



## Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 09:08 AM EST

PDB ID : 6W1N  
EMDB ID : EMD-21513  
Title : Pig Ryanodine Receptor (WT) in 5mM EGTA condition  
Authors : Woll, K.W.; Haji-Ghassemi, O.; Van Petegem, F.  
Deposited on : 2020-03-04  
Resolution : 4.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

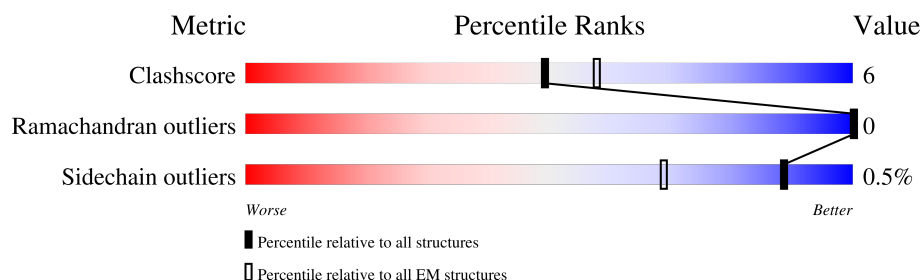
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	110	77% 17% . .
1	C	110	78% 16% . .
1	E	110	76% 18% . .
1	G	110	78% 16% . .
2	B	4624	71% 10% 20%
2	D	4624	71% 10% 20%
2	F	4624	71% 10% 20%
2	H	4624	71% 10% 20%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 105232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	106	Total	C	N	O	S	0	0
			730	465	128	133	4		
1	C	106	Total	C	N	O	S	0	0
			730	465	128	133	4		
1	E	106	Total	C	N	O	S	0	0
			730	465	128	133	4		
1	G	106	Total	C	N	O	S	0	0
			730	465	128	133	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P68106
A	-1	ASN	-	expression tag	UNP P68106
A	0	ALA	-	expression tag	UNP P68106
C	-2	SER	-	expression tag	UNP P68106
C	-1	ASN	-	expression tag	UNP P68106
C	0	ALA	-	expression tag	UNP P68106
E	-2	SER	-	expression tag	UNP P68106
E	-1	ASN	-	expression tag	UNP P68106
E	0	ALA	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	ASN	-	expression tag	UNP P68106
G	0	ALA	-	expression tag	UNP P68106

- Molecule 2 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3719	Total	C	N	O	S	1	0
			25577	16407	4433	4587	150		
2	D	3719	Total	C	N	O	S	1	0
			25577	16407	4433	4587	150		
2	F	3719	Total	C	N	O	S	1	0
			25577	16407	4433	4587	150		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	3719	Total	C	N	O	S	1	0
			25577	16407	4433	4587	150		


- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

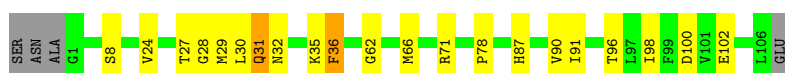
Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	F	1	Total	Zn	0
			1	1	
3	H	1	Total	Zn	0
			1	1	

### 3 Residue-property plots [i](#)


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

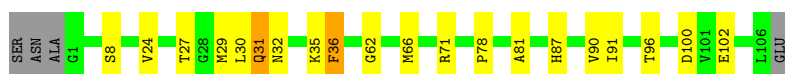
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain C: 




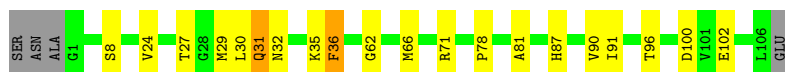
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 



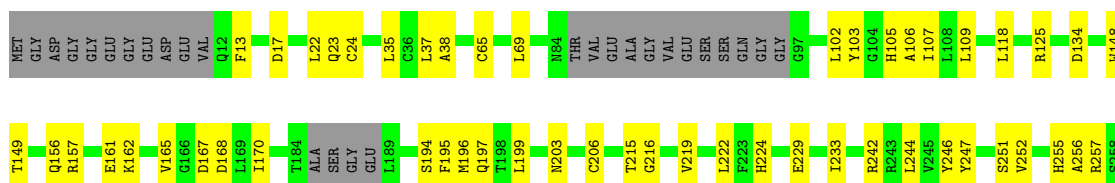
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 



- Molecule 2: Ryanodine Receptor

Chain B: 



L259	L260	L262	L265	G271	R275	R281	T286	T294	E295	D296	L299	C315	L323	ASP	THR	ALA	PRO	K328	Q349	Y359	A360	A361	PRO	PRO	LYS	ALA	LEU	ARG	LEU	GLY	VAL	L372	K373	K374	K375	L378	D385	I404	F414	L436								
G450	E453	N473	S476	Q479	E480	E481	G482	L486	D492	N495	K516	N520	L526	I530	R531	G532	N533	N536	W546	A360	A361	PRO	PRO	LYS	ALA	LEU	ARG	LEU	GLY	VAL	I621	T622	L632	L633	P646	N647	I648	Y659	W662	Y663								
V666	M667	V668	F674	T680	H681	L682	R683	V684	T689	E700	N705	F716	D717	G718	W722	P727	V744	C747	L773	L776	F777	F778	V787	K788	V789	R790	L839	S847	H848	T849	D850	F851	C854	F855	VAL	ASP	THR	VAL	ILE	VAL	LEU	PRO						
PRO	H866	I887	T928	T931	G940	E981	G982	Y989	L970	N994	Y1007	S1008	A1009	V1010	I1013	P1019	N1052	I1053	GLU	PRO	PRO	GLN	GLU	PRO	SER	GLN	VAL	SER	GLN	SER	TRP	ASP	R1071	R1076	A1077	ASP	THR	ALA	GLY	VAL	THR	PRO	LEU	ALA	PRO			
P1111	V1123	Q1130	H1131	W1132	W1143	I1153	D1154	N1158	L1164	G1200	K1240	S1241	L1242	P1243	Q1244	F1245	L1272	R1275	THR	PRO	GLY	GLN	ASN	S1282	L1289	R1290	L1293	Q1296	Q1299	HIS	PHE	ARG	CYS	THR	ALA	GLY	VAL	GLU	GLN	PRO	ALA	PRO	ARG	PRO				
GLY	LEU	GLN	PRO	PRO	ALA	ASP	GLU	ASP	PRO	ASP	TYR	GLU	ASN	LEU	ARG	SER	ALA	TRP	GLY	ALA	GLY	GLN	GLY	GLU	THR	GLY	VAL	GLY	PRO	GLY	THR	ALA	GLN	GLY	VAL	GLU	ALA	GLN	PRO	PRO	ARG	ALA	PRO	ALA				
GLU	ASN	LYS	THR	THR	GLY	LYS	LYS	ARG	PHE	LYS	ALA	LYS	ALA	MET	MET	THR	GLN	PRO	ALA	THR	THR	PRO	ARG	LEU	HIS	VAL	VAL	VAL	PRO	ALA	ARG	ASP	ASP	ILE	L1428	T1432	Y1435											
V1439	V1448	V1449	G1451	W1452	D1456	Y1457	H1458	Q1459	H1460	A1471	V1472	T1473	D1478	GLU	GLN	GLY	S1486	L1487	K1488	N1491	M1494	V1495	V1501	SER	PRO	GLN	GLY	ARG	ILE	SER	HIS	THR	D1513	C1518	L1519	V1520	M1527	T1538	F1539	K1547								
A1551	V1552	F1553	L1555	P1556	V1561	I1562	L1575	F1580	R1594	L1600	W1605	R1618	L1624	L1639	D1649	I1650	H1665	T1666	C1674	A1675	L1676	A1682	H1683	C1686	V1689	L1694	L1698	L1703	P1704	R1708	Y1712	D1713	L1714	S1717	H1718	I1719	L1720											
E1721	R1725	S1732	L1738	T1739	E1741	L1747	F1748	P1749	P1750	GLY	LYS	ARG	THR	GLU	ASN	P1764	S1771	L1772	C1782	F1783	V1784	A1785	P1788	ALA	VAL	GLY	ALA	ALA	E1794	P1801	L1816	F1837	P1841	V1846	S1847	T1848	M1852	G1853	I1854									
V1871	PHE	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	ASP	GLU	GLU	GLU	ALA	ARG	LYS	ASP	GLU	GLY	LYS	LEU	THR	ALA	GLU	GLY	L1816	F1837	P1841	V1846	S1847	T1848	E1925	E1945	E1951									
R1955	V1956	E1957	S1958	L1959	Y1978	K2014	ASP	GLY	GLU	ASP	P2023	C2043	Q2046	GLU	GLY	GLU	GLU	GLU	PRO	GLU	GLU	GLY	SER	ARG	LEU	MET	SER	LEU	GLU	VAL	LYS	VAL	LYS	LYS	GLY	TYR	LEU	GLU	SER	GLU	GLU	GLU	GLU					
PRO	PRO	ALA	GLU	GLU	SER	LYS	L2092	L2095	F2111	V2112	Q2113	S2114	L2117	V2118	N2121	F2122	S2123	L2124	R2127	Q2128	G2131	L2132	L2139	P2140	R2141	A2142	Y2143	P2147	N2154	L2157	L2168	L2198	V2215	L2216	Q2217	GLY	GLY	GLU	SER	GLU	GLU	GLU	GLU					
R2235	S2244	R2245	Q2246	G2263	ILE	GLY	GLY	LEU	MET	GLN	HIS	LEU	G2271	K2298	S2301	P2326	V2347	N2350	L2369	ARG	D2466	L2467	L2473	PRO	LEU	GLN	ILE	PRO	THR	LEU	GLY	ALA	ILE	ARG	ARG	PRO	GLY	VAL	ARG	ARG	ARG	ARG	ARG	GLU				
HIS	PHE	GLY	GLU	PRO	PRO	GLU	GLU	GLU	ASN	ARG	VAL	HIS	LEU	G2420	I2423	I2431	A2451	I2454	L2464	G2465	D2466	L2467	L2473	PRO	LEU	GLN	ILE	PRO	THR	LEU	GLY	LYS	ASP	GLY	VAL	GLN	F2489	R2490	R2491	S2492	A2493	V2496	P2497	D2498	Y2504	L2505	F2506	Y2511

- Molecule 2: Ryanodine Receptor















## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	52289	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.28	0/746	0.56	1/1019 (0.1%)
1	C	0.28	0/746	0.56	1/1019 (0.1%)
1	E	0.28	0/746	0.56	1/1019 (0.1%)
1	G	0.28	0/746	0.56	1/1019 (0.1%)
2	B	0.24	0/24464	0.41	1/33485 (0.0%)
2	D	0.24	0/24464	0.41	1/33485 (0.0%)
2	F	0.24	0/24464	0.41	1/33485 (0.0%)
2	H	0.24	0/24464	0.41	1/33485 (0.0%)
All	All	0.25	0/100840	0.42	8/138016 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	31	GLN	CA-CB-CG	5.80	126.15	113.40
1	A	31	GLN	CA-CB-CG	5.78	126.10	113.40
1	C	31	GLN	CA-CB-CG	5.78	126.11	113.40
1	G	31	GLN	CA-CB-CG	5.77	126.09	113.40
2	H	1554	VAL	C-N-CA	5.62	135.74	121.70
2	D	1554	VAL	C-N-CA	5.59	135.67	121.70
2	F	1554	VAL	C-N-CA	5.59	135.67	121.70
2	B	1554	VAL	C-N-CA	5.58	135.65	121.70

There are no chirality outliers.

There are no planarity outliers.

## 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	730	0	674	14	0
1	C	730	0	674	16	0
1	E	730	0	674	16	0
1	G	730	0	674	15	0
2	B	25577	0	21686	288	0
2	D	25577	0	21686	288	0
2	F	25577	0	21686	279	0
2	H	25577	0	21686	286	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	105232	0	89440	1180	0

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

All (1180) 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)
2:F:1561:VAL:HG12	2:F:1562:ILE:HG12	1.55	0.88
2:H:1561:VAL:HG12	2:H:1562:ILE:HG12	1.55	0.88
2:D:1561:VAL:HG12	2:D:1562:ILE:HG12	1.55	0.88
2:B:1561:VAL:HG12	2:B:1562:ILE:HG12	1.55	0.86
2:H:252:VAL:HA	2:H:255:HIS:HD2	1.45	0.81
2:F:252:VAL:HA	2:F:255:HIS:HD2	1.45	0.80
2:B:252:VAL:HA	2:B:255:HIS:HD2	1.45	0.79
2:D:1452:TRP:HE1	2:D:1518:CYS:HG	1.30	0.79
2:D:252:VAL:HA	2:D:255:HIS:HD2	1.45	0.79
2:H:2128:GLN:HA	2:H:2128:GLN:HE21	1.50	0.77
2:B:2128:GLN:HE21	2:B:2128:GLN:HA	1.50	0.76
2:F:2128:GLN:HE21	2:F:2128:GLN:HA	1.50	0.75
2:D:2128:GLN:HE21	2:D:2128:GLN:HA	1.50	0.74
2:H:3991:PHE:HA	2:H:3994:MET:HG2	1.70	0.74
2:B:3991:PHE:HA	2:B:3994:MET:HG2	1.70	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4706:THR:HG21	2:B:4773:TYR:HB2	1.70	0.74
2:D:4706:THR:HG21	2:D:4773:TYR:HB2	1.70	0.74
2:D:3991:PHE:HA	2:D:3994:MET:HG2	1.70	0.74
2:F:3991:PHE:HA	2:F:3994:MET:HG2	1.70	0.74
2:H:1452:TRP:HE1	2:H:1518:CYS:HG	1.35	0.74
2:F:4706:THR:HG21	2:F:4773:TYR:HB2	1.70	0.73
2:H:4706:THR:HG21	2:H:4773:TYR:HB2	1.70	0.73
1:A:24:VAL:HG13	1:A:102:GLU:H	1.54	0.73
1:C:24:VAL:HG13	1:C:102:GLU:H	1.54	0.73
2:D:252:VAL:HA	2:D:255:HIS:CD2	2.24	0.73
1:E:24:VAL:HG13	1:E:102:GLU:H	1.54	0.73
2:B:252:VAL:HA	2:B:255:HIS:CD2	2.24	0.73
2:F:252:VAL:HA	2:F:255:HIS:CD2	2.24	0.73
1:G:24:VAL:HG13	1:G:102:GLU:H	1.54	0.72
2:B:790:ARG:HD2	2:B:1624:LEU:HB3	1.72	0.72
2:D:790:ARG:HD2	2:D:1624:LEU:HB3	1.72	0.72
2:H:252:VAL:HA	2:H:255:HIS:CD2	2.24	0.71
2:F:790:ARG:HD2	2:F:1624:LEU:HB3	1.72	0.71
2:F:161:GLU:HG2	2:H:3979:ARG:NH2	2.06	0.71
2:B:4940:GLU:OE2	2:D:4942:ARG:NH1	2.24	0.71
2:B:4942:ARG:NH1	2:H:4940:GLU:OE2	2.24	0.71
2:F:4940:GLU:OE2	2:H:4942:ARG:NH1	2.24	0.71
2:B:161:GLU:HG2	2:D:3979:ARG:NH2	2.06	0.71
2:D:161:GLU:HG2	2:F:3979:ARG:NH2	2.06	0.71
2:D:4940:GLU:OE2	2:F:4942:ARG:NH1	2.24	0.71
1:A:29:MET:HG2	1:A:35:LYS:HB3	1.73	0.70
2:H:790:ARG:HD2	2:H:1624:LEU:HB3	1.72	0.70
1:G:29:MET:HG2	1:G:35:LYS:HB3	1.73	0.70
1:E:29:MET:HG2	1:E:35:LYS:HB3	1.73	0.70
2:F:1945:GLU:OE2	2:F:2127:ARG:NH2	2.25	0.70
1:C:29:MET:HG2	1:C:35:LYS:HB3	1.73	0.70
2:H:1945:GLU:OE2	2:H:2127:ARG:NH2	2.25	0.70
1:G:30:LEU:HD23	1:G:32:ASN:H	1.57	0.70
2:B:1452:TRP:HE1	2:B:1518:CYS:HG	1.38	0.69
2:B:1945:GLU:OE2	2:B:2127:ARG:NH2	2.25	0.69
2:B:3979:ARG:NH2	2:H:161:GLU:HG2	2.06	0.69
2:D:1945:GLU:OE2	2:D:2127:ARG:NH2	2.25	0.69
2:B:1555:LEU:HD12	2:B:1556:PRO:HD2	1.75	0.69
2:B:4919:PHE:HA	2:B:4923:ILE:HD13	1.75	0.69
2:H:4919:PHE:HA	2:H:4923:ILE:HD13	1.75	0.69
1:A:30:LEU:HD23	1:A:32:ASN:H	1.57	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1555:LEU:HD12	2:D:1556:PRO:HD2	1.75	0.68
2:D:663:TYR:HD1	2:D:747:CYS:HB2	1.58	0.68
2:B:663:TYR:HD1	2:B:747:CYS:HB2	1.58	0.68
2:D:4919:PHE:HA	2:D:4923:ILE:HD13	1.75	0.68
2:F:1555:LEU:HD12	2:F:1556:PRO:HD2	1.75	0.68
1:C:30:LEU:HD23	1:C:32:ASN:H	1.57	0.68
2:D:850:ASP:OD1	2:D:851:PHE:N	2.24	0.67
2:F:663:TYR:HD1	2:F:747:CYS:HB2	1.58	0.67
2:F:4919:PHE:HA	2:F:4923:ILE:HD13	1.75	0.67
1:E:30:LEU:HD23	1:E:32:ASN:H	1.57	0.67
2:H:663:TYR:HD1	2:H:747:CYS:HB2	1.58	0.67
2:H:1555:LEU:HD12	2:H:1556:PRO:HD2	1.75	0.67
2:B:168:ASP:HB3	2:B:199:LEU:HD11	1.77	0.67
2:F:168:ASP:HB3	2:F:199:LEU:HD11	1.77	0.67
2:D:168:ASP:HB3	2:D:199:LEU:HD11	1.77	0.66
2:F:103:TYR:CD1	2:F:161:GLU:HB2	2.31	0.66
2:D:103:TYR:CD1	2:D:161:GLU:HB2	2.31	0.66
2:H:168:ASP:HB3	2:H:199:LEU:HD11	1.77	0.66
2:H:4177:GLU:OE2	2:H:4981:HIS:NE2	2.29	0.66
2:D:1816:LEU:HD22	2:D:1846:VAL:HG21	1.78	0.66
2:F:850:ASP:OD1	2:F:851:PHE:N	2.24	0.66
2:B:4177:GLU:OE2	2:B:4981:HIS:NE2	2.29	0.65
2:H:103:TYR:CD1	2:H:161:GLU:HB2	2.31	0.65
2:B:103:TYR:CD1	2:B:161:GLU:HB2	2.31	0.65
2:B:887:ILE:HG12	2:B:959:TYR:HA	1.79	0.65
2:D:109:LEU:HD12	2:D:118:LEU:HD23	1.79	0.65
2:D:887:ILE:HG12	2:D:959:TYR:HA	1.79	0.65
2:F:4853:ALA:HA	2:F:4857:PHE:HD2	1.62	0.65
2:H:257:ARG:NH2	2:H:481:GLU:HG3	2.12	0.65
2:B:1816:LEU:HD22	2:B:1846:VAL:HG21	1.78	0.65
2:H:1739:THR:HG22	2:H:1741:GLU:H	1.62	0.65
2:B:257:ARG:NH2	2:B:481:GLU:HG3	2.12	0.65
2:B:1739:THR:HG22	2:B:1741:GLU:H	1.62	0.65
2:H:1816:LEU:HD22	2:H:1846:VAL:HG21	1.78	0.65
2:B:109:LEU:HD12	2:B:118:LEU:HD23	1.79	0.65
2:D:257:ARG:NH2	2:D:481:GLU:HG3	2.12	0.65
2:D:4668:ILE:HG23	2:D:4712:ASN:HD21	1.62	0.65
2:F:257:ARG:NH2	2:F:481:GLU:HG3	2.12	0.65
2:D:1739:THR:HG22	2:D:1741:GLU:H	1.62	0.65
2:F:4177:GLU:OE2	2:F:4981:HIS:NE2	2.29	0.64
2:B:4668:ILE:HG23	2:B:4712:ASN:HD21	1.62	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1739:THR:HG22	2:F:1741:GLU:H	1.62	0.64
2:B:1473:THR:HG22	2:B:1488:LYS:HD3	1.80	0.64
2:D:4177:GLU:OE2	2:D:4981:HIS:NE2	2.29	0.64
2:F:1473:THR:HG22	2:F:1488:LYS:HD3	1.80	0.64
2:H:887:ILE:HG12	2:H:959:TYR:HA	1.79	0.64
2:D:4853:ALA:HA	2:D:4857:PHE:HD2	1.62	0.64
2:H:1473:THR:HG22	2:H:1488:LYS:HD3	1.80	0.64
2:H:4853:ALA:HA	2:H:4857:PHE:HD2	1.62	0.64
2:F:887:ILE:HG12	2:F:959:TYR:HA	1.79	0.64
2:F:1816:LEU:HD22	2:F:1846:VAL:HG21	1.78	0.64
2:H:109:LEU:HD12	2:H:118:LEU:HD23	1.79	0.64
2:D:1473:THR:HG22	2:D:1488:LYS:HD3	1.80	0.64
2:B:850:ASP:OD1	2:B:851:PHE:N	2.24	0.63
2:D:2128:GLN:HE21	2:D:2128:GLN:CA	2.11	0.63
2:F:109:LEU:HD12	2:F:118:LEU:HD23	1.79	0.63
2:B:4560:LEU:HD21	2:B:4654:LEU:HB2	1.81	0.63
2:F:2128:GLN:HE21	2:F:2128:GLN:CA	2.11	0.63
2:F:4668:ILE:HG23	2:F:4712:ASN:HD21	1.62	0.63
2:D:3895:GLN:HB3	2:D:3971:ASN:HD21	1.64	0.63
2:H:4560:LEU:HD21	2:H:4654:LEU:HB2	1.81	0.63
2:H:2128:GLN:HE21	2:H:2128:GLN:CA	2.11	0.63
2:H:4668:ILE:HG23	2:H:4712:ASN:HD21	1.62	0.63
2:F:4560:LEU:HD21	2:F:4654:LEU:HB2	1.81	0.63
2:B:3895:GLN:HB3	2:B:3971:ASN:HD21	1.64	0.63
2:B:4853:ALA:HA	2:B:4857:PHE:HD2	1.62	0.63
2:B:2128:GLN:HE21	2:B:2128:GLN:CA	2.11	0.62
2:D:4560:LEU:HD21	2:D:4654:LEU:HB2	1.81	0.62
2:H:1747:LEU:HG	2:H:1748:PHE:HD1	1.64	0.62
2:B:633:LEU:HD23	2:B:1639:LEU:HD23	1.82	0.62
2:F:3895:GLN:HB3	2:F:3971:ASN:HD21	1.64	0.62
2:F:1738:LEU:HB2	2:F:2147:PRO:HD3	1.81	0.62
2:F:1747:LEU:HG	2:F:1748:PHE:HD1	1.65	0.62
2:D:1738:LEU:HB2	2:D:2147:PRO:HD3	1.82	0.62
2:B:1747:LEU:HG	2:B:1748:PHE:HD1	1.64	0.62
2:D:1747:LEU:HG	2:D:1748:PHE:HD1	1.64	0.62
2:H:850:ASP:OD1	2:H:851:PHE:N	2.24	0.62
2:H:3895:GLN:HB3	2:H:3971:ASN:HD21	1.64	0.62
2:D:495:ASN:HD22	2:D:550:LYS:HE3	1.64	0.62
2:F:1296:GLN:HG2	2:F:1547:LYS:HG2	1.82	0.62
2:F:495:ASN:HD22	2:F:550:LYS:HE3	1.64	0.61
2:F:633:LEU:HD23	2:F:1639:LEU:HD23	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1296:GLN:HG2	2:H:1547:LYS:HG2	1.82	0.61
2:H:1738:LEU:HB2	2:H:2147:PRO:HD3	1.81	0.61
2:B:1296:GLN:HG2	2:B:1547:LYS:HG2	1.82	0.61
2:F:404:ILE:HD13	2:F:481:GLU:HG2	1.82	0.61
2:H:495:ASN:HD22	2:H:550:LYS:HE3	1.64	0.61
2:B:1738:LEU:HB2	2:B:2147:PRO:HD3	1.82	0.61
2:H:633:LEU:HD23	2:H:1639:LEU:HD23	1.82	0.61
2:B:404:ILE:HD13	2:B:481:GLU:HG2	1.82	0.60
2:D:4706:THR:HG22	2:D:4708:SER:H	1.66	0.60
2:B:495:ASN:HD22	2:B:550:LYS:HE3	1.64	0.60
2:D:404:ILE:HD13	2:D:481:GLU:HG2	1.82	0.60
2:D:1296:GLN:HG2	2:D:1547:LYS:HG2	1.82	0.60
2:B:2454:ILE:HD12	2:B:2454:ILE:H	1.66	0.60
2:B:3671:ASP:OD1	2:B:3764:ARG:NH1	2.35	0.60
2:F:4706:THR:HG22	2:F:4708:SER:H	1.66	0.60
2:F:161:GLU:HG2	2:H:3979:ARG:HH22	1.67	0.60
2:F:1076:ARG:NH1	2:F:1077:ALA:O	2.35	0.60
2:H:404:ILE:HD13	2:H:481:GLU:HG2	1.82	0.60
2:H:2454:ILE:H	2:H:2454:ILE:HD12	1.66	0.60
2:H:4706:THR:HG22	2:H:4708:SER:H	1.66	0.60
2:B:1076:ARG:NH1	2:B:1077:ALA:O	2.35	0.60
2:H:4671:ARG:HH11	2:H:4780:VAL:HG13	1.67	0.60
2:B:1708:ARG:NH1	2:B:1837:PHE:O	2.35	0.60
2:D:633:LEU:HD23	2:D:1639:LEU:HD23	1.82	0.60
2:H:1708:ARG:NH1	2:H:1837:PHE:O	2.35	0.60
2:B:4671:ARG:HH11	2:B:4780:VAL:HG13	1.67	0.59
2:B:4706:THR:HG22	2:B:4708:SER:H	1.66	0.59
2:D:23:GLN:OE1	2:D:203:ASN:ND2	2.35	0.59
2:D:4671:ARG:HH11	2:D:4780:VAL:HG13	1.67	0.59
2:B:3985:VAL:HG23	2:B:4046:SER:HB3	1.85	0.59
2:H:3671:ASP:OD1	2:H:3764:ARG:NH1	2.35	0.59
2:F:244:LEU:HD23	2:F:375:LYS:HE3	1.85	0.59
2:D:2454:ILE:HD12	2:D:2454:ILE:H	1.66	0.59
1:E:29:MET:HA	1:E:35:LYS:HA	1.84	0.59
2:D:1076:ARG:NH1	2:D:1077:ALA:O	2.35	0.59
2:H:244:LEU:HD23	2:H:375:LYS:HE3	1.85	0.59
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.35	0.59
2:D:3671:ASP:OD1	2:D:3764:ARG:NH1	2.35	0.59
2:B:161:GLU:HG2	2:D:3979:ARG:HH22	1.67	0.59
2:B:244:LEU:HD23	2:B:375:LYS:HE3	1.85	0.59
2:D:940:GLY:O	2:D:1052:ASN:ND2	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:GLN:OE1	2:H:203:ASN:ND2	2.35	0.59
2:H:1076:ARG:NH1	2:H:1077:ALA:O	2.35	0.59
2:D:3985:VAL:HG23	2:D:4046:SER:HB3	1.85	0.59
2:F:2454:ILE:HD12	2:F:2454:ILE:H	1.66	0.59
2:F:3671:ASP:OD1	2:F:3764:ARG:NH1	2.35	0.59
2:H:359:TYR:HE1	2:H:385:ASP:HB3	1.68	0.59
2:D:359:TYR:HE1	2:D:385:ASP:HB3	1.68	0.59
2:F:359:TYR:HE1	2:F:385:ASP:HB3	1.68	0.58
2:F:1708:ARG:NH1	2:F:1837:PHE:O	2.35	0.58
1:A:29:MET:HA	1:A:35:LYS:HA	1.84	0.58
2:D:1708:ARG:NH1	2:D:1837:PHE:O	2.35	0.58
2:H:940:GLY:O	2:H:1052:ASN:ND2	2.36	0.58
2:D:244:LEU:HD23	2:D:375:LYS:HE3	1.85	0.58
2:F:4671:ARG:HH11	2:F:4780:VAL:HG13	1.67	0.58
1:G:29:MET:HA	1:G:35:LYS:HA	1.84	0.58
2:B:3979:ARG:HH22	2:H:161:GLU:HG2	1.67	0.58
1:C:29:MET:HA	1:C:35:LYS:HA	1.84	0.58
2:F:23:GLN:OE1	2:F:203:ASN:ND2	2.35	0.58
2:F:940:GLY:O	2:F:1052:ASN:ND2	2.36	0.58
2:F:3985:VAL:HG23	2:F:4046:SER:HB3	1.85	0.58
2:B:17:ASP:N	2:B:69:LEU:O	2.32	0.58
2:H:102:LEU:HB2	2:H:105:HIS:HD2	1.69	0.58
2:H:1698:LEU:HA	2:H:1712:TYR:HE1	1.69	0.58
2:B:102:LEU:HB2	2:B:105:HIS:HD2	1.69	0.58
2:D:161:GLU:HG2	2:F:3979:ARG:HH22	1.67	0.58
2:B:940:GLY:O	2:B:1052:ASN:ND2	2.36	0.58
2:B:1698:LEU:HA	2:B:1712:TYR:HE1	1.69	0.58
2:F:1451:GLY:HA3	2:F:1494:MET:HG2	1.85	0.58
2:B:359:TYR:HE1	2:B:385:ASP:HB3	1.68	0.57
2:F:102:LEU:HB2	2:F:105:HIS:HD2	1.69	0.57
2:B:404:ILE:HG21	2:B:481:GLU:HG2	1.86	0.57
2:D:1088:TRP:H	2:D:1153:ILE:HG22	1.69	0.57
2:F:3887:CYS:HB3	2:F:3895:GLN:HE21	1.69	0.57
2:H:1451:GLY:HA3	2:H:1494:MET:HG2	1.85	0.57
2:B:1451:GLY:HA3	2:B:1494:MET:HG2	1.85	0.57
2:H:1088:TRP:H	2:H:1153:ILE:HG22	1.69	0.57
2:D:102:LEU:HB2	2:D:105:HIS:HD2	1.69	0.57
2:D:1698:LEU:HA	2:D:1712:TYR:HE1	1.69	0.57
2:F:1088:TRP:H	2:F:1153:ILE:HG22	1.69	0.57
2:F:1698:LEU:HA	2:F:1712:TYR:HE1	1.69	0.57
2:F:4818:VAL:HB	2:F:4821:LEU:HD23	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:404:ILE:HG21	2:D:481:GLU:HG2	1.86	0.57
2:D:4818:VAL:HB	2:D:4821:LEU:HD23	1.86	0.57
2:B:2112:VAL:HG21	2:B:2118:VAL:HG22	1.87	0.57
2:H:404:ILE:HG21	2:H:481:GLU:HG2	1.86	0.57
2:D:1451:GLY:HA3	2:D:1494:MET:HG2	1.85	0.57
2:H:3985:VAL:HG23	2:H:4046:SER:HB3	1.85	0.57
2:B:1088:TRP:H	2:B:1153:ILE:HG22	1.69	0.57
2:B:3887:CYS:HB3	2:B:3895:GLN:HE21	1.69	0.57
2:B:4922:VAL:HG23	2:B:4923:ILE:HD12	1.86	0.57
2:F:215:THR:OG1	2:F:271:GLY:O	2.23	0.57
2:D:3887:CYS:HB3	2:D:3895:GLN:HE21	1.69	0.56
2:B:479:GLN:HB3	2:B:536:ASN:HD21	1.70	0.56
2:B:215:THR:OG1	2:B:271:GLY:O	2.23	0.56
2:D:2112:VAL:HG21	2:D:2118:VAL:HG22	1.87	0.56
2:H:479:GLN:HB3	2:H:536:ASN:HD21	1.70	0.56
2:D:215:THR:OG1	2:D:271:GLY:O	2.23	0.56
2:D:4922:VAL:HG23	2:D:4923:ILE:HD12	1.86	0.56
2:F:404:ILE:HG21	2:F:481:GLU:HG2	1.86	0.56
2:H:215:THR:OG1	2:H:271:GLY:O	2.23	0.56
2:H:2112:VAL:HG21	2:H:2118:VAL:HG22	1.87	0.56
2:H:473:ASN:O	2:H:476:SER:OG	2.24	0.56
2:H:3887:CYS:HB3	2:H:3895:GLN:HE21	1.69	0.56
2:H:4922:VAL:HG23	2:H:4923:ILE:HD12	1.86	0.56
2:F:216:GLY:HA2	2:F:262:LEU:HD11	1.88	0.56
2:B:4818:VAL:HB	2:B:4821:LEU:HD23	1.86	0.56
2:D:2124:LEU:O	2:D:2128:GLN:HG2	2.06	0.56
2:F:4922:VAL:HG23	2:F:4923:ILE:HD12	1.87	0.56
2:H:2124:LEU:O	2:H:2128:GLN:HG2	2.06	0.56
2:D:473:ASN:O	2:D:476:SER:OG	2.24	0.56
2:H:4818:VAL:HB	2:H:4821:LEU:HD23	1.86	0.56
2:F:2112:VAL:HG21	2:F:2118:VAL:HG22	1.87	0.55
2:H:854:CYS:O	2:H:994:ASN:ND2	2.39	0.55
2:B:1771:SER:OG	2:B:1957:GLU:OE2	2.25	0.55
2:D:854:CYS:O	2:D:994:ASN:ND2	2.39	0.55
2:F:2624:LEU:HA	2:F:2627:LEU:HB2	1.89	0.55
2:D:479:GLN:HB3	2:D:536:ASN:HD21	1.70	0.55
2:F:2124:LEU:O	2:F:2128:GLN:HG2	2.06	0.55
2:H:216:GLY:HA2	2:H:262:LEU:HD11	1.88	0.55
2:B:2624:LEU:HA	2:B:2627:LEU:HB2	1.89	0.55
2:D:414:PHE:HE1	2:D:436:LEU:HD12	1.72	0.55
2:D:1103:GLY:HA3	2:D:1123:VAL:HA	1.89	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1103:GLY:HA3	2:H:1123:VAL:HA	1.89	0.55
2:B:216:GLY:HA2	2:B:262:LEU:HD11	1.88	0.55
2:F:1103:GLY:HA3	2:F:1123:VAL:HA	1.89	0.55
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.89	0.55
2:B:2124:LEU:O	2:B:2128:GLN:HG2	2.06	0.55
2:F:17:ASP:N	2:F:69:LEU:O	2.32	0.55
2:D:2624:LEU:HA	2:D:2627:LEU:HB2	1.89	0.54
2:F:414:PHE:HE1	2:F:436:LEU:HD12	1.72	0.54
2:H:414:PHE:HE1	2:H:436:LEU:HD12	1.72	0.54
2:B:854:CYS:O	2:B:994:ASN:ND2	2.39	0.54
2:B:1154:ASP:O	2:B:1158:ASN:N	2.40	0.54
2:D:17:ASP:N	2:D:69:LEU:O	2.32	0.54
2:D:216:GLY:HA2	2:D:262:LEU:HD11	1.88	0.54
2:D:1771:SER:OG	2:D:1957:GLU:OE2	2.25	0.54
2:D:2326:PRO:HG3	2:D:2423:ILE:HD13	1.90	0.54
2:B:414:PHE:HE1	2:B:436:LEU:HD12	1.72	0.54
2:F:479:GLN:HB3	2:F:536:ASN:HD21	1.70	0.54
2:F:854:CYS:O	2:F:994:ASN:ND2	2.39	0.54
2:F:4664:VAL:HG13	2:F:4781:ILE:HD11	1.89	0.54
2:H:1154:ASP:O	2:H:1158:ASN:N	2.40	0.54
2:H:2624:LEU:HA	2:H:2627:LEU:HB2	1.89	0.54
2:B:473:ASN:O	2:B:476:SER:OG	2.24	0.54
2:D:299:LEU:HD12	2:D:378:LEU:HG	1.90	0.54
2:D:1154:ASP:O	2:D:1158:ASN:N	2.40	0.54
2:D:4861:TYR:HB2	2:D:4874:CYS:HB3	1.90	0.54
2:F:1154:ASP:O	2:F:1158:ASN:N	2.40	0.54
2:F:1771:SER:OG	2:F:1957:GLU:OE2	2.25	0.54
2:D:4664:VAL:HG13	2:D:4781:ILE:HD11	1.89	0.54
2:F:3975:LEU:HD22	2:F:3980:LEU:HD22	1.90	0.54
2:H:17:ASP:N	2:H:69:LEU:O	2.32	0.54
2:H:2244:SER:OG	2:H:2246:GLN:OE1	2.26	0.54
2:B:385:ASP:OD1	2:H:156:GLN:NE2	2.34	0.54
2:B:2326:PRO:HG3	2:B:2423:ILE:HD13	1.90	0.54
2:H:3975:LEU:HD22	2:H:3980:LEU:HD22	1.90	0.54
2:D:257:ARG:HH22	2:D:481:GLU:HG3	1.73	0.53
2:H:4664:VAL:HG13	2:H:4781:ILE:HD11	1.89	0.53
2:B:257:ARG:HH22	2:B:481:GLU:HG3	1.73	0.53
2:B:2244:SER:OG	2:B:2246:GLN:OE1	2.26	0.53
2:H:103:TYR:HD1	2:H:161:GLU:HB2	1.74	0.53
2:D:4976:HIS:HA	2:D:4980:GLU:HB3	1.91	0.53
2:F:2326:PRO:HG3	2:F:2423:ILE:HD13	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4861:TYR:HB2	2:F:4874:CYS:HB3	1.90	0.53
2:H:1771:SER:OG	2:H:1957:GLU:OE2	2.25	0.53
2:B:299:LEU:HD12	2:B:378:LEU:HG	1.90	0.53
2:F:299:LEU:HD12	2:F:378:LEU:HG	1.90	0.53
2:F:2244:SER:OG	2:F:2246:GLN:OE1	2.26	0.53
2:F:257:ARG:HH22	2:F:481:GLU:HG3	1.73	0.53
2:F:492:ASP:OD1	2:F:546:TRP:NE1	2.42	0.53
2:B:479:GLN:NE2	2:B:480:GLU:HG3	2.24	0.53
2:B:4861:TYR:HB2	2:B:4874:CYS:HB3	1.90	0.53
2:D:492:ASP:OD1	2:D:546:TRP:NE1	2.42	0.53
2:F:4976:HIS:HA	2:F:4980:GLU:HB3	1.91	0.53
2:H:479:GLN:NE2	2:H:480:GLU:HG3	2.24	0.53
2:H:4861:TYR:HB2	2:H:4874:CYS:HB3	1.90	0.53
2:D:2244:SER:OG	2:D:2246:GLN:OE1	2.26	0.53
2:H:492:ASP:OD1	2:H:546:TRP:NE1	2.42	0.53
2:B:492:ASP:OD1	2:B:546:TRP:NE1	2.42	0.53
2:B:4664:VAL:HG13	2:B:4781:ILE:HD11	1.89	0.53
2:D:479:GLN:NE2	2:D:480:GLU:HG3	2.24	0.53
2:H:102:LEU:HB2	2:H:105:HIS:CD2	2.44	0.53
2:H:3808:GLN:NE2	2:H:3885:LEU:O	2.42	0.53
2:B:3954:LYS:O	2:B:3958:ASN:ND2	2.42	0.53
2:B:4976:HIS:HA	2:B:4980:GLU:HB3	1.91	0.53
2:H:299:LEU:HD12	2:H:378:LEU:HG	1.90	0.53
2:B:103:TYR:HD1	2:B:161:GLU:HB2	1.74	0.52
2:B:255:HIS:CE1	2:B:480:GLU:OE1	2.62	0.52
2:D:255:HIS:CE1	2:D:480:GLU:OE1	2.63	0.52
2:D:3808:GLN:NE2	2:D:3885:LEU:O	2.42	0.52
2:F:479:GLN:NE2	2:F:480:GLU:HG3	2.24	0.52
2:F:3983:ALA:O	2:F:3987:PHE:HB2	2.10	0.52
2:H:2326:PRO:HG3	2:H:2423:ILE:HD13	1.90	0.52
2:D:2584:LEU:HB3	2:D:2623:LEU:HD22	1.91	0.52
2:F:2584:LEU:HB3	2:F:2623:LEU:HD22	1.92	0.52
2:B:102:LEU:HB2	2:B:105:HIS:CD2	2.44	0.52
2:H:257:ARG:HH22	2:H:481:GLU:HG3	1.73	0.52
2:B:3808:GLN:NE2	2:B:3885:LEU:O	2.42	0.52
2:B:3983:ALA:O	2:B:3987:PHE:HB2	2.10	0.52
2:D:3975:LEU:HD22	2:D:3980:LEU:HD22	1.90	0.52
2:F:102:LEU:HB2	2:F:105:HIS:CD2	2.44	0.52
2:H:4976:HIS:HA	2:H:4980:GLU:HB3	1.91	0.52
2:H:2624:LEU:HA	2:H:2627:LEU:HD12	1.92	0.52
2:B:3975:LEU:HD22	2:B:3980:LEU:HD22	1.90	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1703:LEU:HD12	2:D:1704:PRO:HD2	1.92	0.52
1:E:36:PHE:H	1:E:36:PHE:HD1	1.58	0.52
2:H:255:HIS:CE1	2:H:480:GLU:OE1	2.62	0.52
2:D:1719:HIS:CD2	2:D:1801:PRO:HB2	2.45	0.52
1:E:62:GLY:O	1:E:66:MET:HG3	2.10	0.52
2:F:1719:HIS:CD2	2:F:1801:PRO:HB2	2.45	0.52
2:D:3983:ALA:O	2:D:3987:PHE:HB2	2.10	0.51
2:H:1719:HIS:CD2	2:H:1801:PRO:HB2	2.45	0.51
1:C:62:GLY:O	1:C:66:MET:HG3	2.11	0.51
2:F:1703:LEU:HD12	2:F:1704:PRO:HD2	1.92	0.51
2:F:3808:GLN:NE2	2:F:3885:LEU:O	2.42	0.51
1:G:36:PHE:HD1	1:G:36:PHE:H	1.58	0.51
2:D:3954:LYS:O	2:D:3958:ASN:ND2	2.42	0.51
2:F:255:HIS:CE1	2:F:480:GLU:OE1	2.62	0.51
2:B:1683:HIS:CD2	2:B:1801:PRO:HD3	2.46	0.51
2:B:4876:ASP:O	2:B:4879:THR:OG1	2.24	0.51
2:D:1435:TYR:CD1	2:D:1575:LEU:HD22	2.46	0.51
2:H:2584:LEU:HB3	2:H:2623:LEU:HD22	1.92	0.51
2:H:3954:LYS:O	2:H:3958:ASN:ND2	2.42	0.51
2:B:1435:TYR:CD1	2:B:1575:LEU:HD22	2.46	0.51
2:B:2491:MET:HG3	2:B:2493:ALA:H	1.76	0.51
2:B:2584:LEU:HB3	2:B:2623:LEU:HD22	1.91	0.51
2:D:2624:LEU:HA	2:D:2627:LEU:HD12	1.92	0.51
2:H:1703:LEU:HD12	2:H:1704:PRO:HD2	1.92	0.51
2:D:681:HIS:CD2	2:D:683:ARG:HE	2.29	0.51
2:F:2624:LEU:HA	2:F:2627:LEU:HD12	1.92	0.51
2:H:3983:ALA:O	2:H:3987:PHE:HB2	2.09	0.51
1:A:8:SER:HB3	1:A:71:ARG:H	1.76	0.51
2:F:1435:TYR:CD1	2:F:1575:LEU:HD22	2.46	0.51
2:H:1978:TYR:HD2	2:H:3638:TYR:HE2	1.59	0.51
2:B:294:ILE:HG22	2:B:296:ASP:H	1.76	0.51
2:F:681:HIS:CD2	2:F:683:ARG:HE	2.29	0.51
1:G:62:GLY:O	1:G:66:MET:HG3	2.11	0.51
2:H:666:VAL:HG11	2:H:684:VAL:HG11	1.93	0.51
2:H:2491:MET:HG3	2:H:2493:ALA:H	1.76	0.51
2:B:1719:HIS:CD2	2:B:1801:PRO:HB2	2.45	0.51
1:C:8:SER:HB3	1:C:71:ARG:H	1.76	0.51
2:D:102:LEU:HB2	2:D:105:HIS:CD2	2.44	0.51
2:F:1978:TYR:HD2	2:F:3638:TYR:HE2	1.59	0.51
2:H:1435:TYR:CD1	2:H:1575:LEU:HD22	2.46	0.51
2:H:2043:CYS:HB3	2:H:2131:GLY:HA3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLY:O	1:A:66:MET:HG3	2.11	0.51
2:B:1272:LEU:HD22	2:B:1289:LEU:HD11	1.93	0.51
2:D:666:VAL:HG11	2:D:684:VAL:HG11	1.93	0.51
2:D:1683:HIS:CD2	2:D:1801:PRO:HD3	2.46	0.51
2:D:4876:ASP:O	2:D:4879:THR:OG1	2.24	0.51
2:H:294:ILE:HG22	2:H:296:ASP:H	1.76	0.51
2:H:1683:HIS:CD2	2:H:1801:PRO:HD3	2.46	0.51
2:B:2043:CYS:HB3	2:B:2131:GLY:HA3	1.93	0.50
1:C:36:PHE:HD1	1:C:36:PHE:H	1.58	0.50
2:D:682:LEU:HD13	2:D:787:VAL:HG11	1.94	0.50
2:F:473:ASN:O	2:F:476:SER:OG	2.24	0.50
2:F:3954:LYS:O	2:F:3958:ASN:ND2	2.42	0.50
2:D:2043:CYS:HB3	2:D:2131:GLY:HA3	1.93	0.50
2:D:2491:MET:HG3	2:D:2493:ALA:H	1.76	0.50
2:F:294:ILE:HG22	2:F:296:ASP:H	1.76	0.50
2:H:1272:LEU:HD22	2:H:1289:LEU:HD11	1.93	0.50
2:H:2496:VAL:HG12	2:H:2498:ASP:H	1.76	0.50
2:B:1703:LEU:HD12	2:B:1704:PRO:HD2	1.92	0.50
2:D:294:ILE:HG22	2:D:296:ASP:H	1.76	0.50
2:F:2491:MET:HG3	2:F:2493:ALA:H	1.76	0.50
2:H:102:LEU:HD12	2:H:105:HIS:HE2	1.77	0.50
2:H:681:HIS:CD2	2:H:683:ARG:HE	2.29	0.50
2:B:170:ILE:HD11	2:B:197:GLN:HB2	1.93	0.50
2:B:689:THR:HG22	2:B:776:LEU:H	1.77	0.50
2:B:2496:VAL:HG12	2:B:2498:ASP:H	1.76	0.50
2:D:1095:VAL:HG23	2:D:1096:THR:HG23	1.93	0.50
2:F:2043:CYS:HB3	2:F:2131:GLY:HA3	1.93	0.50
2:D:2496:VAL:HG12	2:D:2498:ASP:H	1.76	0.50
2:F:659:TYR:O	2:F:662:TRP:NE1	2.45	0.50
2:F:1683:HIS:CD2	2:F:1801:PRO:HD3	2.46	0.50
2:B:681:HIS:CD2	2:B:683:ARG:HE	2.29	0.50
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.94	0.50
2:F:666:VAL:HG11	2:F:684:VAL:HG11	1.93	0.50
2:F:682:LEU:HD13	2:F:787:VAL:HG11	1.94	0.50
2:F:1272:LEU:HD22	2:F:1289:LEU:HD11	1.93	0.50
2:B:2624:LEU:HA	2:B:2627:LEU:HD12	1.92	0.50
2:D:4877:MET:HA	2:D:4880:CYS:HB3	1.94	0.50
1:E:8:SER:HB3	1:E:71:ARG:H	1.76	0.50
2:F:482:GLY:O	2:F:486:LEU:HG	2.12	0.50
2:F:1010:VAL:HA	2:F:1019:PRO:HB3	1.94	0.50
2:F:1095:VAL:HG23	2:F:1096:THR:HG23	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2496:VAL:HG12	2:F:2498:ASP:H	1.76	0.50
2:H:1095:VAL:HG23	2:H:1096:THR:HG23	1.93	0.50
2:H:4027:GLU:OE1	2:H:5004:GLN:NE2	2.45	0.50
2:B:666:VAL:HG11	2:B:684:VAL:HG11	1.92	0.50
2:D:1978:TYR:HD2	2:D:3638:TYR:HE2	1.59	0.50
2:F:102:LEU:HD12	2:F:105:HIS:HE2	1.77	0.50
2:F:4027:GLU:OE1	2:F:5004:GLN:NE2	2.45	0.50
2:H:482:GLY:O	2:H:486:LEU:HG	2.12	0.50
1:A:36:PHE:HD1	1:A:36:PHE:H	1.58	0.49
2:B:102:LEU:HD12	2:B:105:HIS:HE2	1.77	0.49
2:B:659:TYR:O	2:B:662:TRP:NE1	2.45	0.49
2:D:516:LYS:O	2:D:520:ASN:ND2	2.44	0.49
2:F:516:LYS:O	2:F:520:ASN:ND2	2.44	0.49
1:G:8:SER:HB3	1:G:71:ARG:H	1.76	0.49
2:H:716:PHE:HD2	2:H:718:GLY:H	1.60	0.49
2:H:1010:VAL:HA	2:H:1019:PRO:HB3	1.94	0.49
2:B:4679:LEU:HD13	2:B:4722:VAL:HB	1.95	0.49
2:D:482:GLY:O	2:D:486:LEU:HG	2.12	0.49
2:F:3964:ILE:HG21	2:F:3975:LEU:HD12	1.95	0.49
2:H:1007:TYR:HE2	2:H:1013:ILE:HD13	1.77	0.49
2:B:1095:VAL:HG23	2:B:1096:THR:HG23	1.93	0.49
2:B:4027:GLU:OE1	2:B:5004:GLN:NE2	2.45	0.49
2:D:1272:LEU:HD22	2:D:1289:LEU:HD11	1.93	0.49
2:F:689:THR:HG22	2:F:776:LEU:H	1.77	0.49
2:F:716:PHE:HD2	2:F:718:GLY:H	1.60	0.49
2:D:170:ILE:HD11	2:D:197:GLN:HB2	1.93	0.49
2:D:689:THR:HG22	2:D:776:LEU:H	1.77	0.49
2:D:1439:VAL:HG11	2:D:1448:VAL:HG11	1.94	0.49
2:F:2504:VAL:HG21	2:F:2558:ALA:HB1	1.94	0.49
2:H:682:LEU:HD13	2:H:787:VAL:HG11	1.94	0.49
2:H:689:THR:HG22	2:H:776:LEU:H	1.77	0.49
2:D:450:GLY:HA2	2:D:453:GLU:OE2	2.12	0.49
2:D:1010:VAL:HA	2:D:1019:PRO:HB3	1.94	0.49
2:F:4679:LEU:HD13	2:F:4722:VAL:HB	1.94	0.49
2:B:450:GLY:HA2	2:B:453:GLU:OE2	2.12	0.49
2:B:4877:MET:HA	2:B:4880:CYS:HB3	1.94	0.49
2:D:102:LEU:HD12	2:D:105:HIS:HE2	1.77	0.49
2:D:1104:TRP:CZ3	2:D:1153:ILE:HB	2.47	0.49
2:D:4027:GLU:OE1	2:D:5004:GLN:NE2	2.45	0.49
2:D:4187:ARG:NH1	2:D:4980:GLU:OE1	2.46	0.49
2:F:170:ILE:HD11	2:F:197:GLN:HB2	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1104:TRP:CZ3	2:B:1153:ILE:HB	2.47	0.49
2:B:4187:ARG:NH1	2:B:4980:GLU:OE1	2.46	0.49
2:D:716:PHE:HD2	2:D:718:GLY:H	1.60	0.49
2:D:4172:TYR:HE1	2:D:4194:GLU:HB2	1.78	0.49
2:H:450:GLY:HA2	2:H:453:GLU:OE2	2.12	0.49
2:B:1978:TYR:HD2	2:B:3638:TYR:HE2	1.59	0.49
2:D:103:TYR:HD1	2:D:161:GLU:HB2	1.74	0.49
2:D:2122:PHE:O	2:D:3721:TYR:OH	2.30	0.49
2:D:4922:VAL:HA	2:D:4926:LEU:HB2	1.95	0.49
2:F:1104:TRP:CZ3	2:F:1153:ILE:HB	2.47	0.49
2:F:4178:ILE:HG23	2:F:5019:PHE:HB2	1.95	0.49
2:F:4187:ARG:NH1	2:F:4980:GLU:OE1	2.46	0.49
2:H:4877:MET:HA	2:H:4880:CYS:HB3	1.94	0.49
2:B:2122:PHE:O	2:B:3721:TYR:OH	2.31	0.49
2:D:156:GLN:NE2	2:F:385:ASP:OD1	2.34	0.49
2:D:2504:VAL:HG21	2:D:2558:ALA:HB1	1.94	0.49
2:H:4187:ARG:NH1	2:H:4980:GLU:OE1	2.46	0.49
2:B:156:GLN:NE2	2:D:385:ASP:OD1	2.34	0.49
2:B:1010:VAL:HA	2:B:1019:PRO:HB3	1.94	0.49
2:D:1764:PRO:HG3	2:D:2095:LEU:HD22	1.94	0.49
2:H:170:ILE:HD11	2:H:197:GLN:HB2	1.93	0.49
2:H:928:THR:O	2:H:931:THR:OG1	2.31	0.49
2:H:4178:ILE:HG23	2:H:5019:PHE:HB2	1.95	0.49
2:B:2504:VAL:HG21	2:B:2558:ALA:HB1	1.94	0.48
2:F:103:TYR:HD1	2:F:161:GLU:HB2	1.74	0.48
2:F:4922:VAL:HA	2:F:4926:LEU:HB2	1.95	0.48
2:H:1764:PRO:HG3	2:H:2095:LEU:HD22	1.94	0.48
2:H:3964:ILE:HG21	2:H:3975:LEU:HD12	1.95	0.48
2:H:4922:VAL:HA	2:H:4926:LEU:HB2	1.95	0.48
2:B:3664:SER:OG	2:B:3664:SER:O	2.30	0.48
2:F:450:GLY:HA2	2:F:453:GLU:OE2	2.12	0.48
2:F:2122:PHE:O	2:F:3721:TYR:OH	2.31	0.48
2:B:722:TRP:CZ3	2:B:727:PRO:HD3	2.49	0.48
2:B:4834:GLN:O	2:B:4838:THR:HG23	2.13	0.48
2:D:4178:ILE:HG23	2:D:5019:PHE:HB2	1.95	0.48
2:H:4015:GLN:HG3	2:H:4134:ILE:HD11	1.95	0.48
2:H:4834:GLN:O	2:H:4838:THR:HG23	2.14	0.48
2:B:219:VAL:HG12	2:B:259:LEU:HD12	1.96	0.48
2:B:1007:TYR:HE2	2:B:1013:ILE:HD13	1.77	0.48
2:B:3964:ILE:HG21	2:B:3975:LEU:HD12	1.95	0.48
2:D:4850:THR:HG1	2:D:4880:CYS:HG	1.56	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4850:THR:HG21	2:D:4881:TYR:HD1	1.79	0.48
2:F:1439:VAL:HG11	2:F:1448:VAL:HG11	1.94	0.48
2:F:4850:THR:HG21	2:F:4881:TYR:HD1	1.79	0.48
2:F:4877:MET:HA	2:F:4880:CYS:HB3	1.94	0.48
2:H:722:TRP:CZ3	2:H:727:PRO:HD3	2.49	0.48
2:H:4679:LEU:HD13	2:H:4722:VAL:HB	1.95	0.48
2:B:4015:GLN:HG3	2:B:4134:ILE:HD11	1.95	0.48
2:B:4172:TYR:HE1	2:B:4194:GLU:HB2	1.78	0.48
2:D:722:TRP:CZ3	2:D:727:PRO:HD3	2.49	0.48
2:F:125:ARG:N	2:F:134:ASP:OD2	2.42	0.48
2:F:1007:TYR:HE2	2:F:1013:ILE:HD13	1.78	0.48
2:H:659:TYR:O	2:H:662:TRP:NE1	2.45	0.48
2:H:1439:VAL:HG11	2:H:1448:VAL:HG11	1.94	0.48
2:H:2122:PHE:O	2:H:3721:TYR:OH	2.31	0.48
2:B:716:PHE:HD2	2:B:718:GLY:H	1.60	0.48
2:B:4178:ILE:HG23	2:B:5019:PHE:HB2	1.95	0.48
2:B:4922:VAL:HA	2:B:4926:LEU:HB2	1.95	0.48
2:D:659:TYR:O	2:D:662:TRP:NE1	2.45	0.48
2:H:1104:TRP:CZ3	2:H:1153:ILE:HB	2.47	0.48
2:B:482:GLY:O	2:B:486:LEU:HG	2.12	0.48
2:F:4172:TYR:HE1	2:F:4194:GLU:HB2	1.78	0.48
2:F:674:PHE:H	2:F:680:THR:HG23	1.79	0.48
2:H:219:VAL:HG12	2:H:259:LEU:HD12	1.95	0.48
2:H:246:TYR:HD1	2:H:375:LYS:HA	1.79	0.48
2:H:2504:VAL:HG21	2:H:2558:ALA:HB1	1.94	0.48
2:B:1007:TYR:CE2	2:B:1013:ILE:HD13	2.49	0.48
2:B:1764:PRO:HG3	2:B:2095:LEU:HD22	1.94	0.48
2:F:722:TRP:CZ3	2:F:727:PRO:HD3	2.49	0.48
2:F:4834:GLN:O	2:F:4838:THR:HG23	2.13	0.48
2:H:4172:TYR:HE1	2:H:4194:GLU:HB2	1.78	0.48
2:B:4850:THR:HG1	2:B:4880:CYS:HG	1.58	0.48
2:D:125:ARG:N	2:D:134:ASP:OD2	2.42	0.48
2:D:3964:ILE:HG21	2:D:3975:LEU:HD12	1.95	0.48
2:F:1764:PRO:HG3	2:F:2095:LEU:HD22	1.94	0.48
2:F:4016:LYS:HE3	2:F:4133:ASP:OD2	2.14	0.48
2:H:2451:ALA:HA	2:H:2454:ILE:HD13	1.96	0.48
2:H:4850:THR:HG21	2:H:4881:TYR:HD1	1.79	0.48
2:B:246:TYR:HD1	2:B:375:LYS:HA	1.79	0.47
2:B:2451:ALA:HA	2:B:2454:ILE:HD13	1.95	0.47
2:D:219:VAL:HG12	2:D:259:LEU:HD12	1.96	0.47
2:H:4016:LYS:HE3	2:H:4133:ASP:OD2	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1439:VAL:HG11	2:B:1448:VAL:HG11	1.94	0.47
2:D:1007:TYR:CE2	2:D:1013:ILE:HD13	2.49	0.47
2:F:2451:ALA:HA	2:F:2454:ILE:HD13	1.96	0.47
2:F:4920:PHE:O	2:F:4925:ILE:HG12	2.14	0.47
2:H:533:ASN:ND2	2:H:536:ASN:OD1	2.42	0.47
2:B:4850:THR:HG21	2:B:4881:TYR:HD1	1.79	0.47
2:D:2451:ALA:HA	2:D:2454:ILE:HD13	1.96	0.47
2:D:2624:LEU:O	2:D:2628:VAL:HG12	2.14	0.47
2:D:4679:LEU:HD13	2:D:4722:VAL:HB	1.94	0.47
2:D:4834:GLN:O	2:D:4838:THR:HG23	2.13	0.47
2:H:674:PHE:H	2:H:680:THR:HG23	1.79	0.47
2:D:1007:TYR:HE2	2:D:1013:ILE:HD13	1.77	0.47
2:F:2624:LEU:O	2:F:2628:VAL:HG12	2.14	0.47
2:F:4015:GLN:HG3	2:F:4134:ILE:HD11	1.95	0.47
2:B:4016:LYS:HE3	2:B:4133:ASP:OD2	2.14	0.47
2:F:1676:LEU:HD22	2:F:2168:ILE:HD12	1.96	0.47
2:H:1007:TYR:CE2	2:H:1013:ILE:HD13	2.49	0.47
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.47
2:B:1618:ARG:HG3	2:B:1618:ARG:HH21	1.80	0.47
2:D:1717:SER:HA	2:D:1721:GLU:HB2	1.97	0.47
2:F:533:ASN:ND2	2:F:536:ASN:OD1	2.42	0.47
2:F:1007:TYR:CE2	2:F:1013:ILE:HD13	2.49	0.47
2:B:4920:PHE:O	2:B:4925:ILE:HG12	2.14	0.47
2:D:674:PHE:H	2:D:680:THR:HG23	1.79	0.47
2:D:3753:MET:O	2:D:3756:GLN:NE2	2.48	0.47
2:D:4015:GLN:HG3	2:D:4134:ILE:HD11	1.95	0.47
2:F:219:VAL:HG12	2:F:259:LEU:HD12	1.95	0.47
2:F:3664:SER:O	2:F:3664:SER:OG	2.30	0.47
2:F:3964:ILE:HG22	2:F:3971:ASN:HB3	1.97	0.47
2:H:125:ARG:N	2:H:134:ASP:OD2	2.42	0.47
2:H:1460:HIS:HB2	2:H:1600:LEU:HD21	1.97	0.47
2:D:1618:ARG:HH21	2:D:1618:ARG:HG3	1.80	0.47
2:D:4016:LYS:HE3	2:D:4133:ASP:OD2	2.14	0.47
2:H:3964:ILE:HG22	2:H:3971:ASN:HB3	1.97	0.47
2:B:1717:SER:HA	2:B:1721:GLU:HB2	1.97	0.47
2:D:668:VAL:HG12	2:D:789:VAL:HG23	1.97	0.47
2:D:4929:ILE:HG23	2:F:4938:PHE:HZ	1.80	0.47
2:H:106:ALA:HA	2:H:149:THR:HA	1.97	0.47
2:H:1618:ARG:HH21	2:H:1618:ARG:HG3	1.80	0.47
2:B:668:VAL:HG12	2:B:789:VAL:HG23	1.97	0.47
2:D:4920:PHE:O	2:D:4925:ILE:HG12	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:668:VAL:HG12	2:H:789:VAL:HG23	1.97	0.47
1:A:90:VAL:HG12	1:A:91:ILE:HG12	1.98	0.46
2:B:106:ALA:HA	2:B:149:THR:HA	1.97	0.46
2:B:2624:LEU:O	2:B:2628:VAL:HG12	2.14	0.46
2:B:4929:ILE:HG23	2:D:4938:PHE:HZ	1.80	0.46
2:D:106:ALA:HA	2:D:149:THR:HA	1.97	0.46
2:D:1676:LEU:HD22	2:D:2168:ILE:HD12	1.96	0.46
2:F:106:ALA:HA	2:F:149:THR:HA	1.97	0.46
2:F:668:VAL:HG12	2:F:789:VAL:HG23	1.97	0.46
2:F:1460:HIS:HB2	2:F:1600:LEU:HD21	1.97	0.46
2:H:1717:SER:HA	2:H:1721:GLU:HB2	1.97	0.46
2:H:3664:SER:O	2:H:3664:SER:OG	2.30	0.46
2:D:246:TYR:HD1	2:D:375:LYS:HA	1.79	0.46
2:F:246:TYR:HD1	2:F:375:LYS:HA	1.79	0.46
2:H:2624:LEU:O	2:H:2628:VAL:HG12	2.14	0.46
2:B:1772:LEU:HD11	2:B:2154:MET:HG3	1.97	0.46
2:D:1772:LEU:HD11	2:D:2154:MET:HG3	1.97	0.46
2:B:194:SER:OG	2:B:195:PHE:N	2.48	0.46
2:H:3753:MET:O	2:H:3756:GLN:NE2	2.48	0.46
2:H:4920:PHE:O	2:H:4925:ILE:HG12	2.14	0.46
2:B:621:ILE:HG13	2:B:622:THR:N	2.31	0.46
2:B:1676:LEU:HD22	2:B:2168:ILE:HD12	1.96	0.46
2:B:3994:MET:HB3	2:B:4011:LEU:HD11	1.97	0.46
2:H:621:ILE:HG13	2:H:622:THR:N	2.31	0.46
2:B:1452:TRP:CZ2	2:B:1520:VAL:HG21	2.51	0.46
1:C:90:VAL:HG12	1:C:91:ILE:HG12	1.98	0.46
2:D:1460:HIS:HB2	2:D:1600:LEU:HD21	1.97	0.46
2:D:2215:VAL:HG13	2:D:2216:LEU:HD12	1.98	0.46
2:F:1717:SER:HA	2:F:1721:GLU:HB2	1.97	0.46
2:F:4929:ILE:HG23	2:H:4938:PHE:HZ	1.80	0.46
2:H:1520:VAL:HG22	2:H:1527:MET:SD	2.56	0.46
2:H:1676:LEU:HD22	2:H:2168:ILE:HD12	1.96	0.46
2:B:103:TYR:OH	2:B:167:ASP:OD2	2.34	0.46
2:B:1293:LEU:HD11	2:B:1594:ARG:HH21	1.81	0.46
2:B:1848:THR:O	2:B:1852:MET:HG3	2.16	0.46
2:D:1293:LEU:HD11	2:D:1594:ARG:HH21	1.81	0.46
2:D:1452:TRP:CZ2	2:D:1520:VAL:HG21	2.51	0.46
2:D:3994:MET:HB3	2:D:4011:LEU:HD11	1.97	0.46
2:F:621:ILE:HG13	2:F:622:THR:N	2.31	0.46
2:F:1293:LEU:HD11	2:F:1594:ARG:HD3	1.98	0.46
1:G:87:HIS:HB3	1:G:90:VAL:HB	1.98	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:VAL:HG12	1:G:91:ILE:HG12	1.98	0.46
2:B:1460:HIS:HB2	2:B:1600:LEU:HD21	1.97	0.46
2:B:2570:PHE:HE2	2:B:2611:LEU:HD11	1.81	0.46
2:B:4664:VAL:O	2:B:4668:ILE:HG22	2.16	0.46
2:B:4938:PHE:HZ	2:H:4929:ILE:HG23	1.80	0.46
2:D:1848:THR:O	2:D:1852:MET:HG3	2.16	0.46
2:F:1848:THR:O	2:F:1852:MET:HG3	2.16	0.46
2:H:1772:LEU:HD11	2:H:2154:MET:HG3	1.97	0.46
2:B:1520:VAL:HG22	2:B:1527:MET:SD	2.56	0.46
2:F:3994:MET:HB3	2:F:4011:LEU:HD11	1.97	0.46
2:H:359:TYR:CE1	2:H:385:ASP:HB3	2.51	0.46
2:H:1848:THR:O	2:H:1852:MET:HG3	2.16	0.46
2:B:436:LEU:H	2:B:436:LEU:HD23	1.81	0.45
2:B:2215:VAL:HG13	2:B:2216:LEU:HD12	1.98	0.45
2:B:3964:ILE:HG22	2:B:3971:ASN:HB3	1.97	0.45
2:D:194:SER:OG	2:D:195:PHE:N	2.48	0.45
2:D:479:GLN:CB	2:D:536:ASN:HD21	2.28	0.45
2:D:621:ILE:HG13	2:D:622:THR:N	2.31	0.45
2:D:1245:PHE:CE2	2:D:1290:ARG:HD3	2.51	0.45
2:D:2117:LEU:O	2:D:2121:MET:HG3	2.17	0.45
2:F:1772:LEU:HD11	2:F:2154:MET:HG3	1.97	0.45
2:F:3753:MET:O	2:F:3756:GLN:NE2	2.48	0.45
2:H:1452:TRP:CZ2	2:H:1520:VAL:HG21	2.51	0.45
2:H:3762:GLN:NE2	2:H:3798:SER:O	2.42	0.45
2:D:436:LEU:HD23	2:D:436:LEU:H	1.82	0.45
2:F:103:TYR:OH	2:F:167:ASP:OD2	2.34	0.45
2:F:359:TYR:CE1	2:F:385:ASP:HB3	2.51	0.45
2:F:1452:TRP:CZ2	2:F:1520:VAL:HG21	2.51	0.45
2:F:2570:PHE:HE2	2:F:2611:LEU:HD11	1.81	0.45
2:F:4192:ILE:HG21	2:F:4197:ARG:HH21	1.82	0.45
2:F:4710:PRO:HB2	2:F:4716:LYS:HA	1.99	0.45
2:H:479:GLN:CB	2:H:536:ASN:HD21	2.28	0.45
2:H:3994:MET:HB3	2:H:4011:LEU:HD11	1.98	0.45
2:H:4664:VAL:O	2:H:4668:ILE:HG22	2.16	0.45
2:H:4710:PRO:HB2	2:H:4716:LYS:HA	1.99	0.45
2:F:479:GLN:CB	2:F:536:ASN:HD21	2.28	0.45
2:F:928:THR:O	2:F:931:THR:OG1	2.31	0.45
2:F:1245:PHE:CE2	2:F:1290:ARG:HD3	2.51	0.45
2:F:1293:LEU:HD11	2:F:1594:ARG:HH21	1.81	0.45
2:F:1520:VAL:HG22	2:F:1527:MET:SD	2.56	0.45
2:H:1245:PHE:CE2	2:H:1290:ARG:HD3	2.51	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1676:LEU:HA	2:H:1725:ARG:HH22	1.82	0.45
2:B:928:THR:O	2:B:931:THR:OG1	2.31	0.45
1:C:87:HIS:HB3	1:C:90:VAL:HB	1.98	0.45
2:D:2570:PHE:HE2	2:D:2611:LEU:HD11	1.81	0.45
2:D:3964:ILE:HG22	2:D:3971:ASN:HB3	1.97	0.45
1:E:90:VAL:HG12	1:E:91:ILE:HG12	1.98	0.45
2:F:1618:ARG:HH21	2:F:1618:ARG:HG3	1.80	0.45
2:F:2117:LEU:O	2:F:2121:MET:HG3	2.17	0.45
2:H:436:LEU:HD23	2:H:436:LEU:H	1.82	0.45
2:H:2570:PHE:HE2	2:H:2611:LEU:HD11	1.82	0.45
2:B:674:PHE:H	2:B:680:THR:HG23	1.79	0.45
2:B:1676:LEU:HA	2:B:1725:ARG:HH22	1.82	0.45
2:D:247:TYR:HB2	2:D:374:LYS:HG3	1.99	0.45
2:D:4192:ILE:HG21	2:D:4197:ARG:HH21	1.82	0.45
2:F:2215:VAL:HG13	2:F:2216:LEU:HD12	1.98	0.45
2:H:1293:LEU:HD11	2:H:1594:ARG:HH21	1.81	0.45
2:B:247:TYR:HB2	2:B:374:LYS:HG3	1.99	0.45
2:D:103:TYR:OH	2:D:167:ASP:OD2	2.34	0.45
2:F:4664:VAL:O	2:F:4668:ILE:HG22	2.16	0.45
2:H:103:TYR:OH	2:H:167:ASP:OD2	2.34	0.45
2:H:194:SER:OG	2:H:195:PHE:N	2.49	0.45
2:H:2117:LEU:O	2:H:2121:MET:HG3	2.17	0.45
2:H:3995:MET:HG2	2:H:4008:LEU:HD11	1.99	0.45
2:B:632:LEU:HD12	2:B:1666:THR:HG23	1.99	0.45
2:D:1293:LEU:HD11	2:D:1594:ARG:HD3	1.98	0.45
2:F:436:LEU:HD23	2:F:436:LEU:H	1.82	0.45
2:B:2117:LEU:O	2:B:2121:MET:HG3	2.17	0.45
2:D:632:LEU:HD12	2:D:1666:THR:HG23	1.99	0.45
2:D:1698:LEU:HA	2:D:1712:TYR:CE1	2.51	0.45
2:F:1432:THR:HA	2:F:1520:VAL:O	2.17	0.45
2:B:479:GLN:CB	2:B:536:ASN:HD21	2.28	0.45
2:B:2111:PHE:HD2	2:B:2113:GLN:HG2	1.82	0.45
2:B:3995:MET:HG2	2:B:4008:LEU:HD11	1.99	0.45
2:B:4659:TYR:OH	2:B:4786:SER:OG	2.31	0.45
2:B:4710:PRO:HB2	2:B:4716:LYS:HA	1.99	0.45
2:D:4710:PRO:HB2	2:D:4716:LYS:HA	1.99	0.45
2:F:1676:LEU:HA	2:F:1725:ARG:HH22	1.82	0.45
2:F:4850:THR:HG1	2:F:4880:CYS:HG	1.62	0.45
2:H:531:ARG:NH2	2:H:562:GLU:OE2	2.49	0.45
2:B:1293:LEU:HD11	2:B:1594:ARG:HD3	1.98	0.45
2:B:2231:THR:O	2:B:2235:ARG:HG2	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4192:ILE:HG21	2:B:4197:ARG:HH21	1.82	0.45
2:F:531:ARG:NH2	2:F:562:GLU:OE2	2.49	0.45
2:F:4942:ARG:HE	2:F:4942:ARG:HB3	1.61	0.45
2:B:1432:THR:HA	2:B:1520:VAL:O	2.17	0.44
2:D:1520:VAL:HG22	2:D:1527:MET:SD	2.56	0.44
2:D:4659:TYR:OH	2:D:4786:SER:OG	2.31	0.44
1:E:87:HIS:HB3	1:E:90:VAL:HB	1.98	0.44
2:F:700:GLU:N	2:F:705:ASN:OD1	2.51	0.44
2:H:2179:MET:HB3	2:H:2179:MET:HE3	1.61	0.44
2:H:2231:THR:O	2:H:2235:ARG:HG2	2.17	0.44
2:H:2464:LEU:HD21	2:H:2511:TYR:CD1	2.52	0.44
2:B:4942:ARG:HE	2:B:4942:ARG:HB3	1.61	0.44
2:D:1471:ALA:HB1	2:D:1488:LYS:HZ1	1.82	0.44
2:D:2111:PHE:HD2	2:D:2113:GLN:HG2	1.82	0.44
2:D:4664:VAL:O	2:D:4668:ILE:HG22	2.16	0.44
2:H:2215:VAL:HG13	2:H:2216:LEU:HD12	1.98	0.44
2:H:4192:ILE:HG21	2:H:4197:ARG:HH21	1.82	0.44
1:A:87:HIS:HB3	1:A:90:VAL:HB	1.98	0.44
2:B:531:ARG:NH2	2:B:562:GLU:OE2	2.49	0.44
2:B:1718:ILE:HG23	2:B:1719:HIS:ND1	2.33	0.44
2:F:3762:GLN:NE2	2:F:3798:SER:O	2.41	0.44
1:G:78:PRO:HD3	1:G:96:THR:HG22	2.00	0.44
2:H:516:LYS:O	2:H:520:ASN:ND2	2.44	0.44
2:B:196:MET:SD	2:B:196:MET:N	2.91	0.44
2:B:1782:CYS:SG	2:B:1785:ALA:HB2	2.58	0.44
2:B:3753:MET:O	2:B:3756:GLN:NE2	2.48	0.44
2:D:1432:THR:HA	2:D:1520:VAL:O	2.17	0.44
2:D:2179:MET:HE1	2:D:2229:MET:HE3	1.99	0.44
2:F:1698:LEU:HA	2:F:1712:TYR:CE1	2.51	0.44
2:F:1782:CYS:SG	2:F:1785:ALA:HB2	2.57	0.44
2:F:2347:VAL:HG12	2:F:2350:ASN:H	1.83	0.44
2:H:1782:CYS:SG	2:H:1785:ALA:HB2	2.58	0.44
2:H:2132:LEU:HD22	2:H:3658:ILE:HG23	1.99	0.44
2:B:233:ILE:HD11	2:B:242:ARG:O	2.18	0.44
2:B:359:TYR:CE1	2:B:385:ASP:HB3	2.51	0.44
2:F:233:ILE:HD11	2:F:242:ARG:O	2.18	0.44
2:H:632:LEU:HD12	2:H:1666:THR:HG23	1.99	0.44
2:B:700:GLU:N	2:B:705:ASN:OD1	2.50	0.44
2:B:1245:PHE:CE2	2:B:1290:ARG:HD3	2.51	0.44
2:B:3762:GLN:NE2	2:B:3798:SER:O	2.41	0.44
2:D:359:TYR:CE1	2:D:385:ASP:HB3	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1686:CYS:HB3	2:D:1783:PHE:HZ	1.83	0.44
2:D:3799:ILE:O	2:D:3804:ASN:ND2	2.51	0.44
2:D:4062:LYS:O	2:D:4066:ILE:HG13	2.17	0.44
2:H:1686:CYS:HB3	2:H:1783:PHE:HZ	1.83	0.44
2:H:2111:PHE:HD2	2:H:2113:GLN:HG2	1.82	0.44
2:B:2464:LEU:HD21	2:B:2511:TYR:CD1	2.52	0.44
2:B:3799:ILE:O	2:B:3804:ASN:ND2	2.51	0.44
2:D:2464:LEU:HD21	2:D:2511:TYR:CD1	2.52	0.44
2:D:3922:GLN:HE21	2:D:3986:GLY:HA3	1.83	0.44
2:F:1718:ILE:HG23	2:F:1719:HIS:ND1	2.33	0.44
2:F:2464:LEU:HD21	2:F:2511:TYR:CD1	2.52	0.44
2:F:3995:MET:HG2	2:F:4008:LEU:HD11	1.99	0.44
2:D:196:MET:SD	2:D:196:MET:N	2.91	0.44
2:F:194:SER:OG	2:F:195:PHE:N	2.48	0.44
2:F:1686:CYS:HB3	2:F:1783:PHE:HZ	1.83	0.44
2:F:2132:LEU:HD22	2:F:3658:ILE:HG23	1.99	0.44
2:H:1293:LEU:HD11	2:H:1594:ARG:HD3	1.98	0.44
2:H:4062:LYS:O	2:H:4066:ILE:HG13	2.17	0.44
2:F:3922:GLN:HE21	2:F:3986:GLY:HA3	1.83	0.44
2:F:4062:LYS:O	2:F:4066:ILE:HG13	2.17	0.44
2:H:196:MET:SD	2:H:196:MET:N	2.91	0.44
2:H:247:TYR:HB2	2:H:374:LYS:HG3	1.99	0.44
2:B:4062:LYS:O	2:B:4066:ILE:HG13	2.17	0.43
2:D:2467:LEU:HD11	2:D:2506:PHE:HD2	1.83	0.43
2:D:3995:MET:HG2	2:D:4008:LEU:HD11	1.99	0.43
1:E:78:PRO:HD3	1:E:96:THR:HG22	2.00	0.43
2:F:156:GLN:NE2	2:H:385:ASP:OD1	2.33	0.43
2:F:3799:ILE:O	2:F:3804:ASN:ND2	2.51	0.43
2:H:1432:THR:HA	2:H:1520:VAL:O	2.17	0.43
2:H:1718:ILE:HG23	2:H:1719:HIS:ND1	2.33	0.43
2:B:516:LYS:O	2:B:520:ASN:ND2	2.44	0.43
2:D:107:ILE:N	2:D:148:TRP:O	2.47	0.43
2:D:700:GLU:N	2:D:705:ASN:OD1	2.50	0.43
2:D:1782:CYS:SG	2:D:1785:ALA:HB2	2.58	0.43
2:H:3799:ILE:O	2:H:3804:ASN:ND2	2.51	0.43
2:D:3664:SER:O	2:D:3664:SER:OG	2.30	0.43
2:D:3762:GLN:NE2	2:D:3798:SER:O	2.41	0.43
2:D:4030:VAL:HG12	2:D:4032:ASN:H	1.83	0.43
2:F:632:LEU:HD12	2:F:1666:THR:HG23	1.99	0.43
2:F:2111:PHE:HD2	2:F:2113:GLN:HG2	1.83	0.43
2:H:4941:LEU:O	2:H:4945:GLN:HG2	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1686:CYS:HB3	2:B:1783:PHE:HZ	1.83	0.43
2:B:4029:ASN:ND2	2:B:4035:ILE:HB	2.34	0.43
2:D:1676:LEU:HA	2:D:1725:ARG:HH22	1.82	0.43
2:F:1290:ARG:HB3	2:F:1551:ALA:HB2	2.01	0.43
2:F:2467:LEU:HD11	2:F:2506:PHE:HD2	1.83	0.43
2:H:2347:VAL:HG12	2:H:2350:ASN:H	1.83	0.43
2:D:1718:ILE:HG23	2:D:1719:HIS:ND1	2.33	0.43
2:F:196:MET:SD	2:F:196:MET:N	2.91	0.43
2:F:206:CYS:HB3	2:F:271:GLY:HA3	2.00	0.43
2:F:247:TYR:HB2	2:F:374:LYS:HG3	1.99	0.43
2:F:2231:THR:O	2:F:2235:ARG:HG2	2.17	0.43
2:H:206:CYS:HB3	2:H:271:GLY:HA3	2.00	0.43
2:H:1130:GLN:HE21	2:H:1132:TRP:HZ3	1.66	0.43
2:H:4882:LEU:HD23	2:H:4882:LEU:HA	1.91	0.43
2:B:1290:ARG:HB3	2:B:1551:ALA:HB2	2.01	0.43
2:B:2132:LEU:HD22	2:B:3658:ILE:HG23	1.99	0.43
2:B:3799:ILE:HG22	2:B:3807:VAL:HG11	2.00	0.43
2:B:4030:VAL:HG12	2:B:4032:ASN:H	1.83	0.43
2:D:1290:ARG:HB3	2:D:1551:ALA:HB2	2.01	0.43
2:D:2347:VAL:HG12	2:D:2350:ASN:H	1.83	0.43
2:H:4029:ASN:ND2	2:H:4035:ILE:HB	2.34	0.43
2:B:257:ARG:HH22	2:B:286:THR:HG21	1.84	0.43
2:B:2347:VAL:HG12	2:B:2350:ASN:H	1.83	0.43
2:B:4941:LEU:O	2:B:4945:GLN:HG2	2.19	0.43
1:C:71:ARG:HH21	2:D:674:PHE:HZ	1.61	0.43
2:D:233:ILE:HD11	2:D:242:ARG:O	2.18	0.43
2:D:4936:ASP:O	2:D:4940:GLU:HG2	2.18	0.43
2:F:1130:GLN:HE21	2:F:1132:TRP:HZ3	1.66	0.43
2:H:2114:SER:O	2:H:2118:VAL:HG23	2.19	0.43
2:H:3799:ILE:HG22	2:H:3807:VAL:HG11	2.00	0.43
2:H:4876:ASP:O	2:H:4879:THR:OG1	2.24	0.43
2:B:22:LEU:HD12	2:B:37:LEU:HD22	2.01	0.43
2:B:3991:PHE:HA	2:B:3994:MET:CG	2.46	0.43
2:B:4936:ASP:O	2:B:4940:GLU:HG2	2.19	0.43
2:B:4990:LEU:HD11	2:B:5012:TYR:CE1	2.54	0.43
2:F:1959:LEU:HD23	2:F:2139:LEU:HD21	2.01	0.43
2:F:4030:VAL:HG12	2:F:4032:ASN:H	1.83	0.43
2:H:222:LEU:HD12	2:H:260:TRP:CD1	2.54	0.43
2:H:1698:LEU:HA	2:H:1712:TYR:CE1	2.51	0.43
2:B:38:ALA:HB2	2:B:65:CYS:HB3	2.01	0.43
2:B:222:LEU:HD12	2:B:260:TRP:CD1	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2467:LEU:HD11	2:B:2506:PHE:HD2	1.84	0.43
2:D:2231:THR:O	2:D:2235:ARG:HG2	2.17	0.43
2:D:4850:THR:OG1	2:D:4880:CYS:SG	2.74	0.43
2:D:4941:LEU:O	2:D:4945:GLN:HG2	2.19	0.43
2:D:4990:LEU:HD11	2:D:5012:TYR:CE1	2.54	0.43
2:F:4941:LEU:O	2:F:4945:GLN:HG2	2.19	0.43
2:H:38:ALA:HB2	2:H:65:CYS:HB3	2.01	0.43
2:H:1290:ARG:HB3	2:H:1551:ALA:HB2	2.01	0.43
2:H:2467:LEU:HD11	2:H:2506:PHE:HD2	1.83	0.43
2:H:4936:ASP:O	2:H:4940:GLU:HG2	2.19	0.43
2:B:3922:GLN:HE21	2:B:3986:GLY:HA3	1.83	0.43
2:D:1712:TYR:HD2	2:D:1841:PRO:HB2	1.84	0.43
2:F:4990:LEU:HD11	2:F:5012:TYR:CE1	2.54	0.43
2:H:700:GLU:N	2:H:705:ASN:OD1	2.50	0.43
2:H:1816:LEU:HD12	2:H:1816:LEU:HA	1.91	0.43
2:B:646:PRO:HB2	2:B:648:ILE:HG12	2.01	0.42
2:B:1143:TRP:HB3	2:B:1164:LEU:HD11	2.01	0.42
2:D:222:LEU:HD12	2:D:260:TRP:CD1	2.54	0.42
2:D:646:PRO:HB2	2:D:648:ILE:HG12	2.01	0.42
2:D:2132:LEU:HD22	2:D:3658:ILE:HG23	1.99	0.42
1:E:8:SER:HB2	1:E:71:ARG:HB2	2.01	0.42
2:H:4990:LEU:HD11	2:H:5012:TYR:CE1	2.54	0.42
1:A:8:SER:HB2	1:A:71:ARG:HB2	2.01	0.42
1:A:78:PRO:HD3	1:A:96:THR:HG22	2.00	0.42
2:B:1130:GLN:HE21	2:B:1132:TRP:HZ3	1.66	0.42
2:B:1649:ASP:OD1	2:B:1650:ILE:N	2.52	0.42
2:D:22:LEU:HD12	2:D:37:LEU:HD22	2.01	0.42
2:D:1245:PHE:CE1	2:D:1600:LEU:HB2	2.54	0.42
2:F:24:CYS:SG	2:F:35:LEU:HB2	2.59	0.42
2:F:951:ARG:H	2:F:970:LEU:HA	1.84	0.42
2:F:1245:PHE:CE1	2:F:1600:LEU:HB2	2.54	0.42
2:F:1649:ASP:OD1	2:F:1650:ILE:N	2.52	0.42
2:H:233:ILE:HD11	2:H:242:ARG:O	2.18	0.42
2:B:3757:ARG:O	2:B:3761:GLN:HG3	2.19	0.42
1:C:78:PRO:HD3	1:C:96:THR:HG22	2.00	0.42
2:D:156:GLN:HG2	2:D:157:ARG:N	2.34	0.42
2:D:1456:ASP:C	2:D:1491:ASN:HD21	2.22	0.42
2:D:1495:VAL:HG12	2:D:1538:THR:HG21	2.02	0.42
2:D:3757:ARG:O	2:D:3761:GLN:HG3	2.19	0.42
2:D:3987:PHE:O	2:D:3990:VAL:HG22	2.19	0.42
2:F:257:ARG:HH22	2:F:286:THR:HG21	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1456:ASP:C	2:F:1491:ASN:HD21	2.22	0.42
2:H:1649:ASP:OD1	2:H:1650:ILE:N	2.52	0.42
2:H:3922:GLN:HE21	2:H:3986:GLY:HA3	1.83	0.42
2:D:650:VAL:O	2:D:777:PHE:N	2.37	0.42
2:D:951:ARG:H	2:D:970:LEU:HA	1.84	0.42
2:D:1143:TRP:HB3	2:D:1164:LEU:HD11	2.01	0.42
2:D:1244:GLN:OE1	2:D:1458:HIS:ND1	2.52	0.42
2:D:2114:SER:O	2:D:2118:VAL:HG23	2.19	0.42
2:D:3804:ASN:HB3	2:D:3807:VAL:HB	2.02	0.42
2:F:222:LEU:HD12	2:F:260:TRP:CD1	2.54	0.42
2:F:1495:VAL:HG12	2:F:1538:THR:HG21	2.02	0.42
2:F:3766:HIS:CE1	2:F:3807:VAL:HA	2.55	0.42
2:F:4876:ASP:O	2:F:4879:THR:OG1	2.24	0.42
2:H:22:LEU:HD12	2:H:37:LEU:HD22	2.01	0.42
2:H:554:LEU:HD23	2:H:554:LEU:H	1.84	0.42
2:H:847:SER:OG	2:H:849:THR:HG22	2.20	0.42
2:H:1517:GLY:N	2:H:1530:THR:O	2.35	0.42
2:B:1245:PHE:CE1	2:B:1600:LEU:HB2	2.54	0.42
2:B:1714:LEU:O	2:B:1718:ILE:HG22	2.20	0.42
2:D:257:ARG:HH22	2:D:286:THR:HG21	1.84	0.42
2:F:156:GLN:HG2	2:F:157:ARG:N	2.34	0.42
2:F:847:SER:OG	2:F:849:THR:HG22	2.20	0.42
2:F:3958:ASN:ND2	2:F:4017:ASP:OD2	2.53	0.42
2:F:4029:ASN:ND2	2:F:4035:ILE:HB	2.34	0.42
2:F:4936:ASP:O	2:F:4940:GLU:HG2	2.19	0.42
1:G:8:SER:HB2	1:G:71:ARG:HB2	2.02	0.42
2:H:257:ARG:HH22	2:H:286:THR:HG21	1.84	0.42
2:H:4059:MET:HA	2:H:4062:LYS:HE2	2.02	0.42
2:B:24:CYS:SG	2:B:35:LEU:HB2	2.60	0.42
2:B:1712:TYR:HD2	2:B:1841:PRO:HB2	1.84	0.42
2:B:1816:LEU:HD12	2:B:1816:LEU:HA	1.91	0.42
2:B:1951:GLU:OE1	2:B:1955:ARG:NH1	2.53	0.42
2:B:3987:PHE:O	2:B:3990:VAL:HG22	2.19	0.42
2:D:554:LEU:H	2:D:554:LEU:HD23	1.84	0.42
2:D:1649:ASP:OD1	2:D:1650:ILE:N	2.52	0.42
2:D:3799:ILE:HG22	2:D:3807:VAL:HG11	2.00	0.42
2:F:22:LEU:HD12	2:F:37:LEU:HD22	2.01	0.42
2:F:592:LYS:HA	2:F:1580:PHE:CE1	2.55	0.42
2:F:1732:SER:OG	2:F:2141:ARG:NH2	2.53	0.42
2:F:2114:SER:O	2:F:2118:VAL:HG23	2.19	0.42
2:F:3799:ILE:HG22	2:F:3807:VAL:HG11	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3974:SER:O	2:F:3978:SER:HB3	2.20	0.42
2:H:1714:LEU:O	2:H:1718:ILE:HG22	2.20	0.42
2:H:3958:ASN:ND2	2:H:4017:ASP:OD2	2.52	0.42
2:H:4030:VAL:HG12	2:H:4032:ASN:H	1.83	0.42
2:B:1450:VAL:HA	2:B:1552:VAL:HG12	2.02	0.42
2:B:1495:VAL:HG12	2:B:1538:THR:HG21	2.02	0.42
2:D:255:HIS:ND1	2:D:480:GLU:OE1	2.53	0.42
2:D:592:LYS:HA	2:D:1580:PHE:CE1	2.55	0.42
2:D:847:SER:OG	2:D:849:THR:HG22	2.20	0.42
2:D:1959:LEU:HD23	2:D:2139:LEU:HD21	2.01	0.42
2:F:1712:TYR:HD2	2:F:1841:PRO:HB2	1.84	0.42
2:H:646:PRO:HB2	2:H:648:ILE:HG12	2.01	0.42
2:H:1450:VAL:HA	2:H:1552:VAL:HG12	2.02	0.42
2:B:206:CYS:HB3	2:B:271:GLY:HA3	2.00	0.42
2:B:3766:HIS:CE1	2:B:3807:VAL:HA	2.55	0.42
2:B:4059:MET:HA	2:B:4062:LYS:HE2	2.02	0.42
2:D:206:CYS:HB3	2:D:271:GLY:HA3	2.00	0.42
2:D:3766:HIS:CE1	2:D:3807:VAL:HA	2.55	0.42
2:F:1143:TRP:HB3	2:F:1164:LEU:HD11	2.01	0.42
2:F:3374:UNK:HA	2:F:3442:ILE:HD11	2.02	0.42
2:F:3757:ARG:O	2:F:3761:GLN:HG3	2.19	0.42
2:H:255:HIS:ND1	2:H:480:GLU:OE1	2.53	0.42
2:H:1495:VAL:HG12	2:H:1538:THR:HG21	2.02	0.42
2:H:1712:TYR:HD2	2:H:1841:PRO:HB2	1.84	0.42
2:H:1959:LEU:HD23	2:H:2139:LEU:HD21	2.01	0.42
2:H:3987:PHE:O	2:H:3990:VAL:HG22	2.20	0.42
2:B:3804:ASN:HB3	2:B:3807:VAL:HB	2.02	0.42
2:D:4029:ASN:ND2	2:D:4035:ILE:HB	2.34	0.42
2:F:1714:LEU:O	2:F:1718:ILE:HG22	2.20	0.42
2:H:1456:ASP:C	2:H:1491:ASN:HD21	2.22	0.42
2:H:1852:MET:HB2	2:H:1854:ILE:HG12	2.02	0.42
2:H:3757:ARG:O	2:H:3761:GLN:HG3	2.19	0.42
2:H:3766:HIS:CE1	2:H:3807:VAL:HA	2.55	0.42
2:B:156:GLN:HG2	2:B:157:ARG:N	2.34	0.42
2:B:951:ARG:H	2:B:970:LEU:HA	1.84	0.42
2:B:3958:ASN:ND2	2:B:4017:ASP:OD2	2.52	0.42
2:B:3974:SER:O	2:B:3978:SER:HB3	2.19	0.42
2:B:4165:ILE:O	2:B:4169:PHE:HD1	2.03	0.42
2:B:4954:THR:O	2:B:4963:SER:OG	2.31	0.42
2:D:1732:SER:OG	2:D:2141:ARG:NH2	2.53	0.42
2:F:646:PRO:HB2	2:F:648:ILE:HG12	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3637:LEU:HD12	2:F:3640:LEU:HD12	2.02	0.42
2:H:1245:PHE:CE1	2:H:1600:LEU:HB2	2.54	0.42
2:H:2139:LEU:HD23	2:H:2139:LEU:HA	1.90	0.42
2:H:4861:TYR:OH	2:H:4884:HIS:NE2	2.49	0.42
1:A:27:THR:HB	1:A:100:ASP:HB3	2.02	0.41
2:B:2114:SER:O	2:B:2118:VAL:HG23	2.19	0.41
2:B:2139:LEU:HD23	2:B:2139:LEU:HA	1.90	0.41
1:C:8:SER:HB2	1:C:71:ARG:HB2	2.01	0.41
2:D:533:ASN:ND2	2:D:536:ASN:OD1	2.41	0.41
2:F:597:HIS:HB2	2:F:1665:HIS:ND1	2.35	0.41
2:F:1450:VAL:HA	2:F:1552:VAL:HG12	2.02	0.41
2:F:3987:PHE:O	2:F:3990:VAL:HG22	2.19	0.41
2:F:4059:MET:HA	2:F:4062:LYS:HE2	2.02	0.41
1:G:27:THR:HB	1:G:100:ASP:HB3	2.02	0.41
2:H:24:CYS:SG	2:H:35:LEU:HB2	2.60	0.41
2:H:107:ILE:N	2:H:148:TRP:O	2.47	0.41
2:H:156:GLN:HG2	2:H:157:ARG:N	2.34	0.41
2:H:4165:ILE:O	2:H:4169:PHE:HD1	2.03	0.41
2:B:255:HIS:ND1	2:B:480:GLU:OE1	2.53	0.41
2:B:1244:GLN:OE1	2:B:1458:HIS:ND1	2.52	0.41
2:B:1456:ASP:C	2:B:1491:ASN:HD21	2.22	0.41
2:D:3637:LEU:HD12	2:D:3640:LEU:HD12	2.02	0.41
2:D:4059:MET:HA	2:D:4062:LYS:HE2	2.02	0.41
1:E:78:PRO:HA	1:E:81:ALA:HB3	2.03	0.41
2:F:38:ALA:HB2	2:F:65:CYS:HB3	2.01	0.41
2:F:1245:PHE:CD2	2:F:1290:ARG:HD3	2.55	0.41
2:F:1951:GLU:OE1	2:F:1955:ARG:NH1	2.53	0.41
2:F:3804:ASN:HB3	2:F:3807:VAL:HB	2.02	0.41
2:H:1143:TRP:HB3	2:H:1164:LEU:HD11	2.01	0.41
2:H:1245:PHE:CD2	2:H:1290:ARG:HD3	2.56	0.41
2:H:3974:SER:O	2:H:3978:SER:HB3	2.20	0.41
2:B:125:ARG:N	2:B:134:ASP:OD2	2.42	0.41
2:B:689:THR:HA	2:B:778:PHE:HE2	1.85	0.41
2:B:1732:SER:OG	2:B:2141:ARG:NH2	2.53	0.41
2:B:1959:LEU:HD23	2:B:2139:LEU:HD21	2.01	0.41
2:D:24:CYS:SG	2:D:35:LEU:HB2	2.60	0.41
2:D:102:LEU:HA	2:D:161:GLU:O	2.20	0.41
2:D:1130:GLN:HE21	2:D:1132:TRP:HZ3	1.66	0.41
2:D:4165:ILE:O	2:D:4169:PHE:HD1	2.03	0.41
2:F:102:LEU:HA	2:F:161:GLU:O	2.21	0.41
2:F:773:LEU:HD23	2:F:773:LEU:H	1.85	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1683:HIS:NE2	2:F:1799:LEU:O	2.36	0.41
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.86	0.41
2:B:1852:MET:HB2	2:B:1854:ILE:HG12	2.02	0.41
2:D:38:ALA:HB2	2:D:65:CYS:HB3	2.01	0.41
2:D:265:LEU:HD13	2:D:281:ARG:HH12	1.85	0.41
2:D:773:LEU:HD23	2:D:773:LEU:H	1.85	0.41
2:D:1155:LEU:HD23	2:D:1155:LEU:HA	1.92	0.41
2:F:255:HIS:ND1	2:F:480:GLU:OE1	2.53	0.41
2:H:1732:SER:OG	2:H:2141:ARG:NH2	2.53	0.41
2:B:1240:LYS:HG2	2:B:1242:LEU:HB3	2.03	0.41
2:D:689:THR:HA	2:D:778:PHE:HE2	1.85	0.41
2:D:1450:VAL:HA	2:D:1552:VAL:HG12	2.02	0.41
2:D:3958:ASN:ND2	2:D:4017:ASP:OD2	2.53	0.41
2:F:265:LEU:HD13	2:F:281:ARG:HH12	1.85	0.41
2:F:1111:PRO:HD3	2:F:1605:TRP:HE1	1.86	0.41
2:F:1240:LYS:HG2	2:F:1242:LEU:HB3	2.03	0.41
2:F:2143:TYR:CD2	2:F:2198:LEU:HD13	2.56	0.41
2:F:4029:ASN:OD1	2:F:4030:VAL:N	2.54	0.41
2:H:265:LEU:HD13	2:H:281:ARG:HH12	1.85	0.41
2:H:592:LYS:HA	2:H:1580:PHE:CE1	2.55	0.41
2:H:4040:VAL:O	2:H:4044:VAL:HG23	2.21	0.41
2:B:256:ALA:HB3	2:B:481:GLU:OE1	2.21	0.41
2:B:385:ASP:CG	2:H:156:GLN:HE22	2.22	0.41
2:B:554:LEU:HD23	2:B:554:LEU:H	1.84	0.41
2:B:1245:PHE:CD2	2:B:1290:ARG:HD3	2.56	0.41
2:B:4029:ASN:OD1	2:B:4030:VAL:N	2.54	0.41
2:B:4569:PHE:CE1	2:B:4811:LEU:HD11	2.56	0.41
2:D:839:LEU:N	2:D:1200:GLY:O	2.54	0.41
2:D:1683:HIS:NE2	2:D:1799:LEU:O	2.36	0.41
2:D:1714:LEU:O	2:D:1718:ILE:HG22	2.20	0.41
2:D:1951:GLU:OE1	2:D:1955:ARG:NH1	2.53	0.41
2:F:554:LEU:H	2:F:554:LEU:HD23	1.85	0.41
2:F:839:LEU:N	2:F:1200:GLY:O	2.54	0.41
2:F:1104:TRP:CD1	2:F:1190:PRO:HA	2.56	0.41
2:H:13:PHE:CD1	2:H:162:LYS:HB3	2.56	0.41
2:H:773:LEU:HD23	2:H:773:LEU:H	1.85	0.41
2:H:1683:HIS:NE2	2:H:1799:LEU:O	2.36	0.41
2:H:4140:VAL:HA	2:H:4143:THR:HG22	2.03	0.41
2:B:773:LEU:H	2:B:773:LEU:HD23	1.85	0.41
2:D:1240:LYS:HG2	2:D:1242:LEU:HB3	2.03	0.41
2:D:4925:ILE:O	2:D:4929:ILE:HG12	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4942:ARG:HE	2:D:4942:ARG:HB3	1.61	0.41
2:F:13:PHE:CD1	2:F:162:LYS:HB3	2.56	0.41
2:F:1244:GLN:OE1	2:F:1458:HIS:ND1	2.52	0.41
2:F:4569:PHE:CE1	2:F:4811:LEU:HD11	2.56	0.41
2:H:951:ARG:H	2:H:970:LEU:HA	1.84	0.41
2:H:1951:GLU:OE1	2:H:1955:ARG:NH1	2.53	0.41
2:B:526:LEU:O	2:B:530:ILE:HG12	2.21	0.41
2:B:839:LEU:N	2:B:1200:GLY:O	2.54	0.41
2:B:2377:LEU:HD11	2:B:2431:ILE:HD11	2.03	0.41
2:B:4925:ILE:O	2:B:4929:ILE:HG12	2.21	0.41
2:D:315:CYS:HB2	2:D:349:GLN:NE2	2.35	0.41
2:D:1104:TRP:CD1	2:D:1190:PRO:HA	2.56	0.41
2:D:3374:UNK:HA	2:D:3442:ILE:HD11	2.02	0.41
2:D:3974:SER:O	2:D:3978:SER:HB3	2.20	0.41
2:D:4976:HIS:CD2	2:D:4981:HIS:HB2	2.55	0.41
2:F:4040:VAL:O	2:F:4044:VAL:HG23	2.21	0.41
2:F:4207:GLU:OE1	2:F:4207:GLU:HA	2.21	0.41
2:H:839:LEU:N	2:H:1200:GLY:O	2.54	0.41
2:H:1104:TRP:CD1	2:H:1190:PRO:HA	2.56	0.41
2:H:1674:CYS:SG	2:H:1682:ALA:HA	2.61	0.41
2:B:224:HIS:N	2:B:229:GLU:O	2.51	0.41
2:B:251:SER:O	2:B:255:HIS:CD2	2.74	0.41
2:B:592:LYS:HA	2:B:1580:PHE:CE1	2.55	0.41
2:B:847:SER:OG	2:B:849:THR:HG22	2.20	0.41
2:B:1674:CYS:SG	2:B:1682:ALA:HA	2.61	0.41
2:B:1689:VAL:HG12	2:B:1694:LEU:HD12	2.03	0.41
2:B:4140:VAL:HA	2:B:4143:THR:HG22	2.03	0.41
2:B:4853:ALA:HA	2:B:4857:PHE:CD2	2.50	0.41
2:B:4976:HIS:CD2	2:B:4981:HIS:HB2	2.55	0.41
1:C:78:PRO:HA	1:C:81:ALA:HB3	2.03	0.41
2:D:224:HIS:N	2:D:229:GLU:O	2.51	0.41
2:D:3910:ILE:HA	2:D:3913:CYS:SG	2.61	0.41
2:D:4029:ASN:OD1	2:D:4030:VAL:N	2.54	0.41
1:E:27:THR:HB	1:E:100:ASP:HB3	2.02	0.41
1:E:36:PHE:N	1:E:36:PHE:CD1	2.89	0.41
2:F:315:CYS:HB2	2:F:349:GLN:NE2	2.35	0.41
1:G:24:VAL:HA	1:G:102:GLU:O	2.21	0.41
1:G:78:PRO:HA	1:G:81:ALA:HB3	2.03	0.41
2:H:1111:PRO:HD3	2:H:1605:TRP:HE1	1.86	0.41
2:H:1689:VAL:HG12	2:H:1694:LEU:HD12	2.03	0.41
2:H:2377:LEU:HD11	2:H:2431:ILE:HD11	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3637:LEU:HD12	2:H:3640:LEU:HD12	2.02	0.41
2:H:4049:ASN:O	2:H:4053:ILE:HD12	2.21	0.41
2:H:4659:TYR:OH	2:H:4786:SER:OG	2.31	0.41
2:B:1471:ALA:HB1	2:B:1488:LYS:HZ1	1.86	0.41
2:B:3411:PRO:HB2	2:B:3412:LEU:H	1.73	0.41
1:C:27:THR:HB	1:C:100:ASP:HB3	2.02	0.41
2:D:666:VAL:HG13	2:D:744:VAL:HB	2.03	0.41
2:D:1811:LYS:HE3	2:D:1811:LYS:HB3	1.87	0.41
2:D:1852:MET:HB2	2:D:1854:ILE:HG12	2.02	0.41
2:D:2378:LEU:HD12	2:D:2466:ASP:HA	2.03	0.41
2:D:3964:ILE:HD12	2:D:4025:LEU:HA	2.03	0.41
2:F:107:ILE:N	2:F:148:TRP:O	2.47	0.41
2:F:256:ALA:HB3	2:F:481:GLU:OE1	2.21	0.41
2:F:1500:PHE:CD1	2:F:1531:ALA:HB2	2.56	0.41
2:H:597:HIS:HB2	2:H:1665:HIS:ND1	2.35	0.41
2:H:4569:PHE:CE1	2:H:4811:LEU:HD11	2.56	0.41
2:H:4698:GLN:O	2:H:4701:ARG:HG2	2.21	0.41
2:B:315:CYS:HB2	2:B:349:GLN:NE2	2.35	0.40
2:B:597:HIS:HB2	2:B:1665:HIS:ND1	2.35	0.40
2:B:1527:MET:O	2:B:1539:PHE:HA	2.21	0.40
2:B:3374:UNK:HA	2:B:3442:ILE:HD11	2.02	0.40
2:B:3637:LEU:HD12	2:B:3640:LEU:HD12	2.02	0.40
1:C:36:PHE:CD1	1:C:36:PHE:N	2.89	0.40
2:D:256:ALA:HB3	2:D:481:GLU:OE1	2.21	0.40
2:D:1245:PHE:CD2	2:D:1290:ARG:HD3	2.56	0.40
2:D:1674:CYS:SG	2:D:1682:ALA:HA	2.61	0.40
2:F:2378:LEU:HD12	2:F:2466:ASP:HA	2.03	0.40
2:H:251:SER:O	2:H:255:HIS:CD2	2.74	0.40
2:H:256:ALA:HB3	2:H:481:GLU:OE1	2.21	0.40
2:H:689:THR:HA	2:H:778:PHE:HE2	1.85	0.40
2:H:1240:LYS:HG2	2:H:1242:LEU:HB3	2.03	0.40
2:H:1244:GLN:OE1	2:H:1458:HIS:ND1	2.52	0.40
2:H:1500:PHE:CD1	2:H:1531:ALA:HB2	2.56	0.40
2:H:3418:ASP:OD1	2:H:3419:ASN:N	2.54	0.40
2:H:4976:HIS:CD2	2:H:4981:HIS:HB2	2.55	0.40
2:B:265:LEU:HD13	2:B:281:ARG:HH12	1.85	0.40
2:B:591:ASP:HA	2:B:1594:ARG:NH1	2.36	0.40
2:B:1720:LEU:HD22	2:B:1852:MET:SD	2.62	0.40
2:B:2143:TYR:CD2	2:B:2198:LEU:HD13	2.56	0.40
2:B:3418:ASP:OD1	2:B:3419:ASN:N	2.54	0.40
2:D:526:LEU:O	2:D:530:ILE:HG12	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4671:ARG:NH1	2:D:4780:VAL:HG13	2.36	0.40
1:E:24:VAL:HA	1:E:102:GLU:O	2.21	0.40
2:F:1720:LEU:HD22	2:F:1852:MET:SD	2.61	0.40
2:F:1816:LEU:HD12	2:F:1816:LEU:HA	1.91	0.40
2:F:3418:ASP:OD1	2:F:3419:ASN:N	2.55	0.40
2:F:4193:SER:HB3	2:F:4196:ASN:ND2	2.37	0.40
2:F:4698:GLN:O	2:F:4701:ARG:HG2	2.22	0.40
2:F:4847:TYR:O	2:F:4850:THR:HG22	2.21	0.40
2:F:4976:HIS:CD2	2:F:4981:HIS:HB2	2.55	0.40
1:G:36:PHE:CD1	1:G:36:PHE:N	2.89	0.40
2:H:1739:THR:O	2:H:1742:THR:OG1	2.32	0.40
2:H:3804:ASN:HB3	2:H:3807:VAL:HB	2.02	0.40
2:H:3957:PHE:HD1	2:H:3957:PHE:HA	1.77	0.40
2:H:4029:ASN:OD1	2:H:4030:VAL:N	2.54	0.40
1:A:24:VAL:HA	1:A:102:GLU:O	2.21	0.40
2:B:13:PHE:CD1	2:B:162:LYS:HB3	2.56	0.40
2:B:666:VAL:HG13	2:B:744:VAL:HB	2.03	0.40
2:B:2298:LYS:O	2:B:2301:SER:OG	2.33	0.40
2:B:4847:TYR:O	2:B:4850:THR:HG22	2.21	0.40
2:D:531:ARG:NH2	2:D:562:GLU:OE2	2.49	0.40
2:D:579:GLN:H	2:D:582:HIS:CD2	2.40	0.40
2:D:591:ASP:HA	2:D:1594:ARG:NH1	2.36	0.40
2:D:1689:VAL:HG12	2:D:1694:LEU:HD12	2.03	0.40
2:D:4207:GLU:OE1	2:D:4207:GLU:HA	2.21	0.40
2:F:1007:TYR:CE2	2:F:1009:ALA:HB3	2.57	0.40
2:F:1674:CYS:SG	2:F:1682:ALA:HA	2.61	0.40
2:F:2443:LEU:O	2:F:2448:LYS:N	2.37	0.40
2:F:4049:ASN:O	2:F:4053:ILE:HD12	2.21	0.40
2:F:4165:ILE:O	2:F:4169:PHE:HD1	2.04	0.40
2:H:3374:UNK:HA	2:H:3442:ILE:HD11	2.02	0.40
1:A:28:GLY:HA2	1:A:98:ILE:O	2.21	0.40
2:B:107:ILE:N	2:B:148:TRP:O	2.47	0.40
2:B:1007:TYR:CE2	2:B:1009:ALA:HB3	2.57	0.40
2:B:1698:LEU:HA	2:B:1712:TYR:CE1	2.51	0.40
2:D:13:PHE:CD1	2:D:162:LYS:HB3	2.56	0.40
2:D:1111:PRO:HD3	2:D:1605:TRP:HE1	1.86	0.40
2:D:4569:PHE:CE1	2:D:4811:LEU:HD11	2.56	0.40
1:E:28:GLY:HA2	1:E:98:ILE:O	2.21	0.40
2:F:689:THR:HA	2:F:778:PHE:HE2	1.85	0.40
2:F:1852:MET:HB2	2:F:1854:ILE:HG12	2.02	0.40
2:H:315:CYS:HB2	2:H:349:GLN:NE2	2.35	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:526:LEU:O	2:H:530:ILE:HG12	2.21	0.40
2:B:2378:LEU:HD12	2:B:2466:ASP:HA	2.03	0.40
2:B:4040:VAL:O	2:B:4044:VAL:HG23	2.21	0.40
1:C:8:SER:HB2	1:C:71:ARG:HH11	1.87	0.40
2:D:2143:TYR:CD2	2:D:2198:LEU:HD13	2.56	0.40
2:D:2377:LEU:HD11	2:D:2431:ILE:HD11	2.03	0.40
2:D:4035:ILE:H	2:D:4035:ILE:HD12	1.86	0.40
2:D:4049:ASN:O	2:D:4053:ILE:HD12	2.21	0.40
2:D:4140:VAL:HA	2:D:4143:THR:HG22	2.03	0.40
2:D:4698:GLN:O	2:D:4701:ARG:HG2	2.21	0.40
2:F:1689:VAL:HG12	2:F:1694:LEU:HD12	2.03	0.40
2:F:4925:ILE:O	2:F:4929:ILE:HG12	2.21	0.40
2:H:575:LEU:HA	2:H:578:ILE:HG12	2.03	0.40
2:H:666:VAL:HG13	2:H:744:VAL:HB	2.03	0.40
2:H:1471:ALA:HB1	2:H:1488:LYS:HZ1	1.86	0.40
2:H:1527:MET:O	2:H:1539:PHE:HA	2.21	0.40
2:H:2378:LEU:HD12	2:H:2466:ASP:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	104/110 (94%)	99 (95%)	5 (5%)	0	100	100
1	C	104/110 (94%)	99 (95%)	5 (5%)	0	100	100
1	E	104/110 (94%)	99 (95%)	5 (5%)	0	100	100
1	G	104/110 (94%)	99 (95%)	5 (5%)	0	100	100
2	B	3319/4624 (72%)	3275 (99%)	44 (1%)	0	100	100
2	D	3319/4624 (72%)	3273 (99%)	46 (1%)	0	100	100
2	F	3319/4624 (72%)	3275 (99%)	44 (1%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	3319/4624 (72%)	3275 (99%)	44 (1%)	0	100	100
All	All	13692/18936 (72%)	13494 (99%)	198 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	67/90 (74%)	65 (97%)	2 (3%)	41	64
1	C	67/90 (74%)	65 (97%)	2 (3%)	41	64
1	E	67/90 (74%)	65 (97%)	2 (3%)	41	64
1	G	67/90 (74%)	65 (97%)	2 (3%)	41	64
2	B	2115/3648 (58%)	2106 (100%)	9 (0%)	91	94
2	D	2115/3648 (58%)	2106 (100%)	9 (0%)	91	94
2	F	2115/3648 (58%)	2106 (100%)	9 (0%)	91	94
2	H	2115/3648 (58%)	2106 (100%)	9 (0%)	91	94
All	All	8728/14952 (58%)	8684 (100%)	44 (0%)	89	93

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	36	PHE
2	B	165	VAL
2	B	275	ARG
2	B	373	LYS
2	B	1087	ARG
2	B	2128	GLN
2	B	2157	LEU
2	B	2628	VAL
2	B	4041	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	4878	MET
1	C	31	GLN
1	C	36	PHE
2	D	165	VAL
2	D	275	ARG
2	D	373	LYS
2	D	1087	ARG
2	D	2128	GLN
2	D	2157	LEU
2	D	2628	VAL
2	D	4041	ASP
2	D	4878	MET
1	E	31	GLN
1	E	36	PHE
2	F	165	VAL
2	F	275	ARG
2	F	373	LYS
2	F	1087	ARG
2	F	2128	GLN
2	F	2157	LEU
2	F	2628	VAL
2	F	4041	ASP
2	F	4878	MET
1	G	31	GLN
1	G	36	PHE
2	H	165	VAL
2	H	275	ARG
2	H	373	LYS
2	H	1087	ARG
2	H	2128	GLN
2	H	2157	LEU
2	H	2628	VAL
2	H	4041	ASP
2	H	4878	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	255	HIS
2	B	495	ASN
2	B	1052	ASN
2	B	4712	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	255	HIS
2	D	495	ASN
2	D	1052	ASN
2	D	4712	ASN
2	F	255	HIS
2	F	495	ASN
2	F	1052	ASN
2	F	1696	HIS
2	F	4712	ASN
2	H	255	HIS
2	H	495	ASN
2	H	1052	ASN
2	H	4712	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	25
2	D	25
2	F	25
2	H	25

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3606:UNK	C	3634:MET	N	44.08
1	D	3606:UNK	C	3634:MET	N	44.08
1	F	3606:UNK	C	3634:MET	N	44.08
1	H	3606:UNK	C	3634:MET	N	44.08
1	B	2939:ARG	C	2956:UNK	N	30.87
1	D	2939:ARG	C	2956:UNK	N	30.87
1	F	2939:ARG	C	2956:UNK	N	30.87
1	H	2939:ARG	C	2956:UNK	N	30.87
1	B	2700:UNK	C	2736:ASP	N	28.31
1	D	2700:UNK	C	2736:ASP	N	28.31
1	F	2700:UNK	C	2736:ASP	N	28.31
1	H	2700:UNK	C	2736:ASP	N	28.31
1	B	3385:UNK	C	3411:PRO	N	28.09
1	D	3385:UNK	C	3411:PRO	N	28.09
1	F	3385:UNK	C	3411:PRO	N	28.09
1	H	3385:UNK	C	3411:PRO	N	28.09
1	B	3555:UNK	C	3564:SER	N	21.04
1	D	3555:UNK	C	3564:SER	N	21.04
1	F	3555:UNK	C	3564:SER	N	21.04
1	H	3555:UNK	C	3564:SER	N	21.04
1	B	2653:UNK	C	2664:UNK	N	18.19
1	D	2653:UNK	C	2664:UNK	N	18.19
1	F	2653:UNK	C	2664:UNK	N	18.19
1	H	2653:UNK	C	2664:UNK	N	18.19
1	B	3238:UNK	C	3278:UNK	N	17.52
1	D	3238:UNK	C	3278:UNK	N	17.52
1	F	3238:UNK	C	3278:UNK	N	17.52

*Continued on next page...*

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	3238:UNK	C	3278:UNK	N	17.52
1	B	3193:UNK	C	3202:UNK	N	17.16
1	D	3193:UNK	C	3202:UNK	N	17.16
1	F	3193:UNK	C	3202:UNK	N	17.16
1	H	3193:UNK	C	3202:UNK	N	17.16
1	B	2978:UNK	C	2999:UNK	N	15.49
1	D	2978:UNK	C	2999:UNK	N	15.49
1	F	2978:UNK	C	2999:UNK	N	15.49
1	H	2978:UNK	C	2999:UNK	N	15.49
1	B	3166:UNK	C	3173:UNK	N	15.27
1	D	3166:UNK	C	3173:UNK	N	15.27
1	F	3166:UNK	C	3173:UNK	N	15.27
1	H	3166:UNK	C	3173:UNK	N	15.27
1	B	3062:UNK	C	3146:UNK	N	14.85
1	D	3062:UNK	C	3146:UNK	N	14.85
1	F	3062:UNK	C	3146:UNK	N	14.85
1	H	3062:UNK	C	3146:UNK	N	14.85
1	B	3448:LYS	C	3509:UNK	N	14.70
1	D	3448:LYS	C	3509:UNK	N	14.70
1	H	3448:LYS	C	3509:UNK	N	14.70
1	F	3448:LYS	C	3509:UNK	N	14.69
1	B	3358:UNK	C	3365:UNK	N	14.66
1	D	3358:UNK	C	3365:UNK	N	14.66
1	F	3358:UNK	C	3365:UNK	N	14.66
1	H	3358:UNK	C	3365:UNK	N	14.66
1	B	3018:UNK	C	3032:UNK	N	13.52
1	D	3018:UNK	C	3032:UNK	N	13.52
1	F	3018:UNK	C	3032:UNK	N	13.52
1	H	3018:UNK	C	3032:UNK	N	13.52
1	B	3046:UNK	C	3051:UNK	N	12.43
1	D	3046:UNK	C	3051:UNK	N	12.43
1	F	3046:UNK	C	3051:UNK	N	12.43
1	H	3046:UNK	C	3051:UNK	N	12.43
1	B	3217:UNK	C	3225:UNK	N	12.35
1	D	3217:UNK	C	3225:UNK	N	12.35
1	F	3217:UNK	C	3225:UNK	N	12.35
1	H	3217:UNK	C	3225:UNK	N	12.35
1	B	4090:LYS	C	4109:UNK	N	11.51
1	D	4090:LYS	C	4109:UNK	N	11.51
1	F	4090:LYS	C	4109:UNK	N	11.51
1	H	4090:LYS	C	4109:UNK	N	11.51
1	B	2683:UNK	C	2688:UNK	N	11.14

*Continued on next page...*

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	2683:UNK	C	2688:UNK	N	11.14
1	F	2683:UNK	C	2688:UNK	N	11.14
1	H	2683:UNK	C	2688:UNK	N	11.14
1	B	3308:UNK	C	3321:UNK	N	10.68
1	D	3308:UNK	C	3321:UNK	N	10.68
1	F	3308:UNK	C	3321:UNK	N	10.68
1	H	3308:UNK	C	3321:UNK	N	10.68
1	B	2632:PRO	C	2641:UNK	N	10.67
1	D	2632:PRO	C	2641:UNK	N	10.67
1	F	2632:PRO	C	2641:UNK	N	10.67
1	H	2632:PRO	C	2641:UNK	N	10.67
1	B	3526:UNK	C	3534:UNK	N	10.45
1	D	3526:UNK	C	3534:UNK	N	10.45
1	F	3526:UNK	C	3534:UNK	N	10.45
1	H	3526:UNK	C	3534:UNK	N	10.45
1	B	4114:UNK	C	4121:GLU	N	9.88
1	D	4114:UNK	C	4121:GLU	N	9.88
1	F	4114:UNK	C	4121:GLU	N	9.88
1	H	4114:UNK	C	4121:GLU	N	9.88
1	B	3335:UNK	C	3346:UNK	N	9.64
1	D	3335:UNK	C	3346:UNK	N	9.64
1	F	3335:UNK	C	3346:UNK	N	9.64
1	H	3335:UNK	C	3346:UNK	N	9.64
1	B	3288:UNK	C	3292:UNK	N	9.19
1	D	3288:UNK	C	3292:UNK	N	9.19
1	F	3288:UNK	C	3292:UNK	N	9.19
1	H	3288:UNK	C	3292:UNK	N	9.19
1	D	3544:UNK	C	3548:UNK	N	8.82
1	H	3544:UNK	C	3548:UNK	N	8.82
1	B	3544:UNK	C	3548:UNK	N	8.81
1	F	3544:UNK	C	3548:UNK	N	8.81