



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 01:11 pm GMT

PDB ID : 5TAN  
EMDB ID: : EMD-8380  
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca<sup>2+</sup> dataset, class 3)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;  
Frank, J.  
Deposited on : 2016-09-10  
Resolution : 4.30 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

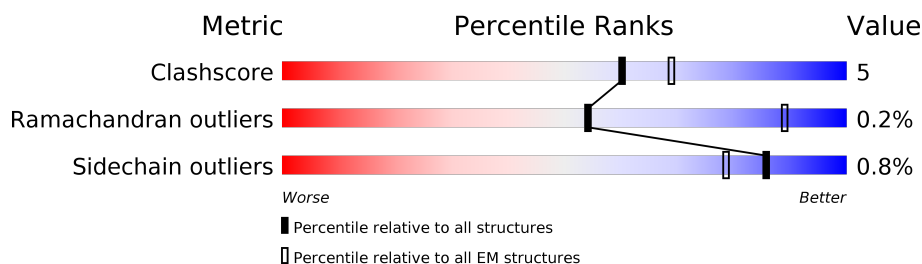
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	108	81% 19% .
1	F	108	81% 19% .
1	H	108	81% 19% .
1	J	108	81% 19% .
2	B	4416	84% 11% 5%
2	E	4416	83% 11% 5%
2	G	4416	83% 11% 5%
2	I	4416	84% 11% 5%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

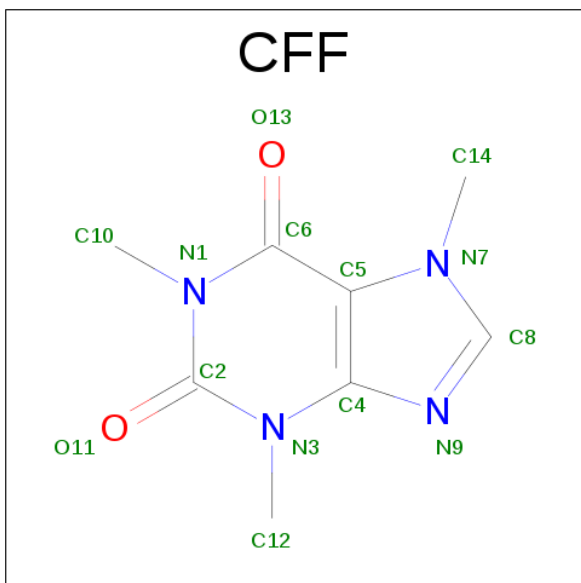
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula:  $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$ ).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

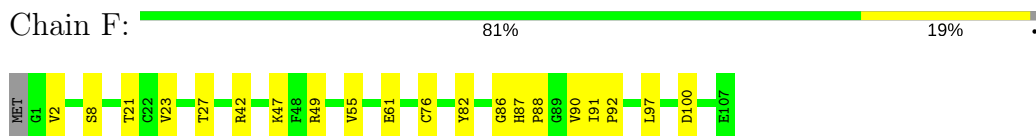
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

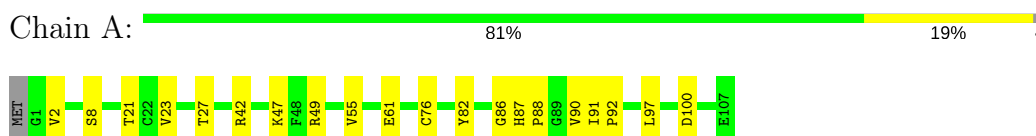
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

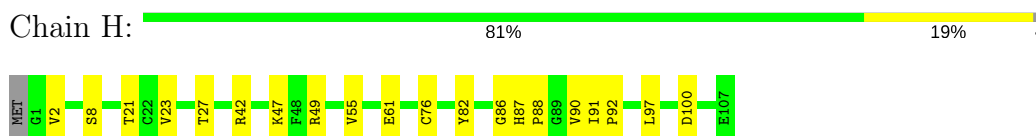
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



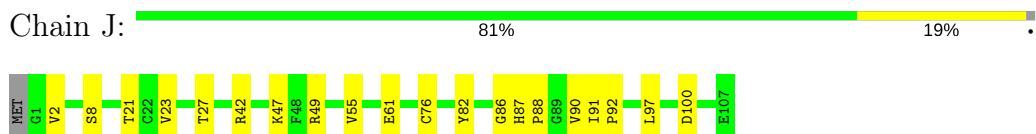
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



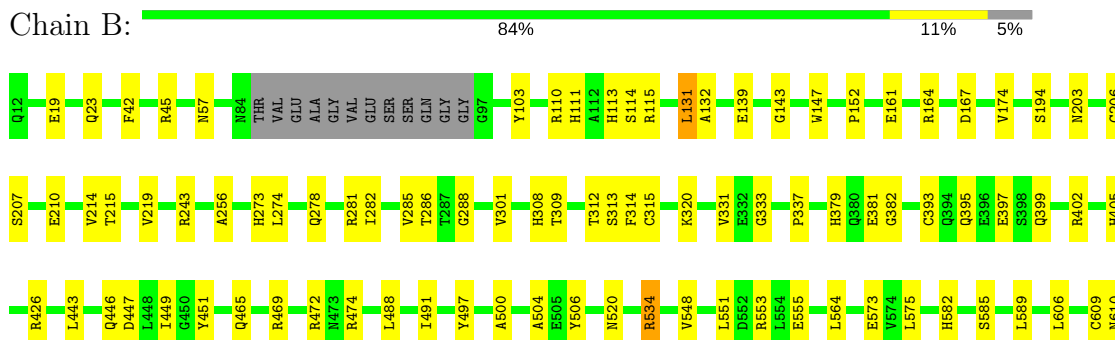
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



- Molecule 2: Ryanodine receptor 1

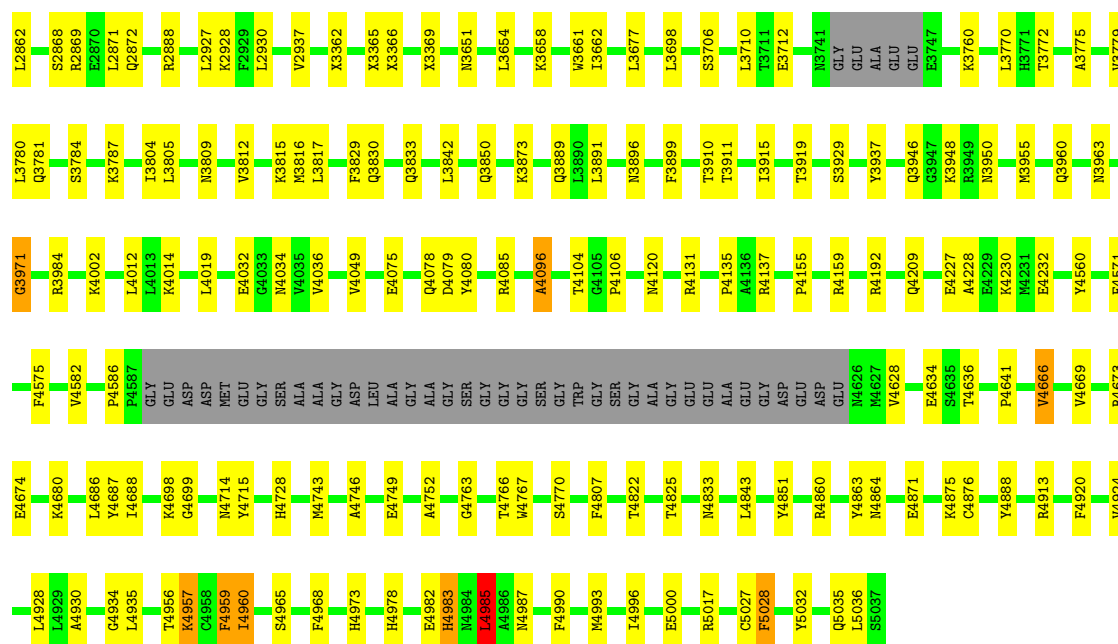



**WORLDWIDE PDB**  
 PROTEIN DATA BANK  

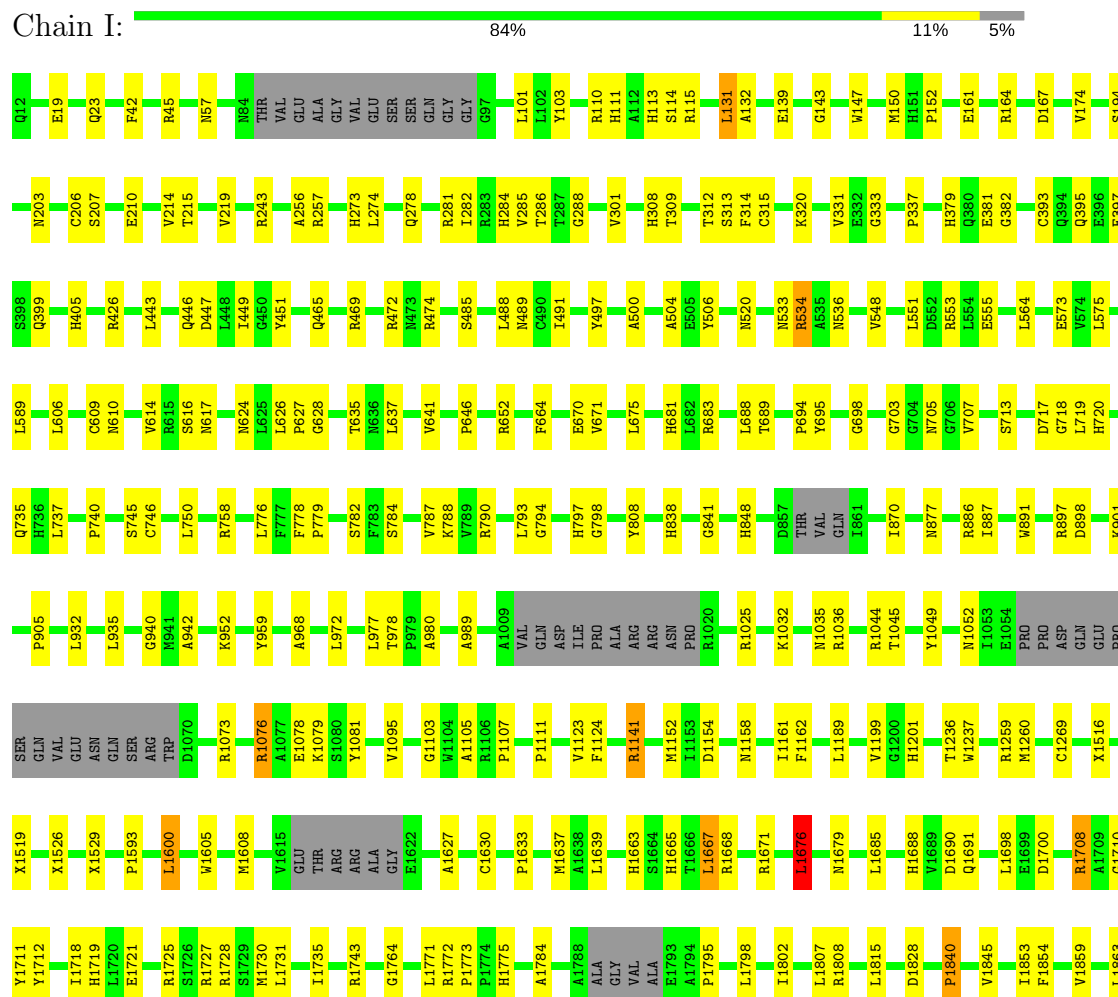
**EMDataBank**  
 Unified Data Resource for 3DEM

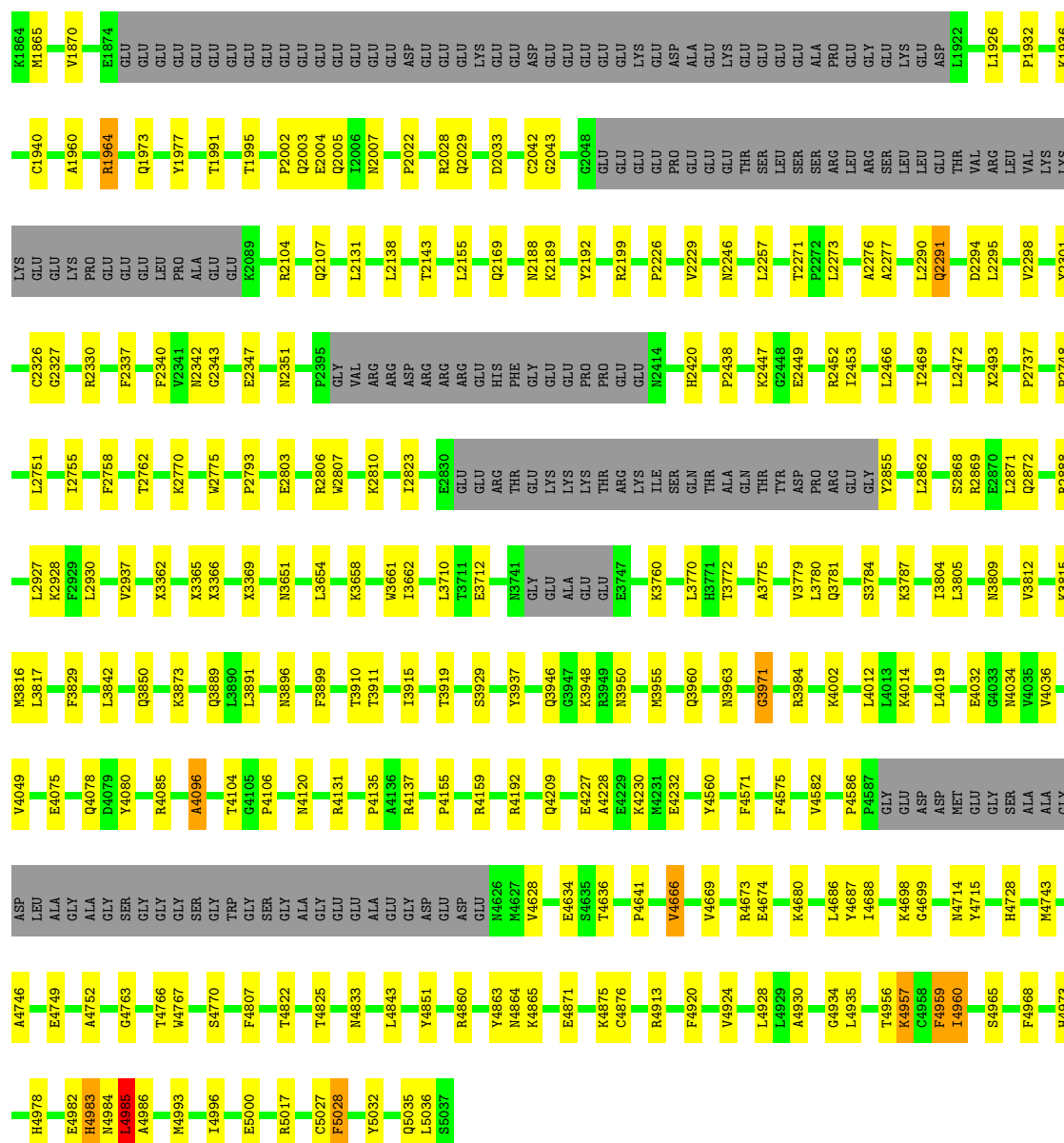






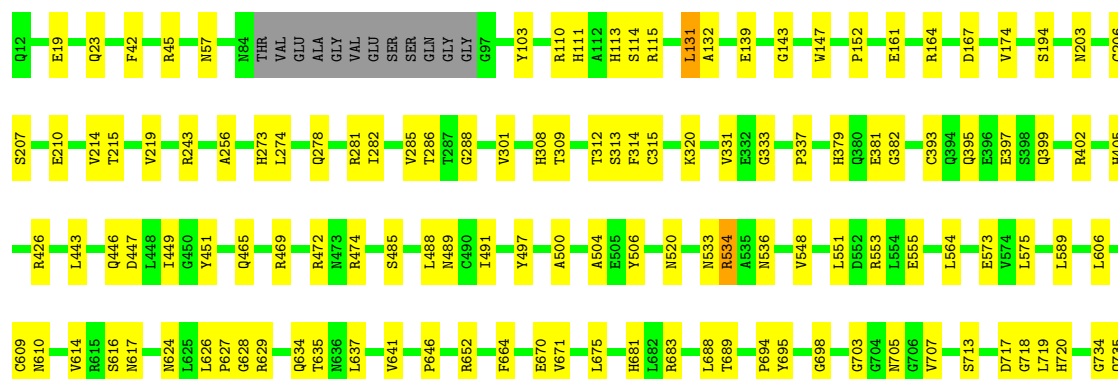
• Molecule 2: Ryanodine receptor 1





### • Molecule 2: Ryanodine receptor 1

Chain G: 83% 11% 5%



A4930	K4680	F4575	S3784	L2862	T2469	D2294	VAL	GLU	Q1691	R1259	GLN	D898	H736
G4934	L4686	V4582	K3787	S2868	L2472	L2295	ARG	ASP	V1845	M1260	GLU		L737
L4935	I4687	K4002	R2869	E2869	L2472	V2298	VAL	L1922	L1698	C1269	PRO	K901	P740
T4956	I4688	P4586	L3804	E2870	X2493	Y2301	LYS	L1926	E1699	X1516	GLN	P905	S745
K4957		F4587	L3805	L2871	Q2872	Y2301	LYS	P1932	R1708	X1516	VAL	L932	C746
K4698		GLY	L4013	Q2872	P2737	C2326	GLU		A1709	X1519	GLU		L750
G4699		GLU	N3809	R2888	P2748	G2327	GLU	K1936	G1710	X1526	GLN	L935	
A4699		ASP	L4014	Q2888	P2748	G2327	LYS	L1863	Y1711	X1526	SER		R758
		ASP	V3812	R2888	P2748	L2330	PRO	C1940	Y1712	X1529	ARG	G940	
S4965		MET	L4019	R2888	P2748	R2330	GLU	A1960	I1718	X1529	TRP	H941	
		GLU	E4032	K2928	L2761	R2330	GLU	A1960	H1719	X1529	D1070	L776	
S4965		GLY	G4033	K2928	L2761	F2337	GLU	L1720	H1719	X1529		F777	
F4968		SER	M3816	F2929	I2755	G2337	LEU	R1964	G1710	X1529		F778	
		ALA	L3817	L2930	F2758	F2340	GLU	E1874	Y1711	X1529		P779	
H4973		ALA	V4036	V2937	F2758	F2340	PRO	GLU	Y1712	X1529			
		GLY	F3829	V2937	F2758	F2340	ALA	GLU	I1721	X1529			
H4978		ASP	Q3830	X3362	T2762	G2343	GLU	Q1973	M1598	X1598	R1076	Y959	
		LEU	Q3833	X3362	K2770	E2347	GLU	GLU	Q1598	X1598	A1077		S782
		ALA	E4075	X3365	K2770	E2347	GLU	GLU	L1600	X1600	E1078	A968	F783
E4982		GLY	L3842	X3366	V2775	N2351	GLU	Y1977	G1727	X1605	K1079		S784
N4984		ALA	Q4078	X3366	V2775	N2351	GLU	T1991	S1080	X1608	GLU	L972	
L4985		GLY	D4079	X3369	P2793	L2368	R2104	GLU	S1728	X1608	GLU	Y1081	V787
A4986		SER	Y4080	X3369	P2793	L2368	GLU	T1995	M1730	X1615	GLU	L977	K788
		GLY	A3853	N3651	E2803	L2376	GLU	GLU	L1731	X1615	GLU	P979	F789
		GLY	K3873	L3654	R2806	L2376	GLU	P2002		GLU	THR	A980	R790
		GLY	R4085	L3654	R2806	F2395	L2131	Q2003	I1735	GLU	G1103		
		SER	A4096	L3654	W2807	GLY	L2138	E2004	ARG	ARG	W1104		L793
		GLY	T4104	L3658	W2807	VAL	T2143	Q2005	ALA	ALA	A1105	A989	G794
		TRP	L3890	X3658	K2810	ARG	T2143	N2007	GLY	GLY	P1107		
		GLY	L3891	W3661	R2810	ASP	ARG	GLU	E1622	E1622	E1108	A1009	H797
		SER	P4106	L3662	L2823	ASP	L2155	ASP	L1109	GLN	GLN	VAL	G798
		GLY	N3896	L3662	L2823	ARG	L2155	GLU	A1627	ASP	ASP	ASP	Y808
		ALA	M4120	X3694	E2830	ARG	Q2169	R2028	P1773	GLU	P1111	ILE	H838
		GLY	F3899	P3695	E2830	ARG	Q2169	GLU	P1774	C1630	GLU	PRO	
		GLU	R4131	P3695	GLU	GLU	N2188	C2042	H1775	GLU	V1123	ALA	
		GLU	T3910	L3710	GLU	HIS	K2189	G2043	P1633	GLU	F1124	ARG	G841
		ALA	T3911	T3711	THR	PHE	K2189	G2043	A1784	ASP	R1141	ARG	
		GLY	A4136	E3712	GLY	GLY	V2192	G2048	M1637	M1637	R1141	ASN	H848
		GLY	R4137	L3915	LYS	GLU	V2192	GLU	A1788	A1638	GLU	PRO	
		ASP	L3915	W3741	LYS	GLU	R2199	GLU	ALA	L1639	M152	R1020	D857
		GLU	T3919	GLY	LYS	PRO	LYS	GLU	GLY	L1639	I1153		THR
		ASP	T3919	GLY	LYS	PRO	THR	GLU	GLU	D1154	D1154	R1025	VAL
		GLU	A4136	ALA	THR	PRO	P2226	GLU	VAL	H1663	GLU	VAL	GLN
		GLU	S3929	GLU	THR	GLU	P2226	PRO	VAL	S1664	N1158	K1032	I861
		GLU	R4192	GLU	LYS	GLU	V2229	GLU	LYS	H1665	GLU		
		GLU	Y3937	GLU	ILE	W2414	V2229	GLU	GLU	T1666	GLU		
			E3747	GLU	SER	N2246	N2246	GLU	ASP	L1667	F1162	N1035	P864
		Q4209	Q3946	E3747	SER	H2420	N2246	THR	ALA	R1668		R1036	
			G3947	K3760	GLN	H2420	L2257	SER	GLU				L867
		E4634	G3947	K3760	THR		L2257	LEU	GLU	R1671	L1189	R1044	
		E4227	K3948	L3770	ALA	P2438	T2271	SER	LYS			T1045	I870
		T4636	R3949	L3770	GLN		T2271	SER	GLU	I1802			
			N3950	H3771	F2272	K2447	P2272	ARG	GLU	Y1199	G1200	Y1049	
		P4641	K4230	T3772	TVR	G2448	L2273	ARG	GLU	L1807	H1201		S877
			W3955	T3772	ASP	E2449	L2273	LEU	GLU	N1679			
			A3775	ASP	PRO			ARG	ALA				
			Q3960	A3775	ARG	R2452	A2276	SER	PRO	L1685	T1236	N1052	R886
			L3780	GLY	GLY	T2453	A2276	LEU	GLU		W1237	I1053	I887
			N3963	Q3781	GLY	L2290	L2290	LEU	GLY	H1688	T1237	E1054	
							Q2291	THR	GLU	W1689	P1247	PRO	W891
								THR	LYS			ASP	

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.32	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.31	0/25428	0.55	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	32/142628 (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	F	0	1
1	H	0	1
1	J	0	1
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.10	133.92	115.30
2	B	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	E	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	G	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	I	4985	LEU	CA-CB-CG	6.89	131.16	115.30
2	B	1600	LEU	CA-CB-CG	6.89	131.15	115.30
2	G	1600	LEU	CA-CB-CG	6.88	131.14	115.30
2	E	1600	LEU	CA-CB-CG	6.88	131.12	115.30
2	G	4985	LEU	CA-CB-CG	6.88	131.12	115.30
2	B	4985	LEU	CA-CB-CG	6.88	131.11	115.30
2	I	1600	LEU	CA-CB-CG	6.87	131.11	115.30
2	E	4985	LEU	CA-CB-CG	6.86	131.08	115.30
2	B	1676	LEU	CA-CB-CG	6.77	130.87	115.30
2	I	1676	LEU	CA-CB-CG	6.77	130.87	115.30
2	E	1676	LEU	CA-CB-CG	6.76	130.85	115.30
2	G	1676	LEU	CA-CB-CG	6.76	130.85	115.30
2	G	977	LEU	CA-CB-CG	6.08	129.29	115.30
2	E	977	LEU	CA-CB-CG	6.07	129.27	115.30
2	B	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	I	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	E	2290	LEU	CA-CB-CG	5.73	128.48	115.30
2	G	2290	LEU	CA-CB-CG	5.72	128.47	115.30
2	B	2290	LEU	CA-CB-CG	5.72	128.46	115.30
2	I	2290	LEU	CA-CB-CG	5.71	128.44	115.30
2	I	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	B	688	LEU	CA-CB-CG	5.40	127.71	115.30
2	E	688	LEU	CA-CB-CG	5.39	127.69	115.30
2	G	688	LEU	CA-CB-CG	5.38	127.68	115.30
2	B	1667	LEU	CA-CB-CG	5.20	127.25	115.30
2	E	1667	LEU	CA-CB-CG	5.20	127.26	115.30
2	G	1667	LEU	CA-CB-CG	5.20	127.25	115.30
2	I	1667	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4096	ALA	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	624	ASN	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4096	ALA	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	624	ASN	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	624	ASN	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4096	ALA	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	624	ASN	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

## 5.2 Too-close contacts [i](#)

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	818	0	824	12	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	12	0
2	B	29499	0	24753	296	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	29499	0	24753	305	0
2	G	29499	0	24753	299	0
2	I	29499	0	24753	295	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102396	1213	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 5.

All (1213) 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:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.32	1.18
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.32	1.17
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.32	1.17
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.32	1.16
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.64	1.16
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.64	1.15
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.64	1.14
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.64	1.14
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.67	1.12
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.67	1.11
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.67	1.10
2:G:5028:PHE:HE1	2:G:5032:TYR:CD2	1.67	1.09
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.54	0.94
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	1.81	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	1.81	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	1.81	0.92
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.54	0.91
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.05	0.90
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.05	0.90
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.05	0.90
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.05	0.90
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	1.81	0.89
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.16	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.16	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.16	0.80
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.16	0.80
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	1.96	0.78
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	1.96	0.78
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	1.96	0.78
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	1.96	0.78
2:E:4192:ARG:HH11	2:E:5028:PHE:HD2	1.36	0.74
2:B:4192:ARG:HH11	2:B:5028:PHE:HD2	1.36	0.73
2:G:4192:ARG:HH11	2:G:5028:PHE:HD2	1.36	0.73
2:I:4192:ARG:HH11	2:I:5028:PHE:HD2	1.36	0.72
2:B:111:HIS:HD2	2:B:114:SER:H	1.41	0.69
2:G:111:HIS:HD2	2:G:114:SER:H	1.41	0.68
2:E:111:HIS:HD2	2:E:114:SER:H	1.41	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.68
2:E:4957:LYS:HB2	2:E:4957:LYS:NZ	2.08	0.68
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.58	0.68
2:G:4957:LYS:NZ	2:G:4957:LYS:HB2	2.08	0.68
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.58	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.58	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:I:111:HIS:HD2	2:I:114:SER:H	1.41	0.68
2:B:4957:LYS:NZ	2:B:4957:LYS:HB2	2.08	0.67
2:E:5028:PHE:HE1	2:E:5032:TYR:HE2	1.39	0.67
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.58	0.67
2:I:4957:LYS:HB2	2:I:4957:LYS:NZ	2.08	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.66
2:E:4230:LYS:HG2	2:E:4959:PHE:HE1	1.60	0.66
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.78	0.66
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.78	0.65
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.15	0.65
2:B:4230:LYS:HG2	2:B:4959:PHE:HE1	1.60	0.65
2:I:4230:LYS:HG2	2:I:4959:PHE:HE1	1.60	0.65
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.78	0.65
2:G:4230:LYS:HD2	2:G:4959:PHE:HD1	1.62	0.65
2:E:161:GLU:HA	2:G:3984:ARG:HH22	1.62	0.64
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.15	0.64
2:G:4230:LYS:HG2	2:G:4959:PHE:HE1	1.61	0.64
2:I:4230:LYS:CD	2:I:4959:PHE:CE1	2.81	0.64
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.31	0.64
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.80	0.64
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.63	0.64
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.31	0.64
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.78	0.63
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.81	0.63
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.80	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:I:4230:LYS:HD2	2:I:4959:PHE:HD1	1.62	0.63
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.15	0.63
2:E:4230:LYS:CD	2:E:4959:PHE:CE1	2.81	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.63
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.80	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:G:4230:LYS:CD	2:G:4959:PHE:CE1	2.81	0.63
2:B:4983:HIS:H	2:B:4983:HIS:CD2	2.15	0.62
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.62
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.62
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.33	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.31	0.62
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.31	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.62
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.62
2:B:4228:ALA:HB2	2:E:4973:HIS:HE1	1.64	0.62
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.61
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.65	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.61
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.33	0.61
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.33	0.61
2:I:331:VAL:HG12	2:I:333:GLY:H	1.65	0.61
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.61
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.83	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.80	0.61
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.33	0.61
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.61
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.82	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.83	0.61
2:B:5028:PHE:HE1	2:B:5032:TYR:HE2	1.39	0.61
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.61
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.61
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.83	0.61
2:G:5028:PHE:HE1	2:G:5032:TYR:HE2	1.39	0.61
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.83	0.60
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.83	0.60
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.60
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.33	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.60
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.84	0.60
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.66	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.60
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.66	0.60
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.90	0.60
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.84	0.60
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.84	0.60
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.84	0.60
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.84	0.60
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.84	0.60
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.84	0.60
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5028:PHE:HE1	2:I:5032:TYR:HE2	1.39	0.60
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.84	0.60
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.60
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.66	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.84	0.59
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.84	0.59
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.84	0.59
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.36	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.59
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.84	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.90	0.59
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.90	0.59
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.84	0.59
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.85	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.66	0.59
2:B:4230:LYS:HD2	2:B:4959:PHE:HD1	1.62	0.59
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.84	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.66	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.85	0.59
2:B:4973:HIS:HE1	2:I:4228:ALA:HB2	1.67	0.59
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.37	0.58
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.58
2:E:4228:ALA:HB2	2:G:4973:HIS:HE1	1.68	0.58
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.37	0.58
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.85	0.58
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.35	0.58
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.90	0.58
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.84	0.58
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.37	0.58
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.36	0.58
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.37	0.58
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.86	0.58
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.83	0.58
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.85	0.58
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.37	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.58
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.86	0.58
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.85	0.58
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.77	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.36	0.58
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.36	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.58
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.85	0.58
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.77	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.37	0.57
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.87	0.57
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.86	0.57
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.77	0.57
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.86	0.57
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.86	0.57
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.57
2:I:4973:HIS:HE1	2:G:4228:ALA:HB2	1.68	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.68	0.57
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.87	0.57
2:I:4983:HIS:N	2:I:4983:HIS:CD2	2.73	0.57
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.86	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.57
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.77	0.57
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.82	0.57
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.73	0.57
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.70	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.56
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.87	0.56
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.87	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.56
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.87	0.56
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.87	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.56
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.56
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.87	0.56
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.39	0.56
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.87	0.56
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.56
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.70	0.56
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.86	0.56
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.71	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.73	0.56
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.39	0.56
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.39	0.56
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.36	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.87	0.56
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.39	0.56
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.56
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.89	0.55
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.87	0.55
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	1.88	0.55
2:E:4230:LYS:HD2	2:E:4959:PHE:HD1	1.62	0.55
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.70	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.87	0.55
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.89	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.88	0.55
2:G:626:LEU:HG	2:G:628:GLY:H	1.71	0.55
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.87	0.55
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.86	0.55
2:I:626:LEU:HG	2:I:628:GLY:H	1.72	0.55
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.40	0.55
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.40	0.55
2:B:626:LEU:HG	2:B:628:GLY:H	1.71	0.55
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.87	0.55
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.38	0.55
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.87	0.55
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.88	0.55
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.89	0.55
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.36	0.55
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.40	0.55
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.55
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.40	0.55
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.88	0.55
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.89	0.55
2:E:626:LEU:HG	2:E:628:GLY:H	1.72	0.55
2:G:3770:LEU:HD21	2:G:3775:ALA:HB3	1.88	0.54
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.88	0.54
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	1.88	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.90	0.54
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.81	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.81	0.54
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.90	0.54
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.40	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.72	0.54
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.73	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.54
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.23	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.90	0.54
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.40	0.54
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.73	0.54
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.38	0.54
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.88	0.54
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.90	0.54
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.54
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.72	0.54
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.73	0.54
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.89	0.54
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.41	0.54
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.81	0.54
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.90	0.54
2:B:309:THR:O	2:B:313:SER:OG	2.26	0.54
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	2.20	0.54
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.41	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.23	0.54
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.73	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.73	0.54
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.90	0.54
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.41	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.90	0.54
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.41	0.54
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.73	0.53
2:E:309:THR:O	2:E:313:SER:OG	2.26	0.53
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	1.88	0.53
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.81	0.53
2:E:5028:PHE:CD1	2:E:5032:TYR:CD2	2.96	0.53
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.90	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:309:THR:O	2:G:313:SER:OG	2.26	0.53
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.42	0.53
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.53
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.91	0.53
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.41	0.53
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.90	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.53
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.41	0.53
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.90	0.53
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.90	0.53
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.91	0.53
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.90	0.53
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.73	0.53
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.90	0.53
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.41	0.53
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.73	0.53
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.40	0.53
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.91	0.53
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.22	0.53
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.91	0.53
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.91	0.53
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.53
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.53
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.38	0.53
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.91	0.53
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.53
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	2.20	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.90	0.53
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.91	0.53
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.53
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.91	0.53
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.91	0.52
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.52
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.52
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.91	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.52
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.91	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:B:4960:ILE:HD13	2:B:4960:ILE:N	2.23	0.52
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.90	0.52
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.36	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.40	0.52
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.43	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.90	0.52
2:B:5028:PHE:CD1	2:B:5032:TYR:CD2	2.96	0.52
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.38	0.52
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.91	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.91	0.52
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
2:I:309:THR:O	2:I:313:SER:OG	2.26	0.52
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:B:3760:LYS:NZ	2:B:5000:GLU:OE1	2.41	0.52
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.43	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.91	0.52
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.52
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.52
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.43	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.91	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.52
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.52
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.91	0.52
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.90	0.52
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.40	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.43	0.52
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.40	0.52
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.92	0.52
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.36	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.91	0.52
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.92	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.40	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.51
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.91	0.51
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:ALA:HA	2:I:194:SER:HB2	1.91	0.51
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.93	0.51
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.51
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.92	0.51
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.76	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.91	0.51
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.76	0.51
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.92	0.51
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.92	0.51
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.44	0.51
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.51
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.51
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.92	0.51
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.92	0.51
2:G:5028:PHE:CD1	2:G:5032:TYR:CD2	2.95	0.51
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.93	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.51
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.91	0.51
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.93	0.51
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.36	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.91	0.51
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.93	0.51
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.91	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.91	0.51
2:B:132:ALA:HA	2:B:194:SER:HB2	1.91	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.91	0.51
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.76	0.51
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.84	0.51
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.44	0.51
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.76	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.92	0.51
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.76	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.51
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.44	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.92	0.51
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.44	0.51
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.43	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.77	0.51
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.77	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.46	0.50
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.44	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.93	0.50
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.92	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.50
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.77	0.50
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.92	0.50
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.76	0.50
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.92	0.50
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.77	0.50
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.84	0.50
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.44	0.50
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.92	0.50
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.93	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.44	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.94	0.50
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.46	0.50
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.77	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.76	0.50
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.76	0.50
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.77	0.50
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.93	0.50
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.92	0.50
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.84	0.50
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.94	0.50
2:I:4956:THR:O	2:I:4965:SER:N	2.42	0.50
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.94	0.50
2:I:5028:PHE:CD1	2:I:5032:TYR:CD2	2.96	0.50
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.77	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.50
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.77	0.50
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.44	0.50
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.40	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.50
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.50
2:G:395:GLN:HG3	2:G:397:GLU:H	1.76	0.49
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.76	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.45	0.49
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.77	0.49
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.94	0.49
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.46	0.49
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.95	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.93	0.49
2:E:3760:LYS:NZ	2:E:5000:GLU:OE1	2.41	0.49
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.93	0.49
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.95	0.49
1:A:21:THR:HA	1:A:49:ARG:HA	1.95	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.94	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.94	0.49
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.84	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.93	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.45	0.49
2:B:320:LYS:NZ	2:B:381:GLU:O	2.42	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.76	0.49
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.94	0.49
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.94	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.49
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.95	0.49
2:E:548:VAL:HG12	2:E:564:LEU:HD22	1.95	0.49
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.94	0.49
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.49
2:B:794:GLY:H	2:B:798:GLY:HA3	1.78	0.49
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.49
1:F:21:THR:HA	1:F:49:ARG:HA	1.95	0.49
2:G:548:VAL:HG12	2:G:564:LEU:HD22	1.95	0.49
2:G:794:GLY:H	2:G:798:GLY:HA3	1.78	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.95	0.49
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.46	0.49
2:E:794:GLY:H	2:E:798:GLY:HA3	1.78	0.49
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.78	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.49
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.77	0.49
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.78	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3760:LYS:NZ	2:I:5000:GLU:OE1	2.41	0.49
2:I:794:GLY:H	2:I:798:GLY:HA3	1.78	0.49
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.94	0.49
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.95	0.49
2:B:548:VAL:HG12	2:B:564:LEU:HD22	1.95	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.95	0.49
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.77	0.49
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.95	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.49
2:I:548:VAL:HG12	2:I:564:LEU:HD22	1.95	0.49
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.95	0.48
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.78	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.95	0.48
2:G:4956:THR:O	2:G:4965:SER:N	2.42	0.48
1:H:21:THR:HA	1:H:49:ARG:HA	1.95	0.48
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.78	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	1.96	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.94	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.77	0.48
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.95	0.48
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.43	0.48
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.95	0.48
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.39	0.48
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.46	0.48
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.95	0.48
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.95	0.48
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.95	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.95	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.95	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.45	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.48
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.96	0.48
2:E:4957:LYS:CB	2:E:4957:LYS:NZ	2.77	0.48
2:G:164:ARG:N	2:G:167:ASP:OD2	2.46	0.48
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.95	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.45	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.95	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.95	0.48
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.46	0.48
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.46	0.48
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.48
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.46	0.48
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.48
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.48
2:B:776:LEU:HG	2:B:848:HIS:HA	1.95	0.48
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.48
2:E:776:LEU:HG	2:E:848:HIS:HA	1.95	0.48
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.96	0.48
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	1.96	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.32	0.48
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.95	0.48
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.48
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.31	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.48
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.48
2:I:4571:PHE:O	2:I:4575:PHE:N	2.47	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.48
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.32	0.47
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.47
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.47	0.47
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.47
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	1.96	0.47
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.96	0.47
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.47
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.95	0.47
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.95	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.47
2:I:4957:LYS:HZ1	2:I:4957:LYS:HB2	1.80	0.47
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.47
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.32	0.47
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.80	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.47	0.47
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.31	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.95	0.47
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.79	0.47
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	2.20	0.47
1:A:27:THR:HB	1:A:100:ASP:HB3	1.97	0.47
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.47
1:F:27:THR:HB	1:F:100:ASP:HB3	1.97	0.47
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.47
2:G:4957:LYS:NZ	2:G:4957:LYS:CB	2.77	0.47
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	2.20	0.47
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.95	0.47
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.47
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.47
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.39	0.47
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.79	0.47
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.32	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.47
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.39	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.47
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.96	0.47
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.95	0.47
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.47
2:I:164:ARG:N	2:I:167:ASP:OD2	2.46	0.47
2:B:164:ARG:N	2:B:167:ASP:OD2	2.46	0.47
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.47
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.80	0.47
2:G:3760:LYS:NZ	2:G:5000:GLU:OE1	2.41	0.47
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.47
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.95	0.47
2:G:320:LYS:NZ	2:G:381:GLU:O	2.42	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.47
2:E:243:ARG:NH1	2:E:301:VAL:O	2.43	0.47
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.47
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.48	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.95	0.47
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.80	0.47
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.97	0.47
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.48	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.48	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:I:215:THR:HG22	2:I:273:HIS:HA	1.97	0.47
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:B:3915:ILE:O	2:B:3919:THR:N	2.47	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.47
2:I:320:LYS:NZ	2:I:381:GLU:O	2.42	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.80	0.47
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.38	0.46
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.95	0.46
2:G:379:HIS:CD2	2:G:381:GLU:H	2.33	0.46
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.48	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.98	0.46
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.97	0.46
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.98	0.46
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.46
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.48	0.46
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.97	0.46
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.31	0.46
2:I:4822:THR:O	2:I:4825:THR:OG1	2.29	0.46
2:B:215:THR:HG22	2:B:273:HIS:HA	1.97	0.46
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.97	0.46
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	1.96	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.48	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:I:379:HIS:CD2	2:I:381:GLU:H	2.33	0.46
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.46
2:I:4957:LYS:NZ	2:I:4957:LYS:CB	2.77	0.46
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.98	0.46
2:E:215:THR:HG22	2:E:273:HIS:HA	1.97	0.46
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.98	0.46
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.48	0.46
2:E:4930:ALA:O	2:E:4934:GLY:N	2.49	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.46
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.96	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.46
2:G:215:THR:HG22	2:G:273:HIS:HA	1.97	0.46
1:J:27:THR:HB	1:J:100:ASP:HB3	1.97	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.43	0.46
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.97	0.46
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.46
2:E:1991:THR:O	2:E:1995:THR:OG1	2.34	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.98	0.46
2:G:4930:ALA:O	2:G:4934:GLY:N	2.49	0.46
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.97	0.46
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.46
1:H:27:THR:HB	1:H:100:ASP:HB3	1.97	0.46
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.98	0.46
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.97	0.46
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.98	0.46
2:B:4957:LYS:CB	2:B:4957:LYS:NZ	2.77	0.46
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.46
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.98	0.46
2:I:4930:ALA:O	2:I:4934:GLY:N	2.49	0.46
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.98	0.46
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.98	0.46
2:G:1991:THR:O	2:G:1995:THR:OG1	2.34	0.46
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.98	0.46
2:G:3915:ILE:O	2:G:3919:THR:N	2.47	0.46
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.98	0.46
1:H:87:HIS:H	1:H:91:ILE:HB	1.81	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.98	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.98	0.46
2:B:4822:THR:O	2:B:4825:THR:OG1	2.29	0.46
2:B:4930:ALA:O	2:B:4934:GLY:N	2.49	0.46
2:B:793:LEU:HB2	2:B:797:HIS:H	1.81	0.46
1:F:87:HIS:H	1:F:91:ILE:HB	1.81	0.46
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.98	0.46
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.97	0.46
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.97	0.46
2:G:243:ARG:NH1	2:G:301:VAL:O	2.43	0.46
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.46
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.98	0.46
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:87:HIS:H	1:J:91:ILE:HB	1.81	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.97	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.47	0.45
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.98	0.45
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.98	0.45
2:I:243:ARG:NH1	2:I:301:VAL:O	2.43	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.45
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.48	0.45
2:B:1936:LYS:O	2:B:1940:CYS:N	2.46	0.45
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.98	0.45
2:G:451:TYR:O	2:G:474:ARG:NH1	2.47	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.45
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.98	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.45
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.45
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.45
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.32	0.45
2:E:4822:THR:O	2:E:4825:THR:OG1	2.29	0.45
2:G:793:LEU:HB2	2:G:797:HIS:H	1.81	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.64	0.45
2:I:451:TYR:O	2:I:474:ARG:NH1	2.47	0.45
1:A:87:HIS:H	1:A:91:ILE:HB	1.81	0.45
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.98	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.33	0.45
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.98	0.45
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.98	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.98	0.45
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.97	0.45
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.98	0.45
2:G:4978:HIS:CD2	2:G:4982:GLU:HB2	2.52	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.45
2:G:206:CYS:SG	2:G:207:SER:N	2.89	0.45
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.80	0.45
2:I:793:LEU:HB2	2:I:797:HIS:H	1.81	0.45
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.31	0.45
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	1.99	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.98	0.45
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.97	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.89	0.45
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.45
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.82	0.45
2:B:940:GLY:O	2:B:1052:ASN:N	2.49	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.33	0.45
2:E:793:LEU:HB2	2:E:797:HIS:H	1.81	0.45
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.98	0.45
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.32	0.45
2:I:4978:HIS:CD2	2:I:4982:GLU:HB2	2.52	0.45
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.50	0.45
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.64	0.45
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.65	0.45
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.98	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:I:1991:THR:O	2:I:1995:THR:OG1	2.34	0.45
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.82	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.45
2:B:1991:THR:O	2:B:1995:THR:OG1	2.34	0.45
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.82	0.45
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	1.99	0.45
2:E:206:CYS:SG	2:E:207:SER:N	2.89	0.45
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.64	0.45
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	1.99	0.45
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.98	0.45
2:B:451:TYR:O	2:B:474:ARG:NH1	2.47	0.45
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.98	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.45
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.98	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.98	0.44
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.50	0.44
2:E:1105:ALA:N	2:E:1189:LEU:O	2.51	0.44
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.82	0.44
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.44
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.82	0.44
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.82	0.44
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.98	0.44
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.65	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.38	0.44
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.82	0.44
2:B:379:HIS:NE2	2:B:381:GLU:OE1	2.50	0.44
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.44
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.44
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.44
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.82	0.44
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.32	0.44
2:E:257:ARG:O	2:E:284:HIS:NE2	2.48	0.44
2:E:4571:PHE:O	2:E:4575:PHE:N	2.47	0.44
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.64	0.44
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.82	0.44
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.39	0.44
2:B:1105:ALA:N	2:B:1189:LEU:O	2.51	0.44
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.44
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.00	0.44
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.44
2:B:4978:HIS:CD2	2:B:4982:GLU:HB2	2.52	0.44
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.44
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.83	0.44
2:B:1663:HIS:O	2:B:1667:LEU:N	2.51	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.89	0.44
2:B:5028:PHE:CG	2:B:5028:PHE:O	2.70	0.44
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.44
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.99	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.44
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.98	0.44
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	1.99	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.99	0.44
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.50	0.44
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.98	0.44
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.00	0.44
2:E:379:HIS:NE2	2:E:381:GLU:OE1	2.50	0.44
2:G:379:HIS:NE2	2:G:381:GLU:OE1	2.50	0.44
2:I:379:HIS:NE2	2:I:381:GLU:OE1	2.50	0.44
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.44
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.44
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.53	0.44
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.65	0.44
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1105:ALA:N	2:G:1189:LEU:O	2.51	0.44
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.83	0.44
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.44
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.98	0.44
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.44
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	2.00	0.44
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.00	0.44
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.83	0.44
2:B:4571:PHE:O	2:B:4575:PHE:N	2.47	0.44
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	2.00	0.44
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.53	0.44
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.00	0.44
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.65	0.44
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.99	0.43
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.43
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.83	0.43
2:E:4978:HIS:CD2	2:E:4982:GLU:HB2	2.52	0.43
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.00	0.43
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.00	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.83	0.43
2:G:4822:THR:O	2:G:4825:THR:OG1	2.29	0.43
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.83	0.43
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.83	0.43
1:A:82:TYR:O	1:A:86:GLY:N	2.51	0.43
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.43
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.42	0.43
2:B:4956:THR:O	2:B:4965:SER:N	2.42	0.43
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.51	0.43
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.00	0.43
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.90	0.43
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	2.00	0.43
2:G:606:LEU:O	2:G:617:ASN:ND2	2.51	0.43
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.43
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.43
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.00	0.43
2:I:606:LEU:O	2:I:617:ASN:ND2	2.51	0.43
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.43
2:B:4996:ILE:HG12	4:B:5102:CFF:H123	2.00	0.43
2:B:606:LEU:O	2:B:617:ASN:ND2	2.51	0.43
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.38	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.00	0.43
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.83	0.43
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.82	0.43
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.43
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.43
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.83	0.43
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.83	0.43
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
1:F:82:TYR:O	1:F:86:GLY:N	2.51	0.43
2:G:1663:HIS:O	2:G:1667:LEU:N	2.51	0.43
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.99	0.43
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.00	0.43
2:I:446:GLN:HA	2:I:449:ILE:HD12	2.01	0.43
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.00	0.43
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.49	0.43
2:E:606:LEU:O	2:E:617:ASN:ND2	2.51	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.52	0.43
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.52	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.43
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.82	0.43
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.53	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.43
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.99	0.43
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	2.00	0.43
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.82	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.83	0.43
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.43
2:G:446:GLN:HA	2:G:449:ILE:HD12	2.01	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.52	0.43
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.52	0.43
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	2.00	0.43
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.52	0.43
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.83	0.43
2:E:485:SER:O	2:E:489:ASN:N	2.38	0.43
2:G:1936:LYS:O	2:G:1940:CYS:N	2.46	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.43
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	2.00	0.43
2:E:278:GLN:N	2:E:315:CYS:SG	2.92	0.43
2:E:446:GLN:HA	2:E:449:ILE:HD12	2.01	0.43
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:101:LEU:HB3	2:I:150:MET:HE1	2.01	0.43
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.01	0.43
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.43
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.01	0.43
2:E:4957:LYS:HB2	2:E:4957:LYS:HZ1	1.83	0.43
2:E:689:THR:H	2:E:778:PHE:HE2	1.67	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:3915:ILE:O	2:I:3919:THR:N	2.47	0.43
2:B:1973:GLN:O	2:B:1977:TYR:N	2.44	0.43
2:B:446:GLN:HA	2:B:449:ILE:HD12	2.01	0.43
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.00	0.43
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	2.01	0.43
2:E:4996:ILE:HG12	4:E:5102:CFF:H123	2.00	0.43
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.54	0.42
2:E:1936:LYS:O	2:E:1940:CYS:N	2.46	0.42
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.53	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.42
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.49	0.42
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.83	0.42
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.54	0.42
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.01	0.42
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.53	0.42
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.84	0.42
2:I:689:THR:H	2:I:778:PHE:HE2	1.66	0.42
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.84	0.42
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.42
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.54	0.42
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.52	0.42
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.42
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.83	0.42
2:I:1973:GLN:O	2:I:1977:TYR:N	2.44	0.42
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.83	0.42
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.52	0.42
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	2.01	0.42
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.85	0.42
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	2.01	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.42
2:I:1105:ALA:N	2:I:1189:LEU:O	2.51	0.42
2:I:2138:LEU:HD11	2:I:3654:LEU:HD11	2.01	0.42
2:I:4996:ILE:HG12	4:I:5102:CFF:H123	2.00	0.42
1:J:82:TYR:O	1:J:86:GLY:N	2.51	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:HIS:O	2:B:399:GLN:NE2	2.53	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	2.01	0.42
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	2.02	0.42
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.52	0.42
2:E:2138:LEU:HD11	2:E:3654:LEU:HD11	2.01	0.42
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.84	0.42
2:G:4996:ILE:HG12	4:G:5102:CFF:H123	2.00	0.42
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.90	0.42
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	2.00	0.42
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.01	0.42
2:E:113:HIS:O	2:E:399:GLN:NE2	2.53	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.84	0.42
1:H:82:TYR:O	1:H:86:GLY:N	2.51	0.42
2:I:1663:HIS:O	2:I:1667:LEU:N	2.51	0.42
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.01	0.42
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.02	0.42
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.01	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:B:4984:ASN:C	2:B:4986:ALA:H	2.23	0.42
2:E:1154:ASP:O	2:E:1158:ASN:N	2.52	0.42
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.85	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.02	0.42
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.53	0.42
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.77	0.42
2:I:1936:LYS:O	2:I:1940:CYS:N	2.46	0.42
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	2.01	0.42
2:B:1154:ASP:O	2:B:1158:ASN:N	2.52	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.42
2:B:4736:ARG:NH1	2:E:4079:ASP:OD1	2.53	0.42
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.02	0.42
2:E:1124:PHE:HB2	2:E:1162:PHE:CE2	2.55	0.42
2:E:670:GLU:HG3	2:E:787:VAL:HG13	2.01	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.02	0.42
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.83	0.42
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.02	0.42
2:B:2138:LEU:HD11	2:B:3654:LEU:HD11	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3677:LEU:O	2:B:3698:LEU:N	2.52	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.53	0.42
2:I:1124:PHE:HB2	2:I:1162:PHE:CE2	2.55	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.01	0.42
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.53	0.42
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	2.02	0.42
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	2.02	0.42
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.32	0.42
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.53	0.42
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.84	0.42
2:B:689:THR:H	2:B:778:PHE:HE2	1.67	0.42
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.02	0.42
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.83	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.02	0.42
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.77	0.42
2:G:278:GLN:N	2:G:315:CYS:SG	2.92	0.42
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	2.02	0.42
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.84	0.42
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.50	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	2.02	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.90	0.42
2:B:1124:PHE:HB2	2:B:1162:PHE:CE2	2.55	0.42
2:B:551:LEU:HD21	2:B:589:LEU:HB2	2.02	0.42
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.85	0.42
2:G:1124:PHE:HB2	2:G:1162:PHE:CE2	2.55	0.42
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	2.01	0.42
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.50	0.42
2:G:614:VAL:HA	2:G:2169:GLN:HB3	2.02	0.42
2:I:1032:LYS:O	2:I:1036:ARG:N	2.47	0.42
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	2.02	0.41
2:B:670:GLU:HG3	2:B:787:VAL:HG13	2.01	0.41
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	2.01	0.41
2:E:3915:ILE:O	2:E:3919:THR:N	2.47	0.41
2:E:4228:ALA:O	2:E:4232:GLU:N	2.52	0.41
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	2.02	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.02	0.41
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.01	0.41
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.85	0.41
2:I:2271:THR:HG22	2:I:2273: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:I:2452:ARG:NH1	2:G:174:VAL:O	2.53	0.41
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.41
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.84	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.01	0.41
2:E:614:VAL:HA	2:E:2169:GLN:HB3	2.02	0.41
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.01	0.41
2:G:2138:LEU:HD11	2:G:3654:LEU:HD11	2.01	0.41
2:G:4080:TYR:CZ	2:G:4096:ALA:HB3	2.55	0.41
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.84	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.41
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.41
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.01	0.41
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.01	0.41
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.53	0.41
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.02	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.01	0.41
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.01	0.41
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	2.01	0.41
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.41
2:G:113:HIS:O	2:G:399:GLN:NE2	2.53	0.41
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.56	0.41
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.86	0.41
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.38	0.41
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.85	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.77	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.86	0.41
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.53	0.41
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.50	0.41
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	2.02	0.41
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.86	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.03	0.41
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	2.02	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.23	0.41
2:G:689:THR:H	2:G:778:PHE:HE2	1.66	0.41
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.02	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.54	0.41
2:I:614:VAL:HA	2:I:2169:GLN:HB3	2.02	0.41
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.84	0.41
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.86	0.41
2:G:1032:LYS:O	2:G:1036:ARG:N	2.47	0.41
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.52	0.41
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.53	0.41
2:I:4863:TYR:HD2	2:I:4875:LYS:HB2	1.86	0.41
2:I:4984:ASN:C	2:I:4986:ALA:H	2.23	0.41
2:I:5027:CYS:O	2:I:5027:CYS:SG	2.79	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.41
2:B:1032:LYS:O	2:B:1036:ARG:N	2.47	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.03	0.41
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.56	0.41
2:E:320:LYS:NZ	2:E:381:GLU:O	2.42	0.41
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	2.02	0.41
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.41
2:G:5027:CYS:SG	2:G:5027:CYS:O	2.79	0.41
2:I:113:HIS:O	2:I:399:GLN:NE2	2.53	0.41
2:I:4014:LYS:HE2	2:I:4135:PRO:HG3	2.03	0.41
2:I:670:GLU:HG3	2:I:787:VAL:HG13	2.02	0.41
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.01	0.41
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.90	0.41
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.53	0.41
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	2.02	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.03	0.41
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	2.02	0.41
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.53	0.41
2:E:4080:TYR:CZ	2:E:4096:ALA:HB3	2.55	0.41
2:E:4014:LYS:HE2	2:E:4135:PRO:HG3	2.03	0.41
2:E:698:GLY:HA2	2:E:703:GLY:HA2	2.03	0.41
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.03	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.01	0.41
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	2.02	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.02	0.41
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.86	0.41
2:E:1663:HIS:O	2:E:1667:LEU:N	2.51	0.41
2:E:3706:SER:OG	2:E:3781:GLN:NE2	2.54	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.56	0.41
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.41
2:G:4863:TYR:HD2	2:G:4875:LYS:HB2	1.86	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.41
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	2.02	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.02	0.41
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.02	0.41
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.49	0.41
2:B:698:GLY:HA2	2:B:703:GLY:HA2	2.03	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.85	0.41
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.02	0.41
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.86	0.41
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.84	0.41
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.52	0.41
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	2.02	0.41
2:G:670:GLU:HG3	2:G:787:VAL:HG13	2.02	0.41
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	2.02	0.41
2:B:4014:LYS:HE2	2:B:4135:PRO:HG3	2.03	0.41
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.85	0.41
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.03	0.41
2:I:257:ARG:O	2:I:284:HIS:NE2	2.48	0.41
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	2.02	0.41
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.56	0.41
2:E:470:SER:O	2:E:474:ARG:NE	2.50	0.41
2:E:4956:THR:O	2:E:4965:SER:N	2.42	0.41
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.56	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.03	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.41
2:G:551:LEU:HD21	2:G:589:LEU:HB2	2.02	0.41
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.56	0.41
2:I:4080:TYR:CZ	2:I:4096:ALA:HB3	2.55	0.41
2:B:4957:LYS:HZ1	2:B:4957:LYS:HB2	1.82	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:551:LEU:HD21	2:E:589:LEU:HB2	2.02	0.40
2:E:582:HIS:O	2:E:585:SER:OG	2.30	0.40
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.56	0.40
2:G:1973:GLN:O	2:G:1977:TYR:N	2.44	0.40
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.02	0.40
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	2.02	0.40
2:G:4929:LEU:HA	2:G:4929:LEU:HD13	1.92	0.40
2:I:551:LEU:HD21	2:I:589:LEU:HB2	2.02	0.40
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.56	0.40
2:B:3706:SER:OG	2:B:3781:GLN:NE2	2.54	0.40
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.55	0.40
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.40
2:B:582:HIS:O	2:B:585:SER:OG	2.30	0.40
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.87	0.40
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.02	0.40
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.87	0.40
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.87	0.40
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.84	0.40
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.02	0.40
2:B:3847:PHE:HE1	2:B:3950:ASN:HD22	1.70	0.40
2:B:5027:CYS:O	2:B:5027:CYS:SG	2.79	0.40
2:B:5028:PHE:CD1	2:B:5028:PHE:O	2.75	0.40
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.40
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.03	0.40
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.03	0.40
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.04	0.40
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.40
2:E:4987:ASN:HA	2:E:4990:PHE:HD2	1.87	0.40
2:E:5028:PHE:O	2:E:5028:PHE:CD1	2.75	0.40
2:E:662:TRP:HZ3	2:E:811:CYS:HA	1.87	0.40
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.40
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.03	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.87	0.40
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	2.02	0.40
2:B:870:ILE:HA	2:B:870:ILE:HD12	1.92	0.40
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.02	0.40
2:E:1705:GLY:HA2	2:E:1709:ALA:HB3	2.04	0.40
2:E:3677:LEU:O	2:E:3698:LEU:N	2.52	0.40
2:E:5027:CYS:O	2:E:5027:CYS:SG	2.79	0.40
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.04	0.40
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.04	0.40
2:G:4014:LYS:HE2	2:G:4135:PRO:HG3	2.03	0.40
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.49	0.40
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.01	0.40
2:I:2029:GLN:O	2:I:2033:ASP:N	2.48	0.40
2:I:2298:VAL:HA	2:I:2301:TYR:HB2	2.03	0.40
2:I:3805:LEU:HG	2:I:3805:LEU:H	1.77	0.40
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.86	0.40
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.40
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.52	0.40
2:E:4863:TYR:HD2	2:E:4875:LYS:HB2	1.86	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.93	0.40
2:G:2298:VAL:HA	2:G:2301:TYR:HB2	2.03	0.40
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	2.04	0.40
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.86	0.40
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.04	0.40
2:G:698:GLY:HA2	2:G:703:GLY:HA2	2.03	0.40
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.56	0.40
2:I:278:GLN:N	2:I:315:CYS:SG	2.92	0.40
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.40
2:I:698:GLY:HA2	2:I:703:GLY:HA2	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	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	51	85
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	51	85
2	G	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	51	85
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	51	85
All	All	13360/18096 (74%)	11941 (89%)	1395 (10%)	24 (0%)	54	85

All (24) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	B	4641	PRO
2	B	4985	LEU
2	E	1932	PRO
2	E	4641	PRO
2	E	4985	LEU
2	I	1932	PRO
2	I	4641	PRO
2	I	4985	LEU
2	G	1932	PRO
2	G	4641	PRO
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	PRO

### 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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2473 (99%)	20 (1%)	85	92
2	E	2493/3022 (82%)	2473 (99%)	20 (1%)	85	92

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	2493/3022 (82%)	2473 (99%)	20 (1%)	85	92
2	I	2493/3022 (82%)	2473 (99%)	20 (1%)	85	92
All	All	10324/12444 (83%)	10244 (99%)	80 (1%)	86	92

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4137	ARG
2	B	4913	ARG
2	B	4957	LYS
2	B	4959	PHE
2	B	4960	ILE
2	B	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	4137	ARG
2	E	4913	ARG
2	E	4957	LYS
2	E	4959	PHE
2	E	4960	ILE
2	E	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4137	ARG
2	I	4913	ARG
2	I	4957	LYS
2	I	4959	PHE
2	I	4960	ILE
2	I	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4137	ARG
2	G	4913	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	4957	LYS
2	G	4959	PHE
2	G	4960	ILE
2	G	4983	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	25	HIS
1	F	87	HIS
1	A	25	HIS
1	A	87	HIS
1	H	25	HIS
1	H	87	HIS
1	J	25	HIS
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	520	ASN
2	B	797	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2007	ASN
2	B	2127	GLN
2	B	2291	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4209	GLN
2	B	4806	ASN
2	B	4933	GLN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	413	GLN
2	E	520	ASN
2	E	797	HIS
2	E	838	HIS
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2127	GLN
2	E	2291	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4201	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	4209	GLN
2	E	4806	ASN
2	E	4933	GLN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	413	GLN
2	I	520	ASN
2	I	797	HIS
2	I	838	HIS
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	2291	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4201	ASN
2	I	4209	GLN
2	I	4806	ASN
2	I	4933	GLN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	405	HIS
2	G	413	GLN
2	G	520	ASN
2	G	797	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	2291	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4201	ASN
2	G	4209	GLN
2	G	4806	ASN
2	G	4933	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
3	ATP	B	5101	-	27,33,33	0.86	1 (3%)	25,52,52	1.70	2 (8%)
4	CFF	B	5102	-	7,15,15	1.94	2 (28%)	8,23,23	1.22	1 (12%)
3	ATP	E	5101	-	27,33,33	0.87	1 (3%)	25,52,52	1.70	2 (8%)
4	CFF	E	5102	-	7,15,15	1.94	2 (28%)	8,23,23	1.21	1 (12%)
3	ATP	G	5101	-	27,33,33	0.86	1 (3%)	25,52,52	1.71	2 (8%)
4	CFF	G	5102	-	7,15,15	1.94	2 (28%)	8,23,23	1.22	1 (12%)
3	ATP	I	5101	-	27,33,33	0.86	1 (3%)	25,52,52	1.70	2 (8%)
4	CFF	I	5102	-	7,15,15	1.93	2 (28%)	8,23,23	1.21	1 (12%)

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
3	ATP	B	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	E	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	G	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	I	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	0/0/0/0	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C6-N1	-3.88	1.32	1.38
4	B	5102	CFF	C6-N1	-3.87	1.32	1.38
4	G	5102	CFF	C6-N1	-3.85	1.32	1.38
4	I	5102	CFF	C6-N1	-3.81	1.32	1.38
4	E	5102	CFF	O13-C6	-2.32	1.18	1.24
4	I	5102	CFF	O13-C6	-2.32	1.18	1.24
4	G	5102	CFF	O13-C6	-2.32	1.18	1.24
4	B	5102	CFF	O13-C6	-2.32	1.18	1.24
3	I	5101	ATP	C5-C4	2.70	1.46	1.40
3	B	5101	ATP	C5-C4	2.72	1.46	1.40
3	G	5101	ATP	C5-C4	2.72	1.46	1.40
3	E	5101	ATP	C5-C4	2.74	1.46	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	N3-C2-N1	-6.45	123.24	128.86
3	I	5101	ATP	N3-C2-N1	-6.43	123.26	128.86
3	B	5101	ATP	N3-C2-N1	-6.43	123.26	128.86
3	E	5101	ATP	N3-C2-N1	-6.43	123.26	128.86
4	E	5102	CFF	C14-N7-C8	-2.86	111.86	125.45
4	B	5102	CFF	C14-N7-C8	-2.86	111.88	125.45
4	I	5102	CFF	C14-N7-C8	-2.85	111.91	125.45
4	G	5102	CFF	C14-N7-C8	-2.85	111.91	125.45
3	B	5101	ATP	C4-C5-N7	-2.27	107.22	109.41
3	E	5101	ATP	C4-C5-N7	-2.25	107.24	109.41
3	I	5101	ATP	C4-C5-N7	-2.24	107.24	109.41
3	G	5101	ATP	C4-C5-N7	-2.24	107.25	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
4	B	5102	CFF	1	0
3	E	5101	ATP	1	0
4	E	5102	CFF	1	0
3	G	5101	ATP	1	0
4	G	5102	CFF	1	0
3	I	5101	ATP	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	5102	CFF	1	0

## 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	G	14
2	B	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	72.44
1	E	4345:UNK	C	4540:PHE	N	72.44
1	I	4345:UNK	C	4540:PHE	N	72.44
1	G	4345:UNK	C	4540:PHE	N	72.44
1	B	3613:UNK	C	3639:THR	N	42.93
1	E	3613:UNK	C	3639:THR	N	42.93
1	I	3613:UNK	C	3639:THR	N	42.93
1	G	3613:UNK	C	3639:THR	N	42.93
1	B	4253:GLU	C	4320:UNK	N	27.35
1	E	4253:GLU	C	4320:UNK	N	27.35
1	I	4253:GLU	C	4320:UNK	N	27.35
1	G	4253:GLU	C	4320:UNK	N	27.35
1	B	3163:UNK	C	3170:UNK	N	16.17
1	E	3163:UNK	C	3170:UNK	N	16.17
1	I	3163:UNK	C	3170:UNK	N	16.17
1	G	3163:UNK	C	3170:UNK	N	16.17
1	B	3063:UNK	C	3134:UNK	N	14.81
1	E	3063:UNK	C	3134:UNK	N	14.81
1	I	3063:UNK	C	3134:UNK	N	14.81
1	G	3063:UNK	C	3134:UNK	N	14.81
1	B	2703:UNK	C	2734:ASN	N	14.74
1	E	2703:UNK	C	2734:ASN	N	14.74

*Continued on next page...*

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	2703:UNK	C	2734:ASN	N	14.74
1	G	2703:UNK	C	2734:ASN	N	14.74
1	B	3468:UNK	C	3511:UNK	N	14.16
1	E	3468:UNK	C	3511:UNK	N	14.16
1	I	3468:UNK	C	3511:UNK	N	14.16
1	G	3468:UNK	C	3511:UNK	N	14.16
1	B	3236:UNK	C	3241:UNK	N	13.24
1	E	3236:UNK	C	3241:UNK	N	13.24
1	I	3236:UNK	C	3241:UNK	N	13.24
1	G	3236:UNK	C	3241:UNK	N	13.24
1	B	2976:UNK	C	2995:UNK	N	12.70
1	E	2976:UNK	C	2995:UNK	N	12.70
1	I	2976:UNK	C	2995:UNK	N	12.70
1	G	2976:UNK	C	2995:UNK	N	12.70
1	B	1564:UNK	C	1573:MET	N	12.34
1	E	1564:UNK	C	1573:MET	N	12.34
1	I	1564:UNK	C	1573:MET	N	12.34
1	G	1564:UNK	C	1573:MET	N	12.34
1	B	3254:UNK	C	3261:UNK	N	8.53
1	E	3254:UNK	C	3261:UNK	N	8.53
1	I	3254:UNK	C	3261:UNK	N	8.53
1	G	3254:UNK	C	3261:UNK	N	8.53
1	B	1297:UNK	C	1430:UNK	N	6.12
1	E	1297:UNK	C	1430:UNK	N	6.12
1	I	1297:UNK	C	1430:UNK	N	6.12
1	G	1297:UNK	C	1430:UNK	N	6.12
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	I	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24
1	B	2939:ARG	C	2942:UNK	N	3.23
1	E	2939:ARG	C	2942:UNK	N	3.23
1	G	2939:ARG	C	2942:UNK	N	3.23
1	I	2939:ARG	C	2942:UNK	N	3.22