



## Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 02:30 AM EDT

PDB ID : 5T9R  
EMDB ID : EMD-8374  
Title : Structure of rabbit RyR1 (Ca<sup>2+</sup>-only dataset, class 3)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;  
Frank, J.  
Deposited on : 2016-09-09  
Resolution : 5.80 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 : 0.0.1.dev43  
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

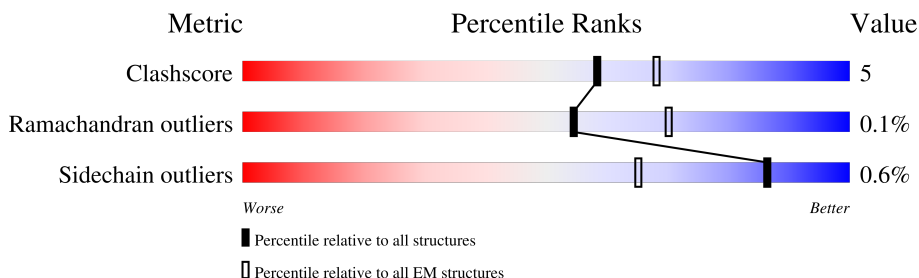
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.80 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	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4676	
2	E	4676	
2	G	4676	
2	I	4676	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- 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	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	


- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

### 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.

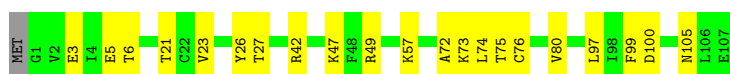
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




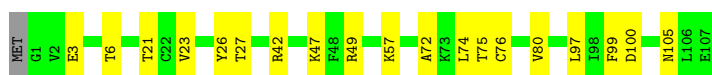
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




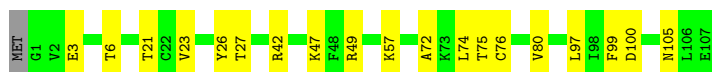
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




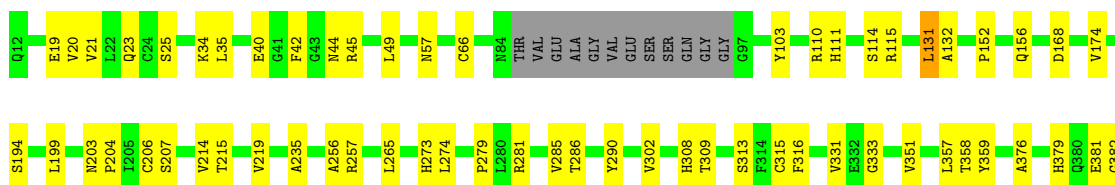
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



- Molecule 2: Ryanodine receptor 1

Chain B: 



C3973	C3974	G3975	N3976	Q3977	Q3978	H3971	T3972	L3780	Q3781	H3988	S3784	K3787	L4002	L4003	L4013	L4019	N4034	V4049	K4067	I4071	E4075	Q4078	R4085	A4096	S4099	Q4102	F4103	G4105	P4106	N4120	E4126	N4130	R4131	E4152	R4159	M4184	I4190	E4191	R4192	Y4193							
GLU	GLU	E3747	H3771	T3772	T3772	L3780	Q3781	S3784	K3787	K3815	M3816	L3817	Q3827	Q3830	Q3833	L3842	R3849	Q3850	A3883	F3880	L3884	Q3889	N3896	N3897	F3899	Q3900	N3901	T3910	T3911	S3929	Y3937	M3955	K3959	Q3960	N3963	N3971	O3972	P3973	T3974	L3975	L3976	L3977					
SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	H2856	P2857	S2868	R2869	Q2872	N2884	R2888	L2927	L2930	X2945	X3362	X3366	X3552	X3556	K3658	V3661	I3662	I3674	D3696	L3710	T3711	E3712	Y3725	I3728	H3741	GLY	GLU	ALA	GLY	GLY	GLY				
L2472	X2517	X2521	X2674	X2675	X2676	P2737	R2738	P2739	P2748	L2751	T2755	F2758	T2762	H2763	E2764	K2770	W2775	G2778	T2787	H2788	P2789	M2790	E2803	R2806	W2807	K2810	I2823	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	ILE	ILE	ILE					
Q2247	L2265	T2271	T2272	L2273	D2274	V2275	A2276	A2277	I2281	E2285	L2290	Q2291	V2299	A2303	C2326	Q2327	R2330	F2337	V2341	N2342	G2343	E2347	N2351	P2395	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	PRO	GLU	N2414	R2452						
PRO	GLU	GLU	THR	SER	LEU	SER	ARG	LEU	ARG	SER	LEU	LEU	VAL	ARG	LEU	VAL	LYS	LYS	LEU	PRG	ALA	GLU	K2089	R2104	Q2107	F2121	L2131	T2152	L2155	L2159	R2163	L2167	L2201	L2236													
GLU	GLU	GLU	LYS	ASP	ALA	GLU	LYS	GLU	GLU	GLU	ALA	PRO	GLY	GLU	LYS	L1922	L1926	L1931	P1932	V1935	A1960	R1964	Y1965	N1972	Q1973	Y1977	P2002	Q2003	E2004	Q2005	N2007	P2024	I2027	C2042	G2043	G2048	GLU	GLU	GLU	GLU	GLU	GLU					
ALA	GLY	VAL	E1793	E1794	P1795	A1796	R1797	L1798	I1802	L1807	R1808	L1812	D1828	P1840	L1848	I1853	F1854	V1859	K1860	Q1861	I1862	M1865	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	LYS	GLU	GLU	ASP	GLU	GLU						
A1627	C1630	D1632	P1633	L1639	D1649	E1652	L1653	Q1660	H1665	L1667	R1668	R1671	L1676	G1677	N1678	M1679	A1682	L1685	H1688	V1689	D1690	L1698	E1699	D1700	R1708	A1709	G1710	Y1711	Y1712	I1718	H1719	L1720	E1721	R1725	R1728	S1729	R1743	A1788									
E1142	W1143	V1148	V1149	M1152	T1161	F1162	T1163	L1164	N1165	V1168	A1178	L1189	V1199	G1200	H1201	A1227	L1267	G1277	N1278	P1279	X1288	X1289	X1290	X1291	X1292	X1293	X1294	X1295	X1296	X1297	X1298	X1299	X1300	X1301	X1302	X1303	X1304	X1305	X1306	X1307	X1308	X1309	X1310	X1311			
N1035	Q1041	R1044	T1045	E1054	PRO	ASP	GLN	GLU	PRO	SER	VAL	ASN	GLN	SER	ARG	T1070	R1073	R1076	A1077	E1078	K1079	F1092	E1093	A1094	T1095	T1096	E1099	G1103	W1104	L1105	R1106	Q1107	E1108	L1109	R1110	P1111	L1120	V1123	G1126	H1127	R1131	R1132	R1133	R1134	R1135		
N877	R886	I887	W891	D898	K901	P914	R918	L932	L935	L950	K951	K952	Y959	A968	P969	L970	D971	L972	L977	T978	P979	A980	T983	R987	L988	A989	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	R1025	K1032	R1033	R1034	R1035	R1036	R1037	R1038	R1039	R1040
G718	L719	H720	P733	G734	Q735	H736	L737	P740	E741	D742	S745	C746	N610	L750	R758	I759	N760	P763	L626	E627	G628	T635	D971	F777	F778	P779	S782	F783	S784	A785	G786	K788	Y808	R820	H838	P842	H848	D857	THR	VAL	GLN	I861	P864	P865			
L575	E580	I583	I586	D591	V599	L600	L606	C609	N610	V614	R615	S616	N617	Q618	E462	L626	E627	G628	T635	D971	F777	F778	P779	S782	F783	S784	A785	G786	K788	Y808	R820	H838	P842	H848	D857	THR	VAL	GLN	I861	P864	P865						
L388	Q395	E396	E397	I404	F414	R426	L436	L443	N610	V614	R615	S616	N617	Q618	E462	L626	E627	G628	T635	D971	F777	F778	P779	S782	F783	S784	A785	G786	K788	Y808	R820	H838	P842	H848	D857	THR	VAL	GLN	I861	P864	P865						







Response	Percentage
Used	78%
Not used	10%
Don't know	11%







E4749	ALA	PRO	ALA	ARG
A4752	GLY	GLU	VAL	LEU
V4767	ASP	LYS	ALA	ARG
S4770	LEU	ALA	ASP	ARG
D4786	ALA	ASP	GLY	LEU
F4808	GLY	GLU	GLY	THR
F4809	GLY	GLU	PRO	ALA
Y4791	GLY	LYS	GLY	ASP
G4802	GLY	GLU	GLY	THR
F4807	SER	GLU	ALA	LEU
F4808	GLY	VAL	GLY	ALA
F4809	TRP	PRO	GLY	ALA
H4812	GLY	ALA	GLY	LEU
D4815	GLY	PRO	GLY	ALA
I4816	GLY	GLU	GLY	ALA
T4840	GLY	SER	GLY	LEU
L4844	GLY	PRO	ASP	LEU
Y4863	GLY	PRO	GLY	THR
Y4888	GLY	PRO	GLY	ALA
I4901	GLY	PRO	GLY	ARG
T4925	GLY	LYS	GLY	ALA
L4928	GLY	LYS	SER	ALA
L4929	GLY	GLU	PRO	ALA
A4930	GLY	ALA	PRO	ALA
I4931	GLY	ALA	GLY	ALA
R4944	GLY	GLY	GLY	ALA
K4957	GLY	GLY	GLY	LEU
C4961	GLY	GLY	GLY	ARG
T4977	GLY	GLY	GLY	LEU
H4978	GLY	GLY	GLY	LEU
E4981	GLY	GLY	GLY	THR
E4982	GLY	GLY	GLY	GLY
H4983	GLY	GLY	GLY	GLY
O5005	GLY	GLY	GLY	VAL
S5037	GLY	GLY	GLY	GLY

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (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: CA, 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	0.29	0/834	0.52	0/1123
1	F	0.29	0/834	0.52	0/1123
1	H	0.29	0/834	0.52	0/1123
1	J	0.29	0/834	0.52	0/1123
2	B	0.30	1/25428 (0.0%)	0.54	8/34534 (0.0%)
2	E	0.29	1/25428 (0.0%)	0.54	8/34534 (0.0%)
2	G	0.30	1/25428 (0.0%)	0.54	8/34534 (0.0%)
2	I	0.30	1/25428 (0.0%)	0.54	8/34534 (0.0%)
All	All	0.29	4/105048 (0.0%)	0.54	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
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	695	TYR	C-N	13.13	1.59	1.34
2	I	695	TYR	C-N	13.12	1.59	1.34
2	B	695	TYR	C-N	13.12	1.59	1.34
2	E	695	TYR	C-N	13.12	1.59	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	LEU	CA-CB-CG	8.21	134.19	115.30
2	I	131	LEU	CA-CB-CG	8.21	134.18	115.30
2	G	131	LEU	CA-CB-CG	8.21	134.17	115.30
2	E	131	LEU	CA-CB-CG	8.20	134.16	115.30
2	E	1600	LEU	CA-CB-CG	7.39	132.30	115.30
2	I	1600	LEU	CA-CB-CG	7.38	132.27	115.30
2	B	1600	LEU	CA-CB-CG	7.37	132.26	115.30
2	G	1600	LEU	CA-CB-CG	7.37	132.26	115.30
2	B	1676	LEU	CA-CB-CG	6.41	130.04	115.30
2	G	1676	LEU	CA-CB-CG	6.40	130.03	115.30
2	E	1676	LEU	CA-CB-CG	6.40	130.03	115.30
2	I	1676	LEU	CA-CB-CG	6.39	130.01	115.30
2	B	2290	LEU	CA-CB-CG	6.08	129.28	115.30
2	E	2290	LEU	CA-CB-CG	6.08	129.27	115.30
2	G	2290	LEU	CA-CB-CG	6.06	129.25	115.30
2	I	2290	LEU	CA-CB-CG	6.06	129.24	115.30
2	I	1667	LEU	CA-CB-CG	5.89	128.84	115.30
2	G	1667	LEU	CA-CB-CG	5.86	128.78	115.30
2	B	1667	LEU	CA-CB-CG	5.85	128.76	115.30
2	E	1667	LEU	CA-CB-CG	5.84	128.74	115.30
2	E	977	LEU	CA-CB-CG	5.77	128.58	115.30
2	I	977	LEU	CA-CB-CG	5.77	128.58	115.30
2	G	977	LEU	CA-CB-CG	5.77	128.58	115.30
2	B	977	LEU	CA-CB-CG	5.75	128.53	115.30
2	G	688	LEU	CA-CB-CG	5.43	127.78	115.30
2	I	688	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	688	LEU	CA-CB-CG	5.41	127.75	115.30
2	E	688	LEU	CA-CB-CG	5.41	127.74	115.30
2	B	2291	GLN	C-N-CA	5.04	134.30	121.70
2	E	2291	GLN	C-N-CA	5.04	134.30	121.70
2	G	2291	GLN	C-N-CA	5.04	134.29	121.70
2	I	2291	GLN	C-N-CA	5.03	134.28	121.70

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	11	0
1	F	818	0	824	12	0
1	H	818	0	824	10	0
1	J	818	0	824	10	0
2	B	29369	0	24721	266	0
2	E	29369	0	24720	263	0
2	G	29369	0	24720	262	0
2	I	29369	0	24720	265	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102177	1083	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 (1083) 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:G:788:LYS:HG2	2:G:1630:CYS:H	1.52	0.74
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.53	0.72
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.53	0.72
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.53	0.72
2:I:379:HIS:HD2	2:I:382:GLY:H	1.41	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.41	0.68
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.28	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.41	0.66
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.79	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.41	0.65
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.78	0.65
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.79	0.65
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.78	0.64
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.79	0.64
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.79	0.64
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.63	0.64
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.79	0.64
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.79	0.63
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.63	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.81	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.63
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.81	0.62
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.81	0.62
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.81	0.62
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.63	0.62
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.81	0.62
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.63	0.62
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.81	0.62
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.61
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.81	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.81	0.61
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.81	0.61
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.83	0.61
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.32	0.61
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.81	0.61
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.61
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.83	0.61
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.83	0.60
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.83	0.60
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.84	0.60

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.84	0.60
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.60
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.84	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.60
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.84	0.60
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.60
1:A:27:THR:HB	1:A:100:ASP:HB3	1.84	0.60
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.82	0.60
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.84	0.60
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.82	0.60
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.84	0.60
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.83	0.60
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.83	0.59
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.59
1:F:27:THR:HB	1:F:100:ASP:HB3	1.84	0.59
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.49	0.59
1:J:27:THR:HB	1:J:100:ASP:HB3	1.84	0.59
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.84	0.59
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.84	0.59
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.85	0.59
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.85	0.59
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.36	0.59
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.68	0.59
2:G:111:HIS:HD2	2:G:114:SER:H	1.49	0.59
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.84	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.49	0.59
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.85	0.59
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.83	0.59
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.85	0.59
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.84	0.59
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.84	0.59
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.85	0.59
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.68	0.59
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.36	0.58
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.36	0.58
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.37	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.86	0.58
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.37	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.84	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.58
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.84	0.58
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.85	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.58
1:H:27:THR:HB	1:H:100:ASP:HB3	1.84	0.58
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.68	0.58
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.58
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.85	0.58
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.36	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.58
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.85	0.58
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.84	0.58
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.58
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.36	0.58
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.85	0.58
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.36	0.58
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.84	0.57
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.36	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.68	0.57
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.86	0.57
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.36	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.36	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.57
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.78	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.86	0.57
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.37	0.57
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.87	0.57
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.84	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.87	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.86	0.57
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.37	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.37	0.57
1:F:3:GLU:HB2	1:F:75:THR:HB	1.86	0.57
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.78	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.57
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.78	0.57
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.86	0.57
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.32	0.57
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.78	0.57
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.37	0.56
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.37	0.56
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.86	0.56
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.39	0.56
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.87	0.56
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.87	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.56
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.86	0.56
2:I:359:TYR:HA	2:I:376:ALA:HA	1.88	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.88	0.56
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.88	0.56
2:B:842:PRO:HD3	2:B:1073:ARG:HG3	1.88	0.56
2:B:4067:LYS:NZ	2:B:4102:GLN:O	2.39	0.56
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.88	0.56
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.86	0.56
1:A:3:GLU:HB2	1:A:75:THR:HB	1.86	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.39	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.87	0.56
2:I:4067:LYS:NZ	2:I:4102:GLN:O	2.39	0.56
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.88	0.56
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.39	0.56
2:B:4928:LEU:HD23	2:B:4931:ILE:HD12	1.87	0.56
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.88	0.56
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.39	0.56
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.79	0.56
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.87	0.56
2:G:4928:LEU:HD23	2:G:4931:ILE:HD12	1.87	0.56
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.88	0.56
2:G:842:PRO:HD3	2:G:1073:ARG:HG3	1.88	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.88	0.56

*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	1.87	0.56
2:I:842:PRO:HD3	2:I:1073:ARG:HG3	1.88	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.87	0.56
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.87	0.56
1:H:3:GLU:HB2	1:H:75:THR:HB	1.86	0.55
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.86	0.55
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.88	0.55
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.39	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.88	0.55
2:E:842:PRO:HD3	2:E:1073:ARG:HG3	1.88	0.55
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.87	0.55
2:E:4067:LYS:NZ	2:E:4102:GLN:O	2.39	0.55
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.40	0.55
1:J:3:GLU:HB2	1:J:75:THR:HB	1.86	0.55
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.88	0.55
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.88	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.31	0.55
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.88	0.55
2:I:385:ASP:HB2	2:G:156:GLN:HE21	1.71	0.55
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.86	0.55
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.89	0.55
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.88	0.55
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.88	0.55
2:E:4928:LEU:HD23	2:E:4931:ILE:HD12	1.87	0.55
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.87	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.89	0.55
2:G:359:TYR:HA	2:G:376:ALA:HA	1.88	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.39	0.55
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.40	0.55
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.89	0.55
2:E:359:TYR:HA	2:E:376:ALA:HA	1.88	0.55
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.88	0.55
2:B:614:VAL:HG22	2:B:616:SER:H	1.72	0.55
2:E:614:VAL:HG22	2:E:616:SER:H	1.72	0.55
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.88	0.55
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.88	0.55
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.40	0.55
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.89	0.55
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.88	0.55
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.55
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.88	0.55
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.55
2:G:4067:LYS:NZ	2:G:4102:GLN:O	2.39	0.55
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.89	0.55
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.88	0.55
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.40	0.55
2:I:614:VAL:HG22	2:I:616:SER:H	1.72	0.55
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.41	0.54
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.88	0.54
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.89	0.54
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.89	0.54
2:G:614:VAL:HG22	2:G:616:SER:H	1.72	0.54
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.88	0.54
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.40	0.54
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.89	0.54
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.89	0.54
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.88	0.54
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.39	0.54
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.54
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.31	0.54
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.41	0.54
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.40	0.54
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.54
2:G:331:VAL:HG12	2:G:333:GLY:H	1.72	0.54
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.90	0.54
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.79	0.54
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.40	0.54
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.89	0.54
2:E:2758:PHE:O	2:E:2762:THR:N	2.41	0.54
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.41	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.73	0.54
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.41	0.54
2:B:2758:PHE:O	2:B:2762:THR:N	2.41	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.73	0.54
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.90	0.54
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.40	0.54
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.90	0.54
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.41	0.54
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.89	0.54
2:I:4928:LEU:HD23	2:I:4931:ILE:HD12	1.87	0.54
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.90	0.54
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.90	0.54
2:I:331:VAL:HG12	2:I:333:GLY:H	1.72	0.54
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.73	0.54
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.39	0.54
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.89	0.53
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.42	0.53
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.88	0.53
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.74	0.53
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.89	0.53
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.41	0.53
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.91	0.53
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.42	0.53
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.90	0.53
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.42	0.53
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.89	0.53
2:B:331:VAL:HG12	2:B:333:GLY:H	1.72	0.53
2:B:1973:GLN:O	2:B:1977:TYR:N	2.42	0.53
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.42	0.53
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.90	0.53
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.42	0.53
2:B:485:SER:O	2:B:489:ASN:N	2.39	0.53
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.90	0.53
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.91	0.53
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.42	0.53
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.42	0.53
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.90	0.53
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.91	0.53
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.90	0.53
2:I:4925:ILE:HA	2:I:4929:LEU:HD13	1.91	0.53
2:B:4925:ILE:HA	2:B:4929:LEU:HD13	1.91	0.53
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.53
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.42	0.53
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.91	0.53
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.91	0.53
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.90	0.53
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.41	0.53
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.91	0.53
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.90	0.53
2:E:331:VAL:HG12	2:E:333:GLY:H	1.72	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.42	0.53
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.90	0.53
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.41	0.53
2:G:1622:GLU:N	2:G:1627:ALA:O	2.42	0.53
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.74	0.53
2:G:4925:ILE:HA	2:G:4929:LEU:HD13	1.91	0.53
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.41	0.53
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.42	0.53
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.53
2:E:4925:ILE:HA	2:E:4929:LEU:HD13	1.91	0.53
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.42	0.53
2:I:2868:SER:O	2:I:2872:GLN:N	2.42	0.53
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.53
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.90	0.52
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.90	0.52
2:B:1622:GLU:N	2:B:1627:ALA:O	2.42	0.52
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.74	0.52
2:E:1973:GLN:O	2:E:1977:TYR:N	2.42	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.91	0.52
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.91	0.52
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.52
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.91	0.52
2:G:168:ASP:HB3	2:G:199:LEU:HD22	1.91	0.52
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.73	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.38	0.52
2:E:168:ASP:HB3	2:E:199:LEU:HD22	1.91	0.52
2:E:1622:GLU:N	2:E:1627:ALA:O	2.42	0.52
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.91	0.52
2:B:168:ASP:HB3	2:B:199:LEU:HD22	1.91	0.52
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.91	0.52
1:H:6:THR:HA	1:H:72:ALA:HA	1.91	0.52
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.91	0.52
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.52
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.91	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.91	0.52
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.40	0.52
2:B:156:GLN:HE21	2:E:385:ASP:HB2	1.74	0.52
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.41	0.52
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.75	0.52
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.74	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1622:GLU:N	2:I:1627:ALA:O	2.42	0.52
1:A:6:THR:HA	1:A:72:ALA:HA	1.91	0.52
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.52
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.42	0.52
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.52
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.75	0.52
2:I:2758:PHE:O	2:I:2762:THR:N	2.41	0.52
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.75	0.51
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.38	0.51
2:I:168:ASP:HB3	2:I:199:LEU:HD22	1.91	0.51
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.51
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.91	0.51
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.75	0.51
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.91	0.51
2:I:1973:GLN:O	2:I:1977:TYR:N	2.42	0.51
2:G:2758:PHE:O	2:G:2762:THR:N	2.41	0.51
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.93	0.51
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.93	0.51
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.92	0.51
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.93	0.51
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.51
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.93	0.51
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.93	0.51
1:F:6:THR:HA	1:F:72:ALA:HA	1.91	0.51
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.93	0.51
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.75	0.51
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.93	0.51
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.93	0.51
2:E:451:TYR:O	2:E:474:ARG:NH1	2.44	0.51
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.44	0.51
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.93	0.51
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.51
2:G:2868:SER:O	2:G:2872:GLN:N	2.42	0.51
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.93	0.51
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.93	0.51
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.93	0.51
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.44	0.51
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.29	0.51
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.29	0.51
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.75	0.51
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.44	0.51
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.29	0.51
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.75	0.51
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.44	0.51
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.92	0.51
2:G:1973:GLN:O	2:G:1977:TYR:N	2.42	0.51
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.75	0.51
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.92	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.29	0.51
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.76	0.50
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.93	0.50
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.50
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.44	0.50
2:E:4942:GLU:HG3	2:G:4944:ARG:HH11	1.77	0.50
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.93	0.50
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.50
1:J:6:THR:HA	1:J:72:ALA:HA	1.91	0.50
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.94	0.50
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.93	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.94	0.50
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.40	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.42	0.50
2:I:451:TYR:O	2:I:474:ARG:NH1	2.44	0.50
2:I:2347:GLU:O	2:I:2351:ASN:N	2.45	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.94	0.50
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.50
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.92	0.50
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.76	0.50
2:E:2347:GLU:O	2:E:2351:ASN:N	2.45	0.50
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.93	0.50
2:G:451:TYR:O	2:G:474:ARG:NH1	2.44	0.50
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.92	0.50
2:G:2347:GLU:O	2:G:2351:ASN:N	2.45	0.50
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.93	0.50
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.76	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.93	0.50
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.94	0.50
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.76	0.50
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.94	0.50
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.93	0.50
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.50
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.38	0.50
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.93	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.42	0.50
2:I:488:LEU:O	2:I:492:ASP:N	2.43	0.50
2:I:1729:SER:HB3	2:I:2163:ARG:HH11	1.77	0.50
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.93	0.50
2:B:1729:SER:HB3	2:B:2163:ARG:HH11	1.77	0.49
2:B:3974:THR:O	2:B:3978:GLN:N	2.40	0.49
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.94	0.49
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.49
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.94	0.49
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.93	0.49
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.44	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.45	0.49
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.94	0.49
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.49
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.44	0.49
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.95	0.49
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.94	0.49
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.78	0.49
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.94	0.49
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.92	0.49
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.44	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.44	0.49
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.93	0.49
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.93	0.49
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.93	0.49
2:E:156:GLN:HE21	2:G:385:ASP:HB2	1.78	0.49
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.95	0.49
2:E:1729:SER:HB3	2:E:2163:ARG:HH11	1.77	0.49
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.95	0.49
2:B:451:TYR:O	2:B:474:ARG:NH1	2.44	0.49
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.94	0.49
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.95	0.49
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.95	0.49
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.94	0.49
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.95	0.49
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1729:SER:HB3	2:G:2163:ARG:HH11	1.77	0.49
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.95	0.49
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.94	0.49
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.95	0.49
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.94	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.46	0.49
2:I:485:SER:O	2:I:489:ASN:N	2.39	0.49
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.95	0.49
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.93	0.49
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.94	0.49
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.95	0.49
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.46	0.49
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.94	0.49
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.95	0.48
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.38	0.48
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.46	0.48
2:E:1516:UNK:N	2:E:1529:UNK:O	2.46	0.48
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.95	0.48
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.46	0.48
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.94	0.48
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.44	0.48
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.95	0.48
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.95	0.48
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.94	0.48
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.95	0.48
2:B:1516:UNK:N	2:B:1529:UNK:O	2.46	0.48
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.95	0.48
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.96	0.48
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.46	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.31	0.48
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.94	0.48
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.95	0.48
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.95	0.48
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.78	0.48
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.46	0.48
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.48
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.48
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.95	0.48
2:G:3974:THR:O	2:G:3978:GLN:N	2.40	0.48
2:G:4184:MET:HB3	2:G:4190:ILE:HD13	1.96	0.48
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.95	0.48
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.94	0.48
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.94	0.48
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.95	0.48
2:E:4184:MET:HB3	2:E:4190:ILE:HD13	1.96	0.48
2:I:21:VAL:HG12	2:I:66:CYS:HA	1.96	0.48
2:I:395:GLN:HG3	2:I:397:GLU:H	1.79	0.48
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.95	0.48
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.46	0.48
2:G:485:SER:O	2:G:489:ASN:N	2.39	0.48
2:G:1516:UNK:N	2:G:1529:UNK:O	2.46	0.48
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.46	0.48
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.78	0.48
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.96	0.48
2:I:3974:THR:O	2:I:3978:GLN:N	2.40	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.79	0.48
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.96	0.48
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.46	0.48
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.95	0.48
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.38	0.48
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.78	0.48
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.95	0.48
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	1.96	0.48
2:G:111:HIS:CD2	2:G:114:SER:H	2.31	0.48
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.95	0.48
2:E:606:LEU:O	2:E:617:ASN:ND2	2.47	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.48
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.96	0.48
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.38	0.48
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.46	0.48
2:I:4184:MET:HB3	2:I:4190:ILE:HD13	1.96	0.48
2:G:206:CYS:SG	2:G:207:SER:N	2.87	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:G:21:VAL:HG12	2:G:66:CYS:HA	1.96	0.48
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.46	0.48
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.44	0.47
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.47	0.47
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.46	0.47
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.46	0.47
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.95	0.47
2:B:206:CYS:SG	2:B:207:SER:N	2.87	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:LEU:O	2:B:617:ASN:ND2	2.47	0.47
2:B:4192:ARG:HH12	2:B:4982:GLU:HG2	1.80	0.47
2:B:4944:ARG:HH11	2:I:4942:GLU:HG3	1.78	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.79	0.47
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.44	0.47
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.95	0.47
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.79	0.47
2:I:206:CYS:SG	2:I:207:SER:N	2.87	0.47
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.42	0.47
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.79	0.47
2:G:606:LEU:O	2:G:617:ASN:ND2	2.47	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.95	0.47
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	1.96	0.47
2:I:606:LEU:O	2:I:617:ASN:ND2	2.47	0.47
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.44	0.47
2:I:1516:UNK:N	2:I:1529:UNK:O	2.47	0.47
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.96	0.47
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.79	0.47
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.95	0.47
2:B:1965:TYR:OH	2:B:2027:ILE:O	2.28	0.47
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.96	0.47
2:E:488:LEU:O	2:E:492:ASP:N	2.43	0.47
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.97	0.47
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.79	0.47
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.47	0.47
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.95	0.47
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.97	0.47
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	1.96	0.47
2:B:4184:MET:HB3	2:B:4190:ILE:HD13	1.96	0.47
2:E:206:CYS:SG	2:E:207:SER:N	2.87	0.47
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.97	0.47
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.96	0.47
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.96	0.47
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.96	0.47
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.97	0.47
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.96	0.47
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.95	0.47
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.47
2:G:978:THR:HB	2:G:980:ALA:H	1.80	0.47
2:G:4192:ARG:HH12	2:G:4982:GLU:HG2	1.80	0.47
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:E:4192:ARG:HH12	2:E:4982:GLU:HG2	1.80	0.47
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.48	0.47
2:I:1238:PHE:O	2:I:1606:SER:N	2.48	0.47
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.47
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.96	0.47
2:B:21:VAL:HG12	2:B:66:CYS:HA	1.96	0.47
2:E:647:ASN:ND2	2:E:820:ARG:O	2.39	0.47
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.47
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.97	0.47
2:I:4192:ARG:HH12	2:I:4982:GLU:HG2	1.80	0.47
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.48	0.47
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.48	0.47
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.79	0.47
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.97	0.47
2:E:21:VAL:HG12	2:E:66:CYS:HA	1.96	0.47
2:G:733:PRO:HD2	2:G:763:PRO:HD2	1.97	0.47
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.47	0.47
2:E:733:PRO:HD2	2:E:763:PRO:HD2	1.97	0.47
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.47
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.47
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	1.96	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:B:309:THR:O	2:B:313:SER:OG	2.33	0.46
2:E:309:THR:O	2:E:313:SER:OG	2.33	0.46
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.46
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.97	0.46
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.46
2:G:488:LEU:O	2:G:492:ASP:N	2.43	0.46
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.38	0.46
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.81	0.46
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.47	0.46
2:E:485:SER:O	2:E:489:ASN:N	2.39	0.46
2:I:733:PRO:HD2	2:I:763:PRO:HD2	1.97	0.46
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.79	0.46
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.46	0.46
2:G:309:THR:O	2:G:313:SER:OG	2.33	0.46
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.79	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.96	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.97	0.46
2:E:1131:ARG:NH1	2:E:1178:ALA:O	2.48	0.46
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.46
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.96	0.46
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.97	0.46
2:B:4661:TYR:OH	2:B:4786:ASP:OD2	2.34	0.46
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.96	0.46
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.81	0.46
2:E:4096:ALA:HA	2:E:4099:SER:HB2	1.98	0.46
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.80	0.46
2:G:4661:TYR:OH	2:G:4786:ASP:OD2	2.34	0.46
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.80	0.46
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.97	0.46
2:I:4228:ALA:O	2:I:4232:GLU:N	2.48	0.46
2:B:111:HIS:CD2	2:B:114:SER:H	2.31	0.46
2:B:733:PRO:HD2	2:B:763:PRO:HD2	1.97	0.46
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.80	0.46
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.97	0.46
2:I:309:THR:O	2:I:313:SER:OG	2.33	0.46
2:I:4096:ALA:HA	2:I:4099:SER:HB2	1.98	0.46
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.80	0.46
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.80	0.46
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.96	0.46
2:B:4228:ALA:O	2:B:4232:GLU:N	2.48	0.46
2:G:495:ASN:HD21	2:G:550:LYS:HG3	1.81	0.46
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.46
2:G:4096:ALA:HA	2:G:4099:SER:HB2	1.98	0.46
2:B:488:LEU:O	2:B:492:ASP:N	2.43	0.46
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.97	0.46
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.48	0.46
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.96	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.79	0.46
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.49	0.46
2:I:495:ASN:HD21	2:I:550:LYS:HG3	1.81	0.46
2:I:4978:HIS:ND1	2:I:4982:GLU:OE1	2.44	0.46
2:G:2869:ARG:HH12	2:G:2945:UNK:C	2.29	0.46
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.46
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.81	0.46
2:B:4096:ALA:HA	2:B:4099:SER:HB2	1.98	0.46
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.46
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.81	0.46
2:I:4661:TYR:OH	2:I:4786:ASP:OD2	2.34	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.51	0.45
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.81	0.45
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.80	0.45
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.46	0.45
2:E:4661:TYR:OH	2:E:4786:ASP:OD2	2.34	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.47	0.45
2:G:2152:THR:HA	2:G:2155:LEU:HB2	1.99	0.45
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.51	0.45
2:E:111:HIS:CD2	2:E:114:SER:H	2.31	0.45
2:E:4228:ALA:O	2:E:4232:GLU:N	2.48	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.97	0.45
2:B:647:ASN:ND2	2:B:820:ARG:O	2.39	0.45
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.97	0.45
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.45
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.51	0.45
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.99	0.45
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.80	0.45
2:I:4071:ILE:HG13	2:I:4103:PHE:HZ	1.81	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:4228:ALA:O	2:G:4232:GLU:N	2.48	0.45
2:E:495:ASN:HD21	2:E:550:LYS:HG3	1.81	0.45
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.98	0.45
2:E:4071:ILE:HG13	2:E:4103:PHE:HZ	1.81	0.45
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.99	0.45
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.45
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.99	0.45
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.99	0.45
2:E:3974:THR:O	2:E:3978:GLN:N	2.40	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.98	0.45
2:G:4071:ILE:HG13	2:G:4103:PHE:HZ	1.81	0.45
2:B:495:ASN:HD21	2:B:550:LYS:HG3	1.81	0.45
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.45
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.82	0.45
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.99	0.45
2:B:2869:ARG:HH12	2:B:2945:UNK:C	2.29	0.45
2:B:4863:TYR:HA	2:B:4901:ILE:HG23	1.98	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2152:THR:HA	2:I:2155:LEU:HB2	1.99	0.45
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.98	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.97	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.51	0.45
2:G:3880:PHE:O	2:G:3884:LEU:N	2.50	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.98	0.45
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.99	0.45
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.99	0.45
2:I:4863:TYR:HA	2:I:4901:ILE:HG23	1.98	0.45
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.97	0.45
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.99	0.45
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.82	0.44
2:B:3880:PHE:O	2:B:3884:LEU:N	2.50	0.44
2:B:4071:ILE:HG13	2:B:4103:PHE:HZ	1.81	0.44
2:B:4978:HIS:ND1	2:B:4982:GLU:OE1	2.44	0.44
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.99	0.44
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.98	0.44
2:B:2152:THR:HA	2:B:2155:LEU:HB2	1.99	0.44
2:E:3880:PHE:O	2:E:3884:LEU:N	2.50	0.44
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.82	0.44
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.53	0.44
2:B:313:SER:HB3	2:B:351:VAL:HB	1.99	0.44
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.83	0.44
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.52	0.44
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.00	0.44
2:I:647:ASN:ND2	2:I:820:ARG:O	2.39	0.44
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.82	0.44
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.99	0.44
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.81	0.44
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.00	0.44
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.82	0.44
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.00	0.44
2:I:1865:MET:SD	2:I:1865:MET:N	2.91	0.44
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.00	0.44
2:G:1238:PHE:O	2:G:1606:SER:N	2.48	0.44
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.99	0.44
2:B:1865:MET:SD	2:B:1865:MET:N	2.91	0.44
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.82	0.44
2:E:1238:PHE:O	2:E:1606:SER:N	2.48	0.44
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.81	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.53	0.44
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.00	0.44
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.47	0.44
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.99	0.44
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.36	0.44
2:E:313:SER:HB3	2:E:351:VAL:HB	1.99	0.44
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.53	0.44
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	2.00	0.44
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.00	0.44
2:E:4863:TYR:HA	2:E:4901:ILE:HG23	1.98	0.44
2:I:3880:PHE:O	2:I:3884:LEU:N	2.50	0.44
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.82	0.44
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.81	0.44
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.36	0.44
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.99	0.44
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.82	0.44
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.44
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.82	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.44	0.44
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.00	0.44
2:I:313:SER:HB3	2:I:351:VAL:HB	1.99	0.44
2:I:460:GLN:HG2	2:I:462:GLU:H	1.83	0.44
2:I:1639:LEU:HD12	2:I:1653:LEU:HD21	2.00	0.44
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.00	0.44
2:G:290:TYR:O	2:G:302:VAL:N	2.51	0.44
2:G:1865:MET:SD	2:G:1865:MET:N	2.91	0.44
2:G:4863:TYR:HA	2:G:4901:ILE:HG23	1.98	0.44
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.82	0.43
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.43
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.43
2:E:2152:THR:HA	2:E:2155:LEU:HB2	1.99	0.43
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	2.00	0.43
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.42	0.43
2:E:290:TYR:O	2:E:302:VAL:N	2.51	0.43
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.43
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.00	0.43
2:I:1271:ARG:HA	2:I:1471:UNK:HA	2.00	0.43
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.43
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.43
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.99	0.43
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1865:MET:SD	2:E:1865:MET:N	2.91	0.43
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.99	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.43
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.00	0.43
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.00	0.43
2:E:460:GLN:HG2	2:E:462:GLU:H	1.83	0.43
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.52	0.43
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.99	0.43
2:G:2281:ILE:HG23	2:G:2341:VAL:HG11	2.00	0.43
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.82	0.43
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.99	0.43
2:B:3696:ASP:OD2	2:B:3771:HIS:NE2	2.52	0.43
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	2.01	0.43
2:E:2281:ILE:HG23	2:E:2341:VAL:HG11	2.00	0.43
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.36	0.43
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.01	0.43
2:I:290:TYR:O	2:I:302:VAL:N	2.51	0.43
2:G:1639:LEU:HD12	2:G:1653:LEU:HD21	2.00	0.43
2:E:2299:VAL:O	2:E:2303:ALA:N	2.52	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.01	0.43
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.01	0.43
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.37	0.43
2:I:3696:ASP:OD2	2:I:3771:HIS:NE2	2.52	0.43
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.82	0.43
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.01	0.43
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.99	0.43
1:J:23:VAL:HB	1:J:105:ASN:HA	2.01	0.43
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.99	0.43
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.01	0.43
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.37	0.43
2:E:3696:ASP:OD2	2:E:3771:HIS:NE2	2.52	0.43
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	2.01	0.43
2:G:3696:ASP:OD2	2:G:3771:HIS:NE2	2.52	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.83	0.43
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.46	0.43
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.52	0.43
2:B:2281:ILE:HG23	2:B:2341:VAL:HG11	2.00	0.43
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.92	0.43
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.83	0.43
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.52	0.43
2:I:2281:ILE:HG23	2:I:2341:VAL:HG11	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.83	0.43
2:G:485:SER:HA	2:G:488:LEU:HB2	2.01	0.43
2:G:838:HIS:HA	2:G:1201:HIS:HB3	2.01	0.43
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.92	0.43
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.01	0.43
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.01	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.00	0.43
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.42	0.43
2:I:2788:HIS:CE1	2:I:2790:MET:HB2	2.54	0.43
2:G:626:LEU:HG	2:G:628:GLY:H	1.84	0.43
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.43
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.52	0.43
2:G:2437:ALA:HA	2:G:2438:PRO:HD3	1.92	0.43
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	2.01	0.43
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.36	0.43
1:H:23:VAL:HB	1:H:105:ASN:HA	2.01	0.42
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.01	0.42
2:E:485:SER:HA	2:E:488:LEU:HB2	2.01	0.42
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	2.01	0.42
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.52	0.42
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.92	0.42
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	2.00	0.42
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.00	0.42
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.92	0.42
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.01	0.42
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.42
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	2.01	0.42
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.37	0.42
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.00	0.42
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	2.01	0.42
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.54	0.42
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	2.01	0.42
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.52	0.42
2:G:2236:LEU:HD23	2:G:2275:VAL:HG11	2.01	0.42
2:G:4840:THR:O	2:G:4844:LEU:N	2.47	0.42
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.42
2:B:2299:VAL:O	2:B:2303:ALA:N	2.52	0.42
2:B:2517:UNK:O	2:B:2521:UNK:N	2.53	0.42
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	2.00	0.42
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.52	0.42
2:E:1804:LEU:O	2:E:1808:ARG:N	2.45	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.42
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.00	0.42
2:E:4918:ILE:HD11	2:G:4888:TYR:HA	2.02	0.42
2:I:485:SER:HA	2:I:488:LEU:HB2	2.01	0.42
2:I:626:LEU:HG	2:I:628:GLY:H	1.85	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:I:4056:GLU:O	2:I:4060:LYS:N	2.52	0.42
2:G:313:SER:HB3	2:G:351:VAL:HB	1.99	0.42
2:G:414:PHE:HE1	2:G:436:LEU:HB3	1.84	0.42
2:G:460:GLN:HG2	2:G:462:GLU:H	1.83	0.42
1:H:21:THR:HA	1:H:49:ARG:HA	2.01	0.42
2:B:460:GLN:HG2	2:B:462:GLU:H	1.83	0.42
2:B:1639:LEU:HD12	2:B:1653:LEU:HD21	2.00	0.42
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.42
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.37	0.42
2:B:2788:HIS:CE1	2:B:2790:MET:HB2	2.54	0.42
2:E:950:LEU:HB3	2:E:970:LEU:HD22	2.02	0.42
2:E:1639:LEU:HD12	2:E:1653:LEU:HD21	2.00	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.02	0.42
2:G:2788:HIS:CE1	2:G:2790:MET:HB2	2.54	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	2.00	0.42
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.52	0.42
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.85	0.42
2:B:914:PRO:O	2:B:918:ARG:N	2.51	0.42
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.01	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.01	0.42
2:E:2236:LEU:HD23	2:E:2275:VAL:HG11	2.01	0.42
2:E:2788:HIS:CE1	2:E:2790:MET:HB2	2.54	0.42
2:I:25:SER:HA	2:I:34:LYS:HA	2.02	0.42
2:I:414:PHE:HE1	2:I:436:LEU:HB3	1.84	0.42
2:I:838:HIS:HA	2:I:1201:HIS:HB3	2.01	0.42
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.42
2:I:2517:UNK:O	2:I:2521:UNK:N	2.52	0.42
2:G:2517:UNK:O	2:G:2521:UNK:N	2.53	0.42
1:F:21:THR:HA	1:F:49:ARG:HA	2.01	0.42
2:B:25:SER:HA	2:B:34:LYS:HA	2.02	0.42
2:E:1227:ALA:HB1	2:E:1230:MET:HG3	2.02	0.42
2:E:2517:UNK:O	2:E:2521:UNK:N	2.53	0.42
2:E:2869:ARG:HH12	2:E:2945:UNK:C	2.32	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.54	0.42
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.83	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.02	0.42
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	2.01	0.42
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.47	0.42
2:G:1227:ALA:HB1	2:G:1230:MET:HG3	2.02	0.42
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.01	0.42
2:B:1238:PHE:O	2:B:1606:SER:N	2.48	0.42
2:E:414:PHE:HE1	2:E:436:LEU:HB3	1.84	0.42
2:E:626:LEU:HG	2:E:628:GLY:H	1.84	0.42
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.85	0.42
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.54	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.02	0.42
2:G:25:SER:HA	2:G:34:LYS:HA	2.02	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.01	0.42
2:G:950:LEU:HB3	2:G:970:LEU:HD22	2.02	0.42
1:A:23:VAL:HB	1:A:105:ASN:HA	2.01	0.42
2:B:626:LEU:HG	2:B:628:GLY:H	1.84	0.42
2:B:950:LEU:HB3	2:B:970:LEU:HD22	2.02	0.42
2:B:983:THR:O	2:B:987:ARG:N	2.51	0.42
2:B:4942:GLU:HG3	2:E:4944:ARG:HH11	1.84	0.42
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.01	0.42
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.01	0.42
2:I:663:TYR:HB2	2:I:808:TYR:HB3	2.02	0.42
2:I:2236:LEU:HD23	2:I:2275:VAL:HG11	2.01	0.42
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.01	0.42
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.02	0.42
2:B:485:SER:HA	2:B:488:LEU:HB2	2.01	0.42
2:E:23:GLN:HE21	2:E:34:LYS:HB3	1.85	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.47	0.42
2:E:838:HIS:HA	2:E:1201:HIS:HB3	2.01	0.42
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.39	0.42
1:J:21:THR:HA	1:J:49:ARG:HA	2.01	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.01	0.41
2:B:414:PHE:HE1	2:B:436:LEU:HB3	1.84	0.41
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.02	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.01	0.41
2:I:1148:VAL:N	2:I:1165:ASN:OD1	2.53	0.41
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.53	0.41
2:I:2299:VAL:O	2:I:2303:ALA:N	2.52	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.02	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.85	0.41
2:B:759:ILE:HG22	2:B:760:ASN:H	1.86	0.41
2:B:1148:VAL:N	2:B:1165:ASN:OD1	2.54	0.41
2:E:25:SER:HA	2:E:34:LYS:HA	2.02	0.41
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.02	0.41
1:F:23:VAL:HB	1:F:105:ASN:HA	2.01	0.41
2:B:663:TYR:HB2	2:B:808:TYR:HB3	2.02	0.41
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.54	0.41
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.85	0.41
2:E:357:LEU:HD12	2:E:388:LEU:HD11	2.03	0.41
2:E:1271:ARG:HA	2:E:1471:UNK:HA	2.02	0.41
2:I:23:GLN:HE21	2:I:34:LYS:HB3	1.85	0.41
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.03	0.41
2:I:759:ILE:HG22	2:I:760:ASN:H	1.86	0.41
2:I:2880:GLU:O	2:I:2884:ASN:N	2.48	0.41
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.02	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:G:4056:GLU:O	2:G:4060:LYS:N	2.52	0.41
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.03	0.41
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.85	0.41
2:B:3994:HIS:O	2:B:3998:HIS:ND1	2.39	0.41
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.03	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.02	0.41
2:E:4840:THR:O	2:E:4844:LEU:N	2.47	0.41
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.19	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.02	0.41
2:I:2437:ALA:HA	2:I:2438:PRO:HD3	1.92	0.41
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.02	0.41
2:B:838:HIS:HA	2:B:1201:HIS:HB3	2.01	0.41
2:B:1041:GLN:O	2:B:1045:THR:OG1	2.30	0.41
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	2.03	0.41
2:B:4918:ILE:HD11	2:E:4888:TYR:HA	2.03	0.41
2:E:759:ILE:HG22	2:E:760:ASN:H	1.86	0.41
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.02	0.41
2:G:759:ILE:HG22	2:G:760:ASN:H	1.86	0.41
2:G:786:GLY:HA2	2:G:1631:GLN:HA	2.01	0.41
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.44	0.41
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.41
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.02	0.41
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.38	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.02	0.41
2:B:4840:THR:O	2:B:4844:LEU:N	2.47	0.41
2:E:663:TYR:HB2	2:E:808:TYR:HB3	2.02	0.41
2:I:950:LEU:HB3	2:I:970:LEU:HD22	2.02	0.41
1:A:21:THR:HA	1:A:49:ARG:HA	2.02	0.41
2:B:290:TYR:O	2:B:302:VAL:N	2.50	0.41
2:E:786:GLY:HA2	2:E:1631:GLN:HA	2.01	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:I:4840:THR:O	2:I:4844:LEU:N	2.47	0.41
2:G:23:GLN:HE21	2:G:34:LYS:HB3	1.85	0.41
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	2.03	0.41
2:G:3552:UNK:O	2:G:3556:UNK:N	2.54	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.19	0.41
2:B:776:LEU:HG	2:B:848:HIS:HA	2.03	0.41
2:B:2236:LEU:HD23	2:B:2275:VAL:HG11	2.01	0.41
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.41
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.02	0.41
2:E:776:LEU:HG	2:E:848:HIS:HA	2.03	0.41
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.53	0.41
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.95	0.41
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	2.02	0.41
2:I:2103:VAL:O	2:I:2107:GLN:N	2.48	0.41
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	2.03	0.41
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.56	0.41
2:G:357:LEU:HD12	2:G:388:LEU:HD11	2.03	0.41
2:G:1148:VAL:N	2:G:1165:ASN:OD1	2.53	0.41
2:G:1804:LEU:O	2:G:1808:ARG:N	2.45	0.41
2:G:2021:CYS:HA	2:G:2022:PRO:HD3	1.94	0.41
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.53	0.41
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.39	0.41
2:G:4977:THR:O	2:G:4981:GLU:N	2.41	0.41
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.03	0.41
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.54	0.41
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.03	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.41
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.38	0.41
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.38	0.41
2:I:2869:ARG:HH12	2:I:2945:UNK:C	2.34	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.54	0.41
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.40
2:B:357:LEU:HD12	2:B:388:LEU:HD11	2.03	0.40
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	2.02	0.40
2:B:3552:UNK:O	2:B:3556:UNK:N	2.54	0.40
2:E:1663:HIS:O	2:E:1667:LEU:N	2.53	0.40
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.03	0.40
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.02	0.40
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.02	0.40
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.04	0.40
2:I:1729:SER:O	2:I:2163:ARG:NH1	2.54	0.40
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.56	0.40
2:G:663:TYR:HB2	2:G:808:TYR:HB3	2.02	0.40
2:G:1271:ARG:HA	2:G:1471:UNK:HA	2.04	0.40
2:G:1595:LEU:HD23	2:G:1595:LEU:HA	1.96	0.40
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.87	0.40
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.56	0.40
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.96	0.40
2:B:1729:SER:O	2:B:2163:ARG:NH1	2.54	0.40
2:B:4809:PHE:HA	2:B:4812:HIS:HD1	1.85	0.40
2:E:3552:UNK:O	2:E:3556:UNK:N	2.54	0.40
2:I:684:VAL:HA	2:I:781:VAL:HA	2.03	0.40
2:I:1657:LEU:HD13	2:I:1657:LEU:HA	1.97	0.40
2:G:1497:UNK:HA	2:G:1535:UNK:HA	2.03	0.40
1:F:5:GLU:HB2	1:F:73:LYS:HB3	2.04	0.40
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.03	0.40
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.04	0.40
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	2.04	0.40
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.86	0.40
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.56	0.40
2:E:1729:SER:O	2:E:2163:ARG:NH1	2.54	0.40
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	2.03	0.40
2:E:4809:PHE:HA	2:E:4812:HIS:HD1	1.85	0.40
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.54	0.40
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.38	0.40
2:I:4809:PHE:HA	2:I:4812:HIS:HD1	1.85	0.40
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.04	0.40
1:A:5:GLU:HB2	1:A:73:LYS:HB3	2.04	0.40
2:E:358:THR:HG21	2:E:382:GLY:HA2	2.04	0.40
2:E:1148:VAL:N	2:E:1165:ASN:OD1	2.54	0.40
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	2.03	0.40
2:I:716:PHE:HE2	2:I:759:ILE:HD11	1.87	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.86	0.40
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.04	0.40
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.04	0.40
2:B:2290:LEU:HB3	2:B:3849:ARG:NH1	2.37	0.40
2:B:3662:ILE:H	2:B:3662:ILE:HG13	1.77	0.40
2:E:3902:TYR:O	2:E:3906:GLN:NE2	2.55	0.40
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	2.02	0.40
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.56	0.40
2:I:358:THR:HG21	2:I:382:GLY:HA2	2.04	0.40
2:I:415:ILE:HA	2:I:418:LEU:HD13	2.04	0.40
2:I:2674:UNK:O	2:I:2676:UNK:N	2.54	0.40
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.86	0.40
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.02	0.40
2:G:1729:SER:O	2:G:2163:ARG:NH1	2.54	0.40
2:G:2034:PHE:O	2:G:2038:LEU:N	2.55	0.40
2:G:4809:PHE:HA	2:G:4812:HIS:HD1	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4676 (69%)	2923 (90%)	308 (10%)	4 (0%)	51	85
2	E	3235/4676 (69%)	2922 (90%)	309 (10%)	4 (0%)	51	85
2	G	3235/4676 (69%)	2922 (90%)	309 (10%)	4 (0%)	51	85

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	3235/4676 (69%)	2924 (90%)	307 (10%)	4 (0%)	51	85
All	All	13360/19136 (70%)	12064 (90%)	1280 (10%)	16 (0%)	54	85

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1840	PRO
2	B	1932	PRO
2	E	1840	PRO
2	E	1932	PRO
2	I	1840	PRO
2	I	1932	PRO
2	G	1840	PRO
2	G	1932	PRO
2	B	4641	PRO
2	E	4641	PRO
2	I	4641	PRO
2	G	4641	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	2493/3202 (78%)	2477 (99%)	16 (1%)	86	92
2	E	2493/3202 (78%)	2477 (99%)	16 (1%)	86	92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	2493/3202 (78%)	2477 (99%)	16 (1%)	86	92
2	I	2493/3202 (78%)	2477 (99%)	16 (1%)	86	92
All	All	10324/13164 (78%)	10260 (99%)	64 (1%)	86	92

All (64) 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	978	THR
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	4957	LYS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	978	THR
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
2	E	4957	LYS
2	I	131	LEU
2	I	534	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	I	553	ARG
2	I	978	THR
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	4957	LYS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	978	THR
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	4957	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	113	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	156	GLN
2	B	273	HIS
2	B	379	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	479	GLN
2	B	495	ASN
2	B	582	HIS
2	B	797	HIS
2	B	838	HIS
2	B	877	ASN
2	B	949	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1693	GLN
2	B	1719	HIS
2	B	1972	ASN
2	B	2005	GLN
2	B	2127	GLN
2	B	2788	HIS
2	B	3830	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	3976	ASN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4142	ASN
2	B	4728	HIS
2	B	4832	HIS
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	156	GLN
2	E	273	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	379	HIS
2	E	395	GLN
2	E	405	HIS
2	E	413	GLN
2	E	479	GLN
2	E	495	ASN
2	E	582	HIS
2	E	797	HIS
2	E	838	HIS
2	E	877	ASN
2	E	949	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1693	GLN
2	E	1719	HIS
2	E	1972	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	2788	HIS
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	3976	ASN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4142	ASN
2	E	4728	HIS
2	E	4832	HIS
2	I	23	GLN
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	113	HIS
2	I	156	GLN
2	I	203	ASN
2	I	273	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	I	379	HIS
2	I	395	GLN
2	I	405	HIS
2	I	413	GLN
2	I	479	GLN
2	I	495	ASN
2	I	582	HIS
2	I	797	HIS
2	I	838	HIS
2	I	877	ASN
2	I	949	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1693	GLN
2	I	1719	HIS
2	I	1972	ASN
2	I	2005	GLN
2	I	2127	GLN
2	I	2788	HIS
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	3976	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4142	ASN
2	I	4728	HIS
2	I	4832	HIS
2	G	23	GLN
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	113	HIS
2	G	156	GLN
2	G	203	ASN
2	G	273	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	379	HIS
2	G	395	GLN
2	G	405	HIS
2	G	413	GLN
2	G	479	GLN
2	G	495	ASN
2	G	582	HIS
2	G	797	HIS
2	G	838	HIS
2	G	877	ASN
2	G	949	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1693	GLN
2	G	1719	HIS
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	2788	HIS
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4728	HIS
2	G	4832	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	12
2	G	12
2	E	12
2	I	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	43.37
1	G	3613:UNK	C	3639:THR	N	43.37
1	E	3613:UNK	C	3639:THR	N	43.34
1	I	3613:UNK	C	3639:THR	N	43.32
1	B	3163:UNK	C	3170:UNK	N	16.45
1	E	3163:UNK	C	3170:UNK	N	16.45
1	I	3163:UNK	C	3170:UNK	N	16.45
1	G	3163:UNK	C	3170:UNK	N	16.45
1	B	3468:UNK	C	3511:UNK	N	15.10

*Continued on next page...*

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3468:UNK	C	3511:UNK	N	15.10
1	I	3468:UNK	C	3511:UNK	N	15.10
1	G	3468:UNK	C	3511:UNK	N	15.10
1	I	3063:UNK	C	3134:UNK	N	14.88
1	B	3063:UNK	C	3134:UNK	N	14.87
1	E	3063:UNK	C	3134:UNK	N	14.87
1	G	3063:UNK	C	3134:UNK	N	14.86
1	I	2703:UNK	C	2734:ASN	N	14.34
1	E	2703:UNK	C	2734:ASN	N	14.33
1	B	2703:UNK	C	2734:ASN	N	14.32
1	G	2703:UNK	C	2734:ASN	N	14.32
1	B	3236:UNK	C	3241:UNK	N	13.55
1	E	3236:UNK	C	3241:UNK	N	13.55
1	I	3236:UNK	C	3241:UNK	N	13.55
1	G	3236:UNK	C	3241:UNK	N	13.55
1	I	1564:UNK	C	1573:MET	N	12.87
1	E	1564:UNK	C	1573:MET	N	12.85
1	G	1564:UNK	C	1573:MET	N	12.85
1	B	1564:UNK	C	1573:MET	N	12.84
1	B	2976:UNK	C	2995:UNK	N	12.50
1	E	2976:UNK	C	2995:UNK	N	12.50
1	I	2976:UNK	C	2995:UNK	N	12.50
1	G	2976:UNK	C	2995:UNK	N	12.50
1	B	3254:UNK	C	3261:UNK	N	8.64
1	E	3254:UNK	C	3261:UNK	N	8.64
1	I	3254:UNK	C	3261:UNK	N	8.64
1	G	3254:UNK	C	3261:UNK	N	8.64
1	I	1297:UNK	C	1430:UNK	N	5.73
1	B	1297:UNK	C	1430:UNK	N	5.72
1	E	1297:UNK	C	1430:UNK	N	5.72
1	G	1297:UNK	C	1430:UNK	N	5.72
1	B	2939:ARG	C	2942:UNK	N	3.71
1	E	2939:ARG	C	2942:UNK	N	3.71
1	I	2939:ARG	C	2942:UNK	N	3.71
1	G	2939:ARG	C	2942:UNK	N	3.71
1	G	2479:LEU	C	2487:UNK	N	3.27
1	B	2479:LEU	C	2487:UNK	N	3.26
1	E	2479:LEU	C	2487:UNK	N	3.26
1	I	2479:LEU	C	2487:UNK	N	3.25

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8374. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.