



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:53 PM GMT

PDB ID : 1HN1
Title : E. COLI (LAC Z) BETA-GALACTOSIDASE (ORTHORHOMBIC)
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2000-12-05
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

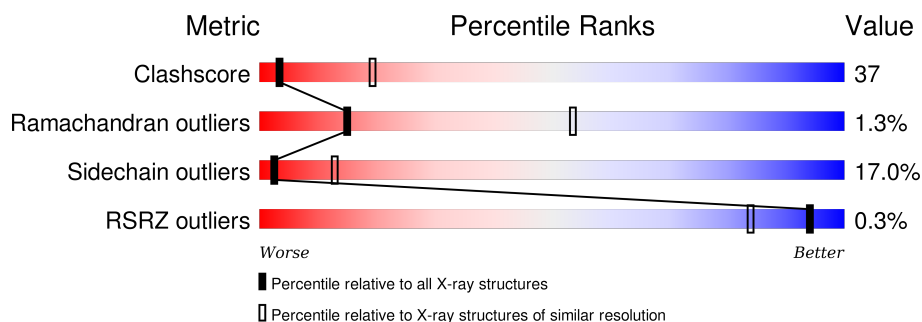
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	1023	<div> <div>32%</div> <div>50%</div> <div>16%</div> <div>..</div> </div>
1	B	1023	<div> <div>30%</div> <div>47%</div> <div>20%</div> <div>..</div> </div>
1	C	1023	<div> <div>33%</div> <div>48%</div> <div>16%</div> <div>..</div> </div>
1	D	1023	<div> <div>35%</div> <div>46%</div> <div>15%</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	MG	A	3001	-	-	-	X
2	MG	C	3001	-	-	-	X
2	MG	D	3001	-	-	-	X
2	MG	D	3002	-	-	-	X
3	NA	A	3101	-	-	-	X
3	NA	A	3102	-	-	-	X
3	NA	B	3102	-	-	-	X
3	NA	C	3101	-	-	-	X
3	NA	C	3102	-	-	-	X
3	NA	D	3102	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32954 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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	2	0
			8136	5145	1443	1510	38			
1	B	1011	Total	C	N	O	S	0	2	0
			8136	5145	1443	1510	38			
1	C	1011	Total	C	N	O	S	0	2	0
			8136	5145	1443	1510	38			
1	D	1011	Total	C	N	O	S	0	1	0
			8130	5141	1441	1510	38			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P00722
A	2	SER	-	CLONING ARTIFACT	UNP P00722
A	3	HIS	-	CLONING ARTIFACT	UNP P00722
A	4	MET	-	CLONING ARTIFACT	UNP P00722
A	5	LEU	-	CLONING ARTIFACT	UNP P00722
A	6	GLU	-	CLONING ARTIFACT	UNP P00722
A	7	ASP	-	CLONING ARTIFACT	UNP P00722
A	8	PRO	-	CLONING ARTIFACT	UNP P00722
B	1	GLY	-	CLONING ARTIFACT	UNP P00722
B	2	SER	-	CLONING ARTIFACT	UNP P00722
B	3	HIS	-	CLONING ARTIFACT	UNP P00722
B	4	MET	-	CLONING ARTIFACT	UNP P00722
B	5	LEU	-	CLONING ARTIFACT	UNP P00722
B	6	GLU	-	CLONING ARTIFACT	UNP P00722
B	7	ASP	-	CLONING ARTIFACT	UNP P00722
B	8	PRO	-	CLONING ARTIFACT	UNP P00722
C	1	GLY	-	CLONING ARTIFACT	UNP P00722
C	2	SER	-	CLONING ARTIFACT	UNP P00722
C	3	HIS	-	CLONING ARTIFACT	UNP P00722
C	4	MET	-	CLONING ARTIFACT	UNP P00722
C	5	LEU	-	CLONING ARTIFACT	UNP P00722

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLU	-	CLONING ARTIFACT	UNP P00722
C	7	ASP	-	CLONING ARTIFACT	UNP P00722
C	8	PRO	-	CLONING ARTIFACT	UNP P00722
D	1	GLY	-	CLONING ARTIFACT	UNP P00722
D	2	SER	-	CLONING ARTIFACT	UNP P00722
D	3	HIS	-	CLONING ARTIFACT	UNP P00722
D	4	MET	-	CLONING ARTIFACT	UNP P00722
D	5	LEU	-	CLONING ARTIFACT	UNP P00722
D	6	GLU	-	CLONING ARTIFACT	UNP P00722
D	7	ASP	-	CLONING ARTIFACT	UNP P00722
D	8	PRO	-	CLONING ARTIFACT	UNP P00722

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Na 2 2	0	0
3	A	2	Total Na 2 2	0	0
3	D	1	Total Na 1 1	0	0
3	C	2	Total Na 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	103	Total O 103 103	0	0

Continued on next page...

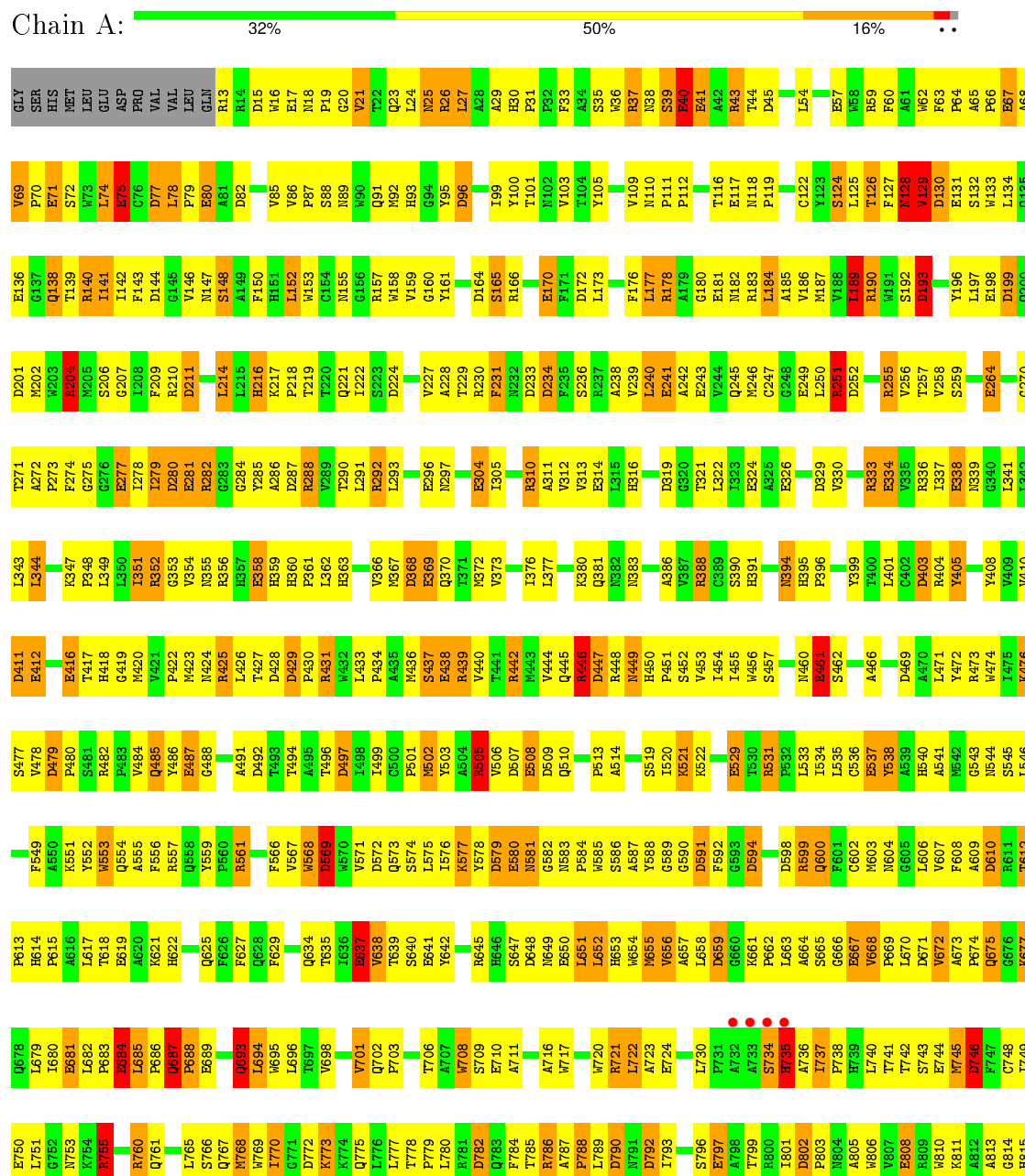
Continued from previous page...

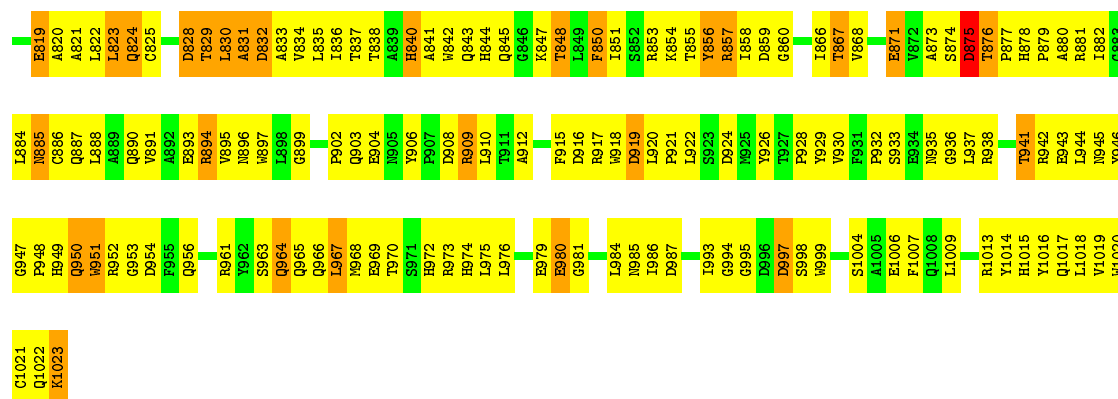
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	92	Total 92	O 92	0	0
4	C	108	Total 108	O 108	0	0
4	D	98	Total 98	O 98	0	0

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.

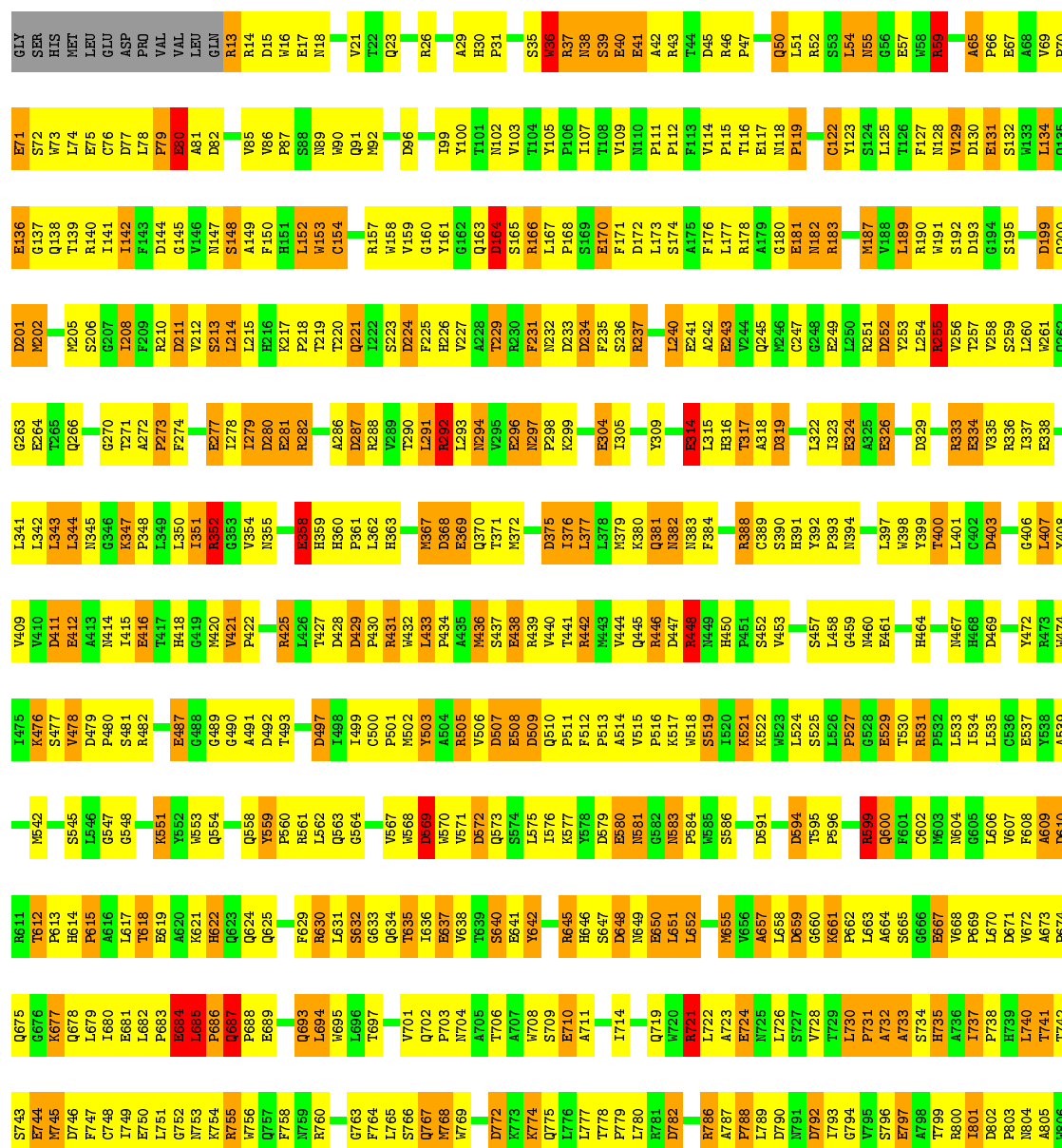
• Molecule 1: BETA-GALACTOSIDASE

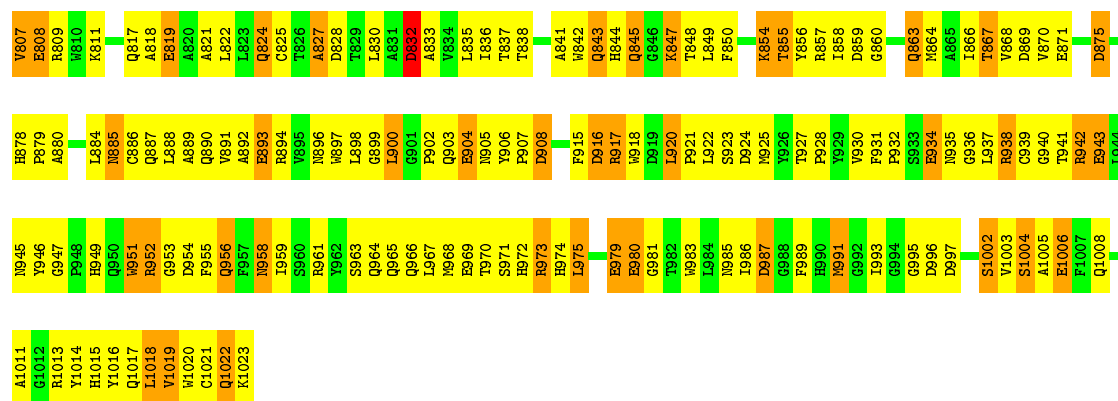




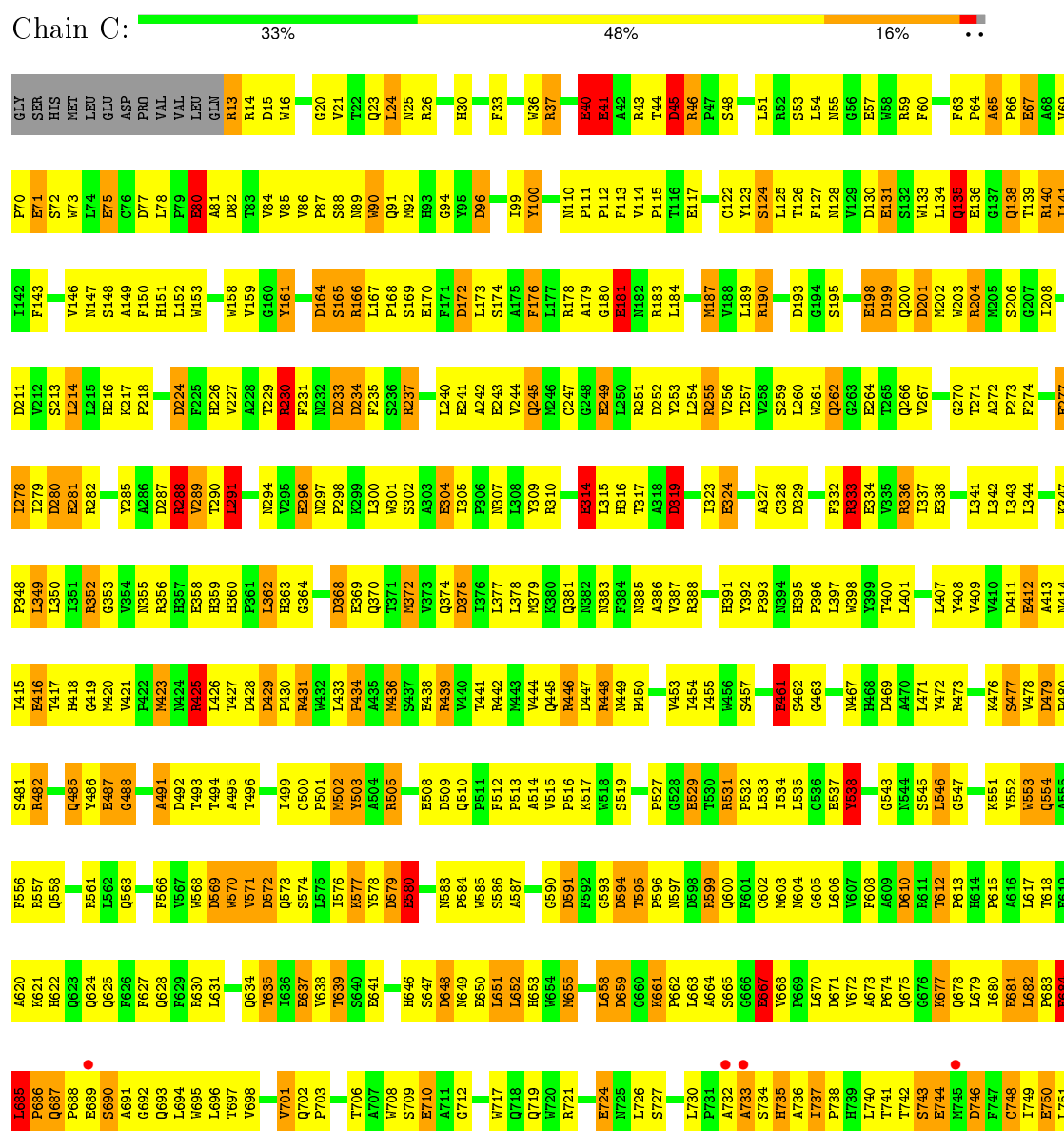
• Molecule 1: BETA-GALACTOSIDASE

Chain B: 30% 47% 20% ..





• Molecule 1: BETA-GALACTOSIDASE





L696	L697	V698	R699	V700	V701	Q702	F703	T706	A707	H708	S709	E710	A711	G712	H713	I714	W717	Q718	W719	W720	R721	L722	A723	E724	N725	L726	S727	N728	T729	L730	P731	A732	A733	S734	E735	H736	A737	I738	H739	L740	T741	T742	S743	E744	M745	D746	F747	C748	I749	E750	L751	R755	W756	F757	N759		
H760	Q761	S762	L765	S766	Q767	M768	W769	T770	G771	D772	K773	K774	Q775	L776	L777	T778	P779	L780	R781	D782	Q783	F784	T785	R786	A787	P788	L789	D790	N791	D792	I793	G794	V795	S796	E797	A798	T799	R800	I801	D802	P803	M804	A805	W806	L807	E808	R809	H815	Y816	Q817	A818	B819	A820	A821	Q824	C825	
T826	A827	D828	T829	L830	A831	D832	A833	L836	T837	T838	A839	H840	A841	M842	Q843	H844	Q845	F850	R853	K854	T855	Y856	R857	L858	D859	G860	L866	T867	V868	D869	V870	E871	V872	D875	T876	P877	H878	P879	A880	R881	L882	G883	L884	Q887	L888	A889	Q890	V891	A892	E893	R894	V895	N896				
L897	L898	G899	L900	G901	P902	Q903	E904	N905	Y906	P907	D908	R909	L910	T911	A912	A913	G914	F915	D916	R917	W918	D919	L920	P921	D924	N925	G926	T927	P928	Y929	V930	F931	P932	S933	E934	N935	G936	L937	R938	C939	G940	T941	A942	E943	Y946	G947	P948	H949	Q950	V951	R952	G953	D954	F955	Q956	F957	N958
I959	S960	R961	E969	T970	S971	H972	R973	H974	L975	A978	E979	E980	G981	T982	W983	L984	R985	L986	D987	G988	F989	H990	N991	D996	D997	S998	S1004	A1005	E1006	F1007	A1011	G1012	R1013	Y1014	Q1017	L1018	Y1019	W1020	C1021	Q1022	K1023																

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.90Å 171.40Å 204.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 29.96 – 2.99	Depositor EDS
% Data completeness (in resolution range)	94.0 (15.00-3.00) 88.8 (29.96-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.00Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.148 , 0.299 0.133 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 132.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 103688 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	32954	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.90 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.08	58/8387 (0.7%)	1.66	166/11442 (1.5%)
1	B	1.07	55/8387 (0.7%)	1.65	170/11442 (1.5%)
1	C	1.07	56/8387 (0.7%)	1.65	157/11442 (1.4%)
1	D	1.09	58/8376 (0.7%)	1.65	168/11427 (1.5%)
All	All	1.08	227/33537 (0.7%)	1.65	661/45753 (1.4%)

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	1	0
1	D	1	0
All	All	2	0

All (227) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	314	GLU	CD-OE2	8.73	1.35	1.25
1	D	304	GLU	CD-OE2	8.61	1.35	1.25
1	D	334	GLU	CD-OE2	8.13	1.34	1.25
1	A	304	GLU	CD-OE2	8.00	1.34	1.25
1	C	461	GLU	CD-OE2	7.99	1.34	1.25
1	D	1006	GLU	CD-OE2	7.93	1.34	1.25
1	C	904	GLU	CD-OE2	7.93	1.34	1.25
1	B	416	GLU	CD-OE2	7.91	1.34	1.25
1	B	326	GLU	CD-OE2	7.86	1.34	1.25
1	D	281	GLU	CD-OE2	7.80	1.34	1.25
1	A	281	GLU	CD-OE2	7.64	1.34	1.25
1	D	170	GLU	CD-OE2	7.59	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	979	GLU	CD-OE2	7.54	1.33	1.25
1	C	334	GLU	CD-OE2	7.36	1.33	1.25
1	C	487	GLU	CD-OE2	7.33	1.33	1.25
1	B	304	GLU	CD-OE2	7.24	1.33	1.25
1	B	334	GLU	CD-OE2	7.20	1.33	1.25
1	B	17	GLU	CD-OE2	7.17	1.33	1.25
1	B	412	GLU	CD-OE2	7.13	1.33	1.25
1	D	416	GLU	CD-OE2	7.07	1.33	1.25
1	B	797	GLU	CD-OE2	7.02	1.33	1.25
1	C	724	GLU	CD-OE2	6.93	1.33	1.25
1	C	750	GLU	CD-OE2	6.91	1.33	1.25
1	B	943	GLU	CD-OE2	6.77	1.33	1.25
1	A	1006	GLU	CD-OE2	6.75	1.33	1.25
1	C	412	GLU	CD-OE2	6.75	1.33	1.25
1	A	537	GLU	CD-OE2	6.72	1.33	1.25
1	D	487	GLU	CD-OE2	6.71	1.33	1.25
1	A	980	GLU	CD-OE2	6.71	1.33	1.25
1	A	358	GLU	CD-OE2	6.70	1.33	1.25
1	A	529	GLU	CD-OE2	6.69	1.33	1.25
1	D	438	GLU	CD-OE2	6.69	1.33	1.25
1	A	487	GLU	CD-OE2	6.69	1.33	1.25
1	C	979	GLU	CD-OE2	6.67	1.32	1.25
1	B	75	GLU	CD-OE2	6.64	1.32	1.25
1	D	324	GLU	CD-OE2	6.61	1.32	1.25
1	D	724	GLU	CD-OE2	6.60	1.32	1.25
1	A	67	GLU	CD-OE2	6.57	1.32	1.25
1	C	281	GLU	CD-OE2	6.52	1.32	1.25
1	D	637	GLU	CD-OE2	6.52	1.32	1.25
1	D	198	GLU	CD-OE2	6.51	1.32	1.25
1	B	508	GLU	CD-OE2	6.47	1.32	1.25
1	D	979	GLU	CD-OE2	6.45	1.32	1.25
1	B	358	GLU	CD-OE2	6.45	1.32	1.25
1	D	508	GLU	CD-OE2	6.41	1.32	1.25
1	D	358	GLU	CD-OE2	6.40	1.32	1.25
1	C	369	GLU	CD-OE2	6.40	1.32	1.25
1	B	1006	GLU	CD-OE2	6.38	1.32	1.25
1	C	438	GLU	CD-OE2	6.36	1.32	1.25
1	A	979	GLU	CD-OE2	6.35	1.32	1.25
1	C	934	GLU	CD-OE2	6.33	1.32	1.25
1	D	537	GLU	CD-OE2	6.31	1.32	1.25
1	C	80	GLU	CD-OE2	6.30	1.32	1.25
1	D	808	GLU	CD-OE2	6.30	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	710	GLU	CD-OE2	6.29	1.32	1.25
1	B	241	GLU	CD-OE2	6.29	1.32	1.25
1	C	529	GLU	CD-OE2	6.29	1.32	1.25
1	C	304	GLU	CD-OE2	6.28	1.32	1.25
1	C	170	GLU	CD-OE2	6.28	1.32	1.25
1	B	41	GLU	CD-OE2	6.27	1.32	1.25
1	A	969	GLU	CD-OE2	6.27	1.32	1.25
1	A	324	GLU	CD-OE2	6.27	1.32	1.25
1	A	338	GLU	CD-OE2	6.24	1.32	1.25
1	D	71	GLU	CD-OE2	6.23	1.32	1.25
1	A	334	GLU	CD-OE2	6.23	1.32	1.25
1	B	296	GLU	CD-OE2	6.22	1.32	1.25
1	A	412	GLU	CD-OE2	6.22	1.32	1.25
1	B	243	GLU	CD-OE2	6.19	1.32	1.25
1	C	181	GLU	CD-OE2	6.17	1.32	1.25
1	B	969	GLU	CD-OE2	6.16	1.32	1.25
1	C	797	GLU	CD-OE2	6.16	1.32	1.25
1	B	724	GLU	CD-OE2	6.15	1.32	1.25
1	C	1006	GLU	CD-OE2	6.15	1.32	1.25
1	C	637	GLU	CD-OE2	6.14	1.32	1.25
1	B	980	GLU	CD-OE2	6.12	1.32	1.25
1	C	324	GLU	CD-OE2	6.12	1.32	1.25
1	D	943	GLU	CD-OE2	6.11	1.32	1.25
1	D	75	GLU	CD-OE2	6.11	1.32	1.25
1	A	681	GLU	CD-OE2	6.10	1.32	1.25
1	B	808	GLU	CD-OE2	6.09	1.32	1.25
1	A	637	GLU	CD-OE2	6.09	1.32	1.25
1	A	508	GLU	CD-OE2	6.06	1.32	1.25
1	C	314	GLU	CD-OE2	6.06	1.32	1.25
1	B	904	GLU	CD-OE2	6.06	1.32	1.25
1	A	80	GLU	CD-OE2	6.05	1.32	1.25
1	C	136	GLU	CD-OE2	6.04	1.32	1.25
1	B	170	GLU	CD-OE2	6.04	1.32	1.25
1	D	296	GLU	CD-OE2	6.04	1.32	1.25
1	A	438	GLU	CD-OE2	6.03	1.32	1.25
1	B	650	GLU	CD-OE2	6.02	1.32	1.25
1	D	80	GLU	CD-OE2	6.01	1.32	1.25
1	D	243	GLU	CD-OE2	6.01	1.32	1.25
1	C	508	GLU	CD-OE2	6.00	1.32	1.25
1	D	117	GLU	CD-OE2	6.00	1.32	1.25
1	B	667	GLU	CD-OE2	6.00	1.32	1.25
1	B	57	GLU	CD-OE2	5.99	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	GLU	CD-OE2	5.99	1.32	1.25
1	D	241	GLU	CD-OE2	5.97	1.32	1.25
1	B	487	GLU	CD-OE2	5.97	1.32	1.25
1	D	871	GLU	CD-OE2	5.96	1.32	1.25
1	B	369	GLU	CD-OE2	5.93	1.32	1.25
1	D	461	GLU	CD-OE2	5.93	1.32	1.25
1	D	326	GLU	CD-OE2	5.92	1.32	1.25
1	A	943	GLU	CD-OE2	5.91	1.32	1.25
1	D	797	GLU	CD-OE2	5.91	1.32	1.25
1	B	710	GLU	CD-OE2	5.90	1.32	1.25
1	B	324	GLU	CD-OE2	5.90	1.32	1.25
1	C	249	GLU	CD-OE2	5.90	1.32	1.25
1	D	57	GLU	CD-OE2	5.89	1.32	1.25
1	C	980	GLU	CD-OE2	5.89	1.32	1.25
1	D	264	GLU	CD-OE2	5.88	1.32	1.25
1	C	338	GLU	CD-OE2	5.88	1.32	1.25
1	B	71	GLU	CD-OE2	5.87	1.32	1.25
1	A	369	GLU	CD-OE2	5.86	1.32	1.25
1	B	580	GLU	CD-OE2	5.86	1.32	1.25
1	D	667	GLU	CD-OE2	5.86	1.32	1.25
1	A	241	GLU	CD-OE2	5.84	1.32	1.25
1	B	819	GLU	CD-OE2	5.83	1.32	1.25
1	D	249	GLU	CD-OE2	5.83	1.32	1.25
1	C	969	GLU	CD-OE2	5.81	1.32	1.25
1	C	117	GLU	CD-OE2	5.81	1.32	1.25
1	B	637	GLU	CD-OE2	5.81	1.32	1.25
1	C	667	GLU	CD-OE2	5.81	1.32	1.25
1	D	338	GLU	CD-OE2	5.81	1.32	1.25
1	A	710	GLU	CD-OE2	5.80	1.32	1.25
1	C	198	GLU	CD-OE2	5.80	1.32	1.25
1	B	893	GLU	CD-OE2	5.79	1.32	1.25
1	B	438	GLU	CD-OE2	5.79	1.32	1.25
1	C	264	GLU	CD-OE2	5.78	1.32	1.25
1	A	750	GLU	CD-OE2	5.75	1.31	1.25
1	C	684	GLU	CD-OE2	5.75	1.31	1.25
1	B	619	GLU	CD-OE2	5.74	1.31	1.25
1	D	819	GLU	CD-OE2	5.74	1.31	1.25
1	A	71	GLU	CD-OE2	5.73	1.31	1.25
1	D	277	GLU	CD-OE2	5.73	1.31	1.25
1	A	17	GLU	CD-OE2	5.73	1.31	1.25
1	D	136	GLU	CD-OE2	5.73	1.31	1.25
1	C	296	GLU	CD-OE2	5.72	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	819	GLU	CD-OE2	5.70	1.31	1.25
1	D	369	GLU	CD-OE2	5.70	1.31	1.25
1	A	243	GLU	CD-OE2	5.69	1.31	1.25
1	A	277	GLU	CD-OE2	5.69	1.31	1.25
1	B	131	GLU	CD-OE2	5.69	1.31	1.25
1	A	264	GLU	CD-OE2	5.69	1.31	1.25
1	A	461	GLU	CD-OE2	5.69	1.31	1.25
1	C	681	GLU	CD-OE2	5.68	1.31	1.25
1	A	131	GLU	CD-OE2	5.68	1.31	1.25
1	A	416	GLU	CD-OE2	5.68	1.31	1.25
1	C	808	GLU	CD-OE2	5.68	1.31	1.25
1	D	980	GLU	CD-OE2	5.67	1.31	1.25
1	D	904	GLU	CD-OE2	5.67	1.31	1.25
1	C	57	GLU	CD-OE2	5.65	1.31	1.25
1	D	969	GLU	CD-OE2	5.64	1.31	1.25
1	B	689	GLU	CD-OE2	5.64	1.31	1.25
1	C	871	GLU	CD-OE2	5.64	1.31	1.25
1	A	797	GLU	CD-OE2	5.64	1.31	1.25
1	D	750	GLU	CD-OE2	5.64	1.31	1.25
1	B	40	GLU	CD-OE2	5.64	1.31	1.25
1	A	667	GLU	CD-OE2	5.63	1.31	1.25
1	B	249	GLU	CD-OE2	5.63	1.31	1.25
1	A	871	GLU	CD-OE2	5.62	1.31	1.25
1	A	41	GLU	CD-OE2	5.62	1.31	1.25
1	B	744	GLU	CD-OE2	5.62	1.31	1.25
1	D	893	GLU	CD-OE2	5.61	1.31	1.25
1	B	80	GLU	CD-OE2	5.60	1.31	1.25
1	B	750	GLU	CD-OE2	5.59	1.31	1.25
1	A	181	GLU	CD-OE2	5.59	1.31	1.25
1	A	819	GLU	CD-OE2	5.59	1.31	1.25
1	A	40	GLU	CD-OE2	5.59	1.31	1.25
1	B	684	GLU	CD-OE2	5.59	1.31	1.25
1	D	181	GLU	CD-OE2	5.58	1.31	1.25
1	B	117	GLU	CD-OE2	5.58	1.31	1.25
1	C	580	GLU	CD-OE2	5.58	1.31	1.25
1	A	296	GLU	CD-OE2	5.56	1.31	1.25
1	C	744	GLU	CD-OE2	5.56	1.31	1.25
1	B	314	GLU	CD-OE2	5.56	1.31	1.25
1	C	641	GLU	CD-OE2	5.55	1.31	1.25
1	C	277	GLU	CD-OE2	5.55	1.31	1.25
1	D	681	GLU	CD-OE2	5.54	1.31	1.25
1	A	580	GLU	CD-OE2	5.53	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	689	GLU	CD-OE2	5.51	1.31	1.25
1	B	264	GLU	CD-OE2	5.50	1.31	1.25
1	C	689	GLU	CD-OE2	5.49	1.31	1.25
1	A	57	GLU	CD-OE2	5.49	1.31	1.25
1	C	71	GLU	CD-OE2	5.48	1.31	1.25
1	A	689	GLU	CD-OE2	5.47	1.31	1.25
1	D	131	GLU	CD-OE2	5.46	1.31	1.25
1	D	684	GLU	CD-OE2	5.46	1.31	1.25
1	D	529	GLU	CD-OE1	-5.45	1.19	1.25
1	A	136	GLU	CD-OE2	5.45	1.31	1.25
1	D	710	GLU	CD-OE2	5.43	1.31	1.25
1	B	338	GLU	CD-OE2	5.42	1.31	1.25
1	C	416	GLU	CD-OE2	5.41	1.31	1.25
1	C	40	GLU	CD-OE2	5.41	1.31	1.25
1	C	893	GLU	CD-OE2	5.41	1.31	1.25
1	C	943	GLU	CD-OE2	5.39	1.31	1.25
1	D	40	GLU	CD-OE2	5.39	1.31	1.25
1	A	641	GLU	CD-OE2	5.39	1.31	1.25
1	A	314	GLU	CD-OE2	5.39	1.31	1.25
1	B	281	GLU	CD-OE2	5.38	1.31	1.25
1	A	198	GLU	CD-OE2	5.35	1.31	1.25
1	B	136	GLU	CD-OE2	5.35	1.31	1.25
1	C	41	GLU	CD-OE2	5.35	1.31	1.25
1	B	181	GLU	CD-OE2	5.34	1.31	1.25
1	D	641	GLU	CD-OE2	5.32	1.31	1.25
1	A	170	GLU	CD-OE2	5.31	1.31	1.25
1	C	67	GLU	CD-OE2	5.31	1.31	1.25
1	A	893	GLU	CD-OE2	5.30	1.31	1.25
1	D	41	GLU	CD-OE2	5.29	1.31	1.25
1	D	580	GLU	CD-OE2	5.27	1.31	1.25
1	A	75	GLU	CD-OE2	5.25	1.31	1.25
1	A	744	GLU	CD-OE2	5.24	1.31	1.25
1	C	243	GLU	CD-OE2	5.24	1.31	1.25
1	D	744	GLU	CD-OE2	5.24	1.31	1.25
1	A	326	GLU	CD-OE2	5.22	1.31	1.25
1	C	131	GLU	CD-OE2	5.21	1.31	1.25
1	A	684	GLU	CD-OE2	5.21	1.31	1.25
1	A	117	GLU	CD-OE2	5.11	1.31	1.25
1	B	277	GLU	CD-OE2	5.11	1.31	1.25
1	D	934	GLU	CD-OE2	5.11	1.31	1.25
1	B	529	GLU	CD-OE2	5.11	1.31	1.25
1	D	17	GLU	CD-OE2	5.11	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	808	GLU	CD-OE2	5.10	1.31	1.25
1	C	241	GLU	CD-OE2	5.09	1.31	1.25
1	B	681	GLU	CD-OE2	5.08	1.31	1.25
1	A	724	GLU	CD-OE2	5.07	1.31	1.25
1	A	249	GLU	CD-OE2	5.05	1.31	1.25

All (661) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	685	LEU	C-N-CD	-21.41	73.50	120.60
1	B	730	LEU	C-N-CD	-21.06	74.26	120.60
1	A	987	ASP	CB-CG-OD2	-13.47	106.18	118.30
1	A	687	GLN	C-N-CD	-12.61	92.86	120.60
1	D	166	ARG	NE-CZ-NH2	-12.33	114.13	120.30
1	C	166	ARG	NE-CZ-NH1	12.03	126.32	120.30
1	D	199	ASP	CB-CG-OD2	-11.98	107.52	118.30
1	C	224	ASP	CB-CG-OD2	-11.61	107.85	118.30
1	C	368	ASP	CB-CG-OD2	-11.41	108.03	118.30
1	C	333	ARG	NE-CZ-NH1	10.97	125.79	120.30
1	C	446	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	D	561	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	C	224	ASP	CB-CG-OD1	10.62	127.86	118.30
1	B	329	ASP	CB-CG-OD2	-10.52	108.83	118.30
1	B	166	ARG	NE-CZ-NH1	10.51	125.56	120.30
1	A	329	ASP	CB-CG-OD2	-10.25	109.07	118.30
1	B	166	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	D	319	ASP	CB-CG-OD2	-9.99	109.31	118.30
1	A	234	ASP	CB-CG-OD2	-9.94	109.36	118.30
1	C	787	ALA	C-N-CD	-9.84	98.95	120.60
1	D	190	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	B	429	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	B	368	ASP	CB-CG-OD2	-9.81	109.47	118.30
1	C	479	ASP	CB-CG-OD2	-9.76	109.52	118.30
1	D	439	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	B	954	ASP	CB-CG-OD1	9.49	126.84	118.30
1	B	193	ASP	CB-CG-OD2	-9.45	109.79	118.30
1	B	987	ASP	CB-CG-OD2	-9.45	109.79	118.30
1	B	329	ASP	CB-CG-OD1	9.40	126.76	118.30
1	A	255	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	509	ASP	CB-CG-OD2	-9.36	109.88	118.30
1	C	987	ASP	CB-CG-OD2	-9.25	109.97	118.30
1	A	507	ASP	CB-CG-OD2	-9.19	110.03	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	C	199	ASP	CB-CG-OD2	-9.13	110.08	118.30
1	C	857	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	A	425	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	C	211	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	C	599	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	B	599	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	D	329	ASP	CB-CG-OD2	-9.05	110.16	118.30
1	D	951	TRP	N-CA-CB	9.03	126.85	110.60
1	D	199	ASP	CB-CG-OD1	9.02	126.42	118.30
1	C	193	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	D	446	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	B	429	ASP	CB-CG-OD1	8.96	126.36	118.30
1	B	446	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	D	978	ALA	N-CA-CB	8.94	122.61	110.10
1	C	838	THR	CA-CB-CG2	-8.91	99.92	112.40
1	D	45	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	D	251	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	B	509	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	D	429	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	D	869	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	B	685	LEU	C-N-CD	-8.78	101.29	120.60
1	C	287	ASP	CB-CG-OD1	8.77	126.19	118.30
1	B	388	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	A	659	ASP	CB-CG-OD1	8.76	126.18	118.30
1	B	224	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	D	204	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	D	439	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	A	479	ASP	CB-CG-OD1	8.69	126.12	118.30
1	C	287	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	D	333	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	C	479	ASP	CB-CG-OD1	8.62	126.06	118.30
1	A	497	ASP	CB-CG-OD1	8.61	126.05	118.30
1	B	954	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	D	569	ASP	CB-CG-OD2	-8.56	110.59	118.30
1	A	199	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	C	234	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	B	292	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	721	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	B	828	ASP	CB-CG-OD1	8.48	125.93	118.30
1	D	492	ASP	CB-CG-OD2	-8.46	110.69	118.30
1	B	164	ASP	CB-CG-OD2	-8.44	110.70	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	908	ASP	CB-CG-OD2	-8.43	110.71	118.30
1	D	96	ASP	CB-CG-OD2	-8.43	110.71	118.30
1	B	828	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	D	557	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	591	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	A	659	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	A	224	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	282	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	45	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	C	832	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	C	790	ASP	CB-CG-OD2	-8.25	110.87	118.30
1	C	594	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	D	648	ASP	CB-CG-OD2	-8.24	110.89	118.30
1	A	211	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	D	494	THR	CA-CB-CG2	-8.22	100.89	112.40
1	A	428	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	C	786	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	954	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	C	492	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	C	856	TYR	CB-CG-CD1	-8.09	116.14	121.00
1	A	234	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	96	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	B	234	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	A	233	ASP	CB-CG-OD1	8.04	125.54	118.30
1	B	234	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	193	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	D	924	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	A	69	VAL	C-N-CD	-7.96	103.10	120.60
1	A	233	ASP	CB-CG-OD2	-7.93	111.17	118.30
1	A	403	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	C	199	ASP	CB-CG-OD1	7.86	125.37	118.30
1	D	193	ASP	CB-CG-OD1	7.86	125.37	118.30
1	B	569	ASP	CB-CG-OD1	7.84	125.35	118.30
1	D	166	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	C	875	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	429	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	A	497	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	A	997	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	D	15	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	A	987	ASP	CB-CG-OD1	7.73	125.26	118.30
1	B	648	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	C	233	ASP	CB-CG-OD2	-7.72	111.35	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	671	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	954	ASP	CB-CG-OD1	7.69	125.22	118.30
1	C	164	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	569	ASP	CB-CG-OD1	7.68	125.22	118.30
1	A	292	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	C	15	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	C	954	ASP	CB-CG-OD1	7.62	125.16	118.30
1	C	446	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	A	505	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	C	859	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	96	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	B	938	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	569	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	172	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	D	802	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	569	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	D	859	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	B	15	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	A	561	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	492	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	A	144	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	A	908	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	A	144	ASP	CB-CG-OD1	7.43	124.99	118.30
1	D	211	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	D	908	ASP	CB-CG-OD1	7.40	124.96	118.30
1	C	987	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	447	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	368	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	A	447	ASP	CB-CG-OD1	7.35	124.92	118.30
1	D	252	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	B	428	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	B	809	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	C	659	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	C	439	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	772	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	782	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	C	832	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	859	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	26	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	446	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	C	671	ASP	CB-CG-OD1	7.25	124.83	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	996	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	D	572	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	B	671	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	C	164	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	D	659	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	C	96	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	B	792	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	B	997	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	82	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	B	509	ASP	CB-CG-OD1	7.15	124.74	118.30
1	B	594	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	A	428	ASP	CB-CG-OD1	7.13	124.71	118.30
1	D	916	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	D	190	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	873	ALA	N-CA-CB	7.07	120.00	110.10
1	B	609	ALA	N-CA-CB	7.07	119.99	110.10
1	A	509	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	507	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	D	164	ASP	CB-CG-OD1	7.06	124.66	118.30
1	A	224	ASP	CB-CG-OD1	7.06	124.66	118.30
1	B	917	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	59	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	786	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	829	THR	CA-CB-CG2	-7.03	102.55	112.40
1	B	255	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	C	531	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	130	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	B	832	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	857	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	446	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	561	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	211	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	45	ASP	CB-CG-OD1	6.96	124.56	118.30
1	D	172	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	C	610	ASP	CB-CG-OD1	6.93	124.54	118.30
1	D	594	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	610	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	C	329	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	366	VAL	CA-CB-CG2	-6.89	100.56	110.90
1	B	411	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	B	859	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	375	ASP	CB-CG-OD2	-6.85	112.14	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	497	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	A	77	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	C	13	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	D	507	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	C	1016	TYR	N-CA-CB	6.81	122.86	110.60
1	C	319	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	802	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	924	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	721	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	594	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	D	782	ASP	CB-CG-OD1	6.77	124.39	118.30
1	C	505	ARG	NE-CZ-NH2	6.75	123.68	120.30
1	B	224	ASP	CB-CG-OD1	6.75	124.38	118.30
1	A	746	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	B	531	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	429	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	926	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	D	919	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	C	233	ASP	CB-CG-OD1	6.73	124.35	118.30
1	D	828	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	D	211	ASP	CB-CG-OD1	6.72	124.34	118.30
1	D	206	SER	N-CA-CB	6.71	120.57	110.50
1	C	769	TRP	CB-CA-C	-6.71	96.98	110.40
1	A	721	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	D	792	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	234	ASP	CB-CG-OD1	6.69	124.33	118.30
1	B	524	LEU	CB-CA-C	-6.69	97.48	110.20
1	C	329	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	D	82	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	130	ASP	CB-CG-OD1	6.68	124.31	118.30
1	C	429	ASP	CB-CG-OD1	6.68	124.31	118.30
1	D	59	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	909	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	37	ARG	N-CA-CB	6.66	122.59	110.60
1	A	280	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	C	82	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	832	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	D	45	ASP	CB-CG-OD1	6.66	124.29	118.30
1	B	199	ASP	CB-CG-OD1	6.65	124.28	118.30
1	C	172	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	B	446	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	C	591	ASP	CB-CG-OD2	-6.63	112.33	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	949	HIS	CA-CB-CG	-6.62	102.34	113.60
1	B	591	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	233	ASP	CB-CG-OD1	6.61	124.25	118.30
1	B	594	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	77	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	252	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	790	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	828	ASP	CB-CG-OD2	-6.58	112.37	118.30
1	C	429	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	193	ASP	CB-CG-OD1	6.55	124.19	118.30
1	D	832	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	C	671	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	C	280	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	D	859	ASP	CB-CG-OD1	6.53	124.17	118.30
1	C	368	ASP	CB-CG-OD1	6.52	124.17	118.30
1	C	425	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	B	908	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	802	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	908	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	287	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	531	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	527	PRO	N-CA-CB	6.47	111.07	103.30
1	D	790	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	352	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	659	ASP	CB-CG-OD1	6.45	124.11	118.30
1	C	919	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	C	252	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	26	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	C	782	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	C	610	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	204	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	579	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	C	77	ASP	CB-CG-OD1	6.37	124.04	118.30
1	D	786	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	C	802	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	B	503	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	D	997	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	D	224	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	671	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	287	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	C	772	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	144	ASP	CB-CG-OD1	6.31	123.98	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	D	130	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	77	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	D	126	THR	CA-CB-CG2	-6.29	103.60	112.40
1	C	561	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	D	730	LEU	C-N-CD	-6.28	106.78	120.60
1	D	26	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	44	THR	CA-CB-CG2	-6.28	103.61	112.40
1	C	291	LEU	N-CA-CB	6.28	122.96	110.40
1	D	645	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	799	THR	CA-CB-CG2	-6.27	103.62	112.40
1	C	594	ASP	CB-CG-OD1	6.27	123.94	118.30
1	D	579	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	450	HIS	CA-CB-CG	6.26	124.24	113.60
1	C	859	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	13	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	C	45	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	C	553	TRP	CA-CB-CG	-6.24	101.84	113.70
1	D	429	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	375	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	233	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	746	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	832	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	C	916	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	924	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	D	685	LEU	C-N-CD	-6.21	106.95	120.60
1	A	166	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	D	699	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	505	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	479	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	C	954	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	D	72	SER	N-CA-CB	-6.20	101.20	110.50
1	B	183	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	65	ALA	N-CA-CB	6.18	118.75	110.10
1	D	594	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C	569	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	D	336	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	D	599	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	479	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	C	37	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	252	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	916	ASP	CB-CG-OD2	-6.15	112.77	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	431	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	96	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	772	ASP	CB-CG-OD1	6.14	123.83	118.30
1	D	721	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	469	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	352	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	C	942	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	D	924	ASP	CB-CG-OD1	6.13	123.81	118.30
1	D	217	LYS	N-CA-CB	6.12	121.62	110.60
1	D	746	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	657	ALA	N-CA-CB	6.12	118.67	110.10
1	C	479	ASP	C-N-CD	-6.11	107.16	120.60
1	C	958	ASN	N-CA-CB	6.11	121.59	110.60
1	D	448	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	599	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	164	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	492	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	919	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	442	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	553	TRP	CA-CB-CG	-6.08	102.15	113.70
1	A	579	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	693	GLN	N-CA-CB	6.07	121.53	110.60
1	D	432	TRP	CA-CB-CG	-6.07	102.16	113.70
1	A	594	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	37	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	A	919	ASP	CB-CG-OD1	6.05	123.75	118.30
1	D	428	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	D	591	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	172	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	411	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	329	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	144	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	C	916	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	855	THR	N-CA-CB	6.02	121.74	110.30
1	D	446	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	788	PRO	N-CA-CB	6.02	110.52	103.30
1	B	411	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	492	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	426	LEU	N-CA-CB	6.00	122.40	110.40
1	C	509	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	938	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	C	172	ASP	CB-CG-OD1	5.99	123.69	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	648	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	D	917	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	919	ASP	CB-CG-OD2	-5.98	112.91	118.30
1	C	439	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	D	509	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	287	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	469	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	C	974	HIS	N-CA-CB	5.97	121.34	110.60
1	D	15	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	403	ASP	CB-CA-C	-5.96	98.49	110.40
1	C	996	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	609	ALA	CB-CA-C	5.95	119.03	110.10
1	C	411	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	648	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	D	875	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	B	403	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	561	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	749	ILE	N-CA-CB	5.93	124.43	110.80
1	C	591	ASP	CB-CG-OD1	5.92	123.62	118.30
1	D	368	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	C	65	ALA	CB-CA-C	5.91	118.97	110.10
1	D	721	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	598	ASP	CB-CG-OD2	-5.91	112.99	118.30
1	A	252	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	772	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	783	GLN	N-CA-CB	5.89	121.21	110.60
1	D	310	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	172	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	77	ASP	CB-CG-OD1	5.89	123.60	118.30
1	C	252	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	164	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	D	411	ASP	CB-CG-OD1	5.88	123.60	118.30
1	C	229	THR	CA-CB-CG2	-5.88	104.17	112.40
1	D	591	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	938	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	938	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	368	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	233	ASP	CB-CG-OD1	5.86	123.58	118.30
1	B	782	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	45	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	280	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	961	ARG	NE-CZ-NH1	5.86	123.23	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	656	VAL	CA-CB-CG2	-5.85	102.12	110.90
1	D	154	CYS	N-CA-CB	5.85	121.13	110.60
1	D	224	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	D	875	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	875	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	B	319	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	172	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	954	ASP	CB-CG-OD1	5.82	123.53	118.30
1	B	439	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	772	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	792	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	166	ARG	CD-NE-CZ	5.79	131.71	123.60
1	A	610	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	D	14	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	382	ASN	N-CA-CB	5.76	120.98	110.60
1	A	447	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	B	509	ASP	N-CA-CB	5.76	120.97	110.60
1	C	746	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	B	579	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	221	GLN	N-CA-CB	-5.75	100.25	110.60
1	A	568	TRP	CA-CB-CG	-5.75	102.78	113.70
1	A	255	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	579	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	C	375	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	105	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	D	287	ASP	CB-CG-OD2	-5.73	113.15	118.30
1	B	59	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	119	PRO	N-CA-CB	5.72	110.17	103.30
1	C	492	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	685	LEU	CA-CB-CG	-5.71	102.16	115.30
1	A	405	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	755	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	201	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	D	634	GLN	N-CA-CB	5.71	120.87	110.60
1	D	204	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	859	ASP	CB-CG-OD2	-5.69	113.17	118.30
1	D	404	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	716	ALA	CB-CA-C	-5.69	101.56	110.10
1	A	230	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	829	THR	CA-CB-CG2	-5.69	104.44	112.40
1	C	667	GLU	N-CA-CB	5.68	120.82	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	828	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	C	352	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	161	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	D	123	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	A	190	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	553	TRP	CA-CB-CG	-5.65	102.96	113.70
1	B	503	TYR	CA-CB-CG	-5.65	102.66	113.40
1	D	312	VAL	CA-CB-CG1	-5.65	102.42	110.90
1	D	193	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	D	130	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	916	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	D	178	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	687	GLN	C-N-CD	-5.63	108.20	120.60
1	B	280	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	D	553	TRP	CA-CB-CG	-5.63	103.01	113.70
1	A	449	ASN	N-CA-CB	5.62	120.72	110.60
1	B	82	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	D	891	VAL	CA-CB-CG1	-5.62	102.48	110.90
1	C	527	PRO	N-CA-CB	5.61	110.03	103.30
1	C	319	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	195	SER	CB-CA-C	5.61	120.75	110.10
1	C	802	ASP	CB-CG-OD1	5.61	123.34	118.30
1	B	847	LYS	N-CA-CB	5.60	120.68	110.60
1	B	802	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	466	ALA	N-CA-CB	5.60	117.94	110.10
1	D	212	VAL	CA-CB-CG2	-5.59	102.52	110.90
1	C	77	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	D	375	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	C	772	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	D	497	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	591	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	359	HIS	CB-CA-C	-5.56	99.28	110.40
1	D	411	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	B	987	ASP	CB-CG-OD1	5.56	123.30	118.30
1	D	428	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	941	THR	CA-CB-CG2	-5.55	104.63	112.40
1	A	964	GLN	N-CA-CB	5.55	120.59	110.60
1	C	572	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	69	VAL	CB-CA-C	5.54	121.92	111.40
1	B	229	THR	CA-CB-CG2	-5.53	104.65	112.40
1	B	109	VAL	CB-CA-C	5.53	121.91	111.40
1	B	869	ASP	CB-CG-OD1	5.53	123.28	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	792	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	D	77	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	439	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	319	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	746	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	436	MET	CG-SD-CE	5.51	109.02	100.20
1	B	572	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	343	LEU	CA-CB-CG	-5.51	102.63	115.30
1	C	894	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	909	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	130	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	227	VAL	N-CA-CB	-5.50	99.41	111.50
1	C	855	THR	N-CA-CB	5.50	120.74	110.30
1	D	557	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	211	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	96	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	234	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	211	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	494	THR	CA-CB-CG2	-5.47	104.74	112.40
1	A	13	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	760	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	610	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	472	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	D	329	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	442	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	183	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	C	301	TRP	CB-CA-C	-5.46	99.48	110.40
1	D	237	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	792	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	B	524	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	C	46	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	201	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	572	ASP	CB-CG-OD1	5.44	123.20	118.30
1	B	869	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	648	ASP	CB-CG-OD1	5.44	123.19	118.30
1	C	857	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	954	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	857	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	642	TYR	N-CA-CB	5.42	120.35	110.60
1	D	889	ALA	CB-CA-C	5.42	118.22	110.10
1	A	557	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	181	GLU	N-CA-CB	5.41	120.34	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	100	TYR	N-CA-CB	5.40	120.33	110.60
1	C	505	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	D	234	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	952	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	840	HIS	CA-CB-CG	5.40	122.78	113.60
1	C	204	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	772	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	873	ALA	CB-CA-C	5.39	118.19	110.10
1	D	635	THR	CA-CB-CG2	-5.39	104.85	112.40
1	B	199	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	C	639	THR	CA-CB-CG2	-5.39	104.86	112.40
1	A	790	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	C	505	ARG	CD-NE-CZ	-5.38	116.07	123.60
1	C	658	LEU	CA-CB-CG	-5.38	102.93	115.30
1	B	371	THR	CA-CB-CG2	-5.38	104.87	112.40
1	D	383	ASN	N-CA-CB	5.38	120.28	110.60
1	D	37	ARG	N-CA-CB	5.37	120.27	110.60
1	C	431	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	221	GLN	CA-CB-CG	-5.37	101.59	113.40
1	C	495	ALA	N-CA-CB	-5.36	102.59	110.10
1	A	832	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	671	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	875	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	827	ALA	N-CA-CB	5.35	117.59	110.10
1	C	571	VAL	N-CA-CB	-5.35	99.73	111.50
1	D	417	THR	CA-CB-CG2	-5.35	104.92	112.40
1	A	231	PHE	CB-CA-C	-5.34	99.71	110.40
1	B	211	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	D	996	ASP	CB-CG-OD1	5.34	123.10	118.30
1	D	782	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	827	ALA	N-CA-CB	5.33	117.56	110.10
1	A	189	LEU	N-CA-CB	5.33	121.05	110.40
1	A	388	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	333	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	365	GLN	CB-CA-C	5.32	121.03	110.40
1	B	973	ARG	CD-NE-CZ	-5.30	116.18	123.60
1	C	469	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	164	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	404	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	77	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	65	ALA	CB-CA-C	5.29	118.03	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	708	TRP	CA-CB-CG	-5.28	103.67	113.70
1	B	448	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	282	ARG	CA-CB-CG	-5.27	101.81	113.40
1	B	622	HIS	CA-CB-CG	-5.27	104.65	113.60
1	C	13	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	772	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	201	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	D	507	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	404	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	446	ARG	CD-NE-CZ	5.23	130.93	123.60
1	C	288	ARG	N-CA-CB	5.23	120.01	110.60
1	A	15	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	551	LYS	CB-CA-C	5.21	120.82	110.40
1	C	612	THR	CA-CB-CG2	-5.21	105.11	112.40
1	D	473	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	C	100	TYR	N-CA-CB	5.20	119.97	110.60
1	A	924	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	439	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	252	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	648	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	216	HIS	CA-CB-CG	-5.19	104.78	113.60
1	D	204	ARG	CD-NE-CZ	5.18	130.86	123.60
1	D	288	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	329	ASP	N-CA-CB	5.18	119.93	110.60
1	A	157	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	782	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	36	TRP	CB-CA-C	-5.17	100.05	110.40
1	D	178	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	967	LEU	CA-CB-CG	-5.17	103.42	115.30
1	A	190	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	958	ASN	N-CA-CB	5.16	119.89	110.60
1	B	802	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	128	ASN	CA-CB-CG	-5.16	102.06	113.40
1	D	668	VAL	C-N-CD	-5.15	109.27	120.60
1	C	491	ALA	N-CA-CB	5.14	117.30	110.10
1	C	96	ASP	CB-CG-OD1	5.14	122.92	118.30
1	D	853	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	635	THR	CA-CB-CG2	-5.14	105.21	112.40
1	B	428	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	659	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	310	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	D	144	ASP	CB-CG-OD2	-5.12	113.69	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	362	LEU	CB-CA-C	-5.12	100.47	110.20
1	C	140	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	924	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	809	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	579	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	648	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	251	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	563	GLN	N-CA-CB	5.09	119.77	110.60
1	B	938	ARG	CB-CA-C	5.09	120.58	110.40
1	D	832	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	610	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	82	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	671	ASP	CB-CG-OD1	5.08	122.88	118.30
1	C	280	ASP	CB-CG-OD1	5.08	122.88	118.30
1	D	828	ASP	N-CA-CB	5.08	119.75	110.60
1	C	538	TYR	CB-CG-CD1	5.08	124.05	121.00
1	C	531	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	47	PRO	N-CA-CB	5.08	109.39	103.30
1	B	317	THR	CA-CB-CG2	-5.08	105.29	112.40
1	C	363	HIS	CA-CB-CG	-5.07	104.98	113.60
1	B	503	TYR	N-CA-CB	5.07	119.72	110.60
1	B	807	VAL	CA-CB-CG2	-5.06	103.30	110.90
1	C	828	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	221	GLN	CB-CA-C	-5.06	100.28	110.40
1	D	790	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	889	ALA	CB-CA-C	5.06	117.69	110.10
1	C	428	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	D	826	THR	CB-CA-C	-5.04	97.99	111.60
1	B	329	ASP	N-CA-CB	5.04	119.67	110.60
1	D	201	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	B	344	LEU	N-CA-CB	5.04	120.47	110.40
1	B	619	GLU	CG-CD-OE2	-5.03	108.24	118.30
1	C	997	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	B	1013	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	193	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	82	ASP	CB-CG-OD1	5.02	122.82	118.30
1	D	869	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	334	GLU	CG-CD-OE2	-5.01	108.28	118.30
1	C	230	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	164	ASP	N-CA-CB	5.00	119.60	110.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	37	ARG	CA
1	D	951	TRP	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8136	0	7723	593	0
1	B	8136	0	7723	660	0
1	C	8136	0	7723	548	0
1	D	8130	0	7720	550	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	103	0	0	2	0
4	B	92	0	0	9	0
4	C	108	0	0	8	0
4	D	98	0	0	6	0
All	All	32954	0	30889	2319	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 37.

All (2319) 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:D:502:MET:HB2	1:D:537:GLU:HB2	1.25	1.18
1:D:734:SER:HB3	1:D:860:GLY:HA3	1.20	1.11
1:B:18:ASN:HD22	1:B:21:VAL:HG23	1.09	1.10
1:B:737:ILE:HD12	1:B:738:PRO:HD2	1.26	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:HG13	1:A:832:ASP:HA	1.35	1.08
1:B:964:GLN:HA	1:B:967:LEU:HD12	1.34	1.08
1:D:232:ASN:ND2	1:D:237:ARG:H	1.51	1.07
1:B:316:HIS:HA	1:B:323:ILE:HD12	1.33	1.07
1:C:823:LEU:HB3	1:D:730:LEU:HD21	1.36	1.07
1:C:986:ILE:HG21	1:C:1018:LEU:HD21	1.37	1.06
1:C:502:MET:HB2	1:C:537:GLU:HG3	1.31	1.06
1:B:786:ARG:HD3	1:B:880:ALA:HB1	1.37	1.05
1:B:412:GLU:HG3	1:B:457:SER:HB3	1.37	1.03
1:B:512:PHE:HE1	1:B:517:LYS:HG3	1.23	1.02
1:A:740:LEU:HD12	1:A:741:THR:H	1.24	1.02
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.20	1.01
1:C:637:GLU:HG3	1:C:679:LEU:HD21	1.40	1.01
1:D:777:LEU:HD11	1:D:889:ALA:HA	1.44	1.00
1:C:344:LEU:HB3	1:C:349:LEU:HD21	1.39	1.00
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.39	1.00
1:A:502:MET:HB2	1:A:537:GLU:HB2	1.42	0.99
1:B:608:PHE:HD1	1:B:612:THR:HG22	1.28	0.98
1:C:746:ASP:HA	1:C:760:ARG:HG2	1.44	0.96
1:B:142:ILE:HG23	1:B:170:GLU:HG2	1.48	0.96
1:B:18:ASN:ND2	1:B:21:VAL:HG23	1.81	0.95
1:D:891:VAL:HG23	1:D:981:GLY:HA2	1.46	0.95
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.31	0.94
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.50	0.93
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.50	0.93
1:D:279:ILE:HG23	1:D:284:GLY:HA2	1.51	0.93
1:D:658:LEU:HG	1:D:661:LYS:HE3	1.51	0.92
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.04	0.92
1:A:608:PHE:HD1	1:A:612:THR:HG22	1.35	0.92
1:A:766:SER:HA	1:A:779:PRO:HB3	1.51	0.92
1:D:232:ASN:HD21	1:D:237:ARG:H	1.01	0.92
1:A:502:MET:HG3	1:A:503:TYR:CD1	2.05	0.91
1:C:942:ARG:HG3	1:C:942:ARG:HH11	1.35	0.91
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.07	0.90
1:B:139:THR:HG21	1:B:177:LEU:HD12	1.53	0.89
1:B:512:PHE:CE1	1:B:517:LYS:HG3	2.08	0.89
1:B:719:GLN:HE22	1:B:915:PHE:H	1.18	0.89
1:C:502:MET:HG3	1:C:503:TYR:CD1	2.07	0.88
1:D:658:LEU:HB3	1:D:661:LYS:HD2	1.56	0.88
1:B:292:ARG:HH11	1:B:292:ARG:HG3	1.38	0.88
1:B:786:ARG:HD3	1:B:880:ALA:CB	2.05	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:HB3	1:A:178:ARG:HH22	1.40	0.87
1:B:930:VAL:HA	1:B:973:ARG:HG2	1.55	0.87
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.56	0.87
1:A:857:ARG:HH11	1:A:857:ARG:HG2	1.38	0.86
1:B:687:GLN:HA	1:B:687:GLN:HE21	1.41	0.86
1:D:655:MET:HB2	1:D:665:SER:HA	1.57	0.86
1:D:524:LEU:HD22	1:D:561:ARG:HB3	1.58	0.85
1:A:36:TRP:CD1	1:A:41:GLU:HB3	2.11	0.85
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.39	0.85
1:C:502:MET:HB2	1:C:537:GLU:CG	2.05	0.85
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.06	0.85
1:D:285:TYR:HB3	1:D:288:ARG:HG3	1.58	0.85
1:C:687:GLN:HE21	1:C:687:GLN:HA	1.41	0.84
1:D:734:SER:HB3	1:D:860:GLY:CA	2.05	0.84
1:D:232:ASN:HD21	1:D:237:ARG:N	1.76	0.84
1:D:654:TRP:NE1	1:D:666:GLY:HA3	1.93	0.83
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.58	0.83
1:A:746:ASP:CA	1:A:760:ARG:HG3	2.09	0.83
1:B:801:ILE:HG22	1:B:803:PRO:HD3	1.61	0.83
1:A:608:PHE:CD1	1:A:612:THR:HG22	2.13	0.82
1:C:943:GLU:HB2	1:C:952:ARG:HG3	1.62	0.82
1:B:758:PHE:CE2	1:B:765:LEU:HB2	2.13	0.82
1:A:848:THR:HG21	1:B:728:VAL:HG11	1.58	0.82
1:B:608:PHE:CD1	1:B:612:THR:HG22	2.15	0.82
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.14	0.82
1:B:245:GLN:HG2	1:B:288:ARG:CG	2.09	0.81
1:D:904:GLU:HG3	1:D:936:GLY:HA2	1.60	0.81
1:A:54:LEU:HD11	1:A:214:LEU:CD2	2.11	0.81
1:D:369:GLU:O	1:D:373:VAL:HG23	1.81	0.81
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.62	0.81
1:B:237:ARG:HG3	1:B:237:ARG:HH11	1.46	0.81
1:B:507:ASP:OD1	1:B:521:LYS:HE2	1.81	0.81
1:D:657:ALA:HB2	1:D:662:PRO:HA	1.62	0.81
1:C:65:ALA:HB1	1:C:67:GLU:OE1	1.81	0.81
1:B:91:GLN:HE21	1:B:190:ARG:NH1	1.77	0.80
1:D:360:HIS:CG	1:D:361:PRO:HD2	2.15	0.80
1:A:37:ARG:HH21	1:A:218:PRO:HD3	1.46	0.80
1:B:13:ARG:NH1	1:C:13:ARG:NH1	2.29	0.80
1:B:406:GLY:O	1:B:407:LEU:HD23	1.82	0.80
1:B:580:GLU:HG3	1:B:581:ASN:OD1	1.82	0.79
1:D:606:LEU:HB3	1:D:617:LEU:HD13	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ARG:HG2	1:C:43:ARG:HH11	1.46	0.79
1:D:157:ARG:NH1	1:D:176:PHE:HA	1.98	0.79
1:B:900:LEU:HB2	1:B:939:CYS:O	1.82	0.79
1:A:354:VAL:HA	1:A:567:VAL:H	1.46	0.79
1:A:942:ARG:HD2	1:A:953:GLY:O	1.81	0.79
1:B:142:ILE:CG2	1:B:170:GLU:HG2	2.11	0.79
1:C:535:LEU:HD22	1:C:538:TYR:HB3	1.65	0.79
1:D:232:ASN:ND2	1:D:237:ARG:N	2.27	0.79
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.63	0.79
1:C:879:PRO:O	1:C:1009:LEU:HD12	1.83	0.79
1:B:274:PHE:HB3	1:B:286:ALA:O	1.83	0.79
1:C:128:ASN:OD1	1:C:180:GLY:HA2	1.82	0.78
1:D:1022:GLN:NE2	1:D:1023:LYS:HB2	1.97	0.78
1:B:958:ASN:OD1	1:B:985:ASN:HB2	1.82	0.78
1:A:668:VAL:HG12	1:A:669:PRO:HD2	1.66	0.78
1:A:101:THR:HG23	1:A:204:ARG:CZ	2.14	0.78
1:A:848:THR:HG21	1:B:728:VAL:CG1	2.12	0.78
1:A:568:TRP:CE2	1:A:569:ASP:HB3	2.19	0.78
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.48	0.78
1:D:926:TYR:O	1:D:928:PRO:HD3	1.83	0.78
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.49	0.78
1:B:631:LEU:HD12	1:B:635:THR:O	1.84	0.78
1:A:310:ARG:HG3	1:A:310:ARG:HH11	1.48	0.78
1:B:629:PHE:CD2	1:B:638:VAL:HG22	2.19	0.78
1:D:577:LYS:HE2	1:D:591:ASP:O	1.84	0.78
1:B:600:GLN:N	1:B:600:GLN:HE21	1.82	0.78
1:B:737:ILE:HD12	1:B:738:PRO:CD	2.11	0.77
1:A:740:LEU:HD12	1:A:741:THR:N	1.99	0.77
1:A:796:SER:HB2	1:A:802:ASP:HB3	1.66	0.77
1:B:360:HIS:CG	1:B:363:HIS:HB2	2.19	0.77
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.65	0.77
1:C:818:ALA:HB1	1:C:842:TRP:HB3	1.66	0.77
1:A:37:ARG:HG3	1:A:37:ARG:HH11	1.48	0.77
1:B:36:TRP:CD1	1:B:41:GLU:HB2	2.20	0.77
1:C:141:ILE:HD13	1:C:143:PHE:CE1	2.20	0.77
1:D:237:ARG:HB3	1:D:237:ARG:NH1	1.97	0.76
1:A:502:MET:HG3	1:A:503:TYR:HD1	1.47	0.76
1:A:843:GLN:HG3	1:A:848:THR:HA	1.65	0.76
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.65	0.76
1:D:69:VAL:HG13	1:D:70:PRO:HD2	1.65	0.76
1:C:487:GLU:HG2	1:C:491:ALA:HB2	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:LEU:O	1:B:651:LEU:HD23	1.86	0.76
1:D:651:LEU:HD11	1:D:653:HIS:HE1	1.48	0.76
1:D:984:LEU:HD21	1:D:986:ILE:HD11	1.66	0.75
1:B:316:HIS:HB3	1:B:322:LEU:HD12	1.67	0.75
1:D:740:LEU:HD12	1:D:741:THR:N	2.00	0.75
1:A:944:LEU:HD12	1:A:945:ASN:N	2.01	0.75
1:D:801:ILE:O	1:D:803:PRO:HD3	1.87	0.75
1:C:128:ASN:HA	1:C:180:GLY:O	1.85	0.75
1:C:786:ARG:HD3	1:C:880:ALA:HB1	1.68	0.75
1:D:99:ILE:HA	1:D:594:ASP:HB2	1.68	0.75
1:D:777:LEU:CD1	1:D:889:ALA:HA	2.15	0.75
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.52	0.75
1:B:43:ARG:HG2	1:B:43:ARG:HH11	1.52	0.75
1:A:944:LEU:HD12	1:A:945:ASN:H	1.51	0.75
1:D:479:ASP:OD1	1:D:481:SER:HB3	1.86	0.75
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.21	0.75
1:D:502:MET:HG3	1:D:503:TYR:CD1	2.22	0.75
1:A:737:ILE:HG12	1:A:738:PRO:HD2	1.67	0.75
1:A:245:GLN:HG2	4:A:4228:HOH:O	1.87	0.75
1:A:486:TYR:CE2	1:A:488:GLY:HA3	2.21	0.75
1:B:610:ASP:OD1	1:B:612:THR:HB	1.87	0.74
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.68	0.74
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.67	0.74
1:B:510:GLN:HB2	1:B:517:LYS:HB2	1.68	0.74
1:A:54:LEU:HD11	1:A:214:LEU:HD21	1.69	0.74
1:D:412:GLU:HG3	1:D:457:SER:OG	1.86	0.74
1:C:942:ARG:HG3	1:C:942:ARG:NH1	2.01	0.74
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.17	0.74
1:C:274:PHE:CD2	1:C:289:VAL:HG12	2.23	0.74
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.00	0.74
1:A:946:TYR:O	1:A:949:HIS:HB2	1.88	0.74
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.70	0.74
1:D:143:PHE:O	1:D:168:PRO:HA	1.87	0.74
1:C:224:ASP:HB3	1:C:245:GLN:HG3	1.69	0.74
1:C:372:MET:HE1	1:C:397:LEU:HB3	1.67	0.74
1:C:85:VAL:O	1:C:88:SER:HB3	1.88	0.74
1:B:763:GLY:O	1:B:838:THR:HG21	1.88	0.74
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.23	0.74
1:A:412:GLU:HB2	1:A:457:SER:HB3	1.69	0.74
1:A:902:PRO:HD3	1:A:918:TRP:CH2	2.21	0.74
1:A:829:THR:C	1:A:830:LEU:HD23	2.08	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:SER:O	1:B:1005:ALA:C	2.21	0.73
1:D:502:MET:HB2	1:D:537:GLU:CB	2.12	0.73
1:A:745:MET:CE	1:A:745:MET:HA	2.18	0.73
1:A:857:ARG:NH1	1:A:857:ARG:HG2	2.03	0.73
1:A:403:ASP:OD1	1:A:451:PRO:HD2	1.88	0.73
1:C:140:ARG:O	1:C:214:LEU:HD12	1.88	0.73
1:B:487:GLU:HG2	1:B:491:ALA:HB2	1.70	0.73
1:D:533:LEU:HD23	1:D:534:ILE:N	2.03	0.73
1:A:767:GLN:HG3	1:A:768:MET:N	2.02	0.73
1:C:24:LEU:HD12	1:C:161:TYR:HB3	1.70	0.73
1:C:53:SER:C	1:C:54:LEU:HD23	2.09	0.73
1:B:506:VAL:HG21	1:B:551:LYS:HG2	1.69	0.73
1:C:510:GLN:HG3	4:C:4005:HOH:O	1.89	0.73
1:C:502:MET:HG3	1:C:503:TYR:HD1	1.52	0.72
1:A:785:THR:O	1:A:881:ARG:HD2	1.87	0.72
1:A:358:GLU:HG2	1:A:367:MET:CG	2.19	0.72
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.52	0.72
1:B:940:GLY:HA2	4:B:4639:HOH:O	1.88	0.72
1:D:685:LEU:HD23	1:D:686:PRO:HD2	1.72	0.72
1:B:599:ARG:HB2	1:B:600:GLN:NE2	2.04	0.72
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.19	0.72
1:C:653[A]:HIS:CE1	1:C:667:GLU:HG2	2.24	0.72
1:B:706:THR:HG23	1:B:709:SER:OG	1.88	0.72
1:B:754:LYS:HD3	1:B:1022:GLN:HG3	1.71	0.72
1:C:261:TRP:CH2	1:C:266:GLN:HB2	2.24	0.72
1:B:780:LEU:HD12	1:B:886:CYS:HB3	1.70	0.72
1:B:942:ARG:HG3	1:B:942:ARG:HH11	1.54	0.72
1:D:354:VAL:HG23	1:D:567:VAL:HB	1.72	0.72
1:D:124:SER:HA	1:D:184:LEU:O	1.89	0.72
1:B:637:GLU:CD	1:B:677:LYS:HE3	2.09	0.72
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.71	0.72
1:D:658:LEU:HG	1:D:661:LYS:CE	2.19	0.72
1:B:928:PRO:HB2	1:B:973:ARG:NH1	2.05	0.72
1:D:655:MET:HG2	1:D:656:VAL:N	2.02	0.72
1:A:472:TYR:CZ	1:A:476:LYS:HD3	2.24	0.71
1:D:656:VAL:HG21	1:D:685:LEU:HD22	1.72	0.71
1:C:989:PHE:CE1	1:C:1014:TYR:HB3	2.25	0.71
1:B:768:MET:HB3	1:B:775:GLN:HB2	1.71	0.71
1:A:651:LEU:HD11	1:A:667:GLU:HG2	1.72	0.71
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.72	0.71
1:B:942:ARG:NH1	1:B:942:ARG:HG3	2.06	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.72	0.71
1:C:167:LEU:HB3	1:C:168:PRO:HD2	1.71	0.71
1:A:71:GLU:O	1:A:74:LEU:HB2	1.89	0.71
1:D:54:LEU:HB2	1:D:212:VAL:HG12	1.72	0.71
1:A:652:LEU:HD11	1:A:698:VAL:HB	1.72	0.71
1:C:995:GLY:H	1:C:1002:SER:HB2	1.55	0.71
1:C:444:VAL:O	1:C:448:ARG:HG2	1.91	0.71
1:B:129:VAL:HG23	1:B:182:ASN:HD21	1.56	0.71
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.26	0.71
1:B:333:ARG:HG2	1:B:333:ARG:HH11	1.54	0.71
1:D:722:LEU:N	1:D:722:LEU:HD23	2.04	0.71
1:D:251:ARG:HH11	1:D:251:ARG:HG3	1.56	0.71
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.73	0.71
1:A:86:VAL:CG1	1:A:87:PRO:HA	2.21	0.70
1:C:554:GLN:HE22	1:C:558:GLN:HB2	1.55	0.70
1:B:502:MET:CB	1:B:537:GLU:HB2	2.21	0.70
1:D:638:VAL:O	1:D:677:LYS:HA	1.92	0.70
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.55	0.70
1:B:251:ARG:O	1:B:254:LEU:HB2	1.91	0.70
1:D:573:GLN:HB2	1:D:602:CYS:O	1.91	0.70
1:D:473:ARG:HH11	1:D:476:LYS:HB3	1.54	0.70
1:C:693:GLN:HB3	1:C:695:TRP:HE1	1.55	0.70
1:B:778:THR:HG22	1:B:779:PRO:HD2	1.73	0.70
1:A:786:ARG:HG2	1:A:880:ALA:HB1	1.74	0.70
1:D:367:MET:CE	1:D:371:THR:HB	2.20	0.70
1:C:939:CYS:HB3	1:C:956:GLN:OE1	1.91	0.70
1:C:906:TYR:CZ	1:C:937:LEU:HB2	2.27	0.70
1:B:974:HIS:O	1:B:975:LEU:HD23	1.91	0.70
1:C:36:TRP:CD1	1:C:41:GLU:HB2	2.26	0.70
1:B:880:ALA:O	1:B:991:MET:HB3	1.92	0.70
1:D:662:PRO:C	1:D:663:LEU:HD23	2.12	0.70
1:A:789:LEU:O	1:A:793:ILE:HD12	1.91	0.70
1:A:383:ASN:ND2	1:A:625:GLN:HA	2.07	0.70
1:B:745:MET:HA	1:B:760:ARG:HB2	1.74	0.70
1:D:502:MET:HG3	1:D:503:TYR:CE1	2.26	0.69
1:A:30:HIS:ND1	1:A:31:PRO:O	2.23	0.69
1:B:142:ILE:HG23	1:B:170:GLU:CG	2.22	0.69
1:D:114:VAL:HG11	1:D:192:SER:N	2.07	0.69
1:C:579:ASP:OD1	1:C:583:ASN:HB2	1.92	0.69
1:A:304:GLU:HG2	1:A:642:TYR:HD2	1.57	0.69
1:B:640:SER:O	1:B:675:GLN:HA	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:LEU:HD12	1:C:635:THR:O	1.92	0.69
1:B:71:GLU:O	1:B:72:SER:C	2.29	0.69
1:C:740:LEU:HD12	1:C:741:THR:N	2.07	0.69
1:A:37:ARG:NH2	1:A:218:PRO:HD3	2.07	0.69
1:B:237:ARG:HG3	1:B:237:ARG:NH1	2.07	0.69
1:B:277:GLU:O	1:B:279:ILE:HD13	1.92	0.69
1:D:748:CYS:C	1:D:749:ILE:HD12	2.12	0.69
1:A:119:PRO:HG2	1:A:190:ARG:HD2	1.74	0.69
1:B:39:SER:O	1:B:42:ALA:HB3	1.93	0.69
1:B:444:VAL:O	1:B:448:ARG:HG2	1.92	0.69
1:A:395:HIS:CG	1:A:396:PRO:HD2	2.28	0.69
1:C:355:ASN:OD1	1:C:388:ARG:HD3	1.93	0.69
1:B:278:ILE:HD12	1:B:278:ILE:H	1.57	0.69
1:C:637:GLU:HG3	1:C:679:LEU:CD2	2.20	0.69
1:B:703:PRO:O	1:B:711:ALA:HB1	1.92	0.69
1:D:942:ARG:HG3	1:D:942:ARG:NH1	2.08	0.69
1:C:887:GLN:NE2	1:C:980:GLU:O	2.26	0.68
1:D:118:ASN:O	1:D:119:PRO:C	2.31	0.68
1:D:773:LYS:HD2	1:D:774:LYS:O	1.93	0.68
1:C:649:ASN:OD1	1:C:703:PRO:HD2	1.92	0.68
1:C:344:LEU:CB	1:C:349:LEU:HD21	2.18	0.68
1:A:153:TRP:CD1	1:A:158:TRP:HA	2.29	0.68
1:D:942:ARG:HG3	1:D:942:ARG:HH11	1.58	0.68
1:C:578:TYR:CE2	1:C:584:PRO:HB3	2.29	0.68
1:A:621:LYS:HD3	1:A:717:TRP:CZ3	2.28	0.68
1:D:333:ARG:NH2	1:D:453:VAL:O	2.26	0.68
1:A:304:GLU:HG2	1:A:642:TYR:CD2	2.28	0.68
1:B:369:GLU:HG3	1:B:397:LEU:HD21	1.75	0.68
1:C:618:THR:HG21	1:C:903[B]:GLN:HG2	1.76	0.68
1:A:134:LEU:HD12	1:A:134:LEU:N	2.08	0.68
1:D:91:GLN:HG3	1:D:96:ASP:OD1	1.93	0.68
1:B:128:ASN:HA	1:B:180:GLY:O	1.93	0.68
1:A:36:TRP:HD1	1:A:41:GLU:HB3	1.55	0.68
1:A:356:ARG:NH1	1:A:356:ARG:HG2	2.06	0.68
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.29	0.68
1:A:180:GLY:O	1:A:182:ASN:ND2	2.27	0.68
1:C:14:ARG:HA	1:C:16:TRP:CZ3	2.28	0.68
1:B:782:ASP:HA	1:B:884:LEU:HD23	1.76	0.68
1:C:706:THR:OG1	1:C:709:SER:N	2.27	0.67
1:B:43:ARG:HG2	1:B:43:ARG:NH1	2.09	0.67
1:C:778:THR:HB	1:C:779:PRO:HD2	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.77	0.67
1:C:54:LEU:N	1:C:54:LEU:HD23	2.09	0.67
1:B:59:ARG:NH1	1:B:81:ALA:O	2.28	0.67
1:A:127:PHE:HE2	1:A:184:LEU:HD23	1.59	0.67
1:D:930:VAL:O	1:D:932:PRO:HD3	1.95	0.67
1:A:358:GLU:HG2	1:A:367:MET:HG3	1.76	0.67
1:C:833:ALA:HB1	1:C:858:ILE:O	1.95	0.67
1:A:608:PHE:N	1:A:612:THR:O	2.27	0.67
1:D:569:ASP:O	1:D:605:GLY:HA2	1.95	0.67
1:D:836:ILE:HB	1:D:856:TYR:HB2	1.75	0.67
1:B:961:ARG:NH2	1:B:979:GLU:O	2.27	0.67
1:D:134:LEU:N	1:D:134:LEU:HD23	2.09	0.67
1:A:919:ASP:O	1:A:920:LEU:HD23	1.95	0.67
1:B:393:PRO:HD3	1:B:412:GLU:O	1.94	0.67
1:D:285:TYR:CB	1:D:288:ARG:HG3	2.25	0.67
1:A:945:ASN:OD1	1:A:950:GLN:NE2	2.27	0.67
1:C:836:ILE:N	1:C:836:ILE:HD13	2.10	0.67
1:B:1011:ALA:HB3	1:B:1014:TYR:CE1	2.30	0.67
1:B:200:GLN:NE2	1:B:391:HIS:O	2.28	0.67
1:B:255:ARG:HB2	1:B:316:HIS:CE1	2.29	0.66
1:B:887:GLN:NE2	1:B:980:GLU:O	2.26	0.66
1:C:59:ARG:NH1	1:C:81:ALA:O	2.27	0.66
1:A:1020:TRP:HD1	1:A:1021:CYS:N	1.93	0.66
1:A:453:VAL:HG12	1:A:482:ARG:HE	1.58	0.66
1:D:577:LYS:O	1:D:584:PRO:HA	1.94	0.66
1:D:656:VAL:HG21	1:D:685:LEU:CD2	2.25	0.66
1:D:927:THR:HG23	1:D:928:PRO:HD2	1.78	0.66
1:C:131:GLU:OE2	1:C:135:GLN:NE2	2.29	0.66
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.77	0.66
1:A:836:ILE:N	1:A:836:ILE:HD13	2.10	0.66
1:D:190:ARG:NH2	1:D:204:ARG:O	2.28	0.66
1:B:891:VAL:HG23	1:B:981:GLY:HA2	1.78	0.66
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.78	0.66
1:C:43:ARG:HG2	1:C:43:ARG:NH1	2.10	0.66
1:C:63:PHE:HB3	1:C:64:PRO:HD2	1.77	0.66
1:A:682:LEU:HD22	1:A:683:PRO:HD2	1.77	0.66
1:A:424:ASN:HD21	1:D:279:ILE:HD11	1.60	0.66
1:D:904:GLU:HG3	1:D:936:GLY:CA	2.26	0.66
1:B:701:VAL:O	1:B:703:PRO:HD3	1.95	0.66
1:C:986:ILE:CG2	1:C:1018:LEU:HD21	2.22	0.66
1:B:767:GLN:OE1	1:B:768:MET:N	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:891:VAL:CG2	1:B:981:GLY:HA2	2.25	0.66
1:B:14:ARG:HG2	1:B:16:TRP:CZ2	2.30	0.66
1:B:830:LEU:HD11	1:B:835:LEU:HB2	1.76	0.66
1:A:43:ARG:HH21	1:A:264:GLU:HA	1.61	0.66
1:C:646:HIS:O	1:C:648:ASP:N	2.28	0.66
1:C:767:GLN:CD	1:C:768:MET:H	2.00	0.66
1:D:853:ARG:NH1	1:D:871:GLU:OE2	2.29	0.66
1:C:146:VAL:HG11	1:C:150:PHE:CD2	2.31	0.66
1:C:608:PHE:HD1	1:C:612:THR:HG22	1.60	0.66
1:A:85:VAL:O	1:A:88:SER:HB3	1.94	0.66
1:A:128:ASN:O	1:A:129:VAL:HG22	1.96	0.65
1:D:948:PRO:O	1:D:1022:GLN:HA	1.95	0.65
1:B:129:VAL:HG23	1:B:182:ASN:ND2	2.11	0.65
1:C:693:GLN:HB3	1:C:695:TRP:NE1	2.11	0.65
1:D:824:GLN:NE2	1:D:837:THR:O	2.29	0.65
1:A:875:ASP:OD2	1:B:723:ALA:HB1	1.97	0.65
1:B:65:ALA:HB1	1:B:67:GLU:OE1	1.96	0.65
1:A:251:ARG:NH1	1:A:251:ARG:HG2	2.08	0.65
1:A:851:ILE:HD11	1:B:728:VAL:HG12	1.78	0.65
1:A:25:ASN:ND2	1:A:159:VAL:O	2.29	0.65
1:C:138:GLN:O	1:C:217:LYS:N	2.26	0.65
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.79	0.65
1:A:146:VAL:HG11	1:A:150:PHE:CD2	2.31	0.65
1:B:646:HIS:O	1:B:648:ASP:N	2.28	0.65
1:D:88:SER:HA	1:D:366:VAL:HG21	1.76	0.65
1:A:354:VAL:HG23	1:A:567:VAL:HB	1.77	0.65
1:C:37:ARG:NH2	1:C:218:PRO:HD3	2.12	0.65
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.76	0.65
1:D:69:VAL:CG1	1:D:70:PRO:HD2	2.25	0.65
1:D:129:VAL:HG22	1:D:134:LEU:HD21	1.78	0.65
1:A:420:MET:HE1	1:A:426:LEU:HD21	1.77	0.65
1:D:78:LEU:O	1:D:80:GLU:N	2.30	0.65
1:A:23:GLN:HB3	1:A:26:ARG:NH2	2.11	0.65
1:B:257:THR:HA	1:B:270:GLY:O	1.96	0.65
1:D:427:THR:HG21	1:D:462:SER:HB3	1.78	0.65
1:C:133:TRP:CZ3	1:C:216:HIS:HB2	2.32	0.65
1:A:138:GLN:OE1	1:A:140:ARG:NH2	2.29	0.65
1:C:377:LEU:HB3	1:C:381:GLN:HE22	1.62	0.65
1:A:684:GLU:OE1	1:A:685:LEU:N	2.30	0.65
1:B:282:ARG:HH21	1:C:419:GLY:C	1.99	0.65
1:B:502:MET:HB2	1:B:537:GLU:HB2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1022:GLN:HE22	1:D:1023:LYS:HB2	1.60	0.65
1:D:215:LEU:HD12	1:D:216:HIS:H	1.62	0.65
1:D:215:LEU:HD12	1:D:216:HIS:N	2.12	0.65
1:A:701:VAL:O	1:A:703:PRO:HD3	1.97	0.65
1:C:893:GLU:O	1:C:921:PRO:HA	1.97	0.65
1:B:1003:VAL:HG12	1:B:1008:GLN:HG2	1.78	0.65
1:B:751:LEU:CD1	1:B:860:GLY:HA2	2.27	0.64
1:B:513:PRO:O	1:B:515:VAL:N	2.29	0.64
1:B:398:TRP:HA	1:B:401:LEU:HD12	1.78	0.64
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.78	0.64
1:D:801:ILE:HD12	1:D:808:GLU:CD	2.18	0.64
1:B:464:HIS:HB2	1:B:489:GLY:HA3	1.78	0.64
1:B:72:SER:OG	1:B:73:TRP:N	2.30	0.64
1:D:770:ILE:O	1:D:773:LYS:HB3	1.98	0.64
1:B:794:GLY:HA3	4:B:4251:HOH:O	1.96	0.64
1:B:899:GLY:O	1:B:918:TRP:NE1	2.30	0.64
1:B:687:GLN:HA	1:B:687:GLN:NE2	2.11	0.64
1:A:279:ILE:C	1:A:279:ILE:HD12	2.18	0.64
1:B:928:PRO:O	1:B:973:ARG:NH1	2.30	0.64
1:A:304:GLU:O	1:A:305:ILE:HG12	1.97	0.64
1:C:377:LEU:HB3	1:C:381:GLN:NE2	2.12	0.64
1:C:706:THR:HB	4:C:4484:HOH:O	1.98	0.64
1:A:236:SER:O	1:A:297:ASN:N	2.29	0.64
1:A:706:THR:OG1	1:A:709:SER:N	2.29	0.64
1:C:237:ARG:HB2	1:C:237:ARG:NH1	2.12	0.64
1:B:141:ILE:CG2	1:B:173:LEU:HD11	2.28	0.64
1:B:573:GLN:HB2	1:B:602:CYS:O	1.98	0.64
1:B:693:GLN:HB3	1:B:695:TRP:CD1	2.32	0.64
1:C:423:MET:HG2	1:C:463:GLY:N	2.13	0.64
1:B:388:ARG:O	1:B:390:SER:N	2.29	0.64
1:A:571:VAL:CG2	1:A:609:ALA:HA	2.27	0.64
1:D:887:GLN:HG3	1:D:983:TRP:CE2	2.32	0.64
1:C:902:PRO:HD2	1:C:903[B]:GLN:HE21	1.63	0.64
1:B:400:THR:HG22	1:B:401:LEU:N	2.12	0.64
1:B:634:GLN:HE22	1:B:684:GLU:HA	1.63	0.64
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.13	0.64
1:A:853:ARG:NH1	1:A:871:GLU:OE2	2.30	0.64
1:C:832:ASP:OD2	1:C:857:ARG:NH2	2.31	0.64
1:D:230:ARG:NH1	1:D:241:GLU:OE1	2.31	0.64
1:B:964:GLN:HA	1:B:967:LEU:CD1	2.22	0.64
1:A:140:ARG:NH1	1:A:170:GLU:OE1	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:PRO:HD3	1:C:412:GLU:O	1.96	0.64
1:D:887:GLN:NE2	1:D:980:GLU:O	2.29	0.63
1:C:847:LYS:HG3	1:C:848:THR:N	2.12	0.63
1:A:801:ILE:O	1:A:803:PRO:HD3	1.97	0.63
1:A:749:ILE:O	1:A:755:ARG:HA	1.98	0.63
1:C:930:VAL:O	1:C:932:PRO:HD3	1.97	0.63
1:B:441:THR:HG22	1:B:474:TRP:CZ3	2.34	0.63
1:C:662:PRO:C	1:C:663:LEU:HD23	2.18	0.63
1:B:634:GLN:NE2	1:B:684:GLU:HA	2.14	0.63
1:C:24:LEU:HD12	1:C:161:TYR:CB	2.29	0.63
1:A:360:HIS:ND1	1:A:363:HIS:N	2.44	0.63
1:B:941:THR:HG22	1:B:955:PHE:CZ	2.33	0.63
1:B:412:GLU:HG2	1:B:459:GLY:HA2	1.81	0.63
1:A:834:VAL:HG12	1:A:835:LEU:N	2.13	0.63
1:D:706:THR:OG1	1:D:709:SER:N	2.31	0.63
1:B:102:ASN:OD1	1:B:201:ASP:HB2	1.98	0.63
1:D:853:ARG:HH11	1:D:853:ARG:HG3	1.64	0.63
1:C:599:ARG:HD2	1:C:600:GLN:OE1	1.99	0.63
1:A:651:LEU:HD11	1:A:653[B]:HIS:CD2	2.33	0.63
1:B:200:GLN:HE21	1:B:391:HIS:HB2	1.64	0.63
1:B:843:GLN:HA	1:B:847:LYS:O	1.97	0.63
1:C:502:MET:HG3	1:C:503:TYR:CE1	2.34	0.63
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.33	0.63
1:C:948:PRO:O	1:C:1022:GLN:HA	1.99	0.63
1:C:436:MET:HE1	1:C:467:ASN:HB2	1.80	0.63
1:C:386:ALA:HB2	1:C:408:TYR:HB2	1.81	0.63
1:A:770:ILE:HG13	1:A:775:GLN:NE2	2.14	0.62
1:D:360:HIS:ND1	1:D:361:PRO:HD2	2.14	0.62
1:B:629:PHE:HD2	1:B:638:VAL:HG22	1.64	0.62
1:C:457:SER:HB2	1:C:485:GLN:HG2	1.79	0.62
1:D:512:PHE:HE1	1:D:517:LYS:HG3	1.63	0.62
1:D:166:ARG:HG3	1:D:392:TYR:CG	2.33	0.62
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.81	0.62
1:C:66:PRO:O	1:C:69:VAL:HG23	1.99	0.62
1:C:23:GLN:O	1:C:24:LEU:HG	1.99	0.62
1:A:210:ARG:HD3	1:A:395:HIS:HB2	1.82	0.62
1:B:920:LEU:HD12	1:B:925:MET:SD	2.38	0.62
1:B:91:GLN:NE2	1:B:190:ARG:NH1	2.44	0.62
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.00	0.62
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.81	0.62
1:A:577:LYS:O	1:A:584:PRO:HA	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:932:PRO:HG3	1:B:970:THR:HG22	1.80	0.62
1:A:202:MET:CB	1:A:573:GLN:HE22	2.12	0.62
1:A:386:ALA:HB2	1:A:408:TYR:HB2	1.80	0.62
1:D:521:LYS:HG2	1:D:559:TYR:CZ	2.34	0.62
1:A:227:VAL:HG13	1:A:240:LEU:HD21	1.82	0.62
1:A:78:LEU:H	1:A:78:LEU:HD12	1.63	0.62
1:B:255:ARG:NH1	1:B:255:ARG:HG2	2.01	0.62
1:B:961:ARG:O	1:B:979:GLU:HG3	1.99	0.62
1:A:453:VAL:HG12	1:A:482:ARG:NE	2.14	0.62
1:B:694:LEU:HB3	1:B:722:LEU:HB2	1.82	0.62
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.82	0.62
1:B:192:SER:O	1:B:195:SER:HB2	2.00	0.62
1:C:687:GLN:NE2	1:C:687:GLN:HA	2.05	0.62
1:D:927:THR:CG2	1:D:928:PRO:HD2	2.30	0.62
1:C:939:CYS:HA	1:C:956:GLN:HB3	1.82	0.62
1:B:123:TYR:CE2	1:B:208:ILE:HG13	2.34	0.62
1:A:66:PRO:HD2	1:A:67:GLU:OE1	2.00	0.62
1:B:510:GLN:O	1:B:517:LYS:N	2.28	0.62
1:C:368:ASP:OD2	1:C:370:GLN:HB2	2.00	0.62
1:C:743:SER:OG	1:C:744:GLU:N	2.29	0.62
1:A:27:LEU:N	1:A:27:LEU:HD23	2.14	0.62
1:D:166:ARG:CG	1:D:392:TYR:HB2	2.27	0.62
1:A:202:MET:HB3	1:A:573:GLN:HE22	1.64	0.62
1:B:128:ASN:OD1	1:B:180:GLY:HA2	1.99	0.62
1:A:505:ARG:CG	1:A:505:ARG:HH11	2.12	0.62
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.00	0.62
1:C:416:GLU:OE2	1:C:418:HIS:HB2	2.00	0.62
1:C:746:ASP:CA	1:C:760:ARG:HG2	2.27	0.62
1:B:600:GLN:H	1:B:600:GLN:HE21	1.46	0.62
1:A:784:PHE:HA	1:A:881:ARG:O	2.00	0.62
1:C:655:MET:HE1	1:C:662:PRO:HB3	1.80	0.62
1:B:153:TRP:HZ3	1:B:187:MET:HB2	1.65	0.62
1:A:222:ILE:CD1	1:A:313:VAL:HG12	2.30	0.62
1:D:354:VAL:HB	1:D:384:PHE:CE2	2.34	0.61
1:D:241:GLU:HG3	1:D:292:ARG:HG2	1.82	0.61
1:A:599:ARG:NH1	1:A:600:GLN:OE1	2.32	0.61
1:C:291:LEU:HD23	1:C:291:LEU:N	2.15	0.61
1:A:438:GLU:O	1:A:442:ARG:HG3	1.99	0.61
1:D:649:ASN:OD1	1:D:703:PRO:HD2	1.99	0.61
1:A:770:ILE:O	1:A:773:LYS:HE3	1.99	0.61
1:B:658:LEU:HD12	1:B:659:ASP:N	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:961:ARG:HB3	1:D:978:ALA:HB1	1.82	0.61
1:A:229:THR:HA	1:A:239:VAL:O	2.00	0.61
1:B:51:LEU:HD13	1:B:215:LEU:HD13	1.83	0.61
1:C:735:HIS:CD2	1:C:735:HIS:H	2.18	0.61
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.27	0.61
1:D:740:LEU:HD12	1:D:741:THR:H	1.66	0.61
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.14	0.61
1:D:930:VAL:HA	1:D:973:ARG:HD3	1.81	0.61
1:B:793:ILE:HA	1:B:807:VAL:HG12	1.82	0.61
1:A:75:GLU:HA	1:A:75:GLU:OE1	2.00	0.61
1:C:415:ILE:HD13	1:C:436:MET:HB3	1.83	0.61
1:B:337:ILE:HG12	1:B:342:LEU:HD13	1.82	0.61
1:D:446:ARG:NH2	1:D:447:ASP:OD2	2.30	0.61
1:B:138:GLN:HG2	1:B:139:THR:N	2.14	0.61
1:A:155:ASN:CB	1:A:178:ARG:HH22	2.12	0.61
1:C:280:ASP:HB2	1:C:281:GLU:OE1	2.00	0.61
1:C:255:ARG:HG2	1:C:255:ARG:HH11	1.65	0.61
1:D:446:ARG:HH21	1:D:447:ASP:CG	2.03	0.61
1:C:44:THR:O	1:C:46:ARG:N	2.33	0.61
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.81	0.61
1:B:258:VAL:HG12	1:B:293:LEU:HD11	1.83	0.61
1:B:429:ASP:OD1	1:B:431:ARG:HG3	2.01	0.61
1:D:654:TRP:CE2	1:D:666:GLY:HA3	2.36	0.60
1:D:104:THR:HG22	1:D:105:TYR:O	2.01	0.60
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.31	0.60
1:B:14:ARG:HA	1:B:16:TRP:CZ3	2.36	0.60
1:D:427:THR:O	1:D:467:ASN:HB2	2.00	0.60
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.36	0.60
1:C:23:GLN:HB3	1:C:26:ARG:NH2	2.15	0.60
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.83	0.60
1:D:129:VAL:CG2	1:D:134:LEU:HD21	2.30	0.60
1:C:750:GLU:HG3	1:C:755:ARG:HB3	1.82	0.60
1:D:1020:TRP:HD1	1:D:1021:CYS:N	1.99	0.60
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.66	0.60
1:B:660:GLY:O	1:B:662:PRO:HD3	2.01	0.60
1:D:479:ASP:N	1:D:480:PRO:HD3	2.16	0.60
1:C:23:GLN:C	1:C:24:LEU:HG	2.22	0.60
1:C:26:ARG:HD3	1:C:169:SER:HB3	1.82	0.60
1:A:222:ILE:HD13	1:A:313:VAL:CG1	2.31	0.60
1:B:352:ARG:NH2	1:B:641:GLU:OE1	2.33	0.60
1:A:277:GLU:H	1:A:277:GLU:CD	2.05	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:NH1	1:A:43:ARG:HG2	2.16	0.60
1:C:237:ARG:HH11	1:C:237:ARG:HB2	1.65	0.60
1:B:78:LEU:HB3	1:B:80:GLU:OE2	2.01	0.60
1:C:577:LYS:HG3	1:C:587:ALA:HB2	1.83	0.60
1:A:423:MET:SD	1:A:461:GLU:HB3	2.42	0.60
1:D:919:ASP:O	1:D:920:LEU:HD23	2.02	0.60
1:D:429:ASP:OD1	1:D:431:ARG:HG3	2.01	0.60
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.82	0.60
1:B:697:THR:OG1	1:B:719:GLN:HG3	2.01	0.60
1:B:43:ARG:NH1	1:B:263:GLY:O	2.35	0.60
1:D:251:ARG:NH1	1:D:251:ARG:HG3	2.12	0.60
1:A:891:VAL:CG2	1:A:981:GLY:HA2	2.32	0.60
1:C:486:TYR:CE2	1:C:488:GLY:HA3	2.36	0.60
1:A:429:ASP:OD1	1:A:430:PRO:HD2	2.02	0.60
1:C:152:LEU:O	1:C:159:VAL:N	2.30	0.60
1:B:849:LEU:N	1:B:849:LEU:HD23	2.16	0.60
1:B:769:TRP:NE1	1:B:774:LYS:HG3	2.15	0.60
1:A:126:THR:HA	1:A:182:ASN:O	2.02	0.60
1:C:300:LEU:HD22	1:C:332:PHE:O	2.01	0.60
1:A:257:THR:HG23	1:A:270:GLY:O	2.02	0.60
1:D:619:GLU:HA	1:D:912:ALA:HB2	1.84	0.60
1:A:187:MET:O	1:A:187:MET:HG2	2.02	0.60
1:B:658:LEU:N	1:B:661:LYS:O	2.30	0.59
1:C:742:THR:HG22	1:C:743:SER:N	2.17	0.59
1:B:341:LEU:HD21	1:B:561:ARG:HG2	1.82	0.59
1:C:446:ARG:HG2	1:C:447:ASP:OD1	2.02	0.59
1:B:74:LEU:N	1:B:74:LEU:HD23	2.17	0.59
1:D:502:MET:HG2	1:D:502:MET:O	2.02	0.59
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.36	0.59
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.82	0.59
1:D:820:ALA:HB2	1:D:842:TRP:NE1	2.16	0.59
1:D:100:TYR:O	1:D:597:ASN:HA	2.02	0.59
1:B:218:PRO:O	1:B:221:GLN:NE2	2.35	0.59
1:D:906:TYR:OH	1:D:935:ASN:HA	2.01	0.59
1:A:502:MET:HG3	1:A:503:TYR:CE1	2.37	0.59
1:A:155:ASN:HB3	1:A:178:ARG:NH2	2.13	0.59
1:B:805:ALA:HB3	1:B:808:GLU:HB2	1.83	0.59
1:B:808:GLU:HA	1:B:808:GLU:OE1	2.02	0.59
1:B:868:VAL:HG11	1:B:1016:TYR:CE2	2.37	0.59
1:C:237:ARG:HG2	1:C:296:GLU:OE1	2.03	0.59
1:A:843:GLN:CG	1:A:848:THR:HA	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:PRO:HD2	1:D:533:LEU:HD21	1.84	0.59
1:C:767:GLN:NE2	1:C:774:LYS:HB3	2.18	0.59
1:B:916:ASP:HB3	1:B:918:TRP:CE2	2.37	0.59
1:D:646:HIS:O	1:D:648:ASP:N	2.34	0.59
1:A:606:LEU:HD13	1:A:617:LEU:HD12	1.85	0.59
1:D:502:MET:HA	1:D:537:GLU:O	2.01	0.59
1:D:578:TYR:HA	1:D:583:ASN:O	2.02	0.59
1:D:36:TRP:CD1	1:D:41:GLU:HB3	2.37	0.59
1:C:84:VAL:HG23	1:C:85:VAL:O	2.03	0.59
1:D:895:VAL:O	1:D:919:ASP:HA	2.03	0.59
1:A:418:HIS:ND1	1:A:461:GLU:OE1	2.35	0.59
1:D:833:ALA:HB1	1:D:858:ILE:O	2.02	0.59
1:B:141:ILE:HG12	1:B:142:ILE:N	2.16	0.59
1:A:54:LEU:HD11	1:A:214:LEU:HD22	1.85	0.59
1:A:62:TRP:CD1	1:A:95:TYR:HB3	2.38	0.59
1:A:751:LEU:HD21	1:A:860:GLY:O	2.02	0.59
1:B:629:PHE:HA	1:B:637:GLU:O	2.02	0.59
1:B:902:PRO:HD2	1:B:903[B]:GLN:HE21	1.68	0.59
1:C:60:PHE:HA	1:C:122:CYS:O	2.03	0.58
1:B:693:GLN:HB3	1:B:695:TRP:NE1	2.18	0.58
1:B:493:THR:HG23	4:B:4020:HOH:O	2.03	0.58
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.84	0.58
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.85	0.58
1:D:610:ASP:OD1	1:D:612:THR:HG23	2.02	0.58
1:D:961:ARG:HG3	1:D:961:ARG:NH1	2.17	0.58
1:D:244:VAL:O	1:D:288:ARG:HA	2.02	0.58
1:B:780:LEU:CD1	1:B:886:CYS:HB3	2.33	0.58
1:D:693:GLN:HG2	1:D:721:ARG:HD3	1.85	0.58
1:D:251:ARG:HH11	1:D:251:ARG:CG	2.15	0.58
1:C:769:TRP:HA	1:C:773:LYS:O	2.03	0.58
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.85	0.58
1:C:190:ARG:HG3	1:C:206:SER:OG	2.03	0.58
1:D:378:LEU:O	1:D:382:ASN:ND2	2.25	0.58
1:B:735:HIS:CD2	1:B:735:HIS:H	2.19	0.58
1:B:38:ASN:OD1	1:B:41:GLU:HG2	2.03	0.58
1:B:655:MET:HE3	1:B:662:PRO:HB3	1.85	0.58
1:C:579:ASP:CG	1:C:583:ASN:HB2	2.23	0.58
1:D:632:SER:N	1:D:635:THR:O	2.27	0.58
1:B:280:ASP:HB2	1:B:281:GLU:OE1	2.03	0.58
1:C:746:ASP:HA	1:C:760:ARG:CG	2.28	0.58
1:B:974:HIS:C	1:B:975:LEU:HD23	2.24	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:ASP:O	1:B:807:VAL:HG12	2.04	0.58
1:B:577:LYS:O	1:B:584:PRO:HA	2.03	0.58
1:D:62:TRP:CD1	1:D:95:TYR:HB3	2.38	0.58
1:C:496:THR:HG23	1:C:531:ARG:NH1	2.18	0.58
1:C:289:VAL:HG22	1:C:291:LEU:CD2	2.33	0.58
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.19	0.58
1:A:189:LEU:HD23	1:A:189:LEU:N	2.18	0.58
1:C:261:TRP:CZ3	1:C:266:GLN:HB2	2.37	0.58
1:D:942:ARG:HA	1:D:953:GLY:O	2.03	0.58
1:B:292:ARG:HH11	1:B:292:ARG:CG	2.15	0.58
1:B:518:TRP:CE3	1:B:522:LYS:HE2	2.39	0.58
1:C:655:MET:HE1	1:C:662:PRO:HA	1.86	0.58
1:B:559:TYR:HB2	1:B:562:LEU:HG	1.86	0.58
1:C:80:GLU:H	1:C:80:GLU:CD	2.05	0.58
1:B:832:ASP:N	1:B:832:ASP:OD1	2.37	0.58
1:C:651:LEU:HD11	1:C:653[A]:HIS:HE1	1.67	0.58
1:B:360:HIS:CE1	1:B:361:PRO:HD2	2.38	0.58
1:D:473:ARG:HD2	1:D:473:ARG:O	2.03	0.58
1:C:658:LEU:O	1:C:659:ASP:C	2.39	0.58
1:C:706:THR:HG23	1:C:709:SER:OG	2.03	0.58
1:D:870:VAL:HG21	1:D:882:ILE:HG23	1.86	0.58
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.39	0.58
1:C:678:GLN:O	1:C:679:LEU:HD23	2.04	0.58
1:A:37:ARG:NH1	1:A:37:ARG:HG3	2.16	0.58
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.85	0.58
1:C:858:ILE:HG12	1:C:864:MET:HB2	1.86	0.58
1:A:193:ASP:O	1:A:196:TYR:HB2	2.04	0.58
1:C:53:SER:O	1:C:54:LEU:HD23	2.04	0.58
1:C:767:GLN:OE1	1:C:767:GLN:HA	2.04	0.58
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.04	0.58
1:A:360:HIS:CE1	1:A:362:LEU:H	2.22	0.58
1:C:945:ASN:OD1	1:C:950:GLN:HG3	2.04	0.58
1:D:990:HIS:HD2	1:D:991:MET:O	1.86	0.58
1:A:344:LEU:N	1:A:347:LYS:O	2.32	0.57
1:A:654:TRP:NE1	1:A:666:GLY:HA3	2.18	0.57
1:B:377:LEU:O	1:B:381:GLN:HB2	2.03	0.57
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.86	0.57
1:A:782:ASP:HB2	1:A:842:TRP:CH2	2.39	0.57
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.86	0.57
1:B:986:ILE:HD11	1:B:1018:LEU:HD21	1.86	0.57
1:D:255:ARG:HH11	1:D:255:ARG:HG2	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:LEU:HD11	1:D:698:VAL:HB	1.86	0.57
1:C:786:ARG:HH21	1:C:792:ASP:CG	2.08	0.57
1:A:118:ASN:O	1:A:119:PRO:C	2.40	0.57
1:A:65:ALA:HB1	1:A:67:GLU:OE1	2.04	0.57
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.69	0.57
1:A:735:HIS:N	1:A:735:HIS:ND1	2.51	0.57
1:B:502:MET:HB3	1:B:537:GLU:HB2	1.86	0.57
1:B:780:LEU:HA	1:B:885:ASN:O	2.05	0.57
1:D:571:VAL:HG23	1:D:607:VAL:HG23	1.86	0.57
1:C:821:ALA:O	1:C:840:HIS:HA	2.05	0.57
1:B:225:PHE:HA	1:B:243:GLU:O	2.04	0.57
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.86	0.57
1:D:697:THR:HG23	1:D:719:GLN:HG2	1.86	0.57
1:C:896:ASN:HD21	1:C:917:ARG:HD2	1.69	0.57
1:B:749:ILE:HD12	1:B:749:ILE:N	2.19	0.57
1:C:176:PHE:N	1:C:176:PHE:CD1	2.71	0.57
1:A:741:THR:HG22	4:A:4722:HOH:O	2.03	0.57
1:C:86:VAL:CG1	1:C:87:PRO:HA	2.35	0.57
1:B:894:ARG:NH1	1:B:921:PRO:HD3	2.19	0.57
1:D:529:GLU:OE2	1:D:531:ARG:N	2.34	0.57
1:D:894:ARG:NE	1:D:919:ASP:OD1	2.37	0.57
1:D:35:SER:O	1:D:50:GLN:HG3	2.04	0.57
1:C:44:THR:O	1:C:45:ASP:C	2.41	0.57
1:C:970:THR:CG2	1:C:975:LEU:HB2	2.34	0.57
1:B:23:GLN:HG2	1:B:26:ARG:HE	1.68	0.57
1:A:1023:LYS:HD2	1:A:1023:LYS:C	2.24	0.57
1:B:316:HIS:CA	1:B:323:ILE:HD12	2.21	0.57
1:D:277:GLU:O	1:D:279:ILE:HG22	2.04	0.57
1:A:29:ALA:HB3	1:A:445:GLN:OE1	2.03	0.57
1:D:579:ASP:OD1	1:D:583:ASN:N	2.27	0.57
1:C:888:LEU:N	1:C:982:THR:O	2.34	0.57
1:D:654:TRP:CE3	1:D:655:MET:HA	2.40	0.57
1:A:651:LEU:CD1	1:A:667:GLU:HG2	2.35	0.57
1:A:43:ARG:O	1:A:310:ARG:HD3	2.05	0.57
1:C:397:LEU:HD12	1:C:400:THR:HB	1.87	0.57
1:B:440:VAL:HG12	1:B:441:THR:N	2.20	0.57
1:A:334:GLU:OE1	1:A:336:ARG:NH1	2.37	0.57
1:D:766:SER:HA	1:D:779:PRO:HB3	1.85	0.57
1:C:343:LEU:HD23	1:C:348:PRO:HA	1.87	0.57
1:A:502:MET:HA	1:A:537:GLU:O	2.05	0.57
1:C:138:GLN:OE1	1:C:140:ARG:NE	2.28	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:PRO:O	1:C:618:THR:HG22	2.05	0.57
1:B:474:TRP:CZ2	1:B:478:VAL:HG11	2.40	0.57
1:A:505:ARG:HG2	1:A:505:ARG:HH11	1.70	0.57
1:B:337:ILE:HA	1:B:341:LEU:O	2.05	0.57
1:B:818:ALA:HB1	1:B:842:TRP:HB3	1.86	0.57
1:C:780:LEU:HD12	1:C:886:CYS:HB3	1.87	0.57
1:D:634:GLN:HB2	1:D:682:LEU:HB2	1.85	0.57
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.86	0.57
1:C:502:MET:HA	1:C:537:GLU:O	2.05	0.57
1:C:679:LEU:C	1:C:680:ILE:HG13	2.25	0.57
1:A:607:VAL:HA	1:A:613:PRO:HA	1.87	0.57
1:B:989:PHE:CE1	1:B:1014:TYR:HB3	2.40	0.57
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.87	0.57
1:A:420:MET:HE2	1:A:426:LEU:HG	1.86	0.57
1:C:759:ASN:OD1	1:C:761:GLN:HB2	2.04	0.57
1:C:198:GLU:CG	1:C:439:ARG:HH12	2.18	0.57
1:C:344:LEU:HB3	1:C:349:LEU:CD2	2.24	0.56
1:D:354:VAL:HA	1:D:567:VAL:H	1.69	0.56
1:C:904:GLU:HG2	1:C:906:TYR:HE1	1.70	0.56
1:C:285:TYR:HB3	1:C:288:ARG:HG3	1.87	0.56
1:B:651:LEU:C	1:B:651:LEU:HD23	2.26	0.56
1:B:952:ARG:NH2	1:B:1019:VAL:HG11	2.20	0.56
1:C:684:GLU:C	1:C:685:LEU:HG	2.25	0.56
1:D:599:ARG:HB2	1:D:600:GLN:OE1	2.05	0.56
1:C:230:ARG:HB2	1:C:230:ARG:HH11	1.69	0.56
1:B:738:PRO:HA	1:B:751:LEU:HB2	1.86	0.56
1:D:730:LEU:O	1:D:731:PRO:C	2.44	0.56
1:D:658:LEU:O	1:D:661:LYS:HG3	2.05	0.56
1:A:769:TRP:HA	1:A:773:LYS:O	2.06	0.56
1:A:599:ARG:HH11	1:A:600:GLN:CD	2.09	0.56
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.40	0.56
1:D:100:TYR:CE2	1:D:602:CYS:HB3	2.39	0.56
1:C:84:VAL:HG23	1:C:85:VAL:N	2.20	0.56
1:A:127:PHE:CE2	1:A:184:LEU:HD23	2.41	0.56
1:B:890:GLN:HG3	1:B:891:VAL:N	2.18	0.56
1:C:750:GLU:HG3	1:C:755:ARG:CB	2.36	0.56
1:C:418:HIS:ND1	1:C:461:GLU:OE1	2.38	0.56
1:A:541:ALA:HA	1:A:545:SER:HB3	1.86	0.56
1:A:765:LEU:O	1:A:765:LEU:HG	2.06	0.56
1:C:100:TYR:HB2	1:C:203:TRP:CD2	2.40	0.56
1:B:995:GLY:H	1:B:1002:SER:HB2	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:GLN:HG3	1:A:768:MET:H	1.69	0.56
1:C:554:GLN:O	1:C:554:GLN:NE2	2.39	0.56
1:D:367:MET:HE1	1:D:371:THR:CG2	2.36	0.56
1:D:571:VAL:CG2	1:D:609:ALA:HA	2.35	0.56
1:A:446:ARG:NE	1:A:447:ASP:OD1	2.38	0.56
1:B:732:ALA:O	1:B:733:ALA:C	2.44	0.56
1:C:630:ARG:NH2	1:C:637:GLU:OE2	2.38	0.56
1:B:985:ASN:ND2	4:B:4166:HOH:O	2.37	0.56
1:A:1015:HIS:CE1	1:B:1015:HIS:CE1	2.94	0.56
1:D:751:LEU:HD23	1:D:751:LEU:C	2.25	0.56
1:B:507:ASP:C	1:B:519:SER:HB2	2.26	0.56
1:C:436:MET:CE	1:C:467:ASN:HB2	2.35	0.56
1:C:417:THR:HB	1:C:420:MET:HG3	1.88	0.56
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.24	0.56
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.20	0.56
1:C:970:THR:HG23	1:C:975:LEU:HB2	1.88	0.56
1:A:272:ALA:HB1	1:A:273:PRO:HD2	1.86	0.56
1:B:706:THR:OG1	1:B:709:SER:N	2.29	0.56
1:A:210:ARG:CD	1:A:395:HIS:HB2	2.34	0.56
1:A:621:LYS:HD3	1:A:717:TRP:CH2	2.41	0.56
1:A:577:LYS:O	1:A:585:TRP:N	2.35	0.56
1:D:756:TRP:CD1	1:D:768:MET:HG3	2.40	0.56
1:A:246:MET:HB3	1:A:274:PHE:CZ	2.41	0.56
1:A:600:GLN:H	1:A:600:GLN:HE21	1.52	0.56
1:A:599:ARG:HD2	1:A:600:GLN:NE2	2.21	0.56
1:C:655:MET:HE1	1:C:662:PRO:CB	2.36	0.56
1:C:590:GLY:H	1:C:594:ASP:CG	2.09	0.56
1:A:43:ARG:HH11	1:A:43:ARG:CG	2.19	0.56
1:C:817:GLN:O	1:C:818:ALA:C	2.44	0.56
1:C:131:GLU:HA	1:C:134:LEU:HD12	1.86	0.56
1:C:768:MET:HG2	1:C:775:GLN:HB2	1.87	0.56
1:B:282:ARG:HH21	1:C:419:GLY:HA2	1.71	0.56
1:A:615:PRO:O	1:A:618:THR:HG22	2.06	0.56
1:C:505:ARG:HG2	1:C:996:ASP:OD2	2.06	0.56
1:B:904:GLU:OE2	1:B:936:GLY:N	2.29	0.56
1:A:866:ILE:O	1:A:1017:GLN:HA	2.05	0.56
1:D:649:ASN:O	1:D:702:GLN:HG2	2.06	0.56
1:D:652:LEU:CD1	1:D:698:VAL:HB	2.36	0.56
1:D:894:ARG:NH1	1:D:921:PRO:HD3	2.21	0.56
1:A:529:GLU:OE2	1:A:531:ARG:HB2	2.06	0.56
1:B:158:TRP:CZ2	1:B:160:GLY:HA2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:NH2	1:C:453:VAL:O	2.38	0.56
1:B:139:THR:HG21	1:B:177:LEU:CD1	2.30	0.55
1:B:649:ASN:OD1	1:B:703:PRO:HD2	2.06	0.55
1:A:649:ASN:O	1:A:702:GLN:HG2	2.06	0.55
1:B:512:PHE:H	1:B:516:PRO:HA	1.71	0.55
1:D:153:TRP:HA	1:D:157:ARG:O	2.06	0.55
1:B:491:ALA:HB2	1:B:501:PRO:HA	1.89	0.55
1:D:512:PHE:CE1	1:D:517:LYS:HG3	2.42	0.55
1:C:254:LEU:O	1:C:255:ARG:NH1	2.38	0.55
1:A:399:TYR:CE1	1:A:446:ARG:NH2	2.74	0.55
1:D:595:THR:HA	1:D:596:PRO:C	2.26	0.55
1:D:322:LEU:HD11	1:D:324:GLU:O	2.06	0.55
1:A:622:HIS:CB	1:A:912:ALA:HB2	2.37	0.55
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.88	0.55
1:B:73:TRP:O	1:B:183:ARG:NH1	2.38	0.55
1:C:600:GLN:NE2	1:C:790:ASP:OD1	2.38	0.55
1:D:73:TRP:O	1:D:183:ARG:NH1	2.32	0.55
1:B:257:THR:HG23	1:B:270:GLY:O	2.05	0.55
1:D:606:LEU:HB3	1:D:617:LEU:CD1	2.36	0.55
1:A:101:THR:HG23	1:A:204:ARG:NH2	2.21	0.55
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.41	0.55
1:B:835:LEU:C	1:B:836:ILE:HD13	2.27	0.55
1:A:571:VAL:HG23	1:A:609:ALA:HA	1.87	0.55
1:B:287:ASP:OD1	1:B:287:ASP:N	2.27	0.55
1:B:793:ILE:HA	1:B:807:VAL:CG1	2.37	0.55
1:B:261:TRP:CH2	1:B:266:GLN:HB2	2.42	0.55
1:B:36:TRP:O	1:B:37:ARG:HD3	2.06	0.55
1:D:696:LEU:HD12	1:D:697:THR:N	2.22	0.55
1:C:696:LEU:HD12	1:C:697:THR:H	1.72	0.55
1:D:899:GLY:HA3	1:D:941:THR:HA	1.89	0.55
1:D:891:VAL:HG12	1:D:891:VAL:O	2.07	0.55
1:A:942:ARG:HA	1:A:953:GLY:O	2.07	0.55
1:A:383:ASN:HD22	1:A:625:GLN:HA	1.72	0.55
1:B:69:VAL:HG13	1:B:70:PRO:HD2	1.89	0.55
1:A:351:ILE:N	1:A:351:ILE:HD13	2.22	0.55
1:B:91:GLN:HE21	1:B:190:ARG:HH12	1.52	0.55
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.42	0.55
1:D:636:ILE:O	1:D:680:ILE:N	2.37	0.55
1:C:533:LEU:C	1:C:533:LEU:HD23	2.27	0.55
1:D:891:VAL:CG2	1:D:981:GLY:HA2	2.29	0.55
1:D:287:ASP:C	1:D:288:ARG:HG2	2.27	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:THR:HB	1:B:887:GLN:H	1.72	0.55
1:C:755:ARG:HD3	1:C:769:TRP:CE3	2.42	0.55
1:A:399:TYR:HE1	1:A:446:ARG:NH2	2.05	0.55
1:D:51:LEU:HD12	1:D:214:LEU:O	2.07	0.55
1:D:872:VAL:N	1:D:1012:GLY:O	2.32	0.55
1:C:883:GLY:HA3	1:C:987:ASP:HA	1.89	0.55
1:B:189:LEU:N	1:B:189:LEU:HD12	2.22	0.55
1:C:433:LEU:HB3	1:C:434:PRO:CD	2.34	0.55
1:D:577:LYS:HB3	1:D:585:TRP:CE2	2.41	0.55
1:C:133:TRP:CE3	1:C:216:HIS:HB2	2.42	0.55
1:A:416:GLU:HA	1:A:460:ASN:O	2.07	0.55
1:A:856:TYR:CD1	1:A:856:TYR:N	2.75	0.55
1:D:663:LEU:N	1:D:663:LEU:HD23	2.22	0.54
1:D:114:VAL:HG11	1:D:192:SER:CA	2.37	0.54
1:D:461:GLU:HG2	4:D:4477:HOH:O	2.08	0.54
1:B:309:TYR:HD1	1:B:309:TYR:H	1.54	0.54
1:D:92:MET:HE2	1:D:92:MET:HA	1.89	0.54
1:A:354:VAL:HA	1:A:567:VAL:N	2.20	0.54
1:B:893:GLU:O	1:B:921:PRO:HA	2.07	0.54
1:D:499:ILE:HD11	1:D:529:GLU:CG	2.36	0.54
1:A:316:HIS:HB2	1:A:321:THR:O	2.08	0.54
1:C:260:LEU:HD12	1:C:310:ARG:O	2.06	0.54
1:A:906:TYR:OH	1:A:935:ASN:HA	2.07	0.54
1:B:412:GLU:HG3	1:B:457:SER:CB	2.25	0.54
1:B:13:ARG:NH1	1:C:13:ARG:HH11	2.05	0.54
1:D:217:LYS:HB3	1:D:218:PRO:HD2	1.89	0.54
1:C:454:ILE:O	1:C:482:ARG:HB3	2.07	0.54
1:D:109:VAL:O	1:D:109:VAL:HG12	2.06	0.54
1:B:13:ARG:HH12	1:C:13:ARG:HH11	1.54	0.54
1:D:741:THR:HG22	1:D:741:THR:O	2.07	0.54
1:B:920:LEU:CB	1:B:921:PRO:HD2	2.38	0.54
1:C:685:LEU:O	1:C:686:PRO:O	2.25	0.54
1:D:599:ARG:HD2	1:D:600:GLN:OE1	2.07	0.54
1:A:176:PHE:CD1	1:A:176:PHE:N	2.74	0.54
1:D:685:LEU:O	1:D:686:PRO:C	2.45	0.54
1:B:652:LEU:O	1:B:668:VAL:N	2.34	0.54
1:D:54:LEU:HB2	1:D:212:VAL:CG1	2.37	0.54
1:B:128:ASN:HB2	1:B:181:GLU:OE2	2.08	0.54
1:B:282:ARG:HH21	1:C:419:GLY:CA	2.21	0.54
1:C:843:GLN:HG2	1:C:848:THR:OG1	2.07	0.54
1:D:870:VAL:HG21	1:D:882:ILE:CG2	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:GLU:OE2	1:C:395:HIS:N	2.34	0.54
1:A:885:ASN:O	1:A:886:CYS:HB3	2.07	0.54
1:C:610:ASP:OD1	1:C:612:THR:HB	2.07	0.54
1:A:853:ARG:HH12	1:A:871:GLU:CD	2.11	0.54
1:A:576:ILE:HD12	1:A:584:PRO:HB2	1.88	0.54
1:C:342:LEU:O	1:C:348:PRO:HA	2.06	0.54
1:A:533:LEU:C	1:A:534:ILE:HG13	2.28	0.54
1:D:749:ILE:N	1:D:749:ILE:HD12	2.22	0.54
1:C:655:MET:HE1	1:C:662:PRO:CA	2.38	0.54
1:B:502:MET:O	1:B:517:LYS:HE3	2.08	0.54
1:D:577:LYS:HD3	1:D:585:TRP:CH2	2.42	0.54
1:D:78:LEU:N	1:D:78:LEU:HD23	2.23	0.54
1:B:932:PRO:HG2	1:B:970:THR:O	2.08	0.54
1:B:37:ARG:NH1	1:B:37:ARG:HG3	2.23	0.54
1:A:158:TRP:CZ2	1:A:160:GLY:HA2	2.42	0.54
1:D:721:ARG:CB	1:D:721:ARG:HH11	2.21	0.54
1:C:905:ASN:N	1:C:937:LEU:O	2.30	0.54
1:B:782:ASP:OD1	1:B:854:LYS:HE3	2.08	0.54
1:D:559:TYR:HB2	1:D:562:LEU:HD12	1.90	0.54
1:D:92:MET:CE	1:D:92:MET:HA	2.38	0.54
1:D:17:GLU:HG2	1:D:113:PHE:HA	1.90	0.54
1:C:959:ILE:O	1:C:959:ILE:HG23	2.06	0.54
1:B:572:ASP:O	1:B:609:ALA:HB2	2.07	0.54
1:D:951:TRP:CE3	1:D:951:TRP:N	2.76	0.54
1:B:433:LEU:HD12	1:B:433:LEU:C	2.28	0.54
1:B:13:ARG:HH12	1:C:13:ARG:NH1	2.04	0.54
1:B:600:GLN:H	1:B:600:GLN:NE2	2.06	0.54
1:D:367:MET:HE1	1:D:371:THR:HB	1.88	0.54
1:D:16:TRP:HB2	1:D:192:SER:HB2	1.89	0.54
1:A:391:HIS:CD2	1:A:460:ASN:HD22	2.25	0.54
1:B:586:SER:HB3	4:B:4091:HOH:O	2.07	0.54
1:D:350:LEU:HD11	1:D:556:PHE:HB3	1.89	0.54
1:D:546:LEU:HA	4:D:4447:HOH:O	2.07	0.54
1:A:655:MET:CE	1:A:662:PRO:HB3	2.38	0.54
1:B:182:ASN:ND2	1:B:182:ASN:N	2.56	0.53
1:C:721:ARG:HB3	1:C:721:ARG:HH11	1.73	0.53
1:A:658:LEU:HD12	1:A:693:GLN:O	2.08	0.53
1:C:153:TRP:CD1	1:C:158:TRP:HA	2.42	0.53
1:C:449:ASN:HB2	4:C:4024:HOH:O	2.07	0.53
1:D:662:PRO:O	1:D:663:LEU:HD23	2.07	0.53
1:A:202:MET:O	1:A:204:ARG:HD3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:LEU:O	1:B:661:LYS:HE3	2.08	0.53
1:B:71:GLU:CD	1:B:71:GLU:H	2.11	0.53
1:B:974:HIS:CD2	1:B:975:LEU:HD23	2.43	0.53
1:A:78:LEU:H	1:A:78:LEU:CD1	2.20	0.53
1:C:742:THR:HG22	1:C:743:SER:O	2.07	0.53
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.89	0.53
1:B:304:GLU:HG2	1:B:642:TYR:CD2	2.42	0.53
1:B:416:GLU:HA	1:B:460:ASN:O	2.08	0.53
1:A:828:ASP:O	1:A:834:VAL:HG13	2.09	0.53
1:B:764:PHE:O	1:B:765:LEU:C	2.43	0.53
1:B:333:ARG:NH1	1:B:333:ARG:HG2	2.21	0.53
1:B:114:VAL:HG11	1:B:192:SER:N	2.23	0.53
1:A:285:TYR:HB3	1:A:288:ARG:HG2	1.90	0.53
1:C:1003:VAL:O	1:C:1008:GLN:NE2	2.41	0.53
1:A:610:ASP:OD1	1:A:612:THR:HB	2.08	0.53
1:D:245:GLN:HB3	1:D:288:ARG:HD3	1.90	0.53
1:A:139:THR:OG1	1:A:216:HIS:HD2	1.92	0.53
1:D:100:TYR:HB2	1:D:203:TRP:CD2	2.44	0.53
1:B:640:SER:HB3	1:B:675:GLN:N	2.23	0.53
1:D:706:THR:HG23	1:D:709:SER:OG	2.09	0.53
1:D:390:SER:HA	1:D:391:HIS:ND1	2.24	0.53
1:D:580:GLU:C	1:D:582:GLY:H	2.12	0.53
1:B:630:ARG:NH2	1:B:637:GLU:OE2	2.42	0.53
1:C:167:LEU:HB3	1:C:168:PRO:CD	2.37	0.53
1:D:254:LEU:C	1:D:255:ARG:HG2	2.29	0.53
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.90	0.53
1:D:866:ILE:HG22	1:D:867:THR:N	2.23	0.53
1:A:417:THR:OG1	1:A:462:SER:HA	2.09	0.53
1:A:835:LEU:CD1	1:A:857:ARG:HB2	2.39	0.53
1:A:745:MET:HE3	1:A:745:MET:HA	1.91	0.53
1:A:1015:HIS:CD2	1:B:1015:HIS:ND1	2.77	0.53
1:D:315:LEU:O	1:D:322:LEU:HD12	2.09	0.53
1:D:224:ASP:OD2	1:D:226:HIS:NE2	2.40	0.53
1:B:870:VAL:HG12	1:B:871:GLU:N	2.23	0.53
1:D:316:HIS:HB2	1:D:321:THR:O	2.09	0.53
1:D:278:ILE:HG22	1:D:278:ILE:O	2.07	0.53
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.90	0.53
1:A:354:VAL:HG22	1:A:355:ASN:N	2.24	0.53
1:B:745:MET:CA	1:B:760:ARG:HB2	2.38	0.53
1:D:48:SER:OG	1:D:50:GLN:HG2	2.09	0.53
1:A:284:GLY:O	1:D:422:PRO:HD3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:HA	1:A:122:CYS:O	2.09	0.53
1:B:382:ASN:O	1:B:383:ASN:HB2	2.09	0.53
1:D:351:ILE:HD13	1:D:351:ILE:N	2.23	0.53
1:D:961:ARG:HH11	1:D:961:ARG:HG3	1.72	0.53
1:D:702:GLN:O	1:D:712:GLY:N	2.40	0.53
1:A:824:GLN:HG3	1:A:825:CYS:N	2.23	0.53
1:A:836:ILE:HG22	1:A:837:THR:N	2.23	0.53
1:A:356:ARG:HH11	1:A:356:ARG:CG	2.19	0.53
1:A:486:TYR:CZ	1:A:488:GLY:HA3	2.44	0.53
1:A:88:SER:HB2	1:A:93:HIS:CE1	2.44	0.53
1:A:751:LEU:HD21	1:A:860:GLY:C	2.29	0.53
1:A:231:PHE:CE1	1:A:334:GLU:HB2	2.44	0.53
1:C:634:GLN:NE2	1:C:684:GLU:HA	2.24	0.53
1:B:409:VAL:HG23	1:B:452:SER:HB2	1.91	0.53
1:C:651:LEU:HD11	1:C:653[A]:HIS:CE1	2.44	0.52
1:B:147:ASN:HD22	1:B:206:SER:HA	1.74	0.52
1:D:53:SER:O	1:D:54:LEU:HD23	2.09	0.52
1:B:916:ASP:OD1	1:B:917:ARG:N	2.41	0.52
1:A:577:LYS:HG3	1:A:587:ALA:HB2	1.90	0.52
1:A:499:ILE:HD11	1:A:529:GLU:CG	2.39	0.52
1:A:658:LEU:O	1:A:659:ASP:C	2.46	0.52
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.38	0.52
1:D:777:LEU:HB2	1:D:887:GLN:HB3	1.89	0.52
1:B:141:ILE:HG21	1:B:173:LEU:HD11	1.91	0.52
1:B:278:ILE:N	1:B:278:ILE:HD12	2.22	0.52
1:C:857:ARG:O	1:C:857:ARG:HG2	2.09	0.52
1:C:735:HIS:HD2	1:C:735:HIS:H	1.56	0.52
1:B:833:ALA:HB1	1:B:858:ILE:O	2.09	0.52
1:B:141:ILE:HG13	1:B:213:SER:O	2.08	0.52
1:C:658:LEU:HG	1:C:661:LYS:NZ	2.23	0.52
1:A:210:ARG:NE	1:A:395:HIS:HB2	2.24	0.52
1:A:1015:HIS:CG	1:B:1015:HIS:ND1	2.77	0.52
1:B:377:LEU:N	1:B:377:LEU:HD23	2.23	0.52
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.91	0.52
1:B:399:TYR:CE1	1:B:446:ARG:NH2	2.77	0.52
1:A:89:ASN:O	1:A:92:MET:HB2	2.09	0.52
1:C:387:VAL:HG13	1:C:409:VAL:HG22	1.91	0.52
1:C:786:ARG:NH2	1:C:792:ASP:OD1	2.33	0.52
1:C:789:LEU:HG	1:C:792:ASP:OD2	2.08	0.52
1:B:127:PHE:N	1:B:127:PHE:CD2	2.77	0.52
1:B:114:VAL:HG11	1:B:192:SER:CA	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:TYR:CZ	1:C:488:GLY:HA3	2.45	0.52
1:C:531:ARG:HB3	1:C:532:PRO:HD2	1.92	0.52
1:D:989:PHE:CE1	1:D:1014:TYR:HB3	2.45	0.52
1:A:581:ASN:OD1	1:A:581:ASN:N	2.42	0.52
1:A:850:PHE:O	1:A:851:ILE:HG13	2.09	0.52
1:B:73:TRP:CH2	1:B:122:CYS:HB3	2.44	0.52
1:C:40:GLU:O	1:C:44:THR:HG23	2.10	0.52
1:A:928:PRO:O	1:A:973:ARG:NH1	2.28	0.52
1:A:390:SER:HA	1:A:391:HIS:ND1	2.25	0.52
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.39	0.52
1:B:309:TYR:N	1:B:309:TYR:CD1	2.77	0.52
1:A:694:LEU:HB3	1:A:722:LEU:HB2	1.91	0.52
1:A:281:GLU:HG3	1:D:515:VAL:HG21	1.92	0.52
1:B:167:LEU:HD13	1:B:442:ARG:HB3	1.90	0.52
1:D:806:TRP:O	1:D:809:ARG:HB2	2.09	0.52
1:A:832:ASP:OD1	1:A:832:ASP:N	2.38	0.52
1:D:871:GLU:HG2	1:D:1013:ARG:HG2	1.92	0.52
1:C:147:ASN:HB3	1:C:206:SER:HA	1.91	0.52
1:D:821:ALA:O	1:D:840:HIS:HA	2.10	0.52
1:A:811:LYS:O	1:A:814:GLY:HA2	2.09	0.52
1:D:576:ILE:O	1:D:576:ILE:HG22	2.08	0.52
1:A:948:PRO:O	1:A:1022:GLN:HA	2.10	0.52
1:A:521:LYS:HB3	1:A:559:TYR:CE2	2.45	0.52
1:D:588:TYR:O	1:D:589:GLY:C	2.47	0.52
1:C:603:MET:O	1:C:604:ASN:ND2	2.43	0.52
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.10	0.52
1:C:823:LEU:CB	1:D:730:LEU:HD21	2.25	0.52
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.45	0.52
1:C:735:HIS:N	1:C:735:HIS:CD2	2.78	0.52
1:D:399:TYR:CZ	1:D:446:ARG:NH2	2.78	0.52
1:D:830:LEU:N	1:D:833:ALA:O	2.38	0.52
1:C:100:TYR:HB2	1:C:203:TRP:CE3	2.44	0.52
1:A:876:THR:OG1	1:A:877:PRO:HD2	2.09	0.52
1:C:736:ALA:O	1:C:860:GLY:HA3	2.10	0.52
1:C:872:VAL:O	1:C:873:ALA:C	2.48	0.52
1:A:742:THR:HG22	1:A:743:SER:N	2.25	0.52
1:D:658:LEU:O	1:D:659:ASP:C	2.48	0.52
1:A:310:ARG:HG3	1:A:310:ARG:NH1	2.17	0.52
1:B:942:ARG:HA	1:B:953:GLY:O	2.10	0.52
1:A:787:ALA:N	1:A:964:GLN:OE1	2.41	0.52
1:D:749:ILE:O	1:D:755:ARG:HA	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:824:GLN:O	1:D:824:GLN:HG3	2.09	0.52
1:A:222:ILE:HD13	1:A:313:VAL:HG12	1.91	0.52
1:D:58:TRP:O	1:D:84:VAL:N	2.40	0.52
1:D:395:HIS:ND1	1:D:396:PRO:HD2	2.24	0.52
1:D:66:PRO:HB3	1:D:187:MET:HE3	1.92	0.52
1:C:421:VAL:O	1:C:425:ARG:NE	2.39	0.52
1:A:734:SER:C	1:A:736:ALA:H	2.11	0.52
1:A:390:SER:HB2	1:A:391:HIS:CE1	2.45	0.52
1:D:737:ILE:HD12	1:D:738:PRO:HD2	1.91	0.52
1:D:437:SER:O	1:D:441:THR:HG23	2.09	0.52
1:A:936:GLY:O	1:A:937:LEU:C	2.44	0.52
1:A:851:ILE:HD12	1:B:726:LEU:HD13	1.91	0.51
1:B:631:LEU:HD13	1:B:636:ILE:HG13	1.92	0.51
1:D:853:ARG:NH1	1:D:853:ARG:HG3	2.23	0.51
1:B:260:LEU:HD11	1:B:309:TYR:CB	2.40	0.51
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.92	0.51
1:A:147:ASN:HB2	1:A:209:PHE:CE2	2.45	0.51
1:B:599:ARG:HB2	1:B:600:GLN:HE21	1.75	0.51
1:B:360:HIS:CB	1:B:363:HIS:HB2	2.39	0.51
1:B:649:ASN:O	1:B:702:GLN:HA	2.10	0.51
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.10	0.51
1:C:659:ASP:OD1	1:C:693:GLN:HB2	2.09	0.51
1:C:634:GLN:HE22	1:C:684:GLU:HA	1.76	0.51
1:C:697:THR:OG1	1:C:719:GLN:HG2	2.11	0.51
1:D:414:ASN:O	1:D:415:ILE:HG13	2.10	0.51
1:D:335:VAL:HG21	1:D:454:ILE:HG22	1.92	0.51
1:C:925:MET:HB3	4:C:4027:HOH:O	2.11	0.51
1:C:926:TYR:CZ	1:C:928:PRO:HA	2.45	0.51
1:D:399:TYR:CE1	1:D:446:ARG:NH2	2.77	0.51
1:D:682:LEU:HB3	1:D:683:PRO:HD2	1.93	0.51
1:D:135:GLN:O	1:D:136:GLU:HG2	2.09	0.51
1:B:837:THR:O	1:B:837:THR:HG22	2.11	0.51
4:B:4291:HOH:O	1:C:20:GLY:HA3	2.10	0.51
1:D:749:ILE:HG22	1:D:750:GLU:N	2.26	0.51
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.40	0.51
1:C:608:PHE:CD1	1:C:612:THR:HG22	2.44	0.51
1:B:304:GLU:HG2	1:B:642:TYR:HD2	1.75	0.51
1:C:513:PRO:O	1:C:514:ALA:HB3	2.10	0.51
1:D:785:THR:O	1:D:881:ARG:HD2	2.10	0.51
1:A:635:THR:CG2	1:A:679:LEU:HD22	2.40	0.51
1:A:755:ARG:HG3	1:A:769:TRP:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:824:GLN:O	1:D:838:THR:HA	2.10	0.51
1:B:403:ASP:OD2	1:B:450:HIS:ND1	2.39	0.51
1:C:496:THR:HG23	1:C:531:ARG:HH11	1.75	0.51
1:C:202:MET:O	1:C:204:ARG:HD3	2.10	0.51
1:C:429:ASP:OD1	1:C:430:PRO:HD2	2.10	0.51
1:B:354:VAL:HG22	1:B:355:ASN:O	2.09	0.51
1:D:363:HIS:HB3	1:D:366:VAL:HB	1.92	0.51
1:B:576:ILE:HG22	1:B:577:LYS:N	2.25	0.51
1:A:337:ILE:HA	1:A:341:LEU:O	2.10	0.51
1:C:317:THR:OG1	1:C:319:ASP:OD1	2.28	0.51
1:C:620:ALA:O	1:C:624:GLN:HG3	2.10	0.51
1:A:578:TYR:HA	1:A:583:ASN:O	2.10	0.51
1:C:543:GLY:O	1:C:545:SER:N	2.44	0.51
1:B:741:THR:O	1:B:741:THR:HG22	2.10	0.51
1:B:945:ASN:HB3	1:B:1023:LYS:NZ	2.26	0.51
1:D:99:ILE:HA	1:D:594:ASP:CB	2.39	0.51
1:A:788:PRO:O	1:A:933:SER:HB2	2.11	0.51
1:C:778:THR:CB	1:C:779:PRO:HD2	2.39	0.51
1:C:749:ILE:O	1:C:755:ARG:HB2	2.10	0.51
1:A:79:PRO:HD2	1:A:80:GLU:OE1	2.11	0.51
1:A:868:VAL:N	1:A:1016:TYR:O	2.37	0.51
1:B:491:ALA:HB1	1:B:501:PRO:N	2.26	0.51
1:C:127:PHE:CD2	1:C:127:PHE:N	2.79	0.51
1:D:254:LEU:O	1:D:255:ARG:HG2	2.11	0.51
1:D:63:PHE:HB3	1:D:64:PRO:CD	2.41	0.51
1:A:687:GLN:O	1:A:688:PRO:O	2.29	0.51
1:B:372:MET:O	1:B:376:ILE:HG13	2.11	0.51
1:A:487:GLU:HG2	1:A:491:ALA:HB2	1.92	0.51
1:A:808:GLU:HA	1:A:808:GLU:OE1	2.10	0.51
1:D:87:PRO:O	1:D:88:SER:HB3	2.11	0.51
1:B:920:LEU:HB2	1:B:921:PRO:HD2	1.92	0.51
1:B:732:ALA:O	1:B:733:ALA:O	2.29	0.51
1:B:383:ASN:HB3	1:B:624:GLN:O	2.10	0.51
1:B:824:GLN:HG3	1:B:825:CYS:N	2.26	0.51
1:B:939:CYS:HA	1:B:956:GLN:HB3	1.92	0.51
1:C:372:MET:CE	1:C:397:LEU:HB3	2.38	0.51
1:B:658:LEU:HB3	1:B:661:LYS:HD2	1.92	0.51
1:A:394:ASN:O	1:A:395:HIS:C	2.46	0.51
1:A:23:GLN:OE1	1:A:26:ARG:N	2.43	0.51
1:B:916:ASP:HB3	1:B:918:TRP:CZ2	2.46	0.51
1:B:441:THR:HG22	1:B:474:TRP:CH2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:767:GLN:OE1	1:D:768:MET:O	2.28	0.51
1:D:89:ASN:O	1:D:92:MET:HB2	2.11	0.51
1:D:393:PRO:HD2	1:D:414:ASN:HB2	1.91	0.51
1:A:687:GLN:O	1:A:688:PRO:C	2.50	0.51
1:C:815:HIS:HE1	1:C:877:PRO:O	1.93	0.51
1:B:491:ALA:CB	1:B:501:PRO:HA	2.41	0.50
1:A:786:ARG:HG2	1:A:880:ALA:CB	2.38	0.50
1:A:24:LEU:O	1:A:25:ASN:C	2.49	0.50
1:A:545:SER:OG	1:A:995:GLY:HA3	2.11	0.50
1:C:572:ASP:HB2	4:C:4093:HOH:O	2.10	0.50
1:A:588:TYR:CD2	1:A:603:MET:CE	2.95	0.50
1:A:242:ALA:O	1:A:290:THR:HA	2.10	0.50
1:C:123:TYR:CD2	1:C:208:ILE:HD12	2.46	0.50
1:C:783:GLN:HG2	1:C:881:ARG:HD2	1.93	0.50
1:A:835:LEU:C	1:A:836:ILE:HD13	2.32	0.50
1:D:524:LEU:HD22	1:D:561:ARG:CB	2.35	0.50
1:C:433:LEU:N	1:C:434:PRO:HD2	2.27	0.50
1:B:13:ARG:CG	1:B:13:ARG:HH11	2.24	0.50
1:B:685:LEU:O	1:B:686:PRO:O	2.29	0.50
1:A:789:LEU:O	1:A:792:ASP:HB2	2.11	0.50
1:D:635:THR:OG1	1:D:681:GLU:OE2	2.27	0.50
1:B:253:TYR:O	1:B:318:ALA:N	2.45	0.50
1:C:92:MET:C	1:C:94:GLY:H	2.12	0.50
1:D:887:GLN:HG3	1:D:983:TRP:CD2	2.46	0.50
1:A:941:THR:HG22	1:A:942:ARG:N	2.25	0.50
1:A:573:GLN:HB2	1:A:602:CYS:O	2.12	0.50
1:B:683:PRO:O	1:B:684:GLU:C	2.49	0.50
1:D:204:ARG:HD3	1:D:204:ARG:N	2.26	0.50
1:C:777:LEU:CD2	1:C:889:ALA:HB2	2.41	0.50
1:B:922:LEU:O	1:B:922:LEU:HG	2.10	0.50
1:B:383:ASN:ND2	1:B:625:GLN:HA	2.26	0.50
1:B:622:HIS:O	1:B:625:GLN:HG3	2.11	0.50
1:D:395:HIS:CG	1:D:396:PRO:HD2	2.46	0.50
1:A:695:TRP:CE2	1:A:915:PHE:CD2	2.99	0.50
1:D:146:VAL:HG11	1:D:150:PHE:CD2	2.46	0.50
1:B:242:ALA:O	1:B:290:THR:HA	2.12	0.50
1:A:614:HIS:N	1:A:614:HIS:CD2	2.76	0.50
1:A:999:TRP:N	1:A:999:TRP:CD2	2.78	0.50
1:D:576:ILE:HD12	1:D:584:PRO:HB2	1.92	0.50
1:C:842:TRP:N	1:C:842:TRP:CE3	2.79	0.50
1:B:652:LEU:HD22	1:B:680:ILE:HD13	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:LEU:N	1:A:830:LEU:HD23	2.26	0.50
1:D:119:PRO:HG2	1:D:190:ARG:HD3	1.94	0.50
1:D:486:TYR:CZ	1:D:488:GLY:HA3	2.46	0.50
1:C:374:GLN:O	1:C:378:LEU:HB2	2.11	0.50
1:B:432:TRP:O	1:B:436:MET:HG3	2.12	0.50
1:C:762:SER:C	1:C:822:LEU:HD22	2.30	0.50
1:D:655:MET:HB2	1:D:665:SER:CA	2.35	0.50
1:B:43:ARG:HD2	1:B:261:TRP:CG	2.46	0.50
1:B:634:GLN:NE2	1:B:685:LEU:HG	2.26	0.50
1:B:830:LEU:CD1	1:B:835:LEU:HB2	2.41	0.50
1:C:843:GLN:HA	1:C:847:LYS:O	2.11	0.50
1:A:891:VAL:HG23	1:A:981:GLY:HA2	1.92	0.50
1:D:842:TRP:HB2	1:D:850:PHE:HD1	1.76	0.50
1:A:258:VAL:HA	1:A:312:VAL:O	2.11	0.50
1:A:629:PHE:HA	1:A:637:GLU:O	2.10	0.50
1:D:511:PRO:HA	1:D:516:PRO:HB3	1.94	0.50
1:B:856:TYR:CD1	1:B:856:TYR:N	2.77	0.50
1:B:176:PHE:N	1:B:176:PHE:CD1	2.78	0.50
1:D:961:ARG:HD2	1:D:981:GLY:O	2.11	0.50
1:B:245:GLN:HG2	1:B:288:ARG:HG3	1.92	0.50
1:C:767:GLN:OE1	1:C:776:LEU:HB2	2.12	0.50
1:D:1020:TRP:CD1	1:D:1021:CYS:N	2.79	0.50
1:B:221:GLN:HA	1:B:315:LEU:CD2	2.41	0.50
1:B:69:VAL:CG1	1:B:70:PRO:HD2	2.42	0.50
1:D:147:ASN:HA	1:D:165:SER:HB3	1.94	0.50
1:B:400:THR:HA	1:B:403:ASP:OD2	2.12	0.50
1:D:226:HIS:HA	1:D:449:ASN:OD1	2.11	0.50
1:C:576:ILE:HA	1:C:585:TRP:O	2.11	0.50
1:C:242:ALA:O	1:C:290:THR:HA	2.12	0.50
1:D:730:LEU:O	1:D:731:PRO:O	2.29	0.50
1:C:652:LEU:CD1	1:C:698:VAL:HB	2.33	0.50
1:A:822:LEU:HD11	1:A:824:GLN:O	2.12	0.50
1:A:843:GLN:HG2	1:A:847:LYS:C	2.31	0.50
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.46	0.50
1:A:127:PHE:N	1:A:127:PHE:CD2	2.79	0.50
1:C:655:MET:CE	1:C:662:PRO:HB3	2.42	0.50
1:D:60:PHE:CE2	1:D:62:TRP:HB2	2.47	0.50
1:B:751:LEU:HD11	1:B:860:GLY:HA2	1.92	0.50
1:D:359:HIS:CD2	1:D:573:GLN:HA	2.47	0.50
1:B:745:MET:C	1:B:760:ARG:HB2	2.33	0.50
1:B:453:VAL:O	1:B:482:ARG:NE	2.35	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:HIS:CG	1:A:460:ASN:HD22	2.30	0.50
1:B:735:HIS:CD2	1:B:735:HIS:N	2.80	0.50
1:B:735:HIS:H	1:B:735:HIS:HD2	1.60	0.50
1:D:461:GLU:HA	4:D:4425:HOH:O	2.12	0.50
1:B:299:LYS:N	1:B:309:TYR:OH	2.37	0.50
1:D:933:SER:O	1:D:934:GLU:C	2.48	0.50
1:A:647:SER:OG	1:A:672:VAL:N	2.34	0.50
1:D:685:LEU:O	1:D:686:PRO:O	2.29	0.49
1:A:39:SER:O	1:A:40:GLU:C	2.49	0.49
1:D:500:CYS:HA	1:D:534:ILE:O	2.12	0.49
1:C:615:PRO:HG3	1:C:927:THR:HG21	1.94	0.49
1:C:767:GLN:HE21	1:C:774:LYS:HG2	1.77	0.49
1:B:409:VAL:N	1:B:452:SER:O	2.45	0.49
1:B:537:GLU:HG2	1:B:568:TRP:HE3	1.76	0.49
1:B:148:SER:HB3	1:B:190:ARG:O	2.12	0.49
1:D:157:ARG:HH11	1:D:176:PHE:HA	1.72	0.49
1:B:570:TRP:CD1	1:B:571:VAL:HG12	2.47	0.49
1:D:305:ILE:HG21	1:D:307:ASN:HD21	1.77	0.49
1:C:512:PHE:H	1:C:516:PRO:HA	1.76	0.49
1:B:533:LEU:HD23	1:B:533:LEU:C	2.32	0.49
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.38	0.49
1:A:499:ILE:HG13	1:A:531:ARG:HB3	1.94	0.49
1:C:732:ALA:O	1:C:733:ALA:O	2.30	0.49
1:B:617:LEU:O	1:B:617:LEU:HG	2.12	0.49
1:D:701:VAL:O	1:D:703:PRO:HD3	2.11	0.49
1:D:587:ALA:HA	1:D:591:ASP:OD2	2.13	0.49
1:B:600:GLN:C	1:B:602:CYS:H	2.16	0.49
1:D:959:ILE:HD12	1:D:984:LEU:HD13	1.94	0.49
1:A:433:LEU:O	1:A:437:SER:HB3	2.12	0.49
1:C:989:PHE:HE1	1:C:1014:TYR:HB3	1.77	0.49
1:D:858:ILE:HG22	1:D:859:ASP:N	2.28	0.49
1:A:890:GLN:NE2	1:A:947:GLY:HA3	2.27	0.49
1:B:296:GLU:O	1:B:297:ASN:C	2.51	0.49
1:A:369:GLU:O	1:A:373:VAL:HG23	2.12	0.49
1:A:830:LEU:O	1:A:831:ALA:C	2.50	0.49
1:B:658:LEU:O	1:B:661:LYS:HG3	2.13	0.49
1:B:972:HIS:CB	1:B:974:HIS:CE1	2.96	0.49
1:A:78:LEU:HD12	1:A:78:LEU:N	2.27	0.49
1:C:417:THR:HG21	1:C:426:LEU:HD12	1.95	0.49
1:A:654:TRP:CE2	1:A:666:GLY:HA3	2.47	0.49
1:B:136:GLU:HG3	1:B:137:GLY:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.30	0.49
1:A:820:ALA:HA	1:A:841:ALA:O	2.12	0.49
1:B:635:THR:HG22	1:B:636:ILE:N	2.27	0.49
1:D:78:LEU:O	1:D:79:PRO:C	2.51	0.49
1:B:118:ASN:HD21	1:B:191:TRP:HB2	1.76	0.49
1:C:359:HIS:NE2	1:C:574:SER:O	2.40	0.49
1:D:946:TYR:O	1:D:949:HIS:HB2	2.11	0.49
1:D:580:GLU:OE1	1:D:580:GLU:HA	2.13	0.49
1:A:147:ASN:HB3	1:A:206:SER:HA	1.93	0.49
1:D:229:THR:HA	1:D:239:VAL:O	2.12	0.49
1:A:455:ILE:HG21	1:A:485:GLN:HG2	1.94	0.49
1:B:780:LEU:HA	1:B:886:CYS:HB3	1.95	0.49
1:C:510:GLN:HB2	1:C:517:LYS:HB2	1.95	0.49
1:B:441:THR:HG22	1:B:474:TRP:CE3	2.46	0.49
1:B:941:THR:HG22	1:B:955:PHE:CE1	2.48	0.49
1:B:559:TYR:HB2	1:B:562:LEU:CG	2.42	0.49
1:C:513:PRO:O	1:C:515:VAL:N	2.38	0.49
1:B:354:VAL:HG22	1:B:355:ASN:N	2.27	0.49
1:A:984:LEU:HG	1:A:985:ASN:N	2.27	0.49
1:A:833:ALA:HB1	1:A:858:ILE:O	2.12	0.49
1:A:867:THR:HG22	1:A:867:THR:O	2.12	0.49
1:C:360:HIS:O	1:C:364:GLY:N	2.44	0.49
1:D:433:LEU:N	1:D:434:PRO:CD	2.75	0.49
1:B:16:TRP:HA	1:B:161:TYR:OH	2.13	0.49
1:B:827:ALA:HA	1:B:836:ILE:HD12	1.93	0.49
1:B:50:GLN:O	1:B:215:LEU:HA	2.13	0.49
1:D:571:VAL:HG22	1:D:609:ALA:HA	1.94	0.49
1:C:807:VAL:HG22	1:C:807:VAL:O	2.13	0.49
1:C:513:PRO:C	1:C:515:VAL:H	2.15	0.49
1:B:154:CYS:N	1:B:157:ARG:O	2.46	0.49
1:C:383:ASN:ND2	1:C:625:GLN:HA	2.26	0.49
1:B:256:VAL:O	1:B:271:THR:HA	2.12	0.49
1:B:147:ASN:ND2	1:B:206:SER:HA	2.28	0.49
1:D:894:ARG:HH12	1:D:921:PRO:HD3	1.77	0.49
1:D:77:ASP:C	1:D:78:LEU:HD23	2.33	0.49
1:C:300:LEU:C	1:C:307:ASN:HB2	2.33	0.49
1:A:16:TRP:CG	1:A:189:LEU:HD12	2.48	0.49
1:A:655:MET:HG3	1:A:656:VAL:N	2.26	0.49
1:A:177:LEU:HD23	1:A:177:LEU:N	2.27	0.49
1:B:181:GLU:OE2	1:B:181:GLU:HA	2.12	0.49
1:B:890:GLN:O	1:B:891:VAL:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:HA	1:A:372:MET:CE	2.42	0.49
1:A:18:ASN:O	1:A:20:GLY:N	2.46	0.49
1:A:21:VAL:HG12	1:A:21:VAL:O	2.12	0.49
1:B:505:ARG:O	1:B:519:SER:HA	2.13	0.48
1:A:651:LEU:HB2	1:A:669:PRO:HA	1.94	0.48
1:D:796:SER:OG	1:D:801:ILE:HA	2.13	0.48
1:A:543:GLY:O	1:A:545:SER:N	2.45	0.48
1:D:377:LEU:HD22	1:D:708:TRP:CB	2.43	0.48
1:C:585:TRP:CG	1:C:974:HIS:CD2	3.01	0.48
1:B:650:GLU:HB3	1:B:670:LEU:HD12	1.94	0.48
1:A:670:LEU:HA	1:A:670:LEU:HD23	1.29	0.48
1:A:848:THR:CG2	1:B:728:VAL:HG11	2.38	0.48
1:B:260:LEU:HD11	1:B:309:TYR:HB3	1.94	0.48
1:B:232:ASN:ND2	1:B:234:ASP:OD1	2.46	0.48
1:A:410:VAL:HG22	1:A:455:ILE:HB	1.94	0.48
1:C:173:LEU:HA	1:C:173:LEU:HD23	1.48	0.48
1:D:777:LEU:HD11	1:D:889:ALA:CA	2.29	0.48
1:A:767:GLN:CG	1:A:768:MET:N	2.73	0.48
1:D:594:ASP:O	1:D:597:ASN:ND2	2.41	0.48
1:D:30:HIS:CB	1:D:31:PRO:HD2	2.38	0.48
1:A:91:GLN:HE21	1:A:190:ARG:CZ	2.26	0.48
1:D:200:GLN:O	1:D:202:MET:N	2.46	0.48
1:D:568:TRP:CG	1:D:569:ASP:HB3	2.49	0.48
1:C:776:LEU:O	1:C:777:LEU:HD23	2.13	0.48
1:B:67:GLU:OE1	1:B:67:GLU:N	2.30	0.48
1:D:37:ARG:NH2	1:D:216:HIS:O	2.42	0.48
1:C:895:VAL:N	1:C:920:LEU:O	2.43	0.48
1:A:279:ILE:HD11	1:A:280:ASP:OD2	2.12	0.48
1:A:576:ILE:CG2	1:A:577:LYS:N	2.75	0.48
1:C:587:ALA:HB1	1:C:591:ASP:HB2	1.95	0.48
1:D:499:ILE:HD11	1:D:529:GLU:CD	2.33	0.48
1:C:343:LEU:HD23	1:C:348:PRO:CA	2.43	0.48
1:B:414:ASN:O	1:B:415:ILE:HG13	2.13	0.48
1:C:901:GLY:N	1:C:914:CYS:O	2.43	0.48
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.48	0.48
1:D:460:ASN:O	1:D:461:GLU:C	2.51	0.48
1:C:450:HIS:O	1:C:482:ARG:NH2	2.46	0.48
1:C:585:TRP:CB	1:C:974:HIS:CD2	2.96	0.48
1:C:553:TRP:O	1:C:557:ARG:HG3	2.13	0.48
1:B:149:ALA:O	1:B:150:PHE:HB3	2.12	0.48
1:D:790:ASP:HB2	4:D:4435:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:765:LEU:HD12	1:D:765:LEU:C	2.33	0.48
1:C:479:ASP:N	1:C:480:PRO:HD3	2.22	0.48
1:C:65:ALA:CB	1:C:66:PRO:HD2	2.42	0.48
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.49	0.48
1:B:41:GLU:HA	1:B:46:ARG:HB2	1.95	0.48
1:D:721:ARG:C	1:D:722:LEU:HD23	2.33	0.48
1:A:222:ILE:HD13	1:A:313:VAL:HG11	1.94	0.48
1:B:740:LEU:HA	1:B:748:CYS:O	2.13	0.48
1:C:395:HIS:ND1	1:C:396:PRO:HD2	2.29	0.48
1:A:815:HIS:HE1	1:A:877:PRO:O	1.97	0.48
1:A:513:PRO:O	1:A:514:ALA:HB3	2.12	0.48
1:A:380:LYS:HE2	1:A:405:TYR:O	2.13	0.48
1:C:679:LEU:O	1:C:680:ILE:HG13	2.13	0.48
1:D:651:LEU:HD23	1:D:703:PRO:HG3	1.96	0.48
1:B:972:HIS:HB2	1:B:974:HIS:CE1	2.48	0.48
1:D:856:TYR:CD1	1:D:856:TYR:N	2.79	0.48
1:A:587:ALA:HB1	1:A:591:ASP:HB2	1.96	0.48
1:A:311:ALA:HB2	1:A:330:VAL:HG21	1.95	0.48
1:A:592:PHE:C	1:A:594:ASP:H	2.16	0.48
1:C:968:MET:HG2	1:C:968:MET:O	2.14	0.48
1:C:473:ARG:HH12	1:C:477:SER:N	2.12	0.48
1:B:507:ASP:O	1:B:519:SER:HB2	2.14	0.48
1:A:651:LEU:HD11	1:A:653[B]:HIS:HD2	1.75	0.48
1:B:966:GLN:NE2	1:B:979:GLU:OE2	2.40	0.48
1:A:24:LEU:HB2	1:A:161:TYR:H	1.78	0.48
1:D:395:HIS:CE1	1:D:397:LEU:HB2	2.48	0.48
1:A:424:ASN:ND2	1:D:279:ILE:HD11	2.26	0.48
1:A:138:GLN:HG2	1:A:139:THR:N	2.29	0.48
1:B:667:GLU:O	1:B:668:VAL:HG23	2.13	0.48
1:A:944:LEU:HG	1:A:951:TRP:CE3	2.49	0.48
1:D:830:LEU:HD23	1:D:830:LEU:N	2.29	0.48
1:C:153:TRP:CD1	1:C:158:TRP:CA	2.97	0.48
1:A:635:THR:HG21	1:A:679:LEU:HD22	1.96	0.48
1:A:456:TRP:O	1:A:484:VAL:HA	2.13	0.48
1:D:420:MET:CE	1:D:425:ARG:HD2	2.43	0.48
1:A:741:THR:O	1:A:741:THR:HG22	2.13	0.48
1:A:775:GLN:OE1	1:A:775:GLN:HA	2.13	0.48
1:A:673:ALA:HB1	1:A:674:PRO:CD	2.36	0.48
1:D:98:PRO:O	1:D:594:ASP:HB3	2.14	0.48
1:D:101:THR:HG23	1:D:204:ARG:NH2	2.29	0.48
1:A:271:THR:HG22	1:A:272:ALA:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:902:PRO:HD3	1:D:918:TRP:CH2	2.48	0.48
1:B:534:ILE:HD11	1:B:563:GLN:HB2	1.96	0.48
1:B:234:ASP:O	1:B:235:PHE:HB2	2.14	0.48
1:C:256:VAL:O	1:C:271:THR:HA	2.14	0.48
1:D:651:LEU:O	1:D:701:VAL:HG23	2.14	0.48
1:A:155:ASN:CG	1:A:178:ARG:HH12	2.17	0.48
1:A:782:ASP:OD1	1:A:854:LYS:HE3	2.14	0.48
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.78	0.48
1:A:43:ARG:NH2	1:A:264:GLU:HA	2.29	0.48
1:B:706:THR:HG1	1:B:708:TRP:H	1.57	0.48
1:B:658:LEU:O	1:B:659:ASP:C	2.49	0.48
1:B:693:GLN:HB3	1:B:695:TRP:HE1	1.78	0.48
1:B:843:GLN:O	1:B:844:HIS:HB2	2.13	0.48
1:D:36:TRP:HD1	1:D:41:GLU:HB3	1.77	0.48
1:A:285:TYR:HB3	1:A:288:ARG:CG	2.44	0.48
1:B:343:LEU:HD23	1:B:348:PRO:HA	1.94	0.48
1:A:588:TYR:CD2	1:A:603:MET:HE2	2.49	0.48
1:A:824:GLN:O	1:A:838:THR:HA	2.14	0.47
1:B:360:HIS:HB3	1:B:363:HIS:HB2	1.95	0.47
1:D:807:VAL:HG13	1:D:808:GLU:N	2.28	0.47
1:B:778:THR:HG23	1:B:779:PRO:HD2	1.94	0.47
1:C:658:LEU:HA	1:C:658:LEU:HD12	1.52	0.47
1:D:333:ARG:HA	1:D:345:ASN:OD1	2.14	0.47
1:C:423:MET:HG2	1:C:462:SER:C	2.34	0.47
1:A:533:LEU:O	1:A:534:ILE:HG13	2.14	0.47
1:B:99:ILE:HD12	1:B:99:ILE:N	2.29	0.47
1:C:234:ASP:O	1:C:235:PHE:HB2	2.13	0.47
1:B:29:ALA:HB3	1:B:445:GLN:OE1	2.14	0.47
1:D:416:GLU:HG2	1:D:418:HIS:HB2	1.97	0.47
1:C:797:GLU:O	1:C:801:ILE:HD13	2.13	0.47
1:D:622:HIS:HE1	1:D:717:TRP:O	1.96	0.47
1:C:353:GLY:C	1:C:566:PHE:HA	2.33	0.47
1:A:38:ASN:O	1:A:39:SER:C	2.52	0.47
1:B:261:TRP:CZ2	1:B:266:GLN:HB2	2.50	0.47
1:B:43:ARG:HD2	1:B:261:TRP:CE3	2.48	0.47
1:D:217:LYS:NZ	1:D:326:GLU:OE2	2.46	0.47
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.28	0.47
1:B:947:GLY:O	1:B:1023:LYS:HE3	2.14	0.47
1:A:638:VAL:O	1:A:677:LYS:HA	2.14	0.47
1:A:369:GLU:HA	1:A:372:MET:HE2	1.96	0.47
1:A:821:ALA:N	1:A:841:ALA:O	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:PRO:HA	1:C:112:PRO:HA	1.39	0.47
1:C:433:LEU:N	1:C:434:PRO:CD	2.77	0.47
1:A:788:PRO:HB2	1:A:793:ILE:HD11	1.97	0.47
1:C:417:THR:O	1:C:418:HIS:C	2.50	0.47
1:D:635:THR:HG22	1:D:635:THR:O	2.08	0.47
1:B:1019:VAL:O	1:B:1019:VAL:HG12	2.13	0.47
1:C:960:SER:O	1:C:983:TRP:HB2	2.14	0.47
1:C:972:HIS:HB2	1:C:974:HIS:ND1	2.29	0.47
1:D:103:VAL:HG22	1:D:418:HIS:CD2	2.48	0.47
1:D:581:ASN:OD1	1:D:581:ASN:N	2.43	0.47
1:A:607:VAL:HB	1:A:612:THR:O	2.14	0.47
1:A:140:ARG:HG2	1:A:141:ILE:N	2.23	0.47
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.49	0.47
1:B:706:THR:HG1	1:B:709:SER:H	1.57	0.47
1:C:898:LEU:HD12	1:C:916:ASP:C	2.35	0.47
1:B:253:TYR:O	1:B:317:THR:HA	2.15	0.47
1:D:376:ILE:HG12	1:D:407:LEU:HD12	1.96	0.47
1:D:262:GLN:HE22	1:D:299:LYS:HD2	1.80	0.47
1:D:543:GLY:O	1:D:545:SER:N	2.48	0.47
1:B:55:ASN:OD1	1:B:55:ASN:N	2.46	0.47
1:A:427:THR:HG21	1:A:462:SER:HB3	1.94	0.47
1:D:157:ARG:HB2	1:D:176:PHE:HD2	1.79	0.47
1:C:535:LEU:H	1:C:535:LEU:HD12	1.78	0.47
1:B:629:PHE:CE2	1:B:638:VAL:HG22	2.49	0.47
1:C:14:ARG:HH11	1:C:14:ARG:HG2	1.79	0.47
1:A:234:ASP:OD2	1:A:236:SER:OG	2.30	0.47
1:B:986:ILE:CD1	1:B:1018:LEU:HD21	2.44	0.47
1:D:354:VAL:HA	1:D:567:VAL:N	2.28	0.47
1:B:986:ILE:HD13	1:B:986:ILE:HG21	1.57	0.47
1:B:748:CYS:C	1:B:749:ILE:HD12	2.35	0.47
1:B:433:LEU:N	1:B:434:PRO:HD2	2.29	0.47
1:A:647:SER:HA	1:A:650:GLU:OE1	2.15	0.47
1:A:69:VAL:HA	1:A:70:PRO:HD2	1.64	0.47
1:C:874:SER:N	1:D:724:GLU:OE1	2.46	0.47
1:B:141:ILE:CG1	1:B:142:ILE:N	2.78	0.47
1:A:766:SER:O	1:A:767:GLN:HB2	2.14	0.47
1:D:656:VAL:CG1	1:D:657:ALA:N	2.78	0.47
1:C:43:ARG:HD2	1:C:261:TRP:CE2	2.48	0.47
1:D:176:PHE:N	1:D:176:PHE:CD1	2.81	0.47
1:C:143:PHE:O	1:C:168:PRO:HA	2.14	0.47
1:A:433:LEU:HB3	1:A:434:PRO:CD	2.42	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LEU:HD12	1:C:214:LEU:HA	1.64	0.47
1:C:14:ARG:HA	1:C:16:TRP:CH2	2.50	0.47
1:B:891:VAL:HA	1:B:946:TYR:OH	2.15	0.47
1:D:893:GLU:O	1:D:921:PRO:HA	2.14	0.47
1:B:898:LEU:HD12	1:B:916:ASP:O	2.15	0.47
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.96	0.47
1:D:414:ASN:O	1:D:439:ARG:NH1	2.46	0.47
1:B:896:ASN:HB3	1:B:945:ASN:HB2	1.97	0.47
1:C:972:HIS:HB3	4:C:4095:HOH:O	2.13	0.47
1:D:420:MET:HE2	1:D:425:ARG:HD2	1.95	0.47
1:C:552:TYR:HB3	1:C:556:PHE:CZ	2.49	0.47
1:C:868:VAL:HG12	1:C:869:ASP:N	2.29	0.47
1:B:229:THR:HG22	1:B:240:LEU:HB2	1.97	0.47
1:A:619:GLU:OE1	1:A:619:GLU:HA	2.14	0.47
1:D:311:ALA:HB2	1:D:330:VAL:HG21	1.96	0.47
1:D:234:ASP:O	1:D:235:PHE:HB2	2.14	0.47
1:C:114:VAL:HB	1:C:115:PRO:HD2	1.97	0.47
1:D:474:TRP:O	1:D:477:SER:HB2	2.14	0.47
1:B:789:LEU:HD11	1:B:993:ILE:HG22	1.96	0.47
1:D:141:ILE:C	1:D:142:ILE:HG13	2.35	0.47
1:C:824:GLN:HG2	1:C:825:CYS:N	2.29	0.47
1:B:142:ILE:O	1:B:212:VAL:HA	2.15	0.47
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.49	0.47
1:B:682:LEU:HA	1:B:683:PRO:HD3	1.78	0.47
1:D:721:ARG:NH1	1:D:721:ARG:HB2	2.30	0.47
1:C:130:ASP:OD2	1:C:131:GLU:N	2.47	0.47
1:C:767:GLN:NE2	1:C:774:LYS:CB	2.78	0.47
1:D:619:GLU:OE1	1:D:619:GLU:HA	2.14	0.47
1:A:147:ASN:HA	1:A:148:SER:HA	1.67	0.47
1:C:855:THR:OG1	1:C:867:THR:HB	2.14	0.47
1:A:520:ILE:HG21	1:A:535:LEU:HD11	1.97	0.47
1:D:627:PHE:HA	1:D:639:THR:O	2.15	0.47
1:B:36:TRP:HD1	1:B:41:GLU:HB2	1.75	0.47
1:C:297:ASN:N	1:C:298:PRO:HD3	2.30	0.47
1:A:904:GLU:OE1	1:A:929:TYR:OH	2.29	0.47
1:D:829:THR:C	1:D:830:LEU:HD23	2.34	0.47
1:D:767:GLN:CG	1:D:768:MET:N	2.78	0.47
1:D:784:PHE:HA	1:D:881:ARG:O	2.15	0.47
1:B:607:VAL:HG12	1:B:613:PRO:HA	1.97	0.47
1:B:513:PRO:C	1:B:515:VAL:H	2.15	0.47
1:A:101:THR:HG23	1:A:204:ARG:NE	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:HIS:N	1:A:367:MET:HE1	2.30	0.47
1:C:906:TYR:CE2	1:C:937:LEU:HB2	2.50	0.47
1:D:749:ILE:N	1:D:749:ILE:CD1	2.78	0.47
1:B:337:ILE:CG1	1:B:342:LEU:HD13	2.45	0.47
1:A:856:TYR:HD1	1:A:856:TYR:N	2.11	0.47
1:C:153:TRP:CH2	1:C:187:MET:HE2	2.50	0.47
1:A:888:LEU:HA	1:A:888:LEU:HD23	1.64	0.47
1:C:344:LEU:N	1:C:347:LYS:O	2.38	0.46
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.14	0.46
1:B:855:THR:OG1	1:B:867:THR:HB	2.14	0.46
1:C:708:TRP:CZ3	1:C:709:SER:HB3	2.50	0.46
1:A:429:ASP:OD1	1:A:431:ARG:HB2	2.14	0.46
1:C:454:ILE:HG13	1:C:455:ILE:HG13	1.97	0.46
1:B:103:VAL:HG22	1:B:418:HIS:CE1	2.50	0.46
1:A:197:LEU:HD12	1:A:439:ARG:HE	1.79	0.46
1:C:251:ARG:HG3	1:C:253:TYR:OH	2.15	0.46
1:C:991:MET:HG2	1:C:992:GLY:O	2.15	0.46
1:A:782:ASP:HA	1:A:884:LEU:HD23	1.98	0.46
1:D:808:GLU:OE1	1:D:808:GLU:HA	2.14	0.46
1:C:85:VAL:HG12	1:C:86:VAL:N	2.30	0.46
1:C:26:ARG:HD2	1:C:442:ARG:HH22	1.80	0.46
1:B:200:GLN:O	1:B:202:MET:N	2.47	0.46
1:C:153:TRP:NE1	1:C:158:TRP:HB2	2.29	0.46
1:B:416:GLU:HG2	1:B:418:HIS:HB2	1.97	0.46
1:A:1018:LEU:HA	1:A:1018:LEU:HD23	1.67	0.46
1:B:634:GLN:NE2	1:B:684:GLU:CA	2.78	0.46
1:A:634:GLN:O	1:A:682:LEU:HB2	2.15	0.46
1:C:278:ILE:N	1:C:278:ILE:CD1	2.78	0.46
1:A:640:SER:O	1:A:675:GLN:HA	2.15	0.46
1:B:778:THR:HG22	1:B:779:PRO:CD	2.43	0.46
1:B:79:PRO:HD2	1:B:80:GLU:OE2	2.15	0.46
1:D:382:ASN:HA	1:D:621:LYS:HG3	1.97	0.46
1:D:529:GLU:OE2	1:D:530:THR:N	2.43	0.46
1:D:490:GLY:HA2	1:D:515:VAL:HG12	1.97	0.46
1:D:397:LEU:HA	1:D:397:LEU:HD12	1.75	0.46
1:B:503:TYR:HD2	1:B:996:ASP:O	1.97	0.46
1:A:275:GLY:HA2	1:A:286:ALA:HA	1.98	0.46
1:A:842:TRP:CB	1:A:850:PHE:HD1	2.29	0.46
1:A:951:TRP:CE3	1:A:951:TRP:N	2.84	0.46
1:C:833:ALA:HB2	1:C:859:ASP:HB3	1.95	0.46
1:C:835:LEU:C	1:C:836:ILE:HD13	2.35	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:ND2	1:B:191:TRP:HB2	2.30	0.46
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.50	0.46
1:B:621:LYS:NZ	1:B:714:ILE:O	2.41	0.46
1:A:1004:SER:O	1:A:1007:PHE:N	2.37	0.46
1:B:722:LEU:O	1:B:723:ALA:HB2	2.16	0.46
1:D:377:LEU:HD22	1:D:708:TRP:CA	2.45	0.46
1:A:455:ILE:CG2	1:A:485:GLN:HG2	2.45	0.46
1:B:751:LEU:HA	4:B:7165:HOH:O	2.15	0.46
1:C:535:LEU:N	1:C:535:LEU:HD12	2.31	0.46
1:B:695:TRP:CZ2	1:B:721:ARG:HG3	2.50	0.46
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.79	0.46
1:B:955:PHE:HB2	1:B:987:ASP:O	2.16	0.46
1:A:577:LYS:CD	1:A:587:ALA:HB2	2.46	0.46
1:B:576:ILE:CG2	1:B:577:LYS:N	2.79	0.46
1:B:236:SER:O	1:B:297:ASN:N	2.48	0.46
1:B:54:LEU:HD21	1:B:214:LEU:HD12	1.97	0.46
1:C:375:ASP:CG	1:C:570:TRP:HE1	2.19	0.46
1:B:751:LEU:O	1:B:754:LYS:O	2.33	0.46
1:B:292:ARG:CG	1:B:292:ARG:NH1	2.77	0.46
1:A:834:VAL:CG1	1:A:835:LEU:N	2.78	0.46
1:D:657:ALA:CB	1:D:662:PRO:HA	2.39	0.46
1:D:524:LEU:CD2	1:D:561:ARG:HB3	2.36	0.46
1:C:69:VAL:HA	1:C:70:PRO:HD3	1.83	0.46
1:A:949:HIS:HB3	1:A:951:TRP:CH2	2.51	0.46
1:C:226:HIS:CD2	1:C:448:ARG:HD3	2.51	0.46
1:D:770:ILE:HB	1:D:775:GLN:HE21	1.81	0.46
1:A:126:THR:HG22	1:A:126:THR:O	2.14	0.46
1:D:326:GLU:HB3	4:D:4424:HOH:O	2.15	0.46
1:C:417:THR:CG2	1:C:426:LEU:HD12	2.46	0.46
1:D:832:ASP:O	1:D:833:ALA:HB2	2.16	0.46
1:D:112:PRO:HD2	1:D:113:PHE:CE1	2.50	0.46
1:A:99:ILE:HG23	1:A:594:ASP:HB2	1.96	0.46
1:D:260:LEU:O	1:D:267:VAL:N	2.38	0.46
1:D:259:SER:OG	1:D:314:GLU:OE1	2.33	0.46
1:D:250:LEU:HA	1:D:250:LEU:HD23	1.78	0.46
1:C:350:LEU:HA	1:C:350:LEU:HD12	1.68	0.46
1:D:651:LEU:CD1	1:D:667:GLU:HB3	2.45	0.46
1:B:13:ARG:CG	1:B:13:ARG:NH1	2.79	0.46
1:A:544:ASN:HB3	1:A:789:LEU:HD22	1.98	0.46
1:A:930:VAL:O	1:A:932:PRO:HD3	2.15	0.46
1:C:531:ARG:CB	1:C:532:PRO:HD2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PHE:CD2	1:A:238:ALA:HB2	2.50	0.46
1:B:253:TYR:HD1	1:B:317:THR:HG22	1.80	0.46
1:B:368:ASP:N	1:B:368:ASP:OD1	2.48	0.46
1:C:360:HIS:ND1	1:C:362:LEU:HB2	2.29	0.46
1:A:945:ASN:CG	1:A:950:GLN:HE21	2.20	0.46
1:A:682:LEU:HD23	1:A:682:LEU:HA	1.67	0.46
1:B:898:LEU:HD12	1:B:916:ASP:C	2.36	0.46
1:C:662:PRO:O	1:C:663:LEU:HD23	2.16	0.46
1:C:457:SER:HA	1:C:485:GLN:O	2.15	0.46
1:B:35:SER:HB2	1:B:217:LYS:HD3	1.98	0.46
1:C:147:ASN:HA	1:C:148:SER:HA	1.56	0.46
1:D:621:LYS:HE2	1:D:714:ILE:O	2.15	0.46
1:C:244:VAL:O	1:C:288:ARG:HB3	2.15	0.46
1:C:327:ALA:O	1:C:328:CYS:HB3	2.14	0.46
1:B:539:ALA:O	1:B:567:VAL:HG13	2.16	0.46
1:A:767:GLN:CG	1:A:768:MET:H	2.29	0.45
1:B:777:LEU:HG	1:B:889:ALA:HA	1.97	0.45
1:B:920:LEU:CB	1:B:921:PRO:CD	2.94	0.45
1:D:272:ALA:HB1	1:D:273:PRO:CD	2.46	0.45
1:D:89:ASN:O	1:D:92:MET:N	2.44	0.45
1:A:897:TRP:CD1	1:A:899:GLY:N	2.85	0.45
1:D:759:ASN:OD1	1:D:762:SER:HB3	2.16	0.45
1:C:595:THR:HA	1:C:596:PRO:HA	1.33	0.45
1:A:627:PHE:HA	1:A:639:THR:O	2.16	0.45
1:B:752:GLY:N	4:B:7165:HOH:O	2.48	0.45
1:B:719:GLN:HE22	1:B:915:PHE:N	1.99	0.45
1:C:899:GLY:HA2	1:C:915:PHE:CD1	2.51	0.45
1:C:134:LEU:HD11	1:C:179:ALA:HA	1.97	0.45
1:C:767:GLN:HE21	1:C:774:LYS:CB	2.28	0.45
1:A:279:ILE:O	1:A:279:ILE:HD12	2.15	0.45
1:B:87:PRO:HA	1:B:208:ILE:O	2.15	0.45
1:A:460:ASN:O	1:A:461:GLU:C	2.54	0.45
1:A:347:LYS:HB3	1:A:348:PRO:HD2	1.99	0.45
1:B:749:ILE:O	1:B:755:ARG:HA	2.17	0.45
1:D:766:SER:O	1:D:767:GLN:HB2	2.16	0.45
1:C:100:TYR:O	1:C:597:ASN:HA	2.16	0.45
1:D:788:PRO:O	1:D:933:SER:HB2	2.17	0.45
1:A:972:HIS:HB3	1:A:974:HIS:ND1	2.31	0.45
1:B:878:HIS:HA	1:B:879:PRO:HD3	1.78	0.45
1:B:314:GLU:HB3	1:B:322:LEU:HD11	1.97	0.45
1:A:30:HIS:CE1	1:A:33:PHE:CD1	3.04	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:ALA:HB2	1:B:662:PRO:HA	1.97	0.45
1:B:693:GLN:HE22	1:B:942:ARG:NH2	2.14	0.45
1:A:702:GLN:HA	1:A:703:PRO:HD2	1.66	0.45
1:A:227:VAL:CG1	1:A:228:ALA:N	2.79	0.45
1:D:608:PHE:CE1	1:D:614:HIS:CD2	3.04	0.45
1:A:890:GLN:HE22	1:A:948:PRO:HD3	1.81	0.45
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.97	0.45
1:C:257:THR:HG23	1:C:270:GLY:O	2.16	0.45
1:A:109:VAL:HG12	1:A:109:VAL:O	2.16	0.45
1:A:575:LEU:HA	1:A:575:LEU:HD23	1.84	0.45
1:B:897:TRP:HB2	1:B:943:GLU:O	2.15	0.45
1:A:941:THR:CG2	1:A:942:ARG:N	2.79	0.45
1:B:636:ILE:HD11	1:B:682:LEU:CD1	2.47	0.45
1:A:993:ILE:HG13	1:A:994:GLY:N	2.30	0.45
1:D:129:VAL:CG1	1:D:182:ASN:ND2	2.78	0.45
1:D:215:LEU:HD21	1:D:217:LYS:HD3	1.98	0.45
1:B:85:VAL:CG1	1:B:86:VAL:N	2.78	0.45
1:D:805:ALA:O	1:D:806:TRP:C	2.53	0.45
1:A:723:ALA:HB1	1:B:875:ASP:OD2	2.17	0.45
1:B:678:GLN:HG2	1:B:679:LEU:N	2.32	0.45
1:B:256:VAL:CG1	1:B:257:THR:N	2.79	0.45
1:B:513:PRO:O	1:B:514:ALA:HB3	2.15	0.45
1:B:245:GLN:CG	1:B:288:ARG:HG2	2.41	0.45
1:A:43:ARG:CG	1:A:43:ARG:NH1	2.78	0.45
1:B:836:ILE:N	1:B:836:ILE:HD13	2.31	0.45
1:C:768:MET:O	1:C:775:GLN:N	2.50	0.45
1:C:663:LEU:O	1:C:664:ALA:HB2	2.16	0.45
1:D:635:THR:HA	1:D:680:ILE:O	2.16	0.45
1:D:595:THR:O	1:D:595:THR:HG23	2.17	0.45
1:D:335:VAL:HG22	1:D:344:LEU:HD13	1.99	0.45
1:B:490:GLY:C	1:B:492:ASP:H	2.20	0.45
1:B:145:GLY:N	1:B:210:ARG:HB2	2.31	0.45
1:A:422:PRO:HG3	1:D:284:GLY:C	2.37	0.45
1:B:518:TRP:O	1:B:519:SER:C	2.53	0.45
1:C:85:VAL:CG1	1:C:86:VAL:N	2.79	0.45
1:C:658:LEU:HG	1:C:661:LYS:HZ1	1.79	0.45
1:B:971:SER:OG	1:B:972:HIS:ND1	2.32	0.45
1:B:974:HIS:CD2	1:B:975:LEU:CD2	2.98	0.45
1:C:14:ARG:HG2	1:C:14:ARG:NH1	2.32	0.45
1:A:386:ALA:HA	1:A:408:TYR:O	2.17	0.45
1:C:742:THR:CG2	1:C:743:SER:N	2.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:HG12	1:B:258:VAL:O	2.12	0.45
1:B:995:GLY:H	1:B:1002:SER:CB	2.29	0.45
1:A:256:VAL:O	1:A:271:THR:HA	2.17	0.45
1:A:780:LEU:HA	1:A:885:ASN:O	2.17	0.45
1:D:395:HIS:HE1	1:D:397:LEU:HB2	1.82	0.45
1:B:414:ASN:C	1:B:415:ILE:HG13	2.36	0.45
1:A:401:LEU:O	1:A:405:TYR:HD1	1.99	0.45
1:D:40:GLU:OE1	1:D:40:GLU:HA	2.16	0.45
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.99	0.45
1:A:474:TRP:O	1:A:478:VAL:HG13	2.16	0.45
1:B:294:ASN:ND2	1:B:294:ASN:H	2.15	0.45
1:D:655:MET:CA	1:D:655:MET:HE3	2.46	0.45
1:B:1004:SER:O	1:B:1006:GLU:N	2.49	0.45
1:B:487:GLU:O	1:B:491:ALA:N	2.46	0.45
1:B:67:GLU:CD	1:B:67:GLU:H	2.17	0.45
1:C:412:GLU:O	1:C:413:ALA:C	2.55	0.45
1:A:390:SER:CB	1:A:391:HIS:CE1	2.99	0.45
1:D:697:THR:HG23	1:D:719:GLN:CG	2.46	0.45
1:C:151:HIS:HB2	1:C:187:MET:HE3	1.99	0.45
1:D:902:PRO:HD2	1:D:903[B]:GLN:NE2	2.31	0.45
1:B:420:MET:HE2	1:B:425:ARG:HG2	1.98	0.45
1:C:571:VAL:H	1:C:571:VAL:HG12	1.38	0.45
1:C:385:ASN:C	1:C:407:LEU:HD23	2.37	0.45
1:C:393:PRO:HD2	1:C:414:ASN:HB2	1.99	0.45
1:C:847:LYS:HG3	1:C:848:THR:H	1.80	0.45
1:C:255:ARG:HB2	1:C:316:HIS:CE1	2.51	0.45
1:D:767:GLN:HG3	1:D:768:MET:N	2.32	0.45
1:C:256:VAL:HA	1:C:314:GLU:O	2.16	0.45
1:C:854:LYS:HG2	1:C:868:VAL:HG22	1.99	0.45
1:C:824:GLN:CG	1:C:825:CYS:N	2.80	0.45
1:A:19:PRO:HD3	1:A:112:PRO:CB	2.47	0.45
1:B:147:ASN:HA	1:B:148:SER:HA	1.49	0.45
1:C:929:TYR:O	1:C:930:VAL:C	2.53	0.45
1:C:681:GLU:HG2	1:C:682:LEU:N	2.31	0.45
1:A:222:ILE:HD11	1:A:313:VAL:HG12	1.98	0.45
1:A:272:ALA:HB1	1:A:273:PRO:CD	2.46	0.45
1:B:595:THR:HA	1:B:596:PRO:C	2.31	0.45
1:D:343:LEU:HA	1:D:347:LYS:O	2.17	0.45
1:A:153:TRP:CD1	1:A:158:TRP:CA	2.99	0.45
1:A:395:HIS:HA	1:A:396:PRO:HD3	1.65	0.45
1:B:855:THR:O	1:B:866:ILE:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ARG:NH2	1:A:1021:CYS:SG	2.90	0.45
1:C:423:MET:HB2	1:C:423:MET:HE2	1.77	0.45
1:B:474:TRP:CE2	1:B:478:VAL:HG11	2.52	0.45
1:B:894:ARG:NH1	1:B:921:PRO:CD	2.79	0.45
1:A:257:THR:HA	1:A:270:GLY:O	2.17	0.45
1:C:898:LEU:HD12	1:C:917:ARG:N	2.31	0.45
1:C:868:VAL:CG1	1:C:869:ASP:N	2.80	0.45
1:C:825:CYS:HA	1:C:838:THR:HG22	1.98	0.45
1:D:193:ASP:O	1:D:196:TYR:HB2	2.15	0.45
1:B:351:ILE:N	1:B:351:ILE:CD1	2.79	0.45
1:A:882:ILE:CD1	1:A:1014:TYR:CD1	3.00	0.45
1:B:959:ILE:HG23	1:B:959:ILE:O	2.16	0.45
1:A:755:ARG:CG	1:A:769:TRP:HB2	2.47	0.44
1:A:54:LEU:CD1	1:A:214:LEU:HD22	2.47	0.44
1:C:60:PHE:HB3	1:C:84:VAL:CG1	2.48	0.44
1:D:367:MET:CE	1:D:367:MET:HA	2.47	0.44
1:A:134:LEU:HD12	1:A:134:LEU:H	1.81	0.44
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.99	0.44
1:D:78:LEU:N	1:D:78:LEU:CD2	2.77	0.44
1:A:391:HIS:CE1	1:A:460:ASN:ND2	2.84	0.44
1:D:111:PRO:HA	1:D:112:PRO:HA	1.69	0.44
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.98	0.44
1:B:870:VAL:CG1	1:B:871:GLU:N	2.80	0.44
1:D:789:LEU:O	1:D:790:ASP:C	2.56	0.44
1:C:936:GLY:O	1:C:938:ARG:NH1	2.46	0.44
1:D:907:PRO:HD3	1:D:939:CYS:SG	2.56	0.44
1:C:315:LEU:O	1:C:323:ILE:HB	2.17	0.44
1:C:580:GLU:H	1:C:580:GLU:HG3	1.42	0.44
1:B:256:VAL:HG12	1:B:257:THR:N	2.32	0.44
1:B:662:PRO:C	1:B:663:LEU:HD23	2.38	0.44
1:C:901:GLY:HA3	1:C:902:PRO:HA	1.75	0.44
1:B:868:VAL:CG1	1:B:1016:TYR:CE2	3.00	0.44
1:D:60:PHE:HB2	1:D:84:VAL:HG22	1.99	0.44
1:B:558:GLN:O	1:B:560:PRO:HD3	2.17	0.44
1:A:622:HIS:HB2	1:A:912:ALA:HB2	1.99	0.44
1:B:672:VAL:HG22	1:B:678:GLN:HB2	1.99	0.44
1:A:110:ASN:N	1:A:111:PRO:HD3	2.32	0.44
1:A:479:ASP:HA	1:A:480:PRO:HD2	1.81	0.44
1:B:742:THR:CG2	1:B:743:SER:N	2.78	0.44
1:B:305:ILE:HD13	1:B:305:ILE:HG21	1.73	0.44
1:B:291:LEU:N	1:B:291:LEU:CD2	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:PHE:N	1:B:516:PRO:HA	2.31	0.44
1:D:980:GLU:O	1:D:981:GLY:O	2.35	0.44
1:B:634:GLN:HE22	1:B:684:GLU:CA	2.29	0.44
1:B:431:ARG:NH2	1:C:26:ARG:O	2.48	0.44
1:C:199:ASP:OD2	1:C:419:GLY:N	2.48	0.44
1:A:360:HIS:ND1	1:A:362:LEU:N	2.63	0.44
1:C:568:TRP:CG	1:C:569:ASP:HB3	2.52	0.44
1:B:559:TYR:CB	1:B:562:LEU:HG	2.47	0.44
1:A:655:MET:HE2	1:A:662:PRO:HB3	1.99	0.44
1:C:429:ASP:OD1	1:C:431:ARG:HG3	2.17	0.44
1:A:965:GLN:O	1:A:966:GLN:C	2.52	0.44
1:D:211:ASP:OD1	1:D:211:ASP:N	2.34	0.44
1:B:458:LEU:HD11	1:B:472:TYR:HB2	1.98	0.44
1:D:154:CYS:O	1:D:155:ASN:HB2	2.17	0.44
1:B:687:GLN:CA	1:B:687:GLN:NE2	2.79	0.44
1:A:37:ARG:HH21	1:A:217:LYS:HA	1.82	0.44
1:D:617:LEU:O	1:D:620:ALA:HB3	2.17	0.44
1:A:896:ASN:OD1	1:A:917:ARG:HD2	2.17	0.44
1:A:472:TYR:O	1:A:476:LYS:HG2	2.18	0.44
1:A:152:LEU:HG	1:A:153:TRP:N	2.26	0.44
1:B:1015:HIS:CD2	1:B:1016:TYR:N	2.86	0.44
1:C:63:PHE:HB3	1:C:64:PRO:CD	2.46	0.44
1:B:1003:VAL:CG1	1:B:1008:GLN:HG2	2.47	0.44
1:A:279:ILE:HG23	1:A:284:GLY:HA2	1.99	0.44
1:B:731:PRO:HB2	1:B:732:ALA:H	1.48	0.44
1:D:866:ILE:CG2	1:D:867:THR:N	2.79	0.44
1:A:485:GLN:HA	1:A:496:THR:OG1	2.17	0.44
1:C:844:HIS:O	1:C:845:GLN:C	2.55	0.44
1:A:538:TYR:HD2	1:A:566:PHE:O	1.99	0.44
1:C:702:GLN:O	1:C:712:GLY:N	2.48	0.44
1:B:85:VAL:HG12	1:B:86:VAL:N	2.31	0.44
1:A:351:ILE:CD1	1:A:351:ILE:N	2.80	0.44
1:D:423:MET:HB3	1:D:463:GLY:N	2.32	0.44
1:D:187:MET:HE3	1:D:189:LEU:HD21	1.99	0.44
1:C:71:GLU:HB2	4:C:5036:HOH:O	2.17	0.44
1:C:908:ASP:OD1	1:C:993:ILE:HG12	2.17	0.44
1:A:471:LEU:HA	1:A:471:LEU:HD23	1.79	0.44
1:A:770:ILE:HG13	1:A:775:GLN:HE21	1.80	0.44
1:C:920:LEU:HA	1:C:921:PRO:HD3	1.89	0.44
1:A:103:VAL:HG22	1:A:418:HIS:CE1	2.53	0.44
1:D:608:PHE:HD1	1:D:612:THR:O	2.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:HA	1:B:343:LEU:HD23	1.68	0.44
1:C:651:LEU:HD12	1:C:667:GLU:HB3	2.00	0.44
1:B:134:LEU:HD21	1:B:177:LEU:HB3	1.99	0.44
1:B:931:PHE:HA	1:B:932:PRO:HD2	1.64	0.44
1:A:824:GLN:HE21	1:A:837:THR:HG22	1.81	0.44
1:A:158:TRP:CH2	1:A:160:GLY:HA2	2.52	0.44
1:A:338:GLU:HB3	1:A:343:LEU:CD1	2.48	0.44
1:A:446:ARG:HG2	1:A:447:ASP:OD1	2.18	0.44
1:B:905:ASN:N	1:B:937:LEU:O	2.35	0.44
1:A:835:LEU:HD12	1:A:857:ARG:HA	1.99	0.44
1:A:141:ILE:HG13	1:A:214:LEU:HD13	1.99	0.44
1:A:37:ARG:NH2	1:A:218:PRO:CD	2.79	0.44
1:D:606:LEU:HD23	1:D:606:LEU:HA	1.78	0.44
1:C:168:PRO:HD3	4:C:4082:HOH:O	2.18	0.44
1:B:663:LEU:O	1:B:664:ALA:HB2	2.18	0.44
1:C:448:ARG:HB2	1:C:448:ARG:HE	1.56	0.44
1:D:367:MET:HE1	1:D:371:THR:CB	2.47	0.44
1:D:202:MET:O	1:D:204:ARG:HD3	2.17	0.44
1:A:105:TYR:CE1	1:A:419:GLY:HA3	2.52	0.44
1:C:897:TRP:O	1:C:917:ARG:HA	2.18	0.44
1:D:528:GLY:O	1:D:530:THR:HG23	2.17	0.44
1:D:423:MET:SD	1:D:461:GLU:HB3	2.58	0.44
1:B:167:LEU:HA	1:B:168:PRO:HD3	1.75	0.44
1:C:972:HIS:N	1:C:972:HIS:ND1	2.66	0.44
1:B:864:MET:O	1:B:1020:TRP:N	2.28	0.44
1:D:178:ARG:HG3	1:D:179:ALA:O	2.18	0.44
1:B:89:ASN:O	1:B:92:MET:HB2	2.17	0.44
1:C:802:ASP:HA	1:C:803:PRO:HD3	1.82	0.44
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.99	0.44
1:C:537:GLU:HA	1:C:566:PHE:O	2.18	0.44
1:C:995:GLY:H	1:C:1002:SER:CB	2.25	0.44
1:C:425:ARG:HD3	1:C:425:ARG:HH11	1.52	0.44
1:D:897:TRP:CH2	1:D:918:TRP:HB2	2.53	0.44
1:A:887:GLN:NE2	1:A:980:GLU:O	2.50	0.44
1:B:344:LEU:N	1:B:347:LYS:O	2.39	0.44
1:C:546:LEU:HD13	1:C:606:LEU:HD21	2.00	0.44
1:D:878:HIS:HA	1:D:879:PRO:HD3	1.92	0.44
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.53	0.44
1:C:240:LEU:HD23	1:C:240:LEU:C	2.38	0.44
1:C:942:ARG:HA	1:C:953:GLY:O	2.18	0.43
1:A:929:TYR:O	1:A:930:VAL:C	2.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:891:VAL:HG22	1:C:982:THR:OG1	2.18	0.43
1:C:837:THR:C	1:C:838:THR:HG23	2.39	0.43
1:A:963:SER:OG	1:A:966:GLN:N	2.41	0.43
1:B:152:LEU:HG	1:B:159:VAL:HB	2.00	0.43
1:D:970:THR:HG22	1:D:972:HIS:O	2.17	0.43
1:A:579:ASP:OD1	1:A:582:GLY:N	2.50	0.43
1:A:910:LEU:HD12	1:A:910:LEU:C	2.38	0.43
1:B:754:LYS:HA	1:B:769:TRP:O	2.18	0.43
1:B:141:ILE:HG22	1:B:173:LEU:HD11	2.00	0.43
1:C:651:LEU:CD1	1:C:667:GLU:HB3	2.47	0.43
1:C:128:ASN:HB2	1:C:181:GLU:OE2	2.17	0.43
1:B:100:TYR:CE2	1:B:602:CYS:HB3	2.52	0.43
1:A:255:ARG:CG	1:A:255:ARG:NH1	2.81	0.43
1:B:663:LEU:N	1:B:663:LEU:HD23	2.33	0.43
1:A:476:LYS:H	1:A:476:LYS:HG2	1.66	0.43
1:A:184:LEU:HA	1:A:184:LEU:HD22	1.84	0.43
1:A:685:LEU:HA	1:A:686:PRO:HD3	1.89	0.43
1:A:68:ALA:O	1:A:70:PRO:HD3	2.18	0.43
1:C:200:GLN:HG2	1:C:391:HIS:HB2	2.00	0.43
1:B:509:ASP:O	1:B:511:PRO:HD3	2.18	0.43
1:D:854:LYS:O	1:D:855:THR:HG22	2.18	0.43
1:A:352:ARG:HG3	1:A:553:TRP:CH2	2.53	0.43
1:D:974:HIS:CE1	1:D:975:LEU:HG	2.53	0.43
1:B:479:ASP:HA	1:B:480:PRO:HD2	1.69	0.43
1:B:845:GLN:N	1:B:845:GLN:OE1	2.50	0.43
1:B:697:THR:HG23	1:B:719:GLN:HB2	2.00	0.43
1:B:636:ILE:HD11	1:B:682:LEU:HD11	1.98	0.43
1:C:217:LYS:HD2	1:C:218:PRO:HD2	1.99	0.43
1:B:153:TRP:CZ3	1:B:187:MET:HB2	2.50	0.43
1:D:950:GLN:N	1:D:1021:CYS:O	2.46	0.43
1:B:433:LEU:HD12	1:B:433:LEU:O	2.19	0.43
1:B:304:GLU:CG	1:B:642:TYR:HD2	2.31	0.43
1:D:786:ARG:O	1:D:788:PRO:HD3	2.17	0.43
1:B:534:ILE:HG23	1:B:564:GLY:C	2.38	0.43
1:D:141:ILE:HG12	1:D:142:ILE:N	2.33	0.43
1:B:421:VAL:HA	1:B:422:PRO:HA	1.42	0.43
1:C:638:VAL:O	1:C:677:LYS:HA	2.19	0.43
1:C:231:PHE:N	1:C:231:PHE:CD1	2.86	0.43
1:D:802:ASP:O	1:D:808:GLU:HG3	2.18	0.43
1:C:397:LEU:O	1:C:398:TRP:C	2.56	0.43
1:B:129:VAL:CG2	1:B:182:ASN:ND2	2.78	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ARG:O	1:D:16:TRP:N	2.51	0.43
1:B:854:LYS:HA	1:B:867:THR:O	2.18	0.43
1:A:952:ARG:HH12	1:A:1019:VAL:HG11	1.82	0.43
1:C:777:LEU:HD21	1:C:889:ALA:HB2	1.99	0.43
1:A:240:LEU:HD23	1:A:241:GLU:N	2.33	0.43
1:B:51:LEU:HD12	1:B:51:LEU:HA	1.69	0.43
1:D:949:HIS:HB3	1:D:951:TRP:CH2	2.53	0.43
1:B:416:GLU:CD	1:B:460:ASN:HD22	2.20	0.43
1:B:500:CYS:HA	1:B:534:ILE:O	2.18	0.43
1:B:503:TYR:N	1:B:503:TYR:CD1	2.85	0.43
1:A:111:PRO:HA	1:A:112:PRO:HA	1.58	0.43
1:B:497:ASP:O	1:B:531:ARG:HG2	2.19	0.43
1:B:140:ARG:HB2	1:B:171:PHE:O	2.18	0.43
1:D:547:GLY:HA2	1:D:908:ASP:O	2.18	0.43
1:B:257:THR:HB	1:B:314:GLU:OE1	2.19	0.43
1:B:930:VAL:O	1:B:932:PRO:HD3	2.19	0.43
1:A:843:GLN:HA	1:A:847:LYS:O	2.19	0.43
1:A:142:ILE:HG12	1:A:170:GLU:HG2	2.01	0.43
1:A:100:TYR:HD2	1:A:589:GLY:HA3	1.84	0.43
1:B:632:SER:N	1:B:635:THR:O	2.43	0.43
1:A:621:LYS:HD3	1:A:717:TRP:HZ3	1.79	0.43
1:C:768:MET:HG3	1:C:769:TRP:N	2.31	0.43
1:B:847:LYS:HG2	1:B:848:THR:N	2.33	0.43
1:B:904:GLU:O	1:B:905:ASN:HB3	2.18	0.43
1:D:310:ARG:HG3	1:D:311:ALA:N	2.34	0.43
1:A:708:TRP:N	1:A:708:TRP:CD1	2.86	0.43
1:D:937:LEU:HA	1:D:957:PHE:O	2.18	0.43
1:C:282:ARG:HD2	1:C:282:ARG:HA	1.86	0.43
1:A:768:MET:HG2	1:A:769:TRP:N	2.34	0.43
1:B:649:ASN:O	1:B:703:PRO:HD2	2.19	0.43
1:A:473:ARG:HD2	1:A:473:ARG:HA	1.70	0.43
1:D:770:ILE:HB	1:D:775:GLN:NE2	2.33	0.43
1:B:854:LYS:HG2	1:B:868:VAL:HG22	2.00	0.43
1:B:86:VAL:HA	1:B:87:PRO:C	2.39	0.43
1:A:62:TRP:CH2	1:A:64:PRO:HA	2.54	0.43
1:D:572:ASP:OD2	1:D:608:PHE:HA	2.18	0.43
1:D:60:PHE:HE2	1:D:95:TYR:CD2	2.36	0.43
1:B:344:LEU:HD22	1:B:408:TYR:CE2	2.53	0.43
1:D:261:TRP:CZ2	1:D:266:GLN:HG3	2.54	0.43
1:C:692:GLY:O	1:C:724:GLU:HA	2.18	0.43
1:D:130:ASP:OD1	1:D:131:GLU:N	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:930:VAL:HA	1:B:973:ARG:CG	2.38	0.43
1:A:829:THR:O	1:A:830:LEU:HD23	2.18	0.43
1:D:637:GLU:HG2	1:D:638:VAL:N	2.33	0.43
1:D:133:TRP:CH2	1:D:216:HIS:HB2	2.54	0.43
1:D:50:GLN:HB3	1:D:216:HIS:HB3	2.01	0.43
1:A:272:ALA:HA	1:A:273:PRO:HD3	1.69	0.43
1:C:110:ASN:ND2	1:C:113:PHE:CD1	2.87	0.43
1:D:815:HIS:HE1	1:D:877:PRO:O	2.02	0.43
1:C:687:GLN:CA	1:C:687:GLN:NE2	2.79	0.43
1:D:936:GLY:O	1:D:938:ARG:HD2	2.19	0.43
1:B:668:VAL:HA	1:B:669:PRO:HD3	1.70	0.43
1:D:100:TYR:CD2	1:D:602:CYS:HB3	2.53	0.43
1:A:469:ASP:O	1:A:472:TYR:HB3	2.18	0.43
1:A:395:HIS:CG	1:A:396:PRO:CD	2.99	0.43
1:A:577:LYS:CG	1:A:587:ALA:HB2	2.49	0.43
1:A:505:ARG:O	1:A:519:SER:HA	2.19	0.43
1:D:830:LEU:HD22	1:D:830:LEU:HA	1.71	0.43
1:D:58:TRP:CG	1:D:86:VAL:HG21	2.53	0.43
1:B:461:GLU:HA	4:B:4042:HOH:O	2.18	0.43
1:D:341:LEU:HB3	1:D:343:LEU:HD21	1.99	0.43
1:C:304:GLU:C	1:C:305:ILE:HG13	2.38	0.43
1:C:441:THR:O	1:C:445:GLN:HG3	2.19	0.43
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.77	0.43
1:A:502:MET:HB3	1:A:502:MET:HE3	1.87	0.43
1:C:687:GLN:HG3	1:C:688:PRO:CD	2.49	0.43
1:A:129:VAL:HG11	1:A:177:LEU:HD12	2.01	0.43
1:B:706:THR:OG1	1:B:708:TRP:N	2.37	0.43
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.40	0.43
1:A:1015:HIS:ND1	1:B:1015:HIS:CE1	2.86	0.43
1:B:961:ARG:NE	1:B:981:GLY:O	2.51	0.43
1:C:134:LEU:CD1	1:C:179:ALA:HA	2.49	0.43
1:C:1021:CYS:HB2	1:C:1022:GLN:H	1.55	0.43
1:B:583:ASN:HA	1:B:584:PRO:HD3	1.89	0.43
1:C:99:ILE:HA	1:C:594:ASP:HB3	2.00	0.43
1:D:490:GLY:CA	1:D:515:VAL:HG12	2.48	0.43
1:D:306:PRO:O	1:D:307:ASN:C	2.56	0.43
1:A:436:MET:O	1:A:439:ARG:HB2	2.19	0.43
1:C:690:SER:HB2	1:C:691:ALA:H	1.24	0.43
1:D:435:ALA:O	1:D:438:GLU:HB2	2.19	0.43
1:C:30:HIS:CE1	1:C:33:PHE:CD1	3.07	0.43
1:D:253:TYR:HD1	1:D:253:TYR:O	2.02	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LYS:HD2	1:B:476:LYS:HA	1.80	0.43
1:A:836:ILE:HG22	1:A:837:THR:H	1.84	0.43
1:A:133:TRP:HZ3	1:A:214:LEU:HB3	1.83	0.43
1:B:636:ILE:CD1	1:B:682:LEU:HG	2.49	0.43
1:D:433:LEU:N	1:D:434:PRO:HD2	2.34	0.43
1:B:747:PHE:CD1	1:B:760:ARG:HG2	2.53	0.43
1:C:1020:TRP:HD1	1:C:1021:CYS:N	2.16	0.43
1:A:343:LEU:HA	1:A:347:LYS:O	2.18	0.43
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.53	0.43
1:A:810:TRP:O	1:A:811:LYS:C	2.57	0.43
1:A:559:TYR:CD1	1:A:559:TYR:N	2.87	0.43
1:B:897:TRP:HA	1:B:943:GLU:O	2.19	0.43
1:D:435:ALA:HB2	4:D:4470:HOH:O	2.19	0.43
1:D:484:VAL:HG12	1:D:485:GLN:N	2.33	0.43
1:A:440:VAL:O	1:A:444:VAL:HG23	2.18	0.43
1:B:568:TRP:CE2	1:B:569:ASP:HB3	2.54	0.42
1:A:130:ASP:O	1:A:133:TRP:HB2	2.19	0.42
1:A:124:SER:HA	1:A:184:LEU:O	2.19	0.42
1:C:467:ASN:O	1:C:471:LEU:HG	2.19	0.42
1:D:429:ASP:OD1	1:D:431:ARG:N	2.52	0.42
1:B:218:PRO:HB2	1:B:220:THR:O	2.19	0.42
1:D:830:LEU:HB2	1:D:833:ALA:O	2.19	0.42
1:D:62:TRP:CD1	1:D:95:TYR:CB	3.02	0.42
1:A:376:ILE:CD1	1:A:401:LEU:HB3	2.48	0.42
1:B:606:LEU:C	1:B:614:HIS:HD2	2.22	0.42
1:A:970:THR:HG22	1:A:972:HIS:O	2.19	0.42
1:C:499:ILE:HD11	1:C:529:GLU:CD	2.38	0.42
1:A:657:ALA:HA	1:A:661:LYS:O	2.18	0.42
1:B:645:ARG:HH11	1:B:645:ARG:HD3	1.68	0.42
1:B:801:ILE:HD12	1:B:808:GLU:OE2	2.19	0.42
1:A:896:ASN:HA	1:A:918:TRP:O	2.19	0.42
1:B:658:LEU:HD12	1:B:693:GLN:O	2.19	0.42
1:D:476:LYS:HD2	1:D:476:LYS:HA	1.67	0.42
1:C:769:TRP:N	1:C:769:TRP:CE3	2.88	0.42
1:D:430:PRO:O	1:D:431:ARG:C	2.54	0.42
1:C:203:TRP:CD1	1:C:573:GLN:HG2	2.53	0.42
1:B:336:ARG:O	1:B:343:LEU:N	2.50	0.42
1:B:607:VAL:CA	1:B:614:HIS:HD2	2.32	0.42
1:B:350:LEU:HD12	1:B:351:ILE:N	2.34	0.42
1:D:304:GLU:HG2	1:D:642:TYR:HD2	1.85	0.42
1:B:499:ILE:HD11	1:B:529:GLU:CD	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ARG:HD3	1:B:525:SER:O	2.18	0.42
1:C:726:LEU:HA	1:C:726:LEU:HD23	1.79	0.42
1:B:537:GLU:HG2	1:B:568:TRP:CE3	2.55	0.42
1:A:388:ARG:NH1	1:A:536:CYS:SG	2.92	0.42
1:D:168:PRO:O	1:D:442:ARG:NH2	2.52	0.42
1:B:777:LEU:HD13	1:B:980:GLU:HB3	2.02	0.42
1:D:942:ARG:HD2	1:D:942:ARG:HA	1.90	0.42
1:A:634:GLN:HE22	1:A:684:GLU:CD	2.23	0.42
1:C:963:SER:HB3	1:C:983:TRP:NE1	2.34	0.42
1:C:959:ILE:HA	1:C:983:TRP:O	2.19	0.42
1:C:807:VAL:HG13	1:C:808:GLU:N	2.33	0.42
1:B:533:LEU:HD23	1:B:534:ILE:N	2.34	0.42
1:C:110:ASN:O	1:C:113:PHE:HD1	2.02	0.42
1:C:356:ARG:HD2	1:C:379:MET:HE1	2.00	0.42
1:A:339:ASN:O	1:B:527:PRO:HB3	2.19	0.42
1:A:77:ASP:HA	1:A:183:ARG:NH2	2.34	0.42
1:C:830:LEU:HD23	1:C:830:LEU:N	2.29	0.42
1:B:805:ALA:HB3	1:B:808:GLU:CG	2.50	0.42
1:D:167:LEU:HA	1:D:168:PRO:HD3	1.96	0.42
1:C:906:TYR:CD1	1:C:906:TYR:N	2.86	0.42
1:D:568:TRP:CE2	1:D:569:ASP:HB3	2.54	0.42
1:D:35:SER:H	1:D:326:GLU:CD	2.22	0.42
1:C:593:GLY:O	1:C:594:ASP:C	2.58	0.42
1:B:825:CYS:HA	1:B:837:THR:O	2.19	0.42
1:A:970:THR:HG23	1:A:975:LEU:HB2	2.01	0.42
1:D:55:ASN:HD21	1:D:211:ASP:HB3	1.84	0.42
1:B:111:PRO:HA	1:B:112:PRO:HA	1.39	0.42
1:B:949:HIS:HB2	1:B:951:TRP:CH2	2.55	0.42
1:B:316:HIS:HA	1:B:323:ILE:CD1	2.25	0.42
1:A:746:ASP:N	1:A:760:ARG:HG3	2.33	0.42
1:A:29:ALA:HB2	1:A:442:ARG:HB3	2.00	0.42
1:C:658:LEU:HB3	1:C:661:LYS:HD2	2.00	0.42
1:B:922:LEU:O	1:B:925:MET:HB2	2.19	0.42
1:A:928:PRO:HB2	1:A:973:ARG:NH1	2.34	0.42
1:A:497:ASP:O	1:A:531:ARG:HG2	2.20	0.42
1:A:970:THR:CG2	1:A:975:LEU:HB2	2.49	0.42
1:A:966:GLN:OE1	1:A:976:LEU:HA	2.19	0.42
1:A:555:ALA:O	1:A:556:PHE:C	2.57	0.42
1:A:823:LEU:HD11	1:B:728:VAL:HB	2.01	0.42
1:B:637:GLU:OE2	1:B:677:LYS:HE3	2.19	0.42
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:PRO:HG2	1:C:324:GLU:HG2	2.02	0.42
1:D:533:LEU:HD23	1:D:533:LEU:C	2.39	0.42
1:C:442:ARG:HH11	1:C:442:ARG:HD3	1.74	0.42
1:B:745:MET:HE3	1:B:745:MET:C	2.39	0.42
1:C:836:ILE:HB	1:C:856:TYR:HB2	2.02	0.42
1:A:685:LEU:HG	1:A:685:LEU:H	1.63	0.42
1:B:986:ILE:O	1:B:986:ILE:HG23	2.19	0.42
1:C:342:LEU:HA	1:C:342:LEU:HD12	1.74	0.42
1:A:207:GLY:O	1:A:209:PHE:HD2	2.03	0.42
1:C:352:ARG:HD3	1:C:383:ASN:O	2.20	0.42
1:C:110:ASN:O	1:C:113:PHE:N	2.38	0.42
1:B:52:ARG:HB2	1:B:214:LEU:HB2	2.01	0.42
1:C:622:HIS:HB3	1:C:912:ALA:HB2	2.00	0.42
1:D:1006:GLU:HG2	1:D:1007:PHE:CE1	2.55	0.42
1:A:549:PHE:O	1:A:552:TYR:HB2	2.20	0.42
1:D:227:VAL:HG12	1:D:228:ALA:N	2.34	0.42
1:B:547:GLY:HA3	1:B:908:ASP:OD2	2.20	0.42
1:B:542:MET:HB2	1:B:604:ASN:HD22	1.85	0.42
1:C:309:TYR:CD1	1:C:309:TYR:N	2.88	0.42
1:B:685:LEU:HA	1:B:686:PRO:HD3	1.58	0.42
1:B:657:ALA:HB1	1:B:661:LYS:C	2.40	0.42
1:A:544:ASN:CB	1:A:789:LEU:HD22	2.49	0.42
1:A:476:LYS:HE3	1:A:476:LYS:HB3	1.24	0.42
1:B:66:PRO:HD2	1:B:67:GLU:OE1	2.18	0.42
1:A:146:VAL:CG1	1:A:150:PHE:CD2	3.03	0.42
1:B:35:SER:O	1:B:50:GLN:NE2	2.52	0.42
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.67	0.42
1:A:655:MET:HE3	1:A:664:ALA:O	2.19	0.42
1:A:742:THR:HG22	1:A:743:SER:H	1.84	0.42
1:C:553:TRP:N	1:C:553:TRP:CD1	2.87	0.42
1:C:878:HIS:CD2	1:C:1010:SER:HA	2.54	0.42
1:D:424:ASN:HB3	1:D:464:HIS:H	1.85	0.42
1:A:967:LEU:HD23	1:A:967:LEU:HA	1.82	0.42
1:D:654:TRP:HE1	1:D:666:GLY:HA3	1.81	0.42
1:B:722:LEU:HA	1:B:722:LEU:HD23	1.62	0.42
1:C:296:GLU:O	1:C:297:ASN:C	2.55	0.42
1:B:123:TYR:CD2	1:B:208:ILE:HG13	2.54	0.42
1:D:394:ASN:O	1:D:399:TYR:HE1	2.03	0.42
1:C:738:PRO:CA	1:C:751:LEU:HD13	2.49	0.42
1:B:280:ASP:HB2	1:B:281:GLU:H	1.53	0.42
1:C:897:TRP:O	1:C:918:TRP:N	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:HIS:CD2	1:C:573:GLN:HA	2.55	0.42
1:C:557:ARG:CZ	1:C:628:GLN:NE2	2.82	0.42
1:B:420:MET:CE	1:B:425:ARG:HG2	2.50	0.42
1:C:337:ILE:HA	1:C:341:LEU:O	2.20	0.42
1:B:107:ILE:HD12	1:B:115:PRO:HD3	2.01	0.42
1:B:651:LEU:HB2	1:B:669:PRO:HA	2.02	0.42
1:A:118:ASN:HA	1:A:119:PRO:HD2	1.94	0.42
1:C:932:PRO:HG3	1:C:973:ARG:HA	2.02	0.42
1:D:521:LYS:HG2	1:D:559:TYR:OH	2.20	0.42
1:B:615:PRO:O	1:B:618:THR:HG23	2.20	0.42
1:C:333:ARG:O	1:C:333:ARG:HD3	2.19	0.42
1:D:914:CYS:O	1:D:918:TRP:HZ2	2.03	0.42
1:A:999:TRP:CE3	1:A:999:TRP:N	2.88	0.42
1:B:534:ILE:HG23	1:B:564:GLY:O	2.20	0.42
1:C:753:ASN:OD1	1:C:753:ASN:N	2.41	0.42
1:A:805:ALA:O	1:A:806:TRP:C	2.58	0.42
1:D:220:THR:HA	1:D:247:CYS:O	2.19	0.42
1:D:448:ARG:HE	1:D:448:ARG:HB2	1.56	0.42
1:D:726:LEU:HD23	1:D:726:LEU:HA	1.80	0.42
1:B:231:PHE:N	1:B:231:PHE:CD1	2.88	0.42
1:B:612:THR:O	1:B:612:THR:HG22	2.20	0.42
1:C:73:TRP:HD1	1:C:78:LEU:CD1	2.33	0.42
1:A:589:GLY:O	1:A:599:ARG:HA	2.20	0.42
1:B:634:GLN:HG2	1:B:682:LEU:O	2.20	0.42
1:C:754:LYS:HA	1:C:769:TRP:O	2.20	0.42
1:B:916:ASP:CG	1:B:917:ARG:H	2.23	0.42
1:A:571:VAL:HG22	1:A:572:ASP:O	2.18	0.42
1:D:446:ARG:NE	1:D:447:ASP:OD1	2.42	0.42
1:D:618:THR:HG22	1:D:912:ALA:HB1	2.01	0.42
1:B:559:TYR:HA	1:B:560:PRO:HD2	1.73	0.42
1:C:897:TRP:CH2	1:C:918:TRP:HB2	2.54	0.42
1:D:767:GLN:CG	1:D:768:MET:H	2.33	0.42
1:D:147:ASN:HA	1:D:148:SER:HA	1.69	0.42
1:A:401:LEU:HA	1:A:401:LEU:HD23	1.84	0.42
1:D:38:ASN:OD1	1:D:40:GLU:N	2.53	0.42
1:C:650:GLU:HA	1:C:701:VAL:O	2.19	0.42
1:A:737:ILE:HG12	1:A:738:PRO:CD	2.43	0.41
1:A:854:LYS:HG2	1:A:868:VAL:HG13	2.02	0.41
1:A:129:VAL:O	1:A:130:ASP:C	2.56	0.41
1:B:885:ASN:HB2	1:B:985:ASN:OD1	2.20	0.41
1:A:600:GLN:H	1:A:600:GLN:NE2	2.16	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:TYR:O	1:A:675:GLN:HG2	2.20	0.41
1:A:786:ARG:HA	1:A:964:GLN:OE1	2.20	0.41
1:D:942:ARG:HH11	1:D:942:ARG:CG	2.25	0.41
1:C:859:ASP:OD1	1:C:861:SER:OG	2.37	0.41
1:D:80:GLU:H	1:D:80:GLU:CD	2.24	0.41
1:D:35:SER:HB2	1:D:217:LYS:HD2	2.02	0.41
1:C:447:ASP:OD1	1:C:447:ASP:N	2.48	0.41
1:D:570:TRP:O	1:D:607:VAL:HG22	2.19	0.41
1:D:673:ALA:O	1:D:676:GLY:N	2.52	0.41
1:B:824:GLN:CG	1:B:825:CYS:N	2.82	0.41
1:C:571:VAL:O	1:C:571:VAL:HG13	2.19	0.41
1:A:878:HIS:HA	1:A:879:PRO:HD3	1.74	0.41
1:D:770:ILE:O	1:D:770:ILE:HG22	2.19	0.41
1:A:972:HIS:HB2	1:A:975:LEU:HG	2.01	0.41
1:C:753:ASN:O	1:C:771:GLY:N	2.53	0.41
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.54	0.41
1:D:380:LYS:HB3	1:D:380:LYS:HE3	1.44	0.41
1:C:986:ILE:HG21	1:C:1018:LEU:CD2	2.27	0.41
1:B:91:GLN:NE2	1:B:190:ARG:CZ	2.83	0.41
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.83	0.41
1:A:30:HIS:CB	1:A:31:PRO:CD	2.96	0.41
1:C:21:VAL:HG11	1:C:24:LEU:HD11	2.02	0.41
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.21	0.41
1:B:114:VAL:HB	1:B:191:TRP:CB	2.50	0.41
1:A:418:HIS:HD2	1:A:418:HIS:O	2.04	0.41
1:A:590:GLY:C	1:A:592:PHE:H	2.23	0.41
1:A:619:GLU:HG2	1:A:909:ARG:HG3	2.02	0.41
1:C:547:GLY:HA2	1:C:908:ASP:O	2.20	0.41
1:D:794:GLY:HA2	1:D:998:SER:O	2.20	0.41
1:B:515:VAL:HA	1:B:516:PRO:HD2	1.85	0.41
1:A:823:LEU:HD23	1:A:823:LEU:N	2.35	0.41
1:D:100:TYR:CZ	1:D:602:CYS:HB3	2.54	0.41
1:B:890:GLN:C	1:B:891:VAL:HG23	2.40	0.41
1:D:893:GLU:HG3	1:D:894:ARG:HG2	2.03	0.41
1:B:69:VAL:HA	1:B:70:PRO:HD3	1.95	0.41
1:B:433:LEU:N	1:B:434:PRO:CD	2.83	0.41
1:A:165:SER:O	1:A:209:PHE:HZ	2.03	0.41
1:A:695:TRP:NE1	1:A:915:PHE:CD2	2.87	0.41
1:B:232:ASN:OD1	1:B:236:SER:N	2.52	0.41
1:B:297:ASN:N	1:B:298:PRO:CD	2.83	0.41
1:C:473:ARG:HH11	1:C:476:LYS:HB2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:934:GLU:O	1:B:935:ASN:HB3	2.20	0.41
1:A:753:ASN:N	1:A:753:ASN:OD1	2.48	0.41
1:B:805:ALA:HB3	1:B:808:GLU:CB	2.49	0.41
1:C:900:LEU:HB2	1:C:939:CYS:O	2.20	0.41
1:C:146:VAL:CG1	1:C:150:PHE:CD2	3.03	0.41
1:D:78:LEU:HA	1:D:78:LEU:HD22	1.77	0.41
1:D:147:ASN:HB2	1:D:209:PHE:CE2	2.55	0.41
1:D:253:TYR:C	1:D:253:TYR:CD1	2.93	0.41
1:C:621:LYS:HE3	1:C:717:TRP:HZ3	1.85	0.41
1:B:568:TRP:HA	1:B:569:ASP:HA	1.73	0.41
1:A:424:ASN:O	1:A:427:THR:N	2.53	0.41
1:D:658:LEU:CD2	1:D:661:LYS:NZ	2.84	0.41
1:B:900:LEU:HD23	1:B:900:LEU:HA	1.58	0.41
1:D:801:ILE:HA	1:D:801:ILE:HD13	1.86	0.41
1:B:127:PHE:CZ	1:B:182:ASN:HB2	2.55	0.41
1:C:695:TRP:CH2	1:C:721:ARG:HB2	2.55	0.41
1:D:599:ARG:HB2	1:D:600:GLN:H	1.39	0.41
1:A:622:HIS:HB3	1:A:912:ALA:HB2	2.02	0.41
1:A:285:TYR:HB2	1:A:288:ARG:HG3	2.02	0.41
1:D:436:MET:O	1:D:439:ARG:HB2	2.20	0.41
1:D:896:ASN:HA	1:D:918:TRP:O	2.20	0.41
1:D:165:SER:OG	1:D:198:GLU:OE1	2.34	0.41
1:B:89:ASN:ND2	1:B:205:MET:HB2	2.35	0.41
1:A:381:GLN:HA	1:A:708:TRP:HZ3	1.86	0.41
1:A:878:HIS:HB3	1:A:1009:LEU:O	2.21	0.41
1:D:626:PHE:O	1:D:641:GLU:HB2	2.20	0.41
1:C:627:PHE:HA	1:C:639:THR:O	2.20	0.41
1:A:349:LEU:HA	1:A:349:LEU:HD23	1.80	0.41
1:A:278:ILE:H	1:A:278:ILE:HD12	1.86	0.41
1:A:895:VAL:O	1:A:919:ASP:HA	2.21	0.41
1:B:282:ARG:HH11	1:B:282:ARG:HD2	1.60	0.41
1:B:450:HIS:O	1:B:482:ARG:NH2	2.54	0.41
1:A:62:TRP:CZ3	1:A:64:PRO:N	2.89	0.41
1:B:418:HIS:ND1	1:B:461:GLU:OE1	2.53	0.41
1:C:429:ASP:HA	1:C:430:PRO:HD2	1.88	0.41
1:C:783:GLN:HG2	1:C:881:ARG:CD	2.51	0.41
1:B:344:LEU:O	1:B:345:ASN:C	2.58	0.41
1:B:787:ALA:HA	1:B:788:PRO:HD2	1.91	0.41
1:B:427:THR:O	1:B:467:ASN:HB2	2.20	0.41
1:D:242:ALA:O	1:D:290:THR:HA	2.21	0.41
1:D:652:LEU:O	1:D:667:GLU:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:LEU:HD12	1:A:857:ARG:HB2	2.02	0.41
1:C:842:TRP:HE3	1:C:842:TRP:H	1.68	0.41
1:C:138:GLN:HG2	1:C:139:THR:N	2.33	0.41
1:C:184:LEU:HA	1:C:184:LEU:HD23	1.89	0.41
1:C:149:ALA:O	1:C:150:PHE:HB3	2.20	0.41
1:C:427:THR:HG21	1:C:462:SER:HB3	2.03	0.41
1:C:336:ARG:O	1:C:343:LEU:N	2.45	0.41
1:D:708:TRP:CD1	1:D:708:TRP:N	2.88	0.41
1:A:351:ILE:HG22	1:A:353:GLY:H	1.86	0.41
1:D:261:TRP:CD1	1:D:261:TRP:N	2.89	0.41
1:B:821:ALA:N	1:B:841:ALA:O	2.53	0.41
1:D:471:LEU:HA	1:D:471:LEU:HD23	1.71	0.41
1:C:866:ILE:HG12	1:C:866:ILE:H	1.20	0.41
1:B:510:GLN:HB3	1:B:512:PHE:CZ	2.55	0.41
1:B:513:PRO:C	1:B:515:VAL:N	2.74	0.41
1:D:166:ARG:CB	1:D:392:TYR:HB2	2.51	0.41
1:D:651:LEU:HD11	1:D:653:HIS:ND1	2.36	0.41
1:B:292:ARG:NH1	1:B:292:ARG:HG3	2.15	0.41
1:C:73:TRP:CD1	1:C:78:LEU:CD1	3.04	0.41
1:B:634:GLN:HE22	1:B:685:LEU:HG	1.86	0.41
1:A:43:ARG:NH2	1:A:264:GLU:CG	2.84	0.41
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.56	0.41
1:D:99:ILE:HG23	1:D:594:ASP:HB2	2.02	0.41
1:C:55:ASN:ND2	1:C:87:PRO:HD3	2.35	0.41
1:D:721:ARG:HB2	1:D:721:ARG:HH11	1.85	0.41
1:C:615:PRO:CG	1:C:927:THR:HG21	2.51	0.41
1:C:773:LYS:HE2	1:C:775:GLN:HE22	1.86	0.41
1:A:703:PRO:O	1:A:711:ALA:HB1	2.21	0.41
1:A:240:LEU:O	1:A:292:ARG:HA	2.21	0.41
1:D:383:ASN:ND2	1:D:621:LYS:O	2.52	0.41
1:A:316:HIS:HB3	1:A:322:LEU:HD12	2.03	0.41
1:A:658:LEU:HD12	1:A:658:LEU:HA	1.79	0.41
1:B:103:VAL:O	1:B:199:ASP:OD2	2.39	0.41
1:B:756:TRP:N	1:B:756:TRP:CE3	2.88	0.41
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.56	0.41
1:D:806:TRP:CE2	1:D:809:ARG:NH2	2.89	0.41
1:D:66:PRO:HB3	1:D:187:MET:CE	2.50	0.41
1:B:372:MET:O	1:B:375:ASP:HB2	2.21	0.41
1:B:548:GLY:N	1:B:908:ASP:O	2.48	0.41
1:D:424:ASN:O	1:D:428:ASP:N	2.53	0.41
1:D:592:PHE:N	1:D:592:PHE:CD1	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LEU:HD23	1:A:720:TRP:CE3	2.56	0.41
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.60	0.41
1:D:804:ASN:HA	1:D:804:ASN:HD22	1.66	0.41
1:B:43:ARG:CD	1:B:261:TRP:CD2	2.97	0.41
1:A:141:ILE:HD13	1:A:143:PHE:CE1	2.56	0.41
1:A:894:ARG:CZ	1:A:921:PRO:HD3	2.50	0.41
1:D:894:ARG:NH2	1:D:919:ASP:OD1	2.53	0.41
1:D:78:LEU:HA	1:D:79:PRO:HD2	1.70	0.41
1:A:505:ARG:HD3	1:A:510:GLN:NE2	2.35	0.41
1:C:569:ASP:O	1:C:605:GLY:HA2	2.20	0.41
1:B:224:ASP:OD1	1:B:225:PHE:N	2.52	0.41
1:B:615:PRO:HG2	1:B:904:GLU:OE1	2.21	0.41
1:D:389:CYS:O	1:D:391:HIS:HA	2.20	0.41
1:A:663:LEU:HD23	1:A:663:LEU:N	2.36	0.41
1:C:787:ALA:HA	1:C:788:PRO:HD3	1.67	0.41
1:C:961:ARG:NH2	1:C:979:GLU:O	2.54	0.41
1:D:905:ASN:HB2	1:D:910:LEU:HB3	2.03	0.41
1:C:262:GLN:HB2	1:C:267:VAL:HG21	2.03	0.41
1:A:38:ASN:O	1:A:41:GLU:HB2	2.22	0.40
1:B:166:ARG:HG3	1:B:392:TYR:CG	2.56	0.40
1:C:124:SER:HA	1:C:184:LEU:O	2.20	0.40
1:C:833:ALA:HB2	1:C:859:ASP:CB	2.51	0.40
1:B:282:ARG:NH2	1:C:419:GLY:HA2	2.33	0.40
1:B:114:VAL:HB	1:B:191:TRP:HB3	2.04	0.40
1:B:217:LYS:NZ	1:B:326:GLU:OE2	2.41	0.40
1:A:16:TRP:HB2	1:A:192:SER:CB	2.51	0.40
1:C:230:ARG:HB2	1:C:230:ARG:NH1	2.34	0.40
1:C:573:GLN:HB3	1:C:602:CYS:O	2.22	0.40
1:D:73:TRP:CH2	1:D:185:ALA:HB1	2.56	0.40
1:C:379:MET:HE3	1:C:570:TRP:CE2	2.56	0.40
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.03	0.40
1:D:900:LEU:HB3	1:D:913:ALA:HB1	2.02	0.40
1:C:125:LEU:HG	1:C:126:THR:N	2.34	0.40
1:C:60:PHE:CB	1:C:84:VAL:CG1	2.99	0.40
1:C:693:GLN:O	1:C:695:TRP:HD1	2.04	0.40
1:C:695:TRP:CE2	1:C:915:PHE:CD2	3.09	0.40
1:C:377:LEU:HD23	1:C:377:LEU:HA	1.80	0.40
1:C:147:ASN:HA	1:C:165:SER:HB3	2.03	0.40
1:B:756:TRP:CE2	1:B:858:ILE:HD13	2.56	0.40
1:A:813:ALA:HB3	1:A:815:HIS:CD2	2.56	0.40
1:A:984:LEU:HD21	1:A:986:ILE:CG1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HG22	1:B:344:LEU:CD1	2.51	0.40
1:D:975:LEU:HD23	1:D:975:LEU:HA	1.80	0.40
1:B:479:ASP:N	1:B:480:PRO:HD3	2.37	0.40
1:B:379:MET:O	1:B:384:PHE:HB2	2.20	0.40
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.47	0.40
1:D:360:HIS:CD2	1:D:361:PRO:HD2	2.53	0.40
1:A:568:TRP:CG	1:A:569:ASP:HB3	2.56	0.40
1:D:98:PRO:HB2	1:D:203:TRP:CE3	2.56	0.40
1:C:26:ARG:HD2	1:C:442:ARG:NH2	2.36	0.40
1:B:767:GLN:HA	1:B:767:GLN:OE1	2.20	0.40
1:D:16:TRP:HB2	1:D:192:SER:CB	2.52	0.40
1:D:770:ILE:HD13	1:D:775:GLN:NE2	2.36	0.40
1:C:63:PHE:CB	1:C:64:PRO:HD2	2.50	0.40
1:A:506:VAL:O	1:A:519:SER:HB2	2.21	0.40
1:D:571:VAL:HG23	1:D:608:PHE:O	2.20	0.40
1:C:147:ASN:O	1:C:206:SER:HB2	2.21	0.40
1:D:634:GLN:NE2	1:D:682:LEU:O	2.55	0.40
1:B:260:LEU:HD11	1:B:309:TYR:HB2	2.03	0.40
1:B:416:GLU:HG3	1:B:460:ASN:O	2.21	0.40
1:B:896:ASN:O	1:B:945:ASN:N	2.53	0.40
1:A:663:LEU:HD11	1:A:688:PRO:HG3	2.03	0.40
1:A:629:PHE:CE2	1:A:638:VAL:HG13	2.56	0.40
1:D:103:VAL:HG22	1:D:418:HIS:CG	2.57	0.40
1:C:71:GLU:O	1:C:72:SER:C	2.60	0.40
1:C:500:CYS:HA	1:C:534:ILE:O	2.22	0.40
1:C:172:ASP:OD1	1:C:174:SER:OG	2.34	0.40
1:C:401:LEU:HD23	1:C:401:LEU:HA	1.80	0.40
1:D:252:ASP:OD2	1:D:252:ASP:N	2.44	0.40
1:D:353:GLY:C	1:D:566:PHE:HA	2.42	0.40
1:A:29:ALA:O	1:A:30:HIS:HB3	2.22	0.40
1:B:975:LEU:HD22	1:B:975:LEU:HA	1.91	0.40
1:C:741:THR:O	1:C:748:CYS:N	2.45	0.40
1:B:278:ILE:H	1:B:278:ILE:CD1	2.31	0.40
1:B:888:LEU:O	1:B:981:GLY:HA3	2.21	0.40
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.84	0.40
1:D:820:ALA:HB2	1:D:842:TRP:CE2	2.57	0.40
1:C:147:ASN:OD1	1:C:148:SER:HB3	2.22	0.40
1:D:636:ILE:HD13	1:D:636:ILE:HG21	1.80	0.40
1:C:260:LEU:HD12	1:C:260:LEU:HA	1.91	0.40
1:C:153:TRP:HH2	1:C:187:MET:HE2	1.86	0.40
1:A:454:ILE:C	1:A:455:ILE:HG13	2.40	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:C	1:A:20:GLY:N	2.75	0.40
1:B:99:ILE:HG23	1:B:594:ASP:HB2	2.04	0.40
1:A:352:ARG:HG3	1:A:553:TRP:HH2	1.87	0.40
1:B:163:GLN:O	1:B:164:ASP:HB3	2.21	0.40
1:B:358:GLU:HB2	1:B:367:MET:HG2	2.04	0.40
1:D:26:ARG:HD2	1:D:169:SER:HA	2.03	0.40
1:B:751:LEU:HD13	1:B:860:GLY:HA2	2.00	0.40
1:C:73:TRP:HD1	1:C:78:LEU:HD12	1.86	0.40
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.98	0.40
1:D:533:LEU:C	1:D:534:ILE:HG13	2.42	0.40
1:A:74:LEU:HA	1:A:74:LEU:HD23	1.65	0.40
1:C:473:ARG:NH1	1:C:476:LYS:HB2	2.37	0.40
1:C:110:ASN:N	1:C:111:PRO:HD3	2.36	0.40
1:D:250:LEU:HD11	1:D:286:ALA:O	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	1011/1023 (99%)	902 (89%)	99 (10%)	10 (1%)	19	61
1	B	1011/1023 (99%)	901 (89%)	96 (10%)	14 (1%)	14	51
1	C	1011/1023 (99%)	904 (89%)	93 (9%)	14 (1%)	14	51
1	D	1010/1023 (99%)	904 (90%)	93 (9%)	13 (1%)	15	53
All	All	4043/4092 (99%)	3611 (89%)	381 (9%)	51 (1%)	15	53

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	425	ARG
1	A	688	PRO
1	B	201	ASP
1	B	647	SER
1	B	686	PRO
1	B	731	PRO
1	B	732	ALA
1	B	733	ALA
1	C	570	TRP
1	C	686	PRO
1	C	733	ALA
1	D	79	PRO
1	B	389	CYS
1	B	633	GLY
1	B	688	PRO
1	C	164	ASP
1	C	647	SER
1	C	882	ILE
1	D	581	ASN
1	D	731	PRO
1	A	461	GLU
1	A	540	HIS
1	C	461	GLU
1	C	937	LEU
1	D	201	ASP
1	D	461	GLU
1	D	647	SER
1	D	686	PRO
1	D	735	HIS
1	C	45	ASP
1	C	135	GLN
1	D	119	PRO
1	D	164	ASP
1	D	174	SER
1	A	735	HIS
1	A	831	ALA
1	B	39	SER
1	B	164	ASP
1	C	90	TRP
1	C	201	ASP
1	A	687	GLN
1	B	79	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	434	PRO
1	A	788	PRO
1	B	273	PRO
1	D	928	PRO
1	B	119	PRO
1	C	488	GLY
1	D	981	GLY
1	A	21	VAL

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	866/875 (99%)	723 (84%)	143 (16%)	3	13
1	B	866/875 (99%)	699 (81%)	167 (19%)	2	9
1	C	866/875 (99%)	732 (84%)	134 (16%)	3	16
1	D	865/875 (99%)	721 (83%)	144 (17%)	3	13
All	All	3463/3500 (99%)	2875 (83%)	588 (17%)	2	13

All (588) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	27	LEU
1	A	35	SER
1	A	39	SER
1	A	40	GLU
1	A	43	ARG
1	A	72	SER
1	A	74	LEU
1	A	75	GLU
1	A	78	LEU
1	A	116	THR
1	A	124	SER
1	A	125	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	126	THR
1	A	128	ASN
1	A	129	VAL
1	A	132	SER
1	A	138	GLN
1	A	140	ARG
1	A	141	ILE
1	A	148	SER
1	A	152	LEU
1	A	165	SER
1	A	177	LEU
1	A	178	ARG
1	A	184	LEU
1	A	186	VAL
1	A	189	LEU
1	A	193	ASP
1	A	204	ARG
1	A	211	ASP
1	A	214	LEU
1	A	219	THR
1	A	240	LEU
1	A	247	CYS
1	A	250	LEU
1	A	251	ARG
1	A	259	SER
1	A	279	ILE
1	A	282	ARG
1	A	288	ARG
1	A	291	LEU
1	A	293	LEU
1	A	333	ARG
1	A	344	LEU
1	A	351	ILE
1	A	352	ARG
1	A	368	ASP
1	A	370	GLN
1	A	377	LEU
1	A	394	ASN
1	A	411	ASP
1	A	431	ARG
1	A	437	SER
1	A	442	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	446	ARG
1	A	448	ARG
1	A	449	ASN
1	A	452	SER
1	A	476	LYS
1	A	477	SER
1	A	485	GLN
1	A	501	PRO
1	A	502	MET
1	A	505	ARG
1	A	508	GLU
1	A	521	LYS
1	A	522	LYS
1	A	531	ARG
1	A	538	TYR
1	A	546	LEU
1	A	551	LYS
1	A	554	GLN
1	A	569	ASP
1	A	574	SER
1	A	577	LYS
1	A	580	GLU
1	A	581	ASN
1	A	586	SER
1	A	599	ARG
1	A	600	GLN
1	A	604	ASN
1	A	612	THR
1	A	637	GLU
1	A	638	VAL
1	A	651	LEU
1	A	652	LEU
1	A	655	MET
1	A	665	SER
1	A	668	VAL
1	A	672	VAL
1	A	675	GLN
1	A	677	LYS
1	A	680	ILE
1	A	681	GLU
1	A	684	GLU
1	A	693	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	694	LEU
1	A	701	VAL
1	A	721	ARG
1	A	722	LEU
1	A	730	LEU
1	A	734	SER
1	A	735	HIS
1	A	737	ILE
1	A	745	MET
1	A	746	ASP
1	A	748	CYS
1	A	755	ARG
1	A	761	GLN
1	A	768	MET
1	A	770	ILE
1	A	773	LYS
1	A	777	LEU
1	A	778	THR
1	A	790	ASP
1	A	797	GLU
1	A	799	THR
1	A	819	GLU
1	A	823	LEU
1	A	824	GLN
1	A	830	LEU
1	A	840	HIS
1	A	848	THR
1	A	850	PHE
1	A	855	THR
1	A	856	TYR
1	A	867	THR
1	A	874	SER
1	A	875	ASP
1	A	876	THR
1	A	885	ASN
1	A	894	ARG
1	A	903[A]	GLN
1	A	903[B]	GLN
1	A	922	LEU
1	A	950	GLN
1	A	951	TRP
1	A	956	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	997	ASP
1	A	998	SER
1	A	1013	ARG
1	A	1023	LYS
1	B	13	ARG
1	B	36	TRP
1	B	38	ASN
1	B	40	GLU
1	B	50	GLN
1	B	54	LEU
1	B	55	ASN
1	B	59	ARG
1	B	76	CYS
1	B	80	GLU
1	B	90	TRP
1	B	116	THR
1	B	122	CYS
1	B	125	LEU
1	B	129	VAL
1	B	131	GLU
1	B	132	SER
1	B	134	LEU
1	B	142	ILE
1	B	148	SER
1	B	152	LEU
1	B	153	TRP
1	B	154	CYS
1	B	165	SER
1	B	174	SER
1	B	178	ARG
1	B	182	ASN
1	B	187	MET
1	B	189	LEU
1	B	202	MET
1	B	208	ILE
1	B	211	ASP
1	B	213	SER
1	B	214	LEU
1	B	219	THR
1	B	223	SER
1	B	226	HIS
1	B	231	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	237	ARG
1	B	240	LEU
1	B	247	CYS
1	B	252	ASP
1	B	255	ARG
1	B	259	SER
1	B	279	ILE
1	B	291	LEU
1	B	292	ARG
1	B	294	ASN
1	B	297	ASN
1	B	314	GLU
1	B	319	ASP
1	B	324	GLU
1	B	333	ARG
1	B	347	LYS
1	B	351	ILE
1	B	352	ARG
1	B	358	GLU
1	B	367	MET
1	B	370	GLN
1	B	376	ILE
1	B	377	LEU
1	B	380	LYS
1	B	381	GLN
1	B	394	ASN
1	B	400	THR
1	B	407	LEU
1	B	421	VAL
1	B	425	ARG
1	B	433	LEU
1	B	437	SER
1	B	438	GLU
1	B	448	ARG
1	B	476	LYS
1	B	477	SER
1	B	478	VAL
1	B	481	SER
1	B	508	GLU
1	B	519	SER
1	B	521	LYS
1	B	530	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	535	LEU
1	B	545	SER
1	B	551	LYS
1	B	554	GLN
1	B	559	TYR
1	B	569	ASP
1	B	581	ASN
1	B	583	ASN
1	B	599	ARG
1	B	600	GLN
1	B	612	THR
1	B	615	PRO
1	B	618	THR
1	B	630	ARG
1	B	632	SER
1	B	640	SER
1	B	645	ARG
1	B	651	LEU
1	B	652	LEU
1	B	655	MET
1	B	661	LYS
1	B	665	SER
1	B	677	LYS
1	B	684	GLU
1	B	685	LEU
1	B	687	GLN
1	B	693	GLN
1	B	694	LEU
1	B	704	ASN
1	B	710	GLU
1	B	721	ARG
1	B	724	GLU
1	B	730	LEU
1	B	734	SER
1	B	735	HIS
1	B	737	ILE
1	B	740	LEU
1	B	741	THR
1	B	744	GLU
1	B	745	MET
1	B	753	ASN
1	B	755	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	766	SER
1	B	767	GLN
1	B	768	MET
1	B	772	ASP
1	B	774	LYS
1	B	786	ARG
1	B	788	PRO
1	B	796	SER
1	B	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	801	ILE
1	B	804	ASN
1	B	811	LYS
1	B	817	GLN
1	B	819	GLU
1	B	824	GLN
1	B	832	ASP
1	B	843	GLN
1	B	845	GLN
1	B	850	PHE
1	B	854	LYS
1	B	863	GLN
1	B	867	THR
1	B	885	ASN
1	B	900	LEU
1	B	920	LEU
1	B	923	SER
1	B	927	THR
1	B	934	GLU
1	B	938	ARG
1	B	942	ARG
1	B	951	TRP
1	B	952	ARG
1	B	956	GLN
1	B	965	GLN
1	B	968	MET
1	B	975	LEU
1	B	991	MET
1	B	1002	SER
1	B	1004	SER
1	B	1017	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1018	LEU
1	B	1019	VAL
1	B	1022	GLN
1	C	24	LEU
1	C	25	ASN
1	C	40	GLU
1	C	41	GLU
1	C	48	SER
1	C	51	LEU
1	C	75	GLU
1	C	80	GLU
1	C	89	ASN
1	C	90	TRP
1	C	124	SER
1	C	135	GLN
1	C	138	GLN
1	C	141	ILE
1	C	165	SER
1	C	176	PHE
1	C	178	ARG
1	C	181	GLU
1	C	187	MET
1	C	189	LEU
1	C	190	ARG
1	C	213	SER
1	C	214	LEU
1	C	227	VAL
1	C	230	ARG
1	C	233	ASP
1	C	237	ARG
1	C	245	GLN
1	C	247	CYS
1	C	249	GLU
1	C	255	ARG
1	C	259	SER
1	C	262	GLN
1	C	277	GLU
1	C	278	ILE
1	C	279	ILE
1	C	288	ARG
1	C	289	VAL
1	C	291	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	294	ASN
1	C	302	SER
1	C	314	GLU
1	C	319	ASP
1	C	333	ARG
1	C	336	ARG
1	C	349	LEU
1	C	372	MET
1	C	423	MET
1	C	425	ARG
1	C	436	MET
1	C	448	ARG
1	C	477	SER
1	C	478	VAL
1	C	481	SER
1	C	482	ARG
1	C	485	GLN
1	C	493	THR
1	C	494	THR
1	C	502	MET
1	C	503	TYR
1	C	519	SER
1	C	538	TYR
1	C	546	LEU
1	C	554	GLN
1	C	577	LYS
1	C	580	GLU
1	C	586	SER
1	C	595	THR
1	C	635	THR
1	C	651	LEU
1	C	652	LEU
1	C	655	MET
1	C	661	LYS
1	C	665	SER
1	C	667	GLU
1	C	668	VAL
1	C	672	VAL
1	C	675	GLN
1	C	677	LYS
1	C	682	LEU
1	C	684	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	685	LEU
1	C	687	GLN
1	C	690	SER
1	C	694	LEU
1	C	701	VAL
1	C	710	GLU
1	C	727	SER
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	743	SER
1	C	748	CYS
1	C	755	ARG
1	C	760	ARG
1	C	765	LEU
1	C	766	SER
1	C	767	GLN
1	C	768	MET
1	C	772	ASP
1	C	781	ARG
1	C	796	SER
1	C	799	THR
1	C	800	ARG
1	C	811	LYS
1	C	828	ASP
1	C	829	THR
1	C	832	ASP
1	C	836	ILE
1	C	857	ARG
1	C	861	SER
1	C	866	ILE
1	C	867	THR
1	C	874	SER
1	C	885	ASN
1	C	886	CYS
1	C	902	PRO
1	C	903[A]	GLN
1	C	903[B]	GLN
1	C	916	ASP
1	C	923	SER
1	C	927	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	937	LEU
1	C	943	GLU
1	C	952	ARG
1	C	956	GLN
1	C	969	GLU
1	C	974	HIS
1	C	982	THR
1	C	997	ASP
1	C	1000	SER
1	C	1002	SER
1	C	1021	CYS
1	D	13	ARG
1	D	22	THR
1	D	40	GLU
1	D	41	GLU
1	D	49	GLN
1	D	50	GLN
1	D	52	ARG
1	D	59	ARG
1	D	71	GLU
1	D	72	SER
1	D	77	ASP
1	D	78	LEU
1	D	85	VAL
1	D	90	TRP
1	D	124	SER
1	D	125	LEU
1	D	129	VAL
1	D	134	LEU
1	D	138	GLN
1	D	152	LEU
1	D	165	SER
1	D	178	ARG
1	D	190	ARG
1	D	211	ASP
1	D	213	SER
1	D	219	THR
1	D	226	HIS
1	D	237	ARG
1	D	245	GLN
1	D	247	CYS
1	D	249	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	250	LEU
1	D	251	ARG
1	D	259	SER
1	D	265	THR
1	D	266	GLN
1	D	267	VAL
1	D	277	GLU
1	D	279	ILE
1	D	288	ARG
1	D	293	LEU
1	D	296	GLU
1	D	302	SER
1	D	310	ARG
1	D	314	GLU
1	D	328	CYS
1	D	333	ARG
1	D	343	LEU
1	D	352	ARG
1	D	370	GLN
1	D	379	MET
1	D	380	LYS
1	D	383	ASN
1	D	392	TYR
1	D	394	ASN
1	D	404	ARG
1	D	426	LEU
1	D	436	MET
1	D	437	SER
1	D	439	ARG
1	D	476	LYS
1	D	481	SER
1	D	502	MET
1	D	505	ARG
1	D	508	GLU
1	D	515	VAL
1	D	521	LYS
1	D	522	LYS
1	D	546	LEU
1	D	551	LYS
1	D	569	ASP
1	D	577	LYS
1	D	581	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	599	ARG
1	D	635	THR
1	D	639	THR
1	D	645	ARG
1	D	651	LEU
1	D	655	MET
1	D	661	LYS
1	D	675	GLN
1	D	679	LEU
1	D	681	GLU
1	D	684	GLU
1	D	685	LEU
1	D	687	GLN
1	D	694	LEU
1	D	701	VAL
1	D	709	SER
1	D	710	GLU
1	D	721	ARG
1	D	727	SER
1	D	729	THR
1	D	730	LEU
1	D	735	HIS
1	D	737	ILE
1	D	743	SER
1	D	745	MET
1	D	746	ASP
1	D	749	ILE
1	D	755	ARG
1	D	757	GLN
1	D	762	SER
1	D	765	LEU
1	D	770	ILE
1	D	774	LYS
1	D	781	ARG
1	D	782	ASP
1	D	795	VAL
1	D	797	GLU
1	D	799	THR
1	D	800	ARG
1	D	804	ASN
1	D	817	GLN
1	D	824	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	830	LEU
1	D	843	GLN
1	D	845	GLN
1	D	855	THR
1	D	858	ILE
1	D	869	ASP
1	D	870	VAL
1	D	875	ASP
1	D	876	THR
1	D	884	LEU
1	D	887	GLN
1	D	893	GLU
1	D	898	LEU
1	D	910	LEU
1	D	914	CYS
1	D	917	ARG
1	D	927	THR
1	D	934	GLU
1	D	951	TRP
1	D	956	GLN
1	D	960	SER
1	D	974	HIS
1	D	980	GLU
1	D	982	THR
1	D	1004	SER
1	D	1017	GLN
1	D	1018	LEU
1	D	1022	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	93	HIS
1	A	216	HIS
1	A	226	HIS
1	A	266	GLN
1	A	363	HIS
1	A	370	GLN
1	A	460	ASN
1	A	510	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	573	GLN
1	A	600	GLN
1	A	624	GLN
1	A	634	GLN
1	A	687	GLN
1	A	702	GLN
1	A	761	GLN
1	A	824	GLN
1	A	844	HIS
1	A	945	ASN
1	A	950	GLN
1	A	977	HIS
1	A	1008	GLN
1	B	50	GLN
1	B	135	GLN
1	B	147	ASN
1	B	200	GLN
1	B	216	HIS
1	B	294	ASN
1	B	381	GLN
1	B	394	ASN
1	B	464	HIS
1	B	600	GLN
1	B	604	ASN
1	B	614	HIS
1	B	628	GLN
1	B	634	GLN
1	B	653	HIS
1	B	675	GLN
1	B	687	GLN
1	B	702	GLN
1	B	713	HIS
1	B	718	GLN
1	B	719	GLN
1	B	735	HIS
1	B	783	GLN
1	B	843	GLN
1	B	965	GLN
1	B	1022	GLN
1	C	110	ASN
1	C	135	GLN
1	C	226	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	262	GLN
1	C	297	ASN
1	C	381	GLN
1	C	554	GLN
1	C	624	GLN
1	C	634	GLN
1	C	687	GLN
1	C	702	GLN
1	C	704	ASN
1	C	713	HIS
1	C	735	HIS
1	C	757	GLN
1	C	824	GLN
1	C	844	HIS
1	C	878	HIS
1	C	1017	GLN
1	D	135	GLN
1	D	232	ASN
1	D	262	GLN
1	D	307	ASN
1	D	394	ASN
1	D	583	ASN
1	D	653	HIS
1	D	687	GLN
1	D	702	GLN
1	D	761	GLN
1	D	783	GLN
1	D	804	ASN
1	D	815	HIS
1	D	843	GLN
1	D	956	GLN
1	D	977	HIS
1	D	990	HIS
1	D	1022	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 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1011/1023 (98%)	-0.82	4 (0%) 93 80	10, 35, 92, 211	0
1	B	1011/1023 (98%)	-0.77	0 100 100	8, 38, 101, 212	0
1	C	1011/1023 (98%)	-0.79	5 (0%) 91 76	14, 34, 91, 214	0
1	D	1011/1023 (98%)	-0.82	2 (0%) 95 87	5, 34, 93, 210	0
All	All	4044/4092 (98%)	-0.80	11 (0%) 94 84	5, 35, 94, 214	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	689	GLU	3.0
1	A	735	HIS	2.7
1	A	733	ALA	2.7
1	C	733	ALA	2.5
1	C	800	ARG	2.2
1	A	732	ALA	2.1
1	C	732	ALA	2.1
1	A	734	SER	2.1
1	D	734	SER	2.0
1	C	745	MET	2.0
1	D	732	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(Å ²)	Q<0.9
3	NA	C	3101	1/1	0.94	0.43	10.24	49,49,49,49	0
2	MG	D	3001	1/1	0.98	0.29	10.20	26,26,26,26	0
2	MG	A	3001	1/1	0.96	0.26	8.12	29,29,29,29	0
2	MG	C	3001	1/1	0.97	0.26	8.10	25,25,25,25	0
3	NA	A	3102	1/1	0.96	0.38	7.18	24,24,24,24	0
3	NA	A	3101	1/1	0.94	0.25	6.95	52,52,52,52	0
3	NA	D	3102	1/1	0.99	0.30	6.92	47,47,47,47	0
3	NA	C	3102	1/1	0.96	0.23	3.45	24,24,24,24	0
3	NA	B	3102	1/1	0.93	0.21	2.92	32,32,32,32	0
2	MG	D	3002	1/1	0.98	0.22	2.09	30,30,30,30	0
2	MG	C	3002	1/1	0.99	0.18	1.68	25,25,25,25	0
2	MG	B	3001	1/1	0.99	0.15	0.58	13,13,13,13	0
2	MG	B	3002	1/1	0.94	0.12	0.12	30,30,30,30	0
3	NA	B	3103	1/1	0.96	0.13	0.02	45,45,45,45	0
2	MG	A	3002	1/1	0.98	0.08	-1.89	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.