



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:58 AM GMT

PDB ID : 3CU7
Title : Human Complement Component 5
Authors : Fredslund, F.; Andersen, G.R.
Deposited on : 2008-04-16
Resolution : 3.10 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

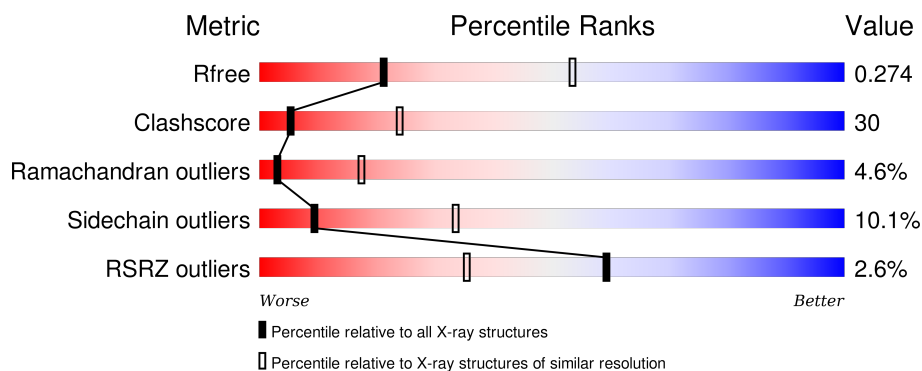
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	1676	<div> <div>3%</div> <div>45%</div> <div>44%</div> <div>8%</div> <div>..</div> </div>
1	B	1676	<div> <div>2%</div> <div>42%</div> <div>39%</div> <div>6%</div> <div>12%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24655 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1625	Total	C	N	O	S	0	0	0
			12861	8239	2111	2458	53			
1	B	1481	Total	C	N	O	S	0	0	0
			11701	7493	1930	2232	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	802	ILE	VAL	SEE REMARK 999	UNP P01031
B	802	ILE	VAL	SEE REMARK 999	UNP P01031

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

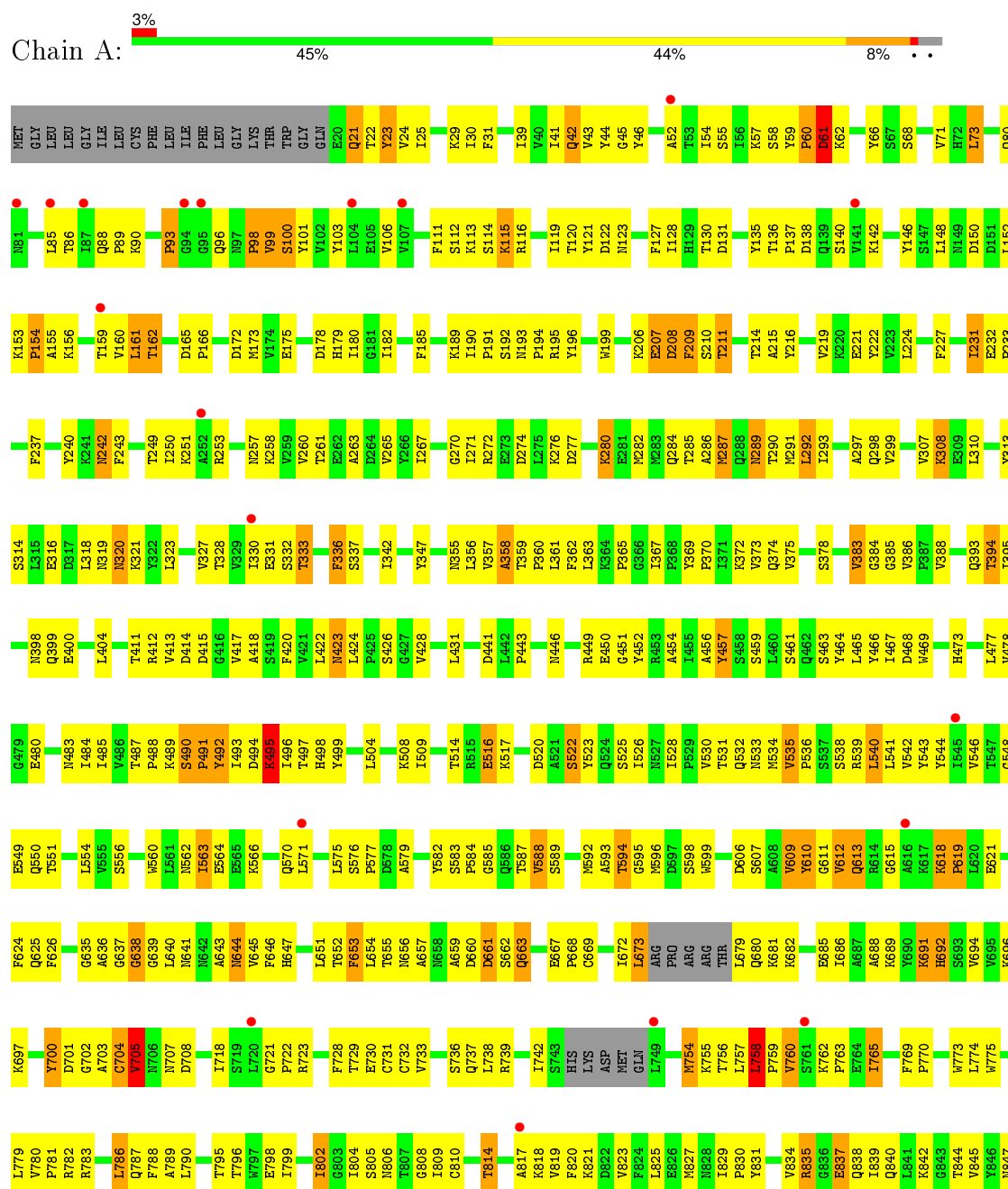
- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Cd	0	0
			4	4		
4	A	5	Total	Cd	0	0
			5	5		

3 Residue-property plots

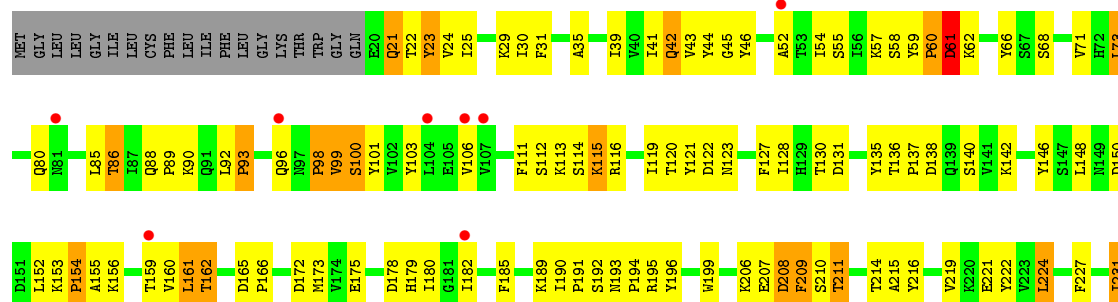
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Complement C5





Chain B: 



G1321	A1322	L1323	H1324	L1325	Y1326	M1332	F1333	L1334	G1335	V1338	E1339	V1340	L1341	L1342	N1343	D1344	D1345	L1346	S1349	T1350	G1351	F1352	G1355	L1356	V1359	H1360	V1361	T1362	H1363	H1366	T1370	S1371	E1372	E1373	F1377	Y1378	L1379	T1383	Q1384	D1385	L1386	GLU	ALA	SER	HIS	TYR	ARG	GLY	TYR			
T1251	A1252	Y1253	A1254	L1255	T1257	S1258	L1259	M1260	L1261	I1264	N1265	Y1266	V1267	M1268	P1269	V1270	I1271	K1272	W1273	L1274	S1275	E1276	E1277	Q1278	R1279	Y1280	G1283	F1284	S1285	S1286	T1287	Q1288	D1289	T1290	I1291	N1292	S1293	L1294	E1295	G1296	L1297	T1298	E1299	Y1300	L1303	V1304	Q1306	L1309	Y1317	K1318	H1319	K1320
D1165	T1166	K1170	N1173	F1174	L1175	L1176	N1177	M1178	T1179	L1180	F1186	I1187	I1190	Y1193	S1196	K1200	T1201	H1202	P1203	Q1204	F1205	L1206	S1207	I1208	L1209	S1210	K1213	A1216	L1217	V1218	K1219	Y1225	W1228	M1231	D1236	S1237	P1240	G1243	T1244	A1245	R1246	M1247	K1248	E1249	T1250							
K1091	Y1092	N1096	S1099	I1100	L1104	L1105	W1106	L1107	V1108	E1109	M1110	Y1111	Q1112	L1113	D1114	N1115	F1118	K1119	E1120	N1121	S1122	Q1123	Y1124	Q1125	P1126	S1127	K1128	L1129	T1132	L1133	P1134	V1135	N1140	L1144	T1145	A1146	F1147	L1148	V1149	I1150	G1151	I1152	F1156	D1157	I1158	G1159	P1160	L1161	V1162	K1163	I1164	
H1002	L1003	A1008	L1012	V1015	V1016	P1017	W1018	F1019	R1020	V1021	F1022	H1023	Y1024	L1025	G1028	T943	W1029	L944	I949	T952	I953	S954	R955	R956	K957	P958	F959	P960	Y961	L967	V968	P969	R970	T971	D1063	S1065	Y1066	S1067	V1068	W1069	K1070	S1075	T1076	W1077	L1078	R1084	G1085	L1086	G1087	Q1088	Y1089	N1090
Y848	R849	T850	S851	G852	M853	Q854	F855	R856	S857	S860	A861	V862	C866	T867	S868	E869	S870	VAL	ILE	ASP	HIS	GLN	GLY	THR	LYS	SER	SER	K882	Q886	K887	V888	H884	T889	V900	P902	L903	I905	G906	L907	H908	E886	I910	N911	S913	L914	E915	T916	W917	I922			
L779	V780	F781	R782	R783	L786	Q787	F788	L789	T795	T796	W797	E798	T799	I802	G803	L804	S805	N806	T807	G808	L809	C810	T814	A817	K818	F819	K820	K821	L823	D824	L825	E826	N827	N828	L829	P830	Y831	V834	R835	E836	E837	Q838	L839	Q840	L841	K842	E843	T844	W845	H846	N847	
K925	F626	G635	A636	G637	G638	G639	L640	R641	N642	A643	W644	V645	H647	L651	T652	F653	L654	T655	N656	A579	Y582	S583	G585	Q586	Y587	W588	S589	M592	A593	Y594	G595	M596	D597	S598	W599	D606	S607	A608	V609	G611	V612	Q613	R614	G615	A616	K617	K618	K619	L620	E621	F624	
E549	Q550	T551	A552	S556	W560	L561	N562	I563	E564	A643	W644	V645	H647	L651	T652	F653	L654	T655	N656	A579	Y582	S583	G585	Q586	Y587	W588	S589	M592	A593	Y594	G595	M596	D597	S598	W599	D606	S607	A608	V609	G611	V612	Q613	R614	G615	A616	K617	K618	K619	L620	E621	F624	
Q625	F626	G635	A636	G637	G638	G639	L640	R641	N642	A643	W644	V645	H647	L651	T652	F653	L654	T655	N656	A579	Y582	S583	G585	Q586	Y587	W588	S589	M592	A593	Y594	G595	M596	D597	S598	W599	D606	S607	A608	V609	G611	V612	Q613	R614	G615	A616	K617	K618	K619	L620	E621	F624	
K697	Y700	D701	G702	A703	C704	Y705	N706	N707	D708	I718	S719	L720	P722	R723	F728	T729	E730	C731	C732	W733	S736	Q737	L738	R739	I742	S743	HIS	LYS	ASP	MET	GLN	L749	G750	R751	L752	H753	W754	K755	L756	L757	R758	P759	V760	I765	F769	P770	W773	L774	W775			
L779	V780	F781	R782	R783	L786	Q787	F788	L789	T795	T796	W797	E798	T799	I802	G803	L804	S805	N806	T807	G808	L809	C810	T814	A817	K818	F819	K820	K821	L823	D824	L825	E826	N827	N828	L829	P830	Y831	V834	R835	E836	E837	Q838	L839	Q840	L841	K842	E843	T844	W845	H846	N847	
Y848	R849	T850	S851	G852	M853	Q854	F855	R856	S857	S860	A861	V862	C866	T867	S868	E869	S870	VAL	ILE	ASP	HIS	GLN	GLY	THR	LYS	SER	SER	K882	Q886	K887	V888	H884	T889	V900	P902	L903	I905	G906	L907	H908	E886	I910	N911	S913	L914	E915	T916	W917	I922			
K925	T926	L927	R928	V929	R930	P931	E932	G933	C934	K935	R936	E937	S938	Y939	S940	G941	V942	T943	L944	I949	T952	I953	S954	R955	R956	K957	P958	F959	P960	Y961	L967	V968	P969	R970	T971	R975	I976	L977	K980	G981	L982	W984	L987	L988	V991	G996	L1000	T1001				

PHE	ASN	ASN	THR	THR	ASN	I1479	ASN
	ALA	ALA	ARG	ARG	ASP	F1480	SER
	GLU	GLU	LYS	LYS	GLN	F1483	ASP
	ASP	LEU	THR	THR	ALA	E1484	
	PHE	VAL	ALA	ALA	VAL	Y1485	
	LEU	LYS	CYS	CYS	LYS	F1486	
	ASN	GLY	ARG	ARG	PRO	F1487	
	GLY	ARG	GLN	GLN	GLU	L1488	
	CYS	THR	THR	THR	THR	S1489	
		LEU	LEU	ILE	ILE	P1490	
PHE	ALA	ALA	LEU	LEU	ALA	I1491	
	GLU	LEU	THR	THR	THR	T1492	
	ASP	GLY	GLN	GLN	ALA	F1493	
	PHE	GLY	GLY	GLY	THR	T1494	
	LEU	GLY	GLY	GLY	LYS	Y1495	
	ASN	GLY	GLU	GLU	VAL	Y1496	
	GLY	ALA	SER	SER	SER	E1497	
	CYS	GLU	ILE	ILE	ILE	Y1498	
		GLN	GLN	THR	THR	H1499	
	PHE	ASN	LYS	LYS	LYS	ILE	P1500
GLU		THR	THR	THR	THR	D1502	
ASP		ASN	VAL	VAL	VAL	K1503	
PHE		PHE	GLU	GLU	GLU	M1507	
SER		SER	ASN	ASN	ASN	F1508	
GLU		PHE	VAL	VAL	VAL	Y1509	
ASP		ARG	PHE	PHE	VAL	S1510	
LEU		THR	THR	THR	VAL	T1511	
SER		ILE	ILE	ILE	LYS	S1512	
GLU		THR	THR	THR	THR	N1513	
PHE	LEU	PRO	LYS	LYS	LYS	N1514	
	ASP	LEU	ALA	ALA	ALA	K1515	
	SER	SER	THR	THR	THR	I1516	
	GLU	LEU	LEU	LEU	LEU	Q1517	
	THR	THR	ASP	ASP	ASP	K1518	
	TRP	THR	ILE	ILE	ILE	V1519	
	ILE	ILE	THR	THR	THR	C1520	
	GLU	GLU	LYS	LYS	LYS	F1524	
	THR	THR	THR	THR	THR	A1524	
	TRP	TRP	GLY	GLY	GLY	C1525	
PHE	PRO	GLU	GLU	GLU	GLU	K1526	
	ARG	ARG	ALA	ALA	ALA	C1527	
	ASP	ASP	VAL	VAL	VAL	C1532	
	THR	THR	ALA	ALA	ALA	G1532	
	THR	THR	GLY	GLY	GLY	GLY	
	CYS	CYS	LYS	LYS	LYS	GLN	
	SER	SER	ASP	ASP	ASP	MET	
	SER	SER	SER	SER	SER	GLN	
	CYS	CYS	GLU	GLU	GLU	L1462	
	ALA	ALA	ILE	ILE	ILE	L1464	
PHE	ALA	ALA	THR	THR	THR	LEU	
	PHE	PHE	PHE	PHE	PHE	ASP	
	LEU	LEU	ILE	ILE	ILE	LEU	
	ALA	ALA	LYS	LYS	LYS	THR	
	ASN	ASN	LYS	LYS	LYS	ILE	
	LEU	LEU	VAL	VAL	VAL	SER	
	ASP	ASP	THR	THR	THR	GLU	
	GLU	GLU	CYS	CYS	CYS	F1477	
	THR	THR	THR	THR	THR	P1477	
	ASN	ASN	THR	THR	THR	V1475	
PHE	GLU	GLU	THR	THR	THR	I1467	
	ASP	ASP	GLU	GLU	GLU	S1466	
	GLY	GLY	LEU	LEU	LEU	ASP	
	CYS	CYS	LEU	LEU	LEU	L1465	
	GLU	GLU	GLN	GLN	GLN	Q1463	
	THR	THR	SER	SER	SER	L1462	
	LEU	LEU	GLN	GLN	GLN	I1461	
	ASP	ASP	LYS	LYS	LYS	H1459	
	THR	THR	ALA	ALA	ALA	G1458	
	GLU	GLU	VAL	VAL	VAL	D1457	

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	144.26 Å 144.26 Å 241.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.29 – 3.10 29.29 – 3.11	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.29-3.10) 97.4 (29.29-3.11)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.11 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.236 , 0.281 0.229 , 0.274	Depositor DCC
R_{free} test set	4916 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	94.3	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 91.1	EDS
Estimated twinning fraction	0.008 for -h,-k,l 0.468 for h,-h-k,-l 0.009 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 100380 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24655	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/13137	0.47	1/17820 (0.0%)
1	B	0.26	0/11954	0.47	1/16219 (0.0%)
All	All	0.26	0/25091	0.47	2/34039 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1488	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	1488	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12861	0	12817	794	0
1	B	11701	0	11669	700	0
2	A	28	0	25	2	0
2	B	28	0	25	2	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
All	All	24655	0	24562	1484	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 30.

All (1484) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1538:GLU:HG2	1:A:1539:LEU:HG	1.31	1.12
1:A:253:ARG:HH22	1:A:257:ASN:HA	1.13	1.11
1:B:253:ARG:HH22	1:B:257:ASN:HA	1.12	1.10
1:A:1279:ARG:HG3	1:A:1284:PHE:HB2	1.30	1.08
1:B:1279:ARG:HG3	1:B:1284:PHE:HB2	1.31	1.06
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.38	1.05
1:B:535:VAL:HG23	1:B:536:PRO:HD3	1.38	1.04
1:B:270:GLY:HA3	1:B:282:MET:HE1	1.41	1.02
1:A:543:TYR:HB3	1:A:556:SER:HB3	1.41	1.02
1:A:835:ARG:HG2	1:A:835:ARG:HH11	1.22	1.01
1:B:543:TYR:HB3	1:B:556:SER:HB3	1.42	1.01
1:A:270:GLY:HA3	1:A:282:MET:HE1	1.42	1.01
1:B:835:ARG:HG2	1:B:835:ARG:HH11	1.23	0.99
1:A:1429:PRO:HG2	1:A:1511:THR:HB	1.44	0.99
1:B:1429:PRO:HG2	1:B:1511:THR:HB	1.45	0.99
1:B:59:TYR:CG	1:B:60:PRO:HD2	1.98	0.98
1:A:1539:LEU:HD13	1:A:1657:CYS:HB3	1.45	0.97
1:A:59:TYR:CG	1:A:60:PRO:HD2	1.98	0.97
1:A:1612:VAL:HB	1:A:1615:ARG:HD2	1.51	0.91
1:A:160:VAL:HG22	1:A:175:GLU:HB3	1.53	0.90
1:A:1632:SER:O	1:A:1633:PHE:HB2	1.72	0.90
1:B:829:ILE:HG13	1:B:925:LYS:HG2	1.53	0.89
1:A:829:ILE:HG13	1:A:925:LYS:HG2	1.53	0.89
1:B:160:VAL:HG22	1:B:175:GLU:HB3	1.52	0.89
1:B:473:HIS:HE1	1:B:477:LEU:HG	1.38	0.88
1:B:653:PHE:CZ	1:B:660:ASP:HA	2.08	0.88
1:A:473:HIS:HE1	1:A:477:LEU:HG	1.40	0.87
1:A:773:TRP:HZ3	1:A:788:PHE:HE1	1.18	0.87
1:A:1096:ASN:HD22	1:A:1099:SER:H	1.18	0.87
1:A:653:PHE:CZ	1:A:660:ASP:HA	2.08	0.87
1:B:773:TRP:HZ3	1:B:788:PHE:HE1	1.18	0.86
1:B:1096:ASN:HD22	1:B:1099:SER:H	1.18	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:NH2	1:A:257:ASN:HA	1.92	0.85
1:B:977:LEU:HD12	1:B:1361:VAL:HG22	1.58	0.84
1:B:639:GLY:H	1:B:645:VAL:HG22	1.42	0.84
1:A:977:LEU:HD12	1:A:1361:VAL:HG22	1.58	0.84
1:B:253:ARG:NH2	1:B:257:ASN:HA	1.92	0.83
1:A:639:GLY:H	1:A:645:VAL:HG22	1.43	0.83
1:B:1500:ARG:HD3	1:B:1503:LYS:HD3	1.61	0.82
1:A:1202:HIS:HD2	1:A:1204:GLN:H	1.28	0.82
1:A:1673:LEU:HB3	1:B:258:LYS:NZ	1.95	0.82
1:B:25:ILE:HB	1:B:654:LEU:HB3	1.62	0.81
1:B:981:GLY:HA3	1:B:1333:PHE:HB2	1.60	0.81
1:B:1023:HIS:HD2	1:B:1092:TYR:OH	1.64	0.81
1:A:981:GLY:HA3	1:A:1333:PHE:HB2	1.61	0.81
1:B:640:LEU:H	1:B:644:ASN:HB3	1.46	0.81
1:B:504:LEU:HD21	1:B:651:LEU:HG	1.62	0.81
1:A:1500:ARG:HD3	1:A:1503:LYS:HD3	1.61	0.81
1:A:362:PHE:HD1	1:A:638:GLY:O	1.64	0.81
1:A:1023:HIS:HD2	1:A:1092:TYR:OH	1.64	0.80
1:A:25:ILE:HB	1:A:654:LEU:HB3	1.64	0.80
1:B:886:GLN:HG3	1:B:887:LYS:H	1.47	0.80
1:A:1541:LEU:HD21	1:A:1659:ALA:HB1	1.64	0.80
1:A:640:LEU:H	1:A:644:ASN:HB3	1.46	0.80
1:B:1096:ASN:ND2	1:B:1099:SER:H	1.79	0.79
1:A:1244:THR:HG22	1:A:1247:MET:H	1.47	0.79
1:A:468:ASP:O	1:A:484:ILE:HG13	1.83	0.79
1:B:770:PRO:HG2	1:B:795:THR:HG21	1.65	0.79
1:B:468:ASP:O	1:B:484:ILE:HG13	1.83	0.79
1:A:1096:ASN:ND2	1:A:1099:SER:H	1.79	0.79
1:B:934:VAL:HG22	1:B:1366:HIS:CD2	2.18	0.79
1:B:1202:HIS:HD2	1:B:1204:GLN:H	1.28	0.79
1:B:362:PHE:HD1	1:B:638:GLY:O	1.66	0.79
1:B:115:LYS:HG2	1:B:654:LEU:HD13	1.66	0.78
1:A:922:ILE:HD12	2:A:2001:NAG:H82	1.65	0.78
1:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.18	0.78
1:B:1244:THR:HG22	1:B:1247:MET:H	1.48	0.78
1:A:504:LEU:HD21	1:A:651:LEU:HG	1.64	0.78
1:A:1497:GLU:HB3	1:A:1500:ARG:HG3	1.66	0.78
1:A:886:GLN:HG3	1:A:887:LYS:H	1.47	0.78
1:B:838:GLN:HB3	1:B:1486:GLY:HA3	1.64	0.78
1:A:770:PRO:HG2	1:A:795:THR:HG21	1.65	0.77
1:B:1497:GLU:HB3	1:B:1500:ARG:HG3	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:ARG:HG3	1:B:1284:PHE:CB	2.13	0.77
1:A:1565:ILE:HD11	1:A:1614:GLY:H	1.50	0.77
1:A:128:ILE:HB	1:A:215:ALA:HB2	1.65	0.77
1:B:961:TYR:OH	1:B:1343:ASN:HA	1.85	0.76
1:A:961:TYR:OH	1:A:1343:ASN:HA	1.84	0.76
1:B:473:HIS:CE1	1:B:477:LEU:HG	2.21	0.76
1:A:707:ASN:HB3	1:A:739:ARG:HH12	1.50	0.76
1:B:128:ILE:HB	1:B:215:ALA:HB2	1.65	0.76
1:B:707:ASN:HB3	1:B:739:ARG:HH12	1.49	0.76
1:A:115:LYS:HG2	1:A:654:LEU:HD13	1.65	0.76
1:A:576:SER:HB2	1:A:577:PRO:HD3	1.68	0.76
1:A:1290:THR:O	1:A:1294:ILE:HG12	1.84	0.76
1:B:576:SER:HB2	1:B:577:PRO:HD3	1.68	0.76
1:A:635:GLY:HA2	1:A:672:ILE:HG23	1.67	0.76
1:B:359:THR:HG21	1:B:372:LYS:H	1.50	0.76
1:B:1290:THR:O	1:B:1294:ILE:HG12	1.84	0.76
1:B:635:GLY:HA2	1:B:672:ILE:HG23	1.68	0.75
1:A:838:GLN:HB3	1:A:1486:GLY:HA3	1.65	0.75
1:A:359:THR:HG21	1:A:372:LYS:H	1.51	0.75
1:B:987:ILE:HD13	1:B:1294:ILE:HG23	1.69	0.75
1:B:566:LYS:HE2	1:B:570:GLN:HE22	1.52	0.75
1:B:23:TYR:HE1	1:B:656:ASN:H	1.35	0.74
1:A:1108:VAL:HG11	1:A:1164:ILE:HG22	1.70	0.74
1:A:55:SER:HB3	1:A:68:SER:HB3	1.69	0.74
1:A:987:ILE:HD13	1:A:1294:ILE:HG23	1.69	0.74
1:B:1056:ILE:HD11	1:B:1066:TYR:CE2	2.23	0.74
1:B:1383:THR:HG21	1:B:1511:THR:HA	1.70	0.74
1:B:1219:LYS:HB2	1:B:1225:TYR:HB2	1.70	0.73
1:A:1279:ARG:HG3	1:A:1284:PHE:CB	2.12	0.73
1:A:1056:ILE:HD11	1:A:1066:TYR:CE2	2.23	0.73
1:A:1219:LYS:HB2	1:A:1225:TYR:HB2	1.70	0.73
1:A:1383:THR:HG21	1:A:1511:THR:HA	1.71	0.73
1:A:23:TYR:HE1	1:A:656:ASN:H	1.37	0.73
1:B:231:ILE:HD12	1:B:327:VAL:HG23	1.71	0.73
1:B:263:ALA:HB3	1:B:292:LEU:HB3	1.71	0.73
1:B:1108:VAL:HG11	1:B:1164:ILE:HG22	1.69	0.73
1:B:57:LYS:HD3	1:B:62:LYS:HB3	1.71	0.73
1:A:467:ILE:HD12	1:A:484:ILE:HD11	1.71	0.72
1:A:566:LYS:HE2	1:A:570:GLN:HE22	1.53	0.72
1:B:1264:ILE:HG12	1:B:1303:LEU:HD11	1.72	0.72
1:B:55:SER:HB3	1:B:68:SER:HB3	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:HIS:CE1	1:A:477:LEU:HG	2.22	0.72
1:B:1132:THR:HB	1:B:1134:PRO:HD2	1.72	0.72
1:B:516:GLU:H	1:B:516:GLU:CD	1.91	0.72
1:A:640:LEU:HB3	1:A:644:ASN:OD1	1.90	0.72
1:B:640:LEU:HB3	1:B:644:ASN:OD1	1.89	0.72
1:A:1132:THR:HB	1:A:1134:PRO:HD2	1.72	0.71
1:B:1000:LEU:HD11	1:B:1017:PRO:HG3	1.72	0.71
1:B:415:ASP:HB3	1:B:417:VAL:H	1.54	0.71
1:A:57:LYS:HD3	1:A:62:LYS:HB3	1.72	0.71
1:A:1516:ILE:HG22	1:A:1517:GLN:H	1.55	0.71
1:A:516:GLU:H	1:A:516:GLU:CD	1.91	0.71
1:A:535:VAL:HA	1:A:563:ILE:HD11	1.73	0.71
1:B:467:ILE:HD12	1:B:484:ILE:HD11	1.72	0.71
1:A:1193:TYR:CE1	1:A:1256:LEU:HB3	2.26	0.71
1:A:1567:SER:HB2	1:A:1578:LYS:HD3	1.73	0.71
1:A:415:ASP:HB3	1:A:417:VAL:H	1.54	0.71
1:A:231:ILE:HD12	1:A:327:VAL:HG23	1.70	0.71
1:A:1668:ALA:O	1:A:1671:ILE:HG22	1.90	0.70
1:A:1000:LEU:HD11	1:A:1017:PRO:HG3	1.73	0.70
1:B:956:ARG:HG2	1:B:1349:SER:HB3	1.71	0.70
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.72	0.70
1:A:862:VAL:HG21	1:A:909:ASN:O	1.91	0.70
1:A:956:ARG:HG2	1:A:1349:SER:HB3	1.72	0.70
1:B:1259:LEU:HD11	1:B:1300:TYR:HB2	1.73	0.70
1:B:1304:VAL:HG12	1:B:1305:LYS:N	2.07	0.70
1:A:1264:ILE:HG12	1:A:1303:LEU:HD11	1.71	0.70
1:B:285:THR:HG23	1:B:681:LYS:HD3	1.73	0.70
1:A:612:VAL:HG23	1:A:613:GLN:H	1.55	0.70
1:B:1193:TYR:CE1	1:B:1256:LEU:HB3	2.26	0.70
1:A:835:ARG:CG	1:A:835:ARG:HH11	2.00	0.69
1:B:1246:ARG:O	1:B:1250:THR:HG23	1.92	0.69
1:A:1304:VAL:HG12	1:A:1305:LYS:N	2.06	0.69
1:A:667:GLU:N	1:A:668:PRO:HD3	2.06	0.69
1:B:612:VAL:HG23	1:B:613:GLN:H	1.55	0.69
1:A:1629:TYR:CZ	1:A:1632:SER:HB2	2.27	0.69
1:A:123:ASN:H	1:A:211:THR:HG23	1.57	0.69
1:A:1259:LEU:HD11	1:A:1300:TYR:HB2	1.73	0.69
1:B:535:VAL:HA	1:B:563:ILE:HD11	1.73	0.69
1:B:123:ASN:H	1:B:211:THR:HG23	1.58	0.69
1:A:1246:ARG:O	1:A:1250:THR:HG23	1.92	0.69
1:B:862:VAL:HG21	1:B:909:ASN:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:835:ARG:CG	1:B:835:ARG:HH11	2.00	0.68
1:A:285:THR:HG23	1:A:681:LYS:HD3	1.74	0.68
1:B:232:GLU:OE2	1:B:251:LYS:HE2	1.93	0.68
1:B:667:GLU:N	1:B:668:PRO:HD3	2.06	0.68
1:A:361:LEU:O	1:A:454:ALA:HA	1.94	0.67
1:B:1488:LEU:O	1:B:1488:LEU:HD12	1.95	0.67
1:B:1247:MET:O	1:B:1251:THR:HG23	1.94	0.67
1:A:1488:LEU:HD12	1:A:1488:LEU:O	1.95	0.67
1:A:232:GLU:OE2	1:A:251:LYS:HE2	1.94	0.67
1:B:1000:LEU:CD1	1:B:1017:PRO:HG3	2.24	0.67
1:A:280:LYS:HG3	1:A:282:MET:HE3	1.77	0.67
1:A:704:CYS:O	1:A:705:VAL:HG13	1.95	0.67
1:B:988:LEU:HD23	1:B:1021:VAL:HG22	1.77	0.67
1:B:280:LYS:HG3	1:B:282:MET:HE3	1.77	0.67
1:B:96:GLN:O	1:B:98:PRO:HD3	1.95	0.67
1:A:1068:VAL:HA	1:A:1078:LEU:HD13	1.77	0.67
1:A:1090:ASN:HD22	1:A:1158:ILE:HD13	1.59	0.67
1:B:123:ASN:N	1:B:211:THR:HG23	2.11	0.66
1:A:242:ASN:ND2	1:A:242:ASN:H	1.93	0.66
1:A:1462:LEU:HD11	1:A:1475:VAL:HG21	1.78	0.66
1:B:1090:ASN:HD22	1:B:1158:ILE:HD13	1.59	0.66
1:A:1000:LEU:CD1	1:A:1017:PRO:HG3	2.25	0.66
1:A:641:ASN:H	1:A:644:ASN:HB2	1.61	0.66
1:A:886:GLN:HE22	1:A:1623:GLU:HG2	1.59	0.66
1:A:54:ILE:HG12	1:A:106:VAL:HG22	1.78	0.66
1:B:361:LEU:O	1:B:454:ALA:HA	1.96	0.66
1:A:96:GLN:O	1:A:98:PRO:HD3	1.95	0.66
1:B:488:PRO:O	1:B:491:PRO:HD2	1.95	0.66
1:B:242:ASN:ND2	1:B:242:ASN:H	1.93	0.66
1:A:1570:VAL:O	1:A:1571:GLU:HB2	1.94	0.66
1:B:386:VAL:H	1:B:411:THR:CG2	2.09	0.66
1:A:1673:LEU:HB3	1:B:258:LYS:HZ2	1.60	0.66
1:A:123:ASN:N	1:A:211:THR:HG23	2.10	0.65
1:B:704:CYS:O	1:B:705:VAL:HG13	1.95	0.65
1:A:496:ILE:HD12	1:A:496:ILE:H	1.61	0.65
1:B:1068:VAL:HA	1:B:1078:LEU:HD13	1.77	0.65
1:B:1462:LEU:HD11	1:B:1475:VAL:HG21	1.78	0.65
1:A:386:VAL:H	1:A:411:THR:CG2	2.09	0.65
1:A:988:LEU:HD23	1:A:1021:VAL:HG22	1.77	0.65
1:A:1247:MET:O	1:A:1251:THR:HG23	1.95	0.65
1:A:1304:VAL:HG12	1:A:1305:LYS:H	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:PRO:O	1:A:491:PRO:HD2	1.95	0.65
1:B:54:ILE:HG12	1:B:106:VAL:HG22	1.79	0.65
1:B:412:ARG:HD2	1:B:415:ASP:HB2	1.78	0.65
1:A:1019:PHE:CZ	1:A:1088:GLN:HB3	2.32	0.65
1:A:120:THR:HG22	1:A:122:ASP:H	1.62	0.65
1:A:52:ALA:HB3	1:A:73:LEU:HD21	1.79	0.65
1:A:1669:GLU:O	1:A:1673:LEU:HG	1.96	0.65
1:B:1019:PHE:CZ	1:B:1088:GLN:HB3	2.32	0.65
1:A:820:PHE:HE2	1:A:848:TYR:HD2	1.45	0.65
1:B:1200:LYS:HE3	1:B:1261:LEU:HD23	1.79	0.65
1:B:464:TYR:H	1:B:491:PRO:HD3	1.62	0.65
1:A:59:TYR:CD2	1:A:60:PRO:HD2	2.32	0.64
1:A:1633:PHE:CD2	1:A:1634:ARG:HB2	2.33	0.64
1:A:412:ARG:HD2	1:A:415:ASP:HB2	1.78	0.64
1:B:59:TYR:CD2	1:B:60:PRO:HD2	2.32	0.64
1:B:829:ILE:CG1	1:B:925:LYS:HG2	2.24	0.64
1:A:1598:ILE:HG13	1:A:1599:THR:H	1.61	0.64
1:B:496:ILE:H	1:B:496:ILE:HD12	1.61	0.64
1:B:120:THR:HG22	1:B:122:ASP:H	1.63	0.64
1:B:754:MET:O	1:B:755:LYS:HG2	1.98	0.64
1:B:499:TYR:CE2	1:B:517:LYS:HG2	2.32	0.64
1:B:641:ASN:H	1:B:644:ASN:HB2	1.61	0.64
1:B:1304:VAL:HG12	1:B:1305:LYS:H	1.62	0.64
1:A:618:LYS:HB2	1:A:621:GLU:HB2	1.79	0.64
1:A:1503:LYS:N	1:A:1503:LYS:HD2	2.13	0.64
1:A:820:PHE:CE2	1:A:848:TYR:HD2	2.15	0.64
1:A:375:VAL:HG12	1:A:383:VAL:HG13	1.80	0.64
1:B:52:ALA:HB3	1:B:73:LEU:HD21	1.79	0.64
1:A:829:ILE:CG1	1:A:925:LYS:HG2	2.24	0.64
1:A:560:TRP:CH2	1:A:562:ASN:HB2	2.33	0.64
1:B:367:ILE:HD11	1:B:489:LYS:HB3	1.80	0.64
1:A:464:TYR:H	1:A:491:PRO:HD3	1.62	0.64
1:B:1323:LEU:HD12	1:B:1324:HIS:H	1.63	0.64
1:A:855:PHE:CE2	1:A:888:VAL:HG13	2.33	0.64
1:A:1200:LYS:HE3	1:A:1261:LEU:HD23	1.79	0.64
1:A:560:TRP:CZ3	1:A:562:ASN:HB2	2.33	0.63
1:A:1630:ASN:O	1:A:1631:PHE:HB2	1.98	0.63
1:A:647:HIS:CD2	1:A:662:SER:HB2	2.33	0.63
1:A:1673:LEU:HB3	1:B:258:LYS:HZ3	1.63	0.63
1:A:499:TYR:CE2	1:A:517:LYS:HG2	2.33	0.63
1:A:1638:PRO:O	1:A:1639:LEU:HB3	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:VAL:HG22	1:B:847:ASN:HA	1.80	0.63
1:B:1503:LYS:N	1:B:1503:LYS:HD2	2.13	0.62
1:B:1399:TYR:OH	1:B:1478:ARG:HD3	1.98	0.62
1:B:271:ILE:HG22	1:B:272:ARG:H	1.65	0.62
1:B:855:PHE:CE2	1:B:888:VAL:HG13	2.33	0.62
1:A:367:ILE:HD11	1:A:489:LYS:HB3	1.81	0.62
1:B:618:LYS:HB2	1:B:621:GLU:HB2	1.79	0.62
1:B:560:TRP:CZ3	1:B:562:ASN:HB2	2.34	0.62
1:A:1669:GLU:HG3	1:A:1672:PHE:CZ	2.34	0.62
1:A:271:ILE:HG22	1:A:272:ARG:H	1.64	0.62
1:A:1614:GLY:O	1:B:1519:VAL:HG21	2.00	0.62
1:B:647:HIS:CD2	1:B:662:SER:HB2	2.34	0.62
1:A:1399:TYR:OH	1:A:1478:ARG:HD3	1.99	0.62
1:B:702:GLY:HA2	1:B:728:PHE:CE1	2.35	0.62
1:A:1488:LEU:HD21	1:A:1511:THR:HG22	1.82	0.62
1:A:1631:PHE:O	1:A:1632:SER:HB3	1.98	0.62
1:B:1488:LEU:HD21	1:B:1511:THR:HG22	1.81	0.62
1:B:707:ASN:HB3	1:B:739:ARG:NH1	2.15	0.62
1:B:647:HIS:HE1	1:B:667:GLU:HG3	1.65	0.62
1:A:696:LYS:HE3	1:A:700:TYR:HD2	1.65	0.62
1:A:1323:LEU:HD12	1:A:1324:HIS:H	1.64	0.62
1:A:647:HIS:HE1	1:A:667:GLU:HG3	1.65	0.61
1:B:153:LYS:HG2	1:B:806:ASN:O	2.00	0.61
1:B:487:THR:HG22	1:B:523:TYR:HB3	1.82	0.61
1:B:39:ILE:HG13	1:B:85:LEU:HD23	1.82	0.61
1:A:39:ILE:HG13	1:A:85:LEU:HD23	1.83	0.61
1:A:153:LYS:HG2	1:A:806:ASN:O	2.00	0.61
1:A:823:VAL:HG22	1:A:847:ASN:HA	1.80	0.61
1:B:560:TRP:CH2	1:B:562:ASN:HB2	2.35	0.61
1:A:1056:ILE:HD11	1:A:1066:TYR:HE2	1.64	0.61
1:A:702:GLY:HA2	1:A:728:PHE:CE1	2.35	0.61
1:B:172:ASP:OD2	1:B:173:MET:N	2.32	0.61
1:A:1431:GLY:HA3	1:A:1483:PHE:CE1	2.36	0.61
1:A:172:ASP:OD2	1:A:173:MET:N	2.32	0.61
1:A:487:THR:HG22	1:A:523:TYR:HB3	1.81	0.61
1:B:1186:PHE:HD1	1:B:1250:THR:HG22	1.65	0.61
1:B:820:PHE:CE2	1:B:848:TYR:HD2	2.19	0.61
1:A:1204:GLN:O	1:A:1208:ILE:HG13	2.00	0.61
1:B:1056:ILE:HD11	1:B:1066:TYR:HE2	1.64	0.61
1:A:21:GLN:NE2	1:A:45:GLY:HA2	2.16	0.61
1:B:820:PHE:HE2	1:B:848:TYR:HD2	1.49	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HA	1:A:655:THR:HG1	1.67	0.60
1:B:375:VAL:HG12	1:B:383:VAL:HG13	1.81	0.60
1:B:773:TRP:HZ3	1:B:788:PHE:CE1	2.10	0.60
1:B:1204:GLN:O	1:B:1208:ILE:HG13	2.01	0.60
1:A:857:VAL:HA	1:A:913:SER:O	2.01	0.60
1:A:534:MET:HB3	1:A:538:SER:OG	2.01	0.60
1:B:733:VAL:HG13	1:B:737:GLN:HE21	1.67	0.60
1:B:21:GLN:NE2	1:B:45:GLY:HA2	2.16	0.60
1:B:857:VAL:HA	1:B:913:SER:O	2.02	0.60
1:B:1431:GLY:HA3	1:B:1483:PHE:CE1	2.37	0.60
1:B:696:LYS:HE3	1:B:700:TYR:HD2	1.65	0.60
1:A:944:LEU:HD22	1:A:1350:THR:HG22	1.84	0.60
1:A:576:SER:OG	1:A:589:SER:HB2	2.02	0.60
1:B:534:MET:HB3	1:B:538:SER:OG	2.01	0.60
1:B:942:VAL:HG23	1:B:1359:VAL:HB	1.83	0.60
1:A:1186:PHE:HD1	1:A:1250:THR:HG22	1.66	0.60
1:B:576:SER:OG	1:B:589:SER:HB2	2.01	0.60
1:B:412:ARG:HB3	1:B:415:ASP:HB2	1.83	0.60
1:A:961:TYR:CZ	1:A:1343:ASN:HA	2.37	0.60
1:B:956:ARG:CG	1:B:1349:SER:HB3	2.32	0.60
1:A:956:ARG:CG	1:A:1349:SER:HB3	2.32	0.60
1:B:961:TYR:CZ	1:B:1343:ASN:HA	2.37	0.60
1:B:647:HIS:CE1	1:B:667:GLU:HG3	2.37	0.60
1:A:885:ARG:NH2	1:A:1628:LYS:HD2	2.17	0.60
1:A:733:VAL:HG13	1:A:737:GLN:HE21	1.66	0.60
1:A:154:PRO:HB3	1:A:180:ILE:O	2.01	0.59
1:B:532:GLN:O	1:B:535:VAL:HG22	2.02	0.59
1:B:944:LEU:HD22	1:B:1350:THR:HG22	1.84	0.59
1:B:1003:LEU:HB3	1:B:1498:TYR:CE1	2.37	0.59
1:A:773:TRP:HZ3	1:A:788:PHE:CE1	2.10	0.59
1:B:982:LEU:HD23	1:B:1309:LEU:HD11	1.83	0.59
1:A:707:ASN:HB3	1:A:739:ARG:NH1	2.15	0.59
1:B:154:PRO:HB3	1:B:180:ILE:O	2.01	0.59
1:A:313:TYR:HE2	1:A:321:LYS:HZ1	1.51	0.59
1:A:982:LEU:HD23	1:A:1309:LEU:HD11	1.83	0.59
1:A:1565:ILE:HD11	1:A:1614:GLY:N	2.17	0.59
1:A:320:ASN:HD22	1:A:320:ASN:N	1.99	0.59
1:A:1485:VAL:CG2	1:A:1488:LEU:HB3	2.32	0.59
1:B:320:ASN:HD22	1:B:320:ASN:N	2.00	0.59
1:A:942:VAL:HG23	1:A:1359:VAL:HB	1.84	0.59
1:A:609:VAL:HG23	1:A:610:TYR:H	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1562:LYS:HG3	1:A:1648:TRP:CE3	2.38	0.59
1:A:412:ARG:HB3	1:A:415:ASP:HB2	1.85	0.58
1:A:647:HIS:CE1	1:A:667:GLU:HG3	2.37	0.58
1:A:41:ILE:O	1:A:80:GLN:HA	2.04	0.58
1:B:641:ASN:HB2	1:B:644:ASN:H	1.68	0.58
1:B:576:SER:CB	1:B:577:PRO:HD3	2.33	0.58
1:B:1485:VAL:CG2	1:B:1488:LEU:HB3	2.33	0.58
1:A:543:TYR:CB	1:A:556:SER:HB3	2.27	0.58
1:A:1649:PRO:HG2	1:A:1661:LEU:HG	1.84	0.58
1:B:272:ARG:O	1:B:321:LYS:HB2	2.04	0.58
1:B:356:LEU:HG	1:B:452:TYR:CZ	2.38	0.58
1:B:284:GLN:NE2	1:B:310:LEU:HD22	2.19	0.58
1:A:1003:LEU:HB3	1:A:1498:TYR:CE1	2.38	0.58
1:A:641:ASN:HB2	1:A:644:ASN:H	1.68	0.58
1:B:231:ILE:HD12	1:B:327:VAL:CG2	2.34	0.58
1:A:532:GLN:O	1:A:535:VAL:HG22	2.02	0.58
1:A:1084:ARG:O	1:A:1088:GLN:HG3	2.03	0.58
1:A:1001:THR:HG22	1:A:1002:HIS:H	1.69	0.58
1:A:1669:GLU:HG3	1:A:1672:PHE:HZ	1.67	0.58
1:B:609:VAL:HG23	1:B:610:TYR:H	1.68	0.58
1:A:1255:LEU:HD22	1:A:1270:VAL:HG12	1.86	0.58
1:A:1274:LEU:C	1:A:1276:GLU:H	2.07	0.58
1:B:1271:ILE:C	1:B:1271:ILE:HD12	2.24	0.58
1:B:41:ILE:O	1:B:80:GLN:HA	2.03	0.57
1:A:884:VAL:HG12	1:A:1625:LEU:HB3	1.86	0.57
1:A:1271:ILE:C	1:A:1271:ILE:HD12	2.24	0.57
1:A:272:ARG:O	1:A:321:LYS:HB2	2.04	0.57
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.40	0.57
1:A:386:VAL:O	1:A:411:THR:HG22	2.04	0.57
1:A:323:LEU:HB2	1:A:347:TYR:CE2	2.39	0.57
1:B:323:LEU:HB2	1:B:347:TYR:CE2	2.39	0.57
1:A:1554:LYS:HD2	1:A:1555:PRO:HD2	1.85	0.57
1:B:786:LEU:HD23	1:B:786:LEU:N	2.19	0.57
1:A:138:ASP:OD1	1:A:192:SER:HA	2.04	0.57
1:A:365:PRO:HG2	1:A:464:TYR:CZ	2.38	0.57
1:B:138:ASP:OD1	1:B:192:SER:HA	2.04	0.57
1:A:786:LEU:N	1:A:786:LEU:HD23	2.19	0.57
1:B:981:GLY:CA	1:B:1333:PHE:HB2	2.34	0.57
1:B:908:HIS:HB3	1:B:926:THR:HB	1.86	0.57
1:A:356:LEU:HG	1:A:452:TYR:CZ	2.40	0.57
1:B:365:PRO:HG2	1:B:464:TYR:CZ	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:VAL:O	1:B:411:THR:HG22	2.04	0.57
1:B:541:LEU:HD21	1:B:646:PHE:CZ	2.40	0.57
1:A:641:ASN:H	1:A:644:ASN:CB	2.17	0.57
1:B:782:ARG:O	1:B:783:ARG:HG3	2.04	0.57
1:A:1550:GLN:C	1:A:1552:ALA:H	2.06	0.57
1:B:1001:THR:HG22	1:B:1002:HIS:H	1.70	0.57
1:B:1213:LYS:HG3	1:B:1266:TYR:OH	2.05	0.57
1:B:641:ASN:H	1:B:644:ASN:CB	2.18	0.57
1:B:961:TYR:HH	1:B:1343:ASN:HA	1.69	0.57
1:B:1084:ARG:O	1:B:1088:GLN:HG3	2.04	0.57
1:A:885:ARG:HH22	1:A:1628:LYS:HD2	1.69	0.57
1:A:782:ARG:O	1:A:783:ARG:HG3	2.04	0.57
1:B:718:ILE:HG12	1:B:1446:VAL:HG12	1.85	0.57
1:A:284:GLN:NE2	1:A:310:LEU:HD22	2.19	0.57
1:B:968:VAL:HG22	1:B:1366:HIS:O	2.04	0.57
1:B:59:TYR:CG	1:B:60:PRO:CD	2.82	0.57
1:A:576:SER:CB	1:A:577:PRO:HD3	2.33	0.57
1:A:908:HIS:HB3	1:A:926:THR:HB	1.86	0.57
1:A:1557:ILE:HG22	1:A:1559:TYR:O	2.04	0.57
1:B:1320:LYS:HG3	1:B:1321:GLY:N	2.20	0.57
1:B:99:VAL:HB	1:B:121:TYR:OH	2.05	0.57
1:A:1411:SER:H	1:A:1414:GLU:HG3	1.70	0.57
1:B:42:GLN:HG3	1:B:80:GLN:HE21	1.70	0.57
1:A:231:ILE:HD12	1:A:327:VAL:CG2	2.34	0.57
1:A:1433:SER:HB2	1:A:1480:PHE:CD1	2.40	0.57
1:A:42:GLN:HG3	1:A:80:GLN:HE21	1.70	0.56
1:A:1025:LEU:HD13	1:A:1031:TRP:CZ3	2.40	0.56
1:A:894:HIS:CE1	1:A:1589:GLU:OE2	2.59	0.56
1:A:739:ARG:HD3	1:A:754:MET:SD	2.45	0.56
1:A:478:VAL:HG11	1:A:566:LYS:HD3	1.87	0.56
1:B:1255:LEU:HB2	1:B:1270:VAL:HG11	1.88	0.56
1:A:834:VAL:O	1:A:837:GLU:HB2	2.05	0.56
1:B:834:VAL:O	1:B:837:GLU:HB2	2.06	0.56
1:A:839:ILE:HD11	1:A:1483:PHE:CZ	2.40	0.56
1:A:1557:ILE:HD12	1:A:1621:GLY:HA2	1.86	0.56
1:A:1624:ALA:HA	1:A:1637:TYR:HA	1.87	0.56
1:B:700:TYR:CZ	1:B:758:LEU:HD12	2.40	0.56
1:A:1127:ILE:HD13	1:A:1129:LEU:HG	1.87	0.56
1:B:1411:SER:H	1:B:1414:GLU:HG3	1.70	0.56
1:B:1025:LEU:HD13	1:B:1031:TRP:CZ3	2.40	0.56
1:B:1127:ILE:HD13	1:B:1129:LEU:HG	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:PRO:HG3	1:A:1483:PHE:CE2	2.40	0.56
1:B:59:TYR:CD1	1:B:60:PRO:HD2	2.41	0.56
1:A:1554:LYS:HE3	1:A:1556:GLU:HG2	1.87	0.56
1:B:1433:SER:HB2	1:B:1480:PHE:CD1	2.41	0.56
1:B:237:PHE:CE1	1:B:378:SER:HB2	2.41	0.56
1:A:835:ARG:HD3	1:A:903:LEU:O	2.05	0.56
1:A:1669:GLU:HA	1:A:1672:PHE:CE1	2.41	0.56
1:B:1274:LEU:C	1:B:1276:GLU:H	2.08	0.56
1:A:1320:LYS:HG3	1:A:1321:GLY:N	2.20	0.56
1:B:835:ARG:HG2	1:B:835:ARG:NH1	2.04	0.56
1:A:981:GLY:CA	1:A:1333:PHE:HB2	2.35	0.56
1:A:855:PHE:CZ	1:A:886:GLN:HB3	2.41	0.56
1:A:1554:LYS:HE3	1:A:1556:GLU:CG	2.36	0.56
1:A:804:ILE:HG22	1:A:809:ILE:HA	1.88	0.56
1:B:1255:LEU:HD22	1:B:1270:VAL:HG12	1.87	0.56
1:A:1213:LYS:HG3	1:A:1266:TYR:OH	2.05	0.56
1:B:496:ILE:HG23	1:B:544:TYR:HB2	1.88	0.56
1:A:541:LEU:HD21	1:A:646:PHE:CZ	2.41	0.56
1:A:1255:LEU:HB2	1:A:1270:VAL:HG11	1.86	0.56
1:B:24:VAL:HA	1:B:655:THR:HG1	1.71	0.56
1:B:835:ARG:HD3	1:B:903:LEU:O	2.05	0.56
1:A:59:TYR:CG	1:A:60:PRO:CD	2.82	0.56
1:B:1450:PHE:CZ	1:B:1475:VAL:HB	2.40	0.56
1:B:88:GLN:HB3	1:B:89:PRO:HD2	1.88	0.56
1:A:1107:LEU:H	1:A:1107:LEU:HD12	1.71	0.56
1:A:88:GLN:HB3	1:A:89:PRO:HD2	1.88	0.56
1:B:385:GLY:N	1:B:411:THR:HG23	2.21	0.56
1:A:885:ARG:HH12	1:A:1628:LYS:HZ3	1.53	0.56
1:A:625:GLN:HG3	1:A:626:PHE:N	2.21	0.56
1:B:697:LYS:HE3	1:B:701:ASP:OD2	2.06	0.56
1:B:478:VAL:HG11	1:B:566:LYS:HD3	1.87	0.55
1:B:955:ARG:O	1:B:956:ARG:HG3	2.05	0.55
1:A:99:VAL:HB	1:A:121:TYR:OH	2.06	0.55
1:A:1590:ALA:O	1:A:1591:VAL:HG12	2.06	0.55
1:B:855:PHE:CZ	1:B:886:GLN:HB3	2.41	0.55
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.88	0.55
1:B:357:VAL:O	1:B:359:THR:HG23	2.07	0.55
1:B:1320:LYS:HG2	1:B:1342:LEU:HD12	1.89	0.55
1:B:696:LYS:HE3	1:B:700:TYR:CD2	2.41	0.55
1:B:250:ILE:HD11	1:B:265:VAL:HG21	1.89	0.55
1:B:587:THR:HG22	1:B:789:ALA:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ILE:HG23	1:A:544:TYR:HB2	1.88	0.55
1:A:385:GLY:N	1:A:411:THR:HG23	2.21	0.55
1:A:955:ARG:O	1:A:956:ARG:HG3	2.07	0.55
1:A:1069:TRP:HH2	1:A:1465:ASN:OD1	1.88	0.55
1:B:489:LYS:O	1:B:490:SER:HB2	2.07	0.55
1:B:804:ILE:HG22	1:B:809:ILE:HA	1.88	0.55
1:B:625:GLN:HG3	1:B:626:PHE:N	2.21	0.55
1:A:967:LEU:HD12	1:A:1366:HIS:O	2.06	0.55
1:B:640:LEU:HD12	1:B:640:LEU:O	2.07	0.55
1:A:968:VAL:HG22	1:A:1366:HIS:O	2.06	0.55
1:B:1056:ILE:HG12	1:B:1056:ILE:O	2.07	0.55
1:B:1069:TRP:HH2	1:B:1465:ASN:OD1	1.89	0.55
1:A:1652:THR:HG21	1:B:868:SER:OG	2.07	0.55
1:A:237:PHE:CE1	1:A:378:SER:HB2	2.41	0.55
1:A:1570:VAL:O	1:A:1571:GLU:CB	2.55	0.55
1:B:938:SER:OG	1:B:1279:ARG:CZ	2.55	0.55
1:B:967:LEU:HD12	1:B:1366:HIS:O	2.07	0.55
1:B:271:ILE:HG22	1:B:272:ARG:N	2.22	0.54
1:A:308:LYS:HG3	1:A:314:SER:HB3	1.89	0.54
1:A:1202:HIS:CD2	1:A:1203:PRO:HD2	2.41	0.54
1:A:243:PHE:CD1	1:A:316:GLU:HG3	2.43	0.54
1:A:271:ILE:HG22	1:A:272:ARG:N	2.23	0.54
1:B:639:GLY:N	1:B:645:VAL:HG22	2.18	0.54
1:B:1202:HIS:CD2	1:B:1203:PRO:HD2	2.42	0.54
1:A:357:VAL:O	1:A:359:THR:HG23	2.06	0.54
1:A:696:LYS:HE3	1:A:700:TYR:CD2	2.41	0.54
1:B:692:HIS:HD2	1:B:694:VAL:HG23	1.72	0.54
1:A:1516:ILE:HG22	1:A:1517:GLN:N	2.20	0.54
1:A:1599:THR:HG22	1:A:1600:PHE:H	1.72	0.54
1:A:692:HIS:HD2	1:A:694:VAL:HG23	1.72	0.54
1:B:465:LEU:HD12	1:B:466:TYR:H	1.72	0.54
1:A:1076:THR:CG2	1:A:1120:GLU:HA	2.37	0.54
1:B:1107:LEU:HD12	1:B:1107:LEU:H	1.71	0.54
1:B:161:LEU:HD11	1:B:185:PHE:CD1	2.43	0.54
1:A:1056:ILE:HG12	1:A:1056:ILE:O	2.07	0.54
1:A:1320:LYS:HG2	1:A:1342:LEU:HD12	1.89	0.54
1:B:331:GLU:OE2	1:B:333:THR:HG23	2.08	0.54
1:A:697:LYS:HE3	1:A:701:ASP:OD2	2.07	0.54
1:B:308:LYS:HG3	1:B:314:SER:HB3	1.89	0.54
1:A:307:VAL:CG1	1:A:313:TYR:HB2	2.38	0.54
1:A:489:LYS:O	1:A:490:SER:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:765:ILE:HG23	1:B:765:ILE:O	2.08	0.54
1:B:1115:ASN:HD22	1:B:1115:ASN:H	1.54	0.54
1:B:839:ILE:HD11	1:B:1483:PHE:CZ	2.42	0.54
1:A:103:TYR:HA	1:A:115:LYS:O	2.08	0.54
1:B:823:VAL:HG21	1:B:853:MET:SD	2.48	0.54
1:B:191:PRO:HD2	1:B:194:PRO:HB3	1.89	0.54
1:B:1001:THR:HG23	1:B:1284:PHE:CD2	2.43	0.54
1:A:29:LYS:HG3	1:A:30:ILE:HG12	1.89	0.54
1:A:1554:LYS:HG3	1:A:1556:GLU:HG2	1.88	0.54
1:B:1255:LEU:O	1:B:1255:LEU:HD12	2.07	0.54
1:B:191:PRO:O	1:B:194:PRO:HG3	2.08	0.54
1:A:1146:ALA:O	1:A:1150:ILE:HG13	2.08	0.54
1:A:465:LEU:HD12	1:A:466:TYR:H	1.72	0.54
1:B:830:PRO:HG3	1:B:1483:PHE:CE2	2.43	0.54
1:B:42:GLN:HG2	1:B:43:VAL:N	2.23	0.54
1:A:263:ALA:HB3	1:A:292:LEU:CB	2.38	0.54
1:A:1019:PHE:CE2	1:A:1088:GLN:HB3	2.43	0.54
1:A:1638:PRO:O	1:A:1639:LEU:CB	2.55	0.54
1:A:161:LEU:HD11	1:A:185:PHE:CD1	2.43	0.54
1:B:1525:CYS:O	1:B:1526:LYS:HG2	2.08	0.54
1:B:307:VAL:CG1	1:B:313:TYR:HB2	2.38	0.54
1:B:103:TYR:HA	1:B:115:LYS:O	2.07	0.54
1:A:509:ILE:HD11	1:A:651:LEU:HD21	1.89	0.54
1:A:1565:ILE:HD11	1:A:1613:LYS:HA	1.89	0.54
1:B:544:TYR:CE2	1:B:546:VAL:HG23	2.43	0.54
1:A:191:PRO:HD2	1:A:194:PRO:HB3	1.90	0.54
1:A:42:GLN:HG2	1:A:43:VAL:N	2.23	0.53
1:A:718:ILE:HG12	1:A:1446:VAL:HG12	1.89	0.53
1:B:540:LEU:C	1:B:540:LEU:HD12	2.29	0.53
1:A:606:ASP:O	1:A:609:VAL:HG22	2.09	0.53
1:A:544:TYR:CE2	1:A:546:VAL:HG23	2.43	0.53
1:B:1411:SER:HB2	1:B:1414:GLU:HG2	1.90	0.53
1:A:191:PRO:O	1:A:194:PRO:HG3	2.08	0.53
1:B:29:LYS:HG3	1:B:30:ILE:HG12	1.89	0.53
1:A:938:SER:OG	1:A:1279:ARG:CZ	2.57	0.53
1:A:59:TYR:CD1	1:A:60:PRO:HD2	2.41	0.53
1:A:653:PHE:N	1:A:653:PHE:CD2	2.76	0.53
1:B:263:ALA:HB3	1:B:292:LEU:CB	2.37	0.53
1:A:823:VAL:HG21	1:A:853:MET:SD	2.48	0.53
1:B:1213:LYS:HG3	1:B:1266:TYR:CZ	2.43	0.53
1:B:243:PHE:CD1	1:B:316:GLU:HG3	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1146:ALA:O	1:B:1150:ILE:HG13	2.08	0.53
1:A:274:ASP:OD2	1:A:277:ASP:HB2	2.07	0.53
1:B:1111:TYR:HD1	1:B:1119:LYS:HG3	1.73	0.53
1:A:1001:THR:HG23	1:A:1284:PHE:CD2	2.43	0.53
1:A:162:THR:HB	1:A:173:MET:HG3	1.90	0.53
1:A:394:THR:HG23	1:A:428:VAL:HG23	1.89	0.53
1:A:540:LEU:HD12	1:A:540:LEU:C	2.29	0.53
1:A:24:VAL:HA	1:A:655:THR:OG1	2.09	0.53
1:B:274:ASP:OD2	1:B:277:ASP:HB2	2.08	0.53
1:A:827:MET:HE3	1:A:842:LYS:O	2.09	0.53
1:B:509:ILE:HD11	1:B:651:LEU:HD21	1.89	0.53
1:A:640:LEU:O	1:A:640:LEU:HD12	2.08	0.53
1:B:394:THR:HG23	1:B:428:VAL:HG23	1.89	0.53
1:A:250:ILE:HD11	1:A:265:VAL:HG21	1.89	0.53
1:A:1629:TYR:OH	1:A:1632:SER:HB2	2.07	0.53
1:A:845:VAL:HG12	1:A:894:HIS:O	2.09	0.53
1:B:356:LEU:HG	1:B:452:TYR:CE1	2.42	0.53
1:A:1111:TYR:HD1	1:A:1119:LYS:HG3	1.73	0.53
1:B:1019:PHE:CE2	1:B:1088:GLN:HB3	2.44	0.53
1:A:1560:ALA:HA	1:A:1620:MET:HG2	1.90	0.53
1:A:443:PRO:HA	1:B:443:PRO:HA	1.90	0.53
1:A:1627:ILE:HD13	1:A:1627:ILE:H	1.73	0.53
1:A:765:ILE:HG23	1:A:765:ILE:O	2.08	0.53
1:B:1076:THR:CG2	1:B:1120:GLU:HA	2.39	0.53
1:B:307:VAL:HG12	1:B:313:TYR:O	2.09	0.53
1:B:543:TYR:CB	1:B:556:SER:HB3	2.27	0.53
1:A:739:ARG:HB3	1:A:754:MET:SD	2.49	0.53
1:A:1255:LEU:O	1:A:1255:LEU:HD12	2.09	0.53
1:A:1411:SER:HB2	1:A:1414:GLU:HG2	1.90	0.53
1:B:1063:ASP:O	1:B:1064:TYR:HB2	2.09	0.53
1:A:494:ASP:C	1:A:496:ILE:HD12	2.30	0.53
1:B:131:ASP:HB3	1:B:142:LYS:HB2	1.91	0.53
1:A:796:THR:HA	1:A:818:LYS:HA	1.91	0.53
1:A:331:GLU:OE2	1:A:333:THR:HG23	2.09	0.53
1:A:1063:ASP:O	1:A:1064:TYR:HB2	2.09	0.53
1:B:796:THR:HA	1:B:818:LYS:HA	1.91	0.53
1:A:1581:LEU:O	1:A:1595:ASP:HA	2.09	0.53
1:B:162:THR:HB	1:B:173:MET:HG3	1.90	0.52
1:B:1213:LYS:HD2	1:B:1266:TYR:CE2	2.44	0.52
1:B:922:ILE:HD12	2:B:2001:NAG:H82	1.91	0.52
1:B:313:TYR:HE2	1:B:321:LYS:HZ1	1.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:LYS:HG3	1:A:1266:TYR:CZ	2.44	0.52
1:B:24:VAL:HA	1:B:655:THR:OG1	2.08	0.52
1:A:639:GLY:N	1:A:645:VAL:HG22	2.18	0.52
1:B:606:ASP:O	1:B:609:VAL:HG22	2.09	0.52
1:B:661:ASP:OD2	1:B:663:GLN:HG2	2.09	0.52
1:A:1535:MET:HB2	1:A:1645:ILE:HD11	1.92	0.52
1:A:1372:GLU:HG3	1:A:1373:GLU:H	1.75	0.52
1:B:1283:GLY:O	1:B:1285:TYR:N	2.42	0.52
1:A:1115:ASN:HD22	1:A:1115:ASN:H	1.54	0.52
1:B:739:ARG:HD3	1:B:754:MET:SD	2.50	0.52
1:A:661:ASP:OD2	1:A:663:GLN:HG2	2.09	0.52
1:A:1670:ASP:HA	1:A:1673:LEU:HD12	1.92	0.52
1:B:1084:ARG:NE	1:B:1088:GLN:OE1	2.39	0.52
1:B:494:ASP:C	1:B:496:ILE:HD12	2.29	0.52
1:B:835:ARG:HH21	1:B:971:THR:HG22	1.75	0.52
1:B:1377:PHE:CE1	1:B:1467:ILE:HD12	2.45	0.52
1:A:1652:THR:OG1	1:B:868:SER:HB3	2.10	0.52
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.10	0.52
1:B:1068:VAL:HG13	1:B:1069:TRP:CE3	2.45	0.52
1:A:489:LYS:C	1:A:491:PRO:HD2	2.30	0.52
1:B:835:ARG:CG	1:B:835:ARG:NH1	2.67	0.52
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.73	0.52
1:A:356:LEU:HG	1:A:452:TYR:CE1	2.44	0.52
1:B:700:TYR:CE1	1:B:758:LEU:HD12	2.45	0.52
1:A:942:VAL:HG22	1:A:957:LYS:HD3	1.92	0.52
1:A:1522:GLY:O	1:A:1523:ALA:HB3	2.10	0.52
1:B:739:ARG:HB3	1:B:754:MET:SD	2.50	0.52
1:A:1599:THR:HB	1:A:1636:ILE:HD12	1.91	0.52
1:B:492:TYR:CD2	1:B:493:ILE:N	2.78	0.52
1:B:1166:THR:O	1:B:1170:LYS:HG2	2.10	0.52
1:A:131:ASP:HB3	1:A:142:LYS:HB2	1.91	0.51
1:A:307:VAL:HG12	1:A:313:TYR:O	2.10	0.51
1:A:1068:VAL:HG13	1:A:1069:TRP:CE3	2.45	0.51
1:A:1111:TYR:CE1	1:A:1121:ASN:HB2	2.45	0.51
1:B:1243:GLY:HA3	1:B:1285:TYR:OH	2.10	0.51
1:B:531:THR:HG23	1:B:533:ASN:H	1.75	0.51
1:B:1034:PHE:CZ	1:B:1041:GLU:HG2	2.45	0.51
1:A:208:ASP:O	1:A:209:PHE:HB2	2.10	0.51
1:B:489:LYS:C	1:B:491:PRO:HD2	2.30	0.51
1:B:587:THR:HA	1:B:789:ALA:HA	1.92	0.51
1:B:1372:GLU:HG3	1:B:1373:GLU:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:HG3	1:B:199:TRP:CD1	2.46	0.51
1:B:968:VAL:HG23	1:B:971:THR:OG1	2.10	0.51
1:B:60:PRO:HD3	1:B:103:TYR:HE1	1.76	0.51
1:B:640:LEU:H	1:B:644:ASN:CB	2.21	0.51
1:A:1213:LYS:HD2	1:A:1266:TYR:CE2	2.45	0.51
1:B:1111:TYR:CE1	1:B:1121:ASN:HB2	2.45	0.51
1:A:1166:THR:O	1:A:1170:LYS:HG2	2.10	0.51
1:A:1034:PHE:CZ	1:A:1041:GLU:HG2	2.45	0.51
1:A:968:VAL:HG23	1:A:971:THR:OG1	2.09	0.51
1:B:566:LYS:HE2	1:B:570:GLN:NE2	2.23	0.51
1:A:909:ASN:H	1:A:926:THR:HG22	1.75	0.51
1:A:39:ILE:CG1	1:A:85:LEU:HD23	2.40	0.51
1:A:1003:LEU:HD11	1:A:1286:SER:HA	1.92	0.51
1:A:1274:LEU:O	1:A:1276:GLU:N	2.44	0.51
1:A:1243:GLY:HA3	1:A:1285:TYR:OH	2.11	0.51
1:A:1283:GLY:O	1:A:1285:TYR:N	2.43	0.51
1:B:827:MET:HE3	1:B:842:LYS:O	2.10	0.51
1:B:749:LEU:HG	1:B:750:GLY:H	1.76	0.51
1:B:59:TYR:CD1	1:B:60:PRO:CD	2.94	0.51
1:A:981:GLY:O	1:A:982:LEU:HD23	2.10	0.51
1:A:357:VAL:HG23	1:A:374:GLN:HB2	1.93	0.51
1:B:1024:TYR:OH	1:B:1306:GLN:NE2	2.44	0.51
1:B:44:TYR:CE1	1:B:497:THR:HG21	2.46	0.51
1:A:855:PHE:HD2	1:A:888:VAL:HG22	1.76	0.51
1:A:492:TYR:CD2	1:A:493:ILE:N	2.78	0.51
1:B:39:ILE:CG1	1:B:85:LEU:HD23	2.40	0.51
1:A:153:LYS:HB3	1:A:154:PRO:HD2	1.93	0.51
1:A:182:ILE:HG12	1:A:804:ILE:HD11	1.93	0.51
1:A:1115:ASN:HD22	1:A:1115:ASN:N	2.09	0.51
1:A:1673:LEU:HD22	1:B:258:LYS:HG2	1.93	0.51
1:B:1204:GLN:HA	1:B:1204:GLN:OE1	2.10	0.51
1:A:916:THR:HG22	1:A:917:TRP:H	1.75	0.51
1:A:1377:PHE:CE1	1:A:1467:ILE:HD12	2.46	0.51
1:B:916:THR:HG22	1:B:917:TRP:H	1.75	0.51
1:B:1123:GLN:NE2	1:B:1123:GLN:H	2.09	0.51
1:A:227:PHE:HB2	1:A:253:ARG:O	2.10	0.51
1:A:1001:THR:HG23	1:A:1284:PHE:HD2	1.75	0.51
1:B:886:GLN:HG2	1:B:894:HIS:CD2	2.46	0.51
1:A:635:GLY:CA	1:A:672:ILE:HG23	2.39	0.51
1:A:839:ILE:HD12	1:A:1485:VAL:HG12	1.93	0.51
1:B:855:PHE:HD2	1:B:888:VAL:HG22	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:LEU:HD11	1:B:1286:SER:HA	1.92	0.51
1:A:1028:GLY:C	1:A:1029:ASN:HD22	2.15	0.51
1:B:1429:PRO:HB3	1:B:1488:LEU:HD22	1.93	0.50
1:A:498:HIS:HB3	1:A:514:THR:HG23	1.94	0.50
1:A:60:PRO:HD3	1:A:103:TYR:HE1	1.76	0.50
1:B:1186:PHE:CD1	1:B:1250:THR:HG22	2.46	0.50
1:B:909:ASN:H	1:B:926:THR:HG22	1.75	0.50
1:A:1084:ARG:NE	1:A:1088:GLN:OE1	2.39	0.50
1:B:942:VAL:HG22	1:B:957:LYS:HD3	1.92	0.50
1:A:1076:THR:HG22	1:A:1120:GLU:HA	1.93	0.50
1:B:227:PHE:HB2	1:B:253:ARG:O	2.11	0.50
1:B:653:PHE:N	1:B:653:PHE:CD2	2.76	0.50
1:A:362:PHE:CD1	1:A:638:GLY:O	2.54	0.50
1:B:292:LEU:HD13	1:B:293:ILE:N	2.27	0.50
1:A:1577:TYR:HB2	1:A:1600:PHE:O	2.12	0.50
1:B:544:TYR:HE2	1:B:546:VAL:HG23	1.76	0.50
1:A:733:VAL:O	1:A:737:GLN:HG2	2.11	0.50
1:B:363:LEU:HD12	1:B:456:ALA:HA	1.93	0.50
1:B:855:PHE:HA	1:B:915:GLU:O	2.11	0.50
1:B:733:VAL:O	1:B:737:GLN:HG2	2.10	0.50
1:A:587:THR:HA	1:A:789:ALA:HA	1.93	0.50
1:A:131:ASP:OD1	1:A:135:TYR:OH	2.21	0.50
1:A:1024:TYR:OH	1:A:1306:GLN:NE2	2.44	0.50
1:B:1028:GLY:C	1:B:1029:ASN:HD22	2.15	0.50
1:A:1016:VAL:HG12	1:A:1017:PRO:N	2.26	0.50
1:A:1637:TYR:CE1	1:A:1639:LEU:HA	2.46	0.50
1:A:1378:TYR:O	1:A:1406:ALA:HA	2.11	0.50
1:B:1378:TYR:O	1:B:1406:ALA:HA	2.12	0.50
1:A:1207:SER:O	1:A:1210:SER:HB3	2.12	0.50
1:A:938:SER:O	1:A:940:SER:N	2.45	0.50
1:B:1016:VAL:HG12	1:B:1017:PRO:N	2.27	0.50
1:B:1304:VAL:CG1	1:B:1305:LYS:H	2.25	0.50
1:A:798:GLU:HG3	1:A:814:THR:OG1	2.11	0.50
1:A:1123:GLN:NE2	1:A:1123:GLN:H	2.09	0.50
1:B:743:SER:OG	1:B:752:LEU:HD22	2.12	0.50
1:B:1207:SER:O	1:B:1210:SER:HB3	2.12	0.50
1:A:830:PRO:HG3	1:A:1483:PHE:HE2	1.77	0.50
1:B:357:VAL:HG23	1:B:374:GLN:HB2	1.93	0.50
1:A:363:LEU:HD12	1:A:456:ALA:HA	1.93	0.50
1:A:166:PRO:HG3	1:A:199:TRP:CD1	2.46	0.50
1:A:680:GLN:HG3	1:A:756:THR:HG23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ARG:CZ	1:A:1284:PHE:CD1	2.94	0.50
1:B:1001:THR:HG23	1:B:1284:PHE:HD2	1.75	0.50
1:A:44:TYR:CE1	1:A:497:THR:HG21	2.47	0.50
1:A:700:TYR:CE1	1:A:758:LEU:HD12	2.47	0.50
1:A:531:THR:HG23	1:A:533:ASN:H	1.75	0.50
1:B:1279:ARG:CZ	1:B:1284:PHE:CD1	2.95	0.50
1:B:208:ASP:O	1:B:209:PHE:HB2	2.11	0.50
1:B:1115:ASN:N	1:B:1115:ASN:HD22	2.09	0.50
1:B:196:TYR:HD1	1:B:219:VAL:HG12	1.77	0.50
1:A:584:PRO:HG2	1:A:821:LYS:HB2	1.94	0.50
1:A:1585:TYR:CD1	1:A:1671:ILE:HG21	2.47	0.50
1:A:292:LEU:HD13	1:A:293:ILE:N	2.26	0.50
1:A:981:GLY:O	1:A:1309:LEU:HD21	2.12	0.49
1:B:1300:TYR:CZ	1:B:1304:VAL:HG21	2.47	0.49
1:B:1385:ASP:O	1:B:1399:TYR:HD2	1.94	0.49
1:A:1385:ASP:O	1:A:1399:TYR:HD2	1.94	0.49
1:B:1274:LEU:O	1:B:1276:GLU:N	2.45	0.49
1:A:835:ARG:HH21	1:A:971:THR:HG22	1.77	0.49
1:B:498:HIS:HB3	1:B:514:THR:HG23	1.93	0.49
1:A:43:VAL:HG22	1:A:44:TYR:N	2.27	0.49
1:A:982:LEU:CD2	1:A:1309:LEU:HD11	2.41	0.49
1:B:373:VAL:HG21	1:B:388:VAL:HG11	1.93	0.49
1:A:1300:TYR:CZ	1:A:1304:VAL:HG21	2.48	0.49
1:B:153:LYS:HB3	1:B:154:PRO:HD2	1.93	0.49
1:B:1076:THR:HG22	1:B:1120:GLU:HA	1.94	0.49
1:B:798:GLU:HG3	1:B:814:THR:OG1	2.11	0.49
1:A:114:SER:O	1:A:115:LYS:HE2	2.12	0.49
1:A:1304:VAL:CG1	1:A:1305:LYS:H	2.24	0.49
1:B:233:PRO:HG3	1:B:342:ILE:HD13	1.94	0.49
1:A:1286:SER:OG	1:A:1287:THR:N	2.45	0.49
1:A:136:THR:HG21	1:A:222:TYR:HB2	1.95	0.49
1:B:1003:LEU:HB3	1:B:1498:TYR:HE1	1.77	0.49
1:A:240:TYR:HB3	1:A:446:ASN:ND2	2.28	0.49
1:A:360:PRO:HA	1:A:636:ALA:HB3	1.95	0.49
1:B:953:ILE:O	1:B:953:ILE:HG13	2.11	0.49
1:A:930:VAL:HG12	1:A:931:PRO:O	2.12	0.49
1:A:1429:PRO:HB3	1:A:1488:LEU:HD22	1.93	0.49
1:B:115:LYS:HA	1:B:115:LYS:HE2	1.95	0.49
1:B:886:GLN:HG3	1:B:887:LYS:N	2.23	0.49
1:A:1066:TYR:N	1:A:1066:TYR:CD1	2.81	0.49
1:A:820:PHE:HZ	1:A:848:TYR:HB2	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:PRO:HA	1:B:932:GLU:OE1	2.13	0.49
1:B:114:SER:O	1:B:115:LYS:HE2	2.13	0.49
1:A:1578:LYS:HA	1:A:1599:THR:HG23	1.94	0.49
1:B:384:GLY:HA2	1:B:411:THR:HG23	1.94	0.49
1:A:373:VAL:HG21	1:A:388:VAL:HG11	1.94	0.49
1:A:703:ALA:HB2	1:A:732:CYS:HA	1.95	0.49
1:A:1293:ALA:O	1:A:1297:LEU:HD12	2.12	0.49
1:A:931:PRO:HA	1:A:932:GLU:OE1	2.12	0.49
1:A:59:TYR:CD1	1:A:60:PRO:CD	2.94	0.49
1:B:982:LEU:CD2	1:B:1309:LEU:HD11	2.42	0.49
1:B:635:GLY:CA	1:B:672:ILE:HG23	2.40	0.49
1:A:233:PRO:HG3	1:A:342:ILE:HD13	1.94	0.49
1:A:196:TYR:HD1	1:A:219:VAL:HG12	1.78	0.49
1:B:271:ILE:O	1:B:280:LYS:HB2	2.13	0.49
1:A:1584:ILE:HG22	1:A:1585:TYR:N	2.27	0.49
1:B:1309:LEU:HD23	1:B:1355:GLY:HA3	1.94	0.49
1:A:855:PHE:HA	1:A:915:GLU:O	2.12	0.49
1:A:1289:ASP:OD2	1:A:1290:THR:N	2.46	0.49
1:A:544:TYR:HE2	1:A:546:VAL:HG23	1.77	0.49
1:B:592:MET:HB3	1:B:780:VAL:HG11	1.94	0.49
1:A:1053:MET:CE	1:A:1086:LEU:HD13	2.43	0.49
1:A:708:ASP:OD2	1:A:1401:ARG:NH2	2.46	0.49
1:B:1053:MET:CE	1:B:1086:LEU:HD13	2.43	0.49
1:A:592:MET:HB3	1:A:780:VAL:HG11	1.94	0.49
1:A:595:GLY:O	1:A:596:MET:HB2	2.13	0.49
1:A:835:ARG:HG2	1:A:835:ARG:NH1	2.04	0.49
1:B:43:VAL:HG22	1:B:44:TYR:N	2.28	0.49
1:A:267:ILE:HG12	1:A:327:VAL:HG13	1.94	0.49
1:B:938:SER:O	1:B:940:SER:N	2.45	0.48
1:B:267:ILE:HG12	1:B:327:VAL:HG13	1.94	0.48
1:B:412:ARG:HG2	1:B:413:VAL:N	2.28	0.48
1:A:384:GLY:HA2	1:A:411:THR:HG23	1.95	0.48
1:B:52:ALA:CB	1:B:73:LEU:HD21	2.43	0.48
1:A:1637:TYR:CD2	1:A:1638:PRO:HD2	2.47	0.48
1:B:757:LEU:O	1:B:758:LEU:HB2	2.12	0.48
1:B:584:PRO:HG2	1:B:821:LYS:HB2	1.94	0.48
1:A:1622:LYS:HG3	1:A:1623:GLU:H	1.78	0.48
1:A:1598:ILE:HG13	1:A:1599:THR:N	2.29	0.48
1:B:1193:TYR:O	1:B:1196:SER:HB3	2.13	0.48
1:B:489:LYS:O	1:B:490:SER:CB	2.61	0.48
1:A:386:VAL:N	1:A:411:THR:HG22	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:ALA:HB2	1:B:732:CYS:HA	1.95	0.48
1:A:1572:ASN:O	1:A:1573:VAL:HG22	2.12	0.48
1:A:835:ARG:NH1	1:A:835:ARG:CG	2.68	0.48
1:B:981:GLY:O	1:B:1309:LEU:HD21	2.13	0.48
1:A:640:LEU:H	1:A:644:ASN:CB	2.21	0.48
1:B:1289:ASP:OD2	1:B:1290:THR:N	2.46	0.48
1:A:906:GLY:O	1:A:908:HIS:CE1	2.66	0.48
1:A:942:VAL:HG13	1:A:957:LYS:HD2	1.95	0.48
1:A:831:TYR:CE1	1:A:1457:ASP:HB3	2.47	0.48
1:A:953:ILE:HG13	1:A:953:ILE:O	2.12	0.48
1:A:271:ILE:O	1:A:280:LYS:HB2	2.13	0.48
1:B:981:GLY:O	1:B:982:LEU:HD23	2.12	0.48
1:B:845:VAL:HG12	1:B:894:HIS:O	2.14	0.48
1:B:1176:LEU:HB3	1:B:1204:GLN:HG2	1.95	0.48
1:A:1589:GLU:HB2	1:A:1623:GLU:OE1	2.13	0.48
1:B:736:SER:O	1:B:739:ARG:HG2	2.14	0.48
1:B:708:ASP:OD2	1:B:1401:ARG:NH2	2.46	0.48
1:B:1293:ALA:O	1:B:1297:LEU:HD12	2.13	0.48
1:A:1673:LEU:CA	1:B:258:LYS:HG3	2.43	0.48
1:B:484:ILE:HG22	1:B:526:ILE:O	2.14	0.48
1:A:1652:THR:O	1:A:1658:GLN:HB2	2.13	0.48
1:B:692:HIS:CD2	1:B:694:VAL:HG23	2.48	0.48
1:B:595:GLY:O	1:B:596:MET:HB2	2.13	0.48
1:B:127:PHE:HB2	1:B:146:TYR:HB2	1.96	0.48
1:B:831:TYR:CE1	1:B:1457:ASP:HB3	2.49	0.48
1:B:930:VAL:HG12	1:B:931:PRO:O	2.14	0.48
1:A:1309:LEU:HD23	1:A:1355:GLY:HA3	1.94	0.48
1:B:386:VAL:N	1:B:411:THR:HG22	2.27	0.48
1:B:686:ILE:C	1:B:688:ALA:H	2.17	0.48
1:A:1340:VAL:HG21	1:A:1346:LEU:HD22	1.96	0.48
1:A:1279:ARG:CZ	1:A:1284:PHE:HD1	2.27	0.48
1:A:922:ILE:HG21	2:A:2001:NAG:C7	2.44	0.48
1:B:1244:THR:HG22	1:B:1246:ARG:N	2.28	0.48
1:A:566:LYS:HE2	1:A:570:GLN:NE2	2.24	0.48
1:A:1132:THR:H	1:A:1135:VAL:HB	1.79	0.48
1:A:412:ARG:HG2	1:A:413:VAL:N	2.28	0.48
1:A:182:ILE:CG1	1:A:804:ILE:HD11	2.43	0.48
1:B:849:ARG:HG3	1:B:851:SER:H	1.78	0.48
1:A:115:LYS:HA	1:A:115:LYS:HE2	1.94	0.48
1:B:589:SER:HA	1:B:787:GLN:HA	1.96	0.48
1:B:182:ILE:HG12	1:B:804:ILE:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1320:LYS:HD2	1:B:1321:GLY:H	1.78	0.48
1:B:136:THR:HG21	1:B:222:TYR:HB2	1.95	0.48
1:A:156:LYS:HB3	1:A:178:ASP:O	2.13	0.48
1:A:480:GLU:O	1:A:530:VAL:HG12	2.13	0.48
1:A:563:ILE:HG13	1:A:564:GLU:N	2.28	0.48
1:A:1176:LEU:HB3	1:A:1204:GLN:HG2	1.95	0.48
1:A:1180:LEU:HA	1:A:1180:LEU:HD23	1.52	0.48
1:B:362:PHE:CD1	1:B:638:GLY:O	2.56	0.48
1:A:736:SER:O	1:A:739:ARG:HG2	2.13	0.48
1:B:1304:VAL:CG1	1:B:1305:LYS:N	2.73	0.48
1:B:490:SER:O	1:B:491:PRO:C	2.51	0.48
1:B:182:ILE:CG1	1:B:804:ILE:HD11	2.44	0.48
1:A:1320:LYS:HD2	1:A:1321:GLY:H	1.79	0.48
1:A:1378:TYR:O	1:A:1379:LEU:HD23	2.13	0.48
1:B:1378:TYR:O	1:B:1379:LEU:HD23	2.14	0.48
1:B:480:GLU:O	1:B:530:VAL:HG12	2.14	0.48
1:A:849:ARG:HG3	1:A:851:SER:H	1.78	0.48
1:A:1244:THR:HG22	1:A:1246:ARG:N	2.28	0.48
1:A:1193:TYR:O	1:A:1196:SER:HB3	2.14	0.48
1:B:493:ILE:CG2	1:B:495:LYS:HE2	2.44	0.48
1:B:942:VAL:HG13	1:B:957:LYS:HD2	1.95	0.48
1:B:1076:THR:HA	1:B:1106:TRP:HZ3	1.79	0.48
1:A:127:PHE:HB2	1:A:146:TYR:HB2	1.96	0.48
1:A:931:PRO:HB2	1:A:1366:HIS:CD2	2.49	0.47
1:A:1565:ILE:O	1:A:1565:ILE:HD12	2.14	0.47
1:B:1066:TYR:N	1:B:1066:TYR:CD1	2.82	0.47
1:A:702:GLY:HA2	1:A:728:PHE:CD1	2.49	0.47
1:B:760:VAL:HG21	1:B:1444:GLU:OE2	2.14	0.47
1:B:1320:LYS:CG	1:B:1321:GLY:N	2.77	0.47
1:B:156:LYS:HB3	1:B:178:ASP:O	2.14	0.47
1:A:987:ILE:HG22	1:A:1021:VAL:HG23	1.96	0.47
1:A:54:ILE:O	1:A:68:SER:HA	2.14	0.47
1:A:490:SER:O	1:A:491:PRO:C	2.50	0.47
1:B:679:LEU:HD13	1:B:742:ILE:HD13	1.96	0.47
1:A:1633:PHE:CE2	1:A:1634:ARG:HD2	2.49	0.47
1:A:1585:TYR:HB3	1:A:1671:ILE:HG12	1.95	0.47
1:A:1258:SER:HB3	1:A:1267:VAL:HG23	1.96	0.47
1:B:931:PRO:HB2	1:B:1366:HIS:CD2	2.49	0.47
1:B:123:ASN:HB3	1:B:209:PHE:CD2	2.49	0.47
1:B:1286:SER:OG	1:B:1287:THR:N	2.44	0.47
1:B:1525:CYS:SG	1:B:1526:LYS:N	2.87	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1576:LYS:HE3	1:A:1601:ILE:HG21	1.97	0.47
1:A:330:ILE:O	1:A:330:ILE:HG13	2.14	0.47
1:B:266:TYR:CE2	1:B:755:LYS:HB2	2.49	0.47
1:B:54:ILE:O	1:B:68:SER:HA	2.15	0.47
1:B:1132:THR:H	1:B:1135:VAL:HB	1.78	0.47
1:B:386:VAL:N	1:B:411:THR:CG2	2.77	0.47
1:A:1003:LEU:HB3	1:A:1498:TYR:HE1	1.78	0.47
1:A:1320:LYS:HG2	1:A:1342:LEU:CD1	2.44	0.47
1:A:1146:ALA:HB1	1:A:1190:ILE:HG22	1.97	0.47
1:B:1379:LEU:HB2	1:B:1507:MET:CE	2.44	0.47
1:B:1379:LEU:HD21	1:B:1495:VAL:CG1	2.44	0.47
1:A:1326:TYR:N	1:A:1326:TYR:CD2	2.83	0.47
1:B:330:ILE:HG13	1:B:330:ILE:O	2.15	0.47
1:B:829:ILE:HG13	1:B:925:LYS:CG	2.35	0.47
1:A:489:LYS:O	1:A:490:SER:CB	2.62	0.47
1:A:1576:LYS:HG3	1:A:1601:ILE:HG22	1.97	0.47
1:A:484:ILE:HG22	1:A:526:ILE:O	2.14	0.47
1:A:123:ASN:HB3	1:A:209:PHE:CD2	2.50	0.47
1:A:757:LEU:HG	1:A:759:PRO:HD3	1.97	0.47
1:A:760:VAL:HG12	1:A:760:VAL:O	2.15	0.47
1:B:820:PHE:HZ	1:B:848:TYR:HB2	1.79	0.47
1:B:760:VAL:O	1:B:760:VAL:HG12	2.15	0.47
1:B:598:SER:HA	1:B:805:SER:OG	2.15	0.47
1:A:457:TYR:HE2	1:A:459:SER:HB2	1.80	0.47
1:A:1561:TYR:O	1:A:1561:TYR:HD2	1.98	0.47
1:B:1326:TYR:N	1:B:1326:TYR:CD2	2.83	0.47
1:A:258:LYS:HD3	1:A:258:LYS:HA	1.59	0.47
1:A:465:LEU:HD21	1:A:542:VAL:HG12	1.97	0.47
1:B:839:ILE:HD12	1:B:1485:VAL:HG12	1.97	0.47
1:B:838:GLN:HA	1:B:901:LEU:HB2	1.97	0.47
1:A:1290:THR:O	1:A:1294:ILE:CG1	2.58	0.47
1:B:987:ILE:HG22	1:B:1021:VAL:HG23	1.96	0.47
1:A:493:ILE:CG2	1:A:495:LYS:HG2	2.45	0.47
1:A:52:ALA:CB	1:A:73:LEU:HD21	2.43	0.47
1:B:702:GLY:HA2	1:B:728:PHE:CD1	2.49	0.47
1:A:1379:LEU:HB2	1:A:1507:MET:CE	2.44	0.47
1:B:423:ASN:ND2	1:B:423:ASN:N	2.63	0.47
1:A:1186:PHE:CD1	1:A:1250:THR:HG22	2.47	0.47
1:B:906:GLY:O	1:B:908:HIS:CE1	2.67	0.47
1:A:493:ILE:CG2	1:A:495:LYS:HE2	2.45	0.47
1:B:493:ILE:CG2	1:B:495:LYS:HG2	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:TRP:HB2	1:A:804:ILE:O	2.15	0.47
1:A:1370:THR:O	1:A:1370:THR:HG22	2.15	0.47
1:A:1034:PHE:CE1	1:A:1041:GLU:HG2	2.50	0.47
1:A:1144:LEU:O	1:A:1148:THR:HG22	2.15	0.47
1:B:1340:VAL:HG21	1:B:1346:LEU:HD22	1.97	0.47
1:A:829:ILE:HG13	1:A:925:LYS:CG	2.35	0.47
1:B:1146:ALA:HB1	1:B:1190:ILE:HG22	1.96	0.47
1:A:598:SER:HA	1:A:805:SER:OG	2.15	0.47
1:A:404:LEU:N	1:A:404:LEU:HD23	2.30	0.47
1:A:423:ASN:ND2	1:A:423:ASN:N	2.63	0.47
1:B:563:ILE:HG13	1:B:564:GLU:N	2.28	0.46
1:A:692:HIS:CD2	1:A:694:VAL:HG23	2.48	0.46
1:B:465:LEU:HD21	1:B:542:VAL:HG12	1.96	0.46
1:A:1180:LEU:CD2	1:A:1208:ILE:HG12	2.44	0.46
1:A:467:ILE:HG13	1:A:467:ILE:O	2.15	0.46
1:A:1193:TYR:HE1	1:A:1256:LEU:HB3	1.77	0.46
1:B:214:THR:HG22	1:B:216:TYR:CE2	2.50	0.46
1:B:363:LEU:O	1:B:363:LEU:HD12	2.14	0.46
1:A:1379:LEU:HD21	1:A:1495:VAL:CG1	2.45	0.46
1:B:1144:LEU:O	1:B:1148:THR:HG22	2.16	0.46
1:A:1546:GLU:HG2	1:A:1547:THR:N	2.30	0.46
1:A:686:ILE:C	1:A:688:ALA:H	2.17	0.46
1:A:679:LEU:HD13	1:A:742:ILE:HD13	1.96	0.46
1:B:1180:LEU:CD2	1:B:1208:ILE:HG12	2.45	0.46
1:B:1290:THR:O	1:B:1294:ILE:CG1	2.58	0.46
1:A:546:VAL:HG12	1:A:546:VAL:O	2.14	0.46
1:B:546:VAL:HG12	1:B:546:VAL:O	2.14	0.46
1:B:1320:LYS:HG2	1:B:1342:LEU:CD1	2.44	0.46
1:A:1320:LYS:CG	1:A:1321:GLY:N	2.77	0.46
1:B:1034:PHE:CE1	1:B:1041:GLU:HG2	2.50	0.46
1:A:363:LEU:O	1:A:363:LEU:HD12	2.14	0.46
1:B:152:LEU:O	1:B:808:GLY:HA2	2.16	0.46
1:B:457:TYR:HE2	1:B:459:SER:HB2	1.80	0.46
1:A:838:GLN:HA	1:A:901:LEU:HB2	1.97	0.46
1:A:618:LYS:HA	1:A:619:PRO:HD3	1.73	0.46
1:A:1076:THR:HA	1:A:1106:TRP:HZ3	1.80	0.46
1:B:1015:VAL:HG22	1:B:1015:VAL:O	2.15	0.46
1:B:1303:LEU:HD13	1:B:1303:LEU:C	2.35	0.46
1:A:1264:ILE:HG12	1:A:1303:LEU:CD1	2.43	0.46
1:A:360:PRO:HB3	1:A:637:GLY:O	2.15	0.46
1:B:1319:HIS:HD2	1:B:1344:ASP:OD1	1.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:TYR:CB	1:B:819:VAL:HG12	2.46	0.46
1:B:360:PRO:HA	1:B:636:ALA:HB3	1.97	0.46
1:A:589:SER:HA	1:A:787:GLN:HA	1.96	0.46
1:B:1457:ASP:O	1:B:1459:HIS:HD2	1.98	0.46
1:A:286:ALA:O	1:A:287:MET:C	2.53	0.46
1:B:286:ALA:O	1:B:287:MET:C	2.53	0.46
1:B:473:HIS:HE1	1:B:477:LEU:CG	2.20	0.46
1:A:1559:TYR:CD2	1:A:1559:TYR:C	2.89	0.46
1:A:587:THR:CG2	1:A:789:ALA:HB2	2.45	0.46
1:B:1015:VAL:HG23	1:B:1049:LEU:HD12	1.98	0.46
1:A:152:LEU:O	1:A:808:GLY:HA2	2.16	0.46
1:A:1641:SER:C	1:A:1643:THR:H	2.18	0.46
1:A:412:ARG:HD3	1:A:414:ASP:OD2	2.16	0.46
1:A:1303:LEU:C	1:A:1303:LEU:HD13	2.35	0.46
1:B:1520:CYS:HA	1:B:1525:CYS:CB	2.46	0.46
1:B:1258:SER:HB3	1:B:1267:VAL:HG23	1.97	0.46
1:A:1015:VAL:O	1:A:1015:VAL:HG22	2.16	0.46
1:A:838:GLN:HB3	1:A:1486:GLY:CA	2.40	0.46
1:B:830:PRO:HG3	1:B:1483:PHE:HE2	1.80	0.46
1:B:599:TRP:CZ3	1:B:779:LEU:HB2	2.51	0.46
1:A:781:PRO:C	1:A:783:ARG:H	2.19	0.46
1:B:594:THR:HG21	1:B:598:SER:HB3	1.98	0.46
1:B:360:PRO:HB3	1:B:637:GLY:O	2.15	0.46
1:B:369:TYR:HA	1:B:370:PRO:HD3	1.70	0.46
1:B:485:ILE:N	1:B:485:ILE:HD12	2.32	0.46
1:A:441:ASP:OD2	1:A:441:ASP:N	2.46	0.46
1:A:1202:HIS:CD2	1:A:1204:GLN:HB3	2.52	0.45
1:B:232:GLU:HA	1:B:233:PRO:HD3	1.73	0.45
1:B:1370:THR:O	1:B:1370:THR:HG22	2.15	0.45
1:A:1548:ARG:NH2	1:A:1646:GLU:OE1	2.48	0.45
1:A:214:THR:HG22	1:A:216:TYR:CE2	2.51	0.45
1:A:643:ALA:O	1:A:647:HIS:N	2.49	0.45
1:A:93:PRO:HD2	1:A:96:GLN:O	2.16	0.45
1:A:758:LEU:HD22	1:A:760:VAL:H	1.80	0.45
1:A:895:LEU:HD13	1:A:1555:PRO:HB2	1.97	0.45
1:A:1076:THR:N	1:A:1120:GLU:OE2	2.49	0.45
1:B:922:ILE:HG21	2:B:2001:NAG:N2	2.32	0.45
1:B:1012:LEU:O	1:B:1015:VAL:HG12	2.16	0.45
1:B:1408:TYR:O	1:B:1410:PRO:HD3	2.17	0.45
1:B:240:TYR:HB3	1:B:446:ASN:ND2	2.31	0.45
1:B:949:ILE:HG12	1:B:949:ILE:H	1.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PHE:HB2	1:B:119:ILE:HG22	1.98	0.45
1:A:1180:LEU:HD21	1:A:1208:ILE:HG12	1.97	0.45
1:B:599:TRP:HB2	1:B:804:ILE:O	2.16	0.45
1:B:577:PRO:HD3	1:B:588:VAL:HG23	1.98	0.45
1:A:1104:LEU:HD13	1:A:1164:ILE:HD12	1.98	0.45
1:B:905:ILE:HG22	1:B:906:GLY:N	2.32	0.45
1:B:779:LEU:O	1:B:781:PRO:HD3	2.17	0.45
1:B:265:VAL:O	1:B:289:ASN:HA	2.17	0.45
1:B:587:THR:CG2	1:B:789:ALA:HB2	2.46	0.45
1:A:1456:LYS:O	1:A:1457:ASP:C	2.55	0.45
1:A:1457:ASP:O	1:A:1459:HIS:HD2	1.99	0.45
1:B:1318:LYS:HG2	1:B:1319:HIS:NE2	2.31	0.45
1:A:1015:VAL:HG23	1:A:1049:LEU:HD12	1.98	0.45
1:B:66:TYR:OH	1:B:90:LYS:HD2	2.17	0.45
1:A:839:ILE:HD11	1:A:1483:PHE:CE1	2.52	0.45
1:B:909:ASN:HD22	1:B:910:ILE:N	2.14	0.45
1:A:265:VAL:O	1:A:289:ASN:HA	2.17	0.45
1:B:131:ASP:OD1	1:B:135:TYR:OH	2.22	0.45
1:A:1524:ALA:O	1:A:1528:VAL:HG23	2.16	0.45
1:B:541:LEU:HD13	1:B:645:VAL:HG12	1.98	0.45
1:A:1076:THR:HG22	1:A:1120:GLU:OE2	2.16	0.45
1:A:388:VAL:O	1:A:420:PHE:HZ	2.00	0.45
1:A:980:LYS:HB3	1:A:980:LYS:HE3	1.64	0.45
1:B:113:LYS:HG3	1:B:114:SER:N	2.31	0.45
1:A:451:GLY:C	1:A:452:TYR:CD2	2.90	0.45
1:B:1323:LEU:CD1	1:B:1324:HIS:H	2.30	0.45
1:A:1433:SER:HB2	1:A:1480:PHE:HD1	1.81	0.45
1:A:150:ASP:HB2	1:A:508:LYS:NZ	2.31	0.45
1:A:1319:HIS:HD2	1:A:1344:ASP:OD1	1.99	0.45
1:A:949:ILE:HG12	1:A:949:ILE:H	1.56	0.45
1:A:1631:PHE:O	1:A:1632:SER:CB	2.64	0.45
1:B:467:ILE:HG13	1:B:467:ILE:O	2.16	0.45
1:B:1180:LEU:HD21	1:B:1208:ILE:HG12	1.99	0.45
1:A:909:ASN:HD22	1:A:909:ASN:C	2.20	0.45
1:B:560:TRP:CD2	1:B:673:LEU:HD12	2.52	0.45
1:A:599:TRP:CZ3	1:A:779:LEU:HB2	2.51	0.45
1:B:1076:THR:HG22	1:B:1120:GLU:OE2	2.17	0.45
1:B:1076:THR:N	1:B:1120:GLU:OE2	2.50	0.45
1:B:592:MET:HG2	1:B:780:VAL:HG21	1.98	0.45
1:B:1427:SER:HB3	1:B:1492:THR:H	1.82	0.45
1:B:404:LEU:HD23	1:B:404:LEU:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:LEU:CD1	1:A:1657:CYS:HB3	2.31	0.45
1:A:577:PRO:HD3	1:A:588:VAL:HG23	1.98	0.45
1:B:667:GLU:N	1:B:668:PRO:CD	2.79	0.45
1:A:779:LEU:O	1:A:781:PRO:HD3	2.17	0.45
1:A:575:LEU:HD11	1:A:817:ALA:HB2	1.99	0.45
1:A:1665:ASP:O	1:A:1668:ALA:HB3	2.17	0.45
1:A:1497:GLU:OE1	1:A:1500:ARG:HD2	2.17	0.45
1:B:1202:HIS:CD2	1:B:1204:GLN:HB3	2.51	0.45
1:A:190:ILE:HG22	1:A:194:PRO:CG	2.47	0.45
1:B:583:SER:HA	1:B:584:PRO:HD3	1.80	0.45
1:B:738:LEU:HG	1:B:742:ILE:HD11	1.98	0.45
1:B:575:LEU:HD11	1:B:817:ALA:HB2	1.99	0.45
1:A:1408:TYR:O	1:A:1410:PRO:HD3	2.17	0.45
1:A:576:SER:HB2	1:A:588:VAL:HG23	1.98	0.44
1:B:292:LEU:HA	1:B:297:ALA:HB2	1.99	0.44
1:A:909:ASN:HD22	1:A:910:ILE:N	2.15	0.44
1:A:818:LYS:HG3	1:A:818:LYS:O	2.16	0.44
1:B:818:LYS:O	1:B:818:LYS:HG3	2.16	0.44
1:A:1490:PRO:HB3	1:A:1509:TYR:O	2.17	0.44
1:A:1599:THR:HG22	1:A:1600:PHE:N	2.32	0.44
1:B:909:ASN:C	1:B:909:ASN:HD22	2.20	0.44
1:A:1323:LEU:CD1	1:A:1324:HIS:H	2.30	0.44
1:A:319:ASN:C	1:A:320:ASN:HD22	2.20	0.44
1:B:373:VAL:HG22	1:B:418:ALA:HB3	1.99	0.44
1:A:594:THR:HG21	1:A:598:SER:HB3	1.98	0.44
1:A:738:LEU:HG	1:A:742:ILE:HD11	1.99	0.44
1:B:774:LEU:HD23	1:B:774:LEU:HA	1.80	0.44
1:A:535:VAL:CG2	1:A:536:PRO:HD3	2.28	0.44
1:B:61:ASP:CG	1:B:61:ASP:O	2.56	0.44
1:A:539:ARG:NH2	1:A:635:GLY:O	2.50	0.44
1:B:1104:LEU:HD13	1:B:1164:ILE:HD12	1.99	0.44
1:A:260:VAL:HG11	1:A:263:ALA:HB2	1.99	0.44
1:A:292:LEU:HA	1:A:297:ALA:HB2	1.99	0.44
1:A:1090:ASN:HD22	1:A:1158:ILE:CD1	2.27	0.44
1:B:121:TYR:HB2	1:B:210:SER:HB2	2.00	0.44
1:B:388:VAL:O	1:B:420:PHE:HZ	2.01	0.44
1:A:582:TYR:CB	1:A:819:VAL:HG12	2.46	0.44
1:A:1618:LEU:HG	1:A:1618:LEU:O	2.17	0.44
1:A:66:TYR:OH	1:A:90:LYS:HD2	2.17	0.44
1:A:838:GLN:O	1:A:1485:VAL:HA	2.17	0.44
1:B:497:THR:HG23	1:B:498:HIS:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ILE:HG22	1:A:906:GLY:N	2.32	0.44
1:A:1440:LYS:HD2	1:A:1444:GLU:OE1	2.17	0.44
1:B:189:LYS:HE2	1:B:190:ILE:O	2.18	0.44
1:B:190:ILE:HG22	1:B:194:PRO:CG	2.47	0.44
1:B:1053:MET:HE2	1:B:1086:LEU:HD13	1.99	0.44
1:A:1318:LYS:HG2	1:A:1319:HIS:NE2	2.32	0.44
1:A:290:THR:O	1:A:290:THR:HG22	2.17	0.44
1:A:689:LYS:HB3	1:A:689:LYS:HE2	1.76	0.44
1:A:1518:LYS:HE2	1:A:1518:LYS:HB2	1.82	0.44
1:B:1485:VAL:HG23	1:B:1488:LEU:HB3	1.99	0.44
1:A:541:LEU:HD13	1:A:645:VAL:HG12	1.99	0.44
1:B:1309:LEU:CD2	1:B:1356:LEU:H	2.31	0.44
1:B:576:SER:HB2	1:B:588:VAL:HG23	1.98	0.44
1:B:775:TRP:O	1:B:775:TRP:CD1	2.71	0.44
1:A:592:MET:HG2	1:A:780:VAL:HG21	1.98	0.44
1:A:193:ASN:OD1	1:A:1070:LYS:HE2	2.17	0.44
1:A:1626:GLN:HG2	1:A:1635:TYR:CD2	2.52	0.44
1:A:113:LYS:HG3	1:A:114:SER:N	2.32	0.44
1:B:539:ARG:NH2	1:B:635:GLY:O	2.51	0.44
1:B:93:PRO:HD2	1:B:96:GLN:O	2.16	0.44
1:B:1379:LEU:HD21	1:B:1495:VAL:HG11	1.99	0.44
1:A:1484:GLU:OE1	1:A:1484:GLU:N	2.45	0.44
1:A:497:THR:HG23	1:A:498:HIS:N	2.33	0.44
1:B:1180:LEU:HD23	1:B:1180:LEU:HA	1.52	0.44
1:A:681:LYS:H	1:A:681:LYS:HG3	1.67	0.44
1:B:1090:ASN:HD22	1:B:1158:ILE:CD1	2.27	0.44
1:B:733:VAL:HG13	1:B:737:GLN:NE2	2.33	0.44
1:B:781:PRO:C	1:B:783:ARG:H	2.19	0.44
1:A:189:LYS:HE2	1:A:190:ILE:O	2.18	0.44
1:A:775:TRP:O	1:A:775:TRP:CD1	2.71	0.44
1:B:1030:HIS:CE1	1:B:1306:GLN:HE21	2.36	0.44
1:A:1012:LEU:O	1:A:1015:VAL:HG12	2.17	0.44
1:A:1109:GLU:HG2	1:A:1163:LYS:HE2	2.00	0.44
1:A:1216:ALA:HB2	1:A:1228:TRP:CZ2	2.53	0.44
1:A:969:PRO:O	1:A:971:THR:HG23	2.18	0.44
1:B:58:SER:O	1:B:103:TYR:HD1	2.01	0.44
1:B:1264:ILE:HG12	1:B:1303:LEU:CD1	2.44	0.44
1:B:1300:TYR:CD2	1:B:1300:TYR:C	2.90	0.44
1:A:610:TYR:O	1:A:612:VAL:HG22	2.18	0.44
1:B:1266:TYR:O	1:B:1269:PRO:HD2	2.18	0.44
1:B:1109:GLU:HG2	1:B:1163:LYS:HE2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1644:TRP:O	1:A:1644:TRP:CD1	2.71	0.44
1:A:485:ILE:N	1:A:485:ILE:HD12	2.32	0.44
1:B:1279:ARG:CZ	1:B:1284:PHE:HD1	2.29	0.44
1:B:1429:PRO:HB2	1:B:1432:ILE:HG13	2.00	0.44
1:A:61:ASP:O	1:A:61:ASP:CG	2.56	0.44
1:B:260:VAL:HG11	1:B:263:ALA:HB2	1.98	0.44
1:B:412:ARG:HD3	1:B:414:ASP:OD2	2.17	0.44
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.91	0.44
1:B:610:TYR:O	1:B:612:VAL:HG22	2.18	0.44
1:A:544:TYR:HE2	1:A:546:VAL:CG2	2.31	0.44
1:A:885:ARG:HH12	1:A:1628:LYS:NZ	2.16	0.44
1:B:802:ILE:HD11	1:B:809:ILE:HG13	2.00	0.44
1:B:1216:ALA:HB2	1:B:1228:TRP:CZ2	2.53	0.44
1:B:1484:GLU:N	1:B:1484:GLU:OE1	2.45	0.44
1:A:1091:LYS:HB3	1:A:1091:LYS:HE2	1.70	0.44
1:A:58:SER:O	1:A:103:TYR:HD1	2.01	0.43
1:B:1497:GLU:OE1	1:B:1500:ARG:HD2	2.18	0.43
1:A:1309:LEU:CD2	1:A:1356:LEU:H	2.31	0.43
1:B:984:VAL:HG13	1:B:988:LEU:HG	2.00	0.43
1:A:757:LEU:O	1:A:758:LEU:HB2	2.18	0.43
1:B:840:GLN:HG3	1:B:899:THR:CG2	2.48	0.43
1:B:977:LEU:HD12	1:B:1361:VAL:CG2	2.39	0.43
1:B:969:PRO:O	1:B:971:THR:HG23	2.18	0.43
1:A:1584:ILE:CG2	1:A:1585:TYR:N	2.80	0.43
1:A:1673:LEU:HA	1:B:258:LYS:HG3	2.00	0.43
1:B:1202:HIS:CD2	1:B:1204:GLN:H	2.20	0.43
1:A:886:GLN:HG3	1:A:887:LYS:N	2.23	0.43
1:A:1379:LEU:HD21	1:A:1495:VAL:HG11	2.00	0.43
1:A:901:LEU:HA	1:A:902:PRO:HD3	1.78	0.43
1:B:758:LEU:C	1:B:760:VAL:H	2.21	0.43
1:B:142:LYS:HD3	1:B:775:TRP:CG	2.53	0.43
1:A:659:ALA:C	1:A:661:ASP:H	2.22	0.43
1:A:1427:SER:OG	1:A:1491:ALA:HB1	2.18	0.43
1:B:150:ASP:HB2	1:B:508:LYS:NZ	2.33	0.43
1:A:1454:GLN:HG3	1:A:1461:ILE:HB	1.99	0.43
1:A:31:PHE:HB2	1:A:119:ILE:HG22	1.98	0.43
1:A:276:LYS:HA	1:A:276:LYS:HD3	1.89	0.43
1:A:554:LEU:HD23	1:A:554:LEU:HA	1.88	0.43
1:A:1671:ILE:HG23	1:A:1672:PHE:N	2.34	0.43
1:B:504:LEU:N	1:B:504:LEU:HD12	2.33	0.43
1:B:1244:THR:HB	1:B:1247:MET:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:LYS:O	1:B:692:HIS:HB2	2.18	0.43
1:B:571:LEU:HA	1:B:593:ALA:O	2.18	0.43
1:B:1454:GLN:HG3	1:B:1461:ILE:HB	2.00	0.43
1:A:1202:HIS:CD2	1:A:1204:GLN:H	2.20	0.43
1:B:367:ILE:HD12	1:B:489:LYS:HD3	2.00	0.43
1:B:544:TYR:HE2	1:B:546:VAL:CG2	2.30	0.43
1:B:1440:LYS:HD2	1:B:1444:GLU:OE1	2.18	0.43
1:A:691:LYS:O	1:A:692:HIS:HB2	2.18	0.43
1:A:1075:SER:HB2	1:A:1120:GLU:OE1	2.19	0.43
1:A:1318:LYS:HG3	1:A:1318:LYS:O	2.18	0.43
1:B:1516:ILE:HG21	1:B:1518:LYS:HE3	2.00	0.43
1:B:290:THR:HG22	1:B:290:THR:O	2.18	0.43
1:B:980:LYS:HE3	1:B:980:LYS:HB3	1.63	0.43
1:A:1429:PRO:HB2	1:A:1432:ILE:HG13	2.01	0.43
1:A:497:THR:HG23	1:A:498:HIS:H	1.82	0.43
1:B:1186:PHE:CD1	1:B:1246:ARG:HD2	2.53	0.43
1:A:214:THR:HG22	1:A:215:ALA:N	2.34	0.43
1:B:451:GLY:C	1:B:452:TYR:CD2	2.92	0.43
1:A:367:ILE:HD12	1:A:489:LYS:HD3	2.01	0.43
1:B:758:LEU:HD22	1:B:760:VAL:H	1.83	0.43
1:B:1433:SER:HB2	1:B:1480:PHE:HD1	1.82	0.43
1:B:592:MET:HE3	1:B:780:VAL:CG2	2.48	0.43
1:A:1318:LYS:HG2	1:A:1319:HIS:CD2	2.54	0.43
1:A:1174:PHE:O	1:A:1178:ASN:HB2	2.18	0.43
1:A:774:LEU:HA	1:A:774:LEU:HD23	1.80	0.43
1:A:1402:ILE:O	1:A:1476:ARG:HA	2.19	0.43
1:B:1002:HIS:HD1	1:B:1284:PHE:HZ	1.66	0.43
1:A:23:TYR:HA	1:A:43:VAL:HG23	2.01	0.43
1:A:1630:ASN:O	1:A:1631:PHE:CB	2.65	0.43
1:A:906:GLY:H	1:A:929:VAL:HB	1.83	0.43
1:A:1200:LYS:HA	1:A:1205:PHE:CD2	2.54	0.43
1:A:154:PRO:O	1:A:155:ALA:HB3	2.19	0.43
1:B:757:LEU:HG	1:B:758:LEU:N	2.34	0.43
1:A:1649:PRO:CG	1:A:1660:PHE:HD2	2.32	0.43
1:A:1554:LYS:CG	1:A:1556:GLU:HG2	2.49	0.43
1:B:161:LEU:HD21	1:B:185:PHE:CD2	2.54	0.43
1:B:1075:SER:HB2	1:B:1120:GLU:OE1	2.19	0.43
1:A:1535:MET:CG	1:A:1645:ILE:HD11	2.49	0.43
1:B:1243:GLY:HA3	1:B:1285:TYR:CZ	2.54	0.43
1:A:1030:HIS:CE1	1:A:1306:GLN:HE21	2.36	0.43
1:B:1379:LEU:HB2	1:B:1507:MET:HE1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1152:ILE:O	1:B:1156:PHE:HB2	2.19	0.43
1:A:1604:VAL:HG22	1:A:1604:VAL:O	2.19	0.43
1:A:1485:VAL:HG23	1:A:1488:LEU:HB3	1.99	0.43
1:B:838:GLN:HB3	1:B:1486:GLY:CA	2.41	0.43
1:A:1202:HIS:HD2	1:A:1204:GLN:N	2.07	0.43
1:B:258:LYS:HA	1:B:258:LYS:HD3	1.59	0.43
1:A:769:PHE:HA	1:A:770:PRO:HD3	1.82	0.43
1:A:809:ILE:HG12	1:A:810:CYS:N	2.34	0.43
1:B:1456:LYS:O	1:B:1457:ASP:C	2.56	0.43
1:A:682:LYS:O	1:A:685:GLU:HG2	2.18	0.43
1:A:571:LEU:HA	1:A:593:ALA:O	2.18	0.43
1:B:689:LYS:HE2	1:B:689:LYS:HB3	1.76	0.43
1:B:1334:LEU:H	1:B:1334:LEU:HD22	1.83	0.43
1:A:1487:PHE:O	1:A:1488:LEU:C	2.57	0.43
1:B:23:TYR:OH	1:B:656:ASN:HB2	2.18	0.43
1:A:733:VAL:HG13	1:A:737:GLN:NE2	2.32	0.43
1:A:1649:PRO:HB2	1:A:1661:LEU:HD11	2.01	0.43
1:A:1107:LEU:HB3	1:A:1118:PHE:HE2	1.84	0.43
1:A:121:TYR:HB2	1:A:210:SER:HB2	2.00	0.43
1:B:1427:SER:OG	1:B:1491:ALA:HB1	2.18	0.43
1:A:290:THR:HG21	1:A:298:GLN:O	2.19	0.43
1:B:398:ASN:O	1:B:399:GLN:HB2	2.19	0.43
1:A:23:TYR:O	1:A:23:TYR:HD1	2.02	0.43
1:A:1186:PHE:CD1	1:A:1246:ARG:HD2	2.53	0.43
1:B:468:ASP:CG	1:B:469:TRP:H	2.23	0.43
1:A:760:VAL:HG21	1:A:1444:GLU:OE2	2.18	0.43
1:B:1174:PHE:O	1:B:1178:ASN:HB2	2.17	0.43
1:B:548:GLY:C	1:B:549:GLU:HG3	2.38	0.43
1:B:542:VAL:O	1:B:556:SER:HA	2.19	0.42
1:B:25:ILE:HD13	1:B:41:ILE:HG13	2.01	0.42
1:B:497:THR:HG23	1:B:498:HIS:N	2.33	0.42
1:B:1132:THR:HG22	1:B:1133:LEU:H	1.83	0.42
1:B:809:ILE:HG12	1:B:810:CYS:N	2.33	0.42
1:A:1535:MET:CB	1:A:1645:ILE:HD11	2.49	0.42
1:B:1318:LYS:HG3	1:B:1318:LYS:O	2.18	0.42
1:A:287:MET:CE	1:A:299:VAL:HB	2.49	0.42
1:B:287:MET:CE	1:B:299:VAL:HB	2.49	0.42
1:B:959:PHE:HA	1:B:960:PRO:HD3	1.80	0.42
1:A:1152:ILE:O	1:A:1156:PHE:HB2	2.19	0.42
1:B:60:PRO:O	1:B:61:ASP:HB3	2.18	0.42
1:B:1096:ASN:O	1:B:1100:ILE:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:TYR:CZ	1:B:755:LYS:HB2	2.55	0.42
1:B:1200:LYS:HA	1:B:1205:PHE:CD2	2.54	0.42
1:B:290:THR:HG21	1:B:298:GLN:O	2.18	0.42
1:B:682:LYS:O	1:B:685:GLU:HG2	2.18	0.42
1:B:71:VAL:O	1:B:71:VAL:HG23	2.19	0.42
1:B:1487:PHE:N	1:B:1487:PHE:CD2	2.87	0.42
1:A:1244:THR:HB	1:A:1247:MET:HB2	2.01	0.42
1:B:154:PRO:O	1:B:155:ALA:HB3	2.19	0.42
1:B:319:ASN:C	1:B:320:ASN:HD22	2.22	0.42
1:A:802:ILE:HD11	1:A:809:ILE:HG13	2.00	0.42
1:A:161:LEU:HD21	1:A:185:PHE:CD2	2.54	0.42
1:A:548:GLY:C	1:A:549:GLU:HG3	2.38	0.42
1:A:840:GLN:HG3	1:A:899:THR:CG2	2.48	0.42
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.93	0.42
1:A:938:SER:HB2	1:A:1362:THR:HA	2.01	0.42
1:B:886:GLN:CG	1:B:887:LYS:H	2.23	0.42
1:B:611:GLY:O	1:B:612:VAL:C	2.58	0.42
1:A:142:LYS:HD3	1:A:775:TRP:CG	2.54	0.42
1:A:721:GLY:HA2	1:A:722:PRO:HD3	1.87	0.42
1:A:1332:ASN:CG	1:A:1332:ASN:O	2.58	0.42
1:A:938:SER:C	1:A:940:SER:H	2.23	0.42
1:A:940:SER:OG	1:A:1361:VAL:HB	2.19	0.42
1:B:535:VAL:CG2	1:B:536:PRO:HD3	2.28	0.42
1:A:829:ILE:HA	1:A:830:PRO:HD3	1.94	0.42
1:B:773:TRP:CZ3	1:B:788:PHE:HE1	2.11	0.42
1:A:1180:LEU:HD21	1:A:1208:ILE:HA	2.01	0.42
1:B:1180:LEU:HD21	1:B:1208:ILE:HA	2.02	0.42
1:A:504:LEU:HD11	1:A:651:LEU:HD11	2.02	0.42
1:B:137:PRO:O	1:B:138:ASP:HB2	2.19	0.42
1:A:1266:TYR:O	1:A:1269:PRO:HD2	2.18	0.42
1:A:1372:GLU:HG3	1:A:1373:GLU:N	2.34	0.42
1:A:373:VAL:HG22	1:A:418:ALA:HB3	2.00	0.42
1:B:975:ARG:HB3	1:B:1363:THR:HB	2.01	0.42
1:B:938:SER:C	1:B:940:SER:H	2.23	0.42
1:B:839:ILE:HD11	1:B:1483:PHE:CE1	2.55	0.42
1:B:23:TYR:O	1:B:23:TYR:HD1	2.02	0.42
1:A:25:ILE:HD13	1:A:41:ILE:HG13	2.02	0.42
1:A:887:LYS:HD2	1:A:887:LYS:N	2.35	0.42
1:A:1008:ALA:HB3	1:A:1078:LEU:HD11	2.00	0.42
1:A:30:ILE:HG21	1:A:120:THR:OG1	2.20	0.42
1:B:1317:TYR:CB	1:B:1320:LYS:HB3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1274:LEU:C	1:B:1276:GLU:N	2.73	0.42
1:B:1318:LYS:HG2	1:B:1319:HIS:CD2	2.54	0.42
1:B:449:ARG:O	1:B:450:GLU:HG2	2.19	0.42
1:A:71:VAL:HG23	1:A:71:VAL:O	2.19	0.42
1:B:751:ARG:HA	1:B:751:ARG:HD3	1.88	0.42
1:A:1487:PHE:N	1:A:1487:PHE:CD2	2.88	0.42
1:B:23:TYR:HA	1:B:43:VAL:HG23	2.01	0.42
1:A:60:PRO:O	1:A:61:ASP:HB3	2.18	0.42
1:B:983:LEU:HD13	1:B:1356:LEU:HD13	2.02	0.42
1:A:468:ASP:CG	1:A:469:TRP:H	2.22	0.42
1:A:611:GLY:O	1:A:612:VAL:C	2.58	0.42
1:B:643:ALA:O	1:B:647:HIS:N	2.49	0.42
1:A:755:LYS:HD2	1:A:755:LYS:HA	1.82	0.42
1:A:1572:ASN:C	1:A:1574:PHE:H	2.23	0.42
1:B:1402:ILE:O	1:B:1476:ARG:HA	2.19	0.42
1:B:193:ASN:OD1	1:B:1070:LYS:HE2	2.19	0.42
1:B:159:THR:HG22	1:B:160:VAL:N	2.34	0.42
1:B:214:THR:HG22	1:B:215:ALA:N	2.35	0.42
1:B:906:GLY:H	1:B:929:VAL:HB	1.83	0.42
1:B:1200:LYS:H	1:B:1200:LYS:HG2	1.54	0.42
1:A:1637:TYR:HA	1:A:1638:PRO:HD2	1.76	0.42
1:B:487:THR:HG22	1:B:523:TYR:CB	2.49	0.42
1:A:1317:TYR:CB	1:A:1320:LYS:HB3	2.50	0.42
1:A:1379:LEU:CB	1:A:1507:MET:HE1	2.50	0.42
1:B:582:TYR:HB2	1:B:819:VAL:HG12	2.02	0.42
1:A:520:ASP:N	1:A:520:ASP:OD1	2.52	0.42
1:B:1515:LYS:HG3	1:B:1515:LYS:O	2.20	0.42
1:A:504:LEU:HD12	1:A:504:LEU:N	2.34	0.42
1:A:984:VAL:HG13	1:A:988:LEU:HG	2.00	0.42
1:B:907:LEU:HD12	1:B:908:HIS:H	1.84	0.42
1:B:73:LEU:HD23	1:B:73:LEU:N	2.35	0.42
1:A:1557:ILE:HG23	1:A:1621:GLY:N	2.34	0.42
1:B:1320:LYS:CD	1:B:1321:GLY:H	2.33	0.42
1:A:1320:LYS:CD	1:A:1321:GLY:H	2.33	0.42
1:A:1248:VAL:HG21	1:A:1285:TYR:HD2	1.85	0.42
1:B:607:SER:HB3	1:B:798:GLU:HB2	2.01	0.42
1:A:1427:SER:HB3	1:A:1492:THR:H	1.83	0.42
1:A:336:PHE:HB3	1:A:337:SER:H	1.64	0.42
1:A:825:LEU:HD12	1:A:844:THR:O	2.20	0.42
1:B:1487:PHE:O	1:B:1488:LEU:C	2.57	0.42
1:A:1132:THR:HG22	1:A:1133:LEU:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:ASN:ND2	1:B:1158:ILE:HD13	2.33	0.42
1:A:323:LEU:HB2	1:A:347:TYR:HE2	1.85	0.42
1:A:424:LEU:HB3	1:A:428:VAL:HG11	2.02	0.42
1:A:1627:ILE:N	1:A:1627:ILE:HD13	2.35	0.42
1:B:659:ALA:C	1:B:661:ASP:H	2.22	0.42
1:B:1248:VAL:HG21	1:B:1285:TYR:HD2	1.85	0.42
1:A:1243:GLY:HA3	1:A:1285:TYR:CZ	2.55	0.42
1:A:1379:LEU:HB2	1:A:1507:MET:HE1	2.00	0.42
1:A:755:LYS:HE3	1:A:756:THR:H	1.84	0.42
1:B:196:TYR:CZ	1:B:221:GLU:HB2	2.55	0.42
1:B:1412:ARG:HG3	1:B:1413:GLU:CD	2.40	0.42
1:A:398:ASN:O	1:A:399:GLN:HB2	2.20	0.42
1:B:976:ILE:O	1:B:1361:VAL:HA	2.20	0.41
1:A:981:GLY:C	1:A:982:LEU:HD23	2.40	0.41
1:B:888:VAL:HG12	1:B:894:HIS:HB2	2.02	0.41
1:B:991:VAL:HG21	1:B:1017:PRO:O	2.20	0.41
1:A:412:ARG:CG	1:A:413:VAL:N	2.83	0.41
1:B:1008:ALA:HB3	1:B:1078:LEU:HD11	2.01	0.41
1:A:1648:TRP:CZ3	1:A:1664:LEU:HD22	2.55	0.41
1:B:1107:LEU:HB3	1:B:1118:PHE:HE2	1.84	0.41
1:B:1520:CYS:HA	1:B:1525:CYS:HB2	2.01	0.41
1:A:583:SER:HA	1:A:584:PRO:HD3	1.80	0.41
1:A:721:GLY:C	1:A:723:ARG:H	2.24	0.41
1:B:1490:PRO:HB3	1:B:1509:TYR:O	2.18	0.41
1:A:1334:LEU:HD22	1:A:1334:LEU:H	1.84	0.41
1:B:866:CYS:SG	1:B:903:LEU:HD21	2.60	0.41
1:A:1096:ASN:O	1:A:1100:ILE:HG12	2.20	0.41
1:B:504:LEU:HD11	1:B:651:LEU:HD11	2.02	0.41
1:A:907:LEU:HD12	1:A:908:HIS:H	1.85	0.41
1:A:73:LEU:N	1:A:73:LEU:HD23	2.35	0.41
1:B:1190:ILE:HG12	1:B:1253:TYR:CE2	2.56	0.41
1:A:975:ARG:HB3	1:A:1363:THR:HB	2.02	0.41
1:B:860:SER:HB3	1:B:911:ASN:HB2	2.02	0.41
1:B:940:SER:OG	1:B:1361:VAL:HB	2.20	0.41
1:A:1309:LEU:HD23	1:A:1356:LEU:H	1.86	0.41
1:B:412:ARG:CG	1:B:413:VAL:N	2.83	0.41
1:B:906:GLY:N	1:B:929:VAL:HB	2.35	0.41
1:A:1124:TYR:HA	1:A:1465:ASN:OD1	2.19	0.41
1:B:1372:GLU:HG3	1:B:1373:GLU:N	2.34	0.41
1:A:483:ASN:ND2	1:A:525:SER:HB3	2.36	0.41
1:B:825:LEU:HD12	1:B:844:THR:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:LYS:HA	1:A:763:PRO:HD3	1.91	0.41
1:A:977:LEU:HD12	1:A:1361:VAL:CG2	2.40	0.41
1:B:308:LYS:HA	1:B:313:TYR:O	2.20	0.41
1:B:901:LEU:HA	1:B:902:PRO:HD3	1.77	0.41
1:A:357:VAL:O	1:A:358:ALA:C	2.59	0.41
1:A:1193:TYR:CD1	1:A:1256:LEU:HB3	2.55	0.41
1:A:906:GLY:N	1:A:929:VAL:HB	2.35	0.41
1:A:493:ILE:CG2	1:A:494:ASP:N	2.84	0.41
1:B:703:ALA:HB2	1:B:731:CYS:C	2.41	0.41
1:A:860:SER:HB3	1:A:911:ASN:HB2	2.02	0.41
1:B:350:SER:HA	1:B:351:PRO:HD3	1.89	0.41
1:B:938:SER:OG	1:B:1279:ARG:NH1	2.52	0.41
1:A:280:LYS:HG3	1:A:282:MET:CE	2.47	0.41
1:B:834:VAL:HG12	1:B:835:ARG:O	2.20	0.41
1:B:59:TYR:CD1	1:B:103:TYR:CE1	3.08	0.41
1:B:887:LYS:N	1:B:887:LYS:HD2	2.35	0.41
1:B:577:PRO:C	1:B:579:ALA:H	2.23	0.41
1:A:991:VAL:HG21	1:A:1017:PRO:O	2.20	0.41
1:B:618:LYS:HA	1:B:619:PRO:HD3	1.73	0.41
1:A:137:PRO:O	1:A:138:ASP:HB2	2.20	0.41
1:B:1213:LYS:HD2	1:B:1266:TYR:CZ	2.55	0.41
1:B:88:GLN:HE21	1:B:88:GLN:HB3	1.73	0.41
1:B:1024:TYR:HB2	1:B:1298:THR:HG23	2.03	0.41
1:A:196:TYR:CZ	1:A:221:GLU:HB2	2.55	0.41
1:A:1013:MET:HE1	1:A:1081:PHE:HZ	1.86	0.41
1:B:395:ILE:HA	1:B:400:GLU:O	2.21	0.41
1:A:1272:LYS:O	1:A:1272:LYS:HG3	2.20	0.41
1:B:1278:GLN:HA	1:B:1278:GLN:NE2	2.35	0.41
1:A:308:LYS:HA	1:A:313:TYR:O	2.20	0.41
1:A:59:TYR:CD1	1:A:103:TYR:CE1	3.08	0.41
1:B:357:VAL:O	1:B:358:ALA:C	2.58	0.41
1:B:412:ARG:CD	1:B:415:ASP:HB2	2.48	0.41
1:A:356:LEU:HD12	1:A:361:LEU:HD11	2.02	0.41
1:A:857:VAL:HG21	1:A:896:VAL:CG1	2.50	0.41
1:A:1274:LEU:C	1:A:1276:GLU:N	2.73	0.41
1:A:1190:ILE:HG12	1:A:1253:TYR:CE2	2.56	0.41
1:A:1113:LEU:C	1:A:1115:ASN:H	2.24	0.41
1:B:1370:THR:HG23	1:B:1373:GLU:OE1	2.21	0.41
1:A:542:VAL:O	1:A:556:SER:HA	2.20	0.41
1:A:1511:THR:HG23	1:A:1511:THR:O	2.19	0.41
1:B:1511:THR:HG23	1:B:1511:THR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TYR:OH	1:A:656:ASN:HB2	2.20	0.41
1:A:175:GLU:OE1	1:A:206:LYS:HD2	2.20	0.41
1:A:612:VAL:HG23	1:A:613:GLN:N	2.30	0.41
1:B:1124:TYR:HA	1:B:1465:ASN:OD1	2.20	0.41
1:A:1559:TYR:OH	1:A:1637:TYR:CD1	2.73	0.41
1:A:884:VAL:HG12	1:A:1625:LEU:CB	2.50	0.41
1:A:530:VAL:O	1:A:530:VAL:HG13	2.21	0.41
1:A:1333:PHE:C	1:A:1335:GLY:H	2.24	0.41
1:A:1133:LEU:N	1:A:1134:PRO:CD	2.84	0.41
1:A:667:GLU:N	1:A:668:PRO:CD	2.79	0.41
1:A:607:SER:HB3	1:A:798:GLU:HB2	2.03	0.41
1:A:592:MET:HE3	1:A:780:VAL:CG2	2.51	0.41
1:A:1002:HIS:HD1	1:A:1284:PHE:HZ	1.67	0.41
1:A:532:GLN:NE2	1:A:535:VAL:HG11	2.35	0.41
1:B:532:GLN:NE2	1:B:535:VAL:HG11	2.35	0.41
1:A:838:GLN:O	1:A:1486:GLY:N	2.54	0.41
1:B:1225:TYR:CE1	1:B:1272:LYS:HG3	2.56	0.41
1:A:1218:VAL:HA	1:A:1225:TYR:O	2.21	0.41
1:B:327:VAL:HG12	1:B:328:THR:N	2.36	0.41
1:B:356:LEU:HD12	1:B:361:LEU:HD11	2.02	0.41
1:A:487:THR:HG22	1:A:523:TYR:CB	2.48	0.41
1:B:758:LEU:O	1:B:760:VAL:N	2.54	0.41
1:A:243:PHE:CZ	1:A:316:GLU:HB2	2.56	0.41
1:A:1548:ARG:HG2	1:A:1548:ARG:NH1	2.36	0.41
1:B:35:ALA:HA	1:B:150:ASP:OD1	2.21	0.41
1:B:483:ASN:HD21	1:B:525:SER:HB3	1.86	0.41
1:A:449:ARG:O	1:A:450:GLU:HG2	2.21	0.41
1:B:1332:ASN:O	1:B:1332:ASN:CG	2.59	0.41
1:B:1420:SER:O	1:B:1421:HIS:C	2.60	0.41
1:A:1455:ILE:HG13	1:A:1460:VAL:HG22	2.03	0.41
1:A:461:SER:C	1:A:463:SER:N	2.74	0.41
1:B:721:GLY:C	1:B:723:ARG:H	2.23	0.41
1:A:1666:GLU:HA	1:A:1666:GLU:OE2	2.21	0.41
1:A:1412:ARG:HG3	1:A:1413:GLU:CD	2.41	0.41
1:A:834:VAL:HG12	1:A:835:ARG:O	2.21	0.41
1:B:838:GLN:O	1:B:1486:GLY:N	2.54	0.41
1:B:1333:PHE:C	1:B:1335:GLY:H	2.24	0.41
1:B:1008:ALA:HB2	1:B:1059:TYR:CD2	2.55	0.41
1:A:560:TRP:CD2	1:A:673:LEU:HD12	2.55	0.41
1:B:1113:LEU:C	1:B:1115:ASN:H	2.24	0.41
1:B:29:LYS:O	1:B:30:ILE:HD13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:LYS:O	1:B:1119:LYS:HG3	2.20	0.41
1:A:1024:TYR:HB2	1:A:1298:THR:HG23	2.03	0.41
1:B:721:GLY:HA2	1:B:722:PRO:HD3	1.88	0.41
1:B:1039:LEU:HD12	1:B:1039:LEU:HA	1.85	0.41
1:A:1001:THR:HG22	1:A:1002:HIS:N	2.36	0.40
1:A:976:ILE:O	1:A:1361:VAL:HA	2.20	0.40
1:A:159:THR:HG22	1:A:160:VAL:N	2.35	0.40
1:A:1577:TYR:CE2	1:A:1611:LEU:HB3	2.56	0.40
1:B:1193:TYR:HE1	1:B:1256:LEU:HB3	1.78	0.40
1:A:1213:LYS:HD2	1:A:1266:TYR:CZ	2.56	0.40
1:B:530:VAL:HG13	1:B:530:VAL:O	2.22	0.40
1:A:290:THR:O	1:A:291:MET:C	2.60	0.40
1:A:111:PHE:CD2	1:A:112:SER:N	2.89	0.40
1:B:838:GLN:O	1:B:1485:VAL:HA	2.20	0.40
1:A:983:LEU:HD13	1:A:1356:LEU:HD13	2.03	0.40
1:B:495:LYS:HA	1:B:495:LYS:CE	2.51	0.40
1:B:85:LEU:O	1:B:86:THR:HB	2.21	0.40
1:B:323:LEU:HB2	1:B:347:TYR:HE2	1.85	0.40
1:A:1563:VAL:HG12	1:A:1581:LEU:HG	2.03	0.40
1:B:592:MET:HE3	1:B:780:VAL:HG21	2.03	0.40
1:B:1053:MET:CE	1:B:1086:LEU:HD22	2.52	0.40
1:B:290:THR:O	1:B:291:MET:C	2.59	0.40
1:B:1279:ARG:CG	1:B:1284:PHE:HB2	2.23	0.40
1:B:540:LEU:CD1	1:B:542:VAL:HG23	2.51	0.40
1:A:308:LYS:HG3	1:A:314:SER:CB	2.51	0.40
1:A:1615:ARG:NE	1:A:1647:TYR:HE1	2.19	0.40
1:A:987:ILE:HG12	1:A:1294:ILE:HD12	2.03	0.40
1:A:1591:VAL:HG13	1:A:1591:VAL:O	2.20	0.40
1:A:703:ALA:HB2	1:A:731:CYS:C	2.41	0.40
1:A:483:ASN:HD21	1:A:525:SER:HB3	1.86	0.40
1:A:369:TYR:HA	1:A:370:PRO:HD3	1.70	0.40
1:B:520:ASP:N	1:B:520:ASP:OD1	2.52	0.40
1:B:175:GLU:OE1	1:B:206:LYS:HD2	2.21	0.40
1:B:769:PHE:HA	1:B:770:PRO:HD3	1.83	0.40
1:B:1133:LEU:N	1:B:1134:PRO:CD	2.83	0.40
1:A:327:VAL:HG12	1:A:328:THR:N	2.37	0.40
1:B:1193:TYR:CD1	1:B:1256:LEU:HB3	2.55	0.40
1:B:493:ILE:CG2	1:B:494:ASP:N	2.83	0.40
1:A:1557:ILE:HG23	1:A:1621:GLY:CA	2.51	0.40
1:B:1378:TYR:CE2	1:B:1409:LYS:HG2	2.57	0.40
1:A:1053:MET:CE	1:A:1086:LEU:HD22	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ASN:HD22	1:B:423:ASN:H	1.69	0.40
1:A:582:TYR:HB2	1:A:819:VAL:HG12	2.03	0.40
1:A:1085:VAL:O	1:A:1089:VAL:HG23	2.22	0.40
1:B:224:LEU:HA	1:B:224:LEU:HD22	1.90	0.40
1:A:1278:GLN:NE2	1:A:1278:GLN:HA	2.36	0.40
1:A:540:LEU:CD1	1:A:542:VAL:HG23	2.51	0.40
1:A:773:TRP:CZ3	1:A:788:PHE:HE1	2.11	0.40
1:A:577:PRO:C	1:A:579:ALA:H	2.24	0.40
1:A:207:GLU:HB3	1:A:208:ASP:H	1.66	0.40
1:B:493:ILE:HG21	1:B:495:LYS:HG2	2.03	0.40
1:A:1444:GLU:O	1:A:1444:GLU:HG2	2.22	0.40
1:A:21:GLN:HE22	1:A:45:GLY:HA2	1.87	0.40
1:A:1370:THR:HG23	1:A:1373:GLU:OE1	2.21	0.40
1:A:1140:ASN:HA	1:A:1140:ASN:HD22	1.72	0.40
1:B:111:PHE:CD2	1:B:112:SER:N	2.89	0.40
1:B:1091:LYS:HE2	1:B:1091:LYS:HB3	1.69	0.40
1:A:395:ILE:HA	1:A:400:GLU:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1615/1676 (96%)	1282 (79%)	257 (16%)	76 (5%)	3	17
1	B	1471/1676 (88%)	1191 (81%)	214 (14%)	66 (4%)	3	17
All	All	3086/3352 (92%)	2473 (80%)	471 (15%)	142 (5%)	3	17

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	261	THR
1	A	308	LYS
1	A	336	PHE
1	A	490	SER
1	A	612	VAL
1	A	705	VAL
1	A	1275	SER
1	A	1284	PHE
1	A	1352	PHE
1	A	1548	ARG
1	A	1571	GLU
1	A	1633	PHE
1	A	1639	LEU
1	B	60	PRO
1	B	261	THR
1	B	308	LYS
1	B	336	PHE
1	B	490	SER
1	B	612	VAL
1	B	705	VAL
1	B	1275	SER
1	B	1284	PHE
1	B	1352	PHE
1	A	99	VAL
1	A	100	SER
1	A	207	GLU
1	A	638	GLY
1	A	657	ALA
1	A	663	GLN
1	A	996	GLY
1	A	1029	ASN
1	A	1240	PRO
1	A	1286	SER
1	A	1335	GLY
1	A	1419	SER
1	A	1457	ASP
1	A	1632	SER
1	A	1634	ARG
1	A	1657	CYS
1	B	99	VAL
1	B	100	SER
1	B	207	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	638	GLY
1	B	657	ALA
1	B	663	GLN
1	B	996	GLY
1	B	1029	ASN
1	B	1240	PRO
1	B	1286	SER
1	B	1335	GLY
1	B	1419	SER
1	B	1457	ASP
1	A	46	TYR
1	A	93	PRO
1	A	101	TYR
1	A	289	ASN
1	A	704	CYS
1	A	939	TYR
1	A	1126	PRO
1	A	1236	ASP
1	A	1596	SER
1	A	1608	ASN
1	A	1636	ILE
1	A	1640	ASP
1	B	46	TYR
1	B	93	PRO
1	B	101	TYR
1	B	289	ASN
1	B	615	GLY
1	B	704	CYS
1	B	939	TYR
1	B	1126	PRO
1	B	1236	ASP
1	A	61	ASP
1	A	98	PRO
1	A	318	LEU
1	A	522	SER
1	A	613	GLN
1	A	615	GLY
1	A	669	CYS
1	A	691	LYS
1	A	700	TYR
1	A	765	ILE
1	A	868	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1373	GLU
1	A	1650	ARG
1	B	61	ASP
1	B	98	PRO
1	B	318	LEU
1	B	522	SER
1	B	613	GLN
1	B	669	CYS
1	B	691	LYS
1	B	700	TYR
1	B	765	ILE
1	B	868	SER
1	B	1373	GLU
1	B	1519	VAL
1	B	1524	ALA
1	A	86	THR
1	A	231	ILE
1	A	355	ASN
1	A	358	ALA
1	A	491	PRO
1	A	495	LYS
1	A	692	HIS
1	A	730	GLU
1	A	1122	SER
1	A	1573	VAL
1	B	86	THR
1	B	355	ASN
1	B	358	ALA
1	B	491	PRO
1	B	495	LYS
1	B	692	HIS
1	B	730	GLU
1	B	1122	SER
1	B	1525	CYS
1	A	154	PRO
1	A	209	PHE
1	A	287	MET
1	A	551	THR
1	A	619	PRO
1	A	754	MET
1	B	154	PRO
1	B	209	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	231	ILE
1	B	551	THR
1	B	619	PRO
1	B	758	LEU
1	A	760	VAL
1	A	585	GLY
1	B	585	GLY
1	B	760	VAL
1	A	758	LEU
1	A	1160	PRO
1	B	759	PRO
1	B	1160	PRO
1	B	1296	GLY
1	A	618	LYS
1	B	618	LYS

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	1441/1484 (97%)	1294 (90%)	147 (10%)	9	33
1	B	1314/1484 (88%)	1183 (90%)	131 (10%)	9	34
All	All	2755/2968 (93%)	2477 (90%)	278 (10%)	9	33

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	22	THR
1	A	23	TYR
1	A	42	GLN
1	A	61	ASP
1	A	73	LEU
1	A	100	SER
1	A	115	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	116	ARG
1	A	130	THR
1	A	140	SER
1	A	148	LEU
1	A	161	LEU
1	A	162	THR
1	A	165	ASP
1	A	179	HIS
1	A	195	ARG
1	A	208	ASP
1	A	211	THR
1	A	224	LEU
1	A	242	ASN
1	A	249	THR
1	A	280	LYS
1	A	292	LEU
1	A	320	ASN
1	A	332	SER
1	A	333	THR
1	A	383	VAL
1	A	393	GLN
1	A	394	THR
1	A	422	LEU
1	A	423	ASN
1	A	426	SER
1	A	431	LEU
1	A	457	TYR
1	A	492	TYR
1	A	495	LYS
1	A	516	GLU
1	A	522	SER
1	A	528	ILE
1	A	535	VAL
1	A	540	LEU
1	A	550	GLN
1	A	563	ILE
1	A	588	VAL
1	A	594	THR
1	A	609	VAL
1	A	610	TYR
1	A	624	PHE
1	A	644	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	652	THR
1	A	653	PHE
1	A	661	ASP
1	A	673	LEU
1	A	705	VAL
1	A	729	THR
1	A	758	LEU
1	A	786	LEU
1	A	790	LEU
1	A	799	ILE
1	A	802	ILE
1	A	814	THR
1	A	835	ARG
1	A	837	GLU
1	A	867	THR
1	A	886	GLN
1	A	887	LYS
1	A	888	VAL
1	A	895	LEU
1	A	901	LEU
1	A	909	ASN
1	A	914	LEU
1	A	916	THR
1	A	927	LEU
1	A	935	LYS
1	A	936	ARG
1	A	942	VAL
1	A	952	THR
1	A	953	ILE
1	A	968	VAL
1	A	980	LYS
1	A	983	LEU
1	A	984	VAL
1	A	1016	VAL
1	A	1029	ASN
1	A	1056	ILE
1	A	1058	SER
1	A	1067	SER
1	A	1076	THR
1	A	1108	VAL
1	A	1115	ASN
1	A	1123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1128	LYS
1	A	1132	THR
1	A	1140	ASN
1	A	1148	THR
1	A	1161	LEU
1	A	1173	ASN
1	A	1200	LYS
1	A	1218	VAL
1	A	1231	ASN
1	A	1246	ARG
1	A	1251	THR
1	A	1279	ARG
1	A	1280	TYR
1	A	1284	PHE
1	A	1291	ILE
1	A	1306	GLN
1	A	1338	VAL
1	A	1341	LEU
1	A	1345	ASP
1	A	1350	THR
1	A	1363	THR
1	A	1423	VAL
1	A	1443	VAL
1	A	1453	TYR
1	A	1464	LEU
1	A	1476	ARG
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1488	LEU
1	A	1494	THR
1	A	1495	VAL
1	A	1497	GLU
1	A	1500	ARG
1	A	1502	ASP
1	A	1511	THR
1	A	1513	ASN
1	A	1548	ARG
1	A	1551	THR
1	A	1556	GLU
1	A	1561	TYR
1	A	1562	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1566	THR
1	A	1581	LEU
1	A	1602	LYS
1	A	1618	LEU
1	A	1622	LYS
1	A	1623	GLU
1	A	1625	LEU
1	A	1626	GLN
1	A	1627	ILE
1	A	1634	ARG
1	A	1645	ILE
1	A	1654	CYS
1	A	1669	GLU
1	B	21	GLN
1	B	22	THR
1	B	23	TYR
1	B	42	GLN
1	B	61	ASP
1	B	73	LEU
1	B	100	SER
1	B	115	LYS
1	B	116	ARG
1	B	130	THR
1	B	140	SER
1	B	148	LEU
1	B	161	LEU
1	B	162	THR
1	B	165	ASP
1	B	179	HIS
1	B	195	ARG
1	B	208	ASP
1	B	211	THR
1	B	224	LEU
1	B	242	ASN
1	B	249	THR
1	B	280	LYS
1	B	292	LEU
1	B	320	ASN
1	B	332	SER
1	B	333	THR
1	B	383	VAL
1	B	393	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	394	THR
1	B	422	LEU
1	B	423	ASN
1	B	426	SER
1	B	431	LEU
1	B	436	LYS
1	B	457	TYR
1	B	492	TYR
1	B	495	LYS
1	B	522	SER
1	B	528	ILE
1	B	535	VAL
1	B	540	LEU
1	B	550	GLN
1	B	563	ILE
1	B	588	VAL
1	B	594	THR
1	B	609	VAL
1	B	610	TYR
1	B	624	PHE
1	B	644	ASN
1	B	652	THR
1	B	653	PHE
1	B	661	ASP
1	B	673	LEU
1	B	705	VAL
1	B	729	THR
1	B	758	LEU
1	B	786	LEU
1	B	790	LEU
1	B	799	ILE
1	B	802	ILE
1	B	814	THR
1	B	835	ARG
1	B	837	GLU
1	B	867	THR
1	B	886	GLN
1	B	887	LYS
1	B	888	VAL
1	B	894	HIS
1	B	901	LEU
1	B	909	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	914	LEU
1	B	916	THR
1	B	927	LEU
1	B	935	LYS
1	B	936	ARG
1	B	942	VAL
1	B	952	THR
1	B	953	ILE
1	B	968	VAL
1	B	980	LYS
1	B	983	LEU
1	B	984	VAL
1	B	1016	VAL
1	B	1029	ASN
1	B	1056	ILE
1	B	1058	SER
1	B	1067	SER
1	B	1076	THR
1	B	1108	VAL
1	B	1115	ASN
1	B	1123	GLN
1	B	1128	LYS
1	B	1132	THR
1	B	1140	ASN
1	B	1148	THR
1	B	1161	LEU
1	B	1162	VAL
1	B	1173	ASN
1	B	1200	LYS
1	B	1218	VAL
1	B	1231	ASN
1	B	1246	ARG
1	B	1251	THR
1	B	1279	ARG
1	B	1280	TYR
1	B	1284	PHE
1	B	1291	ILE
1	B	1306	GLN
1	B	1338	VAL
1	B	1341	LEU
1	B	1345	ASP
1	B	1350	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1363	THR
1	B	1423	VAL
1	B	1443	VAL
1	B	1464	LEU
1	B	1476	ARG
1	B	1480	PHE
1	B	1483	PHE
1	B	1487	PHE
1	B	1488	LEU
1	B	1494	THR
1	B	1495	VAL
1	B	1497	GLU
1	B	1500	ARG
1	B	1502	ASP
1	B	1511	THR
1	B	1513	ASN
1	B	1520	CYS
1	B	1527	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	42	GLN
1	A	72	HIS
1	A	80	GLN
1	A	81	ASN
1	A	88	GLN
1	A	242	ASN
1	A	289	ASN
1	A	298	GLN
1	A	320	ASN
1	A	381	GLN
1	A	393	GLN
1	A	423	ASN
1	A	446	ASN
1	A	483	ASN
1	A	647	HIS
1	A	656	ASN
1	A	692	HIS
1	A	737	GLN
1	A	787	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	909	ASN
1	A	1023	HIS
1	A	1029	ASN
1	A	1090	ASN
1	A	1096	ASN
1	A	1115	ASN
1	A	1123	GLN
1	A	1140	ASN
1	A	1173	ASN
1	A	1202	HIS
1	A	1221	ASN
1	A	1231	ASN
1	A	1234	HIS
1	A	1278	GLN
1	A	1306	GLN
1	A	1319	HIS
1	A	1366	HIS
1	A	1459	HIS
1	A	1463	GLN
1	A	1536	GLN
1	A	1572	ASN
1	A	1626	GLN
1	B	21	GLN
1	B	42	GLN
1	B	72	HIS
1	B	80	GLN
1	B	81	ASN
1	B	88	GLN
1	B	242	ASN
1	B	289	ASN
1	B	298	GLN
1	B	320	ASN
1	B	381	GLN
1	B	393	GLN
1	B	423	ASN
1	B	446	ASN
1	B	483	ASN
1	B	647	HIS
1	B	656	ASN
1	B	692	HIS
1	B	737	GLN
1	B	787	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	894	HIS
1	B	909	ASN
1	B	1023	HIS
1	B	1029	ASN
1	B	1090	ASN
1	B	1096	ASN
1	B	1115	ASN
1	B	1123	GLN
1	B	1140	ASN
1	B	1173	ASN
1	B	1202	HIS
1	B	1221	ASN
1	B	1231	ASN
1	B	1234	HIS
1	B	1278	GLN
1	B	1306	GLN
1	B	1319	HIS
1	B	1366	HIS
1	B	1459	HIS
1	B	1463	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	2001	1,2	14,14,15	0.49	0	15,19,21	0.80	0
2	NAG	A	2002	2	14,14,15	0.46	0	15,19,21	0.89	1 (6%)
2	NAG	B	2001	1,2	14,14,15	0.49	0	15,19,21	0.81	0
2	NAG	B	2002	2	14,14,15	0.46	0	15,19,21	0.92	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2002	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2002	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2002	NAG	C1-O5-C5	2.26	115.12	112.25
2	A	2002	NAG	C1-O5-C5	2.34	115.22	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2002	NAG	O7-C7-N2-C2
2	B	2002	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	NAG	2	0
2	B	2001	NAG	2	0

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	2003	1	14,14,15	0.56	0	15,19,21	0.80	0
3	NAG	B	2003	1	14,14,15	0.58	0	15,19,21	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2003	1	-	0/6/23/26	0/1/1/1

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1625/1676 (96%)	0.20	54 (3%)	50 26	73, 136, 224, 290	0
1	B	1481/1676 (88%)	0.13	27 (1%)	71 50	75, 131, 205, 267	0
All	All	3106/3352 (92%)	0.16	81 (2%)	59 35	73, 133, 215, 290	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	871	PRO	10.3
1	B	871	PRO	6.3
1	A	1534	GLN	5.0
1	A	1635	TYR	4.3
1	A	1617	TYR	4.3
1	B	1518	LYS	4.2
1	A	1645	ILE	4.1
1	A	1630	ASN	4.1
1	B	81	ASN	3.8
1	B	870	SER	3.7
1	A	1619	ILE	3.7
1	B	104	LEU	3.6
1	B	52	ALA	3.6
1	B	107	VAL	3.5
1	A	1605	THR	3.4
1	B	96	GLN	3.4
1	B	309	GLU	3.4
1	B	1519	VAL	3.3
1	A	1596	SER	3.3
1	A	1543	ILE	3.3
1	A	720	LEU	3.3
1	A	1583	ASP	3.3
1	A	616	ALA	3.2
1	A	1636	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	252	ALA	3.2
1	A	1581	LEU	3.1
1	B	720	LEU	3.1
1	A	1613	LYS	3.1
1	A	330	ILE	3.1
1	B	857	VAL	3.1
1	B	552	ALA	3.1
1	A	1634	ARG	3.0
1	A	749	LEU	2.9
1	A	159	THR	2.8
1	A	1593	GLU	2.8
1	A	85	LEU	2.8
1	A	1646	GLU	2.8
1	A	104	LEU	2.8
1	A	861	ALA	2.8
1	A	545	ILE	2.8
1	A	81	ASN	2.7
1	A	1601	ILE	2.7
1	B	809	ILE	2.7
1	A	1584	ILE	2.6
1	A	817	ALA	2.6
1	A	1523	ALA	2.6
1	B	1236	ASP	2.6
1	B	482	LEU	2.6
1	A	1611	LEU	2.5
1	A	1585	TYR	2.5
1	B	839	ILE	2.5
1	A	1284	PHE	2.4
1	A	870	SER	2.4
1	A	1542	THR	2.4
1	A	94	GLY	2.3
1	B	106	VAL	2.3
1	A	87	ILE	2.3
1	B	1480	PHE	2.2
1	B	182	ILE	2.2
1	A	1638	PRO	2.2
1	B	252	ALA	2.2
1	B	616	ALA	2.2
1	B	329	VAL	2.2
1	A	1647	TYR	2.2
1	A	1579	ALA	2.1
1	A	1561	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	571	LEU	2.1
1	A	997	ILE	2.1
1	A	52	ALA	2.1
1	A	107	VAL	2.1
1	A	95	GLY	2.1
1	B	330	ILE	2.1
1	B	683	ILE	2.1
1	A	1572	ASN	2.1
1	A	937	GLU	2.1
1	A	761	SER	2.1
1	B	159	THR	2.1
1	B	1237	SER	2.0
1	A	141	VAL	2.0
1	A	1573	VAL	2.0
1	A	1600	PHE	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](#)

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
2	NAG	A	2001	14/15	0.81	0.33	-	257,259,270,271	0
2	NAG	B	2001	14/15	0.89	0.38	-	263,269,274,275	0
2	NAG	B	2002	14/15	0.58	0.51	-	251,259,262,262	0
2	NAG	A	2002	14/15	0.79	0.24	-	249,258,261,262	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CD	B	2006	1/1	0.76	0.19	-	183,183,183,183	0
3	NAG	B	2003	14/15	0.81	0.57	-	246,252,259,262	0
4	CD	A	2007	1/1	0.94	0.21	-	184,184,184,184	0
4	CD	B	2007	1/1	0.78	0.13	-	264,264,264,264	0
4	CD	A	2006	1/1	0.68	0.18	-	189,189,189,189	0
4	CD	B	2004	1/1	0.99	0.18	-	239,239,239,239	0
3	NAG	A	2003	14/15	0.85	0.25	-	215,223,233,237	0
4	CD	B	2005	1/1	0.75	0.20	-	181,181,181,181	0
4	CD	A	2005	1/1	0.97	0.16	-	243,243,243,243	0
4	CD	A	2008	1/1	0.73	0.11	-	282,282,282,282	0
4	CD	A	2004	1/1	0.95	0.35	-	123,123,123,123	1

6.5 Other polymers [i](#)

There are no such residues in this entry.