



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 PM GMT

PDB ID : 4AKH
Title : Dynein Motor Domain - AMPPNP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

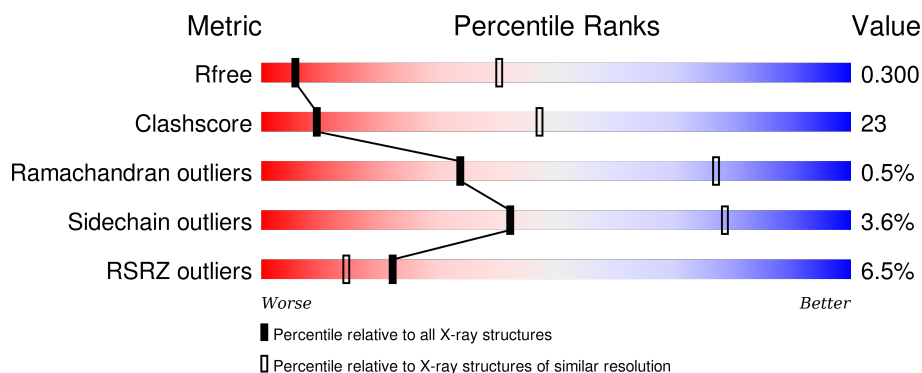
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2695	<div> <div>3%</div> <div>65%</div> <div>31%</div> <div>..</div> </div>
1	B	2695	<div> <div>10%</div> <div>67%</div> <div>30%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	B	5093	-	-	X	-
4	SO4	A	5095	-	-	X	-
4	SO4	B	5096	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 41642 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

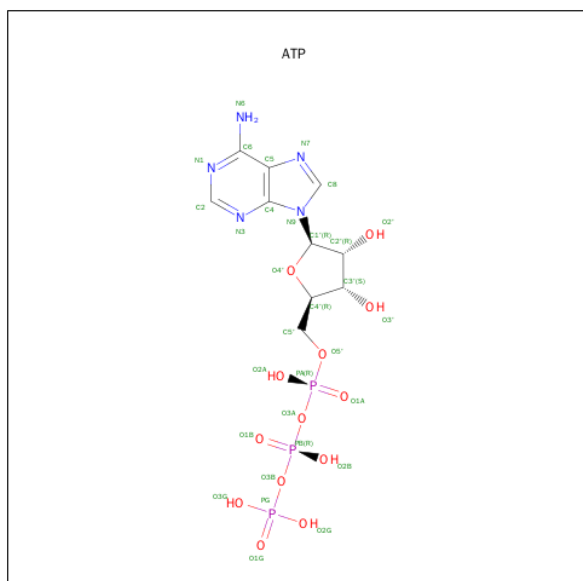
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			
1	B	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			

There are 4 discrepancies between the modelled and reference sequences:

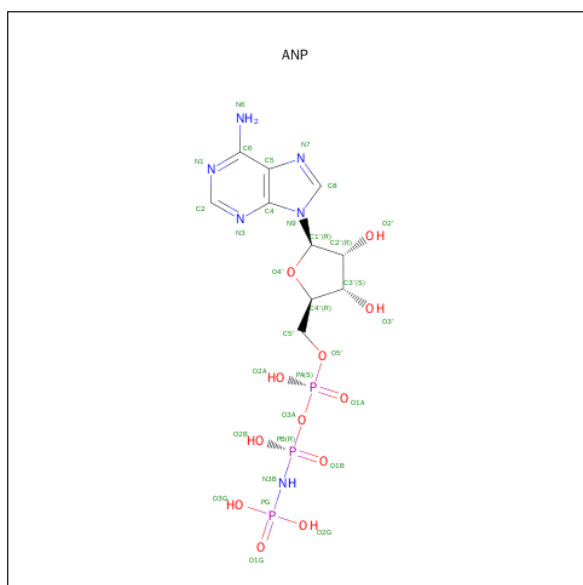
Chain	Residue	Modelled	Actual	Comment	Reference
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	1630	ILE	LEU	CONFLICT	UNP P36022
B	3782	ASP	GLU	CONFLICT	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

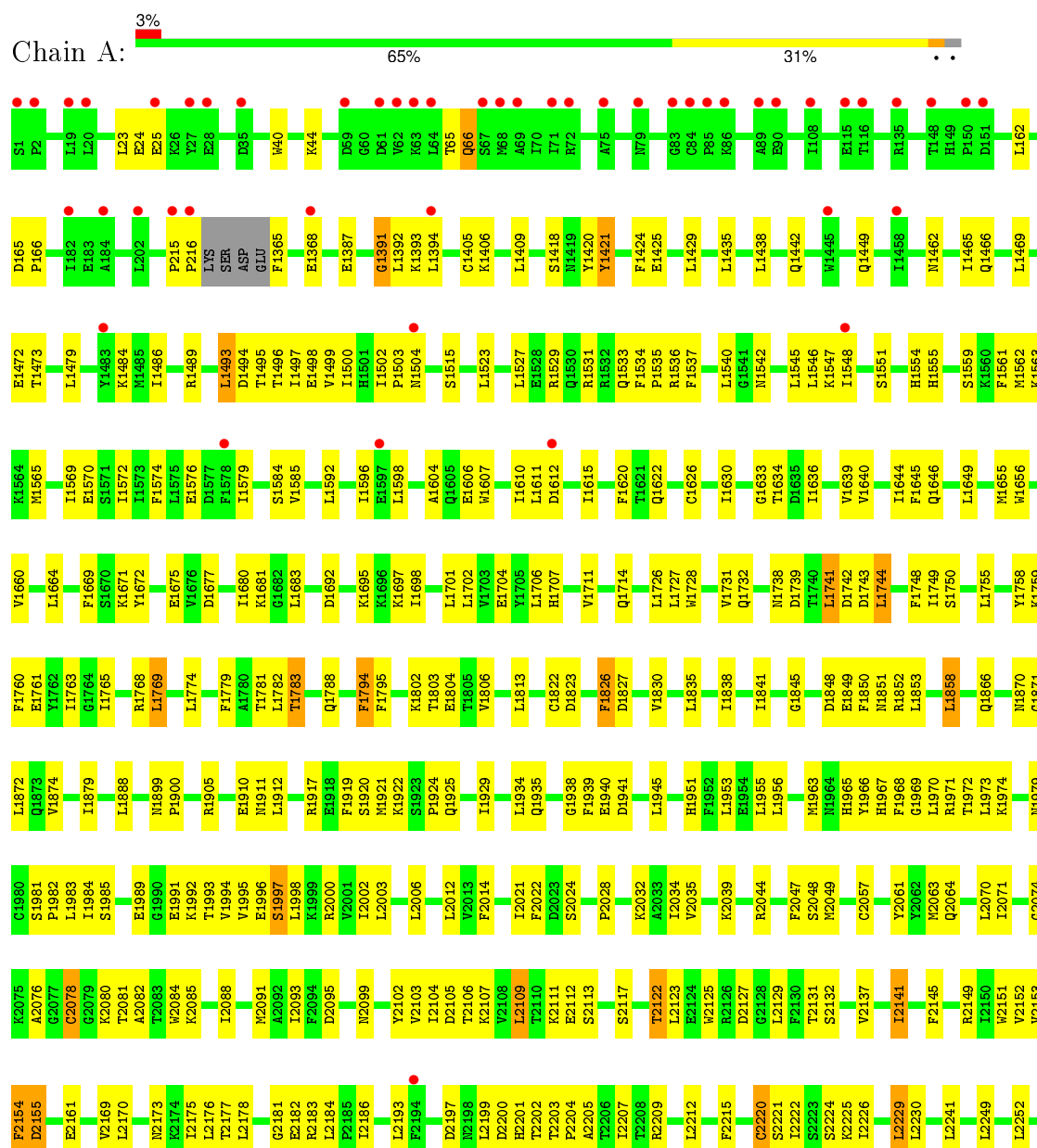
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

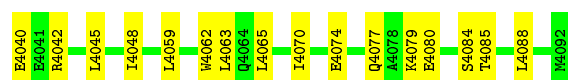
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

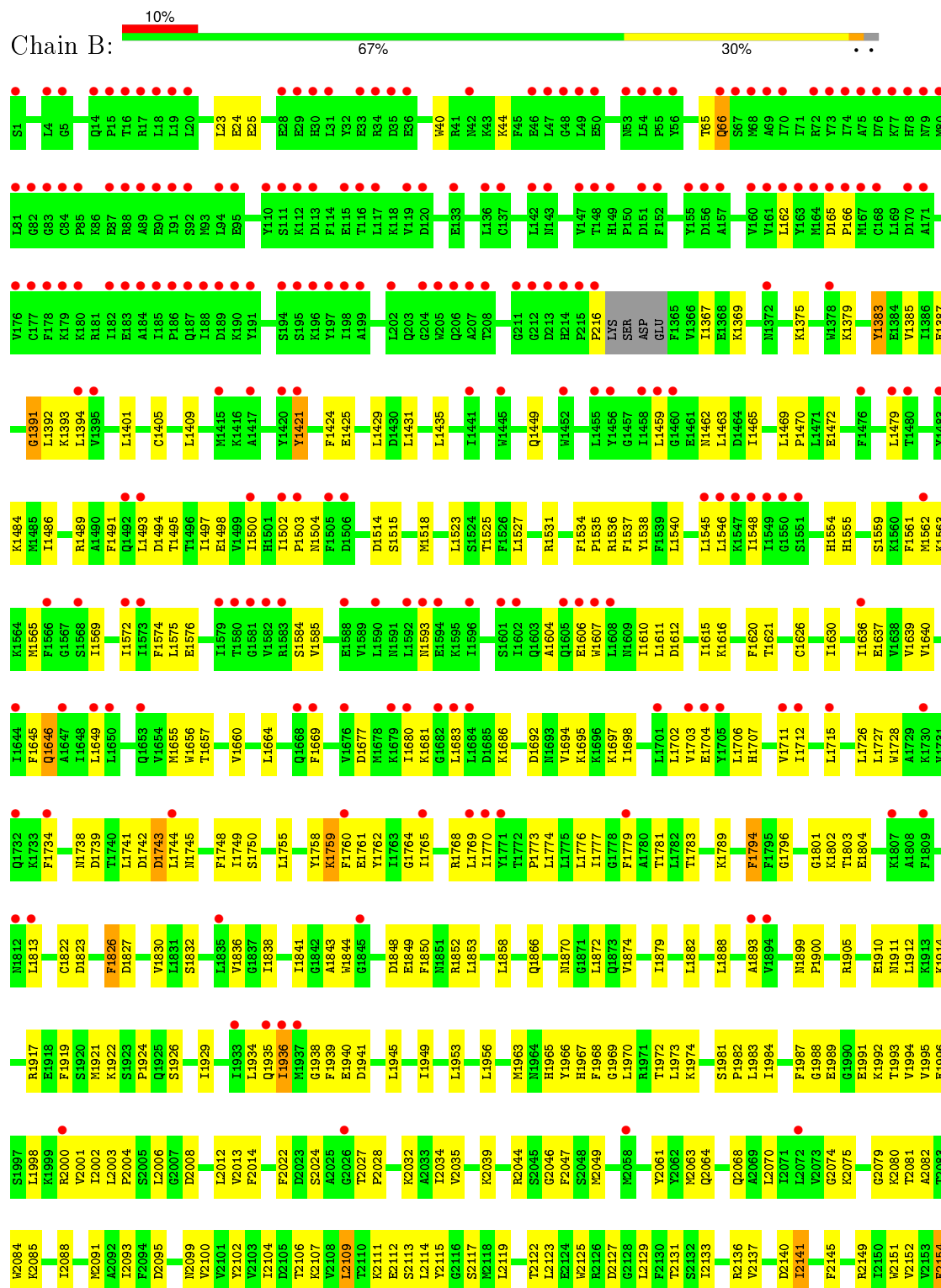
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



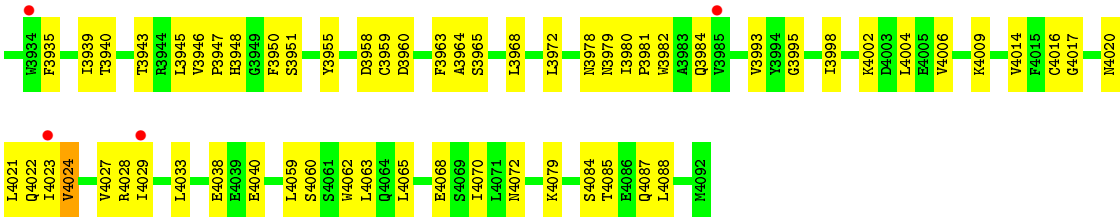




• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



Y3854	W3772	K3541	K3393	VAL	L2840	H2741	G2584	L2476	V2386	I2282	D2155
L3855	N3773	K3544	S3400	PRO	P2841	R2744	K2565	S2477	D2389	K2283	S2156
H3858	I3774	K3544	K3303	GLU	D2842	I2745	S2566	I2478	I2390	E2285	E2161
V3859	V3777	D3547	F3406	ASN	Q2845	D2746	E2571	L2482	V2391	V2288	Y2162
T3862	A3778	L3548	K3306	LYS	G2846	A2748	E2572	V2483	T2394	Q2269	V2169
A3865	N3780	K3550	I3409	GLU	Y2849	L3507	I2573	L2484	T2395	L2290	
E3866	V3656	L3551	K3425	LEU	Q2751	Q2751	Y2574	F2485	T2397	H2293	M2173
F3867	F3657	E3554	V3426	VAL	L2853	V2752	A2577	E2488	T2397	K2174	K2175
N3784	L3658	Y3555	T3427	THR	G2754	Q2753	L2578	I2489	F2404	L2294	L2176
K3870	L3310	K3311	L3428	GLU	L2856	G2754	E2590	V2490	F2404	T2177	T2177
F3871	L3312	Q3312	L3428	PRO	T2860	H2755	E2590	V2490	F2404	L2178	
N3786	L3313	F3313	S3450	ILE	T2860	M2756	E2590	V2490	F2404		
A3872	F3313	E3319	F3431	GLN	T2860	M2756	E2590	V2490	F2404		
M3873	E3319	L3320	F3431	T2960	L2865	M2757	R2620	F2492	L2407	F2302	
K3874	L3320	L3320	K3430	I2961	L2865	L2758	R2620	F2492	L2407	L2305	G2181
M3875	L3321	L3321	K3430	I2962	L2866	L2758	T2623	F2492	L2407	D2306	E2182
T3876	G3322	G3322	S3463	D2963	L2867	G2760	T2623	L2495	K2411	D2307	R2183
C3877	N3323	N3323	S3463	L2968	E2870	T2769	R2627	V2496	K2412		
H3878	L3329	L3329	K3464	L2969	Q2871	L2770	Y2630	V2497		L2310	I2186
D3882	F3330	F3330	K3464	T2965	L2871	K2766	Y2630	V2497		K2311	
K3883	F3334	F3334	L3466	I2966	L2872	L2769	T2631	S2499		D2312	L2193
L3884	N3338	N3338	A3473	D2985	L2873	T2770	T2635	V2503		V2313	L2193
L3885	E3341	E3341	R3476	D2986	E2883	R2771	G2636	L2506		L2314	T2195
A3886	L3346	L3346	K3473	T2988	K2883	L2779	P2637	L2507		L2317	E2196
F3887	F3347	F3347	K3473	D2989	H2886	K2780	Q2638	Q2507		L2318	D2197
L3888	L3348	L3348	R3476	T2990	E2886	L2786	T2640	Q2508		S2321	H2201
L3889	L3349	L3349	K3473	D2990	F2888	K2787	S2643	T2510		T2202	T2202
Q3890	F3356	F3356	K3502	L3002	L2900	R2788	E2643	K2512		T2203	P2204
R3894	K3357	K3357	S3502	L3010	T2890	F2789	S2643	K2512		L2322	A2205
F3895	V3358	V3358	K3502	L3010	L2891	L2799	L2660	K2517		Q2332	L2212
Y3897	K3359	K3359	D3482	V3017	C2892	L2808	V2661	T2518		Q2335	W2214
E3898	L3360	L3360	D3482	N3018	C2892	L2808	V2661	T2518		R2336	
D3899	F3361	F3361	K3502	V3019	C2912	L2812	V2661	T2518		I2339	
L3900	D3361	D3361	K3502	K3023	N2915	T2813	L2681	T2518		Q2351	S2224
P3901	L3370	L3370	K3502	L3024	N2916	T2813	L2681	T2518		K2352	K2225
T3906	F3371	F3371	K3502	L3024	N2916	T2813	L2681	T2518		Q2351	S2224
W3911	V3372	V3372	K3502	L3024	N2916	T2813	L2681	T2518		K2352	S2224
S3912	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		Q2351	S2224
Q3913	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		K2352	S2224
F3915	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		Q2351	S2224
F3916	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		K2352	S2224
T3917	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		Q2351	S2224
G3918	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		K2352	S2224
K3919	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		Q2351	S2224
V3923	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		K2352	S2224
W3924	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		Q2351	S2224
S3925	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		K2352	S2224
W3926	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		Q2351	S2224
Y3927	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		K2352	S2224
F3930	F3372	F3372	K3502	L3024	N2916	T2813	L2681	T2518		Q2351	S2224



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.56Å 118.13Å 201.02Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 70.46 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.60) 99.2 (70.46-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.302 0.236 , 0.300	Depositor DCC
R_{free} test set	4766 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	127.5	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 117.1	EDS
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 94922 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41642	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, SO4, 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 > 5$	RMSZ	# $ Z > 5$
1	A	0.53	0/21146	0.77	7/28618 (0.0%)
1	B	0.46	2/21146 (0.0%)	0.68	5/28618 (0.0%)
All	All	0.49	2/42292 (0.0%)	0.73	12/57236 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3306	TRP	CE3-CZ3	-6.25	1.27	1.38
1	B	3306	TRP	CE2-CZ2	-5.22	1.30	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2012	LEU	CA-CB-CG	7.99	133.67	115.30
1	A	1741	LEU	CB-CG-CD1	6.69	122.38	111.00
1	A	3792	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	1782	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	B	2460	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	2865	LEU	CB-CG-CD1	-5.47	101.69	111.00
1	A	2866	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	2494	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	A	2220	CYS	CA-CB-SG	-5.22	104.60	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2279	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	B	3306	TRP	N-CA-C	-5.02	97.43	111.00
1	B	1463	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2119	LEU	Peptide
1	B	2620	ARG	Sidechain

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	20748	0	20206	952	0
1	B	20748	0	20206	909	0
2	A	31	0	12	8	0
2	B	31	0	12	17	0
3	A	31	0	13	7	0
3	B	31	0	13	7	0
4	A	10	0	0	3	0
4	B	10	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41642	0	40462	1861	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 23.

All (1861) 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)
1:A:216:PRO:CB	1:A:1365:PHE:CE1	2.05	1.38
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	1.67	1.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.25
1:A:1368:GLU:HG2	1:A:1424:PHE:CZ	1.69	1.24
1:B:2467:THR:HB	1:B:2473:LEU:CD1	1.66	1.23
1:A:2061:TYR:CE1	1:A:2091:MET:SD	2.35	1.20
1:A:2061:TYR:HE1	1:A:2091:MET:SD	1.65	1.19
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.80	1.16
1:A:1970:LEU:HD13	1:A:1974:LYS:HE3	1.25	1.16
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.58	1.16
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.18	1.14
1:B:3023:LYS:CD	1:B:3567:LEU:HD21	1.77	1.14
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.23	1.14
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	1.27	1.14
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.61	1.13
1:B:2470:GLY:HA3	1:B:2473:LEU:HD21	1.29	1.13
1:A:215:PRO:CB	1:A:3475:ASN:HD22	1.61	1.13
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.84	1.12
1:B:1970:LEU:CD2	1:B:1974:LYS:HE2	1.77	1.12
1:B:2404:PHE:CZ	1:B:2428:MET:SD	2.43	1.12
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	1.49	1.12
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.22	1.11
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.13	1.11
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.51	1.10
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.68	1.10
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.32	1.10
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.13	1.10
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.09	1.09
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	1.88	1.09
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.83	1.09
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.50	1.08
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.28	1.08
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.33	1.08
1:B:3023:LYS:CD	1:B:3567:LEU:CD2	2.31	1.08
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.18	1.08
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.22	1.08
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.36	1.08
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.36	1.08
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.83	1.08
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	0.96	1.07
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.37	1.07
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.85	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.10	1.07
1:B:2988:SER:HB3	1:B:2989:PRO:CD	1.84	1.07
1:B:2467:THR:HB	1:B:2473:LEU:HD12	1.32	1.06
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.85	1.06
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.34	1.06
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.86	1.05
1:B:2467:THR:CB	1:B:2473:LEU:HD12	1.86	1.05
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.43	1.05
1:B:2061:TYR:HE1	1:B:2091:MET:CE	1.70	1.05
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.86	1.05
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.86	1.05
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.86	1.04
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	0.90	1.04
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.36	1.03
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.88	1.03
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.58	1.03
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.73	1.03
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.41	1.03
1:B:2386:MET:HB2	1:B:2627:ARG:HD3	1.35	1.03
1:A:2476:LYS:H	1:A:2476:LYS:CD	1.66	1.02
1:B:3023:LYS:HD3	1:B:3567:LEU:HD21	1.37	1.02
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.41	1.02
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.60	1.02
1:B:2061:TYR:CE1	1:B:2091:MET:SD	2.53	1.02
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.03	1.02
1:B:2386:MET:CB	1:B:2627:ARG:HD3	1.90	1.02
1:B:3303:LYS:HD2	1:B:3306:TRP:HD1	0.87	1.02
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.77	1.01
1:B:2391:VAL:HG23	1:B:2426:MET:SD	2.00	1.01
1:A:1983:LEU:HD21	1:A:2000:ARG:HD2	1.36	1.01
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.40	1.01
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.91	1.01
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.58	1.01
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.43	1.00
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	1.02	1.00
1:B:1421:TYR:CE2	1:B:1425:GLU:CG	2.45	1.00
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	1.89	1.00
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.03	1.00
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.41	1.00
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.61	0.99
1:A:1983:LEU:HD22	1:A:1997:SER:OG	1.63	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2081:THR:HB	2:B:5093:ATP:O2A	1.60	0.99
1:B:3023:LYS:HD2	1:B:3567:LEU:CD2	1.92	0.99
1:A:215:PRO:CB	1:A:3475:ASN:ND2	2.24	0.99
1:A:1421:TYR:CE2	1:A:1425:GLU:CG	2.46	0.99
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.44	0.99
1:A:1421:TYR:CE2	1:A:1425:GLU:HG3	1.97	0.99
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.92	0.99
1:B:1421:TYR:CE2	1:B:1425:GLU:HG3	1.97	0.99
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.75	0.98
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.00	0.98
1:B:3645:SER:HB3	1:B:3890:GLN:HE21	1.26	0.97
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.46	0.97
1:B:1970:LEU:HD21	1:B:1974:LYS:HE2	1.46	0.97
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.26	0.97
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.94	0.97
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.93	0.97
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	1.94	0.97
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	1.99	0.97
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	0.98	0.97
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.64	0.97
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.65	0.97
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	1.95	0.96
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.43	0.96
1:B:2988:SER:CB	1:B:2989:PRO:HD2	1.95	0.96
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.31	0.96
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.66	0.96
1:B:1992:LYS:CG	1:B:2024:SER:HB2	1.94	0.96
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	1.95	0.95
1:B:1983:LEU:HG	1:B:1993:THR:HG23	1.45	0.95
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.43	0.95
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.47	0.95
1:B:3023:LYS:HE2	1:B:3567:LEU:HG	1.49	0.95
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.85	0.94
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.66	0.94
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.79	0.94
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.32	0.94
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.50	0.93
1:B:2380:LEU:HD12	1:B:2577:ALA:HB1	1.49	0.93
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.09	0.93
1:A:2380:LEU:HD12	1:A:2577:ALA:CB	1.98	0.93
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	1.98	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1421:TYR:CZ	1:A:1425:GLU:HG3	2.04	0.93
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.69	0.93
1:B:3023:LYS:HD2	1:B:3567:LEU:HD21	1.51	0.92
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.31	0.92
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	1.52	0.92
1:B:1939:PHE:CD2	1:B:1940:GLU:O	2.23	0.92
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.52	0.92
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.03	0.92
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	2.04	0.92
1:B:1535:PRO:C	1:B:1841:ILE:HD11	1.90	0.92
1:B:2061:TYR:HE1	1:B:2091:MET:SD	1.91	0.91
1:A:2787:HIS:HA	1:A:3460:PRO:CD	1.99	0.91
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.52	0.91
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.85	0.91
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.24	0.91
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.06	0.91
1:B:1421:TYR:CZ	1:B:1425:GLU:HG3	2.05	0.91
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	2.00	0.91
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.01	0.91
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.90
1:A:1983:LEU:HD21	1:A:2000:ARG:CD	2.01	0.90
1:B:2380:LEU:CD1	1:B:2577:ALA:CB	2.49	0.90
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.00	0.90
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.20	0.90
1:B:2380:LEU:HD12	1:B:2577:ALA:CB	2.01	0.90
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.60	0.90
1:B:2061:TYR:HE1	1:B:2091:MET:HE1	1.37	0.90
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.72	0.90
1:B:3303:LYS:CD	1:B:3306:TRP:HD1	1.82	0.90
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.60	0.90
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	2.02	0.89
1:B:2404:PHE:HZ	1:B:2428:MET:SD	1.94	0.89
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.72	0.89
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.55	0.89
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.02	0.89
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.54	0.89
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.71	0.89
1:B:2467:THR:HB	1:B:2473:LEU:HD11	1.54	0.89
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	2.00	0.89
1:B:2404:PHE:CE1	1:B:2428:MET:SD	2.66	0.89
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.37	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2757:MET:CE	1:A:2912:CYS:HB2	2.01	0.89
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.26	0.89
1:B:3303:LYS:CD	1:B:3306:TRP:CD1	2.54	0.89
1:A:2563:SER:HB3	1:A:2566:SER:H	1.37	0.88
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.04	0.88
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.53	0.88
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.72	0.88
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.55	0.88
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.53	0.88
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.04	0.88
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.09	0.88
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.04	0.87
1:A:1979:ASN:O	1:A:1983:LEU:HD13	1.73	0.87
1:B:2224:SER:O	2:B:5093:ATP:H2	1.57	0.87
1:A:1535:PRO:C	1:A:1841:ILE:HD11	1.94	0.87
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.74	0.87
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	2.03	0.87
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.11	0.86
1:B:2563:SER:HB3	1:B:2566:SER:H	1.38	0.86
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.05	0.86
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.04	0.86
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.04	0.86
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	2.10	0.86
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.39	0.86
1:A:2412:ARG:HH11	1:A:2412:ARG:HB2	1.41	0.86
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.10	0.85
1:B:1926:SER:CB	1:B:1970:LEU:HD12	2.06	0.85
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.06	0.85
1:B:2745:ILE:HG23	1:B:2756:MET:HE1	1.57	0.85
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.58	0.85
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.76	0.85
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.07	0.85
1:A:1368:GLU:HG2	1:A:1424:PHE:HZ	1.36	0.85
1:A:2380:LEU:CD1	1:A:2577:ALA:CB	2.54	0.85
1:A:2380:LEU:HD12	1:A:2577:ALA:HB1	1.56	0.85
1:B:1425:GLU:OE2	1:B:1429:LEU:HG	1.76	0.85
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.57	0.84
1:A:166:PRO:CB	1:A:3476:ARG:HD3	2.06	0.84
1:B:2081:THR:HB	2:B:5093:ATP:PA	2.17	0.84
1:A:2446:SER:H	1:A:2449:THR:CG2	1.90	0.84
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.77	0.84
1:A:216:PRO:CB	1:A:1365:PHE:CZ	2.59	0.84
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	1.22	0.84
1:A:2061:TYR:CE1	1:A:2091:MET:CE	2.60	0.84
1:B:1425:GLU:OE2	1:B:1429:LEU:CG	2.24	0.84
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.99	0.84
1:A:1368:GLU:CG	1:A:1424:PHE:CZ	2.58	0.83
1:B:2141:ILE:HG22	1:B:2145:PHE:CB	2.06	0.83
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.61	0.83
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	2.08	0.83
1:B:1983:LEU:HD23	1:B:1993:THR:O	1.78	0.83
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.57	0.83
1:B:2623:THR:HG21	3:B:5094:ANP:O3'	1.78	0.83
1:A:2476:LYS:N	1:A:2476:LYS:HD3	1.90	0.83
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.26	0.83
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.13	0.83
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.61	0.83
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.60	0.83
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	2.07	0.83
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.58	0.83
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.93	0.83
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.61	0.83
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.26	0.83
1:B:2920:TRP:CB	1:B:2989:PRO:HG3	2.04	0.83
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.59	0.83
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.61	0.83
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.59	0.83
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.60	0.83
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.77	0.82
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.94	0.82
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	2.08	0.82
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.06	0.82
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.61	0.82
1:B:1421:TYR:CE2	1:B:1425:GLU:HG2	2.13	0.82
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.45	0.82
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.95	0.82
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.59	0.82
1:B:2513:GLN:O	1:B:2526:ILE:HG13	1.78	0.82
1:A:1365:PHE:CZ	1:A:1420:TYR:CD1	2.68	0.82
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.61	0.82
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.62	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.10	0.82
1:A:1421:TYR:CE2	1:A:1425:GLU:HG2	2.14	0.81
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.80	0.81
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.61	0.81
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	1.96	0.81
1:A:1779:PHE:O	1:A:1783:THR:HG22	1.80	0.81
1:A:2224:SER:O	2:A:5093:ATP:H2	1.63	0.81
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.81	0.81
1:A:1970:LEU:HD13	1:A:1974:LYS:CE	2.08	0.81
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.61	0.81
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.21	0.81
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.57	0.80
1:B:1970:LEU:CD2	1:B:1974:LYS:CE	2.59	0.80
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.45	0.80
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.80	0.80
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.29	0.80
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.62	0.80
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	1.96	0.80
1:A:2225:LYS:HA	2:A:5093:ATP:C2	2.16	0.80
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.82	0.80
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.64	0.80
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.62	0.80
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	1.97	0.80
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.12	0.79
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.12	0.79
1:B:2141:ILE:CG2	1:B:2145:PHE:HB2	2.09	0.79
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.22	0.79
1:B:3023:LYS:HD2	1:B:3567:LEU:HD23	1.64	0.79
1:A:2410:SER:C	1:A:2411:LYS:HG3	2.03	0.79
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	1.99	0.78
1:A:2386:MET:CB	1:A:2627:ARG:HD3	2.13	0.78
1:A:2513:GLN:O	1:A:2526:ILE:HG13	1.82	0.78
1:B:1939:PHE:HD2	1:B:1940:GLU:O	1.64	0.78
1:A:3792:ARG:HB2	1:A:3955:TYR:CD2	2.18	0.78
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.61	0.78
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.82	0.78
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.70	0.78
1:A:2631:THR:O	1:A:2635:THR:HG22	1.81	0.78
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.64	0.78
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.83	0.78
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.49	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.84	0.78
1:B:2061:TYR:CE1	1:B:2091:MET:HE1	2.18	0.78
1:A:2552:ARG:HG2	1:A:2552:ARG:HH11	1.48	0.78
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.14	0.77
1:A:1970:LEU:HD12	1:A:1971:ARG:N	1.98	0.77
1:B:1967:HIS:C	1:B:1968:PHE:HD1	1.88	0.77
1:A:1922:LYS:NZ	1:A:4004:LEU:HD12	1.99	0.77
1:B:3919:LYS:HZ3	1:B:4038:GLU:CD	1.87	0.77
1:B:2745:ILE:HG12	1:B:2756:MET:HE3	1.66	0.77
1:A:2757:MET:HE3	1:A:2912:CYS:HB2	1.64	0.77
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.64	0.77
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.20	0.77
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.83	0.77
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.66	0.77
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.84	0.77
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.67	0.77
1:A:2446:SER:H	1:A:2449:THR:HG23	1.49	0.77
1:A:2061:TYR:CD1	1:A:2091:MET:SD	2.78	0.77
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.66	0.77
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.20	0.77
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.32	0.76
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.50	0.76
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.87	0.76
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.59	0.76
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.33	0.76
1:A:2103:VAL:CG1	1:A:2155:ASP:OD1	2.33	0.76
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.84	0.76
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.67	0.76
1:A:216:PRO:CB	1:A:1365:PHE:CD1	2.69	0.76
1:A:1922:LYS:HZ1	1:A:4004:LEU:HD12	1.49	0.76
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.85	0.76
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.66	0.76
1:A:2766:LYS:HE3	1:A:2892:CYS:SG	2.26	0.76
1:B:3019:VAL:O	1:B:3023:LYS:HG3	1.86	0.76
1:B:2380:LEU:HD11	1:B:2577:ALA:CB	2.15	0.76
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.16	0.76
1:A:2061:TYR:CD1	1:A:2091:MET:CE	2.69	0.76
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.14	0.76
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	2.01	0.76
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.65	0.75
1:B:2467:THR:CB	1:B:2473:LEU:CD1	2.50	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.11	0.75
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.68	0.75
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.86	0.75
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.16	0.75
1:B:2446:SER:H	1:B:2449:THR:HG23	1.52	0.75
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.66	0.75
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.66	0.75
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.52	0.75
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.64	0.75
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.86	0.75
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.87	0.75
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.87	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:HB1	2.15	0.74
1:B:3023:LYS:HE2	1:B:3567:LEU:CG	2.16	0.74
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.54	0.74
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.68	0.74
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.27	0.74
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.52	0.74
1:B:2081:THR:CB	2:B:5093:ATP:O2A	2.28	0.74
1:B:2517:LYS:HE2	1:B:2520:GLU:OE1	1.88	0.74
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.69	0.74
1:A:1707:HIS:O	1:A:1711:VAL:HG23	1.88	0.74
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.74	0.74
1:A:1922:LYS:HE2	1:A:3999:ASP:O	1.87	0.74
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.15	0.74
1:B:2220:CYS:CB	2:B:5093:ATP:C6	2.71	0.74
1:A:2152:VAL:HG12	1:A:2154:PHE:HE1	1.51	0.74
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.53	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:HB2	2.18	0.73
1:B:3618:TYR:CD1	1:B:3618:TYR:N	2.51	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.18	0.73
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.51	0.73
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.88	0.73
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.70	0.73
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.36	0.73
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	2.18	0.73
1:B:3792:ARG:HB2	1:B:3955:TYR:CD2	2.23	0.73
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.86	0.73
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.04	0.73
1:A:2425:THR:CG2	3:A:5094:ANP:O3G	2.37	0.73
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.18	0.72
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.88	0.72
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.18	0.72
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.10	0.72
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.71	0.72
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.03	0.72
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.70	0.72
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.89	0.72
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.29	0.72
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.20	0.72
1:B:2446:SER:H	1:B:2449:THR:CG2	2.01	0.72
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.72	0.72
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.71	0.72
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.90	0.72
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.60	0.72
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.36	0.71
1:A:2380:LEU:CD1	1:A:2577:ALA:HB2	2.20	0.71
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.04	0.71
1:B:1706:LEU:HD22	1:B:1935:GLN:HG2	1.72	0.71
1:A:2061:TYR:CE1	1:A:2091:MET:HE1	2.24	0.71
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.38	0.71
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.91	0.71
1:B:3618:TYR:HD1	1:B:3618:TYR:N	1.87	0.71
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.73	0.71
1:B:2061:TYR:CE1	1:B:2091:MET:CE	2.63	0.71
1:B:3792:ARG:HB2	1:B:3955:TYR:CE2	2.26	0.71
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.25	0.71
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.21	0.71
1:B:1852:ARG:HG3	1:B:1852:ARG:O	1.91	0.71
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.72	0.71
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.26	0.71
1:B:2111:LYS:CD	1:B:2161:GLU:HG3	2.10	0.71
1:A:2549:ARG:HE	2:A:5093:ATP:PG	2.13	0.71
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.72	0.71
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.31	0.71
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.11	0.71
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.20	0.71
1:A:2103:VAL:HG13	1:A:2155:ASP:OD1	1.91	0.71
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.91	0.71
1:B:1738:ASN:O	1:B:1739:ASP:OD1	2.09	0.71
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.17	0.70
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.91	0.70
1:B:2420:PRO:HB2	1:B:2620:ARG:NH2	2.06	0.70
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.22	0.70
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.25	0.70
1:B:1938:GLY:O	1:B:1989:GLU:HB3	1.92	0.70
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.21	0.70
1:B:3737:THR:HB	1:B:3740:THR:HG1	1.53	0.70
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	1.73	0.70
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.92	0.70
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.74	0.70
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.92	0.70
1:B:3577:MET:O	1:B:3579:GLU:N	2.24	0.70
1:B:2064:GLN:OE1	1:B:2151:TRP:HH2	1.74	0.70
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.73	0.70
1:A:216:PRO:CB	1:A:1365:PHE:HE1	1.99	0.70
1:A:2225:LYS:HA	2:A:5093:ATP:N3	2.07	0.70
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.73	0.70
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.21	0.70
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	0.81	0.69
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.72	0.69
1:B:3645:SER:CB	1:B:3890:GLN:HE21	2.03	0.69
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.22	0.69
1:B:1698:ILE:O	1:B:1702:LEU:HG	1.92	0.69
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.92	0.69
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.57	0.69
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.74	0.69
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.81	0.69
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.23	0.69
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.73	0.69
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.71	0.69
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.57	0.69
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.21	0.69
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.57	0.69
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.92	0.69
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.73	0.69
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.57	0.69
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.75	0.69
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.13	0.69
1:B:3837:GLY:O	1:B:3871:PHE:HD1	1.75	0.69
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1970:LEU:CD1	1:A:1974:LYS:HE3	2.14	0.69
1:A:1802:LYS:NZ	4:A:5095:SO4:O2	2.26	0.69
1:B:2061:TYR:CD1	1:B:2091:MET:SD	2.86	0.68
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.21	0.68
1:A:1368:GLU:HG2	1:A:1424:PHE:CE2	2.25	0.68
1:B:3023:LYS:CD	1:B:3567:LEU:HD23	2.19	0.68
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.22	0.68
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.73	0.68
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.71	0.68
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.57	0.68
1:A:2109:LEU:HD13	1:A:2129:LEU:HD23	1.75	0.68
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.57	0.68
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.22	0.68
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.75	0.68
1:B:3819:ILE:O	1:B:3823:ASN:HB2	1.93	0.68
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.76	0.68
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	1.93	0.68
1:B:2181:GLY:O	1:B:2182:GLU:HG3	1.93	0.68
1:A:2476:LYS:NZ	1:A:2528:ARG:HD3	2.09	0.68
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.93	0.68
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.93	0.68
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	1.93	0.68
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.59	0.68
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.64	0.68
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.76	0.68
1:A:2846:GLY:O	1:A:2849:TYR:HB3	1.92	0.68
1:B:3612:ASP:O	1:B:3615:VAL:HG22	1.93	0.68
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.24	0.67
1:B:2620:ARG:HH12	1:B:2910:ASN:CG	1.97	0.67
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.47	0.67
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.24	0.67
1:B:1929:ILE:HD13	1:B:1970:LEU:HD11	1.75	0.67
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.29	0.67
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.09	0.67
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.29	0.67
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.28	0.67
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.82	0.67
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.94	0.67
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.94	0.67
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.10	0.67
1:B:1726:LEU:HD13	1:B:3984:GLN:HB3	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1611:LEU:O	1:B:1615:ILE:HG23	1.95	0.67
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.72	0.67
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.15	0.67
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.09	0.67
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.59	0.67
1:A:2380:LEU:HD12	1:A:2577:ALA:HB2	1.75	0.67
1:B:2394:THR:H	1:B:2397:THR:HB	1.59	0.67
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.09	0.67
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.29	0.67
1:A:2757:MET:HE2	1:A:2912:CYS:HB2	1.75	0.67
1:B:3816:LEU:HD23	1:B:3847:SER:OG	1.95	0.67
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.29	0.67
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.10	0.67
1:A:2224:SER:O	2:A:5093:ATP:C2	2.48	0.67
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.77	0.67
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.30	0.67
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.25	0.67
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.10	0.66
1:A:1922:LYS:NZ	1:A:4004:LEU:CD1	2.58	0.66
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.25	0.66
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.77	0.66
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.25	0.66
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.77	0.66
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.25	0.66
1:A:1527:LEU:HD23	1:A:1545:LEU:HD22	1.77	0.66
1:B:2936:ILE:HG22	1:B:2962:ARG:HD3	1.78	0.66
1:A:2081:THR:O	1:A:2085:LYS:HB2	1.96	0.66
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.76	0.66
1:A:2425:THR:HG23	3:A:5094:ANP:O3G	1.95	0.66
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.26	0.66
1:A:1466:GLN:CB	1:A:1473:THR:HG21	2.26	0.66
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.59	0.66
1:A:2495:ASP:O	1:A:2498:GLY:N	2.29	0.66
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.77	0.66
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.25	0.66
1:B:3023:LYS:CE	1:B:3567:LEU:HG	2.25	0.65
1:B:2109:LEU:CD1	1:B:2129:LEU:HD23	2.26	0.65
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	1.77	0.65
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.00	0.65
1:A:3618:TYR:HD1	1:A:3618:TYR:N	1.94	0.65
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.36	0.65
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.76	0.65
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.27	0.65
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.30	0.65
1:B:3850:TRP:NE1	1:B:3854:TYR:HB3	2.12	0.65
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.77	0.65
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.27	0.65
1:A:1706:LEU:HD21	1:A:1935:GLN:HG2	1.79	0.65
1:A:1425:GLU:OE2	1:A:1429:LEU:HD11	1.96	0.65
1:B:3460:PRO:O	1:B:3463:SER:HB3	1.97	0.65
1:B:2508:GLN:HG3	1:B:2512:LYS:HG3	1.77	0.65
1:A:2766:LYS:CE	1:A:2892:CYS:SG	2.84	0.65
1:A:2032:LYS:O	1:A:2035:VAL:HG12	1.96	0.65
1:B:2391:VAL:CG2	1:B:2426:MET:SD	2.83	0.65
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.11	0.65
1:B:2513:GLN:O	1:B:2526:ILE:CG1	2.45	0.65
1:B:1425:GLU:OE2	1:B:1429:LEU:CD2	2.45	0.65
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.32	0.65
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.78	0.64
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.62	0.64
1:B:2109:LEU:HD11	1:B:2129:LEU:HD23	1.79	0.64
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.30	0.64
1:B:2410:SER:C	1:B:2411:LYS:HG3	2.16	0.64
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.27	0.64
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.98	0.64
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	1.78	0.64
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.12	0.64
1:B:3911:TRP:HH2	1:B:3926:VAL:HG12	1.62	0.64
1:B:1726:LEU:CD1	1:B:3984:GLN:CB	2.75	0.64
1:B:2106:THR:HG1	1:B:2154:PHE:HB3	1.62	0.64
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.86	0.64
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.62	0.64
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.32	0.64
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.78	0.64
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.98	0.64
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.56	0.64
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.80	0.64
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.79	0.64
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.13	0.64
1:A:1365:PHE:CZ	1:A:1420:TYR:CE1	2.86	0.63
1:B:3737:THR:OG1	1:B:3740:THR:HB	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1983:LEU:CD2	1:B:1993:THR:O	2.45	0.63
1:B:2623:THR:HB	3:B:5094:ANP:O2'	1.99	0.63
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.29	0.63
1:A:2401:GLU:HG2	1:A:2431:ALA:HB2	1.81	0.63
1:B:2728:LEU:HD12	1:B:2771:ARG:CZ	2.28	0.63
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.61	0.63
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.33	0.63
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.28	0.63
1:A:2552:ARG:HG2	1:A:2552:ARG:NH1	2.14	0.63
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.64	0.63
1:A:3679:TYR:HB3	1:A:3767:PHE:HE1	1.64	0.63
1:B:1744:LEU:HD22	1:B:1760:PHE:CG	2.34	0.63
1:B:2508:GLN:CG	1:B:2512:LYS:HG3	2.28	0.63
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.80	0.63
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.53	0.63
1:B:1421:TYR:O	1:B:1425:GLU:N	2.32	0.63
1:B:2220:CYS:SG	2:B:5093:ATP:C6	2.92	0.62
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.74	0.62
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.13	0.62
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.11	0.62
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.13	0.62
1:B:3925:SER:HB2	1:B:3972:LEU:HD13	1.81	0.62
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.87	0.62
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.87	0.62
1:B:2109:LEU:HD11	1:B:2129:LEU:CD2	2.29	0.62
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.52	0.62
1:B:1425:GLU:OE2	1:B:1429:LEU:HD21	1.98	0.62
1:B:2428:MET:SD	1:B:2532:VAL:HG11	2.39	0.62
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.99	0.62
1:B:1706:LEU:HD11	1:B:1936:ILE:HG12	1.80	0.62
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.81	0.62
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.33	0.62
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.81	0.62
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.30	0.62
1:B:2280:THR:HA	1:B:2283:LYS:HD2	1.81	0.62
1:B:2467:THR:OG1	1:B:2473:LEU:HD12	1.99	0.62
1:B:2677:VAL:HG11	1:B:2686:LEU:HD21	1.82	0.62
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.63	0.62
1:B:1726:LEU:HD12	1:B:3984:GLN:CB	2.29	0.62
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.29	0.62
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2709:LYS:O	1:A:2713:VAL:HG23	1.98	0.62
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.80	0.62
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.63	0.62
1:A:1536:ARG:HD3	1:A:1841:ILE:HD13	1.82	0.62
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.81	0.62
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.65	0.61
1:B:2631:THR:O	1:B:2635:THR:HG22	1.99	0.61
1:B:1965:HIS:HD2	1:B:2212:LEU:HD21	1.65	0.61
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.82	0.61
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.81	0.61
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.63	0.61
1:B:3737:THR:HB	1:B:3740:THR:CB	2.29	0.61
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.82	0.61
1:A:3813:ILE:HG22	1:A:3840:LEU:HD23	1.83	0.61
1:B:2063:MET:HB3	1:B:2070:LEU:HD11	1.82	0.61
1:B:3023:LYS:HD3	1:B:3567:LEU:CD2	2.10	0.61
1:A:2380:LEU:HD11	1:A:2577:ALA:CB	2.30	0.61
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.30	0.61
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.66	0.61
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.83	0.61
1:A:3696:MET:SD	1:A:3760:LEU:HD23	2.41	0.61
1:A:1469:LEU:HD13	1:A:1523:LEU:CD2	2.30	0.61
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.84	0.61
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.82	0.61
1:A:4021:LEU:HD23	1:A:4023:ILE:HG12	1.82	0.61
1:B:3023:LYS:CE	1:B:3567:LEU:CD2	2.79	0.61
1:B:1493:LEU:O	1:B:1494:ASP:HB2	2.00	0.61
1:A:2394:THR:H	1:A:2397:THR:HB	1.65	0.61
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.36	0.60
1:B:2386:MET:HB3	1:B:2627:ARG:HD3	1.77	0.60
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.16	0.60
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.31	0.60
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.31	0.60
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.34	0.60
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.55	0.60
1:B:1744:LEU:HD22	1:B:1760:PHE:CD2	2.36	0.60
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.54	0.60
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.18	0.60
1:B:1983:LEU:HD21	1:B:1996:GLU:HB2	1.84	0.60
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.30	0.60
1:B:1991:GLU:O	1:B:1995:VAL:HG23	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.30	0.60
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.31	0.60
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.90	0.60
1:A:2230:LEU:HD23	1:A:2288:VAL:HG13	1.83	0.60
1:A:2332:GLY:O	1:A:2336:ARG:HG3	2.01	0.60
1:A:2757:MET:HE1	1:A:2909:PHE:HA	1.83	0.60
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.84	0.60
1:B:2107:LYS:CE	1:B:2495:ASP:OD2	2.38	0.60
1:B:1983:LEU:CG	1:B:1993:THR:HG23	2.25	0.60
1:B:2476:LYS:HD2	1:B:2476:LYS:H	1.67	0.60
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.32	0.60
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.01	0.60
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.37	0.60
1:B:3728:GLU:HG3	1:B:4079:LYS:HE2	1.82	0.60
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.64	0.59
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.50	0.59
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.02	0.59
1:A:3819:ILE:O	1:A:3823:ASN:HB2	2.01	0.59
1:A:2446:SER:H	1:A:2449:THR:HG21	1.66	0.59
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.84	0.59
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.02	0.59
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.02	0.59
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.32	0.59
1:A:2757:MET:CE	1:A:2912:CYS:CB	2.77	0.59
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.67	0.59
1:B:3631:MET:HE3	1:B:3698:MET:HG3	1.82	0.59
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.84	0.59
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.50	0.59
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.03	0.59
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.84	0.59
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.01	0.59
1:A:1802:LYS:NZ	4:A:5095:SO4:S	2.75	0.59
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.37	0.59
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	1.83	0.59
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.01	0.59
1:A:1534:PHE:HD2	1:A:1537:PHE:CE1	2.20	0.59
1:B:2423:GLY:N	3:B:5094:ANP:O1B	2.29	0.59
1:B:3877:CYS:SG	1:B:3884:LEU:HD22	2.41	0.59
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.86	0.59
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.51	0.59
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2512:LYS:O	1:B:2513:GLN:CB	2.50	0.59
1:B:3995:GLY:HA2	1:B:3998:ILE:HD13	1.84	0.59
1:A:2080:LYS:HG2	1:A:2215:PHE:CD1	2.38	0.59
1:B:1926:SER:HB2	1:B:1970:LEU:HD12	1.84	0.59
1:A:2757:MET:HE2	1:A:2912:CYS:CB	2.32	0.59
1:B:2266:PHE:HD1	1:B:2326:LEU:HD21	1.67	0.59
1:B:2856:LEU:HD23	1:B:2873:LEU:HB3	1.84	0.59
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.38	0.59
1:B:166:PRO:CB	1:B:1369:LYS:HB3	2.32	0.59
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.19	0.59
1:A:1852:ARG:O	1:A:1852:ARG:HG3	2.03	0.59
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.01	0.59
1:A:3460:PRO:O	1:A:3463:SER:HB3	2.03	0.59
1:B:2274:HIS:CE1	1:B:2326:LEU:O	2.51	0.59
1:A:1965:HIS:CD2	1:A:2212:LEU:HD21	2.38	0.59
1:B:2503:VAL:HA	1:B:2506:LEU:HD12	1.83	0.59
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.37	0.58
1:A:3737:THR:HB	1:A:3740:THR:CB	2.32	0.58
1:A:2425:THR:HG21	3:A:5094:ANP:O3G	2.02	0.58
1:B:3807:SER:O	1:B:3808:LYS:HB2	2.03	0.58
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.84	0.58
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.24	0.58
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.84	0.58
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.84	0.58
1:A:1425:GLU:C	1:A:1425:GLU:OE1	2.42	0.58
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.83	0.58
1:A:1967:HIS:C	1:A:1968:PHE:HD1	2.06	0.58
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.82	0.58
1:A:1368:GLU:CG	1:A:1424:PHE:CE2	2.86	0.58
1:B:2517:LYS:CE	1:B:2520:GLU:OE1	2.50	0.58
1:B:3948:HIS:NE2	1:B:4072:ASN:CG	2.57	0.58
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.24	0.58
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.18	0.58
1:A:2842:ASP:O	1:A:2845:GLN:HG2	2.04	0.58
1:B:2655:ILE:HD11	1:B:2747:ARG:HH22	1.68	0.58
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.85	0.58
1:A:1683:LEU:HD22	1:A:1698:ILE:HG23	1.85	0.58
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.30	0.58
1:A:2563:SER:CB	1:A:2566:SER:OG	2.51	0.58
1:A:1774:LEU:HD21	1:A:1922:LYS:O	2.03	0.58
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.85	0.58
1:B:3530:PHE:HD1	1:B:3618:TYR:HD2	1.49	0.58
1:B:1929:ILE:HD13	1:B:1970:LEU:CD1	2.34	0.58
1:A:1421:TYR:O	1:A:1425:GLU:N	2.36	0.58
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.22	0.58
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.39	0.58
1:A:2755:HIS:O	1:A:2913:ILE:HG13	2.03	0.58
1:A:3792:ARG:HB2	1:A:3955:TYR:CE2	2.39	0.58
1:B:2846:GLY:O	1:B:2849:TYR:HB3	2.02	0.58
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.34	0.58
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.69	0.58
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.04	0.58
1:B:2786:ILE:O	1:B:3460:PRO:HB2	2.04	0.58
1:B:1940:GLU:HG3	1:B:1941:ASP:N	2.19	0.58
1:A:1620:PHE:HA	1:A:1760:PHE:CE1	2.39	0.57
1:A:1409:LEU:CD2	1:A:1435:LEU:HB3	2.24	0.57
1:B:2224:SER:C	2:B:5093:ATP:H2	2.07	0.57
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.33	0.57
1:A:3449:VAL:HG22	1:A:3493:LYS:HB2	1.85	0.57
1:A:2064:GLN:OE1	1:A:2151:TRP:CH2	2.51	0.57
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	1.86	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.57	0.57
1:B:4020:ASN:HB3	1:B:4028:ARG:HH11	1.68	0.57
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.57	0.57
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.69	0.57
1:A:3810:SER:O	1:A:3838:TRP:HB2	2.03	0.57
1:A:2382:ALA:O	1:A:2385:VAL:HG12	2.04	0.57
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.33	0.57
1:A:1611:LEU:O	1:A:1615:ILE:HG23	2.05	0.57
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.86	0.57
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	1.86	0.57
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.20	0.57
1:B:1940:GLU:CB	1:B:1989:GLU:O	2.52	0.57
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.23	0.57
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.87	0.57
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	1.87	0.57
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.87	0.57
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.86	0.57
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.34	0.57
1:A:1698:ILE:O	1:A:1702:LEU:HG	2.05	0.57
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.47	0.57
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.86	0.57
1:B:1620:PHE:CB	1:B:1760:PHE:CE1	2.87	0.57
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.70	0.57
1:B:2563:SER:CB	1:B:2566:SER:OG	2.52	0.57
1:B:2620:ARG:O	1:B:2623:THR:HG22	2.04	0.57
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.39	0.57
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.57
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.20	0.57
1:B:3353:LEU:HD23	1:B:3358:VAL:HG11	1.85	0.57
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.38	0.57
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.70	0.57
1:B:1744:LEU:HA	1:B:1760:PHE:HE2	1.66	0.57
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.51	0.57
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.70	0.57
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.25	0.57
1:A:2047:PHE:CE2	1:A:2082:ALA:HB1	2.40	0.57
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.35	0.57
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.86	0.56
1:B:2755:HIS:CB	1:B:2911:ARG:O	2.47	0.56
1:A:1535:PRO:O	1:A:1841:ILE:HD11	2.05	0.56
1:B:3810:SER:O	1:B:3838:TRP:HB2	2.04	0.56
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.93	0.56
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.69	0.56
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.86	0.56
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.40	0.56
1:A:3618:TYR:O	1:A:3622:GLY:N	2.37	0.56
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.05	0.56
1:A:2517:LYS:HG2	1:A:2520:GLU:HB2	1.87	0.56
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.69	0.56
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.20	0.56
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.86	0.56
1:B:1813:LEU:HD12	1:B:1844:TRP:HH2	1.71	0.56
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.20	0.56
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.20	0.56
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.39	0.56
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.40	0.56
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.87	0.56
1:B:1803:THR:HG21	1:B:1848:ASP:OD1	2.05	0.56
1:A:2581:LEU:HD13	1:A:2633:ILE:HG22	1.87	0.56
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.41	0.56
1:B:1998:LEU:HD11	1:B:2022:PHE:HZ	1.71	0.56
1:B:2225:LYS:HA	2:B:5093:ATP:N3	2.21	0.56
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.69	0.56
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.88	0.56
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.84	0.56
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.32	0.56
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.88	0.56
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.87	0.56
1:B:3440:LEU:HD23	1:B:3462:ILE:HD12	1.87	0.56
1:A:2356:TYR:CE1	1:A:2395:ILE:HG22	2.41	0.56
1:A:2513:GLN:O	1:A:2526:ILE:CG1	2.50	0.56
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.20	0.56
1:A:2741:HIS:HA	1:A:2744:ARG:HD2	1.87	0.56
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.87	0.56
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.87	0.56
1:B:3919:LYS:NZ	1:B:4038:GLU:HG3	2.21	0.56
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.06	0.56
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.70	0.56
1:A:3481:ILE:O	1:A:3483:ASP:N	2.35	0.56
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	2.06	0.56
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.24	0.55
1:A:2380:LEU:CD1	1:A:2577:ALA:HB1	2.30	0.55
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.19	0.55
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.71	0.55
1:B:3930:PHE:HE2	1:B:4029:ILE:HD13	1.71	0.55
1:A:3833:LYS:HZ3	1:A:3862:THR:HG21	1.70	0.55
1:B:216:PRO:CB	1:B:1424:PHE:CG	2.89	0.55
1:B:2225:LYS:HA	2:B:5093:ATP:C2	2.40	0.55
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.87	0.55
1:A:2048:SER:H	2:A:5093:ATP:HN62	1.54	0.55
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.36	0.55
1:B:2728:LEU:HD12	1:B:2771:ARG:NH2	2.21	0.55
1:B:1527:LEU:HD22	1:B:1545:LEU:HD22	1.88	0.55
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.07	0.55
1:A:2762:SER:O	1:A:2763:ARG:HB2	2.06	0.55
1:B:2386:MET:CB	1:B:2627:ARG:CD	2.77	0.55
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.71	0.55
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.72	0.55
1:B:2472:THR:CB	1:B:2524:VAL:HG22	2.37	0.55
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2320:ARG:NH1	1:A:2406:ASP:OD2	2.30	0.55
1:A:1365:PHE:CE2	1:A:1420:TYR:CE2	2.94	0.55
1:A:1922:LYS:HZ2	1:A:4004:LEU:CD1	2.18	0.55
1:A:3998:ILE:HG22	1:A:4004:LEU:HG	1.89	0.55
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	1.87	0.55
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.42	0.55
1:B:1970:LEU:HD23	1:B:1974:LYS:CE	2.35	0.55
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.71	0.55
1:B:2220:CYS:SG	2:B:5093:ATP:N1	2.79	0.55
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.06	0.55
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.39	0.55
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.87	0.55
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.90	0.55
1:B:2495:ASP:O	1:B:2498:GLY:N	2.39	0.55
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.35	0.55
1:B:1534:PHE:HD2	1:B:1537:PHE:CE1	2.25	0.55
1:B:2420:PRO:HB2	1:B:2620:ARG:HH21	1.69	0.55
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.37	0.55
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.42	0.55
1:A:1365:PHE:CD1	1:A:1365:PHE:N	2.74	0.55
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.72	0.55
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.89	0.55
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.88	0.55
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.40	0.55
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.20	0.55
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.07	0.55
1:A:2825:THR:O	1:A:2829:GLU:HG2	2.06	0.55
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.55	0.55
1:B:1970:LEU:HD23	1:B:1974:LYS:HE2	1.78	0.55
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.89	0.55
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.51	0.55
1:B:4065:LEU:HD11	1:B:4070:ILE:CD1	2.34	0.55
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.35	0.55
1:B:2891:ILE:HG21	1:B:2902:MET:HG3	1.89	0.55
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.88	0.55
1:A:2490:ASN:HB3	1:A:2546:MET:CE	2.37	0.55
1:A:1970:LEU:C	1:A:1970:LEU:HD12	2.27	0.55
1:B:1562:MET:CB	1:B:1569:ILE:HD11	2.36	0.55
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.54	0.55
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.37	0.55
1:A:2257:PHE:CD1	1:A:2262:LEU:HD11	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3945:LEU:O	1:A:3948:HIS:O	2.24	0.55
1:B:1462:ASN:HB2	1:B:1465:ILE:HG22	1.89	0.55
1:A:3460:PRO:O	1:A:3463:SER:CB	2.55	0.54
1:B:1802:LYS:NZ	4:B:5096:SO4:O4	2.40	0.54
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.88	0.54
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.72	0.54
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.42	0.54
1:B:3023:LYS:HE2	1:B:3567:LEU:CD2	2.37	0.54
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.24	0.54
1:A:3303:LYS:HD2	1:A:3306:TRP:HD1	1.66	0.54
1:B:3509:LEU:HD12	1:B:3513:VAL:HG21	1.86	0.54
1:A:1540:LEU:HD12	1:A:1548:ILE:CD1	2.37	0.54
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.37	0.54
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.60	0.54
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.72	0.54
1:A:1741:LEU:O	1:A:1742:ASP:HB2	2.07	0.54
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.72	0.54
1:A:1969:GLY:O	1:A:1972:THR:HB	2.07	0.54
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.88	0.54
1:B:2081:THR:O	1:B:2085:LYS:HB2	2.06	0.54
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.65	0.54
1:B:2424:LYS:HE2	1:B:2534:ALA:HB1	1.88	0.54
1:A:4084:SER:O	1:A:4088:LEU:HG	2.07	0.54
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.07	0.54
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.38	0.54
1:A:3797:THR:HG23	1:A:3840:LEU:HD21	1.90	0.54
1:A:2064:GLN:HE22	1:A:2091:MET:HG3	1.73	0.54
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.07	0.54
1:B:1965:HIS:HD2	1:B:2212:LEU:CD2	2.21	0.54
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.07	0.54
1:A:2448:ASP:HB2	1:A:2829:GLU:OE2	2.08	0.54
1:A:2566:SER:O	1:A:2570:ILE:HD12	2.08	0.54
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	2.95	0.54
1:B:3945:LEU:O	1:B:3948:HIS:O	2.25	0.54
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.42	0.54
1:B:1926:SER:HB3	1:B:1970:LEU:HD12	1.86	0.54
1:B:2708:ASN:O	1:B:2712:LEU:HD13	2.08	0.54
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.61	0.54
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.38	0.54
1:B:3964:ALA:HB2	1:B:3993:VAL:HG11	1.90	0.54
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2412:ARG:HH11	1:A:2412:ARG:CB	2.16	0.54
1:B:2420:PRO:CB	1:B:2620:ARG:NH2	2.71	0.54
1:B:3785:TYR:CE2	1:B:3859:VAL:HG22	2.42	0.54
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.90	0.54
1:B:2385:VAL:O	1:B:2574:TYR:HE1	1.91	0.54
1:B:2412:ARG:HH11	1:B:2412:ARG:HB2	1.73	0.54
1:B:2514:GLY:HA3	1:B:2525:THR:HA	1.90	0.53
1:B:2425:THR:HG23	1:B:2485:PHE:HE2	1.71	0.53
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.28	0.53
1:B:1965:HIS:CD2	1:B:2212:LEU:HD21	2.42	0.53
1:A:4020:ASN:HB3	1:A:4028:ARG:HH11	1.73	0.53
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.71	0.53
1:B:1769:LEU:HD11	1:B:1804:GLU:HB3	1.90	0.53
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.89	0.53
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.07	0.53
1:B:3509:LEU:HD11	1:B:3513:VAL:HG21	1.90	0.53
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.90	0.53
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.37	0.53
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.90	0.53
1:B:3612:ASP:C	1:B:3615:VAL:HG22	2.29	0.53
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.83	0.53
1:A:2336:ARG:HA	1:A:2339:ILE:HD12	1.91	0.53
1:A:2391:VAL:HG23	1:A:2426:MET:SD	2.47	0.53
1:A:2154:PHE:HD1	1:A:2154:PHE:N	2.05	0.53
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.89	0.53
1:B:2808:LEU:HD21	1:B:2856:LEU:HD12	1.91	0.53
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.44	0.53
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.24	0.53
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.44	0.53
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.09	0.53
1:A:2410:SER:O	1:A:2411:LYS:CG	2.57	0.53
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.21	0.53
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.55	0.53
1:A:2640:THR:HG23	1:A:2643:SER:H	1.74	0.53
1:B:3683:TYR:O	1:B:3687:SER:HB2	2.09	0.53
1:A:1365:PHE:CE2	1:A:1420:TYR:CZ	2.97	0.53
1:B:2467:THR:O	1:B:2471:LEU:N	2.42	0.53
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.44	0.53
1:B:1425:GLU:OE2	1:B:1429:LEU:CD1	2.57	0.53
1:A:2410:SER:O	1:A:2411:LYS:HG3	2.08	0.53
1:A:2154:PHE:CD1	1:A:2154:PHE:N	2.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.08	0.53
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.44	0.53
1:A:2424:LYS:HE2	3:A:5094:ANP:O1G	2.08	0.53
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.57	0.53
1:B:1879:ILE:HG12	1:B:1888:LEU:HB2	1.89	0.53
1:A:3965:SER:HA	1:A:3968:LEU:HD12	1.91	0.53
1:B:1759:LYS:HE3	1:B:1761:GLU:OE2	2.09	0.53
1:B:1914:LYS:HD3	1:B:3959:CYS:SG	2.48	0.53
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.70	0.53
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.20	0.53
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.30	0.53
1:A:2220:CYS:SG	1:A:2221:SER:N	2.82	0.53
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.73	0.53
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.72	0.53
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.39	0.53
1:B:2224:SER:O	2:B:5093:ATP:C2	2.53	0.53
1:A:1929:ILE:HD12	1:A:1929:ILE:H	1.74	0.53
1:B:4021:LEU:HD23	1:B:4023:ILE:HG12	1.91	0.53
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.90	0.53
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.09	0.53
1:B:2472:THR:HG21	1:B:2524:VAL:CG2	2.39	0.52
1:B:3923:VAL:CG2	1:B:4038:GLU:HA	2.37	0.52
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.09	0.52
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.57	0.52
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.09	0.52
1:B:2354:SER:OG	1:B:2357:SER:HB2	2.10	0.52
1:B:3785:TYR:HE2	1:B:3859:VAL:HG22	1.74	0.52
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.91	0.52
1:B:1963:MET:HB3	1:B:1966:TYR:CD2	2.44	0.52
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.91	0.52
1:A:2673:LEU:O	1:A:2677:VAL:HG23	2.10	0.52
1:A:1983:LEU:HD21	1:A:2000:ARG:NE	2.24	0.52
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.57	0.52
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.70	0.52
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.44	0.52
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.39	0.52
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	1.92	0.52
1:A:2780:LYS:HD3	1:A:2813:THR:HG22	1.92	0.52
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.09	0.52
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.90	0.52
1:B:3632:LEU:HD13	1:B:3644:ILE:HD13	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.91	0.52
1:B:2458:LEU:HD11	1:B:2484:LEU:HD11	1.91	0.52
1:B:3737:THR:CB	1:B:3740:THR:CB	2.87	0.52
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.39	0.52
1:A:1535:PRO:O	1:A:1841:ILE:CD1	2.58	0.52
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ1	1.75	0.52
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.89	0.52
1:B:2476:LYS:CD	1:B:2476:LYS:H	2.23	0.52
1:B:1502:ILE:HG23	1:B:1503:PRO:HD2	1.91	0.52
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.45	0.52
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.10	0.52
1:B:3460:PRO:O	1:B:3463:SER:CB	2.58	0.52
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.31	0.52
1:B:1844:TRP:CD1	1:B:1893:ALA:HB3	2.44	0.52
1:B:2111:LYS:CD	1:B:2161:GLU:CG	2.82	0.52
1:A:2494:LEU:O	1:A:2494:LEU:HD12	2.10	0.52
1:A:1870:ASN:O	1:A:1874:VAL:HG23	2.09	0.52
1:A:1559:SER:HB3	1:A:1572:ILE:CG2	2.40	0.52
1:A:3631:MET:HE3	1:A:3698:MET:HG3	1.91	0.52
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.44	0.52
1:A:2834:LEU:HD21	1:A:2885:LEU:HD21	1.92	0.52
1:B:3618:TYR:O	1:B:3622:GLY:N	2.38	0.52
1:A:1531:ARG:HD3	1:A:1537:PHE:O	2.10	0.52
1:A:2181:GLY:O	1:A:2182:GLU:CG	2.56	0.52
1:A:65:THR:O	1:A:66:GLN:CB	2.57	0.52
1:B:1826:PHE:CE1	1:B:1853:LEU:HD22	2.45	0.51
1:B:2220:CYS:HB2	2:B:5093:ATP:C6	2.45	0.51
1:B:3810:SER:HB3	1:B:3837:GLY:HA2	1.92	0.51
1:A:3566:LEU:CD2	1:A:3587:LEU:HD11	2.41	0.51
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	2.99	0.51
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	2.98	0.51
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.39	0.51
1:B:2867:LEU:HB3	1:B:2872:GLU:HB3	1.92	0.51
1:A:2580:LYS:HG2	1:A:2586:ARG:HH22	1.74	0.51
1:A:2849:TYR:O	1:A:2853:LEU:HB2	2.11	0.51
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.43	0.51
1:B:1563:LYS:HE2	1:B:1585:VAL:HG12	1.91	0.51
1:B:2428:MET:HE2	1:B:2485:PHE:HD1	1.74	0.51
1:B:2428:MET:HE2	1:B:2485:PHE:CD1	2.45	0.51
1:A:1992:LYS:HG2	1:A:2024:SER:CB	2.38	0.51
1:B:3939:ILE:HG23	1:B:3950:PHE:HE2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.10	0.51
1:B:65:THR:O	1:B:66:GLN:CB	2.58	0.51
1:B:2470:GLY:CA	1:B:2473:LEU:HD21	2.20	0.51
1:B:2425:THR:HG23	1:B:2485:PHE:CE2	2.45	0.51
1:B:1968:PHE:N	1:B:1968:PHE:HD1	2.08	0.51
1:B:2154:PHE:CD1	1:B:2154:PHE:N	2.78	0.51
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.93	0.51
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.92	0.51
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.38	0.51
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.25	0.51
1:B:1826:PHE:HE1	1:B:1853:LEU:HD22	1.76	0.51
1:B:2084:TRP:CZ3	1:B:2085:LYS:HG3	2.45	0.51
1:B:3509:LEU:CD1	1:B:3513:VAL:CG2	2.83	0.51
1:A:2385:VAL:O	1:A:2574:TYR:HE1	1.93	0.51
1:A:2655:ILE:HD11	1:A:2747:ARG:HH22	1.76	0.51
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.91	0.51
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.46	0.51
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.41	0.51
1:B:3737:THR:CB	1:B:3740:THR:HB	2.41	0.51
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.91	0.51
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.40	0.51
1:A:3737:THR:CB	1:A:3740:THR:CB	2.88	0.51
1:B:1540:LEU:HD11	1:B:1561:PHE:HB3	1.93	0.51
1:B:3353:LEU:HD23	1:B:3358:VAL:CG1	2.41	0.51
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.76	0.51
1:B:2368:PHE:N	1:B:2368:PHE:CD1	2.77	0.51
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.11	0.51
1:B:2620:ARG:NH1	1:B:2910:ASN:ND2	2.58	0.51
1:B:2382:ALA:O	1:B:2385:VAL:HG12	2.11	0.51
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.51
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.43	0.51
1:B:1744:LEU:CD2	1:B:1760:PHE:CD2	2.94	0.51
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.76	0.51
1:B:3023:LYS:CE	1:B:3567:LEU:HD23	2.41	0.51
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.91	0.51
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.44	0.51
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD13	2.46	0.51
1:B:2472:THR:HB	1:B:2524:VAL:HG22	1.92	0.51
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.46	0.51
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.46	0.51
1:B:1462:ASN:CB	1:B:1465:ILE:HG22	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	2.94	0.50
1:A:3569:GLU:O	1:A:3573:SER:OG	2.22	0.50
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.46	0.50
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.30	0.50
1:B:1929:ILE:HD12	1:B:1929:ILE:H	1.75	0.50
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.11	0.50
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.59	0.50
1:B:2312:ASP:HB3	1:B:2351:GLN:HG3	1.93	0.50
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.32	0.50
1:A:1749:ILE:O	1:A:1755:LEU:HA	2.12	0.50
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.69	0.50
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.59	0.50
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.41	0.50
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	2.95	0.50
1:A:3757:ILE:HD11	1:A:4074:GLU:HG2	1.91	0.50
1:A:1714:GLN:HB3	1:A:1727:LEU:HD11	1.92	0.50
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.93	0.50
1:B:2220:CYS:SG	1:B:2224:SER:HB3	2.51	0.50
1:B:1968:PHE:CD1	1:B:1968:PHE:N	2.79	0.50
1:B:1939:PHE:HD1	1:B:1939:PHE:H	1.58	0.50
1:A:1534:PHE:CE2	1:A:1536:ARG:HB2	2.47	0.50
1:A:2048:SER:H	2:A:5093:ATP:N6	2.08	0.50
1:A:2410:SER:O	1:A:2411:LYS:CB	2.57	0.50
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.25	0.50
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.27	0.50
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.41	0.50
1:A:2514:GLY:HA3	1:A:2525:THR:HA	1.93	0.50
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.25	0.50
1:A:1822:CYS:SG	1:A:1850:PHE:CA	2.97	0.50
1:A:162:LEU:HA	1:A:165:ASP:O	2.11	0.50
1:A:1622:GLN:HE22	1:A:1644:ILE:H	1.59	0.50
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.12	0.50
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.35	0.50
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.12	0.50
1:A:2201:HIS:CE1	1:A:2497:TYR:HB3	2.47	0.50
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	1.94	0.50
1:B:2833:THR:HG21	1:B:2841:PRO:HD2	1.94	0.50
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.93	0.50
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.93	0.50
1:B:4006:VAL:HA	1:B:4009:LYS:HG2	1.93	0.50
1:A:1646:GLN:NE2	1:A:1758:TYR:OH	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2620:ARG:HH12	1:B:2910:ASN:ND2	2.10	0.49
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.94	0.49
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.93	0.49
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.11	0.49
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.25	0.49
1:B:1926:SER:CA	1:B:1970:LEU:HD12	2.42	0.49
1:B:1425:GLU:OE2	1:B:1429:LEU:HD11	2.13	0.49
1:B:1822:CYS:HB2	1:B:1853:LEU:CD2	2.29	0.49
1:B:1536:ARG:HE	1:B:1841:ILE:HD13	1.77	0.49
1:A:2003:LEU:HD23	1:A:2006:LEU:HD12	1.93	0.49
1:A:3848:LEU:CD2	1:A:3852:LYS:HE3	2.41	0.49
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.25	0.49
1:A:2492:PRO:HB2	1:A:2502:VAL:HG11	1.93	0.49
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.47	0.49
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.93	0.49
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.12	0.49
1:A:3737:THR:CB	1:A:3740:THR:HB	2.43	0.49
1:A:2249:LEU:HD21	1:A:2302:PHE:HD2	1.77	0.49
1:B:3979:ASN:O	1:B:3981:PRO:HD2	2.11	0.49
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.27	0.49
1:B:1983:LEU:HD11	1:B:2000:ARG:HH21	1.76	0.49
1:B:3461:ILE:C	1:B:3463:SER:H	2.15	0.49
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.42	0.49
1:A:2563:SER:C	1:A:2565:LYS:H	2.15	0.49
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.12	0.49
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.12	0.49
1:B:2908:LEU:O	1:B:2912:CYS:HB2	2.12	0.49
1:B:1535:PRO:O	1:B:1841:ILE:HD11	2.13	0.49
1:B:2421:GLY:C	3:B:5094:ANP:O1B	2.51	0.49
1:B:4059:LEU:HA	1:B:4063:LEU:HD13	1.93	0.49
1:B:2640:THR:HG23	1:B:2643:SER:H	1.77	0.49
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.33	0.49
1:B:2380:LEU:HD11	1:B:2577:ALA:HB2	1.88	0.49
1:B:2620:ARG:NH1	1:B:2910:ASN:CG	2.65	0.49
1:A:2941:THR:HG22	1:A:2942:ASP:N	2.24	0.49
1:A:2853:LEU:HD21	1:A:2870:GLU:HG3	1.94	0.49
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.48	0.49
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.12	0.49
1:B:2835:LEU:HD23	1:B:2911:ARG:HB2	1.95	0.49
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	1.95	0.49
1:B:4084:SER:O	1:B:4088:LEU:HG	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2936:ILE:HG22	1:A:2962:ARG:HD3	1.95	0.49
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.94	0.49
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	2.47	0.49
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.94	0.49
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.78	0.49
1:A:2080:LYS:O	1:A:2084:TRP:CD1	2.65	0.49
1:A:3461:ILE:C	1:A:3463:SER:H	2.15	0.49
1:B:2154:PHE:N	1:B:2154:PHE:HD1	2.10	0.49
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	1.95	0.49
1:B:2136:ARG:O	1:B:2140:ASP:O	2.30	0.49
1:A:2988:SER:CB	1:A:2989:PRO:CD	2.66	0.49
1:A:2833:THR:HG21	1:A:2841:PRO:HD2	1.94	0.49
1:B:162:LEU:HA	1:B:165:ASP:O	2.12	0.49
1:A:3693:LYS:HE3	1:A:4080:GLU:HB3	1.94	0.49
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.95	0.49
1:B:1375:LYS:HE3	1:B:1431:LEU:HD13	1.94	0.49
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.95	0.49
1:B:1801:GLY:N	4:B:5096:SO4:O4	2.46	0.48
1:A:2152:VAL:HG12	1:A:2154:PHE:CE1	2.39	0.48
1:A:2407:LEU:HB2	1:A:2414:ILE:HD11	1.94	0.48
1:B:2339:ILE:HG23	1:B:2353:LEU:HB3	1.94	0.48
1:A:2878:VAL:HA	1:A:2881:ILE:HD12	1.95	0.48
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.42	0.48
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.94	0.48
1:A:1630:ILE:HA	1:A:1634:THR:HG22	1.95	0.48
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.95	0.48
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.13	0.48
1:B:1802:LYS:NZ	4:B:5096:SO4:S	2.86	0.48
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.94	0.48
1:B:3848:LEU:HD21	1:B:3852:LYS:HE3	1.95	0.48
1:A:2226:ILE:HG23	1:A:2288:VAL:HG21	1.95	0.48
1:B:2441:VAL:HB	1:B:2484:LEU:HD23	1.95	0.48
1:A:2856:LEU:HD23	1:A:2873:LEU:HB3	1.95	0.48
1:A:2305:LEU:HD11	1:A:2368:PHE:CG	2.48	0.48
1:B:2046:GLY:O	1:B:2228:HIS:HB2	2.13	0.48
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.94	0.48
1:B:1926:SER:HA	1:B:1970:LEU:HD12	1.94	0.48
1:A:2109:LEU:CD1	1:A:2129:LEU:CD2	2.92	0.48
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.94	0.48
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.14	0.48
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2122:THR:O	1:B:2123:LEU:C	2.52	0.48
1:A:2822:ILE:O	1:A:2822:ILE:HG13	2.14	0.48
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.79	0.48
1:B:3023:LYS:NZ	1:B:3571:ASN:HD21	2.11	0.48
1:A:1645:PHE:CB	1:A:1765:ILE:HG21	2.41	0.48
1:B:2623:THR:CB	3:B:5094:ANP:O2'	2.61	0.48
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.13	0.48
1:B:2100:VAL:HG12	1:B:2102:TYR:CE2	2.48	0.48
1:A:2175:ILE:HG13	1:A:2184:LEU:C	2.34	0.48
1:B:2833:THR:CG2	1:B:2841:PRO:HD2	2.43	0.48
1:B:2473:LEU:CD2	1:B:2525:THR:HB	2.43	0.48
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.47	0.48
1:A:1826:PHE:O	1:A:1826:PHE:CD1	2.67	0.48
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.13	0.48
1:B:3406:PHE:CZ	1:B:3505:ILE:HG21	2.49	0.48
1:B:2102:TYR:HB2	1:B:2152:VAL:HG22	1.95	0.48
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.96	0.48
1:B:1493:LEU:HD23	1:B:1498:GLU:HB2	1.94	0.48
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.96	0.48
1:A:2314:ILE:HG22	1:A:2318:ILE:HD12	1.96	0.48
1:A:2387:ARG:O	1:A:2390:ILE:HG22	2.13	0.48
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.73	0.48
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.86	0.48
1:B:2755:HIS:CE1	1:B:2835:LEU:HG	2.49	0.48
1:A:2425:THR:OG1	3:A:5094:ANP:O2A	2.31	0.48
1:B:2780:LYS:HB3	1:B:2813:THR:HG22	1.94	0.48
1:B:2290:LEU:HD23	1:B:2321:SER:HA	1.96	0.48
1:B:3348:ILE:HA	1:B:3351:ARG:HG2	1.95	0.48
1:B:1604:ALA:HA	1:B:1607:TRP:HE1	1.75	0.48
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.96	0.48
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.41	0.48
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.81	0.48
1:B:2106:THR:HG1	1:B:2154:PHE:HD2	1.61	0.48
1:B:4022:GLN:HG2	1:B:4022:GLN:O	2.14	0.48
1:B:23:LEU:O	1:B:25:GLU:N	2.47	0.48
1:B:3566:LEU:HD13	1:B:3570:LEU:HD12	1.96	0.47
1:B:2305:LEU:HB3	1:B:2310:LEU:HD12	1.95	0.47
1:B:1803:THR:HG21	1:B:1848:ASP:CG	2.34	0.47
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.96	0.47
1:A:2294:LEU:HB3	1:A:2317:LEU:HD22	1.94	0.47
1:A:1649:LEU:HD13	1:A:1704:GLU:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.54	0.47
1:A:1534:PHE:CD2	1:A:1537:PHE:CE1	3.02	0.47
1:A:1466:GLN:HB3	1:A:1473:THR:HG21	1.95	0.47
1:B:3671:VAL:HA	1:B:3674:ILE:HG22	1.95	0.47
1:A:2354:SER:OG	1:A:2357:SER:CB	2.62	0.47
1:A:2582:VAL:O	1:A:2582:VAL:HG23	2.14	0.47
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.45	0.47
1:B:3978:ASN:O	1:B:3981:PRO:HD2	2.14	0.47
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.14	0.47
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.96	0.47
1:A:1421:TYR:CD2	1:A:1425:GLU:CG	2.97	0.47
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.95	0.47
1:B:2563:SER:CB	1:B:2566:SER:H	2.16	0.47
1:B:2420:PRO:HD3	1:B:2536:ASN:ND2	2.25	0.47
1:A:3812:LYS:HB2	1:A:3839:ILE:HD12	1.97	0.47
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	1.96	0.47
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	1.96	0.47
1:A:3911:TRP:HH2	1:A:3926:VAL:HG13	1.79	0.47
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.14	0.47
1:A:3728:GLU:HG3	1:A:4079:LYS:HE2	1.95	0.47
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.62	0.47
1:B:40:TRP:O	1:B:44:LYS:N	2.48	0.47
1:A:3443:ALA:HB1	1:A:3450:VAL:HG21	1.96	0.47
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.97	0.47
1:A:1495:THR:CG2	1:A:1497:ILE:HG22	2.41	0.47
1:A:1527:LEU:HD21	1:A:1546:LEU:HD23	1.96	0.47
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.95	0.47
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.44	0.47
1:B:2760:GLY:O	1:B:2761:ALA:HB3	2.14	0.47
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.62	0.47
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.15	0.47
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.96	0.47
1:A:2463:ASN:O	1:A:2475:PRO:HD2	2.15	0.47
1:B:2282:ASN:HB3	1:B:2552:ARG:HG3	1.97	0.47
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.14	0.47
1:A:1365:PHE:HE2	1:A:1420:TYR:CZ	2.33	0.47
1:B:1387:GLU:HA	1:B:1393:LYS:HA	1.97	0.47
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.15	0.47
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.15	0.47
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.49	0.47
1:A:2122:THR:O	1:A:2123:LEU:C	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.15	0.47
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.79	0.47
1:A:1822:CYS:SG	1:A:1849:GLU:C	2.93	0.47
1:B:2061:TYR:O	1:B:2064:GLN:HG2	2.14	0.47
1:A:2839:ASP:HB3	1:A:2878:VAL:HG22	1.97	0.47
1:B:2967:ASN:HB3	1:B:3356:PHE:CE2	2.49	0.47
1:B:2785:LYS:HD3	1:B:3482:GLY:O	2.15	0.47
1:B:2472:THR:CG2	1:B:2524:VAL:CG2	2.86	0.47
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.15	0.47
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.29	0.47
1:A:3466:ILE:HD13	1:A:3509:LEU:HD13	1.97	0.47
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.96	0.47
1:A:2761:ALA:O	1:A:2892:CYS:HB3	2.15	0.47
1:A:2422:SER:N	3:A:5094:ANP:O1B	2.47	0.47
1:B:4020:ASN:ND2	1:B:4028:ARG:HD3	2.30	0.47
1:A:1750:SER:HA	1:A:1755:LEU:HD23	1.96	0.47
1:A:3307:LEU:HA	1:A:3310:THR:HB	1.97	0.47
1:B:2276:LEU:CD2	1:B:2415:ILE:HG21	2.45	0.47
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.98	0.46
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.94	0.46
1:A:2757:MET:HE3	1:A:2912:CYS:CB	2.38	0.46
1:A:3844:ILE:HG12	1:A:3851:VAL:HG21	1.96	0.46
1:B:2441:VAL:HG21	1:B:2482:LEU:HD21	1.96	0.46
1:B:2758:LEU:HD23	1:B:2915:ASN:HB3	1.96	0.46
1:B:2155:ASP:O	1:B:2549:ARG:NH1	2.46	0.46
1:B:3307:LEU:HA	1:B:3310:THR:HB	1.97	0.46
1:B:1656:TRP:HE1	1:B:1712:ILE:HD11	1.81	0.46
1:B:2318:ILE:O	1:B:2322:LEU:HB2	2.14	0.46
1:A:3632:LEU:HD13	1:A:3644:ILE:HD13	1.96	0.46
1:A:2178:LEU:HD12	1:A:2182:GLU:HB2	1.97	0.46
1:B:2354:SER:OG	1:B:2357:SER:CB	2.63	0.46
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.97	0.46
1:A:2758:LEU:HD23	1:A:2915:ASN:HB3	1.96	0.46
1:A:2516:TRP:CZ3	1:A:2523:TRP:HB2	2.51	0.46
1:B:2938:MET:SD	1:B:3321:ILE:HG21	2.55	0.46
1:A:1592:LEU:CD1	1:A:1596:ILE:HD12	2.45	0.46
1:B:2860:THR:HG22	1:B:2865:LEU:O	2.15	0.46
1:B:2464:TYR:CE1	1:B:2524:VAL:HG11	2.49	0.46
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.63	0.46
1:B:3372:THR:HG23	1:B:3375:GLU:HB2	1.97	0.46
1:B:1636:ILE:O	1:B:1640:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1871:GLY:HA3	1:A:1879:ILE:HG21	1.98	0.46
1:B:2220:CYS:HG	1:B:2224:SER:HB3	1.80	0.46
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.51	0.46
1:A:1527:LEU:HD21	1:A:1546:LEU:CD2	2.45	0.46
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.84	0.46
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.15	0.46
1:B:2761:ALA:O	1:B:2892:CYS:SG	2.73	0.46
1:B:1593:ASN:HD21	1:B:1621:THR:CB	2.29	0.46
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.16	0.46
1:A:1479:LEU:HD11	1:A:1515:SER:HB3	1.97	0.46
1:A:3869:GLU:O	1:A:3870:LYS:C	2.54	0.46
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.96	0.46
1:B:1367:ILE:HD12	1:B:1367:ILE:H	1.80	0.46
1:B:2137:VAL:O	1:B:2141:ILE:HG23	2.16	0.46
1:A:1744:LEU:HA	1:A:1760:PHE:HE2	1.75	0.46
1:B:1983:LEU:HD13	1:B:2000:ARG:HE	1.80	0.46
1:A:3461:ILE:C	1:A:3463:SER:N	2.67	0.46
1:A:1540:LEU:HD11	1:A:1561:PHE:HB3	1.97	0.46
1:B:1612:ASP:HA	1:B:1615:ILE:CG1	2.46	0.46
1:A:3911:TRP:CH2	1:A:3926:VAL:HG13	2.50	0.46
1:A:2061:TYR:CD1	1:A:2091:MET:HE3	2.47	0.46
1:B:2493:LYS:HG3	1:B:2494:LEU:N	2.30	0.46
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.43	0.46
1:B:1421:TYR:O	1:B:1425:GLU:CA	2.63	0.46
1:B:2112:GLU:HB3	1:B:2117:SER:OG	2.14	0.46
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD3	1.81	0.46
1:B:2464:TYR:HE1	1:B:2524:VAL:HG11	1.80	0.46
1:A:3470:PHE:CE1	1:A:3488:VAL:HG21	2.51	0.46
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.97	0.46
1:A:2084:TRP:CH2	1:A:2153:VAL:HG21	2.50	0.46
1:B:1681:LYS:HE2	1:B:1939:PHE:CZ	2.51	0.46
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.45	0.46
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	1.98	0.46
1:B:1514:ASP:O	1:B:1518:MET:HG2	2.15	0.46
1:B:3869:GLU:O	1:B:3870:LYS:C	2.52	0.46
1:B:1620:PHE:HB2	1:B:1760:PHE:CZ	2.50	0.46
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.46	0.46
1:B:2563:SER:C	1:B:2565:LYS:H	2.18	0.46
1:A:3473:ALA:HB3	1:A:3476:ARG:HG3	1.97	0.46
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	3.01	0.46
1:A:1802:LYS:NZ	4:A:5095:SO4:O1	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.97	0.46
1:B:4017:GLY:HA3	1:B:4021:LEU:HD12	1.97	0.46
1:A:2305:LEU:CD1	1:A:2368:PHE:CD1	2.98	0.46
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.97	0.46
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.15	0.46
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.98	0.46
1:B:3889:LEU:HG	1:B:3894:ARG:HD3	1.97	0.46
1:B:1969:GLY:O	1:B:1972:THR:HB	2.15	0.46
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.94	0.46
1:B:1956:LEU:CB	1:B:1968:PHE:CE2	2.90	0.46
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.45	0.46
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.16	0.46
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.97	0.46
1:A:215:PRO:C	1:A:3475:ASN:ND2	2.69	0.45
1:B:2488:GLU:CG	1:B:2491:LEU:HD12	2.45	0.45
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.56	0.45
1:A:1802:LYS:O	1:A:1806:VAL:HG23	2.16	0.45
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.64	0.45
1:A:1529:ARG:O	1:A:1533:GLN:HG2	2.16	0.45
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	1.98	0.45
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.96	0.45
1:B:2380:LEU:HD12	1:B:2577:ALA:HB2	1.85	0.45
1:B:2420:PRO:CB	1:B:2620:ARG:HH21	2.29	0.45
1:B:1392:LEU:HD22	1:B:1393:LYS:H	1.82	0.45
1:B:2109:LEU:HD13	1:B:2129:LEU:HD23	1.97	0.45
1:B:1813:LEU:HD12	1:B:1844:TRP:CH2	2.50	0.45
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.98	0.45
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.15	0.45
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.98	0.45
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.80	0.45
1:A:3322:GLY:HA2	1:A:3325:ILE:HD12	1.98	0.45
1:B:3338:ASN:HD22	1:B:3341:GLU:HG2	1.81	0.45
1:A:1365:PHE:CZ	1:A:1420:TYR:CG	3.05	0.45
1:A:2563:SER:CB	1:A:2566:SER:H	2.19	0.45
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.98	0.45
1:B:3538:ASN:HB3	1:B:3541:MET:HG2	1.98	0.45
1:A:2490:ASN:HB3	1:A:2546:MET:HE1	1.98	0.45
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.56	0.45
1:A:1365:PHE:HZ	1:A:1420:TYR:CE1	2.31	0.45
1:B:2471:LEU:O	1:B:2473:LEU:HG	2.16	0.45
1:A:2081:THR:HG22	1:A:2085:LYS:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1563:LYS:HA	1:A:1569:ILE:O	2.17	0.45
1:A:1563:LYS:HE2	1:A:1585:VAL:HG12	1.98	0.45
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.49	0.45
1:A:3592:LYS:O	1:A:3596:ASN:N	2.49	0.45
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.16	0.45
1:A:3832:SER:O	1:A:3836:GLY:N	2.43	0.45
1:B:3965:SER:HA	1:B:3968:LEU:HD12	1.98	0.45
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.17	0.45
1:B:2494:LEU:HD12	1:B:2494:LEU:O	2.17	0.45
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.99	0.45
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.50	0.45
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.97	0.45
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	1.99	0.45
1:B:2201:HIS:CE1	1:B:2497:TYR:HB3	2.52	0.45
1:A:3926:VAL:HG11	1:A:4042:ARG:HG2	1.97	0.45
1:B:2839:ASP:O	1:B:2841:PRO:HD3	2.17	0.45
1:A:3342:ARG:NH2	1:A:3393:ASN:OD1	2.47	0.45
1:A:23:LEU:O	1:A:25:GLU:N	2.50	0.45
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.32	0.45
1:B:3461:ILE:C	1:B:3463:SER:N	2.68	0.45
1:B:1940:GLU:CG	1:B:1941:ASP:H	2.18	0.45
1:A:2412:ARG:HD3	1:A:2555:ALA:HB2	1.99	0.45
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.37	0.45
1:B:1495:THR:HB	1:B:1498:GLU:CG	2.47	0.45
1:A:1919:PHE:CD1	1:A:3996:GLY:HA2	2.51	0.45
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.57	0.45
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.98	0.45
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.22	0.45
1:B:3946:VAL:HB	1:B:3947:PRO:HA	1.98	0.45
1:B:1531:ARG:CD	1:B:1538:TYR:HA	2.47	0.45
1:B:1383:TYR:CE2	1:B:1401:LEU:HD13	2.52	0.45
1:A:1934:LEU:HD22	1:A:1945:LEU:HD12	1.98	0.45
1:B:2386:MET:HB3	1:B:2627:ARG:CD	2.45	0.45
1:B:2225:LYS:HG3	2:B:5093:ATP:H1'	1.99	0.45
1:A:3509:LEU:CG	1:A:3513:VAL:HG21	2.46	0.45
1:A:2755:HIS:O	1:A:2913:ILE:N	2.48	0.45
1:A:1984:ILE:CG2	1:A:1989:GLU:HG3	2.46	0.45
1:B:2474:LEU:HB3	1:B:2526:ILE:HG22	1.99	0.45
1:A:3994:TYR:O	1:A:3998:ILE:HD12	2.16	0.45
1:A:3628:ILE:HG22	1:A:3649:PHE:HE2	1.82	0.45
1:A:4022:GLN:O	1:A:4023:ILE:C	2.56	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.98	0.45
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.82	0.45
1:B:2354:SER:H	1:B:2357:SER:HB2	1.81	0.45
1:A:1750:SER:HB2	1:A:1755:LEU:CD2	2.47	0.45
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.17	0.45
1:B:2155:ASP:OD1	1:B:2195:GLU:OE2	2.34	0.45
1:A:3903:ILE:O	1:A:3907:VAL:HG23	2.17	0.45
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.52	0.45
1:A:1998:LEU:HD11	1:A:2022:PHE:HZ	1.82	0.45
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.82	0.45
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.46	0.45
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.52	0.45
1:A:1469:LEU:HD13	1:A:1523:LEU:HD21	1.99	0.45
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.52	0.45
1:A:1365:PHE:CE2	1:A:1420:TYR:CD2	3.04	0.45
1:A:1970:LEU:HD12	1:A:1971:ARG:CA	2.47	0.45
1:B:2447:LYS:HE3	1:B:2493:LYS:HD3	1.98	0.45
1:B:2755:HIS:HD2	1:B:2911:ARG:HB3	1.82	0.45
1:B:2508:GLN:HG2	1:B:2512:LYS:HG3	1.97	0.45
1:B:2104:ILE:O	1:B:2154:PHE:HA	2.16	0.45
1:B:2203:THR:HG23	1:B:2204:PRO:HD2	1.99	0.45
1:A:3330:TYR:CE1	1:A:3334:PHE:CE2	3.04	0.45
1:B:2294:LEU:HB3	1:B:2317:LEU:HD22	1.98	0.45
1:B:2047:PHE:CE2	1:B:2082:ALA:HB1	2.52	0.45
1:B:3862:THR:HB	1:B:3865:ALA:HB2	1.99	0.45
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	1.99	0.45
1:B:1421:TYR:CD2	1:B:1425:GLU:CG	2.98	0.44
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.82	0.44
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.51	0.44
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.50	0.44
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.81	0.44
1:A:2745:ILE:HG12	1:A:2756:MET:CE	2.42	0.44
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	1.99	0.44
1:A:2424:LYS:HA	1:A:2559:LEU:HD12	1.99	0.44
1:A:1527:LEU:HD22	1:A:1545:LEU:HD22	1.97	0.44
1:B:1612:ASP:CA	1:B:1615:ILE:HG12	2.47	0.44
1:B:2109:LEU:HB3	1:B:2113:SER:HB2	2.00	0.44
1:B:3845:GLN:NE2	1:B:3882:ASP:O	2.50	0.44
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.29	0.44
1:B:3481:ILE:O	1:B:3483:ASP:N	2.46	0.44
1:A:3372:THR:HG23	1:A:3375:GLU:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1995:VAL:HG22	1:B:2022:PHE:CD2	2.52	0.44
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.51	0.44
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.87	0.44
1:A:2356:TYR:CE1	1:A:2399:LYS:HD2	2.52	0.44
1:A:3968:LEU:HA	1:A:3971:VAL:HG12	2.00	0.44
1:B:3010:LEU:HD22	1:B:3320:LEU:HD12	1.99	0.44
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.99	0.44
1:A:1849:GLU:CD	1:A:1899:ASN:HD22	2.20	0.44
1:A:1536:ARG:HD3	1:A:1841:ILE:CD1	2.47	0.44
1:A:1392:LEU:CD1	1:A:1392:LEU:C	2.83	0.44
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.32	0.44
1:A:3671:VAL:HA	1:A:3674:ILE:CG2	2.46	0.44
1:A:1982:PRO:O	1:A:1985:SER:HB2	2.18	0.44
1:B:3636:GLY:CA	1:B:3642:TYR:O	2.66	0.44
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.17	0.44
1:B:3998:ILE:HG22	1:B:4004:LEU:HG	1.97	0.44
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.17	0.44
1:B:1779:PHE:O	1:B:1783:THR:HG22	2.18	0.44
1:B:1715:LEU:HG	1:B:1727:LEU:HD22	2.00	0.44
1:B:2421:GLY:CA	3:B:5094:ANP:O1B	2.66	0.44
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.53	0.44
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	2.00	0.44
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.32	0.44
1:A:2423:GLY:N	3:A:5094:ANP:O1B	2.39	0.44
1:A:1706:LEU:HD21	1:A:1935:GLN:CG	2.47	0.44
1:A:2838:ALA:HB3	1:A:2878:VAL:HG13	2.00	0.44
1:A:3798:PHE:HA	1:A:3801:ILE:HG12	2.00	0.44
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.82	0.44
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.17	0.44
1:B:1385:VAL:HG21	1:B:1491:PHE:CD1	2.53	0.44
1:A:1983:LEU:HB3	1:A:1993:THR:HG23	2.00	0.44
1:B:2755:HIS:HB3	1:B:2912:CYS:SG	2.58	0.44
1:A:3473:ALA:CB	1:A:3476:ARG:HG3	2.48	0.44
1:A:2127:ASP:HB3	1:A:2132:SER:HB3	2.00	0.44
1:B:2572:GLU:CG	1:B:2590:GLU:HG3	2.47	0.44
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.71	0.44
1:A:3930:PHE:HE2	1:A:4029:ILE:CD1	2.31	0.44
1:A:1646:GLN:OE1	1:A:1763:ILE:HG12	2.18	0.44
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.18	0.44
1:B:2389:ASP:HB3	1:B:2433:ARG:HH11	1.83	0.44
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	2.00	0.43
1:A:2941:THR:CG2	1:A:2942:ASP:H	2.25	0.43
1:B:1495:THR:CG2	1:B:1497:ILE:HG22	2.48	0.43
1:B:3911:TRP:CH2	1:B:3926:VAL:CG1	3.01	0.43
1:B:4020:ASN:HB3	1:B:4028:ARG:NH1	2.33	0.43
1:A:4045:LEU:O	1:A:4048:ILE:HG22	2.18	0.43
1:A:2383:HIS:CE1	1:A:2384:GLU:HG3	2.53	0.43
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.18	0.43
1:A:1744:LEU:HD22	1:A:1760:PHE:CD2	2.53	0.43
1:A:2565:LYS:O	1:A:2569:GLN:HG3	2.19	0.43
1:A:3845:GLN:NE2	1:A:3882:ASP:O	2.51	0.43
1:A:2201:HIS:CE1	1:A:2497:TYR:O	2.71	0.43
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.33	0.43
1:B:2984:VAL:C	1:B:2986:PRO:HD3	2.39	0.43
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.52	0.43
1:A:2099:ASN:HB3	1:A:2151:TRP:HE1	1.83	0.43
1:A:2760:GLY:O	1:A:2761:ALA:HB3	2.18	0.43
1:B:3848:LEU:O	1:B:3849:SER:C	2.57	0.43
1:B:1540:LEU:HA	1:B:1540:LEU:HD23	1.72	0.43
1:A:2203:THR:HG23	1:A:2204:PRO:HD2	1.99	0.43
1:B:3592:LYS:O	1:B:3596:ASN:N	2.51	0.43
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.17	0.43
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.83	0.43
1:A:3471:ASN:HB2	1:A:3478:THR:HG23	2.00	0.43
1:B:3832:SER:O	1:B:3836:GLY:N	2.46	0.43
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.18	0.43
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.31	0.43
1:B:1535:PRO:O	1:B:1841:ILE:CD1	2.65	0.43
1:A:1536:ARG:CD	1:A:1841:ILE:HD13	2.48	0.43
1:B:2152:VAL:HG12	1:B:2154:PHE:HE1	1.83	0.43
1:A:2104:ILE:O	1:A:2154:PHE:HA	2.18	0.43
1:B:3886:ALA:N	1:B:3887:PRO:CD	2.78	0.43
1:B:2201:HIS:CE1	1:B:2497:TYR:CA	3.01	0.43
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.83	0.43
1:A:4034:LEU:O	1:A:4036:GLN:HG3	2.19	0.43
1:A:1421:TYR:O	1:A:1425:GLU:CA	2.65	0.43
1:A:1934:LEU:HD13	1:A:1945:LEU:HB2	2.01	0.43
1:B:4065:LEU:HD12	1:B:4065:LEU:C	2.39	0.43
1:A:3800:LEU:HA	1:A:3803:LEU:HD12	1.99	0.43
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.19	0.43
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1794:PHE:HB3	1:B:1919:PHE:HB3	2.01	0.43
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.83	0.43
1:B:1826:PHE:O	1:B:1826:PHE:CG	2.71	0.43
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	2.00	0.43
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.49	0.43
1:B:2517:LYS:HD2	1:B:2524:VAL:CG2	2.49	0.43
1:B:3462:ILE:O	1:B:3465:LEU:N	2.51	0.43
1:B:2425:THR:CG2	1:B:2485:PHE:HE2	2.32	0.43
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.65	0.43
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.99	0.43
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.54	0.43
1:A:4021:LEU:CD2	1:A:4023:ILE:HG12	2.49	0.43
1:B:2761:ALA:O	1:B:2892:CYS:HB3	2.19	0.43
1:A:1872:LEU:HG	1:A:1888:LEU:HD21	2.00	0.43
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	2.01	0.43
1:A:1835:LEU:O	1:A:1838:ILE:HG22	2.18	0.43
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.18	0.43
1:B:2220:CYS:SG	1:B:2221:SER:N	2.92	0.43
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	2.01	0.43
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ3	1.81	0.43
1:B:2510:MET:O	1:B:2513:GLN:NE2	2.52	0.43
1:A:2252:LEU:HD22	1:A:2314:ILE:HG13	2.01	0.43
1:B:3930:PHE:CE2	1:B:4029:ILE:HD13	2.51	0.43
1:A:3788:MET:HG3	1:A:3788:MET:O	2.19	0.43
1:A:2141:ILE:HG22	1:A:2145:PHE:CG	2.54	0.43
1:B:3505:ILE:O	1:B:3510:ARG:NH1	2.52	0.43
1:B:2152:VAL:HG12	1:B:2154:PHE:CE1	2.54	0.43
1:A:1953:LEU:HA	1:A:1956:LEU:HD12	2.01	0.43
1:B:2446:SER:H	1:B:2449:THR:HG21	1.80	0.43
1:A:1794:PHE:CD1	1:A:1802:LYS:HB3	2.51	0.43
1:B:2129:LEU:O	1:B:2133:ILE:HG12	2.19	0.43
1:B:1789:LYS:HD3	1:B:1872:LEU:O	2.19	0.43
1:A:2061:TYR:O	1:A:2064:GLN:HG2	2.19	0.43
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.80	0.43
1:B:2034:ILE:CD1	1:B:2061:TYR:CE2	3.02	0.43
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.67	0.43
1:B:2368:PHE:O	1:B:2369:SER:OG	2.25	0.43
1:A:1438:LEU:O	1:A:1442:GLN:HB2	2.19	0.43
1:A:1645:PHE:CZ	1:A:1768:ARG:HD2	2.52	0.42
1:A:2220:CYS:SG	1:A:2224:SER:HB3	2.59	0.42
1:A:1469:LEU:CD1	1:A:1523:LEU:CD2	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4023:ILE:HG13	1:A:4029:ILE:HD12	2.01	0.42
1:B:1616:LYS:HE3	1:B:1761:GLU:HG3	2.01	0.42
1:A:2170:LEU:HB3	1:A:2209:ARG:HD3	2.01	0.42
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	2.00	0.42
1:A:1744:LEU:HD22	1:A:1760:PHE:CG	2.54	0.42
1:B:2151:TRP:CE3	1:B:2193:LEU:HD11	2.54	0.42
1:B:2220:CYS:HB2	2:B:5093:ATP:N6	2.33	0.42
1:B:2220:CYS:SG	2:B:5093:ATP:N6	2.93	0.42
1:B:2001:VAL:O	1:B:2004:PRO:HD2	2.19	0.42
1:A:3326:ILE:HG22	1:A:3330:TYR:CE2	2.54	0.42
1:A:3930:PHE:HE2	1:A:4029:ILE:HD13	1.83	0.42
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.86	0.42
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.85	0.42
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.55	0.42
1:A:3629:PHE:O	1:A:3633:GLU:HB2	2.20	0.42
1:B:1630:ILE:HG21	1:B:1655:MET:SD	2.57	0.42
1:A:3409:ASP:HA	1:A:3410:PRO:HD3	1.93	0.42
1:B:3930:PHE:HE2	1:B:4029:ILE:CD1	2.31	0.42
1:B:1870:ASN:O	1:B:1874:VAL:HG23	2.19	0.42
1:A:3897:TYR:CZ	1:A:3899:ASP:HB3	2.54	0.42
1:A:2742:ILE:HG23	1:A:2773:VAL:HG22	2.00	0.42
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.27	0.42
1:B:2224:SER:C	2:B:5093:ATP:C2	2.92	0.42
1:B:3459:ASP:HB2	1:B:3460:PRO:HD2	2.01	0.42
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	2.01	0.42
1:A:4022:GLN:HG2	1:A:4022:GLN:O	2.19	0.42
1:B:2747:ARG:O	1:B:2751:GLN:HG2	2.19	0.42
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.19	0.42
1:B:3431:PHE:CZ	1:B:3458:PHE:HD1	2.38	0.42
1:A:1365:PHE:HD1	1:A:1365:PHE:N	2.17	0.42
1:A:2707:VAL:HG12	1:A:2708:ASN:N	2.35	0.42
1:A:2109:LEU:HD11	1:A:2129:LEU:CD2	2.50	0.42
1:A:4037:SER:HB3	1:A:4040:GLU:HB3	2.01	0.42
1:A:2378:VAL:HG11	1:A:2392:ILE:HD12	2.00	0.42
1:A:4006:VAL:HG13	1:A:4009:LYS:HE2	2.01	0.42
1:B:4033:LEU:HD23	1:B:4033:LEU:HA	1.84	0.42
1:A:1536:ARG:HD2	1:A:1565:MET:O	2.19	0.42
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.52	0.42
1:B:1656:TRP:O	1:B:1660:VAL:HG12	2.18	0.42
1:B:3813:ILE:HG22	1:B:3840:LEU:HD23	2.01	0.42
1:B:2467:THR:HG22	1:B:2468:SER:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.23	0.42
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.40	0.42
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.80	0.42
1:B:3848:LEU:O	1:B:3851:VAL:N	2.53	0.42
1:B:1459:LEU:HD23	1:B:1465:ILE:HG13	2.02	0.42
1:B:23:LEU:C	1:B:25:GLU:N	2.73	0.42
1:A:2653:TRP:HB3	1:A:2654:ARG:NH1	2.34	0.42
1:A:2737:SER:HB2	1:A:2924:THR:HG21	2.01	0.42
1:A:1672:TYR:O	1:A:1675:GLU:HB3	2.19	0.42
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.55	0.42
1:B:1531:ARG:HD2	1:B:1538:TYR:HA	2.01	0.42
1:B:2114:LEU:HA	1:B:2129:LEU:HB3	2.02	0.42
1:A:1706:LEU:HD23	1:A:1706:LEU:HA	1.90	0.42
1:A:3628:ILE:HD11	1:A:3679:TYR:CZ	2.55	0.42
1:A:4022:GLN:HA	1:A:4028:ARG:HA	2.01	0.42
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.40	0.42
1:B:1660:VAL:CG1	1:B:1728:TRP:CH2	3.02	0.42
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.83	0.42
1:A:3304:GLU:C	1:A:3306:TRP:H	2.23	0.42
1:A:3509:LEU:HG	1:A:3513:VAL:HG21	2.02	0.42
1:B:2106:THR:H	1:B:2156:SER:HB2	1.83	0.42
1:A:3845:GLN:O	1:A:3848:LEU:HB2	2.20	0.42
1:B:1750:SER:CB	1:B:1755:LEU:HD23	2.50	0.42
1:A:2799:LEU:HD13	1:A:2840:ILE:CD1	2.49	0.42
1:A:2354:SER:H	1:A:2357:SER:HB2	1.85	0.42
1:A:3462:ILE:O	1:A:3465:LEU:N	2.48	0.42
1:B:1838:ILE:HG13	1:B:1843:ALA:HB3	2.02	0.42
1:A:1769:LEU:HD11	1:A:1804:GLU:HB3	2.01	0.42
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.55	0.42
1:B:2336:ARG:HG2	1:B:2355:ASP:OD1	2.19	0.42
1:A:3671:VAL:CA	1:A:3674:ILE:HG22	2.49	0.42
1:B:1593:ASN:ND2	1:B:1621:THR:OG1	2.47	0.42
1:A:3600:LYS:HA	1:A:3603:GLU:HG2	2.01	0.42
1:B:3303:LYS:O	1:B:3306:TRP:HD1	2.03	0.41
1:B:2707:VAL:CB	1:B:2712:LEU:CD1	2.76	0.41
1:B:1992:LYS:CG	1:B:2024:SER:CB	2.83	0.41
1:B:1983:LEU:CD1	1:B:2000:ARG:HH21	2.33	0.41
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.19	0.41
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.80	0.41
1:A:3725:VAL:HA	1:A:3730:SER:O	2.19	0.41
1:B:3002:LEU:HD21	1:B:3370:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2965:VAL:HA	1:B:2968:ILE:HD12	2.01	0.41
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.19	0.41
1:A:40:TRP:O	1:A:44:LYS:N	2.53	0.41
1:B:2754:GLY:HA3	1:B:2886:HIS:CE1	2.55	0.41
1:A:2034:ILE:HG13	1:A:2061:TYR:CE2	2.55	0.41
1:A:1823:ASP:HB3	1:A:1852:ARG:O	2.15	0.41
1:A:2755:HIS:NE2	1:A:2835:LEU:HG	2.35	0.41
1:A:3979:ASN:OD1	1:A:3979:ASN:N	2.51	0.41
1:A:2226:ILE:HG23	1:A:2288:VAL:CG2	2.49	0.41
1:A:2828:LEU:HD13	1:A:2902:MET:SD	2.60	0.41
1:B:1479:LEU:HD11	1:B:1515:SER:HB3	2.02	0.41
1:A:3373:LEU:HD13	1:A:3557:LEU:HD13	2.02	0.41
1:B:3901:PRO:HG2	1:B:3906:THR:HG23	2.01	0.41
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.56	0.41
1:A:3946:VAL:HB	1:A:3947:PRO:HA	2.02	0.41
1:B:1939:PHE:CD1	1:B:1939:PHE:N	2.88	0.41
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.55	0.41
1:B:3919:LYS:HZ3	1:B:4038:GLU:CG	2.31	0.41
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.20	0.41
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	2.02	0.41
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	2.02	0.41
1:A:1671:LYS:HD3	1:A:1671:LYS:HA	1.96	0.41
1:B:1934:LEU:HD22	1:B:1945:LEU:HD12	2.01	0.41
1:A:1697:LYS:O	1:A:1701:LEU:HG	2.20	0.41
1:B:1535:PRO:C	1:B:1841:ILE:CD1	2.77	0.41
1:B:1536:ARG:NE	1:B:1841:ILE:HD13	2.35	0.41
1:A:2078:CYS:N	2:A:5093:ATP:O2B	2.49	0.41
1:B:2938:MET:SD	1:B:3321:ILE:CG2	3.09	0.41
1:B:2661:VAL:HG12	1:B:2916:TRP:CD2	2.55	0.41
1:A:2279:ARG:HH11	1:A:2279:ARG:HD2	1.66	0.41
1:A:2099:ASN:HB3	1:A:2151:TRP:NE1	2.34	0.41
1:A:2494:LEU:HD12	1:A:2495:ASP:O	2.20	0.41
1:B:2080:LYS:O	1:B:2081:THR:C	2.59	0.41
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.35	0.41
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	2.02	0.41
1:B:2748:ALA:O	1:B:2751:GLN:HG3	2.19	0.41
1:B:4022:GLN:O	1:B:4023:ILE:C	2.58	0.41
1:A:3024:LEU:HD13	1:A:3303:LYS:HG3	1.92	0.41
1:B:1774:LEU:HA	1:B:1777:ILE:HD12	2.02	0.41
1:A:1392:LEU:N	1:A:1484:LYS:HE2	2.36	0.41
1:A:2761:ALA:O	1:A:2892:CYS:SG	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3584:MET:HA	1:B:3587:LEU:HD12	2.03	0.41
1:B:2181:GLY:C	1:B:2182:GLU:HG3	2.40	0.41
1:A:3930:PHE:CE2	1:A:4029:ILE:HD13	2.55	0.41
1:B:1832:SER:HB3	1:B:1882:LEU:HD22	2.03	0.41
1:A:3367:ILE:O	1:A:3371:VAL:HG22	2.21	0.41
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.85	0.41
1:B:2034:ILE:CD1	1:B:2061:TYR:CZ	3.03	0.41
1:A:1866:GLN:O	1:A:1870:ASN:HB2	2.21	0.41
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.35	0.41
1:B:2464:TYR:CZ	1:B:2474:LEU:HD12	2.55	0.41
1:A:2762:SER:O	1:A:2763:ARG:CB	2.69	0.41
1:B:3924:TRP:CD1	1:B:3924:TRP:C	2.94	0.41
1:B:2290:LEU:HD13	1:B:2407:LEU:HD23	2.02	0.41
1:B:1949:ILE:HD11	1:B:1994:VAL:HG11	2.03	0.41
1:A:1496:THR:O	1:A:1499:VAL:HG23	2.21	0.41
1:A:215:PRO:C	1:A:3475:ASN:HD21	2.24	0.41
1:B:2428:MET:HG2	1:B:2485:PHE:CE1	2.55	0.41
1:B:1826:PHE:CE1	1:B:1853:LEU:CD2	3.04	0.41
1:B:2079:GLY:HA2	2:B:5093:ATP:H5'2	2.02	0.41
1:A:2076:ALA:HB2	1:A:2549:ARG:HG2	2.02	0.41
1:B:3846:MET:HG3	1:B:3847:SER:N	2.35	0.41
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	2.03	0.41
1:A:2316:LEU:HD13	1:A:2351:GLN:HB3	2.01	0.41
1:B:2044:ARG:HH21	1:B:2093:ILE:HD11	1.85	0.41
1:A:1547:LYS:O	1:A:1551:SER:HB3	2.20	0.41
1:A:1795:PHE:CE1	1:A:1920:SER:HB3	2.55	0.41
1:A:1406:LYS:HB3	1:A:1406:LYS:HE2	1.95	0.41
1:B:2230:LEU:HD23	1:B:2288:VAL:HG13	2.03	0.41
1:B:2707:VAL:HG11	1:B:2712:LEU:CD1	2.46	0.41
1:B:2491:LEU:HD23	1:B:2491:LEU:HA	1.78	0.41
1:B:2000:ARG:O	1:B:2004:PRO:HG2	2.21	0.41
1:B:2787:HIS:HB3	1:B:3461:ILE:HG23	2.02	0.41
1:B:2422:SER:N	3:B:5094:ANP:O1B	2.54	0.41
1:B:1702:LEU:O	1:B:1706:LEU:HG	2.21	0.41
1:B:2572:GLU:HG3	1:B:2590:GLU:HG3	2.02	0.41
1:B:2295:ILE:HG12	1:B:2314:ILE:HD12	2.02	0.41
1:B:3462:ILE:O	1:B:3465:LEU:HB3	2.21	0.41
1:A:3772:TRP:HZ3	1:A:3780:ASN:ND2	2.19	0.41
1:A:2938:MET:HG2	1:A:3321:ILE:HG12	2.03	0.41
1:B:1559:SER:HB3	1:B:1572:ILE:HG22	2.02	0.41
1:A:3430:SER:HB2	1:A:3453:GLN:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3551:LEU:HA	1:B:3554:GLU:HB3	2.02	0.41
1:B:2578:ILE:CG2	1:B:2630:TYR:HB2	2.50	0.41
1:A:1620:PHE:CE1	1:A:1743:ASP:HB3	2.55	0.41
1:B:2488:GLU:CD	1:B:2491:LEU:HD11	2.41	0.41
1:A:1535:PRO:C	1:A:1841:ILE:CD1	2.79	0.41
1:A:1968:PHE:CD1	1:A:1968:PHE:N	2.88	0.41
1:A:2320:ARG:O	1:A:2323:LEU:HB3	2.20	0.41
1:B:1637:GLU:HG2	1:B:1686:LYS:HG3	2.03	0.41
1:A:3642:TYR:CD1	1:A:3642:TYR:N	2.87	0.41
1:A:1853:LEU:HB2	1:A:1858:LEU:HD12	2.03	0.40
1:A:1704:GLU:O	1:A:1707:HIS:HB3	2.21	0.40
1:B:2476:LYS:N	1:B:2476:LYS:CD	2.84	0.40
1:A:4065:LEU:O	1:A:4065:LEU:HD12	2.21	0.40
1:A:3848:LEU:O	1:A:3849:SER:C	2.57	0.40
1:B:2178:LEU:HB2	1:B:2182:GLU:H	1.86	0.40
1:A:3862:THR:HB	1:A:3865:ALA:HB2	2.03	0.40
1:A:1838:ILE:HD11	1:A:1845:GLY:N	2.37	0.40
1:B:2115:TYR:OH	1:B:2162:TYR:O	2.28	0.40
1:A:2415:ILE:O	1:A:2556:ILE:HA	2.21	0.40
1:B:2039:LYS:HG2	1:B:2049:MET:HG3	2.02	0.40
1:A:2199:LEU:O	1:A:2200:ASP:C	2.59	0.40
1:B:1743:ASP:C	1:B:1745:ASN:N	2.74	0.40
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.86	0.40
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.89	0.40
1:A:2510:MET:O	1:A:2513:GLN:NE2	2.53	0.40
1:A:3978:ASN:O	1:A:3981:PRO:HD2	2.19	0.40
1:A:1592:LEU:HD13	1:A:1596:ILE:CD1	2.50	0.40
1:B:3784:ASN:ND2	1:B:3865:ALA:O	2.54	0.40
1:B:1987:PHE:HB3	1:B:1988:GLY:H	1.73	0.40
1:B:1664:LEU:HD23	1:B:1669:PHE:HZ	1.86	0.40
1:A:1579:ILE:HG13	1:A:1598:LEU:HD11	2.03	0.40
1:B:2752:VAL:HG13	1:B:2883:LYS:CB	2.50	0.40
1:A:4033:LEU:HD13	1:A:4035:GLN:H	1.87	0.40
1:A:3534:LEU:HD12	1:A:3618:TYR:CZ	2.54	0.40
1:A:1939:PHE:CD1	1:A:1939:PHE:N	2.81	0.40
1:A:2125:TRP:CE2	1:A:2178:LEU:HD13	2.56	0.40
1:B:1734:PHE:CD2	1:B:1749:ILE:HG12	2.56	0.40
1:B:23:LEU:C	1:B:25:GLU:H	2.25	0.40
1:B:2820:SER:O	1:B:2823:LEU:HD12	2.21	0.40
1:B:2012:LEU:HD12	1:B:2013:VAL:N	2.36	0.40
1:B:1826:PHE:CD1	1:B:1826:PHE:O	2.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2071:ILE:HB	1:A:2212:LEU:CD1	2.51	0.40
1:B:1750:SER:HB2	1:B:1755:LEU:HD23	2.03	0.40
1:A:3443:ALA:HB1	1:A:3450:VAL:CG2	2.50	0.40
1:B:2759:ILE:HG21	1:B:2916:TRP:CZ2	2.56	0.40
1:A:3564:LYS:O	1:A:3568:GLU:HG2	2.21	0.40
1:B:3566:LEU:HA	1:B:3583:LEU:HD23	1.96	0.40
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	2.02	0.40
1:B:1796:GLY:O	1:B:1900:PRO:HD3	2.22	0.40
1:A:3939:ILE:CG1	1:A:4010:LEU:CD2	2.99	0.40
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.35	0.40
1:A:2378:VAL:HG11	1:A:2392:ILE:CD1	2.51	0.40
1:B:1832:SER:O	1:B:1836:VAL:HG23	2.21	0.40
1:B:1773:PRO:HA	1:B:1776:LEU:HD12	2.03	0.40
1:B:2463:ASN:O	1:B:2475:PRO:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2640/2695 (98%)	2518 (95%)	110 (4%)	12 (0%)	34	77
1	B	2640/2695 (98%)	2515 (95%)	111 (4%)	14 (0%)	34	77
All	All	5280/5390 (98%)	5033 (95%)	221 (4%)	26 (0%)	34	77

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	B	1391	GLY
1	B	3578	LEU
1	A	24	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1633	GLY
1	A	2513	GLN
1	A	3482	GLY
1	B	24	GLU
1	B	2513	GLN
1	B	2990	GLY
1	B	3482	GLY
1	A	2990	GLY
1	A	66	GLN
1	A	1744	LEU
1	A	2519	PRO
1	B	66	GLN
1	B	3914	GLN
1	B	2519	PRO
1	B	2562	PRO
1	B	3809	GLU
1	A	3980	ILE
1	B	3305	ARG
1	A	2028	PRO
1	B	3980	ILE
1	A	2562	PRO
1	B	1470	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2218/2453 (90%)	2138 (96%)	80 (4%)	42	78
1	B	2218/2453 (90%)	2137 (96%)	81 (4%)	41	77
All	All	4436/4906 (90%)	4275 (96%)	161 (4%)	42	78

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1421	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1486	ILE
1	A	1493	LEU
1	A	1504	ASN
1	A	1769	LEU
1	A	1783	THR
1	A	1788	GLN
1	A	1794	PHE
1	A	1826	PHE
1	A	1858	LEU
1	A	1925	GLN
1	A	1997	SER
1	A	2057	CYS
1	A	2078	CYS
1	A	2109	LEU
1	A	2122	THR
1	A	2141	ILE
1	A	2154	PHE
1	A	2155	ASP
1	A	2202	THR
1	A	2229	LEU
1	A	2295	ILE
1	A	2352	GLU
1	A	2357	SER
1	A	2387	ARG
1	A	2395	ILE
1	A	2397	THR
1	A	2411	LYS
1	A	2412	ARG
1	A	2428	MET
1	A	2476	LYS
1	A	2482	LEU
1	A	2544	ILE
1	A	2548	GLU
1	A	2566	SER
1	A	2576	LYS
1	A	2623	THR
1	A	2626	VAL
1	A	2627	ARG
1	A	2681	LEU
1	A	2689	ILE
1	A	2694	LEU
1	A	2822	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2833	THR
1	A	2843	LEU
1	A	2856	LEU
1	A	2866	LEU
1	A	2967	ASN
1	A	2999	LEU
1	A	3002	LEU
1	A	3301	PHE
1	A	3329	ILE
1	A	3332	THR
1	A	3340	ARG
1	A	3372	THR
1	A	3400	SER
1	A	3560	LYS
1	A	3578	LEU
1	A	3601	LEU
1	A	3618	TYR
1	A	3634	LYS
1	A	3673	GLU
1	A	3677	LEU
1	A	3729	SER
1	A	3737	THR
1	A	3788	MET
1	A	3805	LYS
1	A	3823	ASN
1	A	3871	PHE
1	A	3876	THR
1	A	3899	ASP
1	A	3906	THR
1	A	3940	THR
1	A	3943	THR
1	A	3958	ASP
1	A	3960	ASP
1	A	3980	ILE
1	A	3982	TRP
1	A	3997	LYS
1	A	4016	CYS
1	B	1383	TYR
1	B	1421	TYR
1	B	1486	ILE
1	B	1504	ASN
1	B	1525	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1646	GLN
1	B	1694	VAL
1	B	1743	ASP
1	B	1759	LYS
1	B	1794	PHE
1	B	1826	PHE
1	B	1858	LEU
1	B	1936	ILE
1	B	2008	ASP
1	B	2068	GLN
1	B	2075	LYS
1	B	2109	LEU
1	B	2141	ILE
1	B	2154	PHE
1	B	2155	ASP
1	B	2202	THR
1	B	2229	LEU
1	B	2285	GLU
1	B	2295	ILE
1	B	2307	ASP
1	B	2310	LEU
1	B	2351	GLN
1	B	2357	SER
1	B	2368	PHE
1	B	2381	GLU
1	B	2390	ILE
1	B	2395	ILE
1	B	2412	ARG
1	B	2425	THR
1	B	2476	LYS
1	B	2479	ILE
1	B	2496	LYS
1	B	2512	LYS
1	B	2566	SER
1	B	2574	TYR
1	B	2681	LEU
1	B	2689	ILE
1	B	2769	LEU
1	B	2822	ILE
1	B	2829	GLU
1	B	2853	LEU
1	B	2920	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2967	ASN
1	B	2969	LEU
1	B	3305	ARG
1	B	3329	ILE
1	B	3360	TYR
1	B	3372	THR
1	B	3380	LEU
1	B	3391	LEU
1	B	3400	SER
1	B	3502	SER
1	B	3559	LEU
1	B	3581	ASP
1	B	3598	GLU
1	B	3605	GLU
1	B	3618	TYR
1	B	3729	SER
1	B	3737	THR
1	B	3744	LEU
1	B	3811	LEU
1	B	3844	ILE
1	B	3871	PHE
1	B	3899	ASP
1	B	3906	THR
1	B	3917	THR
1	B	3940	THR
1	B	3943	THR
1	B	3958	ASP
1	B	3960	ASP
1	B	3982	TRP
1	B	4016	CYS
1	B	4024	VAL
1	B	4040	GLU
1	B	4068	GLU
1	B	4087	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1533	GLN
1	A	1605	GLN
1	A	1622	GLN
1	A	1646	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1736	GLN
1	A	1745	ASN
1	A	1851	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1951	HIS
1	A	1965	HIS
1	A	2064	GLN
1	A	2068	GLN
1	A	2099	ASN
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2351	GLN
1	A	2383	HIS
1	A	2409	ASN
1	A	2444	ASN
1	A	2459	HIS
1	A	2536	ASN
1	A	2601	ASN
1	A	2634	ASN
1	A	2688	ASN
1	A	2896	ASN
1	A	3323	ASN
1	A	3420	ASN
1	A	3475	ASN
1	A	3521	ASN
1	A	3624	HIS
1	A	3780	ASN
1	A	3890	GLN
1	A	3962	GLN
1	A	3970	ASN
1	A	4020	ASN
1	A	4077	GLN
1	B	1501	HIS
1	B	1622	GLN
1	B	1646	GLN
1	B	1707	HIS
1	B	1736	GLN
1	B	1864	ASN
1	B	1873	GLN
1	B	1899	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1951	HIS
1	B	2068	GLN
1	B	2274	HIS
1	B	2282	ASN
1	B	2293	HIS
1	B	2409	ASN
1	B	2444	ASN
1	B	2536	ASN
1	B	2598	HIS
1	B	2634	ASN
1	B	2751	GLN
1	B	2753	GLN
1	B	2755	HIS
1	B	2896	ASN
1	B	2910	ASN
1	B	3323	ASN
1	B	3338	ASN
1	B	3471	ASN
1	B	3521	ASN
1	B	3542	GLN
1	B	3571	ASN
1	B	3624	HIS
1	B	3685	GLN
1	B	3780	ASN
1	B	3783	ASN
1	B	3890	GLN
1	B	3962	GLN
1	B	3970	ASN
1	B	4020	ASN
1	B	4077	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 10 ligands modelled in this entry, 2 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$
2	ATP	A	5093	5	24,33,33	1.06	2 (8%)	31,52,52	2.00	5 (16%)
3	ANP	A	5094	-	27,33,33	3.06	6 (22%)	30,52,52	1.99	5 (16%)
4	SO4	A	5095	-	4,4,4	0.69	0	6,6,6	0.89	0
4	SO4	A	5096	-	4,4,4	0.54	0	6,6,6	0.21	0
2	ATP	B	5093	5	24,33,33	1.04	2 (8%)	31,52,52	1.98	5 (16%)
3	ANP	B	5094	-	27,33,33	3.12	6 (22%)	30,52,52	1.89	4 (13%)
4	SO4	B	5095	-	4,4,4	0.47	0	6,6,6	0.42	0
4	SO4	B	5096	-	4,4,4	0.44	0	6,6,6	0.19	0

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
2	ATP	A	5093	5	-	0/18/38/38	0/3/3/3
3	ANP	A	5094	-	-	0/12/38/38	0/3/3/3
4	SO4	A	5095	-	-	0/0/0/0	0/0/0/0
4	SO4	A	5096	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5093	5	-	0/18/38/38	0/3/3/3
3	ANP	B	5094	-	-	1/12/38/38	0/3/3/3
4	SO4	B	5095	-	-	0/0/0/0	0/0/0/0
4	SO4	B	5096	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-O3G	-2.96	1.48	1.56
3	A	5094	ANP	PG-O3G	-2.91	1.48	1.56
3	A	5094	ANP	O4'-C1'	2.04	1.43	1.41
2	A	5093	ATP	O4'-C1'	2.07	1.43	1.41
3	B	5094	ANP	PB-O1B	2.13	1.48	1.46
2	B	5093	ATP	O4'-C1'	2.37	1.44	1.41
3	A	5094	ANP	C5-C4	3.04	1.47	1.40
3	B	5094	ANP	C5-C4	3.15	1.47	1.40
2	B	5093	ATP	C5-C4	3.26	1.47	1.40
2	A	5093	ATP	C5-C4	3.39	1.48	1.40
3	A	5094	ANP	PB-N3B	4.29	1.74	1.63
3	B	5094	ANP	PB-N3B	4.55	1.75	1.63
3	A	5094	ANP	PG-N3B	4.60	1.75	1.63
3	B	5094	ANP	PG-N3B	4.61	1.75	1.63
3	A	5094	ANP	PG-O1G	13.08	1.61	1.46
3	B	5094	ANP	PG-O1G	13.34	1.61	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5094	ANP	N3-C2-N1	-7.14	123.42	128.89
3	B	5094	ANP	N3-C2-N1	-6.72	123.75	128.89
2	A	5093	ATP	N3-C2-N1	-6.69	123.77	128.89
2	B	5093	ATP	N3-C2-N1	-6.53	123.89	128.89
2	B	5093	ATP	PA-O3A-PB	-4.48	120.16	132.73
2	A	5093	ATP	PA-O3A-PB	-4.18	120.98	132.73
2	B	5093	ATP	PB-O3B-PG	-3.75	120.08	132.67
2	A	5093	ATP	PB-O3B-PG	-3.63	120.49	132.67
3	B	5094	ANP	PA-O3A-PB	-3.62	120.54	132.67
2	A	5093	ATP	C2'-C1'-N9	-3.57	108.83	114.29
3	A	5094	ANP	PA-O3A-PB	-3.48	120.99	132.67
3	A	5094	ANP	C4-C5-N7	-3.29	106.46	109.48
2	B	5093	ATP	C2'-C1'-N9	-3.24	109.35	114.29
3	A	5094	ANP	C2'-C1'-N9	-3.19	109.42	114.29
3	B	5094	ANP	C4-C5-N7	-3.16	106.57	109.48
2	B	5093	ATP	C4-C5-N7	-3.13	106.60	109.48
2	A	5093	ATP	C4-C5-N7	-3.06	106.66	109.48
3	B	5094	ANP	C2'-C1'-N9	-3.02	109.68	114.29
3	A	5094	ANP	C2'-C3'-C4'	2.57	107.90	102.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5094	ANP	O1G-PG-N3B-PB

There are no ring outliers.

6 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	8	0
3	A	5094	ANP	7	0
4	A	5095	SO4	3	0
2	B	5093	ATP	17	0
3	B	5094	ANP	7	0
4	B	5096	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2650/2695 (98%)	0.13	68 (2%) 59 44	69, 151, 281, 423	0
1	B	2650/2695 (98%)	0.66	278 (10%) 8 6	92, 193, 357, 500	0
All	All	5300/5390 (98%)	0.40	346 (6%) 22 14	69, 172, 321, 500	0

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	ASP	25.0
1	B	164	MET	22.5
1	B	213	ASP	20.8
1	B	29	GLU	20.0
1	B	163	TYR	19.5
1	B	84	CYS	19.3
1	B	161	VAL	19.1
1	B	49	LEU	16.6
1	B	214	HIS	15.4
1	B	142	LEU	15.3
1	B	206	GLN	14.6
1	B	166	PRO	13.9
1	B	80	MET	13.9
1	B	48	GLY	13.8
1	B	168	CYS	13.6
1	B	143	ASN	13.1
1	B	69	ALA	12.3
1	B	19	LEU	12.1
1	B	162	LEU	12.1
1	A	2	PRO	12.1
1	B	18	LEU	12.0
1	B	151	ASP	11.8
1	B	83	GLY	11.6
1	B	53	ASN	11.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	215	PRO	10.8
1	B	70	ILE	10.7
1	B	76	ASP	10.7
1	B	78	HIS	10.2
1	B	212	GLY	9.9
1	B	4	LEU	9.7
1	B	1683	LEU	9.5
1	A	2364	ASP	9.0
1	B	30	HIS	8.9
1	B	1572	ILE	8.7
1	B	184	ALA	8.6
1	B	120	ASP	8.3
1	B	90	GLU	8.2
1	B	167	MET	8.2
1	B	197	TYR	8.1
1	B	73	TYR	7.9
1	B	185	ILE	7.9
1	A	63	LYS	7.9
1	B	115	GLU	7.8
1	B	208	THR	7.8
1	B	1549	ILE	7.7
1	B	188	ILE	7.7
1	A	1	SER	7.5
1	B	148	THR	7.5
1	B	205	TRP	7.5
1	B	1644	ILE	7.4
1	B	1937	MET	7.3
1	A	115	GLU	7.3
1	B	216	PRO	7.2
1	A	1483	TYR	7.2
1	B	14	GLN	7.1
1	B	68	MET	7.0
1	B	74	ILE	7.0
1	B	186	PRO	7.0
1	B	79	ASN	6.9
1	B	92	SER	6.8
1	B	133	GLU	6.8
1	B	1459	LEU	6.7
1	B	189	ASP	6.6
1	B	160	VAL	6.6
1	A	71	ILE	6.5
1	A	28	GLU	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	6.4
1	B	171	ALA	6.3
1	B	1680	ILE	6.3
1	B	1590	LEU	6.3
1	B	1582	VAL	6.2
1	B	50	GLU	6.2
1	B	67	SER	6.2
1	B	1732	GLN	6.2
1	B	1679	LYS	6.1
1	B	157	ALA	6.1
1	B	177	CYS	6.1
1	B	116	THR	6.1
1	B	46	GLU	6.0
1	B	33	GLU	5.9
1	B	1684	LEU	5.8
1	B	147	VAL	5.7
1	B	1550	GLY	5.7
1	B	1669	PHE	5.7
1	B	190	LYS	5.7
1	B	1581	GLY	5.6
1	B	91	ILE	5.6
1	B	82	GLY	5.6
1	B	111	SER	5.6
1	B	3580	ASN	5.4
1	A	85	PRO	5.4
1	B	207	ALA	5.4
1	B	75	ALA	5.4
1	A	27	TYR	5.3
1	B	194	SER	5.3
1	A	86	LYS	5.3
1	B	34	ARG	5.2
1	B	1601	SER	5.2
1	B	1458	ILE	5.2
1	B	3555	TYR	5.2
1	B	180	LYS	5.1
1	B	195	SER	5.1
1	B	77	LYS	5.0
1	A	3563	GLU	5.0
1	B	119	VAL	5.0
1	B	1705	TYR	4.9
1	B	1596	ILE	4.9
1	B	1730	LYS	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	35	ASP	4.8
1	B	1606	GLU	4.8
1	B	196	LYS	4.8
1	B	1545	LEU	4.8
1	B	1649	LEU	4.8
1	B	16	THR	4.7
1	B	66	GLN	4.7
1	B	1452	TRP	4.7
1	B	3866	GLU	4.7
1	B	1483	TYR	4.7
1	B	1456	TYR	4.7
1	B	1566	PHE	4.7
1	A	216	PRO	4.6
1	B	47	LEU	4.5
1	A	215	PRO	4.5
1	B	85	PRO	4.5
1	B	54	LEU	4.4
1	B	1771	TYR	4.4
1	B	1415	MET	4.4
1	B	1647	ALA	4.4
1	B	170	ASP	4.3
1	B	204	GLY	4.3
1	A	25	GLU	4.3
1	A	3580	ASN	4.2
1	B	17	ARG	4.2
1	A	35	ASP	4.2
1	B	179	LYS	4.2
1	B	1893	ALA	4.1
1	B	1476	PHE	4.1
1	B	1770	ILE	4.1
1	B	117	LEU	4.1
1	B	1548	ILE	4.0
1	B	28	GLU	3.9
1	B	3304	GLU	3.9
1	A	62	VAL	3.9
1	B	3482	GLY	3.9
1	B	1894	VAL	3.9
1	B	3393	ASN	3.9
1	A	84	CYS	3.8
1	B	1394	LEU	3.8
1	A	151	ASP	3.8
1	B	3588	ASN	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	116	THR	3.7
1	B	1701	LEU	3.7
1	B	15	PRO	3.7
1	B	211	GLY	3.7
1	A	148	THR	3.6
1	B	2938	MET	3.6
1	B	1460	GLY	3.6
1	B	1546	LEU	3.6
1	B	183	GLU	3.6
1	B	3846	MET	3.5
1	A	3979	ASN	3.5
1	B	56	TYR	3.4
1	A	61	ASP	3.4
1	A	1597	GLU	3.4
1	B	1734	PHE	3.4
1	A	20	LEU	3.4
1	B	1933	ILE	3.4
1	A	83	GLY	3.4
1	A	1394	LEU	3.4
1	A	69	ALA	3.3
1	B	187	GLN	3.3
1	B	1441	ILE	3.3
1	B	1	SER	3.3
1	B	112	LYS	3.2
1	B	178	PHE	3.2
1	B	152	PHE	3.2
1	A	3330	TYR	3.2
1	B	89	ALA	3.2
1	B	4023	ILE	3.2
1	A	90	GLU	3.2
1	A	2918	GLY	3.1
1	B	191	TYR	3.1
1	B	1653	GLN	3.1
1	B	1835	LEU	3.1
1	B	1812	ASN	3.1
1	B	1445	TRP	3.1
1	B	1636	ILE	3.1
1	A	64	LEU	3.1
1	A	72	ARG	3.1
1	B	1760	PHE	3.1
1	B	1935	GLN	3.0
1	B	1372	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1676	VAL	3.0
1	B	1845	GLY	3.0
1	B	202	LEU	3.0
1	B	2213	LEU	3.0
1	B	198	ILE	3.0
1	B	5	GLY	3.0
1	B	1608	LEU	3.0
1	B	2000	ARG	3.0
1	B	1602	ILE	2.9
1	B	1650	LEU	2.9
1	B	3726	LEU	2.9
1	B	42	ASN	2.9
1	B	1579	ILE	2.9
1	B	2669	PHE	2.9
1	B	155	TYR	2.9
1	B	1744	LEU	2.9
1	B	1395	VAL	2.9
1	B	3391	LEU	2.8
1	B	1605	GLN	2.8
1	B	1715	LEU	2.8
1	B	113	ASP	2.8
1	B	87	GLU	2.8
1	B	1704	GLU	2.8
1	B	3326	ILE	2.8
1	B	36	GLU	2.8
1	A	3334	PHE	2.8
1	B	110	TYR	2.8
1	B	1813	LEU	2.8
1	A	79	ASN	2.8
1	B	1765	ILE	2.8
1	B	1703	VAL	2.8
1	A	1368	GLU	2.7
1	B	1378	TRP	2.7
1	B	1682	GLY	2.7
1	B	1936	ILE	2.7
1	B	1562	MET	2.7
1	B	2770	THR	2.7
1	B	3589	ASN	2.7
1	A	2194	PHE	2.7
1	B	1607	TRP	2.7
1	B	1420	TYR	2.7
1	A	59	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1548	ILE	2.7
1	B	1506	ASP	2.7
1	A	3418	ILE	2.7
1	B	3841	LEU	2.7
1	B	1568	SER	2.7
1	B	3325	ILE	2.7
1	B	1593	ASN	2.6
1	B	1493	LEU	2.6
1	B	3847	SER	2.6
1	B	1592	LEU	2.6
1	B	3788	MET	2.6
1	A	202	LEU	2.6
1	B	3919	LYS	2.6
1	A	67	SER	2.6
1	B	199	ALA	2.6
1	A	3495	PHE	2.6
1	A	3564	LYS	2.6
1	B	156	ASP	2.6
1	A	1458	ILE	2.6
1	B	72	ARG	2.5
1	B	55	PRO	2.5
1	B	1711	VAL	2.5
1	A	75	ALA	2.5
1	A	89	ALA	2.5
1	B	20	LEU	2.5
1	B	2353	LEU	2.5
1	B	1505	PHE	2.5
1	B	2428	MET	2.5
1	A	3784	ASN	2.5
1	B	3839	ILE	2.5
1	A	3567	LEU	2.5
1	B	3714	GLN	2.5
1	B	31	LEU	2.4
1	B	1479	LEU	2.4
1	B	94	LEU	2.4
1	B	3024	LEU	2.4
1	B	4029	ILE	2.4
1	B	1492	GLN	2.4
1	B	1809	PHE	2.4
1	B	136	LEU	2.4
1	A	68	MET	2.4
1	A	135	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	3590	LEU	2.3
1	B	2918	GLY	2.3
1	B	3785	TYR	2.3
1	B	2058	MET	2.3
1	B	1421	TYR	2.3
1	B	2072	LEU	2.3
1	A	182	ILE	2.3
1	B	137	CYS	2.3
1	B	2026	GLY	2.3
1	A	2928	VAL	2.3
1	A	1445	TRP	2.3
1	B	182	ILE	2.3
1	B	1551	SER	2.3
1	B	1417	ALA	2.3
1	A	108	ILE	2.3
1	B	3618	TYR	2.3
1	B	3694	PHE	2.3
1	B	1500	ILE	2.3
1	B	3425	LYS	2.3
1	B	3597	ILE	2.3
1	A	1504	ASN	2.3
1	B	1547	LYS	2.3
1	B	1503	PRO	2.2
1	B	1573	ILE	2.3
1	B	2214	TRP	2.2
1	B	3560	LYS	2.2
1	A	184	ALA	2.2
1	B	1712	ILE	2.2
1	B	176	VAL	2.2
1	B	1580	THR	2.2
1	B	1588	GLU	2.2
1	B	3571	ASN	2.2
1	A	3321	ILE	2.2
1	B	3927	TYR	2.2
1	B	3915	PHE	2.2
1	B	3427	VAL	2.2
1	B	95	GLU	2.2
1	B	3466	ILE	2.2
1	B	1583	ARG	2.2
1	B	3591	LYS	2.2
1	A	3494	LEU	2.2
1	B	1807	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	3934	TRP	2.1
1	B	3327	SER	2.1
1	B	2212	LEU	2.1
1	A	1578	PHE	2.1
1	A	19	LEU	2.1
1	B	1502	ILE	2.1
1	B	1769	LEU	2.1
1	B	149	HIS	2.1
1	B	2889	PHE	2.1
1	B	88	ARG	2.1
1	B	2660	LEU	2.1
1	B	3884	LEU	2.1
1	B	1480	THR	2.1
1	A	3546	GLU	2.1
1	A	1612	ASP	2.1
1	B	3985	VAL	2.1
1	B	3330	TYR	2.0
1	A	3329	ILE	2.0
1	B	3564	LYS	2.0
1	B	3797	THR	2.0
1	B	1668	GLN	2.0
1	B	1779	PHE	2.0
1	A	150	PRO	2.0
1	A	3025	ASN	2.0
1	B	1455	LEU	2.0
1	B	3844	ILE	2.0
1	B	1594	GLU	2.0
1	A	3865	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	5095	5/5	0.96	0.25	0.94	84,98,104,105	0
2	ATP	A	5093	31/31	0.95	0.29	0.19	88,123,185,204	0
3	ANP	B	5094	31/31	0.89	0.29	-0.05	112,145,237,257	0
3	ANP	A	5094	31/31	0.94	0.27	-0.31	111,140,238,248	0
2	ATP	B	5093	31/31	0.92	0.24	-0.35	99,141,184,200	0
4	SO4	B	5096	5/5	0.95	0.14	-0.78	155,168,174,176	0
5	MG	A	5097	1/1	0.99	0.22	-1.10	62,62,62,62	0
4	SO4	B	5095	5/5	0.84	0.18	-1.17	152,154,166,167	0
4	SO4	A	5096	5/5	0.96	0.20	-1.50	115,130,143,145	0
5	MG	B	5097	1/1	0.97	0.18	-	66,66,66,66	0

6.5 Other polymers

There are no such residues in this entry.