



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2021 – 12:06 PM EST

PDB ID : 6WOY
Title : Thermus thermophilus RNA polymerase initially transcribing complex with 3'dCTP
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2020-04-26
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17

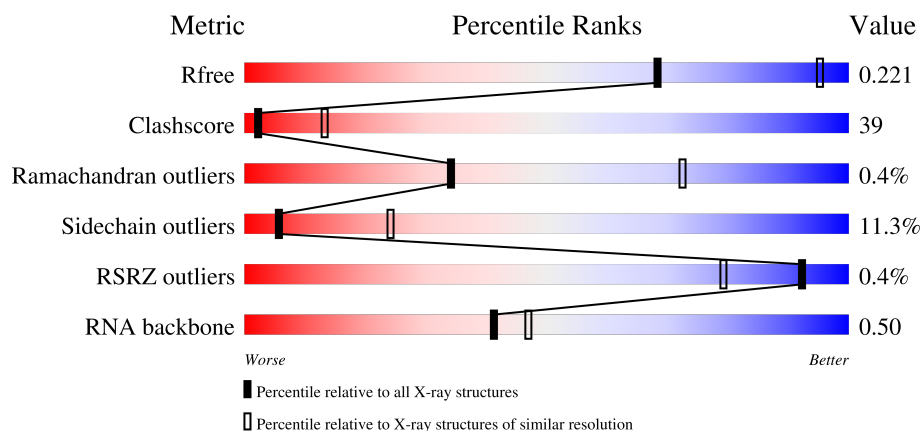
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	
1	B	315	
2	C	1119	
3	D	1505	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>45%</div><div>43%</div><div>6%</div><div>5%</div></div>
5	F	423	<div><div>3%</div><div></div><div>33%</div><div>43%</div><div>6%</div><div>18%</div></div>
6	G	22	<div><div></div><div>14%</div><div>55%</div><div>9%</div><div>23%</div></div>
7	H	27	<div><div></div><div>30%</div><div>59%</div><div></div><div>7%</div></div>
8	I	3	<div><div></div><div>33%</div><div>67%</div></div>

2 Entry composition

There are 11 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			

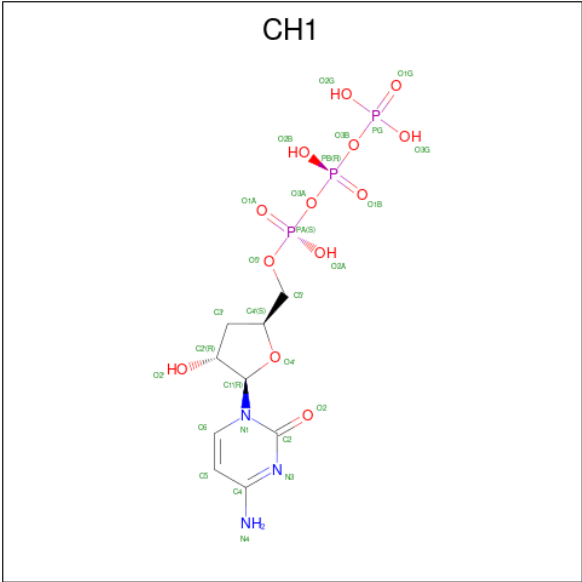
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Mg	0	0
			2	2		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula: C₉H₁₆N₃O₁₃P₃).

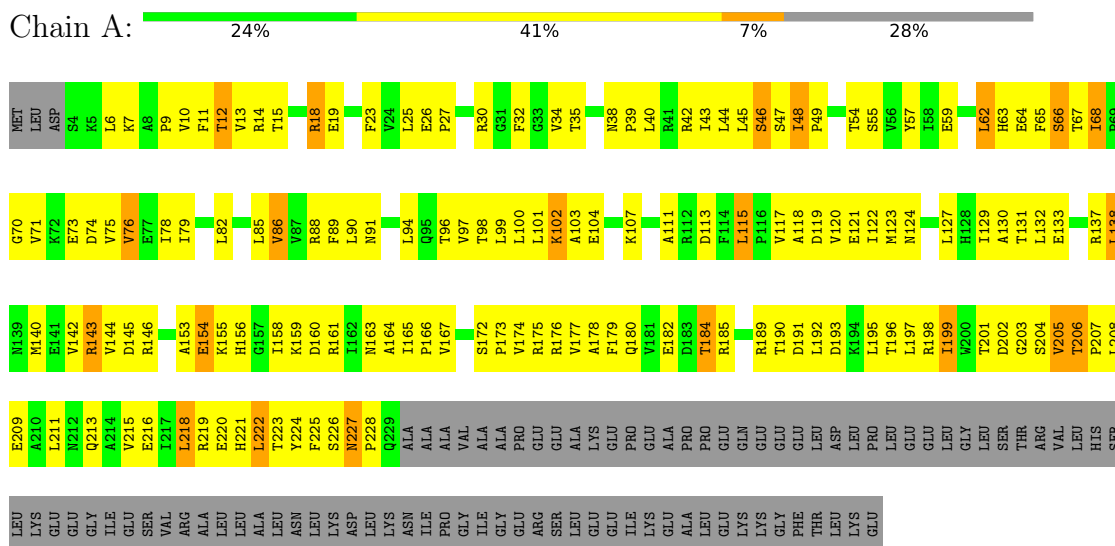


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
11	I	1	40	9	12	3	13	3	0	0

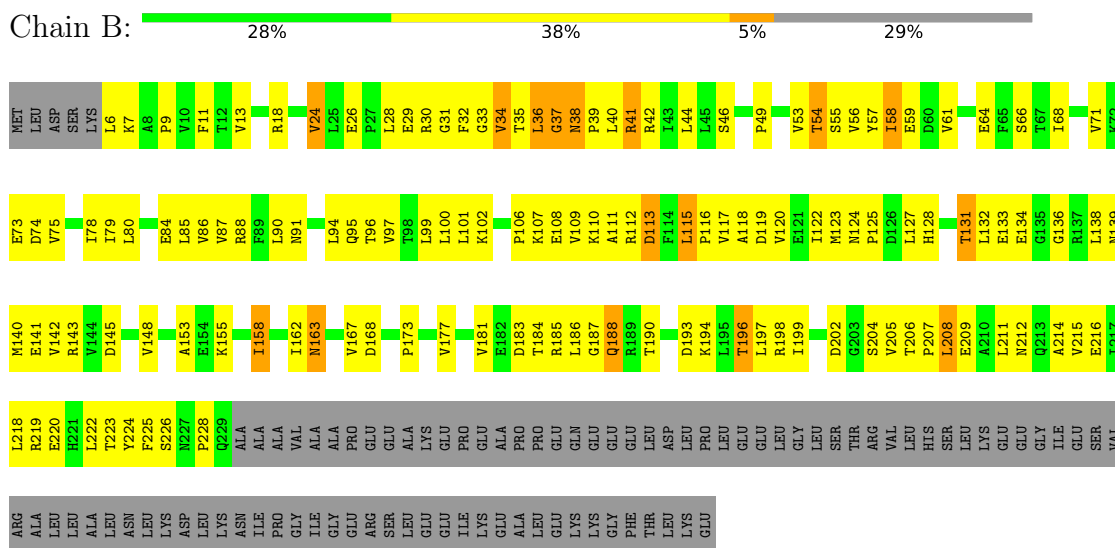
3 Residue-property plots

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



- Molecule 2: DNA-directed RNA polymerase subunit beta

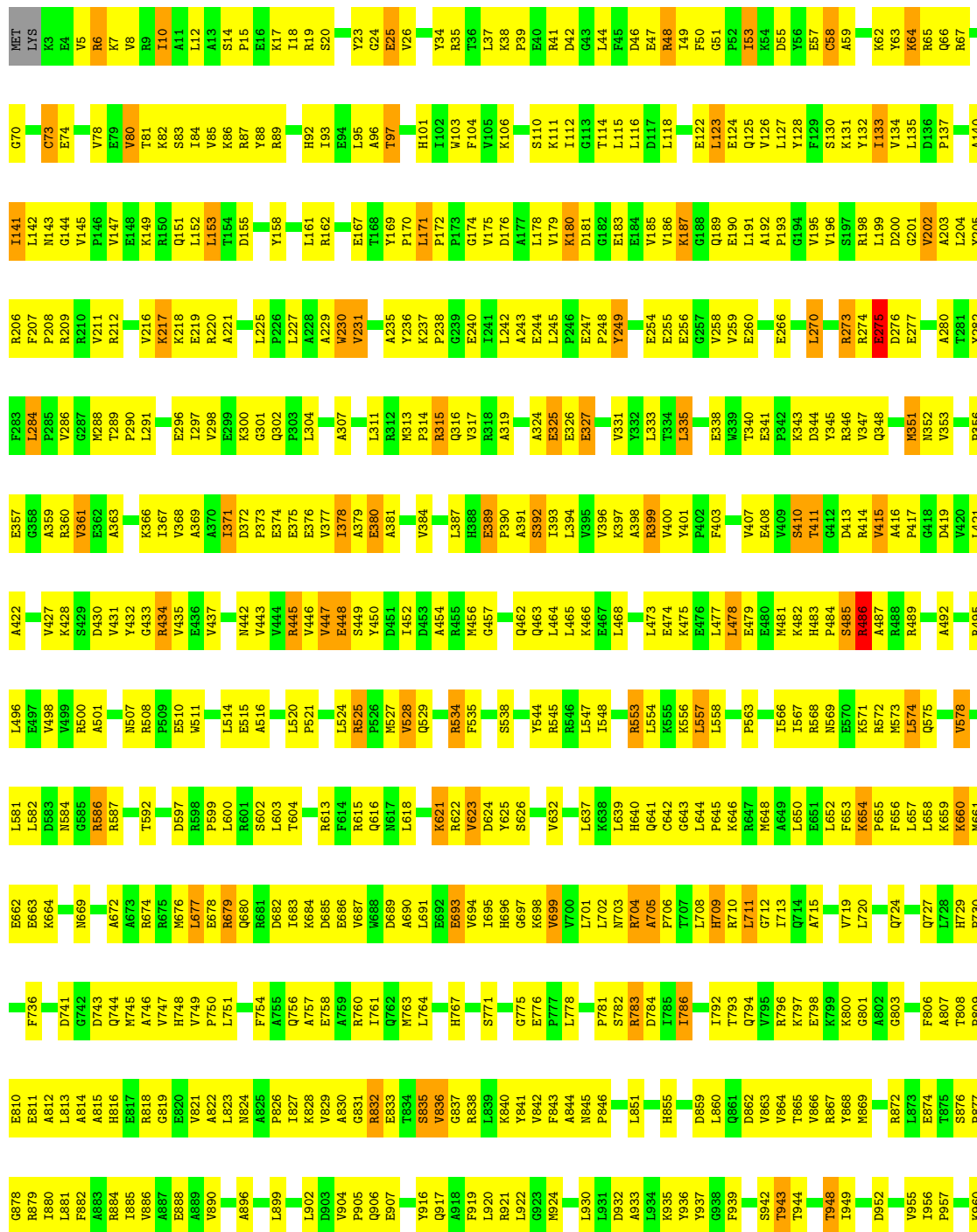
Chain C:  41% 51% 7%

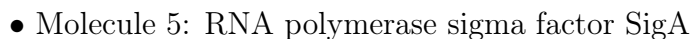
M1005	M1006	A1007	R1008	S1009	P1012	Y1013	S1014	L1015	I1016	Q1019	P1020	L1021	K1024	G1028	G1029	Q1030	R1031	T954	M1035	E1036	Y1037	W1038	Y1043	G1044	A1045	A1046	H1047	M1052	L1053	G1054	L1055	D1058	I1059	I1060	E1061	G1062	R1063	N1064	A1065	A1066	Y1067	E1068	A1069	I1070	I1071	K1072	G1073	E1074	P1077	E1078	D1003	K1004								
E932	G933	F934	G935	V936	D937	K938	R939	E940	V941	E942	V943	L944	R945	R946	A947	K948	E949	G950	L951	L952	V953	T954	K957	T958	P959	E960	E961	Q962	L963	K964	L968	Q969	G970	K971	T979	I983	E984	G985	P986	I987	V988	A1065	A1066	Y1067	E1068	A1069	I1070	I1071	K1072	G1073	E1074	P1077	E1078	D1003	K1004					
G864	T865	P866	F867	D868	G869	L870	L871	N872	P873	L874	G875	S878	R879	M880	N881	L882	G883	Q884	L885	L886	E887	T888	H889	L890	G891	L892	A893	L897	Q898	Q899	Y901	I902	S903	P904	I905	F906	D907	E908	A909	K910	I914	K915	E916	L917	L918	A919	Q920	V985	D987	M988	K928	R929	K930	T931	D932					
V792	P793		T796	G797	G798	I799	V800	L801	R802	T803	V804	R805	L806	R807	G808	D810	P811	G812	V813	E814	L815	K816		V819	R820	E821	V822	E823	R824	Q825		A828	Q829	R830	R831	K832	L833	Q834		K838			N841	G844	K845	K846			I852	L853	A919	Q920	V985	D987	M988	K928	R929	K930	T931	D932
G864	T865	P866	F867	D868	G869	L870	L871	N872	P873	L874	G875	S878	R879	M880	N881	L882	G883	Q884	L885	L886	E887	T888	H889	L890	G891	L892	A893	L897	Q898	Q899	Y901	I902	S903	P904	I905	F906	D907	E908	A909	K910	I914	K915	E916	L917	L918	A919	Q920	V985	D987	M988	K928	R929	K930	T931	D932					
D725	T726	P727	H728	L729	S730	D736	L737	D738	R739	E740		G741	V742	L743	V744	R745	G746	A747	E748	G749	K750	L751	G752	D753	I754	R755	V756	T759	S760	F761	K762		S765	T766	P767	R768	D769	E770	T771	R772	L773	L774	T775	S776	I777		E780	K781	L853	A919	Q920	V985	D987	M988	K928	R929	K930	T931	D932	
L583	E584	R507	E585	R586	V587	V588	R589	D590	R591	L592	E593	A594	L595	Y596	E597	E598	E599		E602	V603	A604	K605	V606	D607	G608	N609	R610	V613	R614	Y615	E616	D617	G618	R619	Y623	R626	R627	F628	Y629	R630	S631	N632	Q633		Q639	R640	P641	R642	V643	V644	P645	G646	Q647	R648	V649	R650				
K651	L654	L655	A656	G664	F665	L666	A667	L668	N671	V672	L673	V674	A675	F679	D680	G681	Y682	N683	F684	E685	V689	L690	E693	K696	R697	D698	F699	Y700	T701	S702	I703	H704	E705	E706	R707	Y708	E709	I710	A711	R712	R713	T714	T715	K716	L717	G718	P719	E720	R721	I722	T723	R724								
L503	R507	I508	V513	V514	A515	R516	K517	K518	E520	P521	V524	E528	V529	D533	V534	S535	P536	K537	S538	Q538	V539	F540	S541	V542	N543	T544	N545	L546	I547	E551	H552	D553	D554	R557	A558	L559	M560	M564	Q565	Q567	A568	P569	V570	L571	I572	P577	V578	M580												
V427	R428	H431	T432	H434	Y435	G436	I437	I438	E442	T443	P444	A445	G446	A447	N448	I449	G450	L451	I452	S453	S454	L455	R460	V461	D462	I467	R468	Y471	R472	R473	V474	T480	D481	E482	Y485	M486	T487	A488	T489	E490	E491	D492	R493	T495	Q498	A499	N500	T501	P502											
E357	R358	M359	L360	M361	G362	S363	E364	D365	F366	L367	T368	A370	K371	L372	R376	P377	L378	E379	A380	E384	F385	F386	S387	R388	S389	Q390	L391	S392	Q393	F394	K395	D396	E397	S402	S403	L404	R405	G337	H406	K407	R408	R409	A412	L413	Q414	L418	T419	R420	E421	A423	G424	F425	D426							
R284	L285	L290	A291	R292	F293	E297	F298	K299	D300	E301	L304	P305	T306	L307	R308	Y309	L310	F311	A312	G316	V317	P318	M179	G319	H320	E321	V322	D323	D326	H327	R331	R332	T333	L260	L261	A262	D263	P264	R265	R266	Y267	D268	L269	Q270	E271	K276	E278	E279	K280	L281	T283									
S143	P144	V146	T149	P150	R154	R157	I162	I163	P164	P166	K167	R168	I172	D173	L174	E175	V176	E177	P178	M179	G180	V181	L182	V183	S183	M184	E185	V186	R189	K190	F191	L193	V194	L196	L197	R198	V199	L200	G201	D203	E205	D133	I136	R209	E210	L211	G212	A213												
L69	E70	Y71	G74	E75	P76	R84	E85	K86	D87	L88	Q91	A92	P93	E97	L98	Q99	L100	I101	H102	K103	D104	T105	G106	L107	V108	K109	E110	D111	E112	L115	G116	H117	I118	L119	M121	T122	E123	D124	F127	I128	N129	G131	A132	D133	I136	V137	I140	H141	R142											
M1	E2	I3	F6	G7	R8	I9	R10	E11	V12	P16	P17	L18	T19	E20	I21	O22	V23	E24	S25	R28	A29	L30	Q31	P35	P36	E37	K38	R39	N41	I44	Q45	A46	R49	E50	T51	F52	P53	E55	E56	GLU	ASP	LYS	GLY	GLY	L64	V65	L66	D67	F68											

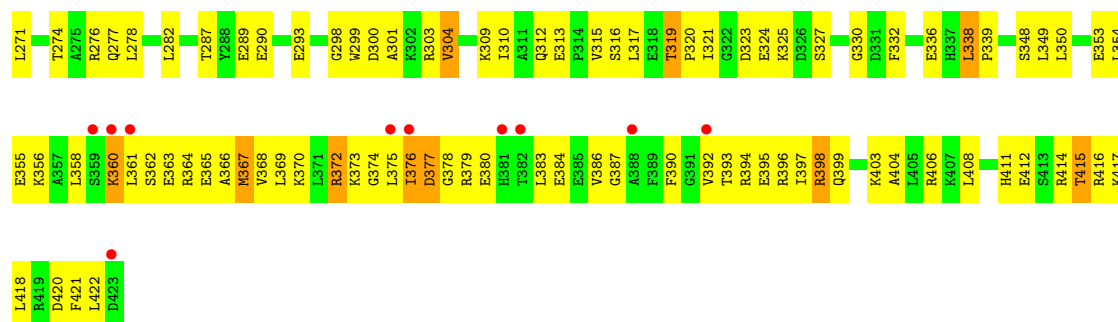


● Molecule 3: DNA-directed RNA polymerase subunit beta'

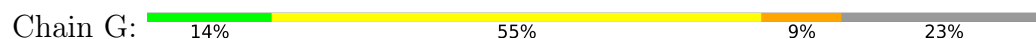
Chain D: 44% 48% 7%







- 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')



- Molecule 7: DNA (25-MER)



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.98Å 102.47Å 296.04Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	29.98 – 3.00 29.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.98-3.00) 96.5 (29.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.206 , 0.219 0.207 , 0.221	Depositor DCC
R_{free} test set	2002 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, CH1

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	0.46	0/1814	0.67	0/2466
1	B	0.45	0/1799	0.63	0/2447
2	C	0.47	0/8937	0.63	1/12087 (0.0%)
3	D	0.51	1/11927 (0.0%)	0.66	0/16127
4	E	0.43	0/775	0.58	0/1045
5	F	0.45	0/2852	0.61	0/3837
6	G	1.12	3/393 (0.8%)	1.11	3/605 (0.5%)
7	H	0.98	0/580	1.02	1/895 (0.1%)
8	I	0.80	0/69	1.46	0/106
All	All	0.51	4/29146 (0.0%)	0.67	5/39615 (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	A	0	1
1	B	0	2
2	C	0	2
3	D	0	6
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	GLY	C-N	7.26	1.50	1.34
6	G	12	DG	C3'-O3'	-5.67	1.36	1.44
6	G	13	DA	C3'-O3'	-5.53	1.36	1.44
6	G	14	DG	C3'-O3'	-5.10	1.37	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	5	DA	O4'-C1'-N9	6.27	112.39	108.00
6	G	16	DG	OP1-P-OP2	6.14	128.81	119.60
6	G	16	DG	O4'-C4'-C3'	-6.01	102.10	104.50
2	C	107	LEU	CA-CB-CG	5.90	128.87	115.30
6	G	13	DA	O4'-C4'-C3'	-5.80	102.18	104.50

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	SER	Peptide
1	B	46	SER	Peptide
1	B	58	ILE	Peptide
2	C	268	ASP	Peptide
2	C	766	GLU	Peptide
3	D	273	ARG	Peptide
3	D	275	GLU	Peptide
3	D	64	LYS	Peptide
3	D	704	ARG	Peptide
3	D	711	LEU	Peptide
3	D	782	SER	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	173	0
1	B	1767	0	1816	186	0
2	C	8770	0	8874	732	1
3	D	11721	0	11941	967	2
4	E	761	0	778	59	0
5	F	2807	0	2882	263	1
6	G	351	0	192	19	0
7	H	516	0	283	28	0
8	I	62	0	34	3	0
9	D	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	2	0	0	0	0
11	I	28	12	11	2	0
All	All	28569	12	28645	2219	2

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 39.

All (2219) 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)
7:H:15:DT:H2''	7:H:16:DC:H5'	1.22	1.16
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.21	1.13
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.24	1.11
3:D:203:ALA:HB1	3:D:393:ILE:HD11	1.31	1.10
2:C:1012:PRO:HB2	2:C:1021:LEU:HD13	1.32	1.08
2:C:200:LEU:HD22	2:C:300:ASP:HB2	1.24	1.06
3:D:65:ARG:HB3	5:F:377:ASP:HA	1.37	1.05
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.30	1.05
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.37	1.04
3:D:1060:SER:HB3	3:D:1063:GLU:HG3	1.39	1.04
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.36	1.04
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.38	1.03
5:F:361:LEU:HD11	5:F:411:HIS:HB2	1.39	1.03
3:D:170:PRO:HA	3:D:392:SER:HB2	1.40	1.01
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.43	1.01
3:D:1234:THR:HB	3:D:1235:GLN:HB2	1.41	1.00
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.44	0.99
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.44	0.99
3:D:216:VAL:HA	3:D:340:THR:HG22	1.41	0.99
1:A:88:ARG:HB3	1:A:123:MET:HE3	1.41	0.98
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.46	0.98
1:B:107:LYS:NZ	1:B:113:ASP:OD2	1.97	0.97
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.26	0.97
3:D:582:LEU:O	3:D:604:THR:HG23	1.65	0.97
3:D:1047:LYS:HG2	3:D:1048:PRO:HD2	1.46	0.97
1:B:128:HIS:HE1	1:B:131:THR:HG22	1.28	0.96
5:F:338:LEU:HD23	5:F:339:PRO:CD	1.94	0.96
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.44	0.96
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.47	0.95
5:F:362:SER:HB3	5:F:365:GLU:HG2	1.44	0.95
3:D:646:LYS:HB3	3:D:720:LEU:HD23	1.47	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.47	0.95
3:D:116:LEU:HB2	3:D:118:LEU:HD12	1.48	0.95
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.02	0.94
2:C:888:THR:HG22	2:C:990:GLY:HA3	1.49	0.94
3:D:1236:LEU:HD22	3:D:1359:GLN:HG3	1.48	0.94
5:F:358:LEU:HB3	5:F:366:ALA:HB1	1.49	0.94
2:C:853:LEU:HB2	2:C:858:MET:CE	1.96	0.94
2:C:755:LEU:HD11	2:C:792:VAL:HG12	1.47	0.94
1:A:222:LEU:HD23	1:B:215:VAL:HG13	1.50	0.94
3:D:1042:ARG:HB3	3:D:1057:VAL:HG13	1.50	0.93
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.50	0.93
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.51	0.93
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.51	0.93
2:C:3:ILE:HD12	2:C:900:ARG:HB2	1.48	0.92
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.49	0.92
1:A:198:ARG:O	1:A:199:ILE:HG12	1.69	0.92
3:D:1234:THR:CB	3:D:1235:GLN:HB2	2.00	0.91
3:D:236:TYR:H	3:D:319:ALA:HB3	1.36	0.91
3:D:558:LEU:HD23	3:D:567:ILE:CD1	2.01	0.90
3:D:986:ARG:HH11	3:D:986:ARG:HB2	1.36	0.90
5:F:109:GLY:O	5:F:113:ILE:HG13	1.68	0.90
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.54	0.90
5:F:319:THR:HG22	5:F:320:PRO:HD2	1.52	0.90
3:D:798:GLU:HG3	3:D:824:ASN:HB2	1.53	0.90
3:D:97:THR:HG21	3:D:571:LYS:CD	2.02	0.90
3:D:650:LEU:HD12	3:D:657:LEU:HD23	1.53	0.90
1:A:159:LYS:HB3	1:A:164:ALA:HB3	1.54	0.89
3:D:413:ASP:O	3:D:435:VAL:HG12	1.72	0.89
2:C:211:LEU:HD23	2:C:218:VAL:HG22	1.55	0.89
2:C:880:MET:HE3	3:D:1037:GLN:HB2	1.55	0.89
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.54	0.88
2:C:234:ALA:HA	2:C:237:ARG:HB2	1.55	0.88
3:D:203:ALA:HB1	3:D:393:ILE:CD1	2.03	0.88
3:D:254:GLU:O	3:D:255:GLU:HG2	1.73	0.88
3:D:284:LEU:HD23	3:D:290:PRO:HG3	1.53	0.88
2:C:102:HIS:HB2	2:C:107:LEU:HB3	1.54	0.88
2:C:666:LEU:HD11	2:C:668:LEU:HD21	1.53	0.88
3:D:411:THR:HG22	5:F:178:ARG:HB3	1.53	0.88
1:A:99:LEU:O	1:A:100:LEU:HD23	1.72	0.88
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.54	0.88
2:C:1012:PRO:HB2	2:C:1021:LEU:CD1	2.02	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:807:ALA:O	3:D:830:ALA:HB2	1.74	0.87
3:D:374:GLU:O	3:D:375:GLU:HG2	1.75	0.87
3:D:401:TYR:OH	3:D:430:ASP:HB2	1.74	0.87
4:E:83:ASP:HA	4:E:86:GLN:HG2	1.57	0.87
7:H:20:DG:H2''	7:H:21:DA:H5'	1.57	0.87
3:D:65:ARG:HD3	5:F:377:ASP:H	1.39	0.87
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.08	0.86
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.09	0.86
1:B:86:VAL:HG12	1:B:124:ASN:OD1	1.76	0.86
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.09	0.86
3:D:1263:PHE:O	3:D:1375:MET:HE2	1.76	0.86
5:F:289:GLU:HG3	5:F:301:ALA:HB2	1.58	0.86
3:D:407:VAL:HG13	3:D:422:ALA:HB2	1.57	0.85
5:F:95:THR:HG22	5:F:98:GLU:CG	2.06	0.85
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.55	0.85
2:C:948:GLU:HG3	2:C:953:VAL:HG23	1.55	0.85
2:C:905:ILE:HG23	2:C:906:PHE:HD1	1.41	0.85
3:D:885:ILE:HD13	3:D:937:TYR:CD1	2.12	0.85
3:D:204:LEU:O	3:D:393:ILE:HG13	1.76	0.84
1:A:206:THR:CG2	1:A:209:GLU:HG3	2.06	0.84
2:C:760:SER:HB2	2:C:788:THR:HG21	1.58	0.84
3:D:65:ARG:CB	5:F:377:ASP:HA	2.06	0.84
3:D:434:ARG:O	3:D:447:VAL:HG23	1.78	0.84
3:D:767:HIS:HA	3:D:924:MET:HE3	1.59	0.84
2:C:195:LEU:HD11	2:C:237:ARG:HB3	1.59	0.84
2:C:474:VAL:HG11	2:C:529:VAL:HG12	1.58	0.84
3:D:1172:HIS:HA	3:D:1175:ILE:HD12	1.60	0.84
5:F:163:LEU:HB3	5:F:174:LEU:HD13	1.60	0.83
5:F:153:PRO:HA	5:F:156:VAL:HG12	1.59	0.83
1:B:124:ASN:ND2	1:B:127:LEU:HD12	1.93	0.83
2:C:1021:LEU:H	2:C:1021:LEU:HD12	1.41	0.83
3:D:93:ILE:HD11	3:D:548:ILE:HD11	1.59	0.83
3:D:1376:MET:HE1	3:D:1421:LEU:HD13	1.61	0.83
2:C:317:VAL:HB	2:C:320:HIS:CD2	2.14	0.83
3:D:520:LEU:O	3:D:525:ARG:NH1	2.10	0.83
3:D:185:VAL:HG13	3:D:189:GLN:OE1	1.78	0.83
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.08	0.83
3:D:956:ILE:HD13	3:D:1039:CYS:O	1.79	0.83
3:D:473:LEU:HD21	3:D:495:ARG:NH2	1.94	0.82
3:D:1232:PRO:O	3:D:1235:GLN:HB3	1.78	0.82
3:D:1422:MET:HE3	3:D:1426:LYS:HG2	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:VAL:HG23	2:C:221:LEU:HA	1.61	0.82
2:C:815:LEU:HD12	2:C:819:VAL:HG23	1.60	0.82
3:D:209:ARG:HH21	3:D:391:ALA:HA	1.44	0.82
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	1.62	0.82
5:F:95:THR:H	5:F:98:GLU:HG3	1.45	0.82
1:B:36:LEU:O	1:B:38:ASN:N	2.13	0.82
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.10	0.82
3:D:275:GLU:O	3:D:277:GLU:N	2.12	0.82
5:F:267:THR:O	5:F:270:LYS:HB2	1.80	0.82
1:A:30:ARG:HB2	1:A:191:ASP:O	1.80	0.82
2:C:585:GLU:O	2:C:588:VAL:HG12	1.79	0.82
5:F:392:VAL:HG21	5:F:396:ARG:HG2	1.62	0.81
3:D:367:ILE:HB	3:D:377:VAL:HG23	1.62	0.81
3:D:683:ILE:CG2	3:D:687:VAL:HG11	2.10	0.81
3:D:180:LYS:O	3:D:183:GLU:HB2	1.80	0.81
3:D:1234:THR:CA	3:D:1235:GLN:HB2	2.10	0.81
1:A:39:PRO:O	1:A:43:ILE:HG13	1.81	0.81
5:F:383:LEU:HD12	5:F:384:GLU:HG3	1.61	0.81
1:B:108:GLU:HG2	1:B:131:THR:HB	1.60	0.81
2:C:206:THR:HA	2:C:209:ARG:HB3	1.60	0.81
3:D:1479:ASP:OD1	3:D:1482:ARG:NH1	2.13	0.81
3:D:217:LYS:NZ	3:D:341:GLU:HG3	1.95	0.81
2:C:597:ALA:HB2	2:C:655:LEU:HD11	1.64	0.80
3:D:1485:GLN:NE2	4:E:82:GLU:OE1	2.13	0.80
7:H:21:DA:H1'	7:H:22:DT:H5'	1.63	0.80
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.16	0.80
2:C:808:ARG:HD3	2:C:814:GLU:HG3	1.64	0.80
3:D:843:PHE:HE2	3:D:864:VAL:HG11	1.46	0.80
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.12	0.80
2:C:194:VAL:HA	2:C:197:LEU:HD13	1.62	0.80
5:F:260:ILE:HG13	5:F:265:VAL:CG2	2.12	0.80
5:F:96:LEU:O	5:F:100:VAL:HG23	1.80	0.80
1:A:206:THR:HB	1:A:209:GLU:OE1	1.81	0.80
3:D:658:LEU:HD23	3:D:661:MET:HE3	1.62	0.79
3:D:986:ARG:HB2	3:D:986:ARG:NH1	1.96	0.79
5:F:104:ARG:O	5:F:108:GLU:HG3	1.83	0.79
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.14	0.79
2:C:180:GLY:O	2:C:217:LEU:HD22	1.81	0.79
5:F:171:LYS:HD3	5:F:175:HIS:HE1	1.47	0.79
7:H:15:DT:C2'	7:H:16:DC:H5'	2.11	0.79
3:D:103:TRP:HE1	3:D:604:THR:HG21	1.44	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:217:LYS:HZ2	3:D:341:GLU:HG3	1.45	0.79
2:C:755:LEU:HD11	2:C:792:VAL:CG1	2.12	0.79
2:C:136:ILE:HG21	2:C:336:VAL:HG23	1.65	0.79
5:F:112:ALA:O	5:F:116:LEU:HB2	1.83	0.79
2:C:540:PHE:HB3	2:C:544:THR:CG2	2.12	0.79
1:A:155:LYS:O	1:A:155:LYS:NZ	2.13	0.79
3:D:1236:LEU:CD2	3:D:1359:GLN:HG3	2.13	0.79
6:G:6:DA:H2''	6:G:7:DT:O5'	1.83	0.79
5:F:129:GLU:HG2	5:F:144:ILE:HG13	1.65	0.78
5:F:166:LEU:HB2	5:F:171:LYS:HB2	1.65	0.78
2:C:560:MET:O	2:C:564:MET:HG3	1.83	0.78
4:E:50:THR:HG22	4:E:53:GLY:O	1.84	0.78
2:C:674:VAL:HG23	2:C:869:VAL:HB	1.64	0.78
3:D:709:HIS:O	3:D:711:LEU:N	2.16	0.78
2:C:938:LYS:O	2:C:941:VAL:HG22	1.84	0.78
2:C:367:LEU:HD12	2:C:371:LYS:NZ	1.98	0.78
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.65	0.78
5:F:120:THR:HG21	5:F:122:LEU:HD22	1.65	0.78
2:C:337:GLY:O	2:C:341:THR:HG23	1.84	0.77
2:C:428:ARG:NH2	2:C:447:ALA:O	2.16	0.77
3:D:1213:ARG:HG3	3:D:1214:PRO:HD2	1.65	0.77
3:D:697:GLY:O	3:D:760:ARG:NH1	2.17	0.77
1:A:222:LEU:HD21	1:B:218:LEU:CD2	2.13	0.77
1:B:36:LEU:O	1:B:39:PRO:HD2	1.84	0.77
2:C:317:VAL:HG13	2:C:318:PRO:HD2	1.66	0.77
5:F:299:TRP:CZ3	5:F:303:ARG:HG2	2.19	0.77
1:A:206:THR:HG22	1:A:209:GLU:H	1.47	0.77
1:B:71:VAL:HG22	1:B:132:LEU:CD1	2.14	0.77
2:C:25:SER:OG	2:C:335:THR:OG1	2.00	0.77
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.66	0.77
3:D:122:GLU:HG2	3:D:152:LEU:HD11	1.65	0.77
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.17	0.77
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.15	0.77
3:D:650:LEU:HD12	3:D:657:LEU:CD2	2.14	0.77
2:C:65:VAL:HG22	2:C:101:ILE:HG23	1.65	0.77
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.66	0.77
2:C:425:PHE:HE2	3:D:1086:LEU:HD12	1.50	0.77
2:C:751:PRO:HA	2:C:792:VAL:CG2	2.14	0.77
3:D:110:SER:O	3:D:114:THR:HG23	1.84	0.77
5:F:260:ILE:HG13	5:F:265:VAL:HG22	1.67	0.77
5:F:364:ARG:HA	5:F:367:MET:HG2	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:OE1	1:B:73:GLU:N	2.18	0.76
2:C:833:LEU:HD12	2:C:834:GLN:H	1.51	0.76
3:D:767:HIS:HA	3:D:924:MET:CE	2.15	0.76
3:D:684:LYS:O	3:D:687:VAL:HG12	1.84	0.76
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.68	0.76
1:B:128:HIS:CE1	1:B:131:THR:HG22	2.16	0.76
2:C:193:LEU:HG	2:C:197:LEU:HD11	1.68	0.76
3:D:245:LEU:HD13	3:D:307:ALA:HB1	1.68	0.76
2:C:535:SER:OG	2:C:537:LYS:HG3	1.84	0.76
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.26	0.76
6:G:3:DT:H2"	6:G:4:DG:C8	2.21	0.76
2:C:808:ARG:NH2	2:C:808:ARG:HB3	2.00	0.76
3:D:572:ARG:NH1	5:F:83:GLN:HG2	2.01	0.76
2:C:751:PRO:HA	2:C:792:VAL:HG23	1.67	0.75
3:D:171:LEU:HD12	3:D:171:LEU:O	1.86	0.75
3:D:26:VAL:HG12	3:D:548:ILE:HD13	1.67	0.75
3:D:1042:ARG:HB3	3:D:1057:VAL:CG1	2.17	0.75
2:C:140:ILE:HD13	2:C:331:ARG:HH11	1.51	0.75
3:D:828:LYS:HE2	3:D:831:GLY:H	1.52	0.75
2:C:715:THR:HG22	2:C:717:LEU:H	1.50	0.75
2:C:805:ARG:HG3	2:C:823:VAL:HG23	1.69	0.75
3:D:496:LEU:HD23	3:D:1390:LEU:HD13	1.68	0.75
2:C:51:THR:HG21	2:C:348:LEU:HB3	1.67	0.75
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.02	0.75
1:B:86:VAL:CG1	1:B:123:MET:HB2	2.17	0.75
2:C:196:LEU:HD13	2:C:200:LEU:HD11	1.68	0.75
2:C:751:PRO:HD3	2:C:796:GLU:O	1.87	0.75
2:C:460:ARG:HD2	2:C:485:TYR:CE1	2.22	0.74
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.68	0.74
3:D:7:LYS:HD3	3:D:1456:LYS:NZ	2.01	0.74
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.70	0.74
2:C:498:GLN:HE21	3:D:1068:LEU:HD12	1.53	0.74
3:D:95:LEU:HD22	3:D:574:LEU:HD21	1.69	0.74
3:D:411:THR:HG22	5:F:178:ARG:CB	2.17	0.74
2:C:766:GLU:HG2	2:C:767:PRO:HD2	1.70	0.74
2:C:811:PRO:O	2:C:813:VAL:HG12	1.88	0.74
2:C:815:LEU:HB2	2:C:819:VAL:CG2	2.17	0.74
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.53	0.74
5:F:95:THR:HG22	5:F:98:GLU:HG2	1.69	0.74
1:A:201:THR:HG22	1:A:203:GLY:H	1.53	0.74
3:D:645:PRO:HG2	3:D:724:GLN:O	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:265:VAL:O	5:F:269:ASN:ND2	2.20	0.74
3:D:680:GLN:HA	3:D:683:ILE:CD1	2.18	0.73
2:C:710:ILE:HG22	2:C:823:VAL:HG12	1.70	0.73
2:C:861:LEU:H	2:C:861:LEU:HD12	1.53	0.73
3:D:236:TYR:N	3:D:319:ALA:HB3	2.02	0.73
3:D:566:ILE:HD11	5:F:192:LEU:CD2	2.17	0.73
2:C:84:ARG:HD3	2:C:629:TYR:OH	1.89	0.73
3:D:646:LYS:CB	3:D:720:LEU:HD23	2.17	0.73
5:F:123:ASP:OD1	5:F:126:LEU:N	2.19	0.73
1:A:222:LEU:CD1	1:B:218:LEU:HD23	2.18	0.73
3:D:982:PHE:O	3:D:983:LEU:HG	1.88	0.73
3:D:1271:LYS:HD2	3:D:1331:ASP:HB2	1.69	0.73
2:C:626:ARG:HD3	2:C:629:TYR:HD2	1.54	0.73
3:D:474:GLU:OE2	3:D:1388:ARG:NH2	2.21	0.73
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.24	0.73
3:D:1312:LEU:HD21	3:D:1327:ARG:HE	1.52	0.73
3:D:1444:THR:O	3:D:1448:THR:HG23	1.87	0.73
5:F:367:MET:CE	5:F:368:VAL:HG13	2.18	0.73
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.22	0.73
2:C:551:GLU:N	2:C:551:GLU:OE2	2.19	0.73
2:C:888:THR:HG22	2:C:990:GLY:CA	2.19	0.73
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.71	0.73
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.70	0.73
5:F:393:THR:HG22	5:F:394:ARG:H	1.53	0.73
2:C:312:ALA:HB1	2:C:317:VAL:HG21	1.69	0.72
3:D:939:PHE:O	3:D:942:SER:OG	2.06	0.72
3:D:1389:LEU:C	3:D:1390:LEU:HD23	2.09	0.72
2:C:498:GLN:NE2	3:D:1068:LEU:HD12	2.04	0.72
2:C:603:VAL:HG23	2:C:647:GLN:O	1.90	0.72
3:D:421:LEU:HD13	3:D:428:LYS:HA	1.71	0.72
3:D:1234:THR:H	3:D:1235:GLN:CB	2.02	0.72
1:A:196:THR:HG21	2:C:934:PHE:CE1	2.25	0.72
2:C:260:LEU:C	2:C:261:ILE:HD12	2.10	0.72
1:A:94:LEU:O	1:A:146:ARG:NH1	2.22	0.72
2:C:564:MET:HE3	2:C:846:LYS:HG2	1.70	0.72
3:D:704:ARG:HB2	3:D:745:MET:CE	2.18	0.72
2:C:28:ARG:O	2:C:28:ARG:HG2	1.90	0.72
2:C:748:GLU:HG3	2:C:799:ILE:HD11	1.72	0.72
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.18	0.72
3:D:1127:GLU:HB3	3:D:1130:ARG:HH12	1.55	0.72
5:F:392:VAL:CG2	5:F:396:ARG:HG2	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:211:LEU:HB3	2:C:218:VAL:HG22	1.72	0.72
2:C:988:VAL:HG23	3:D:948:THR:CG2	2.20	0.72
2:C:673:LEU:HD23	2:C:867:VAL:HA	1.71	0.72
7:H:16:DC:H2"	7:H:17:DA:C8	2.24	0.71
1:B:53:VAL:HG12	1:B:167:VAL:HG11	1.72	0.71
2:C:211:LEU:HB3	2:C:218:VAL:CG2	2.20	0.71
3:D:209:ARG:NH2	3:D:391:ALA:HA	2.05	0.71
2:C:727:PRO:HB2	2:C:728:HIS:CD2	2.26	0.71
5:F:386:VAL:HA	5:F:390:PHE:CE1	2.24	0.71
5:F:408:LEU:HA	5:F:411:HIS:HB3	1.72	0.71
2:C:946:ARG:HH21	2:C:946:ARG:HG3	1.54	0.71
3:D:1283:ILE:HG13	3:D:1315:ASP:OD2	1.87	0.71
3:D:1234:THR:N	3:D:1235:GLN:HB2	2.05	0.71
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.55	0.71
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.72	0.71
1:B:26:GLU:OE2	1:B:194:LYS:HE3	1.90	0.71
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.73	0.71
5:F:126:LEU:HD12	5:F:126:LEU:O	1.90	0.71
1:A:18:ARG:HH11	1:A:18:ARG:HG3	1.54	0.71
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.73	0.71
3:D:1295:GLU:OE1	3:D:1300:SER:HB3	1.89	0.71
3:D:348:GLN:H	3:D:351:MET:HG3	1.55	0.71
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.72	0.70
2:C:367:LEU:HD12	2:C:371:LYS:HZ2	1.54	0.70
3:D:809:PRO:O	3:D:813:LEU:HD12	1.92	0.70
5:F:193:ARG:HB3	7:H:7:DG:H5"	1.72	0.70
2:C:681:GLY:HA2	3:D:939:PHE:CE1	2.25	0.70
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.71	0.70
5:F:369:LEU:CD2	5:F:372:ARG:HB2	2.21	0.70
1:B:58:ILE:HB	1:B:61:VAL:HG21	1.73	0.70
3:D:348:GLN:H	3:D:351:MET:HE2	1.55	0.70
1:B:38:ASN:OD1	2:C:979:THR:HG22	1.92	0.70
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.73	0.70
1:A:73:GLU:OE2	1:A:130:ALA:HA	1.92	0.70
2:C:317:VAL:CG1	2:C:318:PRO:HD2	2.21	0.70
3:D:413:ASP:HB2	3:D:435:VAL:HG11	1.73	0.70
1:A:101:LEU:HD23	1:A:102:LYS:N	2.06	0.70
1:A:206:THR:HG23	1:A:208:LEU:H	1.56	0.70
5:F:338:LEU:CD2	5:F:339:PRO:HD2	2.12	0.70
5:F:362:SER:HB3	5:F:365:GLU:CG	2.19	0.70
3:D:1060:SER:CB	3:D:1063:GLU:HG3	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:520:GLU:HG3	2:C:521:PRO:HD2	1.72	0.69
6:G:6:DA:H5"	6:G:6:DA:C8	2.27	0.69
2:C:197:LEU:HB3	2:C:202:TYR:HD2	1.57	0.69
3:D:175:VAL:CG1	3:D:193:PRO:HG2	2.22	0.69
3:D:581:LEU:HD23	3:D:582:LEU:CD2	2.22	0.69
5:F:153:PRO:HA	5:F:156:VAL:CG1	2.21	0.69
2:C:102:HIS:HB2	2:C:107:LEU:CB	2.22	0.69
5:F:163:LEU:HB3	5:F:174:LEU:CD1	2.22	0.69
2:C:569:VAL:HG21	2:C:1000:MET:CE	2.23	0.69
2:C:680:ASP:OD2	3:D:943:THR:HG21	1.92	0.69
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.07	0.69
5:F:287:THR:OG1	5:F:290:GLU:HG3	1.92	0.69
2:C:689:VAL:HG11	2:C:870:ILE:HD12	1.74	0.69
3:D:689:ASP:HB3	4:E:51:LEU:HD13	1.72	0.69
3:D:970:LYS:HA	3:D:973:GLN:HB3	1.75	0.69
1:A:88:ARG:CB	1:A:123:MET:HE3	2.20	0.69
2:C:237:ARG:O	2:C:240:THR:OG1	2.11	0.69
2:C:808:ARG:HG3	2:C:814:GLU:HA	1.74	0.69
3:D:65:ARG:HD3	5:F:377:ASP:N	2.07	0.69
3:D:298:VAL:HG12	3:D:302:GLN:CD	2.12	0.69
1:A:138:LEU:HD11	1:A:140:MET:HE3	1.75	0.69
1:B:106:PRO:HD3	1:B:134:GLU:HG2	1.75	0.69
1:B:185:ARG:NH1	1:B:187:GLY:O	2.26	0.69
2:C:587:VAL:HG11	2:C:666:LEU:HD22	1.74	0.69
2:C:971:LYS:HA	2:C:987:ILE:O	1.92	0.69
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.28	0.69
3:D:201:GLY:HA3	3:D:396:VAL:O	1.92	0.69
2:C:262:ALA:O	2:C:264:PRO:HD3	1.93	0.69
2:C:906:PHE:CE2	3:D:1067:VAL:HA	2.28	0.69
3:D:835:SER:HB3	3:D:838:ARG:HE	1.58	0.69
1:A:117:VAL:O	1:A:120:VAL:HG22	1.93	0.69
2:C:54:ILE:HG21	2:C:355:VAL:HG23	1.75	0.69
2:C:513:VAL:HG21	2:C:529:VAL:HG21	1.74	0.69
3:D:134:VAL:CG1	3:D:153:LEU:HD11	2.23	0.69
1:B:37:GLY:HA2	1:B:40:LEU:HG	1.75	0.68
3:D:486:ARG:HG3	3:D:489:ARG:NH2	2.08	0.68
1:A:184:THR:HG22	1:A:192:LEU:HB2	1.74	0.68
2:C:683:ASN:CB	2:C:872:ASN:HB2	2.21	0.68
5:F:316:SER:O	5:F:319:THR:OG1	2.11	0.68
1:A:115:LEU:O	1:A:115:LEU:HD23	1.93	0.68
1:A:201:THR:HG21	1:A:205:VAL:O	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HG13	1:B:163:ASN:HD22	1.58	0.68
2:C:540:PHE:HB3	2:C:544:THR:HG21	1.74	0.68
3:D:1394:VAL:HG22	3:D:1420:LEU:CD2	2.24	0.68
1:A:62:LEU:HA	1:A:163:ASN:HB3	1.74	0.68
2:C:926:PHE:O	2:C:929:ARG:HB3	1.93	0.68
5:F:234:LYS:HD3	7:H:5:DA:OP2	1.94	0.68
5:F:354:LEU:HD12	5:F:355:GLU:N	2.09	0.68
2:C:376:ARG:HD3	5:F:276:ARG:HD2	1.76	0.68
2:C:690:ILE:HG13	2:C:852:ILE:HG23	1.75	0.68
4:E:39:VAL:HG21	4:E:72:ARG:HB3	1.74	0.68
6:G:6:DA:H2'	6:G:7:DT:C7	2.24	0.68
1:B:143:ARG:HD3	1:B:158:ILE:HD11	1.76	0.68
2:C:260:LEU:CB	2:C:261:ILE:HD12	2.23	0.68
3:D:93:ILE:HD13	3:D:548:ILE:HG12	1.75	0.68
1:B:38:ASN:HB3	1:B:39:PRO:CD	2.23	0.68
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.29	0.68
3:D:1422:MET:HE3	3:D:1426:LYS:CG	2.22	0.68
1:A:9:PRO:HB3	1:A:27:PRO:O	1.94	0.67
1:A:67:THR:HG21	2:C:609:ASN:OD1	1.94	0.67
1:A:180:GLN:HG3	2:C:934:PHE:CD1	2.28	0.67
1:B:197:LEU:HD12	1:B:198:ARG:N	2.07	0.67
3:D:185:VAL:HG13	3:D:189:GLN:CD	2.13	0.67
5:F:390:PHE:CD2	5:F:397:ILE:HG12	2.30	0.67
2:C:424:GLY:O	2:C:428:ARG:HD2	1.94	0.67
3:D:1273:VAL:H	3:D:1326:THR:CG2	2.06	0.67
1:A:222:LEU:HD11	1:B:218:LEU:CD2	2.24	0.67
2:C:49:ARG:O	2:C:49:ARG:HD3	1.94	0.67
3:D:1057:VAL:HG21	3:D:1065:LEU:HD21	1.75	0.67
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.24	0.67
2:C:878:SER:HA	3:D:1034:GLN:NE2	2.10	0.67
3:D:65:ARG:CD	5:F:377:ASP:HA	2.24	0.67
3:D:348:GLN:N	3:D:351:MET:HE2	2.08	0.67
5:F:206:GLY:O	5:F:207:LEU:HD23	1.95	0.67
3:D:977:ALA:O	3:D:982:PHE:HB3	1.94	0.67
3:D:1047:LYS:HG3	3:D:1053:PHE:CZ	2.30	0.67
1:B:87:VAL:HG12	1:B:122:ILE:HD13	1.77	0.67
3:D:236:TYR:HB3	3:D:313:MET:HG3	1.76	0.67
3:D:335:LEU:H	3:D:335:LEU:HD12	1.58	0.67
3:D:140:ALA:HA	3:D:450:TYR:CD1	2.30	0.67
3:D:701:LEU:HD13	3:D:763:MET:HE1	1.76	0.67
6:G:6:DA:H5''	6:G:6:DA:H8	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASP:O	1:B:78:ILE:HG13	1.95	0.67
2:C:689:VAL:CG1	2:C:870:ILE:HD12	2.25	0.67
3:D:998:GLU:O	3:D:1002:LYS:HG3	1.95	0.67
6:G:11:DT:H2"	6:G:12:DG:H5"	1.77	0.67
1:B:66:SER:O	1:B:75:VAL:HG23	1.94	0.66
3:D:645:PRO:CG	3:D:724:GLN:O	2.42	0.66
2:C:149:THR:HA	2:C:322:VAL:HG13	1.78	0.66
2:C:716:LYS:HE2	3:D:37:LEU:HD11	1.77	0.66
2:C:197:LEU:HA	2:C:200:LEU:CD1	2.25	0.66
2:C:431:HIS:ND1	2:C:433:THR:OG1	2.29	0.66
3:D:972:LEU:HA	3:D:975:GLU:HB3	1.77	0.66
3:D:1045:MET:HA	3:D:1045:MET:CE	2.24	0.66
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.77	0.66
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.77	0.66
1:B:106:PRO:CD	1:B:134:GLU:HG2	2.26	0.66
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.77	0.66
1:A:10:VAL:HG12	1:A:26:GLU:O	1.96	0.66
2:C:425:PHE:HE2	3:D:1086:LEU:CD1	2.09	0.66
2:C:892:LEU:HD13	2:C:989:VAL:O	1.96	0.66
3:D:7:LYS:HD3	3:D:1456:LYS:HZ3	1.59	0.66
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	1.95	0.66
1:A:164:ALA:O	1:A:166:PRO:HD3	1.96	0.66
1:B:80:LEU:HB3	3:D:844:ALA:HB2	1.76	0.66
2:C:1070:ILE:HG21	3:D:655:PRO:CB	2.25	0.66
3:D:558:LEU:CD2	3:D:567:ILE:HD12	2.25	0.66
3:D:885:ILE:HG23	3:D:937:TYR:CD1	2.31	0.66
5:F:369:LEU:HD22	5:F:372:ARG:HB2	1.76	0.66
2:C:880:MET:CE	3:D:1037:GLN:HB2	2.27	0.65
2:C:719:PRO:HD2	2:C:761:PHE:CE1	2.31	0.65
1:A:198:ARG:C	1:A:199:ILE:HG12	2.15	0.65
3:D:1433:SER:OG	3:D:1464:GLU:HG2	1.96	0.65
5:F:321:ILE:HG21	5:F:332:PHE:HE1	1.61	0.65
6:G:3:DT:H2"	6:G:4:DG:H8	1.62	0.65
1:B:24:VAL:HG13	1:B:196:THR:OG1	1.96	0.65
1:B:220:GLU:O	1:B:223:THR:OG1	2.14	0.65
2:C:578:VAL:HA	2:C:900:ARG:HD2	1.78	0.65
3:D:676:MET:HE3	3:D:684:LYS:H	1.62	0.65
2:C:756:VAL:HG21	2:C:823:VAL:HG11	1.78	0.65
2:C:875:GLY:O	2:C:879:ARG:HD3	1.97	0.65
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.78	0.65
3:D:367:ILE:HB	3:D:377:VAL:CG2	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:879:ARG:HB3	3:D:902:LEU:HD11	1.78	0.65
3:D:904:VAL:HG22	3:D:905:PRO:CD	2.27	0.65
5:F:412:GLU:CG	5:F:418:LEU:HD13	2.27	0.65
1:A:107:LYS:NZ	1:A:113:ASP:OD2	2.28	0.65
1:B:211:LEU:O	1:B:215:VAL:HG23	1.96	0.65
3:D:46:ASP:OD1	3:D:48:ARG:HG2	1.97	0.65
1:A:86:VAL:HG21	1:A:202:ASP:HB2	1.78	0.65
2:C:446:GLY:O	2:C:449:ILE:HG22	1.96	0.65
3:D:203:ALA:CB	3:D:393:ILE:HD11	2.19	0.65
3:D:618:LEU:HD12	3:D:1467:ILE:HG23	1.77	0.65
3:D:1065:LEU:HD23	3:D:1069:GLU:CB	2.26	0.65
2:C:203:ASP:HB3	2:C:206:THR:HG22	1.79	0.65
2:C:250:ARG:HD2	2:C:250:ARG:O	1.95	0.65
2:C:1072:LYS:HD2	2:C:1074:GLU:OE2	1.97	0.65
3:D:266:GLU:OE2	3:D:315:ARG:NE	2.30	0.65
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.11	0.65
2:C:905:ILE:CG2	2:C:906:PHE:HD1	2.10	0.65
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.32	0.65
1:B:226:SER:O	1:B:228:PRO:HD3	1.97	0.64
2:C:768:THR:HG23	2:C:771:GLU:OE1	1.97	0.64
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.78	0.64
2:C:880:MET:HE3	3:D:1037:GLN:CB	2.27	0.64
2:C:405:ARG:HD2	2:C:442:GLU:OE2	1.97	0.64
2:C:513:VAL:HG22	2:C:524:VAL:O	1.97	0.64
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.79	0.64
3:D:112:ILE:HG23	3:D:465:LEU:HD11	1.78	0.64
3:D:776:GLU:OE2	3:D:1362:LYS:HD3	1.98	0.64
4:E:26:ARG:HE	4:E:30:LEU:HD11	1.63	0.64
4:E:61:VAL:O	4:E:65:MET:HG3	1.98	0.64
7:H:21:DA:H1'	7:H:22:DT:C5'	2.27	0.64
3:D:431:VAL:HG21	3:D:448:GLU:OE1	1.97	0.64
3:D:864:VAL:HG12	3:D:865:THR:N	2.13	0.64
2:C:109:LYS:HD2	2:C:110:GLU:H	1.63	0.64
3:D:65:ARG:HB3	5:F:377:ASP:CA	2.22	0.64
3:D:351:MET:HB3	3:D:369:ALA:O	1.97	0.64
3:D:411:THR:O	5:F:178:ARG:HD2	1.97	0.64
3:D:703:ASN:HA	3:D:712:GLY:O	1.98	0.64
5:F:271:LEU:H	5:F:271:LEU:HD12	1.63	0.64
2:C:1062:GLY:HA2	2:C:1065:ALA:HB3	1.77	0.64
3:D:170:PRO:HA	3:D:392:SER:CB	2.22	0.64
3:D:1489:GLN:NE2	3:D:1492:LEU:HD12	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:398:ARG:NH2	5:F:399:GLN:HG3	2.13	0.64
1:A:32:PHE:HA	1:A:35:THR:HB	1.78	0.64
1:B:40:LEU:O	1:B:44:LEU:HD12	1.97	0.64
2:C:112:GLU:HG3	2:C:112:GLU:O	1.96	0.64
2:C:436:GLY:HA2	2:C:538:GLN:O	1.98	0.64
3:D:1293:PHE:CE1	3:D:1302:GLU:HB2	2.32	0.64
2:C:958:THR:HG23	2:C:961:GLU:CD	2.18	0.64
2:C:988:VAL:HG23	3:D:948:THR:HG21	1.80	0.64
2:C:1066:ALA:O	2:C:1069:ALA:N	2.31	0.64
3:D:1499:ARG:NH1	4:E:84:ARG:HG2	2.13	0.64
1:A:79:ILE:HD12	1:A:167:VAL:HG22	1.78	0.64
3:D:209:ARG:O	3:D:346:ARG:HD3	1.96	0.64
3:D:975:GLU:O	3:D:979:GLU:HB2	1.98	0.64
3:D:1087:ARG:NH1	3:D:1236:LEU:O	2.31	0.64
2:C:260:LEU:HB3	2:C:261:ILE:CD1	2.26	0.64
2:C:367:LEU:HA	2:C:371:LYS:HZ2	1.61	0.64
3:D:259:VAL:HG13	3:D:270:LEU:HD21	1.78	0.64
3:D:343:LYS:NZ	3:D:380:GLU:OE2	2.31	0.64
4:E:42:PRO:HA	4:E:45:ARG:HG3	1.80	0.64
5:F:368:VAL:HG11	5:F:397:ILE:HD11	1.80	0.64
1:A:97:VAL:HG12	1:A:98:THR:H	1.63	0.63
1:B:96:THR:HG22	1:B:97:VAL:N	2.13	0.63
2:C:890:LEU:HB2	2:C:914:ILE:HD12	1.80	0.63
3:D:187:LYS:HD2	3:D:200:ASP:OD2	1.98	0.63
3:D:311:LEU:O	3:D:311:LEU:HD12	1.99	0.63
3:D:1376:MET:CE	3:D:1421:LEU:HD13	2.28	0.63
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.80	0.63
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.80	0.63
3:D:1191:PRO:HD2	3:D:1369:GLU:OE1	1.98	0.63
3:D:1493:LYS:HA	3:D:1493:LYS:CE	2.29	0.63
5:F:362:SER:CB	5:F:365:GLU:HG2	2.22	0.63
2:C:474:VAL:HG11	2:C:529:VAL:CG1	2.28	0.63
2:C:861:LEU:HD12	2:C:865:THR:O	1.97	0.63
3:D:135:LEU:HD23	3:D:135:LEU:O	1.97	0.63
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.30	0.63
2:C:948:GLU:HG3	2:C:953:VAL:CG2	2.28	0.63
5:F:364:ARG:HA	5:F:367:MET:CG	2.27	0.63
5:F:398:ARG:HH21	5:F:399:GLN:HG3	1.64	0.63
7:H:21:DA:H2"	7:H:22:DT:OP2	1.98	0.63
1:A:222:LEU:CD2	1:B:218:LEU:HD23	2.29	0.63
1:B:64:GLU:O	1:B:75:VAL:HB	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:879:ARG:HB3	3:D:902:LEU:CD1	2.28	0.63
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.33	0.63
5:F:219:GLY:O	5:F:222:ARG:HB2	1.96	0.63
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.80	0.63
2:C:54:ILE:HG21	2:C:355:VAL:CG2	2.29	0.63
3:D:24:GLY:HA3	3:D:49:ILE:HG23	1.79	0.63
3:D:1028:ALA:O	3:D:1029:ARG:HG2	1.97	0.63
4:E:95:VAL:O	4:E:95:VAL:HG12	1.98	0.63
2:C:910:LYS:O	2:C:914:ILE:HG22	1.99	0.63
3:D:50:PHE:O	3:D:89:ARG:HD2	1.97	0.63
3:D:1114:THR:HG23	3:D:1189:ARG:HH21	1.62	0.63
3:D:70:GLY:H	3:D:80:VAL:HG23	1.63	0.63
3:D:134:VAL:HG22	3:D:151:GLN:H	1.63	0.63
3:D:1489:GLN:HE22	3:D:1492:LEU:HD12	1.62	0.63
5:F:372:ARG:HA	5:F:372:ARG:HE	1.64	0.63
2:C:12:VAL:HG21	2:C:472:ARG:NE	2.14	0.63
2:C:474:VAL:CG1	2:C:529:VAL:HG12	2.28	0.63
3:D:544:TYR:O	3:D:547:LEU:N	2.31	0.63
3:D:827:ILE:HG13	3:D:829:VAL:HG23	1.81	0.63
3:D:1234:THR:N	3:D:1235:GLN:CB	2.62	0.63
5:F:93:LEU:HD21	5:F:193:ARG:HD3	1.80	0.63
1:A:216:GLU:OE1	1:A:219:ARG:NH2	2.32	0.62
3:D:371:ILE:HG13	3:D:372:ASP:N	2.13	0.62
3:D:916:TYR:CE1	3:D:920:LEU:HD21	2.34	0.62
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.14	0.62
3:D:1003:VAL:O	3:D:1007:VAL:HG23	1.98	0.62
3:D:123:LEU:O	3:D:127:LEU:HB2	1.99	0.62
3:D:134:VAL:HG13	3:D:153:LEU:HD11	1.80	0.62
3:D:202:VAL:O	3:D:202:VAL:HG22	1.98	0.62
3:D:245:LEU:CD1	3:D:307:ALA:HB1	2.28	0.62
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.25	0.62
3:D:1057:VAL:HG23	3:D:1069:GLU:CD	2.19	0.62
3:D:1273:VAL:H	3:D:1326:THR:HG22	1.64	0.62
5:F:301:ALA:O	5:F:304:VAL:HG13	1.98	0.62
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.34	0.62
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.80	0.62
3:D:586:ARG:HG2	3:D:586:ARG:HH11	1.63	0.62
3:D:1394:VAL:HG22	3:D:1420:LEU:HD21	1.81	0.62
5:F:88:ILE:HG23	5:F:193:ARG:HG2	1.81	0.62
1:A:89:PHE:HB2	1:A:146:ARG:HH22	1.63	0.62
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.81	0.62
2:C:773:LEU:O	2:C:777:ILE:HD12	1.99	0.62
1:A:121:GLU:HB3	1:A:123:MET:HE2	1.81	0.62
2:C:140:ILE:CD1	2:C:331:ARG:HH11	2.11	0.62
3:D:558:LEU:HD23	3:D:567:ILE:HD11	1.81	0.62
3:D:844:ALA:HB1	3:D:867:ARG:NH1	2.14	0.62
5:F:372:ARG:O	5:F:373:LYS:HG2	2.00	0.62
5:F:373:LYS:HD3	5:F:380:GLU:OE1	2.00	0.62
2:C:619:ARG:HH21	2:C:619:ARG:HB2	1.64	0.62
2:C:683:ASN:HB3	2:C:872:ASN:CB	2.25	0.62
2:C:929:ARG:NH2	2:C:940:GLU:OE2	2.26	0.62
3:D:169:TYR:O	3:D:392:SER:HB2	1.98	0.62
3:D:314:PRO:HB2	3:D:317:VAL:CG1	2.30	0.62
3:D:557:LEU:HD13	3:D:566:ILE:CG2	2.30	0.62
3:D:1047:LYS:CG	3:D:1048:PRO:HD2	2.27	0.62
3:D:1198:TYR:CE2	3:D:1460:ILE:HD13	2.35	0.62
3:D:97:THR:CG2	3:D:571:LYS:HD3	2.20	0.62
3:D:206:ARG:HG2	3:D:392:SER:O	2.00	0.62
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.31	0.62
3:D:1442:ASN:O	3:D:1446:VAL:HG23	2.00	0.62
3:D:242:LEU:HD21	3:D:311:LEU:HD13	1.82	0.62
3:D:955:VAL:HG23	3:D:955:VAL:O	1.98	0.62
3:D:1127:GLU:HA	3:D:1130:ARG:HB3	1.81	0.62
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.14	0.62
1:B:117:VAL:HG12	1:B:118:ALA:N	2.15	0.62
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.82	0.62
5:F:300:ASP:O	5:F:304:VAL:HG12	2.00	0.62
2:C:605:LYS:O	2:C:606:VAL:HG23	2.00	0.61
3:D:378:ILE:H	3:D:378:ILE:HD12	1.64	0.61
2:C:230:ARG:H	2:C:233:GLU:HG3	1.65	0.61
2:C:267:TYR:OH	2:C:290:LEU:HD21	2.00	0.61
3:D:97:THR:HG22	3:D:554:LEU:HD21	1.82	0.61
3:D:175:VAL:HG11	3:D:193:PRO:HG2	1.80	0.61
3:D:216:VAL:HA	3:D:340:THR:CG2	2.23	0.61
5:F:260:ILE:CG1	5:F:265:VAL:HG22	2.30	0.61
3:D:291:LEU:HB2	3:D:304:LEU:O	1.99	0.61
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.00	0.61
4:E:80:VAL:HG12	4:E:81:PRO:O	2.00	0.61
1:B:94:LEU:HD21	1:B:96:THR:O	2.01	0.61
2:C:355:VAL:HG12	2:C:372:LEU:O	2.01	0.61
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:666:LEU:HD11	2:C:668:LEU:CD2	2.27	0.61
3:D:23:TYR:CE2	3:D:89:ARG:HD3	2.36	0.61
3:D:672:ALA:HB2	5:F:420:ASP:OD1	2.00	0.61
1:B:31:GLY:N	1:B:193:ASP:OD1	2.30	0.61
2:C:1085:PHE:CE1	3:D:1468:LEU:HD22	2.35	0.61
3:D:574:LEU:O	3:D:578:VAL:HG12	2.00	0.61
1:A:64:GLU:HA	1:A:165:ILE:HD13	1.82	0.61
2:C:281:LEU:HD22	2:C:308:ARG:HH22	1.65	0.61
2:C:743:VAL:HG23	2:C:800:VAL:HG11	1.83	0.61
1:B:94:LEU:HD23	1:B:95:GLN:N	2.15	0.61
2:C:221:LEU:O	2:C:221:LEU:HD22	2.00	0.61
2:C:596:TYR:C	2:C:655:LEU:HD13	2.21	0.61
2:C:879:ARG:N	2:C:879:ARG:HD2	2.16	0.61
3:D:613:ARG:O	3:D:618:LEU:HD23	2.00	0.61
3:D:658:LEU:HD23	3:D:661:MET:CE	2.29	0.61
5:F:309:LYS:O	5:F:312:GLN:HB2	2.01	0.61
3:D:371:ILE:HG13	3:D:372:ASP:H	1.64	0.61
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.35	0.61
3:D:1045:MET:HA	3:D:1045:MET:HE3	1.83	0.61
1:A:211:LEU:O	1:A:215:VAL:HG23	2.01	0.61
2:C:211:LEU:CD2	2:C:218:VAL:HG22	2.31	0.61
3:D:1389:LEU:O	3:D:1390:LEU:HD23	2.01	0.61
3:D:93:ILE:HD11	3:D:548:ILE:CD1	2.31	0.60
2:C:143:SER:HB2	2:C:332:ARG:HD2	1.83	0.60
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.37	0.60
1:B:117:VAL:HG12	1:B:118:ALA:H	1.65	0.60
2:C:905:ILE:HG23	2:C:906:PHE:CD1	2.31	0.60
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.82	0.60
3:D:394:LEU:HG	3:D:396:VAL:HG23	1.82	0.60
3:D:284:LEU:CD2	3:D:290:PRO:HG3	2.29	0.60
3:D:581:LEU:HD23	3:D:582:LEU:HD23	1.84	0.60
1:A:68:ILE:O	1:A:71:VAL:HG22	2.01	0.60
1:B:108:GLU:HG2	1:B:131:THR:CB	2.31	0.60
2:C:390:GLN:NE2	2:C:414:GLY:HA2	2.16	0.60
3:D:230:TRP:HA	3:D:243:ALA:CB	2.31	0.60
3:D:575:GLN:O	3:D:578:VAL:HG13	2.02	0.60
1:B:33:GLY:C	1:B:181:VAL:HG21	2.22	0.60
2:C:226:VAL:O	2:C:229:MET:HG3	2.01	0.60
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.01	0.60
3:D:172:PRO:HB2	3:D:175:VAL:CG2	2.32	0.60
3:D:417:PRO:HB3	3:D:430:ASP:O	2.01	0.60

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	1.84	0.60
1:A:44:LEU:HD13	1:A:199:ILE:HD13	1.83	0.60
2:C:626:ARG:H	2:C:639:GLN:NE2	1.99	0.60
2:C:736:ASP:O	2:C:744:ARG:HG2	2.02	0.60
2:C:944:LEU:HD11	2:C:963:LEU:HD21	1.82	0.60
3:D:478:LEU:HD12	3:D:479:GLU:H	1.67	0.60
3:D:662:GLU:OE2	3:D:669:ASN:HA	2.02	0.60
1:B:109:VAL:C	1:B:110:LYS:HD2	2.21	0.60
3:D:808:THR:O	3:D:811:GLU:HG2	2.02	0.60
1:A:63:HIS:HB2	2:C:799:ILE:HG21	1.84	0.60
2:C:223:ASP:O	2:C:226:VAL:HG23	2.01	0.60
3:D:315:ARG:H	3:D:315:ARG:HD2	1.66	0.60
3:D:860:LEU:HD22	3:D:878:GLY:HA2	1.83	0.60
3:D:1336:LEU:HD12	3:D:1336:LEU:O	2.02	0.60
5:F:102:LEU:HD23	5:F:183:ALA:HB1	1.83	0.60
2:C:41:ASN:OD1	2:C:46:ALA:HA	2.01	0.59
3:D:500:ARG:NH1	3:D:1390:LEU:HD21	2.17	0.59
3:D:659:LYS:NZ	3:D:663:GLU:OE1	2.25	0.59
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.02	0.59
5:F:368:VAL:CG1	5:F:397:ILE:HD11	2.32	0.59
2:C:654:LEU:HD11	2:C:656:ALA:O	2.02	0.59
2:C:745:ILE:HD11	2:C:802:ARG:HA	1.84	0.59
3:D:1486:VAL:HA	4:E:74:VAL:O	2.03	0.59
5:F:120:THR:CG2	5:F:122:LEU:HD22	2.31	0.59
5:F:282:LEU:N	5:F:282:LEU:HD23	2.15	0.59
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.84	0.59
2:C:626:ARG:H	2:C:639:GLN:HE21	1.50	0.59
2:C:897:LEU:HD21	2:C:921:ALA:HB2	1.84	0.59
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.36	0.59
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.01	0.59
1:A:44:LEU:O	1:A:174:VAL:HG21	2.02	0.59
1:A:111:ALA:HB2	1:A:127:LEU:HB3	1.84	0.59
1:A:117:VAL:HB	1:A:120:VAL:HG21	1.85	0.59
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.34	0.59
3:D:134:VAL:CG2	3:D:151:GLN:H	2.16	0.59
3:D:1111:ASP:OD2	3:D:1203:LYS:HE2	2.02	0.59
3:D:216:VAL:CA	3:D:340:THR:HG22	2.24	0.59
5:F:173:TYR:HA	5:F:176:ILE:HG12	1.85	0.59
1:A:97:VAL:HG12	1:A:98:THR:N	2.17	0.59
1:A:159:LYS:HG2	1:A:166:PRO:HD3	1.85	0.59
2:C:197:LEU:CA	2:C:200:LEU:HD12	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:724:ARG:HD2	2:C:739:GLU:HA	1.85	0.59
2:C:1019:GLN:NE2	3:D:621:LYS:HE3	2.17	0.59
2:C:284:ARG:O	2:C:285:LEU:HD22	2.03	0.59
3:D:178:LEU:HD12	3:D:190:GLU:O	2.02	0.59
3:D:1190:SER:OG	3:D:1191:PRO:HD2	2.03	0.59
3:D:1281:VAL:HG22	3:D:1316:GLY:N	2.18	0.59
2:C:136:ILE:CG2	2:C:336:VAL:HG23	2.32	0.59
2:C:229:MET:HB3	2:C:233:GLU:HB2	1.85	0.59
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.84	0.59
5:F:131:VAL:HG11	5:F:177:ALA:HB1	1.83	0.59
2:C:367:LEU:HA	2:C:371:LYS:NZ	2.18	0.59
2:C:547:ILE:O	2:C:905:ILE:HD11	2.01	0.59
3:D:116:LEU:HD12	3:D:118:LEU:CD1	2.33	0.59
3:D:816:HIS:HB2	3:D:836:VAL:HG11	1.85	0.59
3:D:1233:GLY:HA2	3:D:1236:LEU:HG	1.85	0.59
3:D:1394:VAL:CG2	3:D:1420:LEU:HD21	2.33	0.59
1:A:6:LEU:HD23	1:A:7:LYS:N	2.17	0.59
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.67	0.59
3:D:1281:VAL:HG22	3:D:1316:GLY:H	1.66	0.59
5:F:200:LYS:CG	5:F:201:LYS:HG3	2.32	0.59
2:C:644:VAL:HG22	2:C:645:VAL:N	2.18	0.58
2:C:958:THR:HG23	2:C:961:GLU:CG	2.33	0.58
5:F:361:LEU:CD1	5:F:411:HIS:HB2	2.26	0.58
2:C:290:LEU:O	2:C:301:GLU:HB2	2.03	0.58
2:C:1031:ARG:HB2	3:D:622:ARG:NH1	2.18	0.58
1:B:117:VAL:CG1	1:B:118:ALA:H	2.16	0.58
1:B:185:ARG:HB2	1:B:190:THR:OG1	2.03	0.58
3:D:122:GLU:HG2	3:D:152:LEU:CD1	2.32	0.58
3:D:475:LYS:O	3:D:478:LEU:HD12	2.03	0.58
4:E:26:ARG:NE	4:E:30:LEU:HD11	2.19	0.58
2:C:154:ARG:NH1	2:C:175:GLU:OE2	2.36	0.58
1:A:153:ALA:C	1:A:155:LYS:H	2.07	0.58
1:B:58:ILE:HB	1:B:61:VAL:CG2	2.33	0.58
2:C:35:PRO:CG	2:C:38:LYS:HD3	2.34	0.58
2:C:339:LEU:HD13	2:C:391:LEU:HD12	1.86	0.58
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.34	0.58
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.84	0.58
3:D:496:LEU:HG	3:D:500:ARG:HD2	1.85	0.58
3:D:573:MET:SD	5:F:210:LEU:HB3	2.43	0.58
3:D:1041:LEU:O	3:D:1041:LEU:HD23	2.03	0.58
3:D:1198:TYR:CZ	3:D:1460:ILE:HD13	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:367:MET:HE3	5:F:368:VAL:HG13	1.85	0.58
5:F:374:GLY:HA3	5:F:378:GLY:H	1.68	0.58
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.85	0.58
2:C:433:THR:CG2	2:C:488:ALA:HB1	2.34	0.58
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.38	0.58
3:D:683:ILE:HG22	3:D:687:VAL:HG11	1.84	0.58
3:D:699:VAL:CG1	3:D:760:ARG:HG3	2.32	0.58
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.34	0.58
1:A:101:LEU:O	1:A:102:LYS:HG2	2.03	0.58
2:C:167:LYS:HG2	7:H:12:DC:C5	2.39	0.58
3:D:144:GLY:O	3:D:145:VAL:HG23	2.03	0.58
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.86	0.58
3:D:270:LEU:HD13	3:D:304:LEU:HD13	1.86	0.58
5:F:364:ARG:O	5:F:367:MET:HG3	2.04	0.58
5:F:412:GLU:HG3	5:F:418:LEU:HD13	1.84	0.58
3:D:709:HIS:C	3:D:711:LEU:H	2.07	0.58
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.85	0.58
1:A:79:ILE:HD12	1:A:167:VAL:CG2	2.34	0.58
2:C:128:ILE:C	2:C:129:ILE:HD12	2.24	0.58
2:C:767:PRO:HB2	2:C:772:ARG:HG3	1.86	0.58
3:D:1147:ARG:HB3	3:D:1188:VAL:HG22	1.86	0.58
2:C:214:TYR:CD2	2:C:218:VAL:HG23	2.39	0.58
2:C:767:PRO:HB2	2:C:772:ARG:CG	2.34	0.58
3:D:204:LEU:HD11	3:D:445:ARG:HE	1.69	0.58
3:D:1486:VAL:HB	4:E:22:VAL:HG13	1.86	0.58
3:D:297:ILE:HD12	3:D:297:ILE:N	2.19	0.57
3:D:586:ARG:HG2	3:D:586:ARG:NH1	2.19	0.57
1:A:6:LEU:HD23	1:A:7:LYS:O	2.04	0.57
3:D:360:ARG:HA	3:D:384:VAL:HG12	1.86	0.57
5:F:203:THR:O	5:F:205:ARG:HG2	2.04	0.57
2:C:214:TYR:HD2	2:C:218:VAL:HG23	1.69	0.57
3:D:618:LEU:HB3	3:D:1467:ILE:HG23	1.87	0.57
3:D:1205:TYR:CZ	3:D:1366:LYS:HE2	2.39	0.57
3:D:1426:LYS:HE3	7:H:20:DG:OP1	2.04	0.57
2:C:713:ARG:HG2	2:C:720:GLU:OE1	2.05	0.57
3:D:842:VAL:HG22	3:D:865:THR:HB	1.87	0.57
3:D:970:LYS:HA	3:D:973:GLN:CB	2.33	0.57
3:D:1271:LYS:CD	3:D:1331:ASP:HB2	2.33	0.57
1:A:63:HIS:O	1:A:66:SER:OG	2.23	0.57
1:A:222:LEU:HD21	1:B:218:LEU:HD22	1.84	0.57
2:C:127:PHE:O	2:C:133:ASP:HA	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:LEU:H	2:C:197:LEU:HD12	1.69	0.57
2:C:630:ARG:HB2	2:C:705:ILE:HD12	1.86	0.57
2:C:654:LEU:C	2:C:655:LEU:HD12	2.24	0.57
3:D:132:TYR:OH	3:D:568:ARG:NH2	2.38	0.57
3:D:324:ALA:HB1	3:D:331:VAL:HG21	1.86	0.57
3:D:361:VAL:HG21	3:D:379:ALA:CB	2.34	0.57
3:D:1314:LYS:HE2	3:D:1317:ASP:OD2	2.04	0.57
5:F:95:THR:HG22	5:F:98:GLU:OE2	2.04	0.57
1:A:143:ARG:NH1	1:A:160:ASP:OD1	2.37	0.57
2:C:128:ILE:O	2:C:129:ILE:HD12	2.03	0.57
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.85	0.57
2:C:679:PHE:N	2:C:683:ASN:OD1	2.38	0.57
2:C:712:ALA:HB3	2:C:821:GLU:HG2	1.85	0.57
2:C:775:ARG:HH11	5:F:422:LEU:HD23	1.70	0.57
3:D:137:PRO:HB3	3:D:147:VAL:HG23	1.85	0.57
3:D:352:ASN:HB3	5:F:104:ARG:NH1	2.19	0.57
5:F:200:LYS:HG3	5:F:201:LYS:HG3	1.86	0.57
1:A:224:TYR:CG	1:B:9:PRO:HG2	2.39	0.57
2:C:557:ARG:NH1	2:C:844:GLY:O	2.38	0.57
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.38	0.57
3:D:174:GLY:HA2	3:D:389:GLU:CD	2.24	0.57
3:D:378:ILE:HD12	3:D:378:ILE:N	2.20	0.57
3:D:885:ILE:HG23	3:D:937:TYR:CE1	2.39	0.57
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.38	0.57
2:C:172:ILE:HG12	2:C:186:VAL:CG2	2.35	0.57
2:C:765:SER:O	2:C:765:SER:OG	2.22	0.57
2:C:438:ILE:HD11	2:C:467:ILE:HD12	1.86	0.57
2:C:587:VAL:O	2:C:591:SER:HB3	2.05	0.57
3:D:221:ALA:O	3:D:335:LEU:HD12	2.05	0.57
3:D:291:LEU:N	3:D:304:LEU:O	2.36	0.57
3:D:764:LEU:HD23	3:D:767:HIS:NE2	2.18	0.57
3:D:1090:ASP:N	3:D:1090:ASP:OD1	2.37	0.57
2:C:1001:VAL:HB	3:D:724:GLN:HB2	1.86	0.57
3:D:135:LEU:CD1	3:D:463:GLN:HG2	2.35	0.57
3:D:764:LEU:HB3	3:D:767:HIS:CD2	2.40	0.57
3:D:823:LEU:HD11	3:D:837:GLY:CA	2.35	0.57
3:D:1031:ASN:OD1	3:D:1034:GLN:HG3	2.05	0.57
2:C:2:GLU:O	2:C:3:ILE:HD13	2.04	0.56
2:C:1021:LEU:HD12	2:C:1021:LEU:N	2.16	0.56
3:D:983:LEU:HB3	3:D:987:GLU:OE2	2.04	0.56
2:C:718:GLY:HA3	2:C:761:PHE:CD1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:743:VAL:HG13	2:C:755:LEU:O	2.04	0.56
3:D:361:VAL:HG21	3:D:379:ALA:HB1	1.86	0.56
3:D:556:LYS:HD3	5:F:218:GLN:OE1	2.05	0.56
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.34	0.56
1:B:162:ILE:HG13	1:B:163:ASN:ND2	2.20	0.56
2:C:297:GLU:HG3	2:C:299:LYS:NZ	2.20	0.56
2:C:559:LEU:C	2:C:559:LEU:HD23	2.25	0.56
2:C:690:ILE:CD1	2:C:852:ILE:HG23	2.35	0.56
2:C:747:ALA:O	2:C:799:ILE:HA	2.05	0.56
2:C:756:VAL:HG21	2:C:823:VAL:CG1	2.35	0.56
2:C:897:LEU:HB2	2:C:899:GLN:HG3	1.88	0.56
3:D:38:LYS:HB3	3:D:39:PRO:HD2	1.87	0.56
3:D:229:ALA:HB1	3:D:244:GLU:O	2.05	0.56
3:D:563:PRO:HB3	5:F:189:GLU:HG2	1.87	0.56
3:D:828:LYS:CE	3:D:831:GLY:H	2.16	0.56
3:D:864:VAL:CG1	3:D:865:THR:N	2.68	0.56
3:D:1281:VAL:CG2	3:D:1315:ASP:HA	2.36	0.56
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.20	0.56
2:C:958:THR:HG23	2:C:961:GLU:OE1	2.05	0.56
3:D:236:TYR:CE1	3:D:242:LEU:HB2	2.41	0.56
2:C:193:LEU:O	2:C:197:LEU:HD12	2.06	0.56
1:A:10:VAL:N	1:A:26:GLU:O	2.29	0.56
2:C:874:LEU:HD12	3:D:784:ASP:OD1	2.06	0.56
3:D:1126:ASP:O	3:D:1130:ARG:HA	2.06	0.56
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.39	0.56
5:F:153:PRO:CA	5:F:156:VAL:HG12	2.33	0.56
5:F:202:TYR:HE1	5:F:248:ASN:HD21	1.54	0.56
5:F:240:THR:O	5:F:244:ARG:HG2	2.06	0.56
5:F:350:LEU:HD13	5:F:421:PHE:CD2	2.41	0.56
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.41	0.56
2:C:725:ASP:N	2:C:726:ILE:HD12	2.21	0.56
2:C:1004:LYS:HD3	3:D:744:GLN:HE22	1.70	0.56
2:C:1092:LEU:CD1	2:C:1099:VAL:HG21	2.35	0.56
3:D:437:VAL:HG11	5:F:175:HIS:HD2	1.70	0.56
1:B:85:LEU:HD11	1:B:122:ILE:HD12	1.88	0.56
1:B:124:ASN:HD21	1:B:127:LEU:HD12	1.68	0.56
2:C:8:ARG:HB3	2:C:8:ARG:CZ	2.36	0.56
2:C:23:VAL:HG23	2:C:24:GLU:H	1.71	0.56
2:C:35:PRO:HG2	2:C:38:LYS:HB2	1.88	0.56
2:C:719:PRO:HD2	2:C:761:PHE:HE1	1.70	0.56
2:C:762:LYS:HE2	2:C:786:LYS:HG3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:63:TYR:OH	3:D:74:GLU:OE1	2.23	0.56
3:D:618:LEU:CG	3:D:1467:ILE:HG23	2.36	0.56
3:D:693:GLU:HG3	4:E:48:MET:HE2	1.87	0.56
4:E:50:THR:HG23	4:E:53:GLY:H	1.71	0.56
2:C:292:ARG:NH1	2:C:301:GLU:OE2	2.39	0.56
2:C:578:VAL:HG13	2:C:671:ASN:CG	2.26	0.56
4:E:39:VAL:O	4:E:72:ARG:HD2	2.06	0.56
2:C:22:GLN:O	2:C:121:MET:HE1	2.06	0.56
2:C:715:THR:HB	2:C:718:GLY:O	2.07	0.56
3:D:185:VAL:CG1	3:D:186:VAL:N	2.69	0.55
3:D:683:ILE:HG23	3:D:687:VAL:HG11	1.88	0.55
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.34	0.55
3:D:1301:LYS:HG2	3:D:1302:GLU:H	1.71	0.55
1:A:184:THR:HG23	1:A:185:ARG:N	2.21	0.55
2:C:143:SER:HB2	2:C:332:ARG:CD	2.36	0.55
2:C:368:THR:OG1	2:C:371:LYS:HG2	2.06	0.55
3:D:529:GLN:HG3	3:D:535:PHE:CZ	2.42	0.55
3:D:764:LEU:HD23	3:D:767:HIS:HD2	1.69	0.55
3:D:823:LEU:HD11	3:D:837:GLY:HA2	1.89	0.55
3:D:1353:GLN:OE1	3:D:1353:GLN:HA	2.06	0.55
5:F:101:GLU:O	5:F:105:LYS:HG3	2.06	0.55
5:F:171:LYS:HD3	5:F:175:HIS:CE1	2.36	0.55
5:F:274:THR:O	5:F:278:LEU:HG	2.07	0.55
1:B:26:GLU:HB3	1:B:194:LYS:CG	2.36	0.55
1:B:197:LEU:HD12	1:B:198:ARG:H	1.69	0.55
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.06	0.55
3:D:1292:VAL:HG13	3:D:1303:TYR:HB2	1.87	0.55
5:F:120:THR:HG23	5:F:122:LEU:HD13	1.88	0.55
2:C:150:PRO:CD	2:C:322:VAL:HG11	2.31	0.55
2:C:194:VAL:HG13	2:C:221:LEU:CD2	2.36	0.55
2:C:409:ARG:HG2	2:C:409:ARG:HH21	1.72	0.55
2:C:743:VAL:CG1	2:C:755:LEU:HA	2.37	0.55
2:C:833:LEU:HD12	2:C:834:GLN:N	2.18	0.55
2:C:1047:HIS:CE1	3:D:1471:LEU:HD21	2.42	0.55
3:D:256:GLU:OE1	3:D:300:LYS:HE2	2.06	0.55
3:D:367:ILE:HD11	3:D:379:ALA:HB2	1.88	0.55
3:D:881:LEU:O	3:D:885:ILE:HG13	2.07	0.55
4:E:34:GLY:O	4:E:35:PHE:HB2	2.07	0.55
2:C:425:PHE:CD1	3:D:1079:LYS:HE3	2.41	0.55
2:C:567:GLN:NE2	2:C:999:HIS:HE2	2.05	0.55
3:D:116:LEU:CB	3:D:118:LEU:HD12	2.31	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:553:ARG:HG3	3:D:553:ARG:O	2.07	0.55
3:D:698:LYS:HB2	3:D:756:GLN:OE1	2.07	0.55
3:D:800:LYS:HB3	3:D:822:ALA:H	1.71	0.55
3:D:1271:LYS:HD2	3:D:1331:ASP:CB	2.37	0.55
1:A:14:ARG:NH1	1:A:14:ARG:HB2	2.22	0.55
1:B:208:LEU:HD12	1:B:208:LEU:O	2.07	0.55
2:C:462:ASP:HB3	2:C:468:ARG:HD3	1.87	0.55
3:D:676:MET:CE	3:D:683:ILE:HA	2.36	0.55
1:A:124:ASN:HD21	1:A:127:LEU:HD22	1.71	0.55
2:C:352:ALA:O	2:C:356:ARG:HD2	2.07	0.55
2:C:422:ARG:NH2	7:H:13:DT:H5'	2.21	0.55
2:C:471:TYR:OH	2:C:516:ARG:NH2	2.39	0.55
3:D:141:ILE:HG13	3:D:142:LEU:N	2.22	0.55
3:D:650:LEU:CD1	3:D:657:LEU:HD23	2.33	0.55
3:D:1024:ALA:HA	3:D:1029:ARG:O	2.07	0.55
3:D:407:VAL:O	5:F:171:LYS:HE2	2.06	0.55
3:D:410:SER:OG	5:F:174:LEU:HD23	2.06	0.55
3:D:1126:ASP:C	3:D:1130:ARG:HA	2.27	0.55
2:C:540:PHE:HB3	2:C:544:THR:HG22	1.85	0.55
2:C:1085:PHE:O	2:C:1088:LEU:HB3	2.06	0.55
3:D:6:ARG:HB3	3:D:6:ARG:HH11	1.72	0.55
3:D:806:PHE:O	3:D:829:VAL:HA	2.06	0.55
2:C:88:LEU:O	2:C:131:GLY:N	2.40	0.55
2:C:194:VAL:HA	2:C:197:LEU:CD1	2.34	0.55
2:C:726:ILE:HD12	2:C:726:ILE:N	2.22	0.55
2:C:846:LYS:HD2	3:D:741:ASP:HB2	1.89	0.55
3:D:65:ARG:HD3	5:F:377:ASP:CA	2.36	0.55
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.89	0.55
3:D:1160:LEU:HD23	3:D:1164:ARG:NH1	2.22	0.55
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.19	0.55
5:F:194:LEU:HB2	7:H:6:DT:C2	2.42	0.55
2:C:53:PRO:HB3	2:C:67:ASP:OD2	2.07	0.54
3:D:185:VAL:HG12	3:D:186:VAL:N	2.22	0.54
3:D:366:LYS:C	3:D:367:ILE:HD13	2.28	0.54
1:B:40:LEU:C	1:B:44:LEU:HD12	2.27	0.54
1:B:96:THR:O	1:B:97:VAL:HG23	2.06	0.54
2:C:195:LEU:CD1	2:C:234:ALA:HB1	2.37	0.54
2:C:598:GLU:O	2:C:599:GLU:HG2	2.08	0.54
2:C:683:ASN:CB	2:C:872:ASN:HD22	2.20	0.54
3:D:116:LEU:HD12	3:D:118:LEU:HD12	1.89	0.54
3:D:212:ARG:HB2	3:D:344:ASP:OD1	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:916:TYR:CE2	3:D:920:LEU:HD11	2.41	0.54
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.07	0.54
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.72	0.54
2:C:808:ARG:HB3	2:C:808:ARG:HH21	1.70	0.54
2:C:1005:MET:SD	3:D:648:MET:HG3	2.48	0.54
3:D:245:LEU:HD13	3:D:307:ALA:CB	2.38	0.54
3:D:781:PRO:HB2	3:D:786:ILE:HG22	1.89	0.54
3:D:860:LEU:HD22	3:D:878:GLY:CA	2.38	0.54
2:C:498:GLN:HG2	2:C:514:VAL:O	2.07	0.54
2:C:723:THR:OG1	2:C:724:ARG:N	2.41	0.54
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.23	0.54
3:D:664:LYS:HE3	3:D:693:GLU:OE2	2.06	0.54
3:D:1004:THR:OG1	3:D:1036:ARG:HD3	2.08	0.54
3:D:1088:THR:HG21	6:G:14:DG:C6	2.43	0.54
5:F:117:SER:O	5:F:121:GLY:N	2.37	0.54
1:A:133:GLU:OE2	2:C:605:LYS:HB3	2.07	0.54
1:A:138:LEU:CD1	1:A:140:MET:HE3	2.36	0.54
1:A:205:VAL:HG23	1:A:206:THR:N	2.22	0.54
2:C:238:LEU:O	2:C:241:LEU:N	2.38	0.54
2:C:507:ARG:HB2	2:C:507:ARG:NH1	2.23	0.54
2:C:690:ILE:CG1	2:C:852:ILE:HG23	2.38	0.54
2:C:1008:ARG:HD2	2:C:1028:GLY:O	2.08	0.54
3:D:65:ARG:HD3	5:F:377:ASP:HA	1.89	0.54
3:D:297:ILE:HD12	3:D:297:ILE:H	1.73	0.54
3:D:367:ILE:HD13	3:D:367:ILE:N	2.22	0.54
3:D:955:VAL:HG22	3:D:1011:PHE:CZ	2.43	0.54
2:C:679:PHE:O	2:C:680:ASP:HB2	2.08	0.54
2:C:715:THR:HG22	2:C:716:LYS:N	2.22	0.54
3:D:18:ILE:HG21	3:D:516:ALA:O	2.08	0.54
3:D:55:ASP:OD1	3:D:83:SER:HB3	2.08	0.54
3:D:801:GLY:HA2	3:D:821:VAL:HG22	1.89	0.54
1:B:59:GLU:OE2	1:B:139:ASN:ND2	2.32	0.54
2:C:281:LEU:HD22	2:C:308:ARG:NH2	2.23	0.54
2:C:312:ALA:HB1	2:C:317:VAL:CG2	2.38	0.54
2:C:437:ARG:HB3	2:C:467:ILE:HG21	1.89	0.54
3:D:704:ARG:HG2	3:D:705:ALA:H	1.73	0.54
2:C:101:ILE:HA	2:C:107:LEU:O	2.08	0.54
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.90	0.54
2:C:983:ILE:O	2:C:985:GLY:N	2.41	0.54
2:C:1008:ARG:CZ	2:C:1020:PRO:HB3	2.38	0.54
3:D:948:THR:HG23	3:D:949:ILE:N	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1079:LYS:O	3:D:1079:LYS:HG3	2.07	0.54
5:F:376:ILE:O	5:F:377:ASP:HB3	2.08	0.54
1:A:40:LEU:HD23	1:A:218:LEU:HD12	1.90	0.54
1:A:216:GLU:CD	1:A:219:ARG:HH22	2.11	0.54
2:C:189:ARG:NH2	2:C:244:PRO:HD2	2.23	0.54
3:D:741:ASP:OD1	3:D:743:ASP:OD1	2.25	0.54
3:D:764:LEU:HB3	3:D:767:HIS:HD2	1.73	0.54
3:D:1040:GLY:O	3:D:1060:SER:HB2	2.08	0.54
3:D:1496:GLU:O	3:D:1500:LYS:HG2	2.08	0.54
5:F:141:VAL:HG22	5:F:151:LEU:O	2.08	0.54
2:C:356:ARG:HA	2:C:359:MET:HB2	1.89	0.53
2:C:418:LEU:HD21	2:C:427:VAL:HG11	1.90	0.53
3:D:93:ILE:CD1	3:D:548:ILE:HG12	2.37	0.53
3:D:135:LEU:HD11	3:D:463:GLN:HG2	1.89	0.53
3:D:566:ILE:HG13	5:F:217:ASN:HD22	1.72	0.53
3:D:581:LEU:HD23	3:D:582:LEU:HD21	1.89	0.53
5:F:159:ILE:O	5:F:163:LEU:HG	2.09	0.53
1:A:11:PHE:CD2	1:B:225:PHE:HA	2.44	0.53
1:B:100:LEU:CD2	1:B:141:GLU:HG2	2.39	0.53
1:B:124:ASN:HD22	1:B:127:LEU:HD12	1.70	0.53
2:C:815:LEU:HB2	2:C:819:VAL:HG22	1.88	0.53
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.43	0.53
3:D:496:LEU:HD23	3:D:1390:LEU:CD1	2.36	0.53
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.24	0.53
3:D:1254:GLN:HB2	3:D:1258:ARG:HB2	1.90	0.53
2:C:11:GLU:OE2	2:C:537:LYS:HE2	2.09	0.53
3:D:135:LEU:HD11	3:D:463:GLN:CG	2.37	0.53
1:A:38:ASN:HB3	1:A:39:PRO:CD	2.38	0.53
1:B:41:ARG:HA	1:B:177:VAL:HG11	1.89	0.53
1:B:143:ARG:HD3	1:B:158:ILE:CD1	2.39	0.53
1:B:219:ARG:O	1:B:222:LEU:HB2	2.08	0.53
2:C:808:ARG:HB3	2:C:808:ARG:CZ	2.39	0.53
3:D:661:MET:HE1	3:D:677:LEU:HD11	1.89	0.53
3:D:1066:THR:OG1	3:D:1069:GLU:HG3	2.09	0.53
1:B:108:GLU:CG	1:B:131:THR:HB	2.35	0.53
1:B:127:LEU:HD23	1:B:127:LEU:C	2.29	0.53
2:C:317:VAL:HB	2:C:320:HIS:HD2	1.70	0.53
3:D:82:LYS:HB2	3:D:84:ILE:HG22	1.90	0.53
3:D:658:LEU:HA	3:D:661:MET:CE	2.38	0.53
3:D:1165:TYR:CE2	3:D:1214:PRO:HB3	2.43	0.53
4:E:39:VAL:CG2	4:E:72:ARG:HB3	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:ILE:HD13	2:C:305:PRO:HB3	1.91	0.53
2:C:355:VAL:HG23	2:C:356:ARG:N	2.24	0.53
3:D:142:LEU:HD13	3:D:161:LEU:HD21	1.91	0.53
3:D:371:ILE:HD11	5:F:232:ARG:NH1	2.24	0.53
3:D:626:SER:HA	3:D:747:VAL:O	2.09	0.53
3:D:1311:LEU:O	3:D:1312:LEU:HD23	2.09	0.53
7:H:17:DA:H2''	7:H:18:DC:H5'	1.90	0.53
1:A:88:ARG:HB2	1:A:204:SER:HA	1.90	0.53
1:B:173:PRO:HB2	1:B:205:VAL:HG12	1.89	0.53
1:B:202:ASP:OD1	1:B:204:SER:HB3	2.08	0.53
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.38	0.53
2:C:888:THR:O	2:C:891:GLY:N	2.41	0.53
3:D:140:ALA:HA	3:D:450:TYR:CE1	2.43	0.53
3:D:1057:VAL:HG21	3:D:1065:LEU:CD2	2.39	0.53
5:F:383:LEU:C	5:F:386:VAL:HG22	2.29	0.53
1:A:220:GLU:O	1:A:223:THR:OG1	2.10	0.53
2:C:564:MET:HE1	2:C:846:LYS:HD3	1.91	0.53
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.43	0.53
2:C:1109:VAL:HG11	3:D:5:VAL:HG22	1.91	0.53
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.44	0.53
3:D:399:ARG:O	3:D:446:VAL:HG12	2.09	0.53
3:D:462:GLN:O	3:D:466:LYS:HB2	2.09	0.53
3:D:625:TYR:CE2	3:D:751:LEU:HD11	2.43	0.53
3:D:882:PHE:CE2	3:D:906:GLN:HG3	2.44	0.53
3:D:1405:GLU:O	3:D:1408:ILE:HG13	2.08	0.53
5:F:198:ILE:HD12	5:F:243:ILE:HG21	1.91	0.53
1:A:18:ARG:HH21	1:A:88:ARG:CZ	2.20	0.53
2:C:293:PHE:HD1	2:C:298:PHE:CE1	2.27	0.53
2:C:390:GLN:HG3	5:F:323:ASP:OD1	2.08	0.53
2:C:468:ARG:HG3	2:C:485:TYR:HB3	1.91	0.53
2:C:916:GLU:O	2:C:920:GLN:HG3	2.09	0.53
3:D:64:LYS:O	3:D:65:ARG:HB2	2.08	0.53
3:D:170:PRO:CA	3:D:392:SER:HB2	2.26	0.53
3:D:970:LYS:O	3:D:973:GLN:HB3	2.08	0.53
3:D:1087:ARG:HD3	3:D:1234:THR:O	2.09	0.53
5:F:197:SER:HA	5:F:200:LYS:HE3	1.90	0.53
1:A:196:THR:CG2	2:C:934:PHE:HE1	2.21	0.53
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.44	0.53
3:D:699:VAL:HG21	3:D:715:ALA:HB1	1.91	0.53
3:D:1301:LYS:HG2	3:D:1302:GLU:N	2.24	0.53
5:F:369:LEU:HD23	5:F:372:ARG:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.44	0.52
1:A:67:THR:HG23	2:C:609:ASN:HD21	1.74	0.52
1:B:80:LEU:HB3	3:D:844:ALA:CB	2.39	0.52
2:C:723:THR:OG1	2:C:725:ASP:N	2.40	0.52
3:D:534:ARG:NH2	5:F:313:GLU:O	2.43	0.52
3:D:1130:ARG:HB3	3:D:1130:ARG:NH1	2.23	0.52
5:F:132:ARG:O	5:F:135:ILE:HG22	2.09	0.52
2:C:195:LEU:O	2:C:199:VAL:HG23	2.09	0.52
2:C:598:GLU:O	2:C:651:LYS:HE3	2.09	0.52
3:D:242:LEU:HD21	3:D:311:LEU:CD1	2.38	0.52
3:D:400:VAL:HG23	3:D:443:VAL:HB	1.90	0.52
5:F:403:LYS:HA	5:F:406:ARG:HB2	1.91	0.52
1:B:32:PHE:HA	1:B:35:THR:HB	1.91	0.52
1:B:205:VAL:HG22	1:B:206:THR:N	2.24	0.52
2:C:361:MET:HG3	2:C:361:MET:O	2.07	0.52
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.75	0.52
2:C:1099:VAL:HG22	3:D:10:ILE:HG13	1.90	0.52
3:D:238:PRO:HB3	3:D:315:ARG:HA	1.90	0.52
3:D:280:ALA:HB1	3:D:282:TYR:CE2	2.44	0.52
3:D:1078:ARG:HG2	3:D:1078:ARG:HH11	1.74	0.52
3:D:1300:SER:OG	3:D:1301:LYS:N	2.42	0.52
5:F:369:LEU:HD22	5:F:369:LEU:O	2.09	0.52
1:A:79:ILE:HG23	1:A:167:VAL:HG22	1.91	0.52
3:D:284:LEU:HG	3:D:288:MET:CE	2.40	0.52
3:D:729:HIS:CE1	3:D:730:PRO:HD2	2.45	0.52
3:D:984:THR:N	3:D:987:GLU:OE2	2.26	0.52
5:F:95:THR:N	5:F:98:GLU:HG3	2.20	0.52
1:B:18:ARG:O	1:B:207:PRO:HD3	2.09	0.52
1:B:37:GLY:HA2	1:B:40:LEU:CG	2.40	0.52
2:C:420:ARG:HG2	2:C:420:ARG:HH11	1.74	0.52
2:C:745:ILE:CD1	2:C:802:ARG:HA	2.39	0.52
3:D:615:ARG:HD2	3:D:1096:ARG:NH2	2.24	0.52
3:D:618:LEU:CD1	3:D:1467:ILE:HG23	2.39	0.52
3:D:1057:VAL:HG23	3:D:1069:GLU:OE2	2.09	0.52
1:A:71:VAL:HG12	1:A:132:LEU:HG	1.90	0.52
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.39	0.52
1:B:188:GLN:HG2	3:D:685:ASP:OD2	2.09	0.52
2:C:230:ARG:N	2:C:233:GLU:HG3	2.24	0.52
2:C:334:ARG:HD2	2:C:338:GLU:OE2	2.10	0.52
2:C:513:VAL:HG21	2:C:529:VAL:CG2	2.40	0.52
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:47:GLU:HB3	3:D:51:GLY:O	2.09	0.52
3:D:672:ALA:HB2	5:F:420:ASP:CG	2.30	0.52
3:D:701:LEU:CD1	3:D:763:MET:HE1	2.40	0.52
4:E:91:ARG:HH11	4:E:92:LEU:HG	1.73	0.52
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.75	0.52
1:B:29:GLU:HG3	1:B:30:ARG:H	1.74	0.52
1:B:96:THR:HG22	1:B:97:VAL:H	1.74	0.52
3:D:1234:THR:HB	3:D:1235:GLN:CB	2.26	0.52
5:F:127:ILE:O	5:F:131:VAL:HG23	2.10	0.52
5:F:213:ILE:HG22	5:F:214:GLN:N	2.24	0.52
2:C:64:LEU:N	2:C:103:LYS:HB2	2.25	0.52
2:C:422:ARG:HH22	7:H:13:DT:H3'	1.73	0.52
2:C:963:LEU:N	2:C:963:LEU:HD23	2.24	0.52
3:D:860:LEU:O	3:D:876:SER:HB2	2.10	0.52
5:F:112:ALA:HB2	5:F:176:ILE:HG21	1.92	0.52
1:A:40:LEU:CD2	1:A:218:LEU:HD12	2.40	0.52
1:B:26:GLU:CB	1:B:194:LYS:HG3	2.40	0.52
2:C:322:VAL:HG12	2:C:323:ASP:N	2.25	0.52
2:C:432:ARG:O	2:C:432:ARG:HG2	2.10	0.52
2:C:564:MET:HE3	2:C:846:LYS:CG	2.38	0.52
2:C:724:ARG:O	2:C:724:ARG:HG2	2.09	0.52
2:C:825:VAL:CG2	2:C:825:VAL:O	2.58	0.52
2:C:928:LYS:O	2:C:932:GLU:HG3	2.10	0.52
3:D:124:GLU:OE2	3:D:587:ARG:NH1	2.43	0.52
2:C:196:LEU:CD1	2:C:200:LEU:HD11	2.37	0.52
2:C:366:SER:O	2:C:366:SER:OG	2.25	0.52
2:C:468:ARG:HB2	2:C:486:MET:O	2.10	0.52
2:C:838:LYS:HD3	2:C:997:LEU:HD12	1.92	0.52
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.58	0.52
3:D:171:LEU:HD11	3:D:390:PRO:O	2.10	0.52
3:D:975:GLU:O	3:D:975:GLU:HG3	2.10	0.52
5:F:412:GLU:HG2	5:F:418:LEU:HD13	1.91	0.52
1:A:218:LEU:O	1:A:222:LEU:HD12	2.11	0.51
1:B:117:VAL:CG1	1:B:118:ALA:N	2.73	0.51
2:C:29:ALA:O	2:C:44:ILE:HB	2.11	0.51
2:C:91:GLN:HA	2:C:119:PRO:HA	1.91	0.51
2:C:206:THR:CA	2:C:209:ARG:HB3	2.38	0.51
2:C:697:ARG:HG3	2:C:699:PHE:CD1	2.45	0.51
3:D:446:VAL:O	3:D:446:VAL:HG13	2.09	0.51
3:D:815:ALA:O	3:D:818:ARG:HB2	2.10	0.51
3:D:832:ARG:HD3	3:D:832:ARG:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASP:OD1	1:A:76:VAL:HB	2.11	0.51
1:A:138:LEU:HD11	1:A:140:MET:CE	2.39	0.51
1:A:176:ARG:HG2	1:A:177:VAL:N	2.25	0.51
1:A:201:THR:HG22	1:A:203:GLY:N	2.22	0.51
2:C:754:ILE:HG12	2:C:791:ARG:HD3	1.92	0.51
3:D:584:ASN:H	3:D:602:SER:HB3	1.76	0.51
3:D:993:LEU:C	3:D:993:LEU:HD12	2.30	0.51
3:D:1235:GLN:O	3:D:1236:LEU:HD23	2.10	0.51
5:F:186:HIS:ND1	5:F:186:HIS:O	2.43	0.51
5:F:271:LEU:HD12	5:F:271:LEU:N	2.23	0.51
1:A:9:PRO:CD	1:B:224:TYR:CD2	2.93	0.51
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.92	0.51
3:D:398:ALA:HB1	3:D:446:VAL:O	2.10	0.51
3:D:477:LEU:O	3:D:481:MET:N	2.43	0.51
5:F:240:THR:O	5:F:240:THR:HG22	2.11	0.51
1:A:34:VAL:CG2	1:B:42:ARG:CZ	2.88	0.51
2:C:425:PHE:CE2	3:D:1086:LEU:CD1	2.89	0.51
2:C:433:THR:HG22	2:C:488:ALA:HB1	1.93	0.51
3:D:479:GLU:OE2	3:D:482:LYS:NZ	2.38	0.51
2:C:97:ARG:HG2	2:C:112:GLU:HB3	1.93	0.51
2:C:595:LEU:HD23	2:C:596:TYR:N	2.25	0.51
3:D:806:PHE:HD2	3:D:812:ALA:HA	1.75	0.51
3:D:1413:THR:HG22	3:D:1414:PRO:HD2	1.93	0.51
5:F:298:GLY:O	5:F:303:ARG:NH1	2.43	0.51
5:F:358:LEU:N	5:F:358:LEU:HD23	2.24	0.51
1:A:42:ARG:NH2	1:B:34:VAL:HG22	2.25	0.51
1:B:33:GLY:O	1:B:181:VAL:HG21	2.11	0.51
1:B:80:LEU:HD22	3:D:844:ALA:N	2.25	0.51
3:D:575:GLN:HA	3:D:578:VAL:CG1	2.41	0.51
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.93	0.51
1:A:9:PRO:HB2	1:A:26:GLU:O	2.10	0.51
1:B:86:VAL:HG13	1:B:86:VAL:O	2.10	0.51
3:D:116:LEU:HB2	3:D:118:LEU:CD1	2.31	0.51
3:D:180:LYS:HG3	3:D:181:ASP:N	2.24	0.51
3:D:1114:THR:CG2	3:D:1189:ARG:HH21	2.24	0.51
3:D:1493:LYS:HA	3:D:1493:LYS:HE2	1.92	0.51
5:F:95:THR:HG22	5:F:98:GLU:CD	2.30	0.51
1:B:49:PRO:CA	1:B:148:VAL:HG12	2.40	0.51
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.26	0.51
5:F:90:GLN:HA	5:F:90:GLN:NE2	2.26	0.51
2:C:627:ARG:HH21	2:C:641:PRO:HD3	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:415:VAL:HG22	3:D:419:ASP:OD2	2.11	0.51
3:D:478:LEU:HD12	3:D:479:GLU:N	2.25	0.51
3:D:699:VAL:HG11	3:D:760:ARG:HG3	1.92	0.51
3:D:955:VAL:O	3:D:957:PRO:HD3	2.10	0.51
3:D:1259:VAL:CG2	3:D:1355:VAL:HG11	2.40	0.51
5:F:135:ILE:HD11	5:F:182:ALA:HB2	1.93	0.51
1:A:47:SER:O	1:A:49:PRO:HD3	2.11	0.51
1:A:226:SER:O	1:A:228:PRO:HD3	2.10	0.51
2:C:815:LEU:CD1	2:C:819:VAL:HG23	2.36	0.51
2:C:952:LEU:HD12	2:C:969:GLN:OE1	2.11	0.51
4:E:8:LYS:HE3	4:E:8:LYS:O	2.10	0.51
5:F:353:GLU:CD	5:F:417:LYS:HD2	2.32	0.51
1:B:102:LYS:HG3	1:B:139:ASN:HB2	1.92	0.50
2:C:36:PRO:HA	2:C:39:ARG:HG3	1.92	0.50
2:C:685:GLU:OE1	2:C:685:GLU:HA	2.10	0.50
2:C:723:THR:O	2:C:741:GLY:HA3	2.11	0.50
2:C:766:GLU:CG	2:C:767:PRO:HD2	2.40	0.50
3:D:748:HIS:O	3:D:750:PRO:HD3	2.10	0.50
5:F:358:LEU:HD12	5:F:370:LYS:HE3	1.92	0.50
2:C:879:ARG:HD2	2:C:879:ARG:H	1.76	0.50
3:D:7:LYS:HD3	3:D:1456:LYS:HZ1	1.74	0.50
3:D:973:GLN:HG3	3:D:973:GLN:O	2.10	0.50
3:D:1335:LEU:HD12	3:D:1335:LEU:O	2.11	0.50
5:F:102:LEU:HD23	5:F:183:ALA:CB	2.40	0.50
6:G:7:DT:H2"	6:G:8:DC:OP2	2.10	0.50
2:C:881:ASN:O	2:C:884:GLN:HG2	2.12	0.50
3:D:131:LYS:N	3:D:456:MET:HE2	2.27	0.50
3:D:411:THR:CG2	5:F:178:ARG:HB3	2.34	0.50
3:D:1389:LEU:HD12	3:D:1389:LEU:N	2.26	0.50
4:E:13:VAL:HG11	4:E:19:LEU:N	2.26	0.50
1:B:41:ARG:HG2	1:B:177:VAL:CG1	2.41	0.50
1:B:120:VAL:O	1:B:120:VAL:HG12	2.10	0.50
2:C:366:SER:O	2:C:371:LYS:NZ	2.42	0.50
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.93	0.50
3:D:172:PRO:HB2	3:D:175:VAL:HG21	1.94	0.50
3:D:767:HIS:CE1	4:E:3:GLU:HB2	2.45	0.50
1:B:101:LEU:HD11	1:B:109:VAL:CG1	2.42	0.50
1:B:143:ARG:CZ	1:B:158:ILE:HD12	2.42	0.50
2:C:793:PRO:HG2	2:C:796:GLU:OE1	2.12	0.50
2:C:807:ARG:O	2:C:813:VAL:HG21	2.12	0.50
3:D:478:LEU:HA	3:D:481:MET:HB2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:HIS:HA	1:A:224:TYR:CE2	2.46	0.50
2:C:54:ILE:HD12	2:C:352:ALA:HB1	1.93	0.50
2:C:124:ASP:HA	2:C:592:LEU:CD1	2.41	0.50
2:C:263:ASP:O	2:C:265:ARG:N	2.41	0.50
2:C:937:ASP:OD1	2:C:939:ARG:HG2	2.12	0.50
3:D:691:LEU:O	3:D:694:VAL:N	2.45	0.50
3:D:978:TYR:HD1	3:D:983:LEU:O	1.94	0.50
3:D:1213:ARG:HG3	3:D:1214:PRO:CD	2.39	0.50
3:D:1272:ALA:HA	3:D:1326:THR:HG23	1.94	0.50
1:B:101:LEU:CD2	1:B:138:LEU:HD23	2.42	0.50
2:C:109:LYS:CG	2:C:368:THR:HG22	2.33	0.50
2:C:537:LYS:HB3	2:C:545:ASN:OD1	2.12	0.50
2:C:805:ARG:C	2:C:806:LEU:HD23	2.32	0.50
5:F:367:MET:HE1	5:F:368:VAL:HG13	1.90	0.50
3:D:218:LYS:O	3:D:219:GLU:HG2	2.12	0.50
3:D:529:GLN:HA	3:D:534:ARG:O	2.12	0.50
3:D:687:VAL:O	3:D:690:ALA:HB3	2.12	0.50
3:D:916:TYR:CZ	3:D:920:LEU:HD11	2.47	0.50
3:D:1122:LEU:O	3:D:1135:ARG:HG3	2.12	0.50
2:C:30:LEU:O	2:C:31:GLN:HB2	2.11	0.50
5:F:94:LEU:HD22	5:F:98:GLU:HB2	1.94	0.50
1:B:112:ARG:HG3	1:B:113:ASP:OD1	2.11	0.49
2:C:717:LEU:HD12	2:C:717:LEU:N	2.27	0.49
2:C:721:ARG:HB2	2:C:759:THR:OG1	2.11	0.49
3:D:691:LEU:O	3:D:694:VAL:HB	2.11	0.49
3:D:729:HIS:ND1	3:D:730:PRO:CD	2.75	0.49
1:A:101:LEU:C	1:A:102:LYS:HG2	2.32	0.49
1:A:153:ALA:O	1:A:155:LYS:N	2.44	0.49
2:C:380:ALA:O	2:C:384:GLU:HB2	2.12	0.49
3:D:274:ARG:O	3:D:275:GLU:C	2.50	0.49
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.93	0.49
3:D:828:LYS:C	3:D:828:LYS:HD3	2.32	0.49
3:D:916:TYR:CZ	3:D:920:LEU:HD21	2.47	0.49
1:A:122:ILE:O	1:A:122:ILE:HG22	2.11	0.49
1:B:100:LEU:HD23	1:B:141:GLU:HG2	1.94	0.49
2:C:283:ILE:HD13	2:C:305:PRO:CB	2.42	0.49
2:C:890:LEU:N	2:C:914:ILE:HD11	2.28	0.49
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.31	0.49
3:D:95:LEU:HB2	3:D:515:GLU:O	2.12	0.49
3:D:399:ARG:HD2	3:D:431:VAL:CG2	2.42	0.49
3:D:1256:LEU:N	3:D:1257:PRO:HD2	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1479:ASP:HA	3:D:1482:ARG:HD3	1.93	0.49
5:F:321:ILE:HG21	5:F:332:PHE:CE1	2.44	0.49
1:A:34:VAL:HG21	1:B:42:ARG:CZ	2.42	0.49
1:A:138:LEU:HD21	1:A:140:MET:HE2	1.94	0.49
2:C:422:ARG:CZ	7:H:13:DT:H5'	2.42	0.49
3:D:500:ARG:NH2	3:D:1388:ARG:HG3	2.27	0.49
3:D:618:LEU:HD12	3:D:1467:ILE:CG2	2.41	0.49
3:D:806:PHE:CD2	3:D:812:ALA:HA	2.47	0.49
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.95	0.49
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.93	0.49
2:C:267:TYR:HE1	2:C:269:LEU:HD13	1.76	0.49
2:C:278:GLU:HG2	2:C:283:ILE:O	2.12	0.49
2:C:351:LEU:O	2:C:355:VAL:HG13	2.13	0.49
2:C:728:HIS:HE1	2:C:775:ARG:NH1	2.11	0.49
2:C:878:SER:HA	3:D:1034:GLN:HE22	1.77	0.49
2:C:897:LEU:HD21	2:C:921:ALA:CA	2.43	0.49
3:D:346:ARG:HG3	3:D:348:GLN:HE21	1.77	0.49
3:D:421:LEU:HD13	3:D:428:LYS:CA	2.40	0.49
3:D:814:ALA:O	3:D:818:ARG:N	2.44	0.49
3:D:1164:ARG:NH2	3:D:1170:ASP:OD1	2.45	0.49
3:D:1213:ARG:CG	3:D:1214:PRO:HD2	2.40	0.49
1:B:41:ARG:HG2	1:B:177:VAL:HG12	1.95	0.49
1:B:173:PRO:CB	1:B:205:VAL:HG12	2.43	0.49
2:C:141:HIS:CE1	2:C:334:ARG:HD3	2.47	0.49
2:C:177:GLU:CG	2:C:178:PRO:HD2	2.37	0.49
2:C:413:LEU:HD11	2:C:448:ASN:OD1	2.13	0.49
2:C:588:VAL:HG11	2:C:664:GLY:O	2.12	0.49
2:C:798:GLY:HA3	2:C:828:ALA:O	2.12	0.49
2:C:1063:ARG:HG2	2:C:1064:ASN:N	2.27	0.49
3:D:85:VAL:C	3:D:87:ARG:H	2.16	0.49
3:D:483:HIS:ND1	3:D:484:PRO:O	2.46	0.49
1:A:103:ALA:HB1	1:A:107:LYS:HD2	1.93	0.49
2:C:103:LYS:O	2:C:103:LYS:HD3	2.12	0.49
2:C:184:MET:HG2	2:C:191:PHE:CE1	2.47	0.49
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.77	0.49
3:D:65:ARG:CD	5:F:377:ASP:CA	2.90	0.49
3:D:508:ARG:NE	3:D:510:GLU:OE2	2.44	0.49
3:D:835:SER:HB3	3:D:838:ARG:NE	2.25	0.49
3:D:1216:SER:HB3	4:E:15:SER:HB2	1.94	0.49
4:E:18:ARG:HA	4:E:21:VAL:HG12	1.95	0.49
1:A:142:VAL:HG12	1:A:143:ARG:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:LEU:HB3	2:C:202:TYR:CD2	2.42	0.49
2:C:198:ARG:NH1	2:C:229:MET:O	2.45	0.49
2:C:234:ALA:HA	2:C:237:ARG:CB	2.34	0.49
2:C:409:ARG:HD3	2:C:452:ILE:CG2	2.42	0.49
2:C:905:ILE:C	2:C:907:ASP:H	2.16	0.49
5:F:194:LEU:HD12	7:H:6:DT:H5'	1.94	0.49
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.47	0.49
1:A:227:ASN:HD22	1:A:227:ASN:C	2.15	0.49
2:C:204:GLN:HB2	2:C:227:PHE:CE1	2.47	0.49
2:C:616:GLU:O	2:C:616:GLU:HG2	2.12	0.49
2:C:760:SER:HB2	2:C:788:THR:CG2	2.37	0.49
3:D:172:PRO:HB2	3:D:175:VAL:HG23	1.95	0.49
3:D:372:ASP:HB3	3:D:374:GLU:OE1	2.13	0.49
5:F:102:LEU:O	5:F:106:VAL:HG23	2.13	0.49
1:B:107:LYS:HG2	1:B:108:GLU:N	2.27	0.49
2:C:144:PRO:CG	2:C:165:LEU:HD23	2.43	0.49
2:C:214:TYR:CD2	2:C:218:VAL:CG2	2.96	0.49
2:C:772:ARG:HG2	2:C:772:ARG:HH11	1.77	0.49
2:C:878:SER:OG	3:D:1029:ARG:HD2	2.13	0.49
2:C:1016:ILE:O	3:D:87:ARG:NH2	2.46	0.49
2:C:1070:ILE:CG2	3:D:655:PRO:CB	2.90	0.49
3:D:674:ARG:O	3:D:678:GLU:HG2	2.12	0.49
3:D:1291:SER:OG	3:D:1302:GLU:HG3	2.13	0.49
3:D:1364:HIS:CD2	3:D:1366:LYS:HD2	2.47	0.49
4:E:67:GLU:HB3	4:E:73:LEU:HD11	1.94	0.49
4:E:75:PHE:H	4:E:75:PHE:HD2	1.61	0.49
2:C:572:ILE:HG23	2:C:701:THR:O	2.13	0.48
4:E:43:GLU:HG2	4:E:44:GLU:N	2.28	0.48
1:B:102:LYS:HA	1:B:138:LEU:O	2.14	0.48
2:C:124:ASP:HA	2:C:592:LEU:HD13	1.94	0.48
2:C:196:LEU:O	2:C:196:LEU:HD22	2.13	0.48
2:C:263:ASP:C	2:C:265:ARG:H	2.16	0.48
2:C:266:ARG:O	2:C:266:ARG:HG3	2.13	0.48
2:C:362:GLY:O	2:C:363:SER:HB3	2.13	0.48
2:C:443:THR:OG1	2:C:444:PRO:CD	2.61	0.48
2:C:937:ASP:OD2	2:C:939:ARG:NH1	2.47	0.48
2:C:1067:TYR:O	2:C:1067:TYR:CD1	2.66	0.48
3:D:248:PRO:HA	3:D:307:ALA:O	2.14	0.48
3:D:371:ILE:HD13	5:F:232:ARG:HD3	1.95	0.48
3:D:572:ARG:HH12	5:F:83:GLN:HG2	1.78	0.48
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1495:ILE:HG12	4:E:88:GLU:HB3	1.95	0.48
5:F:231:ARG:HB3	5:F:233:PHE:CE2	2.48	0.48
5:F:360:LYS:O	5:F:361:LEU:HD23	2.13	0.48
2:C:64:LEU:HD23	2:C:102:HIS:HA	1.95	0.48
2:C:1019:GLN:HE21	3:D:621:LYS:HE3	1.76	0.48
3:D:167:GLU:OE2	3:D:198:ARG:HD3	2.14	0.48
3:D:584:ASN:H	3:D:602:SER:CB	2.26	0.48
3:D:1054:GLU:O	3:D:1056:PRO:HD3	2.13	0.48
3:D:1140:ILE:HG22	3:D:1144:LEU:HD12	1.95	0.48
5:F:368:VAL:HB	5:F:397:ILE:HD11	1.94	0.48
5:F:404:ALA:O	5:F:408:LEU:HG	2.13	0.48
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.94	0.48
3:D:62:LYS:HD2	3:D:63:TYR:CZ	2.49	0.48
3:D:569:ASN:ND2	5:F:84:TYR:CD2	2.81	0.48
3:D:708:LEU:N	3:D:708:LEU:HD23	2.27	0.48
3:D:832:ARG:HD3	3:D:832:ARG:H	1.78	0.48
3:D:1211:MET:HE2	4:E:16:LYS:HD2	1.95	0.48
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.47	0.48
1:B:56:VAL:HG23	1:B:142:VAL:HG22	1.95	0.48
2:C:215:GLY:HA2	2:C:219:GLN:HG3	1.95	0.48
2:C:615:TYR:HH	2:C:623:TYR:HH	1.49	0.48
3:D:131:LYS:H	3:D:456:MET:HE2	1.78	0.48
3:D:1141:GLU:CD	3:D:1168:MET:HE1	2.34	0.48
5:F:172:ARG:HH11	5:F:172:ARG:HG3	1.78	0.48
5:F:361:LEU:HD11	5:F:411:HIS:CB	2.28	0.48
1:A:137:ARG:HG2	1:A:138:LEU:H	1.79	0.48
2:C:516:ARG:HA	2:C:520:GLU:O	2.14	0.48
2:C:807:ARG:HB2	2:C:807:ARG:HE	1.58	0.48
3:D:63:TYR:CE2	3:D:73:CYS:HB2	2.48	0.48
3:D:483:HIS:CD2	3:D:484:PRO:HD2	2.48	0.48
3:D:699:VAL:HG13	3:D:760:ARG:HG3	1.95	0.48
3:D:864:VAL:CG1	3:D:865:THR:H	2.26	0.48
4:E:26:ARG:O	4:E:30:LEU:HD12	2.14	0.48
5:F:274:THR:O	5:F:277:GLN:HG2	2.13	0.48
7:H:3:DT:H2''	7:H:4:DA:H5'	1.96	0.48
1:A:91:ASN:HB2	1:A:119:ASP:OD2	2.14	0.48
1:B:205:VAL:CG2	1:B:209:GLU:HB3	2.44	0.48
2:C:958:THR:HG23	2:C:961:GLU:HG3	1.95	0.48
3:D:42:ASP:N	3:D:46:ASP:OD2	2.33	0.48
3:D:74:GLU:CD	3:D:74:GLU:H	2.17	0.48
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:179:VAL:HG11	3:D:191:LEU:HD22	1.96	0.48
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	2.29	0.48
5:F:153:PRO:C	5:F:156:VAL:HG12	2.34	0.48
5:F:392:VAL:HG21	5:F:396:ARG:CG	2.37	0.48
1:B:87:VAL:CG1	1:B:122:ILE:HD13	2.43	0.48
2:C:86:LYS:O	2:C:88:LEU:HD23	2.14	0.48
2:C:480:THR:HG22	2:C:481:ASP:N	2.28	0.48
3:D:208:PRO:CG	3:D:353:VAL:HG11	2.43	0.48
3:D:625:TYR:CD2	3:D:751:LEU:HD21	2.48	0.48
3:D:1111:ASP:CG	3:D:1203:LYS:HE2	2.34	0.48
1:B:118:ALA:O	1:B:119:ASP:HB2	2.13	0.48
3:D:368:VAL:HG23	3:D:377:VAL:CG2	2.44	0.48
3:D:408:GLU:OE1	3:D:408:GLU:HA	2.13	0.48
3:D:486:ARG:HG3	3:D:489:ARG:CZ	2.44	0.48
5:F:368:VAL:CB	5:F:397:ILE:HD11	2.43	0.48
2:C:554:ASP:HA	3:D:1061:PHE:CZ	2.49	0.48
2:C:755:LEU:HD23	2:C:825:VAL:HG21	1.96	0.48
3:D:63:TYR:HE2	3:D:73:CYS:HB2	1.79	0.48
3:D:82:LYS:O	3:D:85:VAL:HG22	2.14	0.48
3:D:1141:GLU:CG	3:D:1168:MET:HE1	2.43	0.48
3:D:1310:ARG:H	3:D:1310:ARG:HD2	1.79	0.48
3:D:1495:ILE:CG2	4:E:88:GLU:HG3	2.44	0.48
5:F:260:ILE:HG13	5:F:265:VAL:HG23	1.95	0.48
1:A:224:TYR:CD1	1:B:9:PRO:HG2	2.48	0.47
2:C:403:SER:O	2:C:407:LYS:HG3	2.13	0.47
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.49	0.47
3:D:704:ARG:CG	3:D:705:ALA:H	2.27	0.47
4:E:57:ASP:O	4:E:63:TRP:NE1	2.39	0.47
5:F:372:ARG:HA	5:F:372:ARG:NE	2.29	0.47
1:A:42:ARG:NE	1:B:35:THR:OG1	2.46	0.47
2:C:230:ARG:H	2:C:233:GLU:CG	2.26	0.47
2:C:565:GLN:O	2:C:567:GLN:N	2.48	0.47
2:C:725:ASP:C	2:C:726:ILE:HD12	2.35	0.47
3:D:169:TYR:O	3:D:392:SER:CB	2.63	0.47
3:D:1047:LYS:HG3	3:D:1053:PHE:CE2	2.49	0.47
3:D:1271:LYS:HG2	3:D:1272:ALA:O	2.14	0.47
5:F:112:ALA:HB2	5:F:176:ILE:CG2	2.45	0.47
5:F:325:LYS:N	5:F:325:LYS:HD2	2.29	0.47
1:A:18:ARG:HG3	1:A:18:ARG:NH1	2.24	0.47
1:A:64:GLU:O	1:A:75:VAL:HB	2.13	0.47
1:B:80:LEU:CB	3:D:844:ALA:HB2	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HG12	1:B:99:LEU:HD12	1.94	0.47
1:B:205:VAL:HG22	1:B:206:THR:H	1.80	0.47
2:C:195:LEU:CD1	2:C:237:ARG:HB3	2.39	0.47
2:C:882:LEU:HA	2:C:882:LEU:HD23	1.62	0.47
3:D:258:VAL:HA	3:D:296:GLU:O	2.13	0.47
3:D:810:GLU:OE2	3:D:810:GLU:N	2.21	0.47
3:D:868:TYR:CE2	3:D:869:MET:HG3	2.49	0.47
3:D:1057:VAL:HG23	3:D:1069:GLU:HB3	1.97	0.47
5:F:229:TYR:CE1	5:F:230:LYS:HG3	2.48	0.47
1:A:23:PHE:HE2	1:A:208:LEU:HD13	1.79	0.47
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.96	0.47
1:A:138:LEU:HD21	1:A:140:MET:CE	2.44	0.47
1:A:222:LEU:CD2	1:B:215:VAL:HG13	2.33	0.47
1:B:88:ARG:HB2	1:B:88:ARG:HH11	1.79	0.47
3:D:62:LYS:HB3	3:D:63:TYR:CD2	2.50	0.47
3:D:141:ILE:HD12	3:D:145:VAL:C	2.35	0.47
3:D:970:LYS:CA	3:D:973:GLN:HB3	2.42	0.47
5:F:374:GLY:HA3	5:F:378:GLY:N	2.29	0.47
1:A:225:PHE:HA	1:B:11:PHE:CD2	2.50	0.47
1:B:54:THR:HG21	1:B:145:ASP:OD1	2.14	0.47
2:C:144:PRO:HB3	2:C:270:GLY:H	1.80	0.47
2:C:271:GLU:OE1	2:C:271:GLU:O	2.33	0.47
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.95	0.47
5:F:184:ARG:O	5:F:188:ILE:HG13	2.14	0.47
1:A:201:THR:CG2	1:A:203:GLY:H	2.23	0.47
1:B:44:LEU:HD22	1:B:199:ILE:HD13	1.96	0.47
2:C:602:GLU:HG2	2:C:603:VAL:N	2.28	0.47
3:D:189:GLN:C	3:D:196:VAL:HG13	2.35	0.47
1:A:71:VAL:HG12	1:A:132:LEU:CD1	2.44	0.47
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.96	0.47
1:B:30:ARG:HH21	2:C:854:PRO:HB3	1.78	0.47
1:B:58:ILE:CB	1:B:61:VAL:HG21	2.43	0.47
1:B:162:ILE:O	1:B:163:ASN:HB2	2.15	0.47
2:C:425:PHE:HD1	3:D:1079:LYS:HE3	1.79	0.47
2:C:615:TYR:OH	2:C:623:TYR:OH	2.23	0.47
2:C:893:ALA:O	2:C:897:LEU:HG	2.14	0.47
2:C:987:ILE:CG2	2:C:988:VAL:N	2.78	0.47
3:D:103:TRP:HE1	3:D:604:THR:CG2	2.21	0.47
3:D:137:PRO:HG2	3:D:147:VAL:O	2.14	0.47
3:D:231:VAL:O	3:D:236:TYR:OH	2.29	0.47
3:D:363:ALA:HB2	3:D:381:ALA:HA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:485:SER:O	3:D:487:ALA:N	2.48	0.47
3:D:557:LEU:HD13	3:D:566:ILE:HG21	1.95	0.47
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.95	0.47
3:D:885:ILE:CG2	3:D:937:TYR:HD1	2.27	0.47
3:D:932:ASP:O	3:D:935:LYS:HB3	2.15	0.47
3:D:1282:ARG:HD2	3:D:1283:ILE:O	2.14	0.47
3:D:1405:GLU:HA	3:D:1408:ILE:HG12	1.96	0.47
3:D:1410:GLU:OE1	3:D:1412:LYS:HE3	2.15	0.47
5:F:299:TRP:CE3	5:F:303:ARG:HG2	2.49	0.47
2:C:21:ILE:HD11	2:C:461:VAL:HG11	1.96	0.47
2:C:701:THR:HA	2:C:831:ARG:O	2.15	0.47
3:D:689:ASP:HB3	4:E:51:LEU:CD1	2.42	0.47
3:D:767:HIS:CB	3:D:924:MET:HE1	2.45	0.47
3:D:235:ALA:HB1	3:D:319:ALA:O	2.15	0.47
3:D:800:LYS:NZ	3:D:819:GLY:O	2.48	0.47
3:D:885:ILE:HG23	3:D:937:TYR:HD1	1.79	0.47
5:F:278:LEU:O	5:F:282:LEU:HG	2.15	0.47
5:F:315:VAL:HG22	5:F:316:SER:N	2.30	0.47
6:G:6:DA:H2'	6:G:7:DT:H73	1.97	0.47
1:A:9:PRO:HB2	1:A:26:GLU:C	2.36	0.47
1:A:78:ILE:O	1:A:82:LEU:HG	2.14	0.47
2:C:502:PRO:O	2:C:503:LEU:HD23	2.14	0.47
3:D:15:PRO:O	3:D:19:ARG:HG3	2.15	0.47
3:D:217:LYS:CE	3:D:341:GLU:HG3	2.45	0.47
3:D:274:ARG:O	3:D:275:GLU:O	2.32	0.47
3:D:1110:ALA:N	3:D:1217:ILE:HD11	2.30	0.47
3:D:1148:VAL:HG22	3:D:1165:TYR:CD1	2.50	0.47
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.50	0.47
1:B:44:LEU:HD21	1:B:211:LEU:HA	1.97	0.46
2:C:64:LEU:HD23	2:C:64:LEU:HA	1.72	0.46
3:D:185:VAL:CG1	3:D:186:VAL:H	2.27	0.46
3:D:709:HIS:O	3:D:709:HIS:CD2	2.68	0.46
3:D:1057:VAL:HG13	3:D:1057:VAL:O	2.15	0.46
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.14	0.46
5:F:260:ILE:CD1	5:F:265:VAL:HG22	2.45	0.46
1:A:9:PRO:HD3	1:B:224:TYR:CD2	2.49	0.46
2:C:44:ILE:HD12	2:C:344:PHE:CE1	2.51	0.46
2:C:167:LYS:CE	7:H:12:DC:H5	2.28	0.46
2:C:182:VAL:HG23	2:C:193:LEU:HB2	1.96	0.46
3:D:67:ARG:NH2	5:F:377:ASP:OD2	2.48	0.46
3:D:800:LYS:HB3	3:D:822:ALA:CB	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:89:GLY:HA3	7:H:7:DG:C6	2.50	0.46
5:F:206:GLY:C	5:F:207:LEU:HD23	2.34	0.46
1:A:138:LEU:HD22	1:A:140:MET:HG3	1.95	0.46
1:B:96:THR:CG2	1:B:97:VAL:N	2.79	0.46
2:C:267:TYR:CE1	2:C:269:LEU:HD13	2.49	0.46
2:C:939:ARG:HH11	2:C:939:ARG:CG	2.28	0.46
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.80	0.46
2:C:954:THR:HB	2:C:957:LYS:HD2	1.96	0.46
3:D:401:TYR:HE1	3:D:446:VAL:CG1	2.29	0.46
3:D:1395:LEU:HD23	3:D:1395:LEU:N	2.29	0.46
3:D:1489:GLN:OE1	3:D:1493:LYS:HB2	2.16	0.46
3:D:1495:ILE:HG23	4:E:88:GLU:HG3	1.98	0.46
4:E:26:ARG:NE	4:E:67:GLU:OE1	2.47	0.46
5:F:197:SER:HA	5:F:200:LYS:CE	2.46	0.46
7:H:24:DC:H2"	7:H:25:DA:OP2	2.14	0.46
1:B:90:LEU:HD12	1:B:119:ASP:C	2.35	0.46
2:C:540:PHE:CD1	2:C:544:THR:HG21	2.51	0.46
2:C:577:PRO:HB3	2:C:993:PHE:CD1	2.51	0.46
2:C:1019:GLN:NE2	3:D:621:LYS:HB3	2.30	0.46
3:D:403:PHE:CZ	3:D:442:ASN:HA	2.51	0.46
3:D:930:LEU:O	3:D:933:ALA:HB3	2.15	0.46
1:A:86:VAL:HG13	1:A:124:ASN:OD1	2.16	0.46
2:C:165:LEU:HD11	2:C:270:GLY:HA2	1.97	0.46
2:C:567:GLN:HE22	2:C:999:HIS:HE2	1.64	0.46
2:C:1031:ARG:HA	3:D:622:ARG:HA	1.97	0.46
3:D:171:LEU:HD21	3:D:390:PRO:HG2	1.96	0.46
3:D:207:PHE:CZ	5:F:101:GLU:OE2	2.68	0.46
3:D:1267:ARG:NE	3:D:1331:ASP:OD2	2.49	0.46
5:F:235:PHE:O	5:F:236:SER:C	2.54	0.46
1:B:123:MET:O	1:B:125:PRO:HD3	2.16	0.46
2:C:56:GLU:O	2:C:360:LEU:HD21	2.14	0.46
2:C:167:LYS:HE3	7:H:12:DC:C5	2.51	0.46
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.97	0.46
2:C:312:ALA:O	2:C:317:VAL:HG23	2.14	0.46
2:C:322:VAL:HG12	2:C:323:ASP:H	1.80	0.46
2:C:918:LEU:HD23	2:C:918:LEU:HA	1.44	0.46
3:D:227:LEU:HD21	3:D:326:GLU:HG2	1.97	0.46
3:D:586:ARG:HD2	3:D:586:ARG:O	2.16	0.46
3:D:699:VAL:N	3:D:756:GLN:OE1	2.45	0.46
5:F:122:LEU:HB2	5:F:127:ILE:HD11	1.98	0.46
5:F:383:LEU:HD12	5:F:384:GLU:CG	2.39	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.45	0.46
1:B:115:LEU:HA	1:B:115:LEU:HD22	1.57	0.46
2:C:74:GLY:O	2:C:93:PRO:HD2	2.16	0.46
2:C:577:PRO:HG2	2:C:580:MET:CG	2.45	0.46
2:C:884:GLN:HB2	2:C:992:MET:CE	2.46	0.46
3:D:387:LEU:HD22	3:D:387:LEU:N	2.31	0.46
3:D:767:HIS:HA	3:D:924:MET:HE1	1.97	0.46
5:F:123:ASP:OD1	5:F:125:ASP:N	2.49	0.46
2:C:35:PRO:O	2:C:38:LYS:N	2.44	0.46
3:D:12:LEU:HB2	3:D:507:ASN:OD1	2.16	0.46
3:D:245:LEU:HD22	3:D:249:TYR:HB3	1.97	0.46
3:D:357:GLU:HB2	3:D:387:LEU:HD23	1.98	0.46
3:D:838:ARG:HD2	3:D:874:GLU:OE1	2.16	0.46
3:D:955:VAL:HG22	3:D:1011:PHE:CE1	2.50	0.46
1:A:55:SER:HB2	1:A:158:ILE:O	2.16	0.46
2:C:235:LEU:HD12	2:C:235:LEU:O	2.15	0.46
2:C:557:ARG:HA	2:C:560:MET:HG3	1.98	0.46
3:D:702:LEU:O	3:D:713:ILE:HA	2.15	0.46
5:F:375:LEU:HD23	5:F:375:LEU:O	2.15	0.46
5:F:395:GLU:HB3	5:F:398:ARG:HH12	1.80	0.46
2:C:217:LEU:O	2:C:220:GLY:N	2.48	0.46
2:C:409:ARG:HG2	2:C:409:ARG:NH2	2.30	0.46
2:C:626:ARG:HD3	2:C:629:TYR:CD2	2.43	0.46
2:C:897:LEU:HD21	2:C:921:ALA:CB	2.46	0.46
2:C:1097:LEU:HD23	2:C:1097:LEU:HA	1.54	0.46
3:D:58:CYS:SG	3:D:62:LYS:HB2	2.55	0.46
3:D:832:ARG:H	3:D:832:ARG:CD	2.29	0.46
3:D:1305:LEU:HD12	3:D:1305:LEU:O	2.16	0.46
5:F:387:GLY:CA	5:F:394:ARG:HG2	2.46	0.46
2:C:92:ALA:O	2:C:117:HIS:HA	2.16	0.45
2:C:217:LEU:C	2:C:220:GLY:H	2.19	0.45
2:C:304:LEU:HD12	2:C:307:LEU:HD12	1.98	0.45
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.98	0.45
2:C:813:VAL:CG2	2:C:815:LEU:HD21	2.46	0.45
2:C:1083:GLU:OE1	2:C:1086:ARG:HD2	2.16	0.45
3:D:53:ILE:HG12	3:D:86:LYS:HD2	1.97	0.45
3:D:62:LYS:HD2	3:D:63:TYR:CE2	2.50	0.45
3:D:632:VAL:O	3:D:727:GLN:HA	2.15	0.45
3:D:767:HIS:HE1	4:E:6:ILE:HD13	1.81	0.45
3:D:838:ARG:CD	3:D:874:GLU:OE1	2.64	0.45
3:D:1208:ASP:O	3:D:1209:LEU:C	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:VAL:HG23	2:C:24:GLU:N	2.31	0.45
2:C:752:GLY:HA3	3:D:679:ARG:HA	1.99	0.45
2:C:834:GLN:NE2	3:D:724:GLN:HG2	2.31	0.45
2:C:984:GLU:HB2	3:D:944:THR:O	2.16	0.45
2:C:1065:ALA:CB	2:C:1077:PRO:HG3	2.46	0.45
3:D:186:VAL:HA	3:D:200:ASP:HA	1.97	0.45
3:D:236:TYR:CE1	3:D:242:LEU:CB	3.00	0.45
3:D:544:TYR:O	3:D:545:ARG:C	2.54	0.45
3:D:886:VAL:HG12	3:D:896:ALA:HB1	1.98	0.45
3:D:1109:GLU:C	3:D:1217:ILE:HD11	2.36	0.45
5:F:317:LEU:HD23	5:F:317:LEU:HA	1.56	0.45
5:F:353:GLU:HA	5:F:356:LYS:HB3	1.97	0.45
5:F:392:VAL:HG22	5:F:393:THR:H	1.80	0.45
1:A:65:PHE:HE2	2:C:703:ILE:HG23	1.82	0.45
2:C:65:VAL:O	2:C:65:VAL:CG2	2.65	0.45
2:C:214:TYR:O	2:C:218:VAL:HB	2.17	0.45
2:C:443:THR:HG21	3:D:1078:ARG:HE	1.81	0.45
2:C:495:THR:HG23	2:C:517:ARG:HG3	1.97	0.45
2:C:633:GLN:OE1	2:C:633:GLN:N	2.48	0.45
2:C:902:ILE:O	2:C:902:ILE:HG22	2.15	0.45
3:D:437:VAL:O	3:D:437:VAL:HG12	2.15	0.45
3:D:616:GLN:HG3	3:D:616:GLN:O	2.16	0.45
3:D:709:HIS:O	3:D:709:HIS:CG	2.69	0.45
3:D:796:ARG:NH1	3:D:862:ASP:OD1	2.49	0.45
5:F:135:ILE:HG23	5:F:136:LEU:N	2.32	0.45
1:B:101:LEU:HD11	1:B:109:VAL:HG11	1.98	0.45
2:C:831:ARG:NE	2:C:1002:GLU:OE1	2.49	0.45
2:C:1078:GLU:HG3	2:C:1079:PRO:HD2	1.98	0.45
3:D:70:GLY:N	3:D:80:VAL:HG23	2.30	0.45
3:D:314:PRO:HD2	3:D:317:VAL:HG11	1.97	0.45
3:D:324:ALA:HB1	3:D:331:VAL:CG2	2.46	0.45
3:D:377:VAL:HG23	3:D:377:VAL:O	2.17	0.45
3:D:563:PRO:HB3	5:F:189:GLU:CG	2.46	0.45
3:D:640:HIS:CD2	3:D:641:GLN:HG3	2.51	0.45
3:D:736:PHE:CD1	3:D:745:MET:HE2	2.52	0.45
3:D:775:GLY:CA	3:D:1209:LEU:HB3	2.46	0.45
1:A:107:LYS:CE	1:A:113:ASP:OD2	2.65	0.45
1:A:132:LEU:HD21	1:A:138:LEU:HB2	1.98	0.45
2:C:182:VAL:HG22	2:C:221:LEU:HD23	1.98	0.45
2:C:268:ASP:OD1	2:C:269:LEU:O	2.34	0.45
2:C:281:LEU:CD2	2:C:308:ARG:HH22	2.27	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:700:TYR:HB3	2:C:833:LEU:HD22	1.99	0.45
2:C:1001:VAL:HB	3:D:724:GLN:CB	2.46	0.45
3:D:371:ILE:CD1	5:F:232:ARG:NH1	2.79	0.45
3:D:1136:LYS:O	3:D:1140:ILE:HG13	2.17	0.45
3:D:1464:GLU:H	3:D:1464:GLU:HG3	1.60	0.45
5:F:156:VAL:O	5:F:160:ASP:HB2	2.16	0.45
5:F:395:GLU:HB3	5:F:398:ARG:NH1	2.31	0.45
5:F:414:ARG:HA	5:F:414:ARG:HH11	1.81	0.45
1:A:19:GLU:O	1:A:207:PRO:HG3	2.17	0.45
2:C:613:VAL:HG23	2:C:613:VAL:O	2.16	0.45
2:C:880:MET:HE3	3:D:1037:GLN:CD	2.37	0.45
3:D:93:ILE:CD1	3:D:548:ILE:CG1	2.94	0.45
3:D:284:LEU:HA	3:D:288:MET:HE2	1.97	0.45
3:D:286:VAL:CG2	3:D:314:PRO:HG3	2.46	0.45
3:D:397:LYS:HD2	3:D:397:LYS:HA	1.81	0.45
3:D:474:GLU:O	3:D:478:LEU:HG	2.16	0.45
3:D:653:PHE:O	3:D:656:PHE:N	2.49	0.45
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.99	0.45
3:D:1434:TRP:CD1	3:D:1457:ASP:HB2	2.51	0.45
5:F:215:GLU:O	5:F:218:GLN:HB3	2.17	0.45
5:F:412:GLU:OE1	5:F:416:ARG:HA	2.17	0.45
2:C:834:GLN:HE22	3:D:724:GLN:HG2	1.82	0.45
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.81	0.45
3:D:225:LEU:HD21	3:D:311:LEU:HD21	1.97	0.45
3:D:242:LEU:CD2	3:D:311:LEU:CD1	2.95	0.45
3:D:327:GLU:O	3:D:327:GLU:HG3	2.17	0.45
3:D:407:VAL:HA	3:D:422:ALA:CB	2.47	0.45
3:D:422:ALA:O	3:D:427:VAL:HG12	2.15	0.45
3:D:709:HIS:C	3:D:711:LEU:N	2.66	0.45
4:E:19:LEU:HD12	4:E:23:VAL:HG23	1.98	0.45
6:G:17:DC:H2'	6:G:18:DA:C8	2.51	0.45
1:A:118:ALA:O	1:A:119:ASP:HB2	2.17	0.45
2:C:16:PRO:O	2:C:18:LEU:HD23	2.16	0.45
2:C:607:ASP:OD1	2:C:608:GLY:N	2.49	0.45
3:D:796:ARG:HH22	3:D:859:ASP:CG	2.15	0.45
3:D:1057:VAL:HG23	3:D:1069:GLU:CG	2.47	0.45
3:D:1205:TYR:CE2	3:D:1366:LYS:HE2	2.50	0.45
3:D:1402:ALA:O	3:D:1405:GLU:HB3	2.17	0.45
5:F:324:GLU:OE2	6:G:19:DG:N2	2.50	0.45
1:A:89:PHE:CZ	1:A:97:VAL:HG23	2.52	0.45
2:C:9:ILE:HD11	2:C:500:ASN:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:137:VAL:HG21	2:C:393:GLN:NE2	2.32	0.45
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.98	0.45
2:C:214:TYR:HD2	2:C:218:VAL:CG2	2.30	0.45
2:C:539:VAL:O	2:C:539:VAL:CG1	2.65	0.45
2:C:720:GLU:HG2	2:C:760:SER:OG	2.17	0.45
2:C:742:VAL:CG1	2:C:803:THR:HG21	2.47	0.45
2:C:775:ARG:HB3	2:C:780:GLU:O	2.17	0.45
3:D:126:VAL:O	3:D:457:GLY:N	2.42	0.45
3:D:218:LYS:HB3	3:D:338:GLU:HG2	1.99	0.45
3:D:394:LEU:HD21	3:D:396:VAL:CG2	2.47	0.45
3:D:553:ARG:NH2	5:F:211:ASP:HA	2.31	0.45
3:D:650:LEU:CD1	3:D:657:LEU:CD2	2.91	0.45
3:D:876:SER:OG	3:D:879:ARG:HG3	2.17	0.45
3:D:1264:GLU:OE1	3:D:1264:GLU:HA	2.17	0.45
3:D:1405:GLU:HA	3:D:1408:ILE:CG1	2.47	0.45
4:E:37:ASN:OD1	4:E:37:ASN:N	2.38	0.45
5:F:88:ILE:HG13	5:F:192:LEU:HB2	1.98	0.45
1:B:68:ILE:HG21	1:B:71:VAL:HG21	1.98	0.45
2:C:21:ILE:HD12	2:C:455:LEU:HD22	1.99	0.45
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.52	0.45
2:C:480:THR:HG22	2:C:481:ASP:H	1.82	0.45
2:C:718:GLY:HA3	2:C:761:PHE:CE1	2.51	0.45
3:D:127:LEU:HD23	3:D:127:LEU:HA	1.74	0.45
3:D:446:VAL:O	3:D:446:VAL:CG1	2.65	0.45
3:D:528:VAL:O	3:D:535:PHE:HA	2.17	0.45
3:D:749:VAL:HG12	3:D:750:PRO:O	2.17	0.45
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.47	0.45
2:C:99:GLN:O	2:C:99:GLN:HG2	2.17	0.44
2:C:213:ALA:HB3	2:C:214:TYR:CE1	2.51	0.44
2:C:490:GLU:O	2:C:493:ARG:HB2	2.17	0.44
2:C:936:VAL:HG11	2:C:959:PRO:CB	2.47	0.44
3:D:26:VAL:HG12	3:D:548:ILE:CD1	2.44	0.44
3:D:180:LYS:HA	3:D:205:TYR:OH	2.17	0.44
3:D:230:TRP:HA	3:D:243:ALA:HB2	1.98	0.44
3:D:348:GLN:HB2	3:D:351:MET:CE	2.47	0.44
3:D:368:VAL:HB	3:D:377:VAL:HG22	1.98	0.44
3:D:625:TYR:CD2	3:D:751:LEU:HD11	2.51	0.44
3:D:1012:GLU:HB2	3:D:1021:TYR:OH	2.17	0.44
3:D:1129:THR:C	3:D:1131:SER:H	2.21	0.44
3:D:1487:VAL:O	4:E:74:VAL:HG23	2.15	0.44
5:F:114:LYS:HA	5:F:117:SER:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:360:LYS:HB3	5:F:411:HIS:CD2	2.52	0.44
1:A:49:PRO:O	1:A:173:PRO:HG3	2.17	0.44
2:C:598:GLU:N	2:C:615:TYR:OH	2.46	0.44
3:D:645:PRO:HG3	3:D:724:GLN:O	2.17	0.44
3:D:851:LEU:HD11	3:D:855:HIS:HE1	1.82	0.44
3:D:885:ILE:CG2	3:D:937:TYR:CD1	2.99	0.44
3:D:1045:MET:O	3:D:1052:THR:HG23	2.17	0.44
3:D:1108:ARG:NH2	3:D:1198:TYR:HB3	2.32	0.44
4:E:84:ARG:HD3	4:E:84:ARG:HA	1.41	0.44
5:F:287:THR:HG23	5:F:290:GLU:OE2	2.16	0.44
1:A:201:THR:CG2	1:A:205:VAL:O	2.64	0.44
2:C:586:ARG:O	2:C:589:ARG:HB2	2.17	0.44
2:C:769:PRO:HD2	3:D:65:ARG:NH2	2.33	0.44
2:C:880:MET:CE	3:D:1037:GLN:CB	2.93	0.44
2:C:983:ILE:HG22	2:C:985:GLY:H	1.83	0.44
2:C:1008:ARG:CD	2:C:1028:GLY:O	2.65	0.44
2:C:1060:ILE:HD11	2:C:1083:GLU:HB2	2.00	0.44
3:D:25:GLU:HG3	3:D:92:HIS:NE2	2.32	0.44
3:D:85:VAL:C	3:D:87:ARG:N	2.69	0.44
3:D:181:ASP:OD1	3:D:205:TYR:HB2	2.18	0.44
3:D:586:ARG:HD2	3:D:586:ARG:C	2.38	0.44
3:D:845:ASN:C	3:D:845:ASN:OD1	2.56	0.44
3:D:1189:ARG:HH11	3:D:1203:LYS:HD2	1.83	0.44
1:B:36:LEU:HB3	1:B:37:GLY:H	1.57	0.44
1:B:100:LEU:HD23	1:B:141:GLU:CG	2.47	0.44
2:C:495:THR:OG1	2:C:517:ARG:NE	2.50	0.44
2:C:507:ARG:HB2	2:C:507:ARG:HH11	1.82	0.44
2:C:950:LEU:HB2	2:C:952:LEU:HD22	1.99	0.44
2:C:1008:ARG:NE	3:D:624:ASP:OD1	2.50	0.44
3:D:808:THR:HB	3:D:810:GLU:OE2	2.17	0.44
5:F:148:LYS:HD3	5:F:148:LYS:HA	1.48	0.44
1:A:117:VAL:HB	1:A:120:VAL:CG2	2.47	0.44
1:A:201:THR:CG2	1:A:202:ASP:N	2.81	0.44
1:B:108:GLU:HB2	1:B:110:LYS:NZ	2.33	0.44
2:C:17:PRO:O	2:C:20:GLU:HG2	2.17	0.44
2:C:340:MET:SD	2:C:340:MET:C	2.96	0.44
2:C:388:ARG:HG3	2:C:388:ARG:HH11	1.81	0.44
2:C:617:ASP:HB2	2:C:619:ARG:HH22	1.83	0.44
2:C:987:ILE:HG22	2:C:988:VAL:N	2.32	0.44
2:C:1067:TYR:O	2:C:1071:ILE:HD13	2.17	0.44
4:E:14:ASP:OD2	4:E:14:ASP:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:362:SER:O	5:F:366:ALA:CB	2.66	0.44
1:B:86:VAL:HG12	1:B:124:ASN:CG	2.37	0.44
1:B:94:LEU:HD23	1:B:95:GLN:H	1.80	0.44
2:C:193:LEU:HG	2:C:197:LEU:CD1	2.42	0.44
2:C:358:ARG:HE	2:C:358:ARG:HB2	1.51	0.44
2:C:578:VAL:HG13	2:C:671:ASN:OD1	2.17	0.44
3:D:701:LEU:HD13	3:D:763:MET:CE	2.46	0.44
3:D:1374:GLN:OE1	3:D:1374:GLN:HA	2.16	0.44
8:I:2:C:H2'	8:I:3:A:C8	2.53	0.44
1:A:48:ILE:O	1:A:173:PRO:HD3	2.17	0.44
1:B:208:LEU:HD12	1:B:212:ASN:OD1	2.18	0.44
2:C:182:VAL:HG11	2:C:311:PHE:CZ	2.53	0.44
2:C:717:LEU:N	2:C:717:LEU:CD1	2.81	0.44
2:C:751:PRO:CA	2:C:792:VAL:CG2	2.92	0.44
3:D:132:TYR:HE2	3:D:155:ASP:OD2	2.01	0.44
3:D:1097:LYS:HD3	3:D:1425:THR:OG1	2.18	0.44
3:D:1294:VAL:O	3:D:1294:VAL:HG22	2.18	0.44
5:F:317:LEU:HD22	5:F:330:GLY:HA2	1.99	0.44
1:B:84:GLU:OE2	3:D:867:ARG:NH1	2.50	0.44
2:C:44:ILE:HD13	2:C:44:ILE:HA	1.58	0.44
2:C:701:THR:HG23	2:C:831:ARG:O	2.18	0.44
2:C:905:ILE:O	2:C:907:ASP:N	2.51	0.44
2:C:1019:GLN:CD	3:D:621:LYS:HB3	2.38	0.44
3:D:236:TYR:HB2	3:D:319:ALA:CB	2.47	0.44
3:D:396:VAL:HG12	3:D:397:LYS:N	2.31	0.44
3:D:422:ALA:H	3:D:427:VAL:HG13	1.83	0.44
3:D:699:VAL:CG1	3:D:760:ARG:CG	2.96	0.44
3:D:919:PHE:CE2	3:D:924:MET:HG2	2.53	0.44
3:D:1379:VAL:CG1	3:D:1397:LYS:HB2	2.47	0.44
3:D:1485:GLN:O	4:E:75:PHE:HA	2.18	0.44
7:H:2:DA:H2'	7:H:2:DA:O5'	2.18	0.44
1:A:180:GLN:HG3	2:C:934:PHE:HD1	1.78	0.44
1:B:6:LEU:HD13	1:B:6:LEU:C	2.39	0.44
2:C:97:ARG:HG3	2:C:112:GLU:HB2	1.98	0.44
2:C:102:HIS:CB	2:C:107:LEU:HB3	2.37	0.44
2:C:619:ARG:HB2	2:C:619:ARG:NH2	2.30	0.44
3:D:236:TYR:CZ	3:D:242:LEU:HB2	2.53	0.44
3:D:237:LYS:HB3	3:D:237:LYS:HE2	1.82	0.44
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.00	0.44
3:D:1263:PHE:HD2	3:D:1375:MET:HE1	1.81	0.44
4:E:8:LYS:HA	4:E:8:LYS:HD2	1.69	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:6:DA:H2'	6:G:7:DT:H72	1.99	0.44
2:C:140:ILE:HG22	2:C:412:ALA:HA	1.99	0.43
2:C:182:VAL:HG23	2:C:193:LEU:CB	2.48	0.43
3:D:566:ILE:HG22	3:D:567:ILE:N	2.33	0.43
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.21	0.43
4:E:30:LEU:HD23	4:E:35:PHE:HD1	1.83	0.43
1:A:121:GLU:HB3	1:A:123:MET:CE	2.47	0.43
1:A:216:GLU:CD	1:A:219:ARG:NH2	2.72	0.43
2:C:211:LEU:HB3	2:C:218:VAL:HG21	1.99	0.43
2:C:277:ALA:HA	2:C:280:LYS:HB3	1.99	0.43
2:C:503:LEU:HD22	2:C:508:ILE:HA	1.99	0.43
2:C:679:PHE:CE1	2:C:853:LEU:HD11	2.53	0.43
2:C:841:ASN:HD22	2:C:992:MET:CE	2.29	0.43
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.58	0.43
3:D:373:PRO:O	3:D:376:GLU:HG3	2.17	0.43
3:D:982:PHE:O	3:D:983:LEU:CG	2.64	0.43
3:D:1275:SER:O	3:D:1322:GLY:N	2.48	0.43
5:F:201:LYS:HB2	5:F:201:LYS:HE3	1.80	0.43
2:C:69:LEU:HB2	2:C:97:ARG:O	2.18	0.43
3:D:298:VAL:HA	3:D:302:GLN:OE1	2.18	0.43
3:D:396:VAL:CG1	3:D:397:LYS:N	2.82	0.43
3:D:701:LEU:HB2	3:D:748:HIS:HB2	2.00	0.43
3:D:1023:MET:HB2	3:D:1023:MET:HE2	1.73	0.43
5:F:129:GLU:O	5:F:132:ARG:HB3	2.18	0.43
5:F:161:GLN:C	5:F:163:LEU:H	2.21	0.43
1:A:54:THR:HG22	1:A:158:ILE:HB	2.00	0.43
1:B:133:GLU:O	1:B:136:GLY:N	2.52	0.43
2:C:585:GLU:HG3	2:C:665:PHE:CD2	2.53	0.43
3:D:639:LEU:HA	3:D:639:LEU:HD12	1.74	0.43
3:D:646:LYS:HB3	3:D:646:LYS:HE2	1.80	0.43
3:D:652:LEU:HB3	3:D:749:VAL:HG21	1.99	0.43
3:D:676:MET:HE2	3:D:683:ILE:HA	2.00	0.43
3:D:1029:ARG:O	3:D:1030:GLY:O	2.36	0.43
3:D:1057:VAL:CG2	3:D:1069:GLU:HB3	2.48	0.43
5:F:161:GLN:OE1	5:F:164:LYS:NZ	2.49	0.43
5:F:166:LEU:HD13	5:F:170:HIS:HB3	2.00	0.43
5:F:204:GLY:C	5:F:205:ARG:HG2	2.38	0.43
5:F:374:GLY:N	5:F:378:GLY:HA2	2.34	0.43
1:A:65:PHE:CE2	2:C:703:ILE:HG23	2.53	0.43
1:A:115:LEU:HD21	1:A:117:VAL:HG23	2.00	0.43
1:A:176:ARG:CG	1:A:177:VAL:N	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:GLN:HB2	2:C:117:HIS:HB3	2.01	0.43
2:C:109:LYS:HG3	2:C:369:PRO:HD2	2.00	0.43
3:D:508:ARG:HD2	3:D:508:ARG:HA	1.84	0.43
3:D:677:LEU:H	3:D:677:LEU:HG	1.65	0.43
3:D:1273:VAL:N	3:D:1326:THR:CG2	2.80	0.43
5:F:383:LEU:HG	5:F:384:GLU:OE2	2.19	0.43
1:A:23:PHE:CD2	1:A:211:LEU:CD2	3.02	0.43
1:B:106:PRO:HB3	1:B:134:GLU:CG	2.49	0.43
1:B:124:ASN:ND2	1:B:127:LEU:CD1	2.74	0.43
2:C:149:THR:HA	2:C:322:VAL:CG1	2.47	0.43
3:D:658:LEU:HA	3:D:661:MET:HE2	1.99	0.43
3:D:659:LYS:O	3:D:662:GLU:N	2.45	0.43
3:D:828:LYS:HB2	3:D:833:GLU:OE2	2.18	0.43
3:D:1099:VAL:HG13	3:D:1223:ILE:HD13	2.00	0.43
1:B:28:LEU:HD23	1:B:32:PHE:HB3	2.01	0.43
1:B:222:LEU:HA	1:B:222:LEU:HD23	1.80	0.43
2:C:292:ARG:HD3	2:C:299:LYS:HB2	2.00	0.43
2:C:858:MET:HG2	2:C:867:VAL:O	2.19	0.43
2:C:1085:PHE:CE1	3:D:1468:LEU:CD2	3.00	0.43
3:D:828:LYS:HE2	3:D:831:GLY:N	2.27	0.43
3:D:1492:LEU:HD13	3:D:1492:LEU:C	2.39	0.43
5:F:228:GLU:OE2	5:F:231:ARG:NE	2.37	0.43
1:B:7:LYS:NZ	1:B:186:LEU:HD13	2.34	0.43
1:B:29:GLU:HG3	1:B:30:ARG:N	2.33	0.43
2:C:309:TYR:CE2	2:C:320:HIS:HA	2.53	0.43
2:C:715:THR:CG2	2:C:717:LEU:HD13	2.49	0.43
2:C:743:VAL:HG13	2:C:755:LEU:HA	2.00	0.43
2:C:1045:ALA:HB1	3:D:758:GLU:OE2	2.19	0.43
3:D:133:ILE:O	3:D:133:ILE:CG2	2.67	0.43
3:D:401:TYR:HE1	3:D:446:VAL:HG12	1.82	0.43
3:D:1268:PRO:HG3	3:D:1329:ALA:HB3	2.00	0.43
1:A:82:LEU:HD23	1:A:129:ILE:HD12	1.99	0.43
2:C:422:ARG:HH22	7:H:13:DT:C3'	2.31	0.43
2:C:438:ILE:HD11	2:C:467:ILE:CD1	2.49	0.43
2:C:723:THR:CG2	2:C:759:THR:HG23	2.49	0.43
3:D:343:LYS:HG2	3:D:345:TYR:HE2	1.84	0.43
3:D:357:GLU:OE2	3:D:387:LEU:HD23	2.18	0.43
3:D:658:LEU:HD21	3:D:674:ARG:HA	2.01	0.43
3:D:659:LYS:NZ	3:D:663:GLU:HB2	2.34	0.43
3:D:767:HIS:HE1	4:E:3:GLU:HB2	1.84	0.43
3:D:935:LYS:HB3	3:D:935:LYS:HE3	1.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:2:C:H2'	8:I:3:A:H8	1.83	0.43
2:C:343:GLN:HG3	2:C:385:PHE:CB	2.31	0.43
2:C:524:VAL:HG22	2:C:528:GLU:CD	2.39	0.43
2:C:632:ASN:HB2	2:C:633:GLN:OE1	2.19	0.43
2:C:755:LEU:N	2:C:755:LEU:HD12	2.34	0.43
2:C:1072:LYS:O	2:C:1072:LYS:HD3	2.19	0.43
3:D:211:VAL:HG23	3:D:347:VAL:CG2	2.49	0.43
3:D:694:VAL:HG12	3:D:695:ILE:N	2.33	0.43
3:D:921:ARG:O	3:D:921:ARG:HG2	2.19	0.43
5:F:363:GLU:HG3	5:F:363:GLU:O	2.19	0.43
1:B:80:LEU:HD22	3:D:844:ALA:CA	2.49	0.42
1:B:108:GLU:HA	1:B:131:THR:HA	2.00	0.42
2:C:65:VAL:CG2	2:C:101:ILE:HG23	2.41	0.42
2:C:767:PRO:HB2	2:C:772:ARG:HG2	2.00	0.42
2:C:769:PRO:HD2	3:D:65:ARG:CZ	2.49	0.42
2:C:906:PHE:CE2	3:D:1067:VAL:CA	3.01	0.42
2:C:997:LEU:N	2:C:997:LEU:HD23	2.33	0.42
2:C:1031:ARG:HH21	2:C:1031:ARG:HG3	1.84	0.42
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	2.01	0.42
5:F:159:ILE:HD13	5:F:159:ILE:HA	1.82	0.42
5:F:217:ASN:O	5:F:218:GLN:C	2.58	0.42
2:C:1067:TYR:O	2:C:1067:TYR:CG	2.71	0.42
2:C:1109:VAL:HG11	3:D:5:VAL:CG2	2.49	0.42
3:D:597:ASP:O	3:D:599:PRO:HD3	2.19	0.42
3:D:659:LYS:O	3:D:660:LYS:C	2.58	0.42
3:D:949:ILE:HD11	3:D:1023:MET:CE	2.49	0.42
5:F:177:ALA:O	5:F:180:GLY:N	2.52	0.42
5:F:366:ALA:O	5:F:370:LYS:HB2	2.18	0.42
2:C:722:ILE:HD13	2:C:722:ILE:HA	1.85	0.42
2:C:940:GLU:OE1	2:C:963:LEU:HD11	2.20	0.42
2:C:1090:LYS:HE2	2:C:1112:PHE:CE2	2.54	0.42
3:D:413:ASP:N	3:D:435:VAL:CG1	2.82	0.42
3:D:417:PRO:HG3	3:D:430:ASP:O	2.19	0.42
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	2.00	0.42
4:E:3:GLU:OE2	4:E:4:PRO:HD2	2.19	0.42
5:F:194:LEU:HA	7:H:6:DT:O4'	2.19	0.42
5:F:390:PHE:HB3	5:F:397:ILE:HD13	2.00	0.42
1:B:94:LEU:O	1:B:95:GLN:HG3	2.18	0.42
3:D:57:GLU:HG3	3:D:64:LYS:HG2	2.01	0.42
3:D:348:GLN:CG	3:D:351:MET:HE1	2.50	0.42
3:D:984:THR:HG23	3:D:987:GLU:OE2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1264:GLU:O	3:D:1265:ALA:HB3	2.20	0.42
5:F:260:ILE:HG13	5:F:260:ILE:O	2.20	0.42
1:A:70:GLY:H	2:C:607:ASP:CG	2.20	0.42
1:B:109:VAL:O	1:B:110:LYS:HD2	2.19	0.42
1:B:206:THR:OG1	1:B:209:GLU:HB2	2.19	0.42
2:C:461:VAL:O	2:C:461:VAL:HG23	2.18	0.42
2:C:724:ARG:HD2	2:C:738:ASP:O	2.19	0.42
2:C:889:HIS:HE1	2:C:988:VAL:HG13	1.84	0.42
2:C:1055:LEU:HD21	2:C:1079:PRO:HB3	2.00	0.42
2:C:1058:ASP:OD2	2:C:1084:SER:HB2	2.20	0.42
3:D:237:LYS:O	3:D:240:GLU:HB2	2.20	0.42
6:G:4:DG:H2''	6:G:5:DC:O5'	2.20	0.42
2:C:97:ARG:HA	2:C:112:GLU:HA	2.02	0.42
2:C:205:GLU:O	2:C:209:ARG:HB3	2.19	0.42
2:C:206:THR:HA	2:C:209:ARG:CB	2.41	0.42
2:C:480:THR:HG22	2:C:482:GLU:H	1.85	0.42
2:C:946:ARG:HH21	2:C:946:ARG:CG	2.29	0.42
2:C:988:VAL:HG23	3:D:948:THR:HG23	1.98	0.42
3:D:111:LYS:HD2	3:D:1452:ILE:CD1	2.50	0.42
3:D:144:GLY:O	3:D:145:VAL:CG2	2.67	0.42
3:D:417:PRO:CB	3:D:430:ASP:O	2.67	0.42
3:D:465:LEU:HD23	3:D:510:GLU:HA	2.00	0.42
3:D:1041:LEU:H	3:D:1041:LEU:CD2	2.32	0.42
3:D:1045:MET:HG3	3:D:1073:SER:HA	2.01	0.42
3:D:1281:VAL:CG2	3:D:1316:GLY:H	2.33	0.42
4:E:30:LEU:CD2	4:E:35:PHE:HD1	2.31	0.42
1:A:104:GLU:HG3	1:A:137:ARG:HA	2.02	0.42
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.54	0.42
2:C:168:ARG:HE	2:C:345:ARG:NH1	2.18	0.42
2:C:310:LEU:HD12	2:C:310:LEU:O	2.19	0.42
2:C:336:VAL:HG13	2:C:337:GLY:N	2.34	0.42
2:C:744:ARG:NH1	2:C:746:GLY:O	2.53	0.42
2:C:890:LEU:HD12	2:C:890:LEU:O	2.19	0.42
2:C:940:GLU:O	2:C:944:LEU:HD12	2.19	0.42
2:C:1009:SER:HA	3:D:625:TYR:HD1	1.84	0.42
3:D:368:VAL:HG23	3:D:377:VAL:HG21	2.02	0.42
3:D:657:LEU:HG	3:D:661:MET:CE	2.50	0.42
1:A:222:LEU:HD23	1:B:215:VAL:CG1	2.34	0.42
1:B:74:ASP:OD2	3:D:872:ARG:NH1	2.52	0.42
2:C:348:LEU:CD1	2:C:378:LEU:HD22	2.50	0.42
2:C:552:HIS:CD2	2:C:886:LEU:HD22	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:26:VAL:CG1	3:D:548:ILE:HD13	2.43	0.42
3:D:477:LEU:HD22	3:D:492:ALA:HA	2.01	0.42
3:D:524:LEU:HD23	3:D:524:LEU:N	2.33	0.42
3:D:545:ARG:NH1	5:F:254:GLN:O	2.52	0.42
3:D:658:LEU:HA	3:D:661:MET:HE3	2.02	0.42
3:D:704:ARG:HG2	3:D:705:ALA:N	2.35	0.42
3:D:757:ALA:O	3:D:761:ILE:HG13	2.19	0.42
5:F:94:LEU:HD13	5:F:99:GLU:HA	2.02	0.42
5:F:234:LYS:HD3	7:H:5:DA:P	2.59	0.42
5:F:336:GLU:H	5:F:336:GLU:HG2	1.49	0.42
2:C:728:HIS:O	2:C:729:LEU:HD12	2.19	0.42
2:C:808:ARG:CG	2:C:814:GLU:HA	2.46	0.42
2:C:897:LEU:N	2:C:897:LEU:HD23	2.34	0.42
2:C:946:ARG:HG3	2:C:946:ARG:NH2	2.27	0.42
2:C:1036:GLU:CD	2:C:1036:GLU:H	2.23	0.42
3:D:147:VAL:HG12	3:D:151:GLN:HE22	1.85	0.42
3:D:180:LYS:HB2	3:D:205:TYR:OH	2.19	0.42
3:D:325:GLU:O	3:D:325:GLU:CG	2.68	0.42
3:D:394:LEU:CG	3:D:396:VAL:HG23	2.49	0.42
3:D:416:ALA:HB2	3:D:432:TYR:CE1	2.55	0.42
3:D:618:LEU:CB	3:D:1467:ILE:HG23	2.50	0.42
3:D:803:GLY:HA2	3:D:826:PRO:O	2.19	0.42
3:D:1194:CYS:SG	3:D:1200:VAL:HA	2.60	0.42
5:F:88:ILE:CG2	5:F:193:ARG:HG2	2.49	0.42
2:C:99:GLN:O	2:C:99:GLN:CG	2.68	0.42
2:C:378:LEU:HD12	2:C:378:LEU:O	2.20	0.42
2:C:983:ILE:C	2:C:985:GLY:N	2.73	0.42
3:D:247:GLU:HB2	3:D:248:PRO:CD	2.50	0.42
3:D:1234:THR:H	3:D:1235:GLN:HB3	1.80	0.42
5:F:421:PHE:N	5:F:421:PHE:CD1	2.88	0.42
1:A:12:THR:HG22	1:A:13:VAL:H	1.85	0.41
1:A:129:ILE:HD13	1:A:129:ILE:HA	1.87	0.41
1:A:173:PRO:HD2	1:A:174:VAL:HG23	2.01	0.41
1:B:127:LEU:HD23	1:B:128:HIS:O	2.20	0.41
1:B:153:ALA:C	1:B:155:LYS:H	2.23	0.41
2:C:194:VAL:HG13	2:C:221:LEU:HD21	2.02	0.41
2:C:742:VAL:HG12	2:C:743:VAL:O	2.20	0.41
3:D:65:ARG:CG	5:F:377:ASP:HA	2.48	0.41
3:D:192:ALA:O	3:D:193:PRO:C	2.58	0.41
3:D:206:ARG:CG	3:D:392:SER:O	2.68	0.41
3:D:676:MET:O	3:D:682:ASP:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1171:VAL:HG12	3:D:1175:ILE:HD11	2.02	0.41
4:E:30:LEU:HD23	4:E:35:PHE:CD1	2.54	0.41
5:F:310:ILE:C	5:F:312:GLN:H	2.24	0.41
5:F:321:ILE:HB	5:F:327:SER:OG	2.20	0.41
5:F:372:ARG:HE	5:F:372:ARG:CA	2.31	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.82	0.41
1:A:54:THR:O	1:A:156:HIS:HE1	2.02	0.41
1:B:185:ARG:NH2	3:D:689:ASP:OD1	2.45	0.41
1:B:211:LEU:O	1:B:214:ALA:HB3	2.19	0.41
2:C:1006:HIS:CB	2:C:1024:LYS:HG3	2.48	0.41
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	2.03	0.41
3:D:1130:ARG:HB3	3:D:1130:ARG:HH11	1.85	0.41
3:D:1341:PRO:O	3:D:1345:GLU:HG3	2.20	0.41
5:F:271:LEU:H	5:F:271:LEU:CD1	2.29	0.41
1:A:143:ARG:NH1	1:A:143:ARG:HG3	2.35	0.41
1:B:58:ILE:CG2	1:B:61:VAL:HG21	2.50	0.41
2:C:111:ASP:OD1	2:C:112:GLU:N	2.52	0.41
2:C:644:VAL:CG2	2:C:645:VAL:N	2.83	0.41
2:C:806:LEU:HD23	2:C:806:LEU:N	2.34	0.41
2:C:1047:HIS:CE1	3:D:1471:LEU:HD11	2.55	0.41
2:C:1068:GLU:HA	2:C:1071:ILE:HD11	2.02	0.41
3:D:407:VAL:HA	3:D:422:ALA:HB1	2.03	0.41
3:D:450:TYR:CD2	3:D:450:TYR:N	2.88	0.41
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.55	0.41
3:D:976:GLN:HA	3:D:979:GLU:HB3	2.02	0.41
3:D:1141:GLU:HG2	3:D:1168:MET:CE	2.50	0.41
5:F:167:PRO:HD2	5:F:170:HIS:HB2	2.01	0.41
5:F:354:LEU:HD12	5:F:354:LEU:C	2.40	0.41
1:B:96:THR:CG2	1:B:97:VAL:H	2.33	0.41
2:C:115:LEU:HD23	2:C:115:LEU:HA	1.83	0.41
2:C:546:LEU:HA	2:C:546:LEU:HD23	1.78	0.41
2:C:675:ALA:O	2:C:870:ILE:HA	2.20	0.41
2:C:987:ILE:HD13	2:C:987:ILE:HA	1.86	0.41
2:C:1030:GLN:HB2	3:D:626:SER:OG	2.20	0.41
3:D:41:ARG:HA	3:D:46:ASP:CG	2.41	0.41
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.83	0.41
3:D:132:TYR:HD1	3:D:454:ALA:O	2.03	0.41
3:D:162:ARG:O	3:D:414:ARG:NH2	2.44	0.41
3:D:704:ARG:O	3:D:705:ALA:C	2.58	0.41
3:D:1197:ARG:O	3:D:1198:TYR:HB2	2.20	0.41
3:D:1293:PHE:CZ	3:D:1302:GLU:HB2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:171:LYS:CD	5:F:175:HIS:HE1	2.24	0.41
6:G:18:DA:H2'	6:G:19:DG:O5'	2.20	0.41
1:A:9:PRO:HD2	1:B:224:TYR:CD2	2.56	0.41
1:B:26:GLU:CD	1:B:194:LYS:HG3	2.40	0.41
1:B:86:VAL:CG1	1:B:86:VAL:O	2.68	0.41
1:B:112:ARG:NH2	1:B:112:ARG:HB3	2.36	0.41
1:B:115:LEU:HD13	1:B:116:PRO:N	2.35	0.41
2:C:118:ILE:HD13	2:C:340:MET:CE	2.50	0.41
2:C:144:PRO:HD2	2:C:332:ARG:HD3	2.01	0.41
2:C:396:ASP:CG	2:C:402:SER:HB2	2.41	0.41
2:C:438:ILE:CD1	2:C:467:ILE:HD12	2.49	0.41
2:C:1009:SER:HA	3:D:625:TYR:CD1	2.56	0.41
3:D:18:ILE:HD13	3:D:516:ALA:O	2.20	0.41
3:D:64:LYS:O	3:D:65:ARG:CB	2.68	0.41
3:D:206:ARG:HD2	3:D:206:ARG:HA	1.80	0.41
3:D:767:HIS:CE1	4:E:6:ILE:HD13	2.54	0.41
3:D:767:HIS:CE1	4:E:6:ILE:HG12	2.55	0.41
3:D:794:GLN:OE1	3:D:794:GLN:HA	2.21	0.41
3:D:970:LYS:C	3:D:973:GLN:HB3	2.41	0.41
3:D:1208:ASP:C	3:D:1208:ASP:OD1	2.59	0.41
5:F:157:GLU:OE1	5:F:157:GLU:HA	2.20	0.41
1:B:101:LEU:HD21	1:B:109:VAL:HG11	2.01	0.41
2:C:360:LEU:N	2:C:360:LEU:HD22	2.36	0.41
2:C:492:ASP:HB3	2:C:518:LYS:HG3	2.02	0.41
2:C:743:VAL:CG2	2:C:800:VAL:HG11	2.49	0.41
2:C:750:LYS:C	2:C:792:VAL:HG21	2.39	0.41
2:C:890:LEU:HD11	2:C:901:TYR:CD2	2.55	0.41
2:C:961:GLU:O	2:C:964:LYS:HB3	2.20	0.41
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.55	0.41
3:D:111:LYS:HE2	3:D:1449:GLU:HG2	2.03	0.41
3:D:125:GLN:HA	3:D:130:SER:HB3	2.02	0.41
3:D:637:LEU:HD13	3:D:642:CYS:HA	2.03	0.41
3:D:936:TYR:CD2	3:D:936:TYR:C	2.94	0.41
3:D:1262:LEU:HD11	3:D:1351:GLU:HB3	2.02	0.41
3:D:1280:VAL:HG12	3:D:1318:TYR:HA	2.01	0.41
3:D:1482:ARG:NH1	3:D:1483:PHE:CZ	2.89	0.41
4:E:9:LEU:HD23	4:E:9:LEU:HA	1.81	0.41
6:G:6:DA:C2	6:G:7:DT:C2	3.08	0.41
1:B:64:GLU:HG3	1:B:79:ILE:HD12	2.02	0.41
2:C:185:LYS:O	2:C:186:VAL:HG23	2.19	0.41
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:882:LEU:HD11	3:D:1038:LEU:HD22	2.03	0.41
2:C:939:ARG:HG2	2:C:939:ARG:H	1.53	0.41
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.35	0.41
3:D:135:LEU:O	3:D:149:LYS:HE3	2.20	0.41
3:D:348:GLN:HG2	3:D:351:MET:CE	2.51	0.41
3:D:464:LEU:HA	3:D:464:LEU:HD12	1.81	0.41
3:D:492:ALA:O	3:D:496:LEU:HB2	2.20	0.41
3:D:800:LYS:HB3	3:D:822:ALA:HB2	2.03	0.41
3:D:1031:ASN:ND2	3:D:1034:GLN:OE1	2.54	0.41
1:B:57:TYR:O	1:B:140:MET:HB2	2.21	0.41
1:B:96:THR:O	1:B:97:VAL:CG2	2.68	0.41
2:C:76:PRO:HG3	2:C:120:LEU:CD1	2.50	0.41
2:C:85:GLU:OE2	2:C:802:ARG:NH2	2.53	0.41
2:C:626:ARG:N	2:C:639:GLN:HE21	2.17	0.41
2:C:641:PRO:O	2:C:642:ARG:HD3	2.21	0.41
2:C:781:LYS:HB2	2:C:781:LYS:HE3	1.85	0.41
3:D:348:GLN:HG2	3:D:351:MET:HE1	2.02	0.41
3:D:706:PRO:CG	11:I:101:CH1:O2	2.68	0.41
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.65	0.41
3:D:1259:VAL:HG23	3:D:1355:VAL:HG11	2.03	0.41
3:D:1495:ILE:HG12	4:E:88:GLU:CB	2.51	0.41
5:F:387:GLY:HA2	5:F:394:ARG:HG2	2.03	0.41
6:G:12:DG:H5"	6:G:12:DG:H8	1.86	0.41
1:A:154:GLU:H	1:A:154:GLU:CD	2.23	0.41
1:A:221:HIS:ND1	1:A:224:TYR:HE2	2.19	0.41
1:B:31:GLY:O	1:B:34:VAL:HG22	2.21	0.41
1:B:40:LEU:N	1:B:40:LEU:HD23	2.35	0.41
1:B:181:VAL:HG11	1:B:193:ASP:OD2	2.21	0.41
2:C:45:GLN:OE1	2:C:71:TYR:HE2	2.04	0.41
2:C:107:LEU:O	2:C:108:ILE:HD13	2.21	0.41
2:C:355:VAL:CG2	2:C:356:ARG:N	2.84	0.41
2:C:385:PHE:O	2:C:389:SER:HB2	2.21	0.41
2:C:492:ASP:HB3	2:C:518:LYS:CG	2.51	0.41
2:C:588:VAL:HG13	2:C:596:TYR:OH	2.20	0.41
2:C:1067:TYR:CD2	3:D:655:PRO:HG3	2.56	0.41
3:D:24:GLY:HA3	3:D:49:ILE:CG2	2.49	0.41
3:D:128:TYR:CE2	3:D:587:ARG:HD2	2.56	0.41
3:D:174:GLY:HA2	3:D:389:GLU:OE2	2.20	0.41
3:D:351:MET:CB	3:D:369:ALA:O	2.66	0.41
3:D:764:LEU:CD2	3:D:767:HIS:CD2	2.94	0.41
3:D:1015:TYR:CD2	3:D:1015:TYR:N	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1106:VAL:CG1	3:D:1107:VAL:N	2.84	0.41
3:D:1285:GLU:HG3	3:D:1290:LEU:HD22	2.01	0.41
3:D:1403:LEU:C	3:D:1403:LEU:HD12	2.41	0.41
3:D:1422:MET:HB3	3:D:1422:MET:HE2	1.82	0.41
5:F:115:LYS:HA	5:F:115:LYS:HD3	1.89	0.41
6:G:8:DC:H42	7:H:20:DG:H1	1.69	0.41
1:A:39:PRO:HG3	1:B:39:PRO:HG2	2.01	0.41
1:B:153:ALA:HB2	1:B:168:ASP:N	2.35	0.41
2:C:25:SER:HG	2:C:335:THR:HG1	1.50	0.41
2:C:261:ILE:HG22	2:C:291:ALA:HB3	2.03	0.41
2:C:599:GLU:HA	2:C:651:LYS:HG3	2.03	0.41
3:D:433:GLY:HA2	3:D:449:SER:O	2.20	0.41
3:D:498:VAL:O	3:D:501:ALA:HB3	2.21	0.41
3:D:706:PRO:HG2	11:I:101:CH1:O2	2.19	0.41
3:D:1404:ASN:O	3:D:1408:ILE:HG12	2.21	0.41
3:D:1491:THR:HG21	4:E:89:MET:HG2	2.03	0.41
5:F:79:ASP:C	5:F:79:ASP:OD1	2.59	0.41
5:F:210:LEU:O	5:F:211:ASP:C	2.59	0.41
5:F:372:ARG:NE	5:F:372:ARG:CA	2.84	0.41
5:F:393:THR:HG22	5:F:394:ARG:N	2.28	0.41
2:C:326:ASP:OD2	2:C:426:ASP:HB3	2.22	0.40
2:C:431:HIS:CE1	2:C:433:THR:HG1	2.34	0.40
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.34	0.40
2:C:767:PRO:HG2	2:C:782:ALA:CB	2.51	0.40
2:C:910:LYS:HD2	2:C:910:LYS:N	2.35	0.40
3:D:534:ARG:HE	3:D:534:ARG:HB3	1.33	0.40
3:D:563:PRO:CB	5:F:189:GLU:HG2	2.51	0.40
3:D:866:VAL:HG11	3:D:880:ILE:HG13	2.03	0.40
3:D:989:TYR:CE1	3:D:993:LEU:HD23	2.56	0.40
5:F:152:ASP:OD1	5:F:154:LYS:HB3	2.21	0.40
5:F:321:ILE:HD13	5:F:321:ILE:HA	1.80	0.40
5:F:415:THR:O	5:F:415:THR:OG1	2.35	0.40
1:B:26:GLU:CD	1:B:194:LYS:HE3	2.41	0.40
2:C:230:ARG:HB2	2:C:233:GLU:HG3	2.02	0.40
2:C:759:THR:HA	2:C:786:LYS:O	2.21	0.40
2:C:854:PRO:HB2	2:C:856:GLU:OE1	2.21	0.40
3:D:66:GLN:HB3	5:F:376:ILE:HG12	2.03	0.40
3:D:704:ARG:NH2	8:I:3:A:O2'	2.39	0.40
3:D:1148:VAL:CG2	3:D:1165:TYR:CE1	3.04	0.40
4:E:83:ASP:OD2	4:E:83:ASP:N	2.43	0.40
5:F:264:MET:HE3	5:F:264:MET:HB2	1.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:299:TRP:CD2	5:F:303:ARG:NH1	2.89	0.40
5:F:392:VAL:HG12	5:F:397:ILE:HD13	2.03	0.40
1:A:71:VAL:HA	1:A:131:THR:O	2.22	0.40
1:A:221:HIS:CD2	1:B:32:PHE:CD2	3.09	0.40
2:C:18:LEU:HD13	2:C:542:VAL:HG21	2.03	0.40
2:C:146:VAL:HG12	2:C:277:ALA:CB	2.51	0.40
2:C:545:ASN:HB3	2:C:583:LEU:CD2	2.51	0.40
2:C:655:LEU:HD12	2:C:655:LEU:N	2.36	0.40
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.55	0.40
3:D:211:VAL:HG23	3:D:347:VAL:HG23	2.03	0.40
3:D:325:GLU:O	3:D:325:GLU:HG2	2.21	0.40
3:D:462:GLN:O	3:D:462:GLN:HG2	2.20	0.40
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.03	0.40
3:D:657:LEU:HG	3:D:661:MET:HE1	2.03	0.40
3:D:884:ARG:HD2	3:D:888:GLU:OE1	2.20	0.40
3:D:899:LEU:HD22	3:D:917:GLN:HB3	2.02	0.40
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.95	0.40
3:D:1332:PRO:O	3:D:1335:LEU:HB3	2.21	0.40
4:E:14:ASP:OD2	4:E:18:ARG:HD2	2.21	0.40
5:F:193:ARG:HB3	7:H:7:DG:C5'	2.46	0.40
5:F:363:GLU:HA	5:F:366:ALA:HB3	2.03	0.40
1:A:57:TYR:HE2	1:A:59:GLU:HA	1.86	0.40
1:B:127:LEU:C	1:B:127:LEU:CD2	2.90	0.40
2:C:200:LEU:HD22	2:C:300:ASP:CB	2.18	0.40
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.57	0.40
2:C:617:ASP:OD1	2:C:617:ASP:N	2.54	0.40
2:C:874:LEU:HD23	2:C:874:LEU:HA	1.84	0.40
3:D:17:LYS:O	3:D:20:SER:N	2.55	0.40
3:D:116:LEU:CD2	3:D:468:LEU:HD11	2.51	0.40
3:D:1141:GLU:HG2	3:D:1168:MET:HE1	2.03	0.40
3:D:1281:VAL:HA	3:D:1293:PHE:O	2.22	0.40
3:D:1290:LEU:CB	3:D:1307:LYS:HG2	2.52	0.40
3:D:1305:LEU:HD12	3:D:1305:LEU:C	2.42	0.40
5:F:193:ARG:H	5:F:193:ARG:HG3	1.66	0.40
5:F:349:LEU:HD22	5:F:349:LEU:O	2.21	0.40
1:A:178:ALA:HB2	2:C:864:GLY:HA3	2.03	0.40
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.75	0.40
2:C:11:GLU:CD	2:C:537:LYS:HE2	2.41	0.40
2:C:339:LEU:CD1	2:C:391:LEU:HD12	2.51	0.40
2:C:405:ARG:HG3	2:C:543:ASN:OD1	2.22	0.40
2:C:588:VAL:HG22	2:C:594:ALA:HB2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:727:PRO:HB3	2:C:783:ARG:NH1	2.37	0.40
2:C:841:ASN:C	2:C:841:ASN:OD1	2.60	0.40
3:D:237:LYS:O	3:D:240:GLU:CB	2.70	0.40
3:D:284:LEU:N	3:D:284:LEU:CD1	2.84	0.40
3:D:416:ALA:CB	3:D:432:TYR:CE1	3.04	0.40
3:D:680:GLN:O	3:D:683:ILE:HD12	2.22	0.40
3:D:703:ASN:HB3	3:D:746:ALA:HB3	2.03	0.40
3:D:786:ILE:HD11	3:D:1027:GLY:C	2.41	0.40
3:D:882:PHE:CZ	3:D:906:GLN:HG3	2.56	0.40
3:D:1087:ARG:O	3:D:1088:THR:C	2.60	0.40
3:D:1088:THR:CG2	6:G:14:DG:C5	3.04	0.40
3:D:1281:VAL:HG23	3:D:1315:ASP:HA	2.03	0.40
3:D:1347:TYR:CE2	3:D:1351:GLU:HG3	2.57	0.40
5:F:217:ASN:O	5:F:220:LEU:N	2.55	0.40
5:F:260:ILE:HA	5:F:261:PRO:HD2	1.93	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:GLU:OE2	3:D:1151:ARG:NH1[3_545]	2.04	0.16
3:D:296:GLU:OE2	5:F:222:ARG:NH1[4_1149]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/315 (71%)	183 (82%)	40 (18%)	1 (0%)	34	72
1	B	222/315 (70%)	187 (84%)	33 (15%)	2 (1%)	17	55
2	C	1107/1119 (99%)	971 (88%)	133 (12%)	3 (0%)	41	76
3	D	1481/1505 (98%)	1302 (88%)	172 (12%)	7 (0%)	29	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	92/99 (93%)	81 (88%)	11 (12%)	0	100	100
5	F	344/423 (81%)	293 (85%)	51 (15%)	0	100	100
All	All	3470/3776 (92%)	3017 (87%)	440 (13%)	13 (0%)	34	72

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	GLY
3	D	276	ASP
1	A	154	GLU
1	B	36	LEU
3	D	275	GLU
3	D	705	ALA
3	D	486	ARG
3	D	710	ARG
2	C	984	GLU
3	D	783	ARG
3	D	1130	ARG
2	C	316	GLY
2	C	212	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%)	166 (83%)	33 (17%)	2	11
1	B	197/273 (72%)	180 (91%)	17 (9%)	10	37
2	C	936/941 (100%)	823 (88%)	113 (12%)	5	21
3	D	1249/1265 (99%)	1115 (89%)	134 (11%)	6	26
4	E	83/88 (94%)	77 (93%)	6 (7%)	14	45
5	F	301/371 (81%)	268 (89%)	33 (11%)	6	25
All	All	2965/3211 (92%)	2629 (89%)	336 (11%)	6	24

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	15	THR
1	A	18	ARG
1	A	25	LEU
1	A	46	SER
1	A	48	ILE
1	A	62	LEU
1	A	66	SER
1	A	68	ILE
1	A	76	VAL
1	A	85	LEU
1	A	86	VAL
1	A	90	LEU
1	A	96	THR
1	A	102	LYS
1	A	115	LEU
1	A	138	LEU
1	A	143	ARG
1	A	144	VAL
1	A	145	ASP
1	A	172	SER
1	A	175	ARG
1	A	182	GLU
1	A	184	THR
1	A	189	ARG
1	A	190	THR
1	A	199	ILE
1	A	205	VAL
1	A	206	THR
1	A	213	GLN
1	A	218	LEU
1	A	222	LEU
1	A	227	ASN
1	B	24	VAL
1	B	34	VAL
1	B	38	ASN
1	B	41	ARG
1	B	54	THR
1	B	55	SER
1	B	91	ASN
1	B	113	ASP
1	B	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	131	THR
1	B	158	ILE
1	B	163	ASN
1	B	183	ASP
1	B	184	THR
1	B	188	GLN
1	B	196	THR
1	B	208	LEU
2	C	2	GLU
2	C	8	ARG
2	C	21	ILE
2	C	37	GLU
2	C	44	ILE
2	C	49	ARG
2	C	64	LEU
2	C	65	VAL
2	C	75	GLU
2	C	105	THR
2	C	123	GLU
2	C	141	HIS
2	C	142	ARG
2	C	149	THR
2	C	154	ARG
2	C	157	ARG
2	C	162	ILE
2	C	163	ILE
2	C	174	LEU
2	C	177	GLU
2	C	183	SER
2	C	194	VAL
2	C	200	LEU
2	C	209	ARG
2	C	214	TYR
2	C	224	GLU
2	C	235	LEU
2	C	237	ARG
2	C	246	ASP
2	C	266	ARG
2	C	276	LYS
2	C	279	GLU
2	C	284	ARG
2	C	311	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	335	THR
2	C	342	ASP
2	C	351	LEU
2	C	353	ARG
2	C	356	ARG
2	C	364	GLU
2	C	366	SER
2	C	368	THR
2	C	376	ARG
2	C	387	SER
2	C	390	GLN
2	C	403	SER
2	C	404	LEU
2	C	409	ARG
2	C	426	ASP
2	C	427	VAL
2	C	432	ARG
2	C	433	THR
2	C	434	HIS
2	C	454	SER
2	C	460	ARG
2	C	481	ASP
2	C	490	GLU
2	C	493	ARG
2	C	514	VAL
2	C	516	ARG
2	C	533	ASP
2	C	534	VAL
2	C	538	GLN
2	C	542	VAL
2	C	560	MET
2	C	572	ILE
2	C	598	GLU
2	C	605	LYS
2	C	610	ARG
2	C	617	ASP
2	C	649	VAL
2	C	672	VAL
2	C	674	VAL
2	C	680	ASP
2	C	705	ILE
2	C	707	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	717	LEU
2	C	723	THR
2	C	730	SER
2	C	744	ARG
2	C	748	GLU
2	C	780	GLU
2	C	784	ASP
2	C	785	VAL
2	C	808	ARG
2	C	815	LEU
2	C	816	LYS
2	C	823	VAL
2	C	825	VAL
2	C	829	GLN
2	C	846	LYS
2	C	861	LEU
2	C	879	ARG
2	C	888	THR
2	C	897	LEU
2	C	900	ARG
2	C	929	ARG
2	C	930	LYS
2	C	939	ARG
2	C	946	ARG
2	C	952	LEU
2	C	954	THR
2	C	958	THR
2	C	968	LEU
2	C	1001	VAL
2	C	1005	MET
2	C	1014	SER
2	C	1052	MET
2	C	1060	ILE
2	C	1063	ARG
2	C	1080	SER
2	C	1084	SER
2	C	1115	LEU
3	D	6	ARG
3	D	10	ILE
3	D	25	GLU
3	D	48	ARG
3	D	53	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	58	CYS
3	D	73	CYS
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	133	ILE
3	D	141	ILE
3	D	143	ASN
3	D	153	LEU
3	D	171	LEU
3	D	176	ASP
3	D	180	LYS
3	D	187	LYS
3	D	199	LEU
3	D	202	VAL
3	D	217	LYS
3	D	220	ARG
3	D	230	TRP
3	D	231	VAL
3	D	249	TYR
3	D	270	LEU
3	D	275	GLU
3	D	284	LEU
3	D	289	THR
3	D	315	ARG
3	D	316	GLN
3	D	325	GLU
3	D	327	GLU
3	D	333	LEU
3	D	335	LEU
3	D	351	MET
3	D	361	VAL
3	D	371	ILE
3	D	378	ILE
3	D	380	GLU
3	D	389	GLU
3	D	392	SER
3	D	399	ARG
3	D	410	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	411	THR
3	D	415	VAL
3	D	434	ARG
3	D	445	ARG
3	D	447	VAL
3	D	448	GLU
3	D	478	LEU
3	D	485	SER
3	D	486	ARG
3	D	514	LEU
3	D	525	ARG
3	D	527	MET
3	D	528	VAL
3	D	534	ARG
3	D	538	SER
3	D	553	ARG
3	D	557	LEU
3	D	574	LEU
3	D	578	VAL
3	D	586	ARG
3	D	592	THR
3	D	600	LEU
3	D	603	LEU
3	D	621	LYS
3	D	623	VAL
3	D	654	LYS
3	D	660	LYS
3	D	677	LEU
3	D	679	ARG
3	D	686	GLU
3	D	693	GLU
3	D	699	VAL
3	D	709	HIS
3	D	719	VAL
3	D	754	PHE
3	D	771	SER
3	D	778	LEU
3	D	786	ILE
3	D	797	LYS
3	D	832	ARG
3	D	835	SER
3	D	836	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	863	VAL
3	D	907	GLU
3	D	943	THR
3	D	948	THR
3	D	961	LYS
3	D	966	GLU
3	D	968	ASP
3	D	973	GLN
3	D	982	PHE
3	D	986	ARG
3	D	993	LEU
3	D	997	THR
3	D	1015	TYR
3	D	1026	SER
3	D	1034	GLN
3	D	1041	LEU
3	D	1042	ARG
3	D	1065	LEU
3	D	1083	ASP
3	D	1090	ASP
3	D	1100	ASP
3	D	1114	THR
3	D	1126	ASP
3	D	1131	SER
3	D	1188	VAL
3	D	1208	ASP
3	D	1210	SER
3	D	1235	GLN
3	D	1280	VAL
3	D	1281	VAL
3	D	1310	ARG
3	D	1370	ILE
3	D	1376	MET
3	D	1390	LEU
3	D	1394	VAL
3	D	1400	VAL
3	D	1413	THR
3	D	1420	LEU
3	D	1424	VAL
3	D	1431	THR
3	D	1456	LYS
3	D	1468	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1470	ARG
3	D	1489	GLN
3	D	1493	LYS
4	E	8	LYS
4	E	15	SER
4	E	37	ASN
4	E	74	VAL
4	E	75	PHE
4	E	84	ARG
5	F	82	ARG
5	F	83	GLN
5	F	98	GLU
5	F	116	LEU
5	F	122	LEU
5	F	123	ASP
5	F	126	LEU
5	F	148	LYS
5	F	149	GLU
5	F	164	LYS
5	F	170	HIS
5	F	171	LYS
5	F	174	LEU
5	F	186	HIS
5	F	205	ARG
5	F	209	PHE
5	F	211	ASP
5	F	244	ARG
5	F	254	GLN
5	F	257	THR
5	F	293	GLU
5	F	304	VAL
5	F	319	THR
5	F	338	LEU
5	F	348	SER
5	F	360	LYS
5	F	367	MET
5	F	372	ARG
5	F	376	ILE
5	F	377	ASP
5	F	379	ARG
5	F	398	ARG
5	F	415	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	229	GLN
1	B	63	HIS
1	B	128	HIS
1	B	163	ASN
2	C	390	GLN
2	C	498	GLN
2	C	565	GLN
2	C	567	GLN
2	C	639	GLN
2	C	704	HIS
2	C	728	HIS
2	C	834	GLN
2	C	1050	GLN
3	D	294	HIS
3	D	348	GLN
3	D	640	HIS
3	D	703	ASN
3	D	709	HIS
3	D	717	GLN
3	D	767	HIS
3	D	909	ASN
3	D	1031	ASN
3	D	1034	GLN
3	D	1075	HIS
3	D	1195	GLN
3	D	1359	GLN
3	D	1441	GLN
3	D	1442	ASN
4	E	86	GLN
5	F	90	GLN
5	F	175	HIS
5	F	248	ASN
5	F	399	GLN

5.3.3 RNA ⓘ

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 monosaccharides 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	$\# Z > 2$
11	CH1	I	101	9	22,29,29	3.36	8 (36%)	27,45,45	1.63	7 (25%)

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
11	CH1	I	101	9	-	5/20/34/34	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	101	CH1	C3'-C2'	-10.67	1.24	1.52
11	I	101	CH1	O4'-C1'	-9.38	1.28	1.41
11	I	101	CH1	C2-N3	-3.52	1.31	1.38
11	I	101	CH1	C5'-C4'	-2.70	1.42	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	101	CH1	O4'-C4'	2.32	1.49	1.44
11	I	101	CH1	C2'-C1'	2.32	1.56	1.54
11	I	101	CH1	C5-C4	-2.24	1.35	1.41
11	I	101	CH1	C4-N4	2.18	1.41	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	101	CH1	O4'-C4'-C3'	-3.87	100.08	105.07
11	I	101	CH1	C2-N3-C4	3.22	119.61	116.34
11	I	101	CH1	PB-O3A-PA	-2.96	122.68	132.83
11	I	101	CH1	PB-O3B-PG	-2.20	125.28	132.83
11	I	101	CH1	C2'-C3'-C4'	2.06	106.82	102.94
11	I	101	CH1	O2'-C2'-C1'	-2.04	103.31	110.85
11	I	101	CH1	O4'-C4'-C5'	2.04	112.87	109.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	I	101	CH1	O4'-C1'-N1-C6
11	I	101	CH1	C3'-C4'-C5'-O5'
11	I	101	CH1	O4'-C4'-C5'-O5'
11	I	101	CH1	PB-O3A-PA-O1A
11	I	101	CH1	PB-O3A-PA-O2A

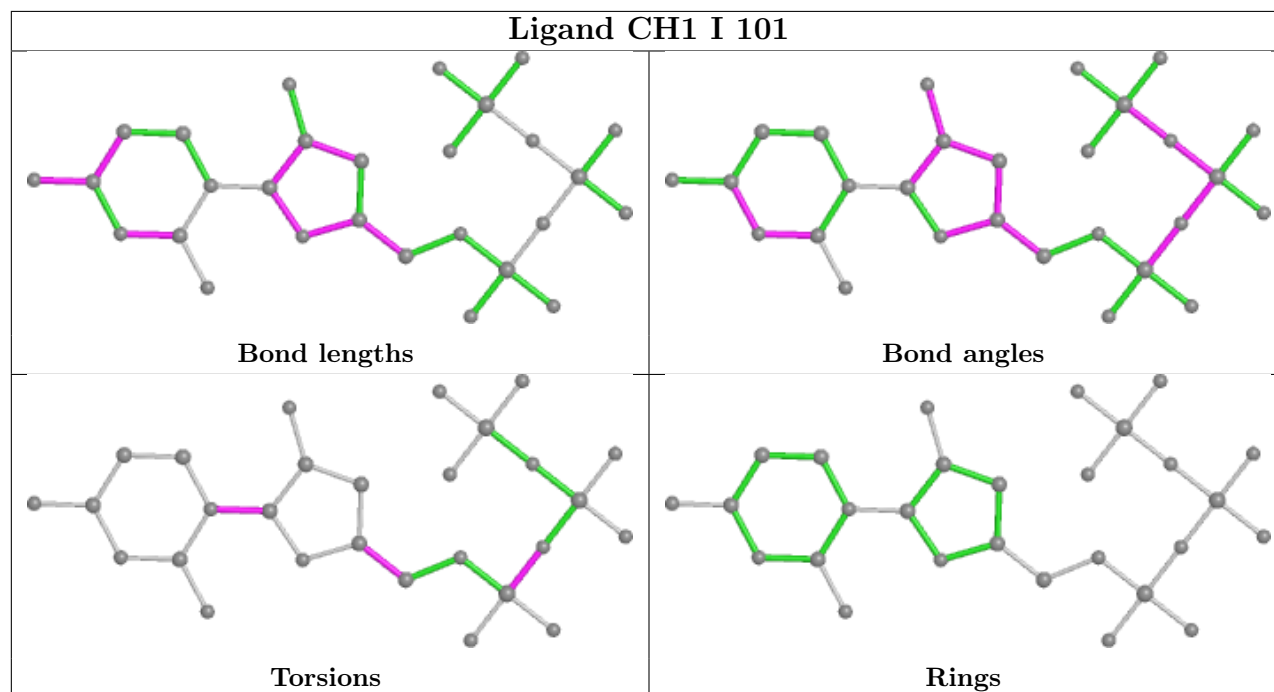
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	101	CH1	2	0

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

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/315 (71%)	-0.53	0 100 100	58, 79, 98, 110	0
1	B	224/315 (71%)	-0.49	0 100 100	59, 85, 110, 122	0
2	C	1111/1119 (99%)	-0.41	2 (0%) 95 87	47, 81, 125, 144	0
3	D	1485/1505 (98%)	-0.44	0 100 100	40, 75, 122, 141	0
4	E	94/99 (94%)	-0.43	0 100 100	57, 90, 116, 121	0
5	F	346/423 (81%)	-0.25	12 (3%) 44 18	57, 88, 138, 150	0
6	G	17/22 (77%)	-0.01	0 100 100	64, 92, 152, 155	0
7	H	25/27 (92%)	-0.32	0 100 100	77, 106, 149, 157	0
8	I	3/3 (100%)	-0.79	0 100 100	72, 72, 73, 75	0
All	All	3531/3828 (92%)	-0.42	14 (0%) 92 79	40, 81, 126, 157	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	360	LYS	3.4
5	F	376	ILE	3.3
5	F	375	LEU	3.2
2	C	219	GLN	3.0
5	F	381	HIS	2.9
5	F	392	VAL	2.6
5	F	382	THR	2.4
5	F	361	LEU	2.2
5	F	388	ALA	2.1
2	C	365	ASP	2.1
5	F	423	ASP	2.1
5	F	145	PRO	2.1
5	F	147	LEU	2.0
5	F	359	SER	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 monosaccharides in this entry.

6.4 Ligands [i](#)

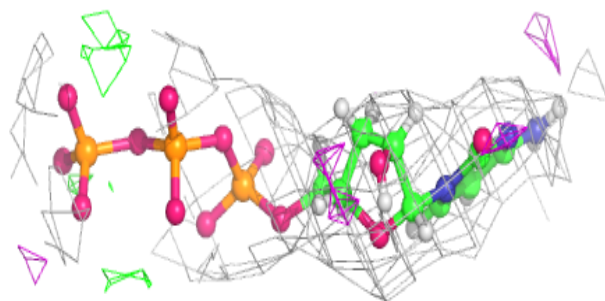
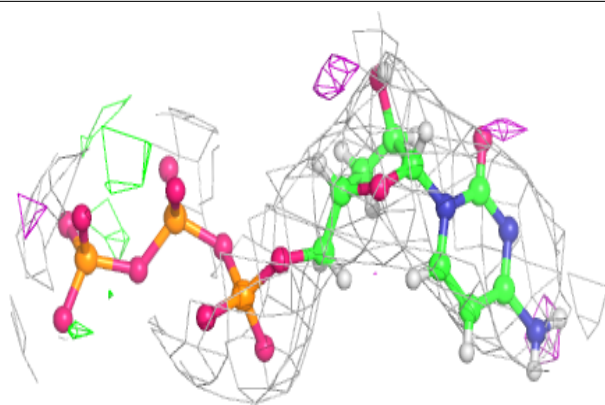
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	MG	D	2002	1/1	0.90	0.18	64,64,64,64	0
11	CH1	I	101	28/28	0.91	0.17	59,77,94,100	0
9	MG	D	2001	1/1	0.97	0.14	47,47,47,47	0
10	ZN	D	2004	1/1	0.98	0.17	76,76,76,76	0
10	ZN	D	2003	1/1	0.98	0.13	96,96,96,96	0

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

Electron density around CH1 I 101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.