER:HA	1.93	0.51
2:C:707:ARG:CB	2:C:707:ARG:HH11	2.23	0.51
2:C:752:GLY:HA3	3:D:679:ARG:HA	1.93	0.51
5:F:156:VAL:O	5:F:160:ASP:HB2	2.11	0.51
5:F:167:PRO:HD2	5:F:170:HIS:HB2	1.91	0.51
1:B:7:LYS:HE3	1:B:186:LEU:HD21	1.91	0.51
2:C:31:GLN:C	2:C:33:ASP:H	2.19	0.51
2:C:390:GLN:NE2	2:C:414:GLY:HA2	2.26	0.51
2:C:1015:LEU:HD11	5:F:333:ILE:CG2	2.40	0.51
2:C:1019:GLN:CD	3:D:621:LYS:HB3	2.35	0.51
3:D:63:TYR:CD2	3:D:73:CYS:HB2	2.46	0.51
3:D:916:TYR:CZ	3:D:920:LEU:HD21	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:PHE:HE2	3:D:1371:VAL:HG11	1.74	0.51
3:D:1376:MET:HE2	3:D:1376:MET:HA	1.92	0.51
1:A:201:THR:HG21	1:A:206:THR:HA	1.93	0.50
2:C:767:PRO:CG	2:C:782:ALA:CB	2.88	0.50
2:C:836:GLY:C	2:C:1001:VAL:HG22	2.35	0.50
2:C:892:LEU:HD13	2:C:989:VAL:O	2.12	0.50
3:D:632:VAL:C	3:D:740:PHE:CE2	2.90	0.50
3:D:1442:ASN:ND2	6:G:11:DT:H4'	2.25	0.50
5:F:79:ASP:C	5:F:79:ASP:OD1	2.53	0.50
5:F:383:LEU:HD12	5:F:384:GLU:HG3	1.93	0.50
1:A:154:GLU:H	1:A:154:GLU:CD	2.19	0.50
2:C:124:ASP:HA	2:C:592:LEU:CD1	2.39	0.50
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.93	0.50
2:C:422:ARG:CZ	7:H:13:DT:H5'	2.42	0.50
3:D:112:ILE:HG12	3:D:512:MET:SD	2.51	0.50
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.93	0.50
3:D:792:ILE:HD13	3:D:941:PHE:CE2	2.46	0.50
3:D:1047:LYS:CG	3:D:1048:PRO:HD2	2.40	0.50
3:D:1310:ARG:CB	3:D:1327:ARG:HD2	2.42	0.50
1:A:34:VAL:O	1:A:36:LEU:N	2.45	0.50
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.38	0.50
1:A:225:PHE:HA	1:B:11:PHE:CD2	2.47	0.50
2:C:263:ASP:C	2:C:265:ARG:H	2.15	0.50
2:C:376:ARG:N	2:C:376:ARG:HD2	2.27	0.50
2:C:886:LEU:HD11	3:D:951:ILE:CD1	2.38	0.50
2:C:1113:GLU:O	2:C:1115:LEU:HD12	2.11	0.50
3:D:956:ILE:HD13	3:D:1039:CYS:O	2.12	0.50
5:F:362:SER:O	5:F:366:ALA:HB3	2.10	0.50
1:A:182:GLU:HG3	1:A:194:LYS:CE	2.41	0.50
1:B:143:ARG:HD3	1:B:158:ILE:CD1	2.41	0.50
2:C:666:LEU:HD11	2:C:668:LEU:CD2	2.41	0.50
2:C:738:ASP:OD2	2:C:742:VAL:HB	2.11	0.50
2:C:1088:LEU:O	2:C:1088:LEU:HG	2.11	0.50
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.47	0.50
3:D:162:ARG:O	3:D:414:ARG:NH2	2.36	0.50
3:D:601:ARG:NH1	3:D:606:ILE:HA	2.26	0.50
3:D:876:SER:OG	3:D:879:ARG:HG3	2.12	0.50
3:D:958:GLU:C	3:D:960:LYS:H	2.20	0.50
3:D:1352:ILE:CG2	3:D:1368:ILE:HD13	2.42	0.50
5:F:198:ILE:HD12	5:F:243:ILE:HG21	1.92	0.50
1:B:20:TYR:OH	1:B:22:GLU:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:OE2	1:B:194:LYS:HE3	2.11	0.50
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.93	0.50
1:B:58:ILE:CG2	1:B:61:VAL:HG21	2.41	0.50
1:B:90:LEU:HD12	1:B:119:ASP:C	2.37	0.50
2:C:230:ARG:HB2	2:C:233:GLU:HG3	1.93	0.50
2:C:739:GLU:H	2:C:739:GLU:CD	2.20	0.50
3:D:499:VAL:HG12	3:D:503:LEU:HD12	1.94	0.50
3:D:703:ASN:HA	3:D:712:GLY:O	2.11	0.50
3:D:805:GLU:HA	3:D:828:LYS:O	2.12	0.50
3:D:885:ILE:HG23	3:D:937:TYR:HE1	1.71	0.50
1:A:62:LEU:HA	1:A:163:ASN:CB	2.34	0.50
2:C:875:GLY:O	2:C:879:ARG:HD3	2.11	0.50
2:C:1006:HIS:ND1	2:C:1007:ALA:N	2.58	0.50
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.93	0.50
3:D:1150:ALA:O	3:D:1151:ARG:HD2	2.10	0.50
3:D:1371:VAL:O	3:D:1372:VAL:C	2.52	0.50
5:F:191:ASN:OD1	7:H:6:DT:N3	2.34	0.50
5:F:247:ILE:CG2	5:F:251:ILE:HD12	2.42	0.50
2:C:148:PHE:CZ	2:C:309:TYR:HB3	2.47	0.50
2:C:988:VAL:HG23	3:D:948:THR:HG21	1.94	0.50
3:D:135:LEU:CD1	3:D:463:GLN:HG2	2.42	0.50
3:D:566:ILE:HD11	5:F:192:LEU:HD22	1.92	0.50
3:D:921:ARG:O	3:D:922:LEU:HD23	2.11	0.50
3:D:1389:LEU:C	3:D:1390:LEU:HD23	2.36	0.50
3:D:1485:GLN:O	4:E:75:PHE:HA	2.12	0.50
5:F:167:PRO:O	5:F:169:GLU:N	2.44	0.50
2:C:328:LEU:HD11	2:C:438:ILE:CD1	2.42	0.50
3:D:116:LEU:O	3:D:118:LEU:HG	2.12	0.50
3:D:486:ARG:HG3	3:D:489:ARG:HH22	1.72	0.50
3:D:1333:HIS:HE1	3:D:1421:LEU:O	1.95	0.50
3:D:1444:THR:O	3:D:1447:LEU:N	2.44	0.50
7:H:13:DT:H2''	7:H:14:DG:OP1	2.11	0.50
1:A:78:ILE:O	1:A:82:LEU:HG	2.12	0.50
1:A:167:VAL:HG12	1:A:168:ASP:N	2.26	0.50
1:B:110:LYS:C	1:B:129:ILE:HD13	2.37	0.50
2:C:9:ILE:HD11	2:C:500:ASN:HB3	1.94	0.50
2:C:422:ARG:HH22	7:H:13:DT:C4'	2.25	0.50
3:D:135:LEU:O	3:D:135:LEU:HD23	2.12	0.50
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.92	0.50
3:D:315:ARG:HG2	3:D:316:GLN:N	2.27	0.50
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:95:THR:H	5:F:98:GLU:CG	2.15	0.50
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.66	0.49
2:C:211:LEU:HB2	2:C:218:VAL:HG13	1.94	0.49
2:C:272:ALA:HA	2:C:464:LEU:HD13	1.93	0.49
2:C:391:LEU:N	2:C:391:LEU:HD23	2.26	0.49
2:C:724:ARG:O	2:C:724:ARG:HG2	2.12	0.49
2:C:783:ARG:HG3	2:C:784:ASP:N	2.27	0.49
2:C:911:GLU:O	2:C:914:ILE:HG23	2.12	0.49
3:D:116:LEU:HD11	3:D:465:LEU:HD13	1.93	0.49
3:D:206:ARG:HG2	3:D:392:SER:O	2.12	0.49
3:D:478:LEU:C	3:D:480:GLU:N	2.69	0.49
5:F:395:GLU:HB3	5:F:398:ARG:HH12	1.77	0.49
2:C:626:ARG:O	2:C:639:GLN:HB2	2.12	0.49
2:C:697:ARG:HG3	2:C:699:PHE:CD1	2.48	0.49
3:D:97:THR:HG21	3:D:571:LYS:CD	2.42	0.49
3:D:284:LEU:CB	3:D:288:MET:HE2	2.41	0.49
4:E:18:ARG:O	4:E:22:VAL:HG23	2.11	0.49
5:F:126:LEU:HD12	5:F:126:LEU:O	2.12	0.49
1:A:198:ARG:C	1:A:199:ILE:HG12	2.36	0.49
1:B:41:ARG:HA	1:B:177:VAL:HG11	1.94	0.49
2:C:773:LEU:O	2:C:777:ILE:HD12	2.12	0.49
3:D:46:ASP:OD1	3:D:48:ARG:HG3	2.12	0.49
3:D:135:LEU:HD13	3:D:455:ARG:NH1	2.27	0.49
3:D:298:VAL:HG12	3:D:302:GLN:OE1	2.12	0.49
3:D:704:ARG:HG2	3:D:705:ALA:N	2.27	0.49
5:F:369:LEU:HD23	5:F:372:ARG:CB	2.38	0.49
2:C:140:ILE:HG22	2:C:412:ALA:HA	1.92	0.49
2:C:157:ARG:HH22	2:C:178:PRO:HA	1.76	0.49
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.94	0.49
2:C:1092:LEU:HD12	2:C:1099:VAL:HG21	1.93	0.49
3:D:191:LEU:HB2	3:D:195:VAL:HG12	1.94	0.49
3:D:1264:GLU:HG3	3:D:1266:ARG:CZ	2.43	0.49
3:D:1310:ARG:O	3:D:1327:ARG:HG2	2.12	0.49
4:E:68:LEU:HD12	4:E:73:LEU:HD12	1.94	0.49
5:F:270:LYS:HG2	5:F:273:ARG:NH2	2.28	0.49
3:D:96:ALA:CB	3:D:554:LEU:HD23	2.40	0.49
3:D:208:PRO:HG2	3:D:353:VAL:HG11	1.95	0.49
3:D:215:TYR:O	3:D:340:THR:HG22	2.12	0.49
3:D:221:ALA:HB2	3:D:281:THR:HG22	1.94	0.49
3:D:222:GLY:HA2	3:D:333:LEU:O	2.11	0.49
3:D:489:ARG:HD2	3:D:1391:GLU:OE1	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:672:ALA:HB2	5:F:420:ASP:OD1	2.13	0.49
5:F:153:PRO:CA	5:F:156:VAL:HG12	2.41	0.49
5:F:387:GLY:HA3	5:F:394:ARG:HG2	1.94	0.49
5:F:400:ILE:HD13	5:F:403:LYS:HB2	1.95	0.49
1:B:50:GLY:HA3	1:B:173:PRO:HD3	1.95	0.49
2:C:45:GLN:OE1	2:C:71:TYR:CE2	2.66	0.49
2:C:55:GLU:HG3	2:C:56:GLU:N	2.28	0.49
2:C:351:LEU:HD12	2:C:374:ASN:O	2.13	0.49
2:C:910:LYS:HD2	2:C:910:LYS:N	2.27	0.49
3:D:367:ILE:CD1	3:D:379:ALA:HB2	2.24	0.49
3:D:500:ARG:NH2	3:D:1388:ARG:HG3	2.28	0.49
2:C:148:PHE:CD2	2:C:160:ALA:HB2	2.48	0.49
2:C:860:HIS:CE1	2:C:975:TYR:HB2	2.47	0.49
3:D:181:ASP:H	3:D:205:TYR:HE1	1.61	0.49
3:D:394:LEU:CG	3:D:396:VAL:HG23	2.41	0.49
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.42	0.49
5:F:88:ILE:C	5:F:90:GLN:H	2.19	0.49
1:A:91:ASN:OD1	1:A:93:SER:N	2.46	0.49
2:C:214:TYR:CD2	2:C:218:VAL:CG2	2.95	0.49
3:D:394:LEU:HD21	3:D:396:VAL:CG2	2.42	0.49
3:D:652:LEU:HB3	3:D:749:VAL:HG21	1.94	0.49
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.48	0.49
3:D:930:LEU:CD1	3:D:934:LEU:CD1	2.91	0.49
3:D:1031:ASN:HB2	3:D:1032:PRO:HD2	1.95	0.49
2:C:443:THR:OG1	2:C:444:PRO:CD	2.60	0.49
2:C:513:VAL:HG21	2:C:529:VAL:CG2	2.42	0.49
2:C:902:ILE:O	2:C:902:ILE:HG22	2.13	0.49
2:C:988:VAL:HG23	3:D:948:THR:OG1	2.13	0.49
3:D:236:TYR:HB2	3:D:319:ALA:CB	2.43	0.49
3:D:923:GLY:O	3:D:927:THR:OG1	2.22	0.49
6:G:18:DA:N6	6:G:19:DG:C2	2.81	0.49
1:B:179:PHE:CB	1:B:197:LEU:HD13	2.41	0.49
2:C:297:GLU:HG3	2:C:299:LYS:NZ	2.28	0.49
2:C:889:HIS:HE1	2:C:988:VAL:HG13	1.77	0.49
3:D:119:SER:HB3	3:D:122:GLU:HG3	1.94	0.49
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	1.94	0.49
5:F:210:LEU:O	5:F:211:ASP:C	2.55	0.49
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.47	0.48
1:B:105:GLY:O	1:B:132:LEU:HB2	2.12	0.48
2:C:3:ILE:HD12	2:C:900:ARG:HB2	1.95	0.48
2:C:86:LYS:O	2:C:88:LEU:HD23	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:LYS:HD2	2:C:110:GLU:N	2.21	0.48
2:C:176:VAL:HG22	2:C:182:VAL:CG1	2.43	0.48
2:C:492:ASP:CB	2:C:518:LYS:HG2	2.43	0.48
2:C:700:TYR:HB3	2:C:833:LEU:HD22	1.96	0.48
3:D:134:VAL:HG22	3:D:151:GLN:H	1.78	0.48
3:D:958:GLU:C	3:D:960:LYS:N	2.71	0.48
3:D:986:ARG:HB2	3:D:986:ARG:CZ	2.43	0.48
3:D:1087:ARG:NH1	3:D:1236:LEU:O	2.46	0.48
6:G:6:DA:H2'	6:G:7:DT:C7	2.42	0.48
1:A:49:PRO:O	1:A:173:PRO:HG3	2.13	0.48
1:A:101:LEU:HD12	1:A:114:PHE:CE1	2.47	0.48
1:B:195:LEU:HD12	1:B:196:THR:N	2.28	0.48
2:C:317:VAL:HB	2:C:320:HIS:HD2	1.76	0.48
2:C:385:PHE:HD2	2:C:386:PHE:CE1	2.32	0.48
2:C:557:ARG:HA	2:C:560:MET:HG3	1.95	0.48
3:D:808:THR:OG1	3:D:811:GLU:HG2	2.12	0.48
3:D:1155:VAL:HB	3:D:1177:ALA:HB1	1.94	0.48
1:A:10:VAL:HG12	1:A:26:GLU:O	2.13	0.48
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.96	0.48
2:C:211:LEU:CB	2:C:218:VAL:HG13	2.44	0.48
2:C:766:GLU:CG	2:C:767:PRO:HD2	2.25	0.48
2:C:861:LEU:CB	2:C:862:PRO:HD2	2.40	0.48
3:D:231:VAL:HG22	3:D:231:VAL:O	2.12	0.48
3:D:1087:ARG:HD3	3:D:1234:THR:O	2.14	0.48
3:D:1088:THR:HG21	6:G:14:DG:C6	2.48	0.48
6:G:7:DT:H3	7:H:21:DA:H61	1.61	0.48
1:A:121:GLU:OE1	1:A:123:MET:HE1	2.14	0.48
1:A:219:ARG:CG	1:B:219:ARG:HG3	2.43	0.48
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.47	0.48
2:C:195:LEU:HD12	2:C:195:LEU:O	2.13	0.48
2:C:685:GLU:OE1	2:C:685:GLU:HA	2.14	0.48
2:C:715:THR:HG22	2:C:716:LYS:N	2.28	0.48
3:D:534:ARG:HE	3:D:534:ARG:HB3	1.27	0.48
3:D:1347:TYR:CE2	3:D:1351:GLU:HG3	2.48	0.48
4:E:88:GLU:OE1	4:E:91:ARG:NH2	2.46	0.48
5:F:286:PRO:HB2	5:F:291:ILE:CD1	2.42	0.48
1:B:205:VAL:HG22	1:B:206:THR:H	1.78	0.48
2:C:267:TYR:CE1	2:C:290:LEU:HG	2.48	0.48
2:C:724:ARG:HB2	2:C:739:GLU:O	2.12	0.48
2:C:734:LEU:HD23	2:C:737:LEU:CD1	2.28	0.48
2:C:974:LEU:HD22	2:C:987:ILE:HG21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:206:ARG:HB2	3:D:392:SER:O	2.13	0.48
3:D:629:SER:HB3	3:D:726:ILE:HG13	1.94	0.48
3:D:1066:THR:OG1	3:D:1069:GLU:HB2	2.13	0.48
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.45	0.48
5:F:128:ARG:HB3	5:F:128:ARG:CZ	2.43	0.48
1:B:93:SER:O	1:B:95:GLN:HG3	2.13	0.48
3:D:131:LYS:H	3:D:456:MET:HE2	1.78	0.48
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.48	0.48
3:D:185:VAL:HG12	3:D:186:VAL:N	2.28	0.48
3:D:1041:LEU:O	3:D:1041:LEU:HD23	2.12	0.48
3:D:1433:SER:OG	3:D:1457:ASP:OD2	2.23	0.48
3:D:1444:THR:O	3:D:1448:THR:HG23	2.13	0.48
1:A:9:PRO:HD2	1:B:224:TYR:CD2	2.48	0.48
1:A:109:VAL:O	1:A:129:ILE:HB	2.14	0.48
1:B:42:ARG:HH21	2:C:981:GLU:HG2	1.78	0.48
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.95	0.48
2:C:915:LYS:CE	2:C:968:LEU:O	2.61	0.48
3:D:93:ILE:HD11	3:D:548:ILE:CD1	2.44	0.48
3:D:134:VAL:CG2	3:D:151:GLN:H	2.27	0.48
3:D:481:MET:O	3:D:489:ARG:HG3	2.13	0.48
3:D:544:TYR:O	3:D:547:LEU:N	2.46	0.48
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.95	0.48
3:D:860:LEU:HD22	3:D:878:GLY:HA2	1.95	0.48
3:D:1404:ASN:O	3:D:1408:ILE:HG13	2.13	0.48
5:F:170:HIS:C	5:F:172:ARG:N	2.70	0.48
2:C:103:LYS:O	2:C:103:LYS:HD3	2.13	0.48
2:C:148:PHE:HD2	2:C:160:ALA:HB2	1.78	0.48
2:C:462:ASP:CB	2:C:468:ARG:HH11	2.27	0.48
2:C:886:LEU:CD1	3:D:951:ILE:HD13	2.39	0.48
2:C:1073:GLY:HA2	3:D:659:LYS:HD3	1.95	0.48
3:D:569:ASN:ND2	5:F:84:TYR:CD2	2.82	0.48
3:D:870:GLY:O	3:D:871:LYS:C	2.56	0.48
3:D:1019:PRO:C	3:D:1023:MET:HE2	2.38	0.48
3:D:1107:VAL:HG23	3:D:1221:VAL:HG13	1.95	0.48
1:A:34:VAL:CG2	1:B:42:ARG:NE	2.77	0.48
1:A:65:PHE:HE2	2:C:703:ILE:CG2	2.26	0.48
1:A:143:ARG:O	1:A:143:ARG:HD3	2.13	0.48
1:A:206:THR:HG23	1:A:208:LEU:H	1.79	0.48
1:B:40:LEU:N	1:B:40:LEU:HD23	2.29	0.48
1:B:180:GLN:HB3	1:B:196:THR:HG22	1.96	0.48
2:C:836:GLY:HA3	2:C:1001:VAL:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1045:MET:HE3	3:D:1046:GLN:N	2.26	0.48
3:D:1259:VAL:HG23	3:D:1355:VAL:HG11	1.96	0.48
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.27	0.48
3:D:1435:LEU:HB2	3:D:1457:ASP:OD2	2.13	0.48
1:B:58:ILE:HG22	1:B:61:VAL:HG23	1.95	0.48
1:B:124:ASN:HD22	1:B:127:LEU:HD12	1.79	0.48
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.96	0.48
2:C:204:GLN:HG2	2:C:227:PHE:CE1	2.48	0.48
2:C:748:GLU:HA	2:C:799:ILE:CD1	2.44	0.48
2:C:983:ILE:HG22	2:C:985:GLY:H	1.78	0.48
3:D:648:MET:CE	3:D:747:VAL:HG21	2.43	0.48
3:D:778:LEU:O	3:D:778:LEU:HD23	2.14	0.48
3:D:1168:MET:HE3	3:D:1172:HIS:CD2	2.48	0.48
5:F:94:LEU:HG	5:F:190:ALA:HB1	1.96	0.48
5:F:198:ILE:CD1	5:F:243:ILE:HG21	2.44	0.48
5:F:300:ASP:O	5:F:304:VAL:HG12	2.14	0.48
1:A:35:THR:OG1	1:B:42:ARG:CD	2.59	0.47
2:C:15:LEU:HD12	2:C:15:LEU:HA	1.70	0.47
2:C:405:ARG:HG3	2:C:543:ASN:OD1	2.14	0.47
2:C:1083:GLU:OE1	2:C:1086:ARG:HD2	2.14	0.47
3:D:1275:SER:O	3:D:1322:GLY:N	2.43	0.47
3:D:1495:ILE:HG12	4:E:88:GLU:HB3	1.96	0.47
4:E:37:ASN:OD1	4:E:37:ASN:N	2.47	0.47
5:F:159:ILE:O	5:F:163:LEU:HD12	2.14	0.47
5:F:217:ASN:O	5:F:218:GLN:C	2.57	0.47
1:B:224:TYR:N	1:B:224:TYR:HD1	2.12	0.47
2:C:436:GLY:HA2	2:C:538:GLN:O	2.14	0.47
2:C:693:GLU:OE1	2:C:696:LYS:HD2	2.13	0.47
2:C:720:GLU:HG2	2:C:760:SER:OG	2.14	0.47
3:D:1121:PRO:O	3:D:1135:ARG:HD3	2.14	0.47
5:F:413:SER:HA	5:F:416:ARG:CZ	2.44	0.47
1:B:80:LEU:HD22	3:D:844:ALA:HA	1.96	0.47
2:C:73:LEU:HD22	2:C:92:ALA:CB	2.43	0.47
2:C:73:LEU:CD2	2:C:92:ALA:HB3	2.43	0.47
2:C:602:GLU:HG2	2:C:603:VAL:N	2.29	0.47
2:C:767:PRO:HG3	2:C:782:ALA:CB	2.42	0.47
2:C:815:LEU:HD12	2:C:819:VAL:CG2	2.37	0.47
2:C:839:LEU:HD23	2:C:996:LYS:HA	1.96	0.47
2:C:1092:LEU:HD21	3:D:607:LEU:HD21	1.95	0.47
3:D:216:VAL:CA	3:D:340:THR:HG22	2.35	0.47
3:D:860:LEU:HD23	3:D:878:GLY:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1034:GLN:HA	3:D:1037:GLN:HE21	1.80	0.47
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.96	0.47
2:C:20:GLU:O	2:C:24:GLU:HB2	2.14	0.47
2:C:176:VAL:HG11	2:C:217:LEU:CD1	2.44	0.47
2:C:726:ILE:HD12	2:C:726:ILE:N	2.28	0.47
2:C:841:ASN:C	2:C:841:ASN:OD1	2.58	0.47
3:D:170:PRO:HA	3:D:392:SER:HB2	1.95	0.47
3:D:558:LEU:CD2	3:D:567:ILE:HD12	2.44	0.47
3:D:575:GLN:HA	3:D:578:VAL:HG13	1.96	0.47
3:D:789:LEU:HD21	3:D:938:GLY:CA	2.45	0.47
3:D:916:TYR:CE1	3:D:920:LEU:HD21	2.48	0.47
4:E:50:THR:HG23	4:E:53:GLY:N	2.27	0.47
5:F:400:ILE:O	5:F:404:ALA:HB2	2.13	0.47
1:A:153:ALA:N	1:A:168:ASP:OD1	2.26	0.47
2:C:224:GLU:C	2:C:226:VAL:H	2.21	0.47
3:D:62:LYS:HE3	3:D:74:GLU:OE2	2.14	0.47
3:D:64:LYS:O	3:D:65:ARG:CB	2.62	0.47
3:D:123:LEU:O	3:D:127:LEU:HB2	2.14	0.47
3:D:134:VAL:CG1	3:D:153:LEU:HD11	2.44	0.47
3:D:237:LYS:O	3:D:240:GLU:HB2	2.15	0.47
3:D:396:VAL:CG1	3:D:397:LYS:N	2.78	0.47
3:D:527:MET:HG3	3:D:535:PHE:HD1	1.80	0.47
3:D:1054:GLU:O	3:D:1056:PRO:HD3	2.13	0.47
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.96	0.47
3:D:1118:ILE:HD13	3:D:1190:SER:HB2	1.96	0.47
3:D:1211:MET:HE1	4:E:16:LYS:HD2	1.95	0.47
3:D:1463:LYS:O	3:D:1464:GLU:C	2.57	0.47
2:C:825:VAL:O	2:C:825:VAL:HG22	2.15	0.47
2:C:858:MET:HG3	2:C:867:VAL:HG23	1.97	0.47
2:C:958:THR:CG2	2:C:961:GLU:HG3	2.33	0.47
2:C:1097:LEU:HD22	3:D:1451:ALA:HB2	1.96	0.47
3:D:242:LEU:CD2	3:D:311:LEU:CD1	2.92	0.47
3:D:401:TYR:HH	3:D:430:ASP:HB2	1.78	0.47
3:D:508:ARG:HB3	3:D:510:GLU:HG2	1.97	0.47
1:A:97:VAL:HG12	1:A:98:THR:H	1.80	0.47
1:A:143:ARG:NH1	1:A:160:ASP:OD1	2.48	0.47
1:B:153:ALA:C	1:B:155:LYS:H	2.22	0.47
2:C:11:GLU:OE2	2:C:537:LYS:HE2	2.13	0.47
2:C:72:ARG:HG2	2:C:95:TYR:HB2	1.96	0.47
2:C:148:PHE:O	2:C:322:VAL:HG13	2.15	0.47
2:C:772:ARG:HG2	2:C:772:ARG:HH11	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:85:VAL:C	3:D:87:ARG:H	2.23	0.47
3:D:314:PRO:CG	3:D:317:VAL:HG11	2.45	0.47
3:D:583:ASP:OD2	3:D:586:ARG:NH1	2.48	0.47
3:D:886:VAL:HG12	3:D:896:ALA:HB1	1.97	0.47
3:D:935:LYS:HE3	3:D:935:LYS:HB3	1.62	0.47
3:D:1103:HIS:HA	3:D:1223:ILE:HD11	1.96	0.47
3:D:1208:ASP:C	3:D:1208:ASP:OD1	2.58	0.47
3:D:1234:THR:H	3:D:1235:GLN:HB3	1.79	0.47
3:D:1379:VAL:C	3:D:1420:LEU:HD22	2.40	0.47
1:A:228:PRO:HB3	1:B:13:VAL:HG23	1.97	0.47
2:C:176:VAL:HG13	2:C:182:VAL:HG12	1.97	0.47
2:C:598:GLU:N	2:C:615:TYR:OH	2.44	0.47
3:D:56:TYR:OH	3:D:82:LYS:HE2	2.15	0.47
3:D:249:TYR:O	3:D:249:TYR:CG	2.68	0.47
3:D:371:ILE:CD1	5:F:232:ARG:NH1	2.78	0.47
3:D:568:ARG:HD2	5:F:87:GLU:OE2	2.14	0.47
3:D:1289:LYS:HZ1	3:D:1304:LYS:HB2	1.78	0.47
5:F:358:LEU:HD13	5:F:366:ALA:HB1	1.97	0.47
5:F:361:LEU:CG	5:F:411:HIS:HD2	2.23	0.47
1:B:13:VAL:HG12	1:B:15:THR:HG22	1.97	0.47
2:C:45:GLN:OE1	2:C:71:TYR:HE2	1.98	0.47
2:C:399:ASN:OD1	2:C:401:LEU:N	2.48	0.47
2:C:419:THR:O	2:C:422:ARG:N	2.47	0.47
2:C:1067:TYR:CD1	2:C:1071:ILE:HD13	2.50	0.47
3:D:135:LEU:HD13	3:D:455:ARG:HH12	1.79	0.47
3:D:557:LEU:HD13	3:D:566:ILE:HG21	1.96	0.47
3:D:789:LEU:CD2	3:D:938:GLY:HA2	2.45	0.47
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.48	0.47
5:F:96:LEU:O	5:F:96:LEU:HD12	2.15	0.47
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.96	0.47
2:C:567:GLN:NE2	2:C:999:HIS:NE2	2.63	0.47
2:C:630:ARG:HD2	2:C:705:ILE:CG2	2.45	0.47
2:C:683:ASN:HB3	2:C:872:ASN:ND2	2.26	0.47
2:C:715:THR:CG2	2:C:716:LYS:N	2.78	0.47
2:C:717:LEU:N	2:C:717:LEU:HD12	2.30	0.47
2:C:949:LYS:HD2	3:D:796:ARG:NE	2.30	0.47
3:D:26:VAL:HG12	3:D:548:ILE:CD1	2.45	0.47
3:D:544:TYR:O	3:D:545:ARG:C	2.57	0.47
3:D:1304:LYS:HG2	3:D:1305:LEU:N	2.29	0.47
3:D:1349:VAL:HG22	3:D:1368:ILE:HG22	1.97	0.47
4:E:85:LEU:HD23	4:E:85:LEU:C	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:235:PHE:O	5:F:236:SER:C	2.56	0.47
5:F:271:LEU:HD12	5:F:271:LEU:N	2.30	0.47
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.97	0.46
1:B:41:ARG:HG2	1:B:177:VAL:CG1	2.45	0.46
1:B:44:LEU:HD13	1:B:199:ILE:HD11	1.97	0.46
1:B:106:PRO:HG3	1:B:134:GLU:CD	2.40	0.46
1:B:143:ARG:HD3	1:B:158:ILE:HD12	1.97	0.46
1:B:219:ARG:O	1:B:222:LEU:HB2	2.14	0.46
2:C:64:LEU:N	2:C:103:LYS:CB	2.77	0.46
2:C:168:ARG:O	2:C:267:TYR:HA	2.16	0.46
2:C:682:TYR:HB2	2:C:689:VAL:CG2	2.45	0.46
3:D:706:PRO:HG2	10:D:1601:DCP:O2	2.14	0.46
3:D:895:VAL:O	3:D:898:GLU:N	2.43	0.46
3:D:998:GLU:O	3:D:1002:LYS:HG3	2.14	0.46
5:F:152:ASP:OD1	5:F:154:LYS:HB3	2.14	0.46
1:A:153:ALA:C	1:A:155:LYS:N	2.69	0.46
1:B:162:ILE:HG13	1:B:163:ASN:HD22	1.80	0.46
2:C:673:LEU:HD23	2:C:867:VAL:HA	1.96	0.46
2:C:712:ALA:HB3	2:C:821:GLU:HG2	1.97	0.46
2:C:741:GLY:O	2:C:756:VAL:HA	2.15	0.46
3:D:7:LYS:HD3	3:D:1456:LYS:HZ1	1.77	0.46
3:D:32:ILE:HG13	3:D:32:ILE:O	2.15	0.46
3:D:203:ALA:O	3:D:204:LEU:HG	2.14	0.46
3:D:259:VAL:CG1	3:D:270:LEU:HD21	2.33	0.46
3:D:484:PRO:C	3:D:486:ARG:H	2.22	0.46
4:E:33:HIS:NE2	4:E:89:MET:HE3	2.30	0.46
5:F:197:SER:HA	5:F:200:LYS:HE3	1.98	0.46
5:F:288:TYR:CE2	5:F:305:GLU:HG3	2.51	0.46
1:A:117:VAL:HB	1:A:120:VAL:HG21	1.96	0.46
1:A:206:THR:O	1:A:207:PRO:C	2.58	0.46
2:C:207:LEU:HB2	2:C:222:MET:HE2	1.96	0.46
2:C:312:ALA:O	2:C:317:VAL:HG23	2.14	0.46
2:C:695:LEU:N	2:C:695:LEU:HD23	2.30	0.46
3:D:207:PHE:CZ	5:F:101:GLU:OE2	2.68	0.46
3:D:269:PHE:CE2	3:D:283:PHE:HD1	2.34	0.46
3:D:394:LEU:CD2	3:D:396:VAL:HG23	2.45	0.46
3:D:786:ILE:HD11	3:D:1027:GLY:C	2.41	0.46
3:D:1263:PHE:CZ	3:D:1352:ILE:HD13	2.49	0.46
5:F:215:GLU:O	5:F:218:GLN:HB3	2.15	0.46
1:A:180:GLN:HG3	2:C:934:PHE:HD1	1.79	0.46
1:B:110:LYS:HD2	1:B:110:LYS:N	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:661:SER:HA	2:C:665:PHE:O	2.16	0.46
3:D:245:LEU:CD2	3:D:307:ALA:HB3	2.45	0.46
3:D:258:VAL:O	3:D:272:LEU:HA	2.15	0.46
3:D:311:LEU:HD12	3:D:311:LEU:O	2.15	0.46
3:D:411:THR:O	5:F:178:ARG:HD2	2.16	0.46
3:D:433:GLY:CA	3:D:447:VAL:O	2.63	0.46
3:D:1487:VAL:HG12	4:E:85:LEU:CD1	2.45	0.46
5:F:136:LEU:HD21	5:F:185:GLN:OE1	2.16	0.46
5:F:291:ILE:HG22	5:F:292:ALA:N	2.30	0.46
5:F:362:SER:O	5:F:366:ALA:CB	2.63	0.46
2:C:262:ALA:HB2	2:C:291:ALA:HB3	1.97	0.46
2:C:461:VAL:O	2:C:461:VAL:CG2	2.64	0.46
2:C:571:LEU:HD13	2:C:669:GLY:HA2	1.97	0.46
2:C:1097:LEU:HD22	3:D:1451:ALA:CB	2.45	0.46
3:D:85:VAL:C	3:D:87:ARG:N	2.72	0.46
3:D:284:LEU:HD13	3:D:284:LEU:N	2.31	0.46
3:D:409:VAL:CG2	3:D:409:VAL:O	2.64	0.46
5:F:369:LEU:HD12	5:F:404:ALA:HB1	1.98	0.46
1:A:5:LYS:HG2	1:A:6:LEU:O	2.15	0.46
1:A:63:HIS:HB2	2:C:799:ILE:HG21	1.98	0.46
1:B:158:ILE:O	1:B:158:ILE:HG13	2.14	0.46
2:C:168:ARG:NH2	2:C:268:ASP:HB2	2.29	0.46
2:C:396:ASP:O	2:C:402:SER:HB2	2.15	0.46
2:C:595:LEU:HD23	2:C:595:LEU:C	2.41	0.46
3:D:25:GLU:CD	3:D:94:GLU:HB3	2.41	0.46
3:D:84:ILE:CD1	3:D:87:ARG:HD3	2.46	0.46
3:D:200:ASP:C	3:D:397:LYS:HD3	2.41	0.46
3:D:1127:GLU:HA	3:D:1130:ARG:HB3	1.96	0.46
3:D:1310:ARG:HB2	3:D:1327:ARG:CD	2.45	0.46
5:F:278:LEU:O	5:F:282:LEU:HG	2.15	0.46
6:G:6:DA:H2'	6:G:7:DT:H72	1.96	0.46
7:H:12:DC:H1'	7:H:13:DT:C6	2.51	0.46
1:A:19:GLU:O	1:A:207:PRO:CG	2.62	0.46
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.45	0.46
1:B:92:PRO:O	1:B:146:ARG:NH1	2.49	0.46
2:C:374:ASN:O	2:C:377:PRO:HD2	2.16	0.46
2:C:409:ARG:HD3	2:C:452:ILE:HG22	1.98	0.46
2:C:836:GLY:HA3	2:C:1001:VAL:HG21	1.98	0.46
2:C:1067:TYR:HE2	3:D:674:ARG:HH21	1.63	0.46
3:D:103:TRP:CE2	3:D:1444:THR:HG22	2.50	0.46
3:D:207:PHE:CE1	5:F:97:GLU:HB3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:583:ASP:O	3:D:584:ASN:C	2.58	0.46
3:D:951:ILE:CD1	3:D:1062:ARG:HG3	2.45	0.46
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.97	0.46
3:D:1499:ARG:HH11	4:E:84:ARG:HG2	1.80	0.46
4:E:14:ASP:CG	4:E:18:ARG:HH11	2.24	0.46
7:H:2:DA:H2'	7:H:2:DA:O5'	2.15	0.46
1:B:197:LEU:HD12	1:B:197:LEU:C	2.38	0.46
2:C:41:ASN:OD1	2:C:46:ALA:HA	2.15	0.46
2:C:211:LEU:O	2:C:213:ALA:N	2.49	0.46
2:C:757:GLY:HA2	2:C:789:SER:OG	2.16	0.46
3:D:131:LYS:HD3	3:D:152:LEU:HB3	1.98	0.46
3:D:1217:ILE:HG21	3:D:1480:PHE:CD2	2.51	0.46
2:C:1:MET:HB2	2:C:898:GLY:O	2.16	0.46
2:C:539:VAL:O	2:C:539:VAL:CG1	2.62	0.46
2:C:666:LEU:HG	2:C:668:LEU:HG	1.98	0.46
2:C:874:LEU:HD13	3:D:783:ARG:CB	2.38	0.46
3:D:396:VAL:HG12	3:D:397:LYS:N	2.31	0.46
3:D:450:TYR:CD2	3:D:450:TYR:N	2.83	0.46
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.31	0.46
3:D:1114:THR:HG23	3:D:1189:ARG:NH2	2.30	0.46
3:D:1234:THR:N	3:D:1235:GLN:HB2	2.31	0.46
3:D:1263:PHE:HD2	3:D:1375:MET:HE3	1.81	0.46
3:D:1491:THR:HG21	4:E:89:MET:CG	2.45	0.46
5:F:88:ILE:HG23	5:F:193:ARG:HG3	1.98	0.46
5:F:194:LEU:HA	7:H:6:DT:O4'	2.16	0.46
1:A:206:THR:H	1:A:209:GLU:HG3	1.81	0.46
1:B:11:PHE:HE1	1:B:23:PHE:HB3	1.80	0.46
1:B:124:ASN:HD21	1:B:127:LEU:HD12	1.81	0.46
2:C:12:VAL:CG2	2:C:472:ARG:HD2	2.46	0.46
2:C:217:LEU:C	2:C:220:GLY:H	2.24	0.46
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.50	0.46
2:C:766:GLU:O	2:C:767:PRO:C	2.59	0.46
2:C:858:MET:HG2	2:C:867:VAL:O	2.15	0.46
2:C:884:GLN:HB2	2:C:992:MET:HE3	1.98	0.46
3:D:93:ILE:CD1	3:D:548:ILE:CG1	2.93	0.46
3:D:192:ALA:HB1	3:D:193:PRO:CD	2.46	0.46
3:D:464:LEU:HA	3:D:464:LEU:HD12	1.36	0.46
3:D:974:ILE:HD11	3:D:991:GLN:OE1	2.16	0.46
3:D:1111:ASP:CG	3:D:1203:LYS:HE2	2.41	0.46
3:D:1149:LEU:HD23	3:D:1149:LEU:HA	1.70	0.46
5:F:170:HIS:C	5:F:172:ARG:H	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:193:ARG:HB3	7:H:6:DT:O3'	2.16	0.46
7:H:3:DT:H2''	7:H:4:DA:H5'	1.98	0.46
1:A:76:VAL:O	1:A:80:LEU:HB2	2.16	0.45
1:A:195:LEU:HD12	1:A:196:THR:N	2.31	0.45
1:B:29:GLU:HG3	1:B:30:ARG:H	1.81	0.45
2:C:238:LEU:HD12	2:C:241:LEU:CB	2.44	0.45
2:C:250:ARG:HH11	2:C:254:VAL:HG21	1.81	0.45
3:D:314:PRO:HD2	3:D:317:VAL:HG13	1.97	0.45
3:D:643:GLY:O	3:D:726:ILE:HA	2.16	0.45
3:D:815:ALA:O	3:D:818:ARG:HB2	2.16	0.45
3:D:1031:ASN:OD1	3:D:1034:GLN:HG3	2.16	0.45
3:D:1192:LEU:HD22	3:D:1192:LEU:HA	1.71	0.45
3:D:1312:LEU:HB2	3:D:1325:LEU:O	2.17	0.45
4:E:65:MET:HE2	4:E:65:MET:HB3	1.83	0.45
5:F:112:ALA:HB2	5:F:176:ILE:HG21	1.97	0.45
1:A:44:LEU:HD22	1:A:199:ILE:HD13	1.98	0.45
1:A:178:ALA:HB2	2:C:864:GLY:CA	2.46	0.45
2:C:546:LEU:HA	2:C:546:LEU:HD23	1.63	0.45
3:D:93:ILE:HD11	3:D:548:ILE:HG12	1.98	0.45
3:D:613:ARG:HG3	3:D:618:LEU:CD2	2.47	0.45
3:D:695:ILE:HD13	3:D:720:LEU:CD1	2.47	0.45
3:D:731:LEU:HD22	3:D:780:LYS:O	2.16	0.45
3:D:957:PRO:CG	3:D:1007:VAL:HG22	2.46	0.45
3:D:958:GLU:O	3:D:960:LYS:N	2.49	0.45
3:D:1281:VAL:HA	3:D:1293:PHE:O	2.16	0.45
3:D:1330:ILE:HD12	3:D:1347:TYR:CE1	2.51	0.45
5:F:239:ALA:C	5:F:241:TRP:N	2.75	0.45
5:F:321:ILE:HG22	5:F:327:SER:OG	2.17	0.45
1:B:128:HIS:HE1	1:B:131:THR:CG2	2.26	0.45
2:C:312:ALA:HB1	2:C:317:VAL:CG2	2.46	0.45
2:C:711:GLU:OE2	2:C:816:LYS:NZ	2.41	0.45
2:C:800:VAL:HG13	2:C:825:VAL:HG23	1.99	0.45
3:D:212:ARG:HB2	3:D:344:ASP:OD1	2.15	0.45
3:D:409:VAL:HG23	3:D:409:VAL:O	2.15	0.45
3:D:1164:ARG:NH2	3:D:1170:ASP:OD1	2.49	0.45
5:F:396:ARG:HG3	5:F:396:ARG:O	2.15	0.45
1:A:54:THR:O	1:A:156:HIS:HE1	1.99	0.45
1:B:38:ASN:CB	1:B:39:PRO:CD	2.94	0.45
2:C:97:ARG:HG2	2:C:112:GLU:HB3	1.98	0.45
2:C:149:THR:HA	2:C:322:VAL:CG1	2.41	0.45
2:C:167:LYS:HG2	7:H:12:DC:C5	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:GLU:O	2:C:282:GLY:N	2.50	0.45
2:C:548:PRO:O	2:C:843:HIS:HE1	1.99	0.45
2:C:594:ALA:HB3	2:C:596:TYR:HE2	1.80	0.45
2:C:677:MET:O	2:C:678:PRO:C	2.59	0.45
2:C:936:VAL:HG11	2:C:959:PRO:CB	2.45	0.45
3:D:46:ASP:OD1	3:D:48:ARG:CG	2.65	0.45
3:D:543:LEU:CD1	3:D:581:LEU:HA	2.47	0.45
3:D:1312:LEU:HD21	3:D:1327:ARG:HH21	1.81	0.45
5:F:361:LEU:HD12	5:F:411:HIS:HB2	1.93	0.45
1:B:157:GLY:O	1:B:158:ILE:C	2.60	0.45
2:C:390:GLN:HE21	2:C:390:GLN:HB3	1.54	0.45
2:C:690:ILE:HD11	2:C:852:ILE:HG23	1.97	0.45
2:C:860:HIS:HB2	2:C:865:THR:O	2.16	0.45
3:D:5:VAL:O	3:D:6:ARG:HG2	2.16	0.45
3:D:97:THR:HG21	3:D:571:LYS:CG	2.46	0.45
3:D:245:LEU:HD21	3:D:307:ALA:HB3	1.99	0.45
3:D:539:ASP:CG	3:D:598:ARG:HH22	2.23	0.45
3:D:671:LYS:HD2	5:F:420:ASP:O	2.16	0.45
3:D:1172:HIS:HA	3:D:1175:ILE:HD12	1.98	0.45
5:F:329:TYR:O	5:F:329:TYR:CD2	2.70	0.45
2:C:534:VAL:HG12	2:C:535:SER:N	2.31	0.45
2:C:737:LEU:HA	2:C:742:VAL:O	2.15	0.45
2:C:745:ILE:CD1	2:C:802:ARG:HA	2.47	0.45
2:C:783:ARG:HG3	2:C:784:ASP:H	1.82	0.45
2:C:1012:PRO:HB3	5:F:334:PRO:HB3	1.99	0.45
3:D:135:LEU:O	3:D:149:LYS:CE	2.64	0.45
3:D:325:GLU:O	3:D:331:VAL:HG23	2.16	0.45
5:F:196:VAL:HG22	5:F:213:ILE:HD11	1.99	0.45
1:A:137:ARG:HG2	1:A:138:LEU:H	1.81	0.45
1:B:112:ARG:NH2	1:B:112:ARG:HB3	2.31	0.45
1:B:146:ARG:HE	1:B:146:ARG:HB2	1.62	0.45
2:C:150:PRO:CD	2:C:322:VAL:HG21	2.46	0.45
2:C:805:ARG:NH2	2:C:821:GLU:OE1	2.50	0.45
3:D:363:ALA:HB2	3:D:381:ALA:HA	1.97	0.45
3:D:1151:ARG:HB3	3:D:1151:ARG:HH21	1.82	0.45
3:D:1166:LEU:N	3:D:1166:LEU:HD23	2.30	0.45
3:D:1447:LEU:HD23	3:D:1447:LEU:HA	1.79	0.45
1:B:162:ILE:HG13	1:B:163:ASN:ND2	2.32	0.45
2:C:239:PHE:HD1	2:C:253:ALA:HA	1.78	0.45
2:C:966:LEU:HD13	2:C:986:PRO:CB	2.47	0.45
2:C:1009:SER:HA	3:D:625:TYR:CD1	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:217:LYS:HZ3	3:D:262:LYS:HZ1	1.64	0.45
3:D:613:ARG:HG3	3:D:618:LEU:HD21	1.99	0.45
3:D:762:GLN:NE2	4:E:17:TYR:HD1	2.15	0.45
3:D:1126:ASP:C	3:D:1130:ARG:HA	2.42	0.45
6:G:4:DG:H2''	6:G:5:DC:O5'	2.17	0.45
1:B:48:ILE:O	1:B:173:PRO:HD2	2.16	0.45
2:C:204:GLN:HG2	2:C:227:PHE:CE2	2.50	0.45
2:C:436:GLY:HA2	2:C:539:VAL:HA	1.98	0.45
2:C:701:THR:HG23	2:C:831:ARG:C	2.42	0.45
2:C:905:ILE:CG2	2:C:906:PHE:HD1	2.26	0.45
2:C:930:LYS:HA	2:C:934:PHE:O	2.16	0.45
2:C:983:ILE:O	2:C:985:GLY:N	2.50	0.45
3:D:128:TYR:CZ	3:D:587:ARG:HD3	2.52	0.45
3:D:1381:VAL:HG12	3:D:1382:THR:N	2.31	0.45
5:F:163:LEU:HB3	5:F:174:LEU:CD1	2.47	0.45
1:A:75:VAL:O	1:A:75:VAL:HG12	2.17	0.45
1:B:101:LEU:HD11	1:B:109:VAL:HG12	1.99	0.45
2:C:64:LEU:N	2:C:103:LYS:HB2	2.32	0.45
2:C:72:ARG:NH2	2:C:95:TYR:CE1	2.85	0.45
2:C:497:ALA:HB3	2:C:532:MET:HG3	1.98	0.45
2:C:760:SER:HB2	2:C:788:THR:HG21	1.99	0.45
3:D:174:GLY:HA2	3:D:389:GLU:CD	2.42	0.45
3:D:1305:LEU:HD12	3:D:1305:LEU:O	2.16	0.45
3:D:1448:THR:OG1	3:D:1449:GLU:N	2.50	0.45
1:B:45:LEU:HD23	1:B:174:VAL:HG11	1.98	0.44
1:B:202:ASP:OD1	1:B:204:SER:CB	2.65	0.44
2:C:168:ARG:HE	2:C:345:ARG:NH1	2.16	0.44
2:C:207:LEU:HD13	2:C:221:LEU:HD12	1.98	0.44
2:C:388:ARG:HG3	2:C:388:ARG:NH1	2.32	0.44
2:C:554:ASP:HA	3:D:1061:PHE:CZ	2.52	0.44
2:C:682:TYR:CE1	2:C:851:LYS:CD	3.01	0.44
2:C:700:TYR:CB	2:C:833:LEU:HD23	2.47	0.44
3:D:58:CYS:SG	3:D:62:LYS:N	2.90	0.44
3:D:374:GLU:O	3:D:375:GLU:HG2	2.17	0.44
3:D:1217:ILE:O	3:D:1217:ILE:HG22	2.17	0.44
5:F:148:LYS:HD3	5:F:148:LYS:HA	1.55	0.44
5:F:208:SER:O	5:F:209:PHE:C	2.59	0.44
1:A:23:PHE:N	1:A:23:PHE:CD1	2.85	0.44
1:A:124:ASN:HD21	1:A:127:LEU:HD22	1.82	0.44
1:A:221:HIS:ND1	1:A:224:TYR:CE2	2.83	0.44
1:B:6:LEU:O	1:B:6:LEU:HD13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD11	1:B:140:MET:HE1	1.99	0.44
2:C:44:ILE:HD13	2:C:44:ILE:HA	1.61	0.44
2:C:767:PRO:HG2	2:C:782:ALA:CB	2.46	0.44
2:C:769:PRO:O	2:C:770:GLU:C	2.60	0.44
2:C:837:ASP:OD1	2:C:1001:VAL:HG23	2.17	0.44
3:D:691:LEU:HD13	3:D:720:LEU:HD21	2.00	0.44
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.99	0.44
3:D:1348:LEU:HD23	3:D:1348:LEU:HA	1.45	0.44
5:F:195:VAL:O	5:F:196:VAL:C	2.60	0.44
5:F:260:ILE:O	5:F:261:PRO:C	2.60	0.44
1:B:94:LEU:HD23	1:B:95:GLN:H	1.80	0.44
2:C:486:MET:HE1	2:C:494:TYR:CE2	2.52	0.44
2:C:501:THR:HG22	2:C:514:VAL:HG23	1.98	0.44
2:C:578:VAL:HA	2:C:900:ARG:HD2	1.99	0.44
2:C:774:LEU:HD21	5:F:421:PHE:HB2	2.00	0.44
2:C:882:LEU:O	2:C:885:ILE:HB	2.17	0.44
3:D:185:VAL:CG1	3:D:186:VAL:H	2.29	0.44
3:D:478:LEU:O	3:D:480:GLU:N	2.50	0.44
3:D:554:LEU:HB2	3:D:570:GLU:CG	2.47	0.44
3:D:1103:HIS:CD2	3:D:1463:LYS:HG3	2.52	0.44
3:D:1191:PRO:C	3:D:1193:THR:H	2.25	0.44
3:D:1273:VAL:HB	3:D:1326:THR:CG2	2.46	0.44
3:D:1432:LYS:HB2	3:D:1432:LYS:HE3	1.80	0.44
5:F:116:LEU:HD12	5:F:173:TYR:C	2.43	0.44
1:A:6:LEU:HD23	1:A:7:LYS:O	2.17	0.44
2:C:177:GLU:OE2	2:C:183:SER:HB3	2.16	0.44
3:D:137:PRO:HG2	3:D:147:VAL:O	2.17	0.44
3:D:211:VAL:HG23	3:D:347:VAL:CG2	2.48	0.44
3:D:367:ILE:C	3:D:368:VAL:HG23	2.42	0.44
3:D:761:ILE:HG21	4:E:19:LEU:HD23	2.00	0.44
3:D:762:GLN:NE2	4:E:17:TYR:CD1	2.86	0.44
3:D:1495:ILE:HG12	4:E:88:GLU:CB	2.47	0.44
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.50	0.44
1:B:58:ILE:HG12	1:B:140:MET:HB2	1.99	0.44
1:B:96:THR:CG2	1:B:97:VAL:H	2.27	0.44
2:C:154:ARG:NH1	2:C:175:GLU:OE2	2.51	0.44
2:C:226:VAL:O	2:C:229:MET:HG3	2.17	0.44
3:D:568:ARG:HE	3:D:568:ARG:HB2	1.56	0.44
3:D:930:LEU:O	3:D:933:ALA:HB3	2.16	0.44
3:D:1280:VAL:HG12	3:D:1318:TYR:HA	2.00	0.44
5:F:154:LYS:HB3	5:F:154:LYS:HE3	1.87	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:387:GLY:HA2	5:F:394:ARG:HG2	1.98	0.44
1:A:79:ILE:HG23	1:A:167:VAL:HG22	1.99	0.44
1:B:37:GLY:HA2	1:B:40:LEU:HB2	1.99	0.44
1:B:123:MET:O	1:B:125:PRO:HD3	2.17	0.44
2:C:606:VAL:HG21	2:C:643:VAL:HG23	2.00	0.44
2:C:822:VAL:HG13	2:C:822:VAL:O	2.17	0.44
2:C:952:LEU:HB3	2:C:966:LEU:CD2	2.48	0.44
3:D:181:ASP:OD1	3:D:205:TYR:HB2	2.17	0.44
3:D:204:LEU:HA	3:D:204:LEU:HD23	1.86	0.44
3:D:644:LEU:HD11	3:D:648:MET:HE2	2.00	0.44
3:D:702:LEU:O	3:D:713:ILE:HA	2.18	0.44
3:D:832:ARG:CD	3:D:832:ARG:N	2.81	0.44
3:D:1127:GLU:HB3	3:D:1130:ARG:HH12	1.83	0.44
3:D:1292:VAL:HG13	3:D:1303:TYR:HB2	1.99	0.44
3:D:1295:GLU:HA	3:D:1300:SER:HB2	2.00	0.44
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.44	0.44
4:E:80:VAL:HG12	4:E:81:PRO:N	2.32	0.44
1:B:74:ASP:OD2	3:D:872:ARG:NH1	2.51	0.44
1:B:109:VAL:O	1:B:110:LYS:HD2	2.17	0.44
1:B:162:ILE:O	1:B:163:ASN:HB2	2.17	0.44
2:C:44:ILE:HD11	2:C:344:PHE:CD2	2.53	0.44
2:C:322:VAL:HG12	2:C:323:ASP:N	2.32	0.44
2:C:355:VAL:CG2	2:C:356:ARG:N	2.80	0.44
2:C:565:GLN:C	2:C:567:GLN:H	2.26	0.44
2:C:583:LEU:O	2:C:585:GLU:N	2.51	0.44
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.33	0.44
2:C:876:VAL:N	2:C:877:PRO:HD2	2.33	0.44
2:C:1048:THR:N	3:D:758:GLU:OE2	2.48	0.44
3:D:119:SER:HB3	3:D:122:GLU:CG	2.48	0.44
3:D:286:VAL:O	3:D:311:LEU:HB2	2.18	0.44
3:D:347:VAL:HA	3:D:351:MET:CE	2.48	0.44
3:D:519:VAL:HG22	3:D:544:TYR:CZ	2.53	0.44
3:D:706:PRO:HB3	3:D:708:LEU:HD21	1.99	0.44
3:D:707:THR:HG22	3:D:707:THR:O	2.16	0.44
3:D:741:ASP:OD1	3:D:741:ASP:N	2.44	0.44
3:D:1140:ILE:CG2	3:D:1144:LEU:HD12	2.47	0.44
3:D:1150:ALA:HB2	3:D:1189:ARG:HG2	2.00	0.44
3:D:1495:ILE:HG23	4:E:88:GLU:HG3	1.99	0.44
5:F:81:VAL:O	5:F:82:ARG:C	2.61	0.44
5:F:363:GLU:HG3	5:F:363:GLU:O	2.17	0.44
5:F:382:THR:HG22	5:F:383:LEU:CG	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HD12	1:A:122:ILE:HA	1.85	0.44
1:A:124:ASN:ND2	1:A:127:LEU:HD22	2.33	0.44
1:A:206:THR:HG22	1:A:209:GLU:H	1.81	0.44
2:C:538:GLN:O	2:C:538:GLN:HG3	2.16	0.44
2:C:607:ASP:HB2	2:C:610:ARG:HH12	1.82	0.44
2:C:853:LEU:CB	2:C:858:MET:HE1	2.40	0.44
3:D:210:ARG:NH2	3:D:212:ARG:HH21	2.15	0.44
3:D:514:LEU:HD22	3:D:517:VAL:HG22	2.00	0.44
3:D:650:LEU:CD1	3:D:657:LEU:HD22	2.43	0.44
3:D:664:LYS:HZ2	3:D:693:GLU:CD	2.13	0.44
3:D:1103:HIS:HA	3:D:1223:ILE:CD1	2.48	0.44
3:D:1145:TYR:CD1	3:D:1146:GLY:N	2.86	0.44
5:F:274:THR:O	5:F:277:GLN:HG2	2.18	0.44
1:A:23:PHE:CD2	1:A:211:LEU:CD2	3.01	0.44
1:A:216:GLU:OE1	1:A:216:GLU:HA	2.18	0.44
1:B:108:GLU:HB2	1:B:110:LYS:NZ	2.32	0.44
2:C:88:LEU:O	2:C:131:GLY:N	2.51	0.44
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.33	0.44
2:C:799:ILE:O	2:C:801:VAL:HG23	2.17	0.44
3:D:132:TYR:HD1	3:D:454:ALA:O	2.00	0.44
3:D:229:ALA:HB1	3:D:244:GLU:O	2.18	0.44
3:D:371:ILE:HG13	3:D:372:ASP:OD1	2.18	0.44
3:D:775:GLY:CA	3:D:1209:LEU:HB3	2.47	0.44
3:D:1231:GLU:N	3:D:1232:PRO:CD	2.81	0.44
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.85	0.44
3:D:1495:ILE:HG23	4:E:88:GLU:CD	2.43	0.44
4:E:9:LEU:HD23	4:E:9:LEU:HA	1.73	0.44
1:A:89:PHE:C	1:A:90:LEU:HD13	2.43	0.43
1:B:208:LEU:HD12	1:B:208:LEU:C	2.42	0.43
2:C:217:LEU:O	2:C:218:VAL:C	2.61	0.43
2:C:905:ILE:HG23	2:C:906:PHE:CD1	2.41	0.43
3:D:187:LYS:CD	3:D:187:LYS:N	2.81	0.43
3:D:828:LYS:CE	3:D:831:GLY:H	2.21	0.43
3:D:838:ARG:HD2	3:D:874:GLU:CD	2.43	0.43
3:D:1234:THR:CA	3:D:1235:GLN:CB	2.96	0.43
3:D:1462:LEU:CD2	3:D:1473:PRO:HD2	2.45	0.43
5:F:86:HIS:O	5:F:90:GLN:HG2	2.17	0.43
5:F:368:VAL:HG11	5:F:397:ILE:HD11	1.98	0.43
1:B:195:LEU:HD12	1:B:195:LEU:C	2.43	0.43
2:C:168:ARG:NE	2:C:345:ARG:NH1	2.65	0.43
2:C:494:TYR:CD2	2:C:531:PHE:CE2	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:63:TYR:HE2	3:D:73:CYS:HB2	1.81	0.43
3:D:247:GLU:HB2	3:D:248:PRO:CD	2.48	0.43
3:D:343:LYS:HG2	3:D:345:TYR:HE2	1.82	0.43
3:D:409:VAL:HG13	3:D:421:LEU:O	2.18	0.43
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.80	0.43
3:D:701:LEU:HD13	3:D:763:MET:HE1	2.00	0.43
3:D:957:PRO:HG3	3:D:1007:VAL:HA	2.00	0.43
3:D:1047:LYS:O	3:D:1048:PRO:C	2.61	0.43
4:E:26:ARG:NH2	4:E:38:THR:HA	2.33	0.43
5:F:219:GLY:O	5:F:222:ARG:HB2	2.18	0.43
5:F:325:LYS:N	5:F:325:LYS:HD2	2.33	0.43
1:A:9:PRO:HD3	1:B:224:TYR:CE2	2.54	0.43
1:B:129:ILE:N	1:B:129:ILE:HD12	2.34	0.43
2:C:564:MET:CG	2:C:997:LEU:HD11	2.44	0.43
2:C:589:ARG:NE	2:C:596:TYR:CE1	2.87	0.43
3:D:230:TRP:CZ2	3:D:232:GLU:HG3	2.53	0.43
3:D:437:VAL:O	3:D:437:VAL:HG12	2.16	0.43
3:D:708:LEU:N	3:D:708:LEU:HD23	2.33	0.43
3:D:804:LEU:HD13	3:D:806:PHE:CZ	2.52	0.43
5:F:116:LEU:HD21	5:F:163:LEU:HD22	2.00	0.43
5:F:143:HIS:HB2	5:F:150:THR:HA	2.01	0.43
1:A:53:VAL:HG11	1:A:82:LEU:O	2.18	0.43
2:C:31:GLN:O	2:C:33:ASP:N	2.51	0.43
2:C:815:LEU:N	2:C:815:LEU:HD23	2.34	0.43
2:C:880:MET:CE	3:D:1037:GLN:CD	2.91	0.43
2:C:890:LEU:N	2:C:914:ILE:HD11	2.32	0.43
2:C:1099:VAL:HG23	3:D:10:ILE:HG13	1.99	0.43
3:D:140:ALA:HB3	3:D:147:VAL:CG2	2.48	0.43
3:D:169:TYR:OH	3:D:198:ARG:HG2	2.17	0.43
3:D:502:PHE:CE2	3:D:512:MET:HE2	2.52	0.43
3:D:821:VAL:O	3:D:821:VAL:HG12	2.17	0.43
3:D:828:LYS:O	3:D:828:LYS:HD3	2.19	0.43
3:D:1209:LEU:N	3:D:1209:LEU:HD23	2.31	0.43
5:F:284:ARG:NH1	5:F:290:GLU:OE2	2.47	0.43
5:F:368:VAL:CG1	5:F:397:ILE:HD11	2.47	0.43
1:B:51:THR:HA	1:B:145:ASP:O	2.18	0.43
1:B:124:ASN:ND2	1:B:127:LEU:CD1	2.79	0.43
2:C:261:ILE:HG22	2:C:291:ALA:HB3	1.99	0.43
2:C:474:VAL:CG1	2:C:530:GLU:C	2.91	0.43
2:C:504:GLU:HG3	2:C:509:ALA:HB2	1.99	0.43
2:C:701:THR:HG23	2:C:831:ARG:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:520:LEU:O	3:D:521:PRO:C	2.61	0.43
3:D:709:HIS:C	3:D:711:LEU:N	2.76	0.43
3:D:907:GLU:OE1	3:D:909:ASN:N	2.43	0.43
3:D:1066:THR:O	3:D:1067:VAL:C	2.62	0.43
3:D:1441:GLN:O	3:D:1442:ASN:C	2.61	0.43
3:D:1495:ILE:HG12	4:E:88:GLU:OE2	2.18	0.43
5:F:100:VAL:O	5:F:104:ARG:HB2	2.18	0.43
1:B:106:PRO:HG3	1:B:134:GLU:OE1	2.18	0.43
2:C:410:ILE:O	2:C:452:ILE:HA	2.17	0.43
2:C:691:SER:HA	2:C:858:MET:HE3	2.00	0.43
2:C:815:LEU:HB2	2:C:819:VAL:CG2	2.49	0.43
2:C:1062:GLY:HA2	2:C:1065:ALA:HB3	2.00	0.43
3:D:230:TRP:HA	3:D:243:ALA:CB	2.49	0.43
3:D:413:ASP:N	3:D:435:VAL:HG12	2.34	0.43
3:D:613:ARG:O	3:D:618:LEU:HD23	2.19	0.43
3:D:638:LYS:HD3	3:D:640:HIS:HE1	1.84	0.43
3:D:757:ALA:O	4:E:20:THR:HG23	2.19	0.43
3:D:961:LYS:NZ	3:D:961:LYS:HB3	2.34	0.43
3:D:1093:TYR:CZ	3:D:1097:LYS:HE2	2.53	0.43
4:E:6:ILE:HD11	4:E:10:PHE:CZ	2.54	0.43
5:F:317:LEU:HD23	5:F:317:LEU:HA	1.81	0.43
5:F:403:LYS:O	5:F:407:LYS:HB2	2.19	0.43
1:A:41:ARG:CG	1:A:177:VAL:HG12	2.49	0.43
1:A:100:LEU:HB2	1:A:115:LEU:HD22	2.01	0.43
1:B:171:PHE:O	1:B:172:SER:C	2.61	0.43
2:C:18:LEU:HD23	2:C:18:LEU:HA	1.81	0.43
2:C:215:GLY:HA2	2:C:219:GLN:HG3	2.01	0.43
2:C:293:PHE:HD1	2:C:298:PHE:CD1	2.37	0.43
2:C:432:ARG:HG3	2:C:519:GLY:HA3	2.00	0.43
2:C:942:GLU:CG	2:C:945:ARG:HH21	2.29	0.43
2:C:1070:ILE:HB	3:D:655:PRO:HB3	2.00	0.43
3:D:361:VAL:HB	3:D:365:ASP:HB2	2.00	0.43
3:D:416:ALA:CB	3:D:432:TYR:CE1	3.01	0.43
3:D:639:LEU:HD12	3:D:639:LEU:HA	1.65	0.43
3:D:691:LEU:O	3:D:694:VAL:N	2.51	0.43
3:D:955:VAL:O	3:D:957:PRO:CD	2.65	0.43
3:D:965:GLU:C	3:D:967:ALA:H	2.26	0.43
3:D:1192:LEU:HD11	3:D:1345:GLU:HB3	1.99	0.43
3:D:1409:ALA:C	3:D:1411:GLY:H	2.25	0.43
5:F:186:HIS:O	5:F:190:ALA:HB2	2.19	0.43
2:C:214:TYR:C	2:C:216:GLU:N	2.74	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:TYR:CZ	2:C:290:LEU:HG	2.54	0.43
2:C:437:ARG:HB3	2:C:467:ILE:HG21	2.01	0.43
2:C:850:ALA:HA	3:D:632:VAL:HG22	2.00	0.43
2:C:1078:GLU:HG3	2:C:1079:PRO:HD2	2.01	0.43
3:D:137:PRO:HA	3:D:452:ILE:HG13	2.00	0.43
3:D:245:LEU:N	3:D:245:LEU:HD12	2.34	0.43
3:D:352:ASN:HB3	5:F:104:ARG:NH1	2.34	0.43
3:D:374:GLU:O	3:D:375:GLU:CB	2.66	0.43
3:D:1153:VAL:HG11	3:D:1183:ILE:CD1	2.49	0.43
3:D:1208:ASP:O	3:D:1209:LEU:C	2.60	0.43
3:D:1256:LEU:N	3:D:1257:PRO:HD2	2.34	0.43
4:E:89:MET:HE3	4:E:89:MET:HB3	1.81	0.43
5:F:99:GLU:OE2	5:F:234:LYS:HG2	2.18	0.43
5:F:118:GLU:OE1	5:F:118:GLU:HA	2.18	0.43
1:A:41:ARG:HG3	1:A:177:VAL:HG12	2.00	0.43
1:A:167:VAL:CG1	1:A:168:ASP:N	2.82	0.43
2:C:177:GLU:HG3	2:C:178:PRO:CD	2.29	0.43
2:C:243:ARG:NH2	7:H:9:DG:O6	2.52	0.43
2:C:405:ARG:HD2	2:C:442:GLU:CD	2.44	0.43
2:C:941:VAL:HG23	2:C:942:GLU:N	2.33	0.43
2:C:974:LEU:HD22	2:C:987:ILE:CG2	2.48	0.43
2:C:1030:GLN:O	3:D:623:VAL:HG22	2.19	0.43
2:C:1073:GLY:CA	3:D:659:LYS:HD3	2.48	0.43
3:D:10:ILE:HG23	3:D:1451:ALA:HA	2.01	0.43
3:D:87:ARG:C	3:D:88:TYR:CD2	2.97	0.43
3:D:348:GLN:CB	3:D:351:MET:HG3	2.44	0.43
3:D:584:ASN:OD1	3:D:585:GLY:N	2.52	0.43
3:D:629:SER:OG	3:D:630:VAL:N	2.51	0.43
3:D:631:ILE:HG22	3:D:726:ILE:HB	2.01	0.43
3:D:783:ARG:H	3:D:783:ARG:HG2	1.57	0.43
3:D:1191:PRO:C	3:D:1193:THR:N	2.75	0.43
3:D:1235:GLN:O	3:D:1236:LEU:HD23	2.19	0.43
5:F:260:ILE:CD1	5:F:265:VAL:HG22	2.48	0.43
5:F:343:ASP:O	5:F:346:THR:N	2.52	0.43
5:F:377:ASP:OD2	5:F:378:GLY:O	2.37	0.43
6:G:12:DG:H8	6:G:12:DG:H5"	1.83	0.43
1:A:159:LYS:HG2	1:A:164:ALA:O	2.19	0.43
1:B:31:GLY:N	1:B:193:ASP:OD1	2.52	0.43
1:B:47:SER:O	1:B:48:ILE:HD13	2.19	0.43
2:C:129:ILE:HG12	2:C:386:PHE:HB3	2.01	0.43
2:C:397:GLU:HG3	2:C:631:SER:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:644:VAL:CG2	2:C:645:VAL:H	2.30	0.43
2:C:707:ARG:HH11	2:C:707:ARG:HB3	1.84	0.43
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.34	0.43
2:C:1046:ALA:HB1	3:D:1471:LEU:HG	2.00	0.43
3:D:185:VAL:HG13	3:D:186:VAL:H	1.83	0.43
3:D:540:LEU:O	3:D:541:ASN:C	2.60	0.43
3:D:684:LYS:O	3:D:687:VAL:CG1	2.65	0.43
3:D:907:GLU:OE1	3:D:908:LYS:N	2.52	0.43
3:D:1263:PHE:HA	3:D:1375:MET:CE	2.39	0.43
3:D:1486:VAL:HG13	3:D:1486:VAL:O	2.17	0.43
1:A:121:GLU:HB3	1:A:123:MET:CE	2.39	0.42
1:B:222:LEU:HA	1:B:222:LEU:HD23	1.78	0.42
2:C:75:GLU:OE2	2:C:76:PRO:CD	2.67	0.42
2:C:879:ARG:HH21	2:C:879:ARG:HD2	1.70	0.42
3:D:207:PHE:HB2	3:D:391:ALA:CB	2.49	0.42
3:D:225:LEU:HA	3:D:249:TYR:CE2	2.54	0.42
3:D:410:SER:O	3:D:435:VAL:CG1	2.61	0.42
3:D:1479:ASP:OD1	3:D:1482:ARG:HD3	2.19	0.42
5:F:321:ILE:HA	5:F:321:ILE:HD13	1.83	0.42
1:B:153:ALA:HB2	1:B:167:VAL:C	2.44	0.42
2:C:336:VAL:HG13	2:C:337:GLY:N	2.33	0.42
2:C:1006:HIS:CD2	2:C:1024:LYS:HA	2.54	0.42
2:C:1092:LEU:CD2	3:D:607:LEU:HD21	2.49	0.42
3:D:231:VAL:O	3:D:236:TYR:OH	2.34	0.42
3:D:245:LEU:HD23	3:D:249:TYR:HB3	2.01	0.42
3:D:954:ALA:O	3:D:1062:ARG:HD2	2.19	0.42
5:F:123:ASP:OD1	5:F:123:ASP:C	2.62	0.42
5:F:128:ARG:HE	5:F:132:ARG:NH2	2.16	0.42
1:A:74:ASP:OD1	1:A:76:VAL:HB	2.20	0.42
2:C:355:VAL:HG23	2:C:356:ARG:H	1.83	0.42
2:C:619:ARG:HH21	2:C:619:ARG:HB2	1.84	0.42
3:D:251:PHE:HE2	3:D:304:LEU:HD12	1.85	0.42
3:D:502:PHE:HZ	3:D:512:MET:HE2	1.84	0.42
3:D:625:TYR:CD2	3:D:751:LEU:HD11	2.54	0.42
3:D:1068:LEU:HD23	3:D:1068:LEU:C	2.44	0.42
3:D:1108:ARG:HH21	3:D:1198:TYR:C	2.24	0.42
3:D:1305:LEU:HD12	3:D:1305:LEU:C	2.44	0.42
3:D:1378:TYR:O	3:D:1420:LEU:HB2	2.19	0.42
1:A:117:VAL:HB	1:A:120:VAL:CG2	2.49	0.42
1:A:133:GLU:OE2	2:C:605:LYS:HB3	2.18	0.42
2:C:31:GLN:C	2:C:33:ASP:N	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:GLN:HA	2:C:227:PHE:CE1	2.55	0.42
2:C:292:ARG:NH1	2:C:301:GLU:OE2	2.52	0.42
2:C:701:THR:HG22	2:C:702:SER:N	2.34	0.42
2:C:820:ARG:HB3	2:C:820:ARG:CZ	2.49	0.42
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.45	0.42
2:C:911:GLU:HA	2:C:914:ILE:CG2	2.49	0.42
2:C:946:ARG:O	2:C:947:ALA:C	2.62	0.42
3:D:217:LYS:HZ3	3:D:262:LYS:NZ	2.17	0.42
3:D:230:TRP:CZ3	3:D:333:LEU:CD2	3.02	0.42
3:D:272:LEU:CD2	3:D:298:VAL:HG21	2.49	0.42
3:D:288:MET:HG3	3:D:307:ALA:HB2	2.02	0.42
3:D:492:ALA:O	3:D:496:LEU:HB2	2.20	0.42
3:D:514:LEU:HD22	3:D:517:VAL:CG2	2.50	0.42
3:D:697:GLY:CA	4:E:59:ASN:HD22	2.33	0.42
3:D:1380:GLU:HB2	3:D:1420:LEU:CD2	2.49	0.42
3:D:1381:VAL:CG1	3:D:1382:THR:N	2.83	0.42
3:D:1386:ASP:OD2	3:D:1412:LYS:HB3	2.19	0.42
4:E:34:GLY:O	4:E:35:PHE:HB2	2.19	0.42
5:F:113:ILE:HD13	5:F:128:ARG:HG3	2.01	0.42
5:F:240:THR:O	5:F:244:ARG:HG2	2.20	0.42
5:F:413:SER:O	5:F:414:ARG:NH1	2.52	0.42
1:A:88:ARG:CD	1:A:123:MET:HE3	2.50	0.42
1:A:111:ALA:CB	1:A:127:LEU:HB3	2.50	0.42
2:C:135:VAL:O	2:C:136:ILE:HD13	2.19	0.42
2:C:612:VAL:HG23	2:C:621:VAL:O	2.19	0.42
2:C:772:ARG:HG2	2:C:772:ARG:NH1	2.34	0.42
2:C:882:LEU:HA	2:C:882:LEU:HD23	1.43	0.42
3:D:56:TYR:HE1	3:D:69:GLU:OE2	2.03	0.42
3:D:296:GLU:CG	3:D:297:ILE:N	2.81	0.42
3:D:832:ARG:N	3:D:832:ARG:HD3	2.35	0.42
3:D:924:MET:O	3:D:925:GLU:C	2.61	0.42
3:D:1342:GLU:HA	3:D:1345:GLU:HB2	2.02	0.42
3:D:1413:THR:HG22	3:D:1414:PRO:CD	2.47	0.42
3:D:1417:TRP:HE3	3:D:1418:LYS:N	2.17	0.42
5:F:102:LEU:HD22	5:F:183:ALA:HA	2.02	0.42
5:F:351:SER:HA	5:F:354:LEU:HD21	2.01	0.42
6:G:7:DT:H2"	6:G:8:DC:OP2	2.19	0.42
1:A:20:TYR:CD1	1:A:21:GLY:N	2.79	0.42
1:A:51:THR:OG1	1:A:87:VAL:O	2.21	0.42
1:B:199:ILE:O	1:B:199:ILE:HG22	2.18	0.42
2:C:170:PRO:HD2	2:C:267:TYR:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.83	0.42
3:D:133:ILE:O	3:D:133:ILE:CG2	2.67	0.42
3:D:648:MET:HE1	3:D:747:VAL:CG2	2.48	0.42
3:D:711:LEU:CD2	3:D:714:GLN:HE21	2.31	0.42
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.54	0.42
3:D:1255:GLY:C	3:D:1257:PRO:HD2	2.44	0.42
3:D:1433:SER:OG	3:D:1464:GLU:HG2	2.20	0.42
3:D:1492:LEU:HD13	3:D:1492:LEU:C	2.45	0.42
5:F:87:GLU:O	5:F:90:GLN:HB2	2.20	0.42
5:F:215:GLU:HG3	5:F:250:ALA:CB	2.50	0.42
5:F:369:LEU:HD11	5:F:405:LEU:HD12	2.01	0.42
1:A:29:GLU:O	1:A:30:ARG:C	2.62	0.42
1:A:62:LEU:HD22	2:C:745:ILE:O	2.20	0.42
2:C:880:MET:HE3	3:D:1037:GLN:CB	2.50	0.42
2:C:921:ALA:O	2:C:922:PHE:C	2.62	0.42
2:C:941:VAL:CG2	2:C:942:GLU:N	2.83	0.42
2:C:1005:MET:HE3	2:C:1005:MET:HB3	1.78	0.42
3:D:34:TYR:CE1	3:D:35:ARG:HG2	2.55	0.42
3:D:201:GLY:HA2	3:D:397:LYS:HD2	2.00	0.42
3:D:201:GLY:HA2	3:D:397:LYS:CD	2.49	0.42
3:D:975:GLU:O	3:D:975:GLU:HG3	2.18	0.42
3:D:1068:LEU:HD23	3:D:1068:LEU:O	2.20	0.42
3:D:1087:ARG:CD	3:D:1234:THR:O	2.68	0.42
3:D:1090:ASP:O	3:D:1091:SER:C	2.63	0.42
3:D:1211:MET:CE	4:E:16:LYS:HD2	2.48	0.42
3:D:1238:MET:CB	3:D:1255:GLY:H	2.32	0.42
3:D:1389:LEU:HD21	3:D:1395:LEU:HD11	2.00	0.42
3:D:1395:LEU:HD23	3:D:1395:LEU:N	2.35	0.42
4:E:14:ASP:CG	4:E:18:ARG:NH1	2.78	0.42
5:F:88:ILE:HD11	5:F:192:LEU:HD13	2.01	0.42
5:F:193:ARG:HG2	7:H:7:DG:C5'	2.50	0.42
5:F:247:ILE:HG22	5:F:251:ILE:HD12	2.02	0.42
5:F:365:GLU:HA	5:F:368:VAL:HG22	2.01	0.42
1:B:28:LEU:HD21	1:B:36:LEU:HD22	2.02	0.42
2:C:364:GLU:HG2	2:C:364:GLU:O	2.19	0.42
2:C:429:ASP:OD1	3:D:1079:LYS:HD2	2.20	0.42
2:C:545:ASN:HB3	2:C:583:LEU:HD22	2.02	0.42
2:C:571:LEU:CD1	2:C:669:GLY:HA2	2.50	0.42
2:C:983:ILE:C	2:C:985:GLY:N	2.77	0.42
2:C:997:LEU:HD23	2:C:997:LEU:HA	1.47	0.42
3:D:10:ILE:O	3:D:10:ILE:CG2	2.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:141:ILE:HG23	3:D:450:TYR:OH	2.20	0.42
3:D:403:PHE:CE2	3:D:442:ASN:C	2.98	0.42
3:D:421:LEU:N	3:D:421:LEU:CD1	2.83	0.42
3:D:433:GLY:HA2	3:D:447:VAL:O	2.20	0.42
3:D:519:VAL:CG2	3:D:544:TYR:CE1	3.02	0.42
3:D:637:LEU:HD13	3:D:642:CYS:HA	2.02	0.42
3:D:676:MET:O	3:D:682:ASP:HB2	2.20	0.42
3:D:695:ILE:HD13	3:D:720:LEU:HD11	2.02	0.42
3:D:879:ARG:HD3	3:D:902:LEU:O	2.19	0.42
3:D:1153:VAL:HG11	3:D:1183:ILE:HD11	2.01	0.42
4:E:46:PRO:HB2	4:E:57:ASP:HB3	2.02	0.42
5:F:231:ARG:HB3	5:F:233:PHE:CE2	2.55	0.42
5:F:307:THR:HG22	5:F:308:LEU:N	2.33	0.42
5:F:403:LYS:HA	5:F:406:ARG:HB2	2.02	0.42
1:A:34:VAL:O	1:A:35:THR:C	2.61	0.42
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.55	0.42
1:A:70:GLY:H	2:C:607:ASP:CG	2.28	0.42
1:B:93:SER:O	1:B:94:LEU:C	2.63	0.42
2:C:115:LEU:HA	2:C:115:LEU:HD23	1.76	0.42
2:C:164:PRO:CA	2:C:269:LEU:HD12	2.48	0.42
2:C:167:LYS:CE	7:H:12:DC:H5	2.32	0.42
2:C:565:GLN:C	2:C:567:GLN:N	2.78	0.42
2:C:726:ILE:HD11	2:C:757:GLY:HA3	2.01	0.42
2:C:793:PRO:HG2	2:C:796:GLU:CD	2.44	0.42
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.94	0.42
2:C:905:ILE:C	2:C:907:ASP:H	2.27	0.42
2:C:1040:LEU:HD12	2:C:1049:LEU:HA	2.02	0.42
3:D:559:ALA:HA	5:F:144:ILE:CD1	2.50	0.42
3:D:941:PHE:HD1	3:D:941:PHE:HA	1.75	0.42
3:D:1167:SER:O	3:D:1168:MET:C	2.61	0.42
5:F:161:GLN:OE1	5:F:164:LYS:NZ	2.25	0.42
5:F:213:ILE:O	5:F:214:GLN:C	2.63	0.42
5:F:241:TRP:CE2	7:H:1:DT:H4'	2.54	0.42
5:F:372:ARG:NE	5:F:372:ARG:CA	2.83	0.42
5:F:415:THR:C	5:F:417:LYS:H	2.28	0.42
1:B:24:VAL:CG1	1:B:196:THR:OG1	2.67	0.42
1:B:127:LEU:HD23	1:B:127:LEU:C	2.43	0.42
2:C:682:TYR:HB2	2:C:689:VAL:HG21	2.02	0.42
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.49	0.42
3:D:207:PHE:CZ	5:F:97:GLU:HB3	2.55	0.42
3:D:512:MET:C	3:D:513:ILE:HG12	2.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:553:ARG:HG2	3:D:570:GLU:OE2	2.19	0.42
3:D:697:GLY:C	4:E:59:ASN:HD22	2.28	0.42
3:D:1012:GLU:O	3:D:1012:GLU:HG2	2.20	0.42
5:F:88:ILE:HD12	5:F:88:ILE:HA	1.62	0.42
5:F:359:SER:OG	5:F:363:GLU:CD	2.63	0.42
1:A:186:LEU:O	1:A:188:GLN:N	2.51	0.41
2:C:96:ALA:HB3	2:C:115:LEU:HD11	2.01	0.41
2:C:134:ARG:NH1	2:C:392:SER:O	2.53	0.41
2:C:140:ILE:CG2	2:C:412:ALA:HA	2.49	0.41
2:C:267:TYR:OH	2:C:290:LEU:HD21	2.20	0.41
2:C:745:ILE:HD11	2:C:802:ARG:HA	2.02	0.41
2:C:999:HIS:CD2	2:C:999:HIS:N	2.88	0.41
3:D:416:ALA:HB1	3:D:432:TYR:CE1	2.55	0.41
3:D:562:ALA:HB2	5:F:221:ILE:HD11	2.02	0.41
3:D:618:LEU:CG	3:D:1467:ILE:HG23	2.50	0.41
3:D:983:LEU:HB3	3:D:987:GLU:CD	2.45	0.41
3:D:1290:LEU:HD23	3:D:1307:LYS:HA	2.01	0.41
1:A:115:LEU:HD23	1:A:115:LEU:C	2.44	0.41
1:B:80:LEU:HD22	3:D:844:ALA:CA	2.49	0.41
2:C:124:ASP:CA	2:C:592:LEU:HD13	2.44	0.41
2:C:203:ASP:O	2:C:206:THR:HG22	2.21	0.41
2:C:376:ARG:N	2:C:377:PRO:HD2	2.34	0.41
2:C:492:ASP:O	2:C:518:LYS:HE3	2.21	0.41
2:C:1055:LEU:HD23	2:C:1055:LEU:H	1.85	0.41
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	2.02	0.41
3:D:223:LEU:HD13	3:D:283:PHE:O	2.20	0.41
3:D:266:GLU:HG3	3:D:314:PRO:HB3	2.00	0.41
3:D:374:GLU:O	3:D:375:GLU:CG	2.68	0.41
3:D:423:ASP:O	3:D:425:GLY:N	2.48	0.41
3:D:610:LYS:HD3	3:D:615:ARG:NH2	2.35	0.41
3:D:780:LYS:HD2	3:D:912:LYS:HG3	2.00	0.41
3:D:1015:TYR:CD2	3:D:1015:TYR:N	2.88	0.41
3:D:1295:GLU:OE1	3:D:1300:SER:HB3	2.20	0.41
7:H:17:DA:C2'	7:H:18:DC:H5'	2.49	0.41
1:A:24:VAL:O	1:A:25:LEU:HD12	2.19	0.41
1:B:87:VAL:CG1	1:B:122:ILE:HD13	2.50	0.41
1:B:209:GLU:O	1:B:210:ALA:C	2.62	0.41
2:C:109:LYS:CD	2:C:110:GLU:H	2.24	0.41
2:C:559:LEU:C	2:C:559:LEU:CD2	2.94	0.41
2:C:580:MET:HE2	2:C:902:ILE:HG12	2.01	0.41
2:C:729:LEU:CD2	2:C:754:ILE:HD11	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1060:ILE:H	2:C:1060:ILE:HG12	1.38	0.41
3:D:58:CYS:SG	3:D:59:ALA:N	2.91	0.41
3:D:219:GLU:HB2	3:D:339:TRP:HH2	1.86	0.41
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.55	0.41
3:D:955:VAL:O	3:D:955:VAL:CG2	2.68	0.41
3:D:972:LEU:HG	3:D:972:LEU:H	1.69	0.41
3:D:1191:PRO:HD2	3:D:1369:GLU:OE1	2.19	0.41
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.60	0.41
1:A:138:LEU:HD21	1:A:140:MET:CE	2.49	0.41
2:C:54:ILE:HG21	2:C:355:VAL:HG21	1.99	0.41
2:C:748:GLU:HG3	2:C:799:ILE:CD1	2.50	0.41
2:C:929:ARG:C	2:C:931:GLY:H	2.29	0.41
3:D:41:ARG:HG2	3:D:48:ARG:HD3	2.02	0.41
3:D:329:GLU:C	3:D:330:THR:HG23	2.45	0.41
3:D:1343:ALA:HA	3:D:1346:ARG:NH1	2.34	0.41
3:D:1486:VAL:HB	4:E:22:VAL:HG13	2.03	0.41
5:F:194:LEU:HB2	7:H:6:DT:C2	2.56	0.41
1:A:30:ARG:HD2	1:A:191:ASP:OD1	2.21	0.41
1:A:34:VAL:HG21	1:B:42:ARG:NE	2.36	0.41
1:A:65:PHE:HE2	2:C:703:ILE:HG23	1.84	0.41
1:A:201:THR:HG23	1:A:202:ASP:N	2.34	0.41
1:A:221:HIS:CD2	1:B:32:PHE:CD2	3.08	0.41
1:B:29:GLU:HG3	1:B:30:ARG:N	2.36	0.41
1:B:96:THR:CG2	1:B:97:VAL:N	2.81	0.41
2:C:333:ILE:HG23	2:C:333:ILE:HD12	1.87	0.41
2:C:588:VAL:HG13	2:C:596:TYR:OH	2.20	0.41
2:C:679:PHE:N	2:C:683:ASN:OD1	2.53	0.41
2:C:939:ARG:HG3	2:C:975:TYR:CE1	2.55	0.41
3:D:101:HIS:CE1	3:D:103:TRP:HB2	2.56	0.41
3:D:142:LEU:HB2	3:D:161:LEU:HD21	2.03	0.41
3:D:150:ARG:HG2	3:D:464:LEU:HD21	2.03	0.41
3:D:201:GLY:HA3	3:D:396:VAL:O	2.21	0.41
3:D:527:MET:HE2	3:D:527:MET:HB2	1.44	0.41
3:D:787:LEU:HD12	3:D:787:LEU:HA	1.88	0.41
3:D:924:MET:HB2	3:D:924:MET:HE2	1.87	0.41
5:F:117:SER:O	5:F:121:GLY:N	2.52	0.41
1:A:162:ILE:HD12	1:A:162:ILE:N	2.36	0.41
1:B:58:ILE:O	1:B:61:VAL:HG23	2.21	0.41
1:B:115:LEU:HD22	1:B:115:LEU:HA	1.58	0.41
2:C:258:TYR:CE1	2:C:263:ASP:HB2	2.55	0.41
2:C:297:GLU:HG3	2:C:299:LYS:HZ2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:314:THR:HG22	2:C:314:THR:O	2.19	0.41
2:C:715:THR:C	2:C:717:LEU:H	2.28	0.41
2:C:863:ASP:OD1	2:C:863:ASP:C	2.63	0.41
2:C:983:ILE:O	2:C:984:GLU:C	2.63	0.41
3:D:50:PHE:O	3:D:89:ARG:HD2	2.21	0.41
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.60	0.41
3:D:187:LYS:N	3:D:187:LYS:HD3	2.36	0.41
3:D:218:LYS:O	3:D:219:GLU:HG2	2.20	0.41
3:D:377:VAL:CG2	3:D:377:VAL:O	2.67	0.41
3:D:638:LYS:O	3:D:639:LEU:C	2.62	0.41
3:D:670:VAL:O	3:D:673:ALA:HB3	2.20	0.41
3:D:1037:GLN:HG2	3:D:1042:ARG:HA	2.01	0.41
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.55	0.41
3:D:1407:LEU:HD13	3:D:1413:THR:O	2.20	0.41
5:F:114:LYS:HG3	5:F:115:LYS:N	2.36	0.41
5:F:132:ARG:HH11	5:F:184:ARG:NH1	2.19	0.41
5:F:152:ASP:O	5:F:154:LYS:N	2.53	0.41
5:F:359:SER:HG	5:F:363:GLU:CD	2.28	0.41
1:A:79:ILE:HG23	1:A:167:VAL:CG2	2.51	0.41
1:B:26:GLU:HB3	1:B:194:LYS:CG	2.46	0.41
1:B:86:VAL:HG21	1:B:202:ASP:CG	2.45	0.41
2:C:97:ARG:HG2	2:C:112:GLU:CB	2.51	0.41
2:C:668:LEU:HD23	2:C:668:LEU:HA	1.75	0.41
2:C:700:TYR:HB3	2:C:833:LEU:CD2	2.50	0.41
3:D:32:ILE:HG13	5:F:258:ILE:HD13	2.01	0.41
3:D:100:ALA:HA	3:D:513:ILE:HG23	2.02	0.41
3:D:144:GLY:O	3:D:145:VAL:HG23	2.20	0.41
3:D:210:ARG:HH21	3:D:212:ARG:HH21	1.69	0.41
3:D:210:ARG:NH1	3:D:388:HIS:HB3	2.36	0.41
3:D:421:LEU:HD13	3:D:428:LYS:C	2.46	0.41
3:D:677:LEU:H	3:D:677:LEU:HG	1.43	0.41
3:D:1400:VAL:HG13	3:D:1401:GLU:N	2.36	0.41
4:E:70:THR:HB	4:E:72:ARG:NE	2.35	0.41
1:A:34:VAL:C	1:A:36:LEU:N	2.75	0.41
1:A:56:VAL:O	1:A:164:ALA:HA	2.20	0.41
1:A:86:VAL:HG21	1:A:202:ASP:CB	2.50	0.41
1:B:205:VAL:CG2	1:B:206:THR:H	2.34	0.41
1:B:205:VAL:CG2	1:B:206:THR:N	2.84	0.41
2:C:390:GLN:C	2:C:391:LEU:HD23	2.46	0.41
2:C:874:LEU:HA	2:C:874:LEU:HD23	1.84	0.41
2:C:941:VAL:O	2:C:942:GLU:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:954:THR:HB	2:C:957:LYS:HD2	2.03	0.41
2:C:1013:TYR:CE2	2:C:1063:ARG:NH1	2.89	0.41
2:C:1110:ASP:OD1	2:C:1110:ASP:C	2.64	0.41
3:D:141:ILE:CD1	3:D:145:VAL:N	2.83	0.41
3:D:298:VAL:HG12	3:D:302:GLN:CG	2.51	0.41
3:D:348:GLN:HB2	3:D:351:MET:CG	2.45	0.41
3:D:377:VAL:HG22	3:D:377:VAL:O	2.21	0.41
3:D:550:ARG:NH2	5:F:211:ASP:OD2	2.53	0.41
3:D:801:GLY:HA2	3:D:821:VAL:HG22	2.03	0.41
3:D:879:ARG:HB3	3:D:902:LEU:HD11	2.01	0.41
3:D:1164:ARG:HG2	3:D:1165:TYR:N	2.35	0.41
3:D:1263:PHE:O	3:D:1375:MET:CE	2.68	0.41
3:D:1448:THR:O	3:D:1449:GLU:C	2.63	0.41
1:A:6:LEU:HD11	1:A:192:LEU:HD13	2.03	0.41
1:A:112:ARG:NH1	1:A:125:PRO:HB2	2.36	0.41
1:A:117:VAL:HG12	1:A:118:ALA:N	2.36	0.41
1:B:58:ILE:CG2	1:B:61:VAL:CG2	2.99	0.41
1:B:58:ILE:HG12	1:B:140:MET:CB	2.51	0.41
1:B:86:VAL:HG13	1:B:86:VAL:O	2.20	0.41
1:B:99:LEU:HD23	1:B:114:PHE:CG	2.55	0.41
1:B:159:LYS:HD3	1:B:164:ALA:O	2.21	0.41
2:C:39:ARG:NH1	2:C:71:TYR:CZ	2.89	0.41
2:C:224:GLU:HA	2:C:227:PHE:H	1.85	0.41
2:C:328:LEU:CD1	2:C:438:ILE:CD1	2.99	0.41
2:C:355:VAL:HG12	2:C:372:LEU:O	2.21	0.41
2:C:492:ASP:HB3	2:C:518:LYS:CG	2.50	0.41
2:C:498:GLN:O	2:C:499:ALA:C	2.63	0.41
2:C:567:GLN:HB2	2:C:997:LEU:HD22	2.03	0.41
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.02	0.41
2:C:916:GLU:O	2:C:920:GLN:HG3	2.21	0.41
2:C:952:LEU:HD22	2:C:952:LEU:N	2.35	0.41
3:D:123:LEU:O	3:D:123:LEU:HD23	2.20	0.41
3:D:144:GLY:O	3:D:145:VAL:CG2	2.69	0.41
3:D:736:PHE:CD1	3:D:745:MET:HE1	2.55	0.41
3:D:828:LYS:HD3	3:D:828:LYS:C	2.45	0.41
3:D:1087:ARG:O	3:D:1088:THR:C	2.63	0.41
3:D:1153:VAL:CG1	3:D:1183:ILE:HD11	2.51	0.41
4:E:83:ASP:OD2	4:E:83:ASP:N	2.41	0.41
5:F:172:ARG:HH11	5:F:172:ARG:HG3	1.86	0.41
5:F:264:MET:HB2	5:F:264:MET:HE2	1.76	0.41
5:F:353:GLU:HG2	5:F:356:LYS:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:O	1:B:130:ALA:HB2	2.20	0.41
2:C:23:VAL:CG2	2:C:24:GLU:H	2.32	0.41
2:C:97:ARG:NH2	2:C:110:GLU:OE1	2.45	0.41
2:C:434:HIS:O	2:C:435:TYR:C	2.64	0.41
2:C:735:ARG:O	2:C:735:ARG:HG3	2.20	0.41
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.56	0.41
3:D:7:LYS:CD	3:D:1456:LYS:NZ	2.82	0.41
3:D:128:TYR:CE2	3:D:587:ARG:HD3	2.55	0.41
3:D:172:PRO:O	3:D:173:PRO:C	2.63	0.41
3:D:463:GLN:O	3:D:466:LYS:N	2.54	0.41
3:D:584:ASN:OD1	3:D:590:PRO:HA	2.22	0.41
3:D:935:LYS:HG2	3:D:939:PHE:CD2	2.56	0.41
3:D:1294:VAL:O	3:D:1294:VAL:HG13	2.21	0.41
5:F:249:ARG:HE	5:F:249:ARG:HB3	1.77	0.41
1:B:43:ILE:HG22	1:B:214:ALA:CB	2.51	0.40
1:B:173:PRO:CG	1:B:205:VAL:HG12	2.51	0.40
2:C:28:ARG:HG2	2:C:28:ARG:O	2.21	0.40
2:C:409:ARG:HH22	2:C:454:SER:HB2	1.86	0.40
2:C:773:LEU:O	2:C:776:SER:HB2	2.21	0.40
3:D:85:VAL:O	3:D:87:ARG:N	2.54	0.40
3:D:111:LYS:HD2	3:D:1452:ILE:HD13	1.98	0.40
3:D:311:LEU:HD12	3:D:311:LEU:C	2.46	0.40
3:D:500:ARG:HH12	3:D:1390:LEU:HD21	1.78	0.40
3:D:610:LYS:HD3	3:D:615:ARG:HH21	1.86	0.40
5:F:94:LEU:HD22	5:F:98:GLU:HB2	2.03	0.40
5:F:143:HIS:O	5:F:145:PRO:HD3	2.20	0.40
5:F:310:ILE:C	5:F:312:GLN:H	2.29	0.40
1:A:34:VAL:CG2	1:A:35:THR:N	2.83	0.40
1:A:90:LEU:HD13	1:A:90:LEU:N	2.36	0.40
2:C:10:ARG:O	2:C:10:ARG:HG2	2.21	0.40
2:C:23:VAL:CG2	2:C:24:GLU:N	2.84	0.40
2:C:172:ILE:HA	2:C:185:LYS:O	2.21	0.40
2:C:1058:ASP:OD1	2:C:1058:ASP:C	2.64	0.40
3:D:38:LYS:HB3	3:D:39:PRO:CD	2.49	0.40
3:D:115:LEU:CD2	3:D:115:LEU:O	2.69	0.40
3:D:313:MET:CE	3:D:319:ALA:HB2	2.51	0.40
3:D:357:GLU:HB2	3:D:387:LEU:HD23	2.03	0.40
3:D:675:ARG:HD2	3:D:675:ARG:HA	1.71	0.40
3:D:687:VAL:HG13	3:D:688:TRP:N	2.35	0.40
3:D:930:LEU:O	3:D:930:LEU:HD12	2.21	0.40
3:D:1108:ARG:HG3	3:D:1199:GLY:HA3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:112:ALA:HB2	5:F:176:ILE:CG2	2.51	0.40
5:F:324:GLU:OE2	6:G:19:DG:N2	2.54	0.40
5:F:407:LYS:O	5:F:411:HIS:HB2	2.21	0.40
1:B:112:ARG:CB	1:B:112:ARG:HH21	2.35	0.40
2:C:214:TYR:HB2	2:C:218:VAL:HG23	2.02	0.40
2:C:438:ILE:HG22	2:C:439:CYS:O	2.22	0.40
2:C:626:ARG:N	2:C:639:GLN:HE21	2.18	0.40
3:D:187:LYS:CD	3:D:187:LYS:H	2.34	0.40
3:D:236:TYR:CE1	3:D:242:LEU:CB	3.02	0.40
3:D:680:GLN:O	3:D:681:ARG:C	2.65	0.40
3:D:1151:ARG:HD2	3:D:1151:ARG:HA	2.01	0.40
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.22	0.40
3:D:1376:MET:HE3	3:D:1376:MET:HB2	1.87	0.40
3:D:1380:GLU:HB2	3:D:1420:LEU:HD21	2.03	0.40
5:F:422:LEU:O	5:F:423:ASP:HB2	2.21	0.40
1:A:75:VAL:O	1:A:75:VAL:CG1	2.70	0.40
1:A:79:ILE:O	1:A:79:ILE:HG22	2.21	0.40
1:B:35:THR:HG22	1:B:36:LEU:HD12	2.04	0.40
1:B:105:GLY:HA2	1:B:134:GLU:HA	2.04	0.40
2:C:49:ARG:NE	2:C:49:ARG:HA	2.35	0.40
2:C:168:ARG:NE	2:C:345:ARG:HH11	2.20	0.40
2:C:168:ARG:HD3	2:C:345:ARG:HH11	1.86	0.40
2:C:487:THR:O	2:C:488:ALA:C	2.65	0.40
2:C:666:LEU:C	2:C:666:LEU:HD12	2.46	0.40
2:C:1013:TYR:O	2:C:1021:LEU:HD11	2.21	0.40
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.21	0.40
4:E:48:MET:HG2	4:E:58:PRO:HD3	2.03	0.40
5:F:417:LYS:C	5:F:418:LEU:HD12	2.47	0.40
1:A:79:ILE:CG2	1:A:167:VAL:HG22	2.51	0.40
2:C:64:LEU:N	2:C:103:LYS:HB3	2.36	0.40
2:C:261:ILE:HD12	2:C:261:ILE:N	2.34	0.40
2:C:428:ARG:O	2:C:429:ASP:C	2.64	0.40
2:C:550:LEU:HD23	2:C:906:PHE:CE1	2.54	0.40
2:C:684:PHE:CD2	3:D:730:PRO:HB3	2.57	0.40
2:C:760:SER:O	2:C:786:LYS:HB2	2.22	0.40
3:D:553:ARG:HE	5:F:214:GLN:CB	2.34	0.40
3:D:625:TYR:HD2	3:D:751:LEU:HD11	1.87	0.40
3:D:695:ILE:CD1	3:D:720:LEU:CD1	2.99	0.40
3:D:796:ARG:NH1	3:D:862:ASP:CG	2.79	0.40
3:D:1494:ALA:HB3	4:E:92:LEU:HD11	2.00	0.40
4:E:37:ASN:HB3	4:E:93:TYR:CD1	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:358:LEU:N	5:F:358:LEU:HD23	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/315 (71%)	192 (86%)	32 (14%)	0	100	100
1	B	222/315 (70%)	192 (86%)	28 (13%)	2 (1%)	14	41
2	C	1107/1119 (99%)	960 (87%)	146 (13%)	1 (0%)	48	76
3	D	1481/1505 (98%)	1255 (85%)	218 (15%)	8 (0%)	24	54
4	E	92/99 (93%)	83 (90%)	9 (10%)	0	100	100
5	F	344/423 (81%)	291 (85%)	51 (15%)	2 (1%)	21	50
All	All	3470/3776 (92%)	2973 (86%)	484 (14%)	13 (0%)	30	59

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	GLY
3	D	276	ASP
1	B	154	GLU
5	F	168	LYS
2	C	212	GLY
3	D	710	ARG
3	D	783	ARG
3	D	1130	ARG
3	D	479	GLU
3	D	705	ALA
3	D	959	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	275	GLU
5	F	378	GLY

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	199/273 (73%)	153 (77%)	46 (23%)	1	3
1	B	197/273 (72%)	162 (82%)	35 (18%)	2	8
2	C	936/941 (100%)	776 (83%)	160 (17%)	2	9
3	D	1249/1265 (99%)	1052 (84%)	197 (16%)	2	10
4	E	83/88 (94%)	72 (87%)	11 (13%)	4	15
5	F	301/371 (81%)	233 (77%)	68 (23%)	1	4
All	All	2965/3211 (92%)	2448 (83%)	517 (17%)	2	8

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	12	THR
1	A	13	VAL
1	A	15	THR
1	A	18	ARG
1	A	19	GLU
1	A	25	LEU
1	A	48	ILE
1	A	62	LEU
1	A	71	VAL
1	A	72	LYS
1	A	76	VAL
1	A	78	ILE
1	A	80	LEU
1	A	85	LEU
1	A	86	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	87	VAL
1	A	90	LEU
1	A	96	THR
1	A	99	LEU
1	A	115	LEU
1	A	122	ILE
1	A	134	GLU
1	A	138	LEU
1	A	143	ARG
1	A	144	VAL
1	A	145	ASP
1	A	151	VAL
1	A	155	LYS
1	A	158	ILE
1	A	170	VAL
1	A	175	ARG
1	A	182	GLU
1	A	184	THR
1	A	189	ARG
1	A	190	THR
1	A	197	LEU
1	A	199	ILE
1	A	201	THR
1	A	204	SER
1	A	205	VAL
1	A	206	THR
1	A	209	GLU
1	A	213	GLN
1	A	216	GLU
1	A	218	LEU
1	B	15	THR
1	B	22	GLU
1	B	24	VAL
1	B	34	VAL
1	B	35	THR
1	B	36	LEU
1	B	39	PRO
1	B	40	LEU
1	B	41	ARG
1	B	47	SER
1	B	55	SER
1	B	58	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	67	THR
1	B	87	VAL
1	B	99	LEU
1	B	109	VAL
1	B	115	LEU
1	B	120	VAL
1	B	128	HIS
1	B	131	THR
1	B	133	GLU
1	B	155	LYS
1	B	156	HIS
1	B	158	ILE
1	B	160	ASP
1	B	162	ILE
1	B	183	ASP
1	B	188	GLN
1	B	196	THR
1	B	197	LEU
1	B	199	ILE
1	B	208	LEU
1	B	223	THR
1	B	226	SER
1	B	227	ASN
2	C	2	GLU
2	C	8	ARG
2	C	10	ARG
2	C	12	VAL
2	C	15	LEU
2	C	21	ILE
2	C	24	GLU
2	C	27	ARG
2	C	30	LEU
2	C	36	PRO
2	C	37	GLU
2	C	38	LYS
2	C	44	ILE
2	C	49	ARG
2	C	51	THR
2	C	65	VAL
2	C	73	LEU
2	C	101	ILE
2	C	105	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	113	VAL
2	C	118	ILE
2	C	138	SER
2	C	149	THR
2	C	154	ARG
2	C	162	ILE
2	C	174	LEU
2	C	177	GLU
2	C	183	SER
2	C	190	LYS
2	C	194	VAL
2	C	196	LEU
2	C	203	ASP
2	C	204	GLN
2	C	207	LEU
2	C	214	TYR
2	C	221	LEU
2	C	224	GLU
2	C	226	VAL
2	C	235	LEU
2	C	246	ASP
2	C	269	LEU
2	C	271	GLU
2	C	285	LEU
2	C	292	ARG
2	C	299	LYS
2	C	311	PHE
2	C	328	LEU
2	C	335	THR
2	C	340	MET
2	C	342	ASP
2	C	348	LEU
2	C	351	LEU
2	C	353	ARG
2	C	356	ARG
2	C	359	MET
2	C	367	LEU
2	C	383	ARG
2	C	384	GLU
2	C	387	SER
2	C	390	GLN
2	C	402	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	403	SER
2	C	409	ARG
2	C	427	VAL
2	C	428	ARG
2	C	442	GLU
2	C	443	THR
2	C	445	GLU
2	C	460	ARG
2	C	461	VAL
2	C	464	LEU
2	C	474	VAL
2	C	475	VAL
2	C	478	VAL
2	C	482	GLU
2	C	493	ARG
2	C	495	THR
2	C	511	GLU
2	C	514	VAL
2	C	529	VAL
2	C	534	VAL
2	C	537	LYS
2	C	538	GLN
2	C	539	VAL
2	C	541	SER
2	C	542	VAL
2	C	559	LEU
2	C	562	SER
2	C	564	MET
2	C	572	ILE
2	C	591	SER
2	C	599	GLU
2	C	616	GLU
2	C	617	ASP
2	C	642	ARG
2	C	649	VAL
2	C	670	GLN
2	C	672	VAL
2	C	674	VAL
2	C	677	MET
2	C	680	ASP
2	C	695	LEU
2	C	702	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	703	ILE
2	C	707	ARG
2	C	717	LEU
2	C	723	THR
2	C	729	LEU
2	C	730	SER
2	C	764	GLU
2	C	770	GLU
2	C	773	LEU
2	C	780	GLU
2	C	785	VAL
2	C	786	LYS
2	C	792	VAL
2	C	796	GLU
2	C	808	ARG
2	C	815	LEU
2	C	823	VAL
2	C	825	VAL
2	C	829	GLN
2	C	833	LEU
2	C	848	VAL
2	C	849	VAL
2	C	851	LYS
2	C	852	ILE
2	C	853	LEU
2	C	861	LEU
2	C	869	VAL
2	C	870	ILE
2	C	880	MET
2	C	888	THR
2	C	897	LEU
2	C	900	ARG
2	C	914	ILE
2	C	916	GLU
2	C	939	ARG
2	C	946	ARG
2	C	954	THR
2	C	958	THR
2	C	959	PRO
2	C	963	LEU
2	C	973	VAL
2	C	974	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	989	VAL
2	C	1001	VAL
2	C	1005	MET
2	C	1008	ARG
2	C	1014	SER
2	C	1052	MET
2	C	1055	LEU
2	C	1056	LYS
2	C	1060	ILE
2	C	1061	GLU
2	C	1063	ARG
2	C	1071	ILE
2	C	1078	GLU
2	C	1084	SER
2	C	1117	SER
3	D	4	GLU
3	D	9	ARG
3	D	10	ILE
3	D	25	GLU
3	D	31	THR
3	D	40	GLU
3	D	53	ILE
3	D	58	CYS
3	D	73	CYS
3	D	74	GLU
3	D	80	VAL
3	D	81	THR
3	D	97	THR
3	D	106	LYS
3	D	115	LEU
3	D	123	LEU
3	D	124	GLU
3	D	133	ILE
3	D	141	ILE
3	D	171	LEU
3	D	176	ASP
3	D	178	LEU
3	D	179	VAL
3	D	187	LYS
3	D	191	LEU
3	D	202	VAL
3	D	212	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	223	LEU
3	D	231	VAL
3	D	232	GLU
3	D	250	LEU
3	D	256	GLU
3	D	270	LEU
3	D	284	LEU
3	D	289	THR
3	D	293	VAL
3	D	298	VAL
3	D	311	LEU
3	D	316	GLN
3	D	333	LEU
3	D	335	LEU
3	D	353	VAL
3	D	361	VAL
3	D	375	GLU
3	D	377	VAL
3	D	378	ILE
3	D	385	VAL
3	D	389	GLU
3	D	393	ILE
3	D	399	ARG
3	D	400	VAL
3	D	409	VAL
3	D	410	SER
3	D	411	THR
3	D	415	VAL
3	D	420	VAL
3	D	428	LYS
3	D	434	ARG
3	D	437	VAL
3	D	440	VAL
3	D	446	VAL
3	D	447	VAL
3	D	448	GLU
3	D	450	TYR
3	D	459	GLU
3	D	464	LEU
3	D	465	LEU
3	D	471	GLU
3	D	475	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	478	LEU
3	D	480	GLU
3	D	491	LYS
3	D	513	ILE
3	D	514	LEU
3	D	517	VAL
3	D	519	VAL
3	D	525	ARG
3	D	527	MET
3	D	534	ARG
3	D	538	SER
3	D	557	LEU
3	D	566	ILE
3	D	567	ILE
3	D	574	LEU
3	D	578	VAL
3	D	586	ARG
3	D	592	THR
3	D	596	SER
3	D	600	LEU
3	D	604	THR
3	D	607	LEU
3	D	608	SER
3	D	621	LYS
3	D	623	VAL
3	D	632	VAL
3	D	638	LYS
3	D	660	LYS
3	D	663	GLU
3	D	677	LEU
3	D	679	ARG
3	D	686	GLU
3	D	691	LEU
3	D	695	ILE
3	D	698	LYS
3	D	704	ARG
3	D	720	LEU
3	D	721	VAL
3	D	722	GLU
3	D	724	GLN
3	D	728	LEU
3	D	731	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	741	ASP
3	D	747	VAL
3	D	754	PHE
3	D	756	GLN
3	D	769	LEU
3	D	786	ILE
3	D	794	GLN
3	D	798	GLU
3	D	821	VAL
3	D	836	VAL
3	D	858	VAL
3	D	863	VAL
3	D	873	LEU
3	D	890	VAL
3	D	904	VAL
3	D	913	ASP
3	D	935	LYS
3	D	936	TYR
3	D	942	SER
3	D	943	THR
3	D	947	ILE
3	D	948	THR
3	D	949	ILE
3	D	966	GLU
3	D	968	ASP
3	D	972	LEU
3	D	973	GLN
3	D	974	ILE
3	D	975	GLU
3	D	995	LEU
3	D	997	THR
3	D	1001	GLU
3	D	1003	VAL
3	D	1004	THR
3	D	1015	TYR
3	D	1018	ASN
3	D	1034	GLN
3	D	1039	CYS
3	D	1057	VAL
3	D	1058	ARG
3	D	1065	LEU
3	D	1067	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1083	ASP
3	D	1088	THR
3	D	1090	ASP
3	D	1100	ASP
3	D	1112	CYS
3	D	1114	THR
3	D	1116	ASN
3	D	1118	ILE
3	D	1119	SER
3	D	1128	VAL
3	D	1129	THR
3	D	1151	ARG
3	D	1183	ILE
3	D	1186	VAL
3	D	1188	VAL
3	D	1192	LEU
3	D	1208	ASP
3	D	1213	ARG
3	D	1216	SER
3	D	1217	ILE
3	D	1235	GLN
3	D	1304	LYS
3	D	1310	ARG
3	D	1320	GLU
3	D	1326	THR
3	D	1335	LEU
3	D	1349	VAL
3	D	1363	LEU
3	D	1376	MET
3	D	1379	VAL
3	D	1394	VAL
3	D	1395	LEU
3	D	1407	LEU
3	D	1413	THR
3	D	1420	LEU
3	D	1426	LYS
3	D	1431	THR
3	D	1448	THR
3	D	1456	LYS
3	D	1468	LEU
3	D	1470	ARG
3	D	1489	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1493	LYS
3	D	1496	GLU
4	E	6	ILE
4	E	15	SER
4	E	21	VAL
4	E	30	LEU
4	E	44	GLU
4	E	54	LEU
4	E	67	GLU
4	E	74	VAL
4	E	75	PHE
4	E	90	GLU
4	E	93	TYR
5	F	78	SER
5	F	79	ASP
5	F	81	VAL
5	F	82	ARG
5	F	83	GLN
5	F	88	ILE
5	F	95	THR
5	F	98	GLU
5	F	100	VAL
5	F	114	LYS
5	F	116	LEU
5	F	122	LEU
5	F	123	ASP
5	F	126	LEU
5	F	131	VAL
5	F	140	ARG
5	F	142	ARG
5	F	148	LYS
5	F	149	GLU
5	F	155	THR
5	F	157	GLU
5	F	164	LYS
5	F	166	LEU
5	F	170	HIS
5	F	171	LYS
5	F	179	GLU
5	F	205	ARG
5	F	207	LEU
5	F	208	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	210	LEU
5	F	211	ASP
5	F	213	ILE
5	F	218	GLN
5	F	251	ILE
5	F	254	GLN
5	F	258	ILE
5	F	270	LYS
5	F	282	LEU
5	F	291	ILE
5	F	304	VAL
5	F	306	GLU
5	F	307	THR
5	F	310	ILE
5	F	319	THR
5	F	323	ASP
5	F	324	GLU
5	F	336	GLU
5	F	338	LEU
5	F	340	SER
5	F	348	SER
5	F	349	LEU
5	F	351	SER
5	F	353	GLU
5	F	358	LEU
5	F	359	SER
5	F	369	LEU
5	F	372	ARG
5	F	376	ILE
5	F	377	ASP
5	F	380	GLU
5	F	386	VAL
5	F	398	ARG
5	F	399	GLN
5	F	400	ILE
5	F	401	GLU
5	F	402	ASN
5	F	415	THR
5	F	423	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	213	GLN
1	A	227	ASN
1	B	63	HIS
1	B	81	ASN
1	B	128	HIS
1	B	163	ASN
1	B	221	HIS
2	C	80	GLN
2	C	390	GLN
2	C	498	GLN
2	C	567	GLN
2	C	639	GLN
2	C	704	HIS
2	C	728	HIS
2	C	834	GLN
2	C	845	ASN
2	C	899	GLN
2	C	991	GLN
2	C	1019	GLN
2	C	1050	GLN
3	D	348	GLN
3	D	462	GLN
3	D	569	ASN
3	D	611	GLN
3	D	617	ASN
3	D	640	HIS
3	D	641	GLN
3	D	680	GLN
3	D	709	HIS
3	D	717	GLN
3	D	748	HIS
3	D	767	HIS
3	D	816	HIS
3	D	855	HIS
3	D	909	ASN
3	D	973	GLN
3	D	976	GLN
3	D	1031	ASN
3	D	1034	GLN
3	D	1075	HIS
3	D	1195	GLN
3	D	1235	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1254	GLN
3	D	1333	HIS
3	D	1334	GLN
3	D	1359	GLN
3	D	1441	GLN
3	D	1442	ASN
3	D	1489	GLN
4	E	86	GLN
5	F	175	HIS
5	F	254	GLN
5	F	269	ASN
5	F	399	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	2/3 (66%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	DCP	D	1601	9	28,29,29	4.27	14 (50%)	41,45,45	1.69	10 (24%)

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
10	DCP	D	1601	9	-	9/22/34/34	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1601	DCP	C2'-C1'	-10.54	1.23	1.52
10	D	1601	DCP	O4'-C4'	-8.64	1.25	1.45
10	D	1601	DCP	O4'-C1'	8.38	1.61	1.42
10	D	1601	DCP	PB-O3B	6.84	1.66	1.59
10	D	1601	DCP	PA-O3A	6.66	1.66	1.59
10	D	1601	DCP	C6-C5	5.52	1.47	1.35
10	D	1601	DCP	PB-O3A	5.01	1.64	1.59
10	D	1601	DCP	C2-N3	4.57	1.45	1.36
10	D	1601	DCP	C4-N3	4.08	1.42	1.34
10	D	1601	DCP	C4-N4	3.88	1.43	1.33
10	D	1601	DCP	O2-C2	-3.88	1.16	1.23
10	D	1601	DCP	C1'-N1	-3.03	1.40	1.48
10	D	1601	DCP	O3'-C3'	-2.97	1.37	1.43
10	D	1601	DCP	C6-N1	2.80	1.44	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1601	DCP	C1'-N1-C2	4.33	125.27	117.83
10	D	1601	DCP	O3G-PG-O3B	3.93	117.81	104.64
10	D	1601	DCP	C4-N3-C2	3.57	125.89	120.26
10	D	1601	DCP	C1'-N1-C6	-2.96	115.71	121.53
10	D	1601	DCP	O4'-C4'-C3'	-2.94	98.95	105.65
10	D	1601	DCP	C2'-C1'-N1	-2.90	106.56	113.81
10	D	1601	DCP	C5-C4-N3	-2.46	117.17	121.32
10	D	1601	DCP	C2'-C3'-C4'	2.40	107.68	102.80
10	D	1601	DCP	N4-C4-N3	2.36	122.14	117.91
10	D	1601	DCP	O4'-C4'-C5'	2.23	116.48	109.33

There are no chirality outliers.

All (9) torsion outliers are listed below:

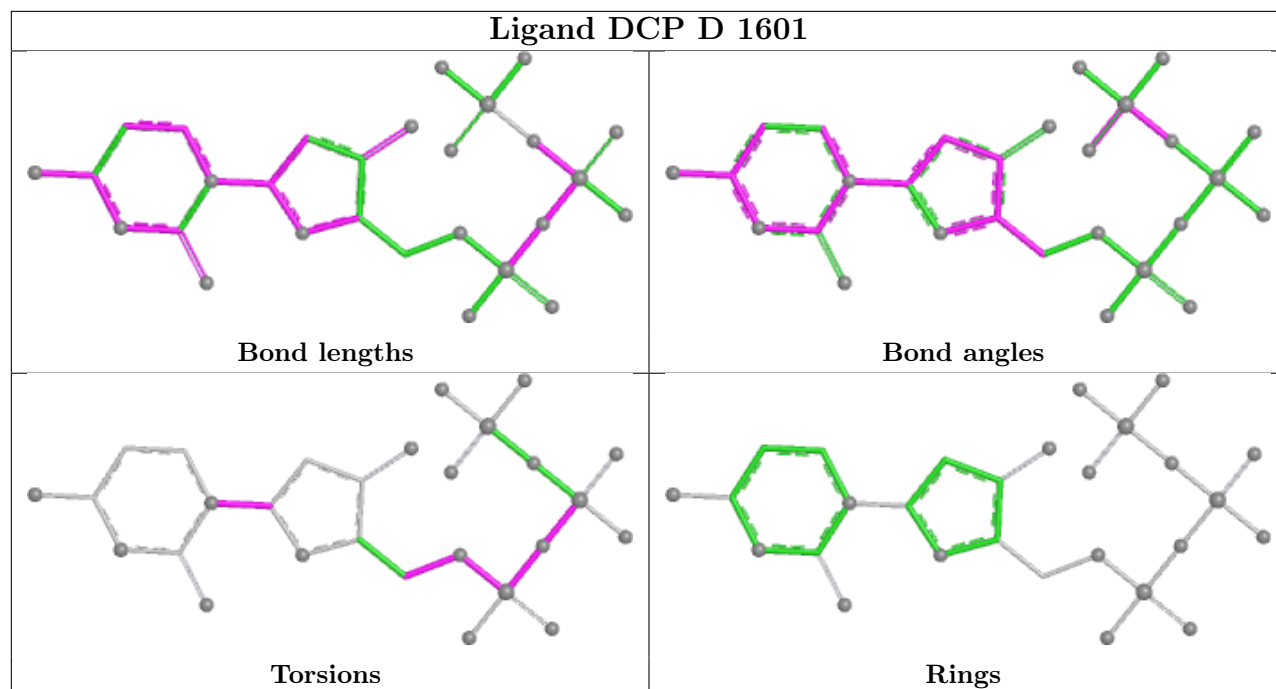
Mol	Chain	Res	Type	Atoms
10	D	1601	DCP	C5'-O5'-PA-O1A
10	D	1601	DCP	C5'-O5'-PA-O3A
10	D	1601	DCP	C2'-C1'-N1-C6
10	D	1601	DCP	PB-O3A-PA-O5'
10	D	1601	DCP	PA-O3A-PB-O1B
10	D	1601	DCP	C2'-C1'-N1-C2
10	D	1601	DCP	C4'-C5'-O5'-PA
10	D	1601	DCP	PB-O3A-PA-O2A
10	D	1601	DCP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1601	DCP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	226/315 (71%)	-0.49	0 100 100	73, 91, 110, 124	0
1	B	224/315 (71%)	-0.53	0 100 100	66, 96, 121, 133	0
2	C	1111/1119 (99%)	-0.55	0 100 100	56, 91, 138, 160	0
3	D	1485/1505 (98%)	-0.55	1 (0%) 92 86	50, 85, 138, 160	0
4	E	94/99 (94%)	-0.51	0 100 100	64, 101, 132, 139	0
5	F	346/423 (81%)	-0.44	2 (0%) 85 70	64, 101, 153, 163	0
6	G	17/22 (77%)	-0.53	0 100 100	69, 95, 169, 171	0
7	H	25/27 (92%)	-0.36	0 100 100	90, 121, 169, 179	0
8	I	3/3 (100%)	-1.05	0 100 100	73, 73, 76, 87	0
All	All	3531/3828 (92%)	-0.54	3 (0%) 92 86	50, 91, 142, 179	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	376	ILE	2.2
3	D	1313	VAL	2.1
5	F	400	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

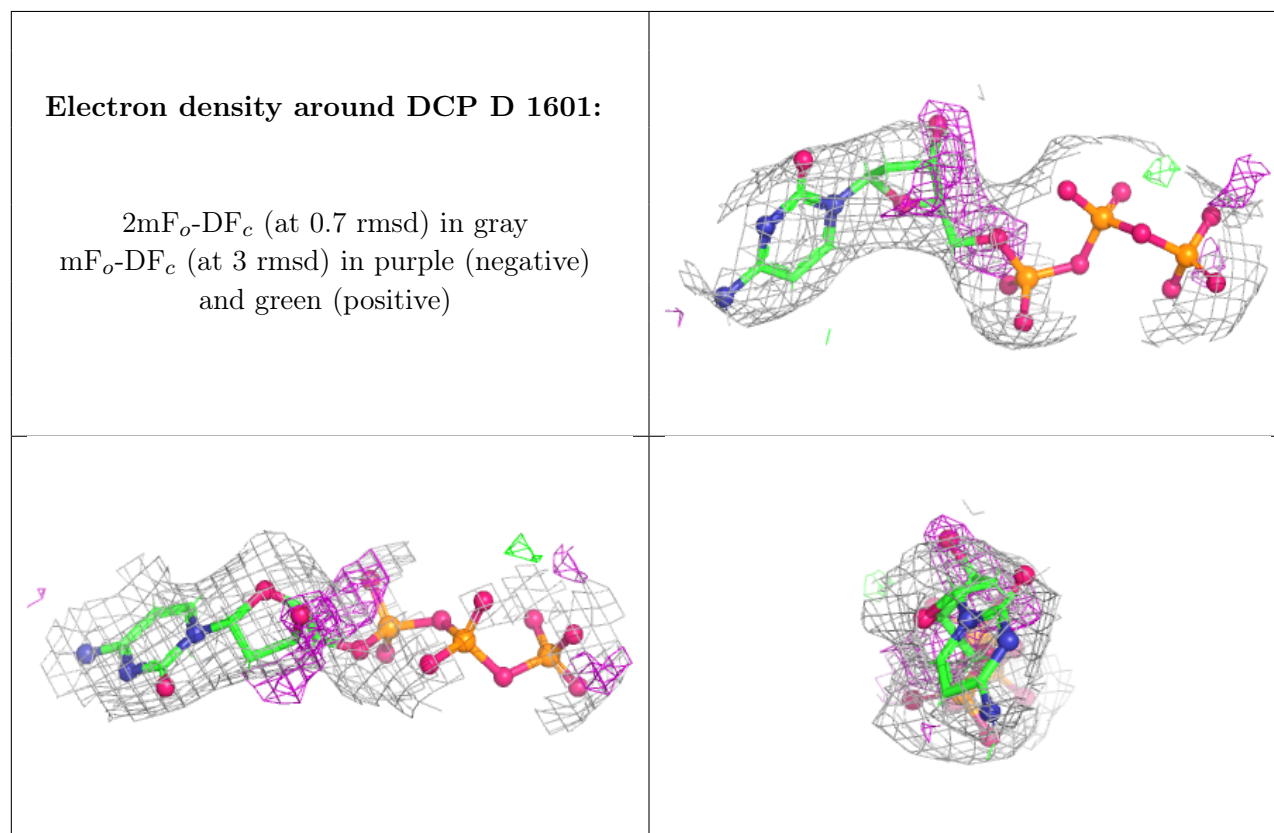
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NA	C	1201	1/1	0.79	0.10	70,70,70,70	0
12	ZN	D	1604	1/1	0.90	0.09	120,120,120,120	0
10	DCP	D	1601	28/28	0.92	0.06	80,93,112,115	0
12	ZN	D	1603	1/1	0.98	0.04	125,125,125,125	0
11	MG	D	1602	1/1	0.98	0.05	67,67,67,67	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.