Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 30, 2017 – 11:01 AM EST

PDB ID	:	5GO9
EMDB ID:	:	EMD-9528
Title	:	Cryo-EM structure of RyR2 in closed state
Authors	:	Peng, W.; Wu, J.P.; Yan, N.
Deposited on	:	2016-07-26
Resolution	:	4.40 Å(reported)

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

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

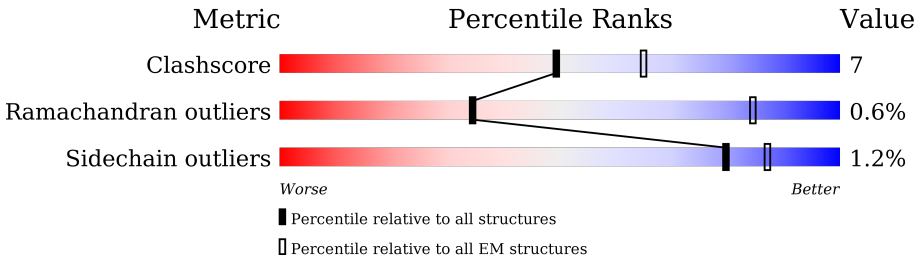
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	4968	54% 14% • 31%
1	B	4968	54% 14% • 31%
1	C	4968	54% 14% • 31%
1	D	4968	54% 14% • 31%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 105068 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3423	Total 26266	C 16740	N 4498	O 4874	S 154	0	0
1	B	3423	Total 26266	C 16740	N 4498	O 4874	S 154	0	0
1	C	3423	Total 26266	C 16740	N 4498	O 4874	S 154	0	0
1	D	3423	Total 26266	C 16740	N 4498	O 4874	S 154	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

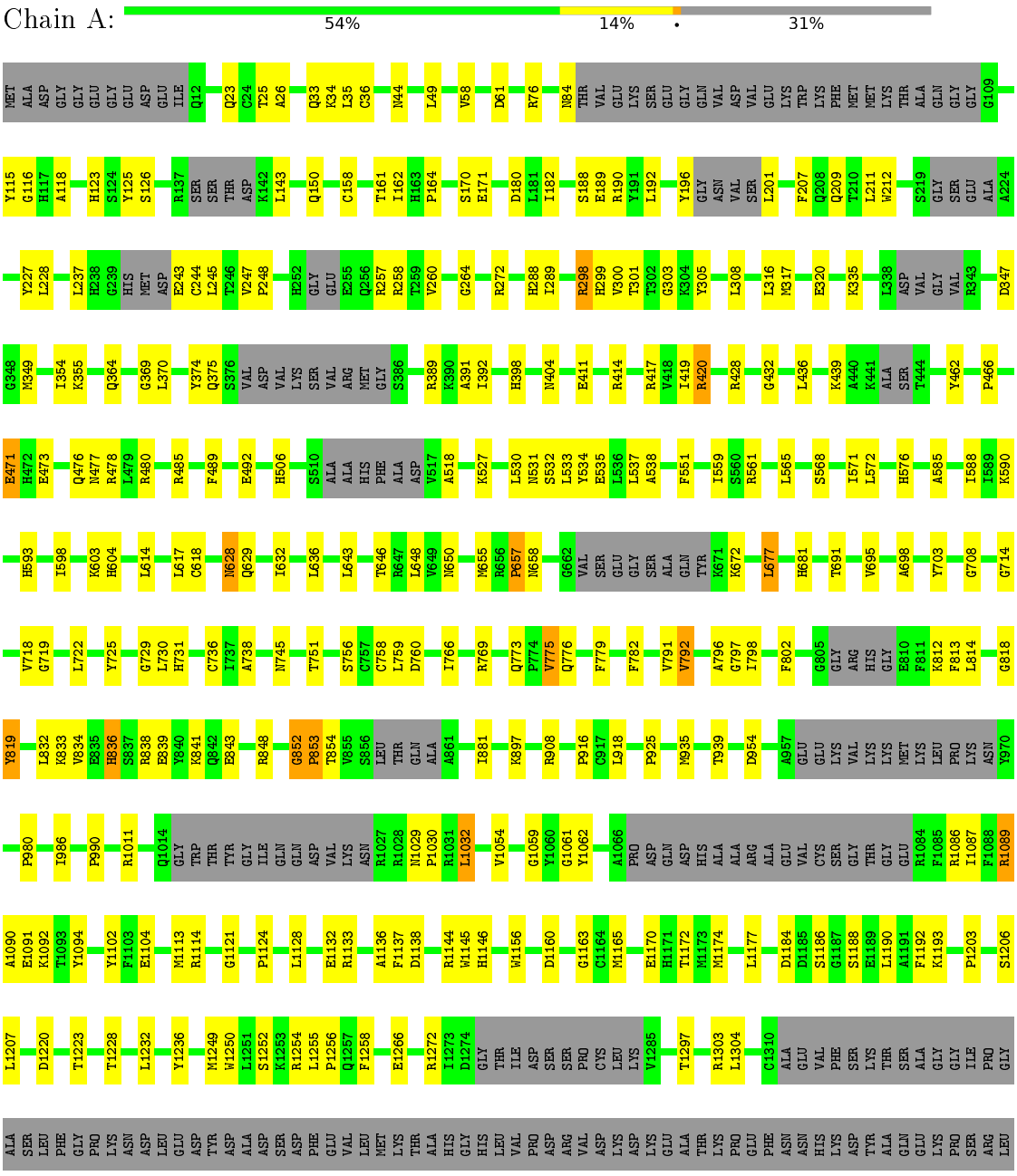
Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total 1	Zn 1	0
2	A	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0

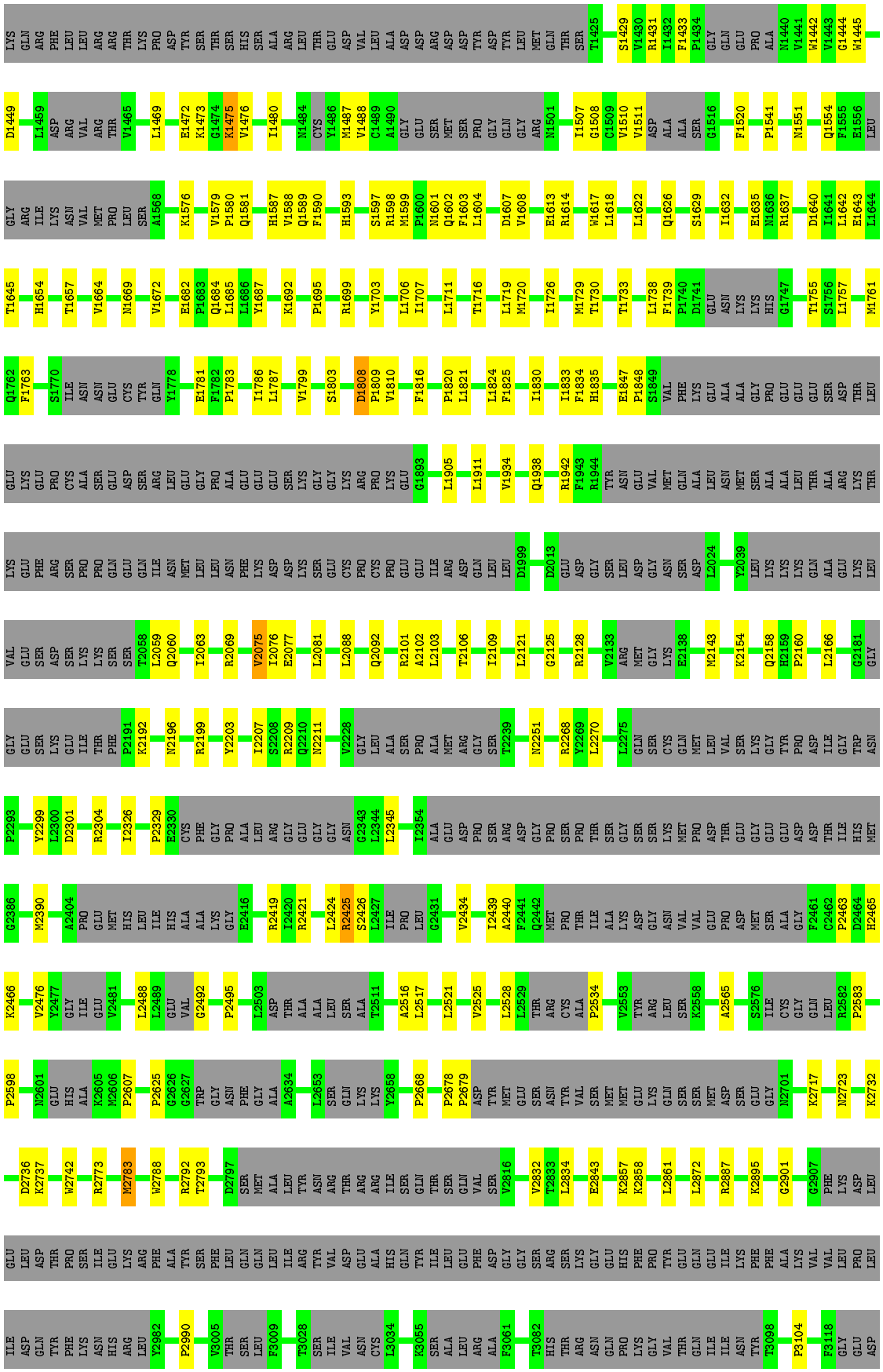
3 Residue-property plots (i)

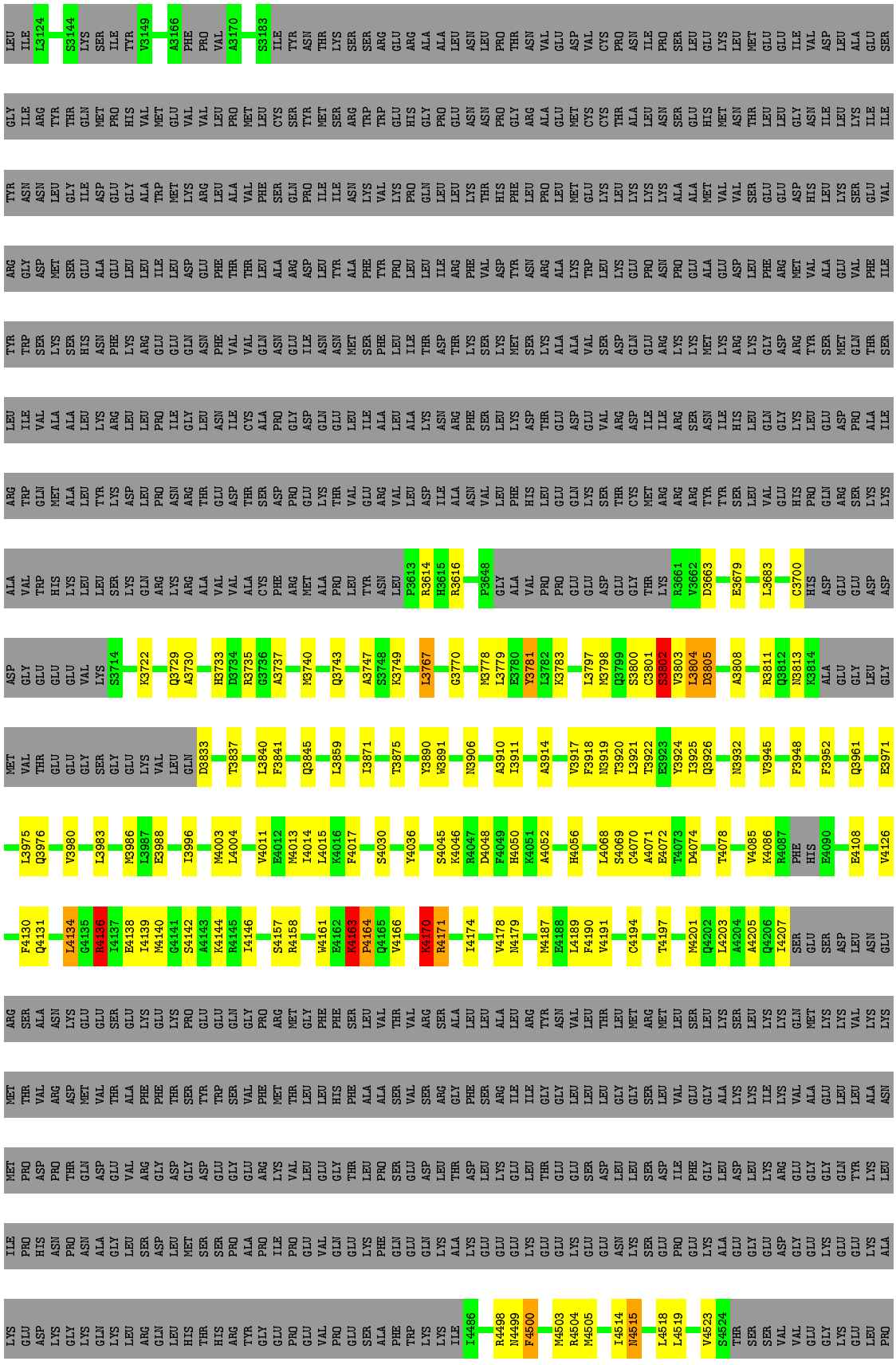
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

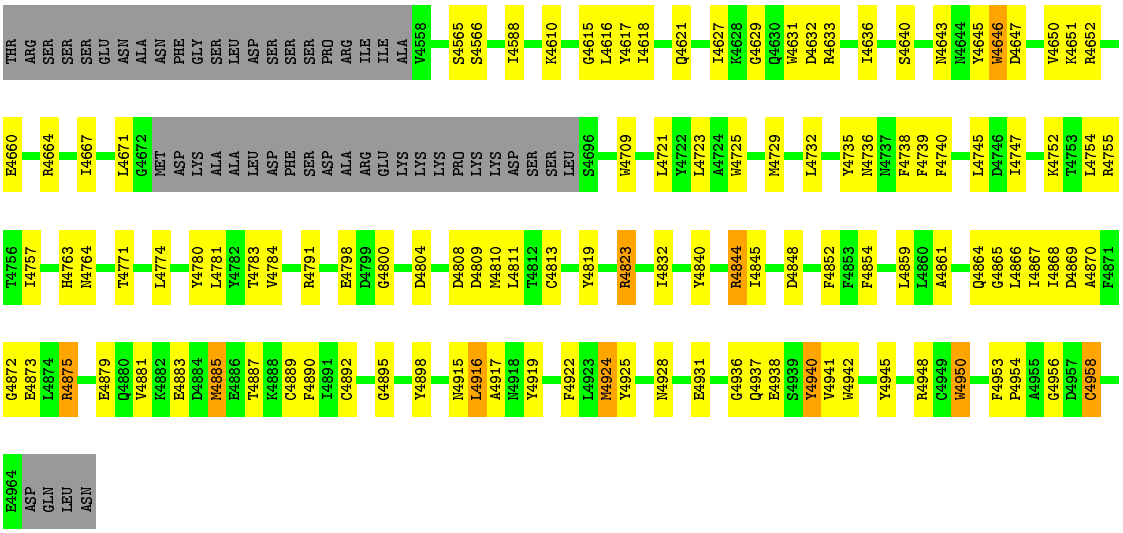
- Molecule 1: RyR2

Chain A:



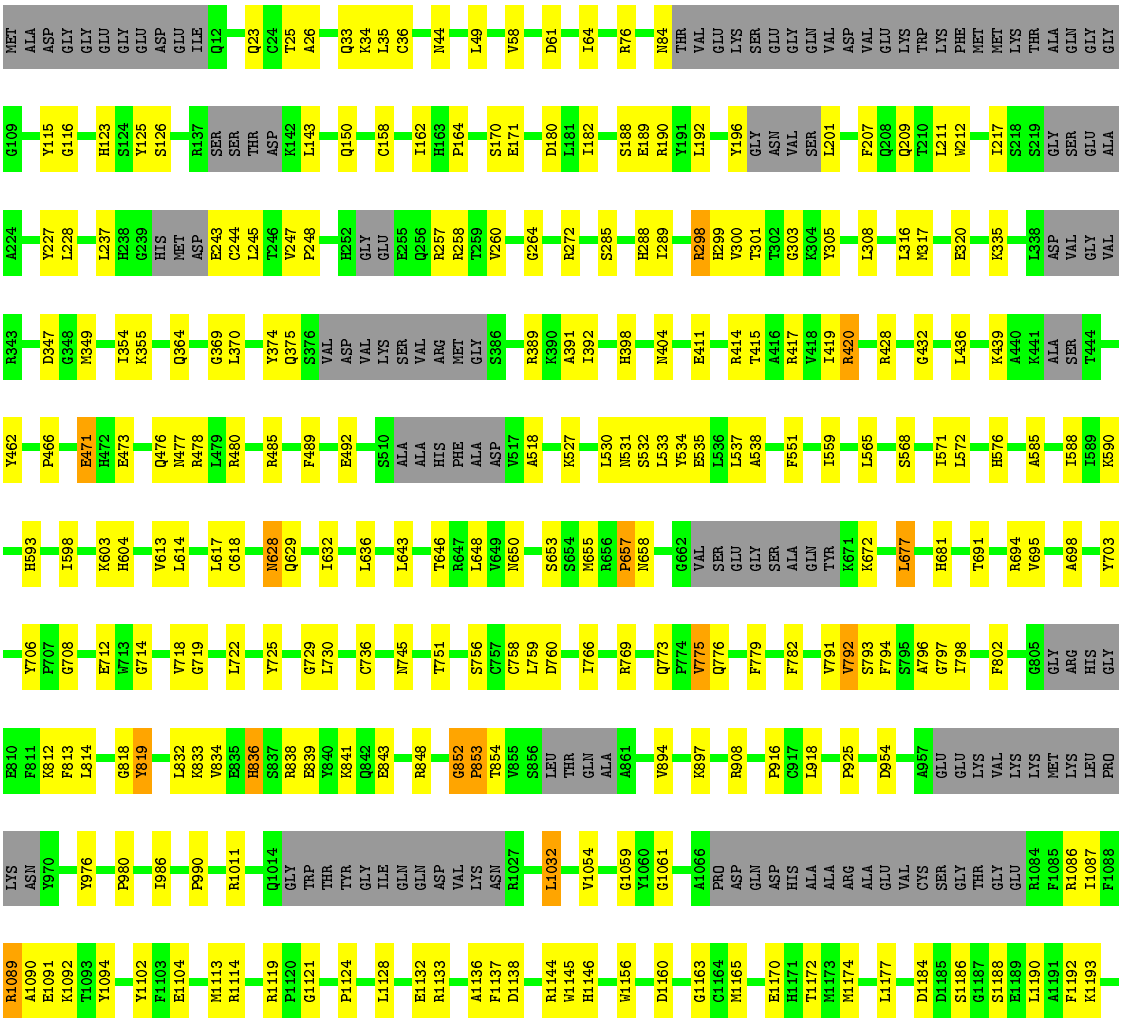


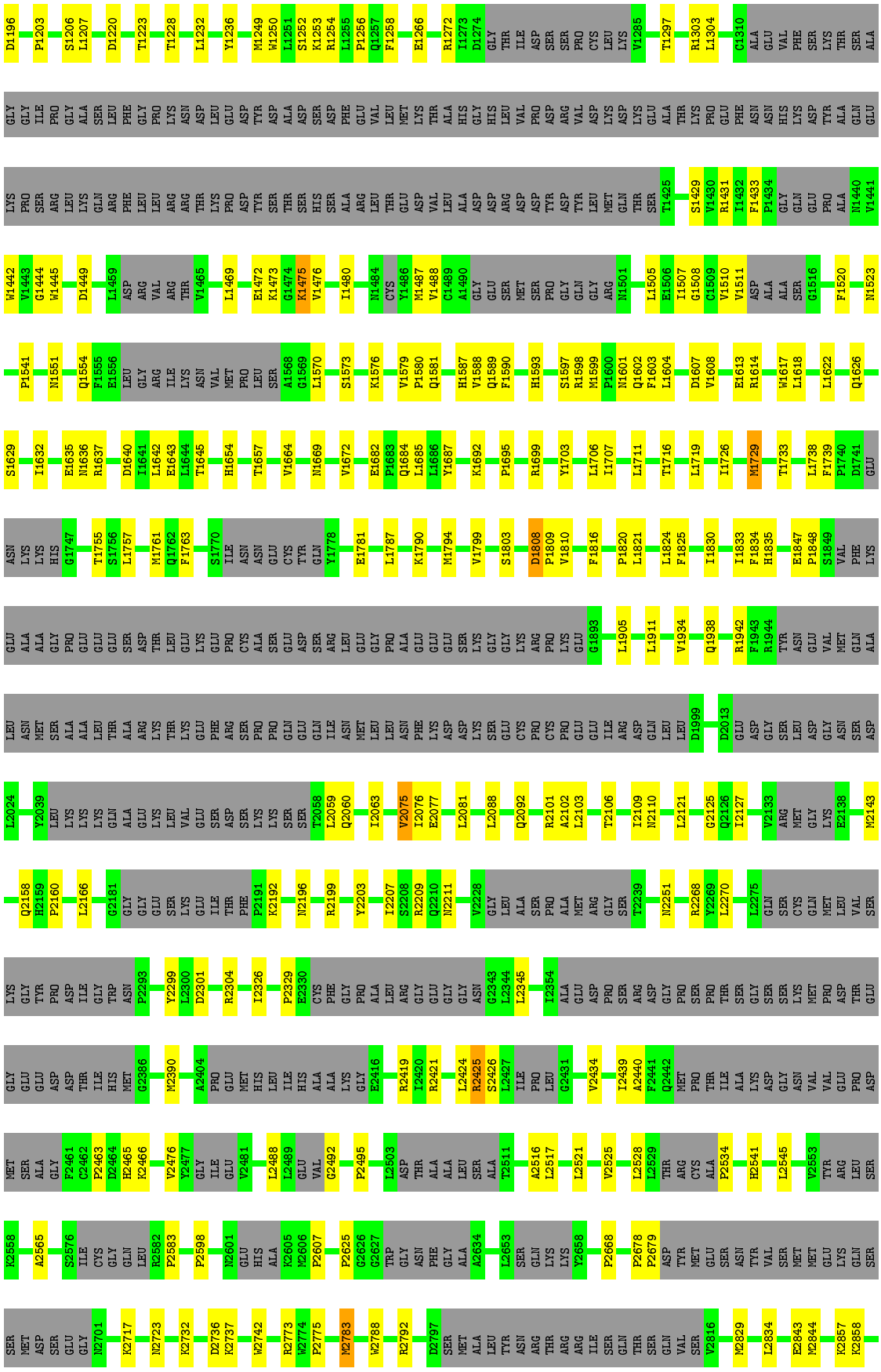


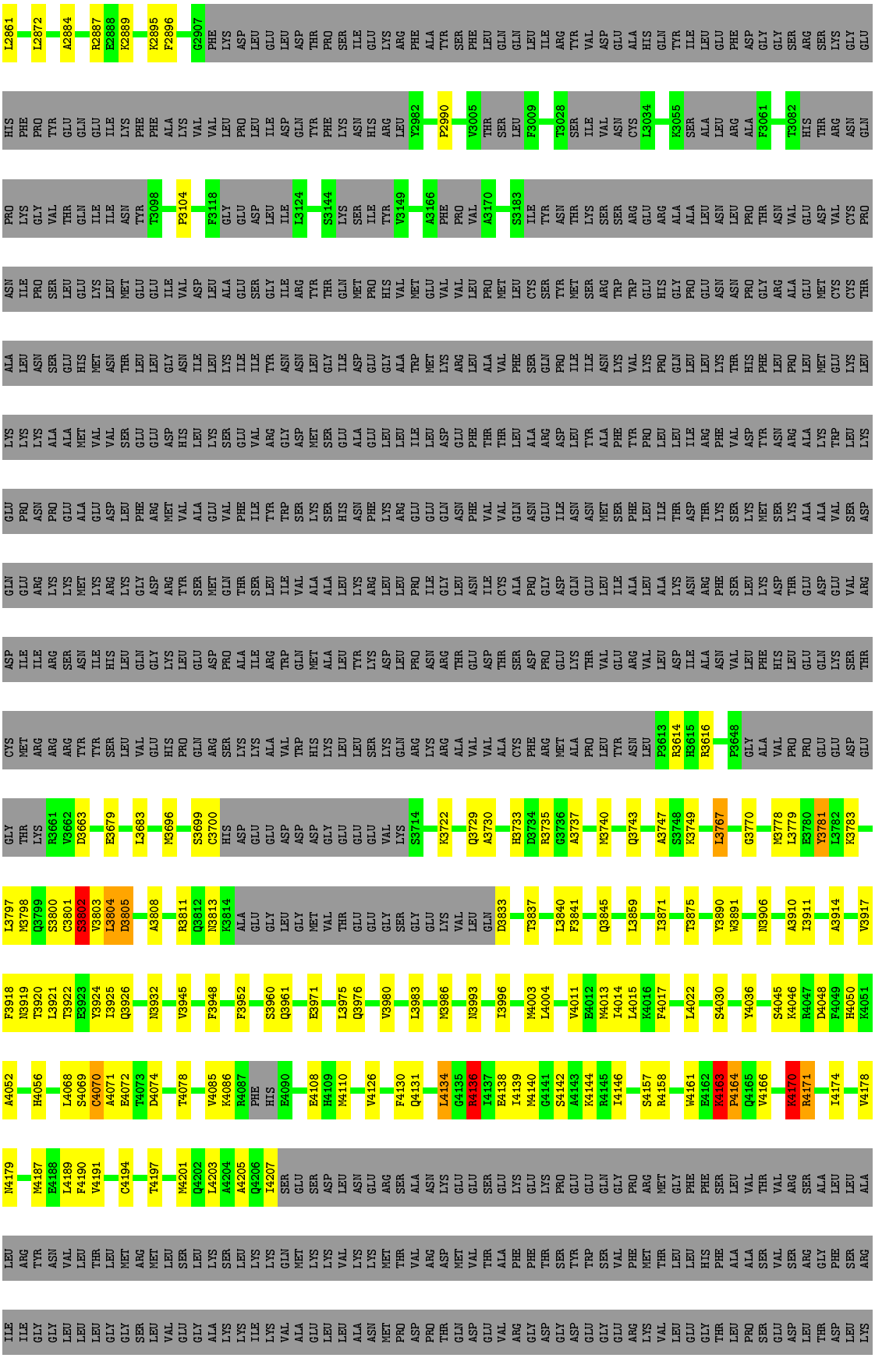


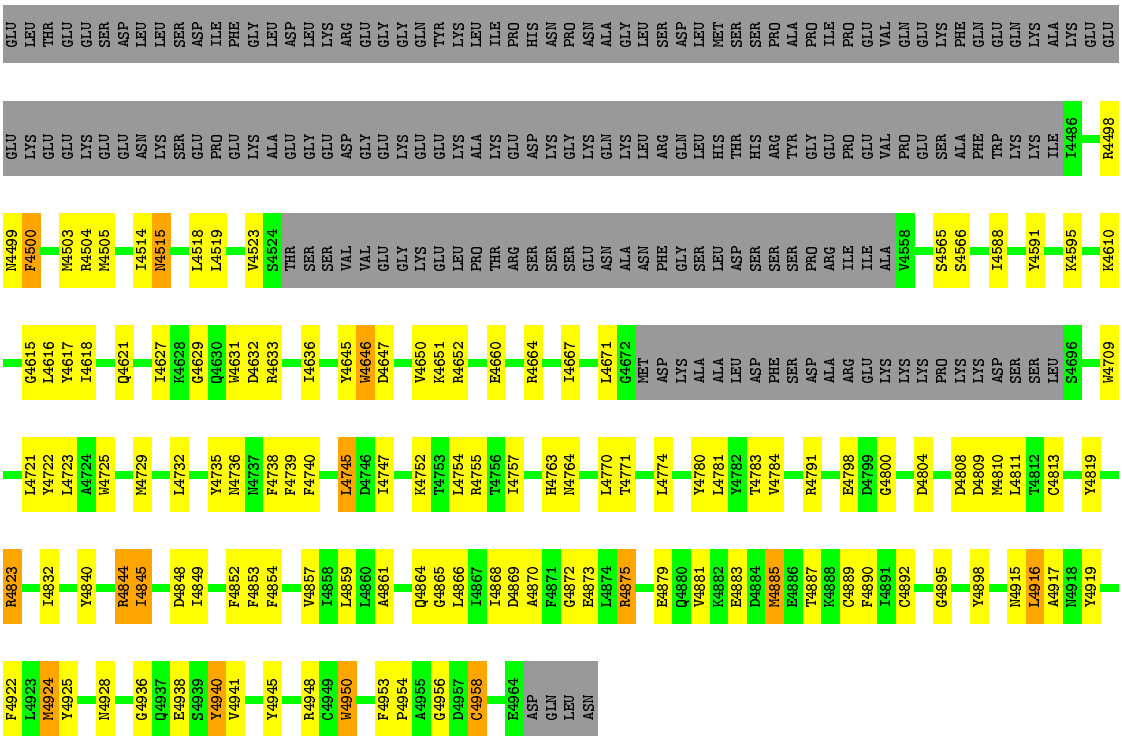
- Molecule 1: RyR2

Chain B:



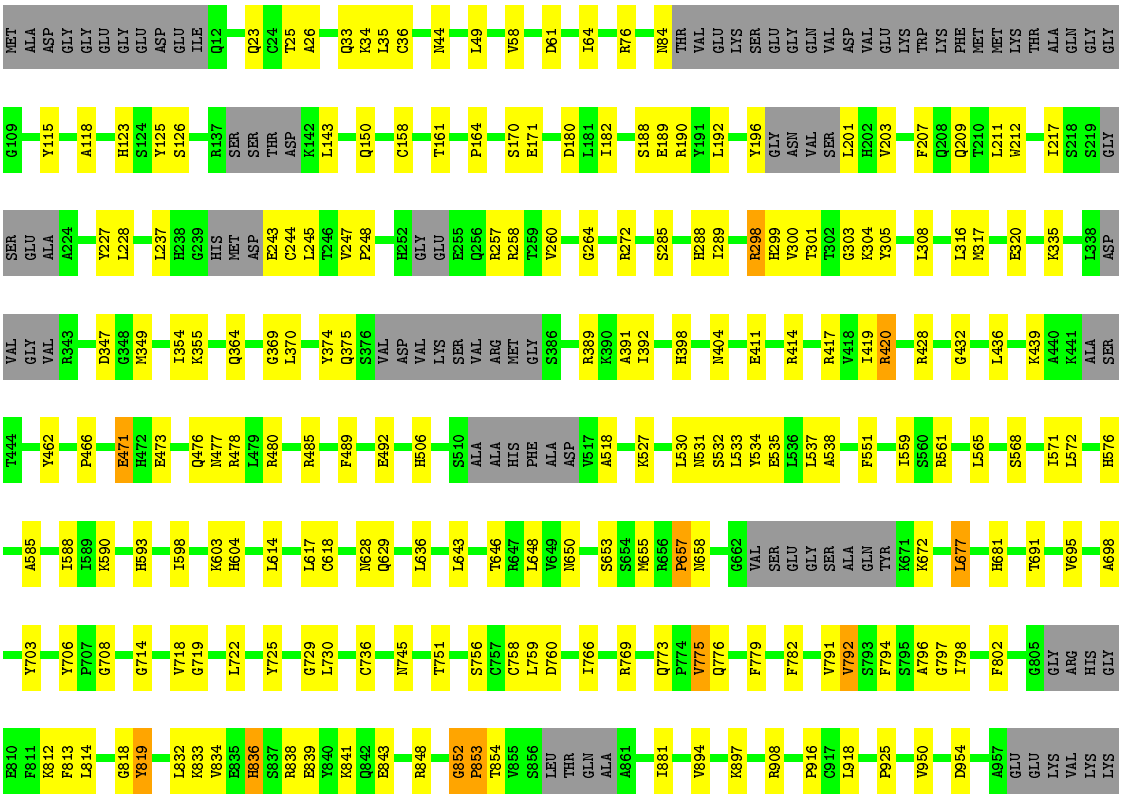

D1196 P1203 S1206 L1207 D1220 T1223 T1228 L1232 Y1236 M1249 W1250 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 F1258 E1266 R1272 I1273 D1274 V1285 T1297 R1303 L1304 C1310
GLY GLY ILE PRO GLY ALA SER LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO LYS ASN ASN HIS LYS ASP TYR ALA GLN GLU
LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP TYR LEU MET GLN THR SER T1425 S1429 V1430 R1431 I1432 F1433 P1434 GLY GLN GLU PRO ALA N1440 V1441
W1442 V1443 G1444 W1445 D1449 L1459 ASP ARG VAL ARG THR V1465 L1469 E1472 K1473 G1474 K1475 V1476 I1480 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO GLY GLN GLY ARG N1501 L1505 E1506 I1507 G1508 C1509 V1510 V1511 ASP ALA ALA SER G1516 F1520 N1523
P1541 N1551 Q1554 F1555 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 L1570 S1573 K1576 V1579 P1580 Q1581 H1587 V1588 Q1589 F1590 H1593 S1597 R1598 M1599 P1600 N1601 Q1602 F1603 L1604 D1607 V1608 E1613 R1614 W1617 L1618 L1622 Q1626
S1629 I1632 E1635 N1636 R1637 D1640 I1641 L1642 E1643 L1644 T1645 H1654 T1657 V1664 N1669 V1672 E1682 P1683 Q1684 L1685 L1686 Y1687 K1692 P1695 R1699 Y1703 L1706 I1707 L1711 T1716 L1719 I1726 M1729 T1733 L1738 F1739 P1740 D1741 GLU
ASN LYS LYS HIS G1747 T1755 S1756 L1757 M1761 Q1762 F1763 S1770 ILE ASN ASN GLU CYS TYR GLN Y1778 E1781 L1787 K1790 M1794 V1799 S1803 D1808 P1809 V1810 F1816 P1820 L1821 L1824 F1825 I1830 I1833 F1834 H1835 E1847 P1848 S1849 VAL PHE LYS
GLU ALA ALA GLY PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU ASP SER ARG LEU GLU GLY PRO ALA GLU GLU GLU SER LYS GLY GLY LYS ARG PRO LYS GLU G1893 L1905 L1911 V1934 Q1938 R1942 F1943 R1944 TYR ASN GLU VAL MET GLN ALA
LEU ASN MET SER ALA ALA LEU THR ALA ARG LYS THR LYS GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO CYS PRO GLU GLU ILE ARG ASP GLN LEU LEU D1999 D2013 GLU ASP GLY SER LEU ASP GLY ASN SER ASP
L2024 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 L2059 Q2060 I2063 V2075 I2076 E2077 L2081 L2088 Q2092 R2101 A2102 L2103 T2106 I2109 N2110 L2121 G2125 Q2126 I2127 V2133 ARG MET GLY LYS E2138 M2143
Q2158 H2159 P2160 L2166 G2181 GLY GLY GLU SER LYS GLU ILE THR PHE P2191 K2192 N2196 R2199 Y2203 I2207 S2208 R2209 Q2210 N2211 V2228 GLY LEU ALA SER PRO ALA MET ARG GLY SER T2239 N2251 R2268 Y2269 L2270 L2275 GLN SER CYS GLN MET LEU VAL SER
LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 Y2299 L2300 D2301 R2304 I2326 P2329 E2330 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 L2344 L2345 I2354 ALA GLU ASP PRO SER ARG ASP GLY PRO SER PRO THR SER GLY SER SER LYS MET PRO ASP THR GLU
GLY GLU GLU ASP ASP THR ILE HIS MET G2386 M2390 A2404 PRO GLU MET HIS LEU ILE HIS ALA ALA LYS GLY E2416 R2419 I2420 R2421 L2424 R2425 S2426 L2427 ILE PRO LEU G2431 V2434 I2439 A2440 F2441 Q2442 MET PRO THR ILE ALA LYS ASP GLY VAL VAL GLU PRO ASP
MET SER ALA GLY F2461 C2462 P2463 D2464 H2465 K2466 V2476 Y2477 GLY ILE GLU V2481 L2488 L2489 GLU VAL G2492 P2495 L2503 ASP THR ALA ALA LEU SER ALA T2511 A2516 L2517 L2521 V2525 L2528 L2529 THR ARG CYS ALA P2534 H2541 L2545 V2553 TYR ARG LEU SER
K2558 A2565 S2576 ILE CYS GLY GLN LEU R2582 P2583 P2598 N2601 GLU HIS ALA K2605 M2606 P2607 P2625 G2626 G2627 TRP GLY ASN PHE GLY ALA A2634 L2653 SER GLN LYS LYS Y2658 P2668 P2678 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER
SER MET ASP SER GLU GLY N2701 K2717 N2723 K2732 D2736 K2737 W2742 R2773 W2774 P2775 M2783 W2788 R2792 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER V2816 M2829 L2834 E2843 M2844 K2857 K2858

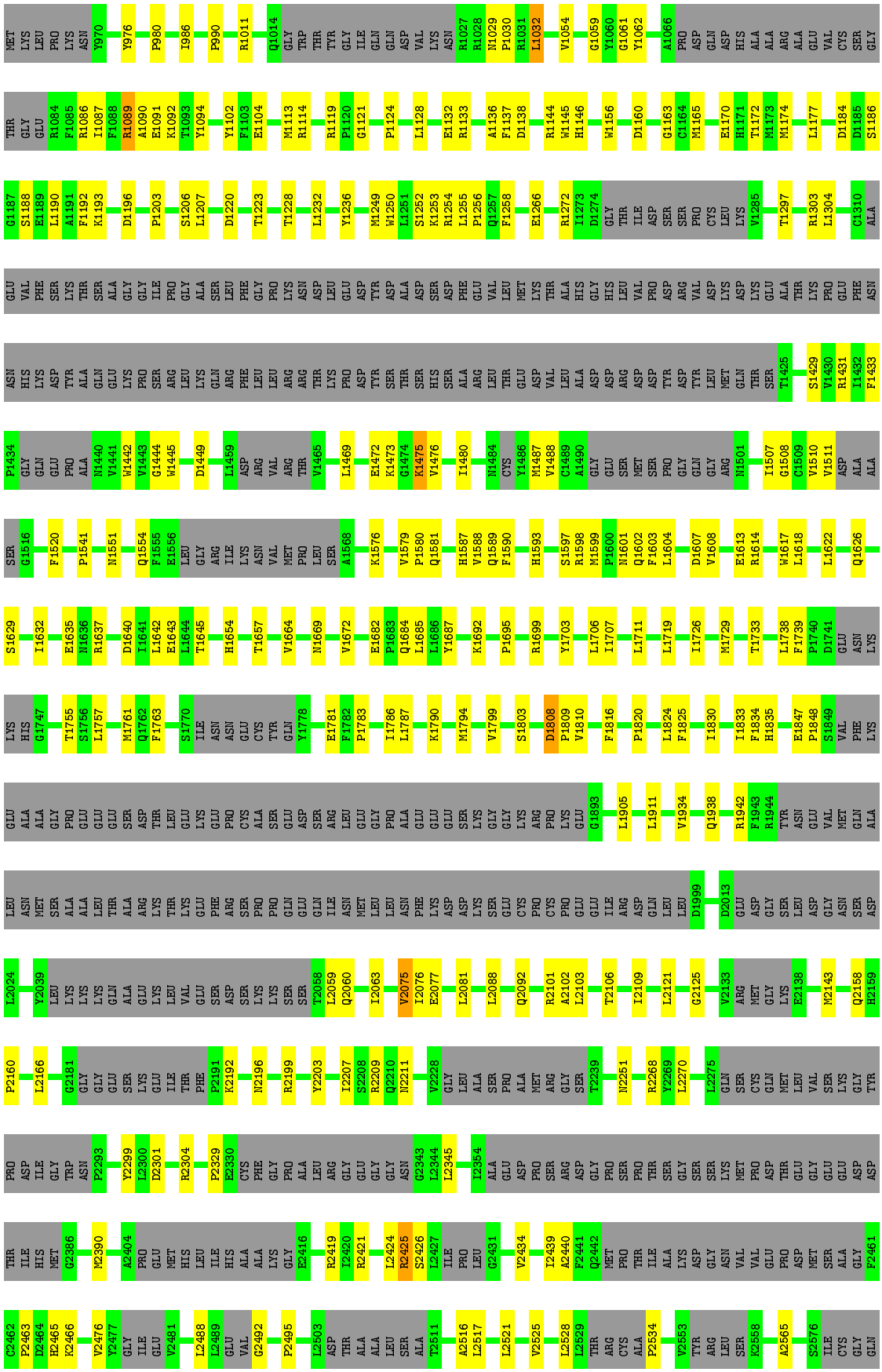


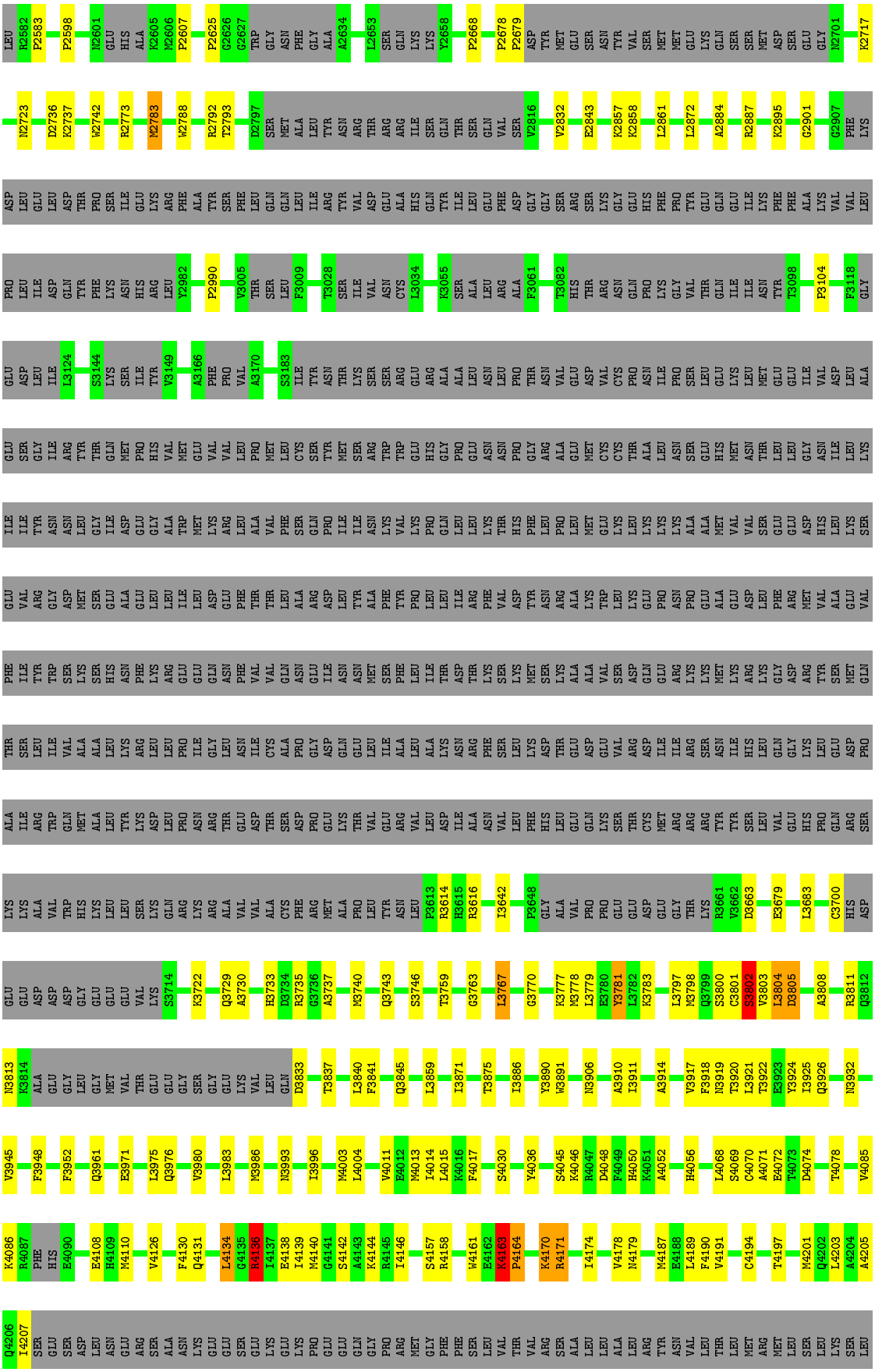


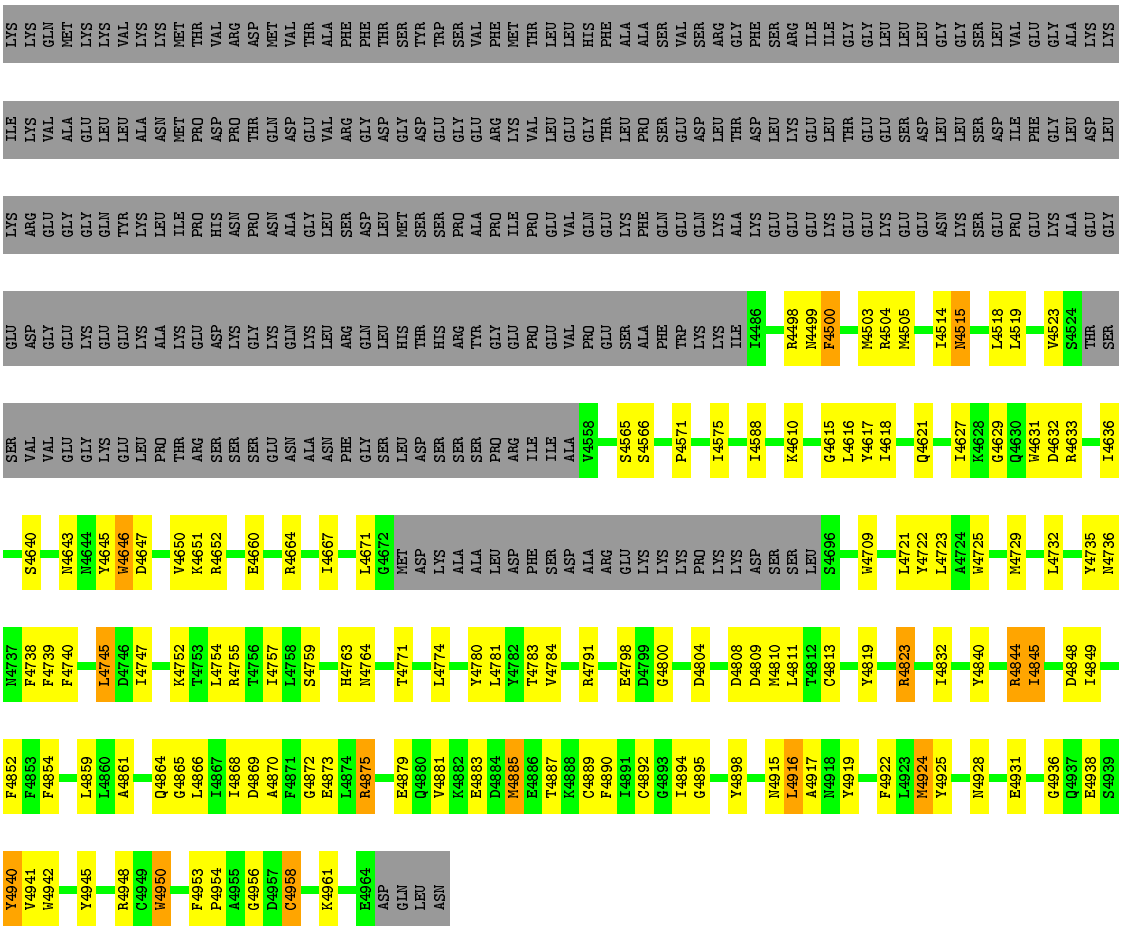
- Molecule 1: RyR2

Chain C:



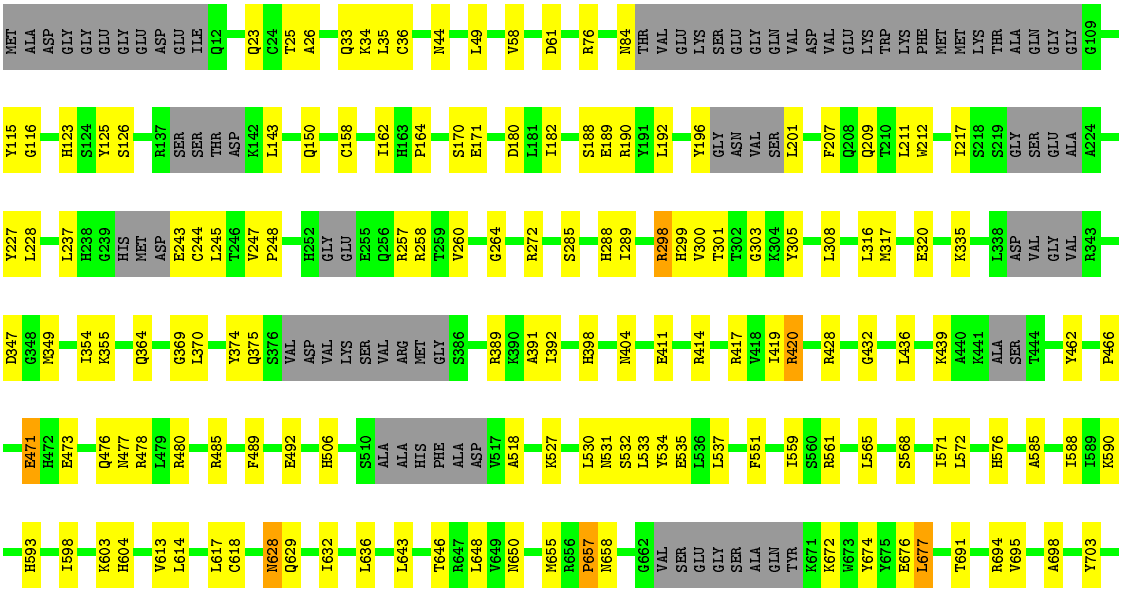


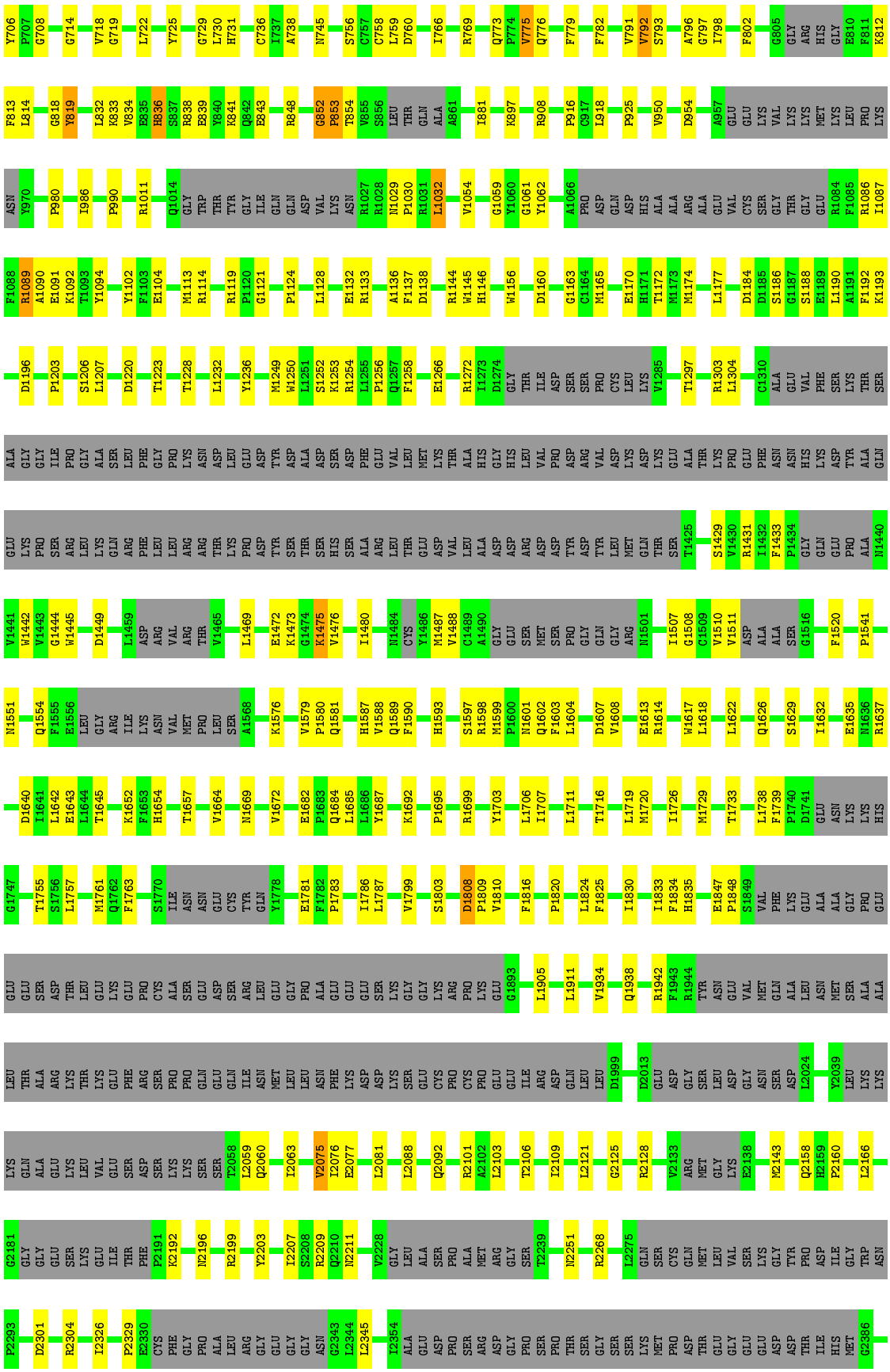


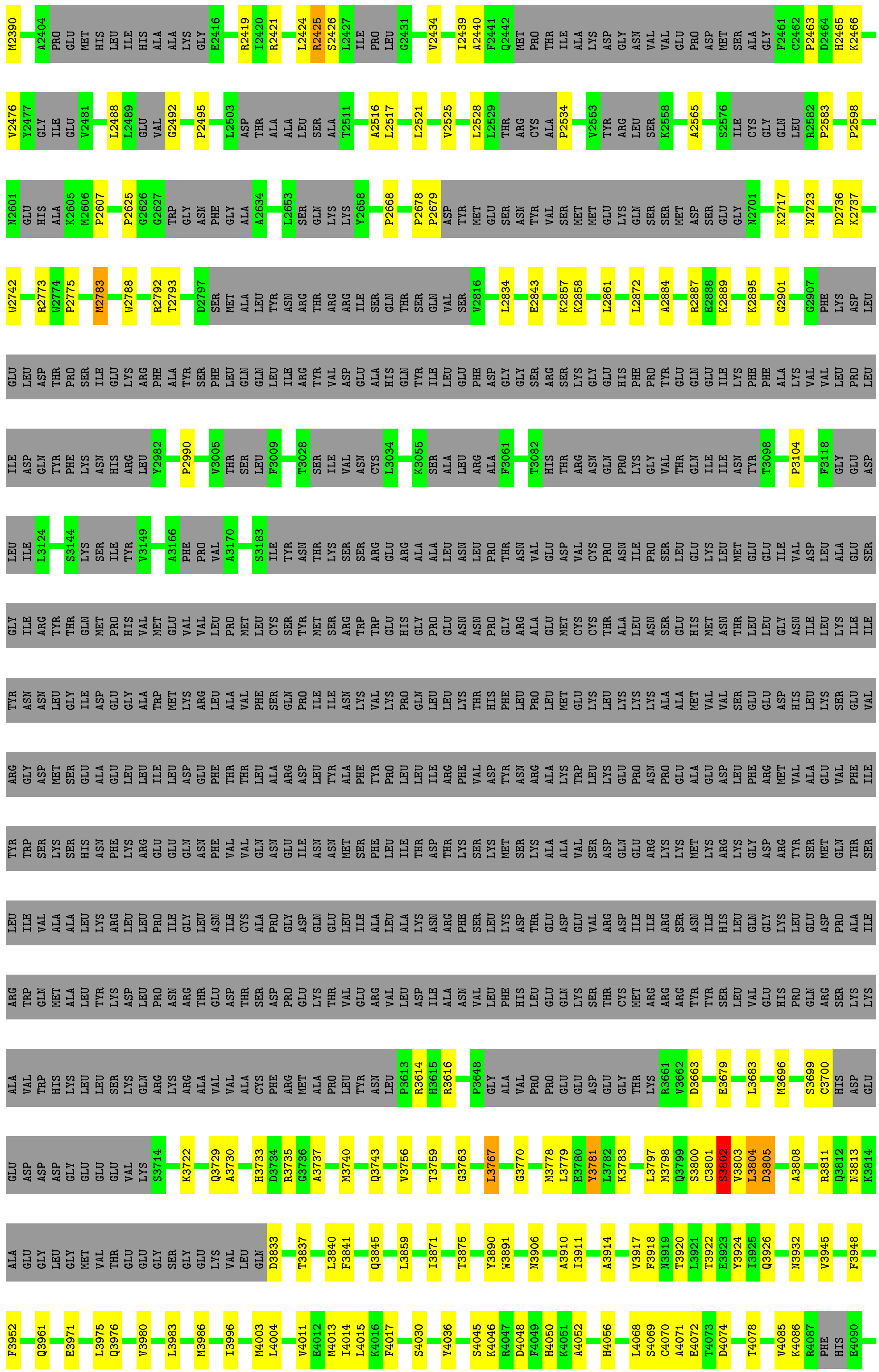


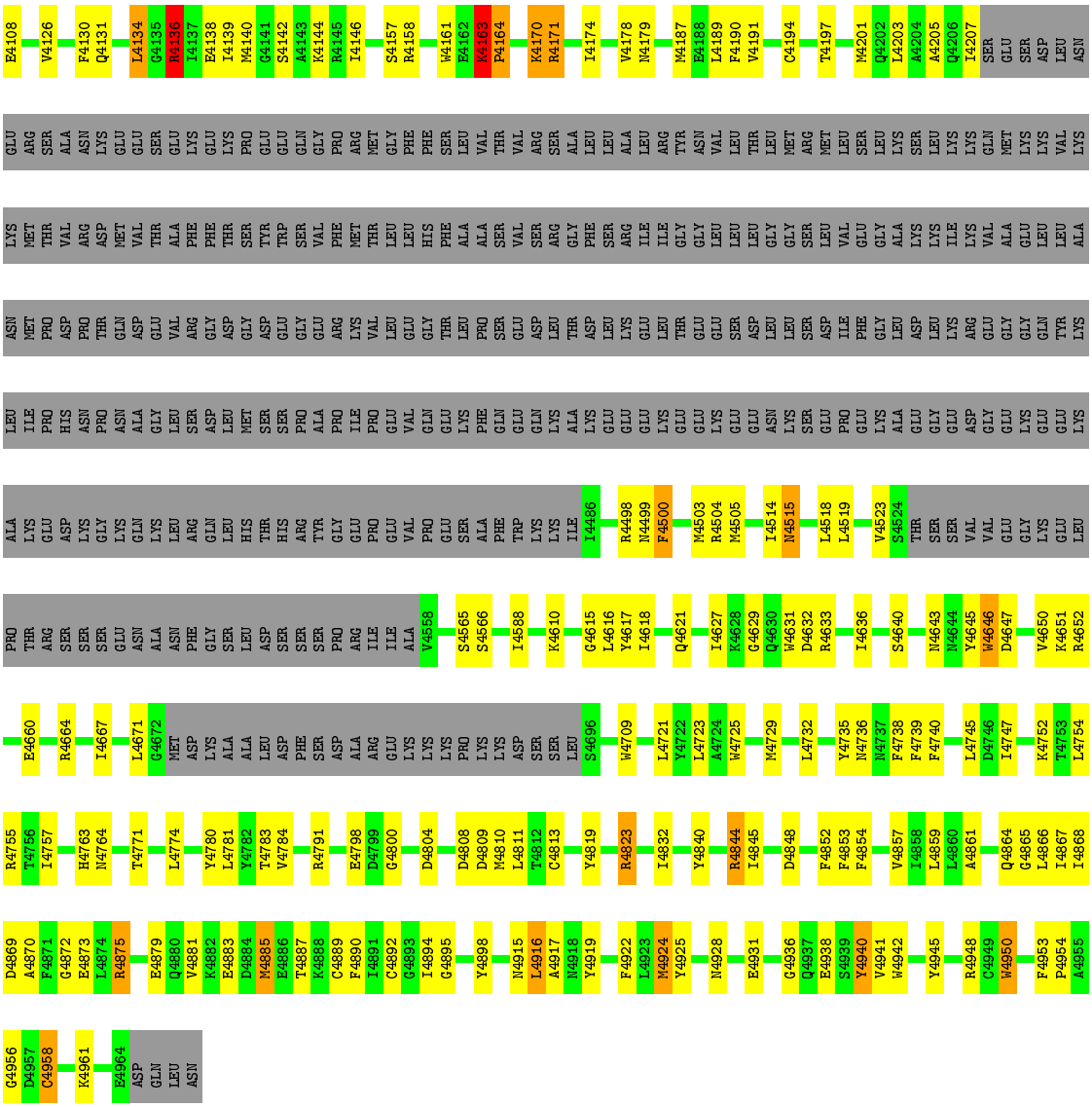
- Molecule 1: RyR2

Chain D:








E4108 V4126 F4130 Q4131 L4134 G4135 R4136 I4137 E4138 I4139 M4140 G4141 S4142 A4143 K4144 R4145 I4146 S4157 R4458 W4161 E4162 K4163 P4164 K4170 R4471 I4174 V4178 N4179 M4187 E4188 L4189 F4190 V4191 C4194 T4197 M4201 Q4202 L4203 A4204 A4205 Q4206 I4207
GLU ARG SER ALA ASN LYS GLU GLU SER GLU LYS GLU LYS PRO GLU GLU GLN GLY PRO ARG MET GLY PHE PHE SER LEU VAL THR VAL ARG SER ALA LEU LEU ALA LEU ARG TYR ASN VAL LEU THR LEU MET ARG MET LEU SER LEU LYS LYS GLN MET LYS LYS VAL LYS
LYS MET THR VAL ARG ASP MET VAL THR ALA PHE PHE THR SER TYR TRP SER VAL PHE MET THR LEU LEU HIS PHE ALA ALA SER VAL SER ARG GLY PHE SER ARG ILE ILE LYS GLY GLY LEU LEU LEU GLY SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA
ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLY ASP GLU GLY GLU ARG LYS VAL LEU GLU GLY THR LEU PRO SER GLU ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS
LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET SER SER PRO ALA PRO ILE PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU LYS GLU GLU ASN LYS SER GLU PRO GLU LYS ALA GLU GLY GLU LYS GLU GLU
ALA LYS GLU ASP LYS GLY LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA PHE TRP LYS LYS ILE I4486 R4498 N4499 F4500 M4503 R4504 M4505 I4514 N4515 L4518 L4519 V4523 S4524 THR SER SER VAL VAL GLU GLY LYS GLU LEU
PRO THR ARG SER SER SER GLU ASN ALA ASN PHE GLY SER LEU ASP SER SER SER PRO ARG ILE ILE ALA V4558 S4565 S4566 I4588 K4610 G4615 L4616 Y4617 I4618 Q4621 I4627 K4628 G4629 Q4630 W4631 D4632 R4633 I4636 S4640 N4643 N4644 Y4645 W4646 D4647 V4650 K4651 R4652
E4660 R4664 I4667 L4671 G4672 MET ASP LYS ALA ALA LEU ASP PHE SER ASP ALA ARG GLU LYS LYS LYS PRO LYS LYS ASP SER SER LEU S4696 W4709 L4721 Y4722 L4723 A4724 W4725 M4729 L4732 Y4735 N4736 N4737 F4738 F4739 F4740 L4745 D4746 I4747 K4752 T4753 L4754
R4755 T4756 I4757 H4763 N4764 T4771 L4774 Y4780 L4781 Y4782 T4783 V4784 R4791 E4798 D4799 G4800 D4804 D4808 D4809 M4810 L4811 T4812 C4813 Y4819 R4823 I4832 Y4840 R4844 I4845 D4848 F4852 F4853 F4854 V4857 I4858 L4859 L4860 A4861 Q4864 G4865 L4866 I4867 I4868
D4869 A4870 F4871 G4872 E4873 L4874 R4875 E4879 Q4880 V4881 K4882 E4883 D4884 M4885 E4886 T4887 K4888 C4889 F4890 I4891 C4892 G4893 I4894 G4895 Y4898 N4915 L4916 A4917 N4918 Y4919 F4922 L4923 M4924 Y4925 N4928 E4931 G4936 Q4937 E4938 S4939 Y4940 V4941 W4942 Y4945 R4948 C4949 W4950 F4953 P4954 A4955
G4956 D4957 C4958 K4961 E4964 ASP GLN LEU ASN

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	48454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	B	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	C	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	D	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
All	All	0.98	116/107004 (0.1%)	0.94	312/144596 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	30
1	B	0	30
1	C	0	30
1	D	0	30
All	All	0	120

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	B	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	C	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	D	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	A	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	B	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	C	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	D	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	A	4190	PHE	CG-CD1	-8.95	1.25	1.38
1	B	4190	PHE	CG-CD1	-8.95	1.25	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4190	PHE	CG-CD1	-8.95	1.25	1.38
1	D	4190	PHE	CG-CD1	-8.95	1.25	1.38
1	A	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	B	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	C	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	D	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	A	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	B	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	C	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	D	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	A	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	B	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	C	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	D	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	A	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	B	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	C	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	D	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	A	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	B	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	C	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	D	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	A	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	B	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	C	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	D	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	A	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	B	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	C	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	D	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	A	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	B	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	C	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	D	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	A	4895	GLY	C-O	-6.48	1.13	1.23
1	B	4895	GLY	C-O	-6.48	1.13	1.23
1	C	4895	GLY	C-O	-6.48	1.13	1.23
1	D	4895	GLY	C-O	-6.48	1.13	1.23
1	A	4136	ARG	C-O	-6.46	1.11	1.23
1	B	4136	ARG	C-O	-6.46	1.11	1.23
1	C	4136	ARG	C-O	-6.46	1.11	1.23
1	D	4136	ARG	C-O	-6.46	1.11	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	B	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	C	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	D	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	A	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	B	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	C	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	D	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	A	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	B	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	C	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	D	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	A	4950	TRP	CB-CG	-5.79	1.39	1.50
1	B	4950	TRP	CB-CG	-5.79	1.39	1.50
1	C	4950	TRP	CB-CG	-5.79	1.39	1.50
1	D	4950	TRP	CB-CG	-5.79	1.39	1.50
1	A	4854	PHE	CG-CD1	5.72	1.47	1.38
1	B	4854	PHE	CG-CD1	5.72	1.47	1.38
1	C	4854	PHE	CG-CD1	5.72	1.47	1.38
1	D	4854	PHE	CG-CD1	5.72	1.47	1.38
1	A	4954	PRO	CA-C	-5.71	1.41	1.52
1	B	4954	PRO	CA-C	-5.71	1.41	1.52
1	C	4954	PRO	CA-C	-5.71	1.41	1.52
1	D	4954	PRO	CA-C	-5.71	1.41	1.52
1	A	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	B	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	C	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	D	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	A	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	B	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	C	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	D	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	A	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	B	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	C	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	D	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	A	4890	PHE	CB-CG	-5.45	1.42	1.51
1	B	4890	PHE	CB-CG	-5.45	1.42	1.51
1	C	4890	PHE	CB-CG	-5.45	1.42	1.51
1	D	4890	PHE	CB-CG	-5.45	1.42	1.51
1	A	471	GLU	CG-CD	5.44	1.60	1.51
1	B	471	GLU	CG-CD	5.44	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	471	GLU	CG-CD	5.44	1.60	1.51
1	D	471	GLU	CG-CD	5.44	1.60	1.51
1	A	4958	CYS	CB-SG	-5.40	1.73	1.81
1	B	4958	CYS	CB-SG	-5.40	1.73	1.81
1	C	4958	CYS	CB-SG	-5.40	1.73	1.81
1	D	4958	CYS	CB-SG	-5.40	1.73	1.81
1	A	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	B	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	C	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	D	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	A	3700	CYS	CB-SG	5.37	1.91	1.82
1	B	3700	CYS	CB-SG	5.37	1.91	1.82
1	C	3700	CYS	CB-SG	5.37	1.91	1.82
1	D	3700	CYS	CB-SG	5.37	1.91	1.82
1	A	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	B	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	C	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	D	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	A	4735	TYR	CG-CD1	-5.18	1.32	1.39
1	B	4735	TYR	CG-CD1	-5.18	1.32	1.39
1	C	4735	TYR	CG-CD1	-5.18	1.32	1.39
1	D	4735	TYR	CG-CD1	-5.18	1.32	1.39

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	B	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	C	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	D	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	A	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	C	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	D	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	B	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	C	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	D	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	A	2583	PRO	N-CA-CB	8.35	113.31	103.30
1	B	2583	PRO	N-CA-CB	8.35	113.31	103.30
1	C	2583	PRO	N-CA-CB	8.35	113.31	103.30
1	D	2583	PRO	N-CA-CB	8.35	113.31	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	B	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	C	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	D	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	A	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	B	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	C	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	D	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	A	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	B	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	C	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	D	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	A	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	B	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	C	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	D	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	A	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	B	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	C	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	D	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	A	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	B	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	C	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	D	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	A	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	C	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	B	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	C	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	D	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	A	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	B	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	C	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	D	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	A	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	B	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	C	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	D	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	A	4745	LEU	CB-CG-CD2	7.06	123.01	111.00
1	B	4745	LEU	CB-CG-CD2	7.06	123.01	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4745	LEU	CB-CG-CD2	7.06	123.01	111.00
1	D	4745	LEU	CB-CG-CD2	7.06	123.01	111.00
1	A	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	B	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	C	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	D	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	A	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	B	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	C	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	D	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	A	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	B	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	C	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	D	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	A	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	B	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	C	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	D	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	A	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	C	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	D	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	B	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	C	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	D	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	A	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	B	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	C	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	D	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	A	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	B	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	C	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	D	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	A	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	B	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	C	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	D	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	A	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	B	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	C	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	D	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	B	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	C	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	D	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	A	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	C	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	D	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	B	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	C	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	D	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	A	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	B	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	C	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	D	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	A	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	B	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	C	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	D	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	A	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	B	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	C	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	D	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	A	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	B	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	C	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	D	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	A	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	B	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	C	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	D	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	A	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	C	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	B	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	C	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	D	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	A	814	LEU	CA-CB-CG	5.81	128.67	115.30
1	B	814	LEU	CA-CB-CG	5.81	128.67	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	814	LEU	CA-CB-CG	5.81	128.67	115.30
1	D	814	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	C	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	D	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	B	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	C	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	D	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	A	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	B	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	C	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	D	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	A	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	B	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	C	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	D	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	A	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	B	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	C	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	D	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	A	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	B	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	C	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	D	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	A	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	B	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	C	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	D	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	A	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	B	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	C	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	D	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	B	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	C	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	D	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	A	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	B	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	C	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	D	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	A	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	B	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	C	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	D	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	A	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	B	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	C	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	D	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	A	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	B	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	C	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	D	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	A	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	C	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	D	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	A	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	C	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	B	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	C	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	D	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	A	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	B	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	C	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	D	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	B	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	C	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	D	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	A	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	4940	TYR	CB-CG-CD2	5.29	124.17	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	4940	TYR	CB-CG-CD2	5.29	124.17	121.00
1	C	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	4940	TYR	CB-CG-CD2	5.29	124.17	121.00
1	D	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	4940	TYR	CB-CG-CD2	5.29	124.17	121.00
1	A	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	B	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	C	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	D	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	A	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	C	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	D	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	B	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	C	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	D	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	A	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	B	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	C	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	D	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	A	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	C	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	C	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	D	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	A	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	4721	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	4721	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	4721	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	4721	LEU	CA-CB-CG	5.20	127.26	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	B	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	D	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	B	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	C	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	D	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	A	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	B	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	C	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	D	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	A	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	B	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	C	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	D	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	A	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	B	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	C	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	D	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	A	3802	SER	C-N-CA	5.13	134.52	121.70
1	B	3802	SER	C-N-CA	5.13	134.52	121.70
1	C	3802	SER	C-N-CA	5.13	134.52	121.70
1	D	3802	SER	C-N-CA	5.13	134.52	121.70
1	A	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	B	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	C	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	D	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	A	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	B	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	C	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	D	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	A	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	B	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	C	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	D	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	A	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	B	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	C	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	D	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	A	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	B	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	D	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00

There are no chirality outliers.

All (120) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1102	TYR	Peptide
1	A	1266	GLU	Peptide
1	A	1297	THR	Peptide
1	A	1475	LYS	Peptide
1	A	1579	VAL	Peptide
1	A	1635	GLU	Peptide
1	A	1739	PHE	Peptide
1	A	1808	ASP	Peptide
1	A	1835	HIS	Peptide
1	A	1847	GLU	Peptide
1	A	2075	VAL	Peptide
1	A	2077	GLU	Peptide
1	A	3767	LEU	Peptide
1	A	3805	ASP	Peptide
1	A	4070	CYS	Peptide
1	A	4144	LYS	Peptide
1	A	4163	LYS	Peptide
1	A	471	GLU	Peptide
1	A	4798	GLU	Peptide
1	A	4956	GLY	Peptide
1	A	4958	CYS	Peptide
1	A	657	PRO	Peptide
1	A	729	GLY	Peptide
1	A	775	VAL	Peptide
1	A	791	VAL	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	Peptide
1	A	838	ARG	Peptide
1	A	852	GLY	Mainchain,Peptide
1	B	1102	TYR	Peptide
1	B	1266	GLU	Peptide
1	B	1297	THR	Peptide
1	B	1475	LYS	Peptide
1	B	1579	VAL	Peptide
1	B	1635	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	1739	PHE	Peptide
1	B	1808	ASP	Peptide
1	B	1835	HIS	Peptide
1	B	1847	GLU	Peptide
1	B	2075	VAL	Peptide
1	B	2077	GLU	Peptide
1	B	3767	LEU	Peptide
1	B	3805	ASP	Peptide
1	B	4070	CYS	Peptide
1	B	4144	LYS	Peptide
1	B	4163	LYS	Peptide
1	B	471	GLU	Peptide
1	B	4798	GLU	Peptide
1	B	4956	GLY	Peptide
1	B	4958	CYS	Peptide
1	B	657	PRO	Peptide
1	B	729	GLY	Peptide
1	B	775	VAL	Peptide
1	B	791	VAL	Peptide
1	B	818	GLY	Peptide
1	B	819	TYR	Peptide
1	B	838	ARG	Peptide
1	B	852	GLY	Mainchain,Peptide
1	C	1102	TYR	Peptide
1	C	1266	GLU	Peptide
1	C	1297	THR	Peptide
1	C	1475	LYS	Peptide
1	C	1579	VAL	Peptide
1	C	1635	GLU	Peptide
1	C	1739	PHE	Peptide
1	C	1808	ASP	Peptide
1	C	1835	HIS	Peptide
1	C	1847	GLU	Peptide
1	C	2075	VAL	Peptide
1	C	2077	GLU	Peptide
1	C	3767	LEU	Peptide
1	C	3805	ASP	Peptide
1	C	4070	CYS	Peptide
1	C	4144	LYS	Peptide
1	C	4163	LYS	Peptide
1	C	471	GLU	Peptide
1	C	4798	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	4956	GLY	Peptide
1	C	4958	CYS	Peptide
1	C	657	PRO	Peptide
1	C	729	GLY	Peptide
1	C	775	VAL	Peptide
1	C	791	VAL	Peptide
1	C	818	GLY	Peptide
1	C	819	TYR	Peptide
1	C	838	ARG	Peptide
1	C	852	GLY	Mainchain,Peptide
1	D	1102	TYR	Peptide
1	D	1266	GLU	Peptide
1	D	1297	THR	Peptide
1	D	1475	LYS	Peptide
1	D	1579	VAL	Peptide
1	D	1635	GLU	Peptide
1	D	1739	PHE	Peptide
1	D	1808	ASP	Peptide
1	D	1835	HIS	Peptide
1	D	1847	GLU	Peptide
1	D	2075	VAL	Peptide
1	D	2077	GLU	Peptide
1	D	3767	LEU	Peptide
1	D	3805	ASP	Peptide
1	D	4070	CYS	Peptide
1	D	4144	LYS	Peptide
1	D	4163	LYS	Peptide
1	D	471	GLU	Peptide
1	D	4798	GLU	Peptide
1	D	4956	GLY	Peptide
1	D	4958	CYS	Peptide
1	D	657	PRO	Peptide
1	D	729	GLY	Peptide
1	D	775	VAL	Peptide
1	D	791	VAL	Peptide
1	D	818	GLY	Peptide
1	D	819	TYR	Peptide
1	D	838	ARG	Peptide
1	D	852	GLY	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26266	0	24898	409	0
1	B	26266	0	24898	421	0
1	C	26266	0	24898	414	0
1	D	26266	0	24898	401	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	105068	0	99592	1515	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 7.

All (1515) 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:4873:GLU:HA	1:B:4875:ARG:NH1	1.62	1.15
1:A:4875:ARG:NH1	1:D:4873:GLU:HA	1.62	1.14
1:B:4873:GLU:HA	1:C:4875:ARG:NH1	1.62	1.13
1:C:4873:GLU:OE1	1:D:4875:ARG:HD3	1.49	1.12
1:C:4873:GLU:HA	1:D:4875:ARG:NH1	1.62	1.12
1:B:4873:GLU:OE1	1:C:4875:ARG:HD3	1.49	1.11
1:A:4873:GLU:OE1	1:B:4875:ARG:HD3	1.49	1.11
1:A:4875:ARG:HD3	1:D:4873:GLU:OE1	1.49	1.10
1:A:4823:ARG:HA	1:D:4852:PHE:CZ	1.98	0.98
1:B:4852:PHE:CZ	1:C:4823:ARG:HA	1.98	0.98
1:A:4852:PHE:CZ	1:B:4823:ARG:HA	1.98	0.98
1:C:4852:PHE:CZ	1:D:4823:ARG:HA	1.98	0.98
1:D:4832:ILE:HG21	1:D:4844:ARG:HH21	1.44	0.83
1:B:4832:ILE:HG21	1:B:4844:ARG:HH21	1.44	0.82
1:C:4832:ILE:HG21	1:C:4844:ARG:HH21	1.44	0.82
1:A:4832:ILE:HG21	1:A:4844:ARG:HH21	1.44	0.80
1:A:4872:GLY:C	1:B:4875:ARG:HH22	1.86	0.79
1:A:4875:ARG:HH22	1:D:4872:GLY:C	1.86	0.78
1:A:4810:MET:HG2	1:B:4518:LEU:O	1.84	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4872:GLY:C	1:C:4875:ARG:HH22	1.86	0.78
1:B:4810:MET:HG2	1:C:4518:LEU:O	1.84	0.78
1:C:4872:GLY:C	1:D:4875:ARG:HH22	1.86	0.78
1:A:4518:LEU:O	1:D:4810:MET:HG2	1.84	0.77
1:C:4810:MET:HG2	1:D:4518:LEU:O	1.84	0.77
1:C:76:ARG:HG2	1:D:3891:TRP:HB3	1.68	0.75
1:B:708:GLY:HA2	1:B:714:GLY:HA3	1.69	0.74
1:B:76:ARG:HG2	1:C:3891:TRP:HB3	1.68	0.74
1:D:708:GLY:HA2	1:D:714:GLY:HA3	1.69	0.74
1:A:708:GLY:HA2	1:A:714:GLY:HA3	1.69	0.73
1:A:76:ARG:HG2	1:B:3891:TRP:HB3	1.68	0.73
1:A:3891:TRP:HB3	1:D:76:ARG:HG2	1.68	0.73
1:C:4872:GLY:C	1:D:4875:ARG:NH2	2.42	0.73
1:C:4873:GLU:OE1	1:D:4875:ARG:CD	2.35	0.73
1:B:4872:GLY:C	1:C:4875:ARG:NH2	2.42	0.73
1:C:708:GLY:HA2	1:C:714:GLY:HA3	1.69	0.72
1:B:4873:GLU:OE1	1:C:4875:ARG:CD	2.35	0.72
1:A:4872:GLY:C	1:B:4875:ARG:NH2	2.42	0.72
1:A:4875:ARG:NH2	1:D:4872:GLY:C	2.42	0.71
1:A:4875:ARG:NH1	1:D:4872:GLY:O	2.24	0.71
1:A:4157:SER:OG	1:A:4924:MET:SD	2.50	0.70
1:A:4872:GLY:O	1:B:4875:ARG:NH2	2.25	0.70
1:A:4872:GLY:O	1:B:4875:ARG:NH1	2.24	0.70
1:A:4875:ARG:NH2	1:D:4872:GLY:O	2.25	0.70
1:B:4157:SER:OG	1:B:4924:MET:SD	2.50	0.70
1:C:4872:GLY:O	1:D:4875:ARG:NH1	2.24	0.70
1:D:4157:SER:OG	1:D:4924:MET:SD	2.50	0.70
1:B:4872:GLY:O	1:C:4875:ARG:NH2	2.25	0.70
1:A:2419:ARG:NH1	1:D:189:GLU:OE1	2.25	0.70
1:B:189:GLU:OE1	1:C:2419:ARG:NH1	2.25	0.70
1:C:4873:GLU:CA	1:D:4875:ARG:NH1	2.51	0.69
1:B:4872:GLY:O	1:C:4875:ARG:NH1	2.24	0.69
1:A:189:GLU:OE1	1:B:2419:ARG:NH1	2.25	0.69
1:C:4157:SER:OG	1:C:4924:MET:SD	2.50	0.69
1:C:189:GLU:OE1	1:D:2419:ARG:NH1	2.25	0.69
1:B:4800:GLY:HA2	1:B:4804:ASP:HB3	1.74	0.68
1:A:4873:GLU:CA	1:B:4875:ARG:NH1	2.51	0.68
1:C:4872:GLY:O	1:D:4875:ARG:NH2	2.25	0.68
1:A:3986:MET:HG2	1:A:3996:ILE:HD11	1.75	0.68
1:D:3986:MET:HG2	1:D:3996:ILE:HD11	1.75	0.68
1:A:4875:ARG:NH1	1:D:4873:GLU:CA	2.51	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4011:VAL:HA	1:A:4014:ILE:HG12	1.76	0.68
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.76	0.68
1:C:4011:VAL:HA	1:C:4014:ILE:HG12	1.76	0.68
1:B:4873:GLU:CA	1:C:4875:ARG:NH1	2.51	0.68
1:D:4800:GLY:HA2	1:D:4804:ASP:HB3	1.74	0.68
1:C:1645:THR:HG22	1:C:1695:PRO:HG3	1.76	0.67
1:C:4873:GLU:HA	1:D:4875:ARG:HH12	1.59	0.67
1:D:1138:ASP:HB2	1:D:1145:TRP:HE1	1.60	0.67
1:D:4011:VAL:HA	1:D:4014:ILE:HG12	1.76	0.67
1:A:1138:ASP:HB2	1:A:1145:TRP:HE1	1.60	0.67
1:C:1138:ASP:HB2	1:C:1145:TRP:HE1	1.60	0.67
1:C:4800:GLY:HA2	1:C:4804:ASP:HB3	1.74	0.67
1:A:4800:GLY:HA2	1:A:4804:ASP:HB3	1.74	0.67
1:B:1645:THR:HG22	1:B:1695:PRO:HG3	1.76	0.67
1:B:4873:GLU:HA	1:C:4875:ARG:HH12	1.59	0.67
1:C:3986:MET:HG2	1:C:3996:ILE:HD11	1.75	0.67
1:B:3986:MET:HG2	1:B:3996:ILE:HD11	1.75	0.67
1:B:4011:VAL:HA	1:B:4014:ILE:HG12	1.76	0.67
1:B:1138:ASP:HB2	1:B:1145:TRP:HE1	1.60	0.67
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.76	0.67
1:D:35:LEU:HD13	1:D:49:LEU:HD22	1.77	0.66
1:A:299:HIS:HE2	1:A:301:THR:HG1	1.43	0.66
1:B:35:LEU:HD13	1:B:49:LEU:HD22	1.77	0.66
1:A:4875:ARG:CD	1:D:4873:GLU:OE1	2.35	0.65
1:A:4873:GLU:HA	1:B:4875:ARG:HH12	1.59	0.65
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.62	0.65
1:A:35:LEU:HD13	1:A:49:LEU:HD22	1.77	0.65
1:B:248:PRO:HG2	1:B:257:ARG:HA	1.79	0.65
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.62	0.65
1:A:248:PRO:HG2	1:A:257:ARG:HA	1.79	0.65
1:A:4873:GLU:OE1	1:B:4875:ARG:CD	2.35	0.65
1:C:35:LEU:HD13	1:C:49:LEU:HD22	1.77	0.65
1:D:248:PRO:HG2	1:D:257:ARG:HA	1.79	0.65
1:B:243:GLU:HA	1:B:264:GLY:HA2	1.79	0.65
1:B:1602:GLN:HE22	1:B:1642:LEU:HB3	1.62	0.65
1:A:1602:GLN:HE22	1:A:1642:LEU:HB3	1.62	0.65
1:B:299:HIS:HE2	1:B:301:THR:HG1	1.45	0.65
1:C:243:GLU:HA	1:C:264:GLY:HA2	1.79	0.65
1:C:248:PRO:HG2	1:C:257:ARG:HA	1.79	0.64
1:D:1602:GLN:HE22	1:D:1642:LEU:HB3	1.62	0.64
1:A:243:GLU:HA	1:A:264:GLY:HA2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1602:GLN:HE22	1:C:1642:LEU:HB3	1.62	0.64
1:D:3875:THR:HG21	1:D:3924:TYR:HE2	1.62	0.64
1:D:243:GLU:HA	1:D:264:GLY:HA2	1.79	0.64
1:B:1304:LEU:HB3	1:B:1541:PRO:HG2	1.80	0.64
1:B:3875:THR:HG21	1:B:3924:TYR:HE2	1.62	0.63
1:A:227:TYR:HE1	1:A:355:LYS:HG2	1.64	0.63
1:A:4868:ILE:HG12	1:D:4865:GLY:HA3	1.81	0.63
1:B:3845:GLN:HB2	1:B:3920:THR:HG22	1.81	0.63
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.64	0.63
1:D:227:TYR:HE1	1:D:355:LYS:HG2	1.64	0.63
1:C:227:TYR:HE1	1:C:355:LYS:HG2	1.64	0.63
1:D:1304:LEU:HB3	1:D:1541:PRO:HG2	1.80	0.63
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.64	0.62
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.64	0.62
1:A:3922:THR:O	1:A:3926:GLN:N	2.32	0.62
1:A:4865:GLY:HA3	1:B:4868:ILE:HG12	1.81	0.62
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.64	0.62
1:C:3922:THR:O	1:C:3926:GLN:N	2.32	0.62
1:A:1304:LEU:HB3	1:A:1541:PRO:HG2	1.80	0.62
1:A:3845:GLN:HB2	1:A:3920:THR:HG22	1.81	0.62
1:C:1304:LEU:HB3	1:C:1541:PRO:HG2	1.80	0.62
1:B:3922:THR:O	1:B:3926:GLN:N	2.32	0.62
1:B:227:TYR:HE1	1:B:355:LYS:HG2	1.64	0.62
1:D:3922:THR:O	1:D:3926:GLN:N	2.32	0.62
1:B:4865:GLY:HA3	1:C:4868:ILE:HG12	1.81	0.62
1:D:3845:GLN:HB2	1:D:3920:THR:HG22	1.81	0.62
1:C:4865:GLY:HA3	1:D:4868:ILE:HG12	1.81	0.62
1:B:1272:ARG:NH1	1:B:1587:HIS:O	2.34	0.61
1:D:1272:ARG:NH1	1:D:1587:HIS:O	2.34	0.61
1:D:299:HIS:HE2	1:D:301:THR:HG1	1.46	0.61
1:C:4072:GLU:HB3	1:C:4074:ASP:HB2	1.83	0.61
1:C:1272:ARG:NH1	1:C:1587:HIS:O	2.34	0.61
1:B:3841:PHE:HB3	1:B:3920:THR:HG21	1.82	0.61
1:A:4875:ARG:HH12	1:D:4873:GLU:HA	1.59	0.61
1:D:779:PHE:HB3	1:D:782:PHE:HE2	1.66	0.61
1:A:3841:PHE:HB3	1:A:3920:THR:HG21	1.82	0.60
1:B:4072:GLU:HB3	1:B:4074:ASP:HB2	1.83	0.60
1:D:3841:PHE:HB3	1:D:3920:THR:HG21	1.82	0.60
1:A:4140:MET:HG2	1:A:4146:ILE:HG12	1.82	0.60
1:B:1258:PHE:HB2	1:B:1593:HIS:HB3	1.83	0.60
1:D:4140:MET:HG2	1:D:4146:ILE:HG12	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HG22	1:A:34:LYS:HG2	1.83	0.60
1:A:779:PHE:HB3	1:A:782:PHE:HE2	1.66	0.60
1:C:3802:SER:OG	1:C:3833:ASP:O	2.18	0.60
1:C:779:PHE:HB3	1:C:782:PHE:HE2	1.66	0.60
1:A:954:ASP:HB3	1:A:1061:GLY:HA3	1.84	0.60
1:B:779:PHE:HB3	1:B:782:PHE:HE2	1.66	0.60
1:D:954:ASP:HB3	1:D:1061:GLY:HA3	1.84	0.60
1:A:1469:LEU:HG	1:A:1480:ILE:HD11	1.84	0.60
1:A:3802:SER:OG	1:A:3833:ASP:O	2.18	0.60
1:B:143:LEU:HD23	1:C:2426:SER:HB3	1.84	0.60
1:C:123:HIS:HD2	1:C:126:SER:H	1.50	0.60
1:C:3845:GLN:HB2	1:C:3920:THR:HG22	1.81	0.60
1:D:1469:LEU:HG	1:D:1480:ILE:HD11	1.84	0.60
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.84	0.60
1:B:954:ASP:HB3	1:B:1061:GLY:HA3	1.84	0.60
1:C:802:PHE:HB2	1:C:1617:TRP:HB2	1.84	0.60
1:C:4140:MET:HG2	1:C:4146:ILE:HG12	1.82	0.60
1:D:25:THR:HG22	1:D:34:LYS:HG2	1.83	0.60
1:A:1258:PHE:HB2	1:A:1593:HIS:HB3	1.83	0.60
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.84	0.60
1:C:1137:PHE:HA	1:C:1144:ARG:HA	1.82	0.60
1:A:1272:ARG:NH1	1:A:1587:HIS:O	2.34	0.60
1:B:123:HIS:HD2	1:B:126:SER:H	1.50	0.60
1:B:25:THR:HG22	1:B:34:LYS:HG2	1.83	0.60
1:B:4140:MET:HG2	1:B:4146:ILE:HG12	1.82	0.60
1:C:1258:PHE:HB2	1:C:1593:HIS:HB3	1.83	0.60
1:A:4072:GLU:HB3	1:A:4074:ASP:HB2	1.83	0.60
1:A:756:SER:HB3	1:A:769:ARG:HB2	1.84	0.60
1:B:4617:TYR:OH	1:B:4629:GLY:O	2.20	0.60
1:B:672:LYS:HA	1:B:760:ASP:HA	1.84	0.60
1:D:1113:MET:HG3	1:D:1156:TRP:HZ2	1.67	0.60
1:B:756:SER:HB3	1:B:769:ARG:HB2	1.84	0.59
1:D:123:HIS:HD2	1:D:126:SER:H	1.50	0.59
1:A:1137:PHE:HA	1:A:1144:ARG:HA	1.82	0.59
1:D:4072:GLU:HB3	1:D:4074:ASP:HB2	1.83	0.59
1:A:4617:TYR:OH	1:A:4629:GLY:O	2.20	0.59
1:A:672:LYS:HA	1:A:760:ASP:HA	1.84	0.59
1:B:1469:LEU:HG	1:B:1480:ILE:HD11	1.84	0.59
1:B:802:PHE:HB2	1:B:1617:TRP:HB2	1.84	0.59
1:C:954:ASP:HB3	1:C:1061:GLY:HA3	1.84	0.59
1:D:1137:PHE:HA	1:D:1144:ARG:HA	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3802:SER:OG	1:D:3833:ASP:O	2.18	0.59
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.85	0.59
1:B:1137:PHE:HA	1:B:1144:ARG:HA	1.82	0.59
1:D:1445:TRP:HE1	1:D:1508:GLY:HA3	1.67	0.59
1:C:3914:ALA:HA	1:C:3917:VAL:HG12	1.85	0.59
1:A:2426:SER:HB3	1:D:143:LEU:HD23	1.84	0.59
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.85	0.59
1:A:123:HIS:HD2	1:A:126:SER:H	1.50	0.59
1:A:143:LEU:HD23	1:B:2426:SER:HB3	1.84	0.59
1:A:3914:ALA:HA	1:A:3917:VAL:HG12	1.85	0.59
1:D:3914:ALA:HA	1:D:3917:VAL:HG12	1.85	0.59
1:C:143:LEU:HD23	1:D:2426:SER:HB3	1.84	0.59
1:D:3924:TYR:O	1:D:3932:ASN:ND2	2.36	0.59
1:B:3914:ALA:HA	1:B:3917:VAL:HG12	1.85	0.59
1:C:25:THR:HG22	1:C:34:LYS:HG2	1.83	0.59
1:C:3841:PHE:HB3	1:C:3920:THR:HG21	1.82	0.59
1:D:1258:PHE:HB2	1:D:1593:HIS:HB3	1.83	0.59
1:A:1113:MET:HG3	1:A:1156:TRP:HZ2	1.67	0.59
1:C:1469:LEU:HG	1:C:1480:ILE:HD11	1.84	0.59
1:C:756:SER:HB3	1:C:769:ARG:HB2	1.84	0.59
1:B:1113:MET:HG3	1:B:1156:TRP:HZ2	1.67	0.58
1:C:1113:MET:HG3	1:C:1156:TRP:HZ2	1.67	0.58
1:C:672:LYS:HA	1:C:760:ASP:HA	1.84	0.58
1:A:3924:TYR:O	1:A:3932:ASN:ND2	2.36	0.58
1:C:4883:GLU:O	1:C:4887:THR:HG23	2.04	0.58
1:B:1445:TRP:HE1	1:B:1508:GLY:HA3	1.67	0.58
1:C:1706:LEU:HD21	1:C:1787:LEU:HD21	1.85	0.58
1:B:3802:SER:OG	1:B:3833:ASP:O	2.18	0.58
1:C:4617:TYR:OH	1:C:4629:GLY:O	2.20	0.58
1:D:756:SER:HB3	1:D:769:ARG:HB2	1.84	0.58
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.85	0.58
1:B:3924:TYR:O	1:B:3932:ASN:ND2	2.36	0.58
1:C:897:LYS:HD3	1:C:918:LEU:HD21	1.86	0.58
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.85	0.58
1:D:672:LYS:HA	1:D:760:ASP:HA	1.84	0.58
1:B:1706:LEU:HD21	1:B:1787:LEU:HD21	1.85	0.58
1:B:897:LYS:HD3	1:B:918:LEU:HD21	1.86	0.58
1:D:4617:TYR:OH	1:D:4629:GLY:O	2.20	0.58
1:A:247:VAL:O	1:A:272:ARG:NH1	2.36	0.58
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.85	0.58
1:A:4883:GLU:O	1:A:4887:THR:HG23	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:LYS:HD3	1:A:918:LEU:HD21	1.86	0.58
1:C:1104:GLU:HA	1:C:1163:GLY:HA2	1.85	0.58
1:D:4883:GLU:O	1:D:4887:THR:HG23	2.04	0.58
1:D:897:LYS:HD3	1:D:918:LEU:HD21	1.86	0.58
1:A:1445:TRP:HE1	1:A:1508:GLY:HA3	1.67	0.57
1:C:3924:TYR:O	1:C:3932:ASN:ND2	2.36	0.57
1:C:4915:ASN:O	1:C:4917:ALA:N	2.38	0.57
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.85	0.57
1:A:1124:PRO:HB2	1:A:1252:SER:HB3	1.86	0.57
1:A:4915:ASN:O	1:A:4917:ALA:N	2.38	0.57
1:C:1445:TRP:HE1	1:C:1508:GLY:HA3	1.67	0.57
1:D:247:VAL:O	1:D:272:ARG:NH1	2.36	0.57
1:B:4915:ASN:O	1:B:4917:ALA:N	2.38	0.57
1:C:1114:ARG:HB2	1:C:1206:SER:HB3	1.86	0.57
1:D:1706:LEU:HD21	1:D:1787:LEU:HD21	1.85	0.57
1:B:1114:ARG:HB2	1:B:1206:SER:HB3	1.86	0.57
1:D:1124:PRO:HB2	1:D:1252:SER:HB3	1.86	0.57
1:D:4915:ASN:O	1:D:4917:ALA:N	2.38	0.57
1:B:4883:GLU:O	1:B:4887:THR:HG23	2.04	0.57
1:C:299:HIS:HE2	1:C:301:THR:HG1	1.51	0.57
1:C:530:LEU:HD23	1:C:533:LEU:HD12	1.87	0.57
1:C:1429:SER:HA	1:C:1507:ILE:HG12	1.87	0.57
1:D:1429:SER:HA	1:D:1507:ILE:HG12	1.87	0.57
1:A:530:LEU:HD23	1:A:533:LEU:HD12	1.87	0.57
1:C:1433:PHE:HD2	1:C:1551:ASN:HB3	1.70	0.57
1:D:530:LEU:HD23	1:D:533:LEU:HD12	1.87	0.57
1:A:1429:SER:HA	1:A:1507:ILE:HG12	1.87	0.57
1:B:1104:GLU:HA	1:B:1163:GLY:HA2	1.85	0.57
1:A:1706:LEU:HD21	1:A:1787:LEU:HD21	1.85	0.56
1:A:1433:PHE:HD2	1:A:1551:ASN:HB3	1.70	0.56
1:D:1442:TRP:HD1	1:D:1488:VAL:HG13	1.71	0.56
1:C:1442:TRP:HD1	1:C:1488:VAL:HG13	1.71	0.56
1:C:473:GLU:OE2	1:C:477:ASN:ND2	2.39	0.56
1:C:1124:PRO:HB2	1:C:1252:SER:HB3	1.86	0.56
1:C:1699:ARG:NH1	1:C:1816:PHE:O	2.39	0.56
1:B:4791:ARG:NE	1:C:4523:VAL:HG11	2.20	0.56
1:D:1433:PHE:HD2	1:D:1551:ASN:HB3	1.70	0.56
1:B:1429:SER:HA	1:B:1507:ILE:HG12	1.87	0.56
1:C:4015:LEU:HD22	1:C:4126:VAL:HG21	1.87	0.56
1:C:58:VAL:HG22	1:C:320:GLU:HA	1.87	0.56
1:D:473:GLU:OE2	1:D:477:ASN:ND2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:TRP:HD1	1:A:1488:VAL:HG13	1.71	0.56
1:A:1114:ARG:HB2	1:A:1206:SER:HB3	1.86	0.56
1:B:4161:TRP:HD1	1:B:4201:MET:HE1	1.71	0.56
1:B:530:LEU:HD23	1:B:533:LEU:HD12	1.87	0.56
1:D:4015:LEU:HD22	1:D:4126:VAL:HG21	1.87	0.56
1:A:1121:GLY:O	1:A:1133:ARG:NH1	2.38	0.56
1:C:2060:GLN:NE2	1:C:2092:GLN:O	2.39	0.56
1:D:1114:ARG:HB2	1:D:1206:SER:HB3	1.86	0.56
1:A:4015:LEU:HD22	1:A:4126:VAL:HG21	1.87	0.56
1:B:58:VAL:HG22	1:B:320:GLU:HA	1.87	0.56
1:D:1121:GLY:O	1:D:1133:ARG:NH1	2.38	0.56
1:A:58:VAL:HG22	1:A:320:GLU:HA	1.87	0.56
1:B:1699:ARG:NH1	1:B:1816:PHE:O	2.39	0.56
1:B:4015:LEU:HD22	1:B:4126:VAL:HG21	1.87	0.56
1:A:4791:ARG:NE	1:B:4523:VAL:HG11	2.20	0.56
1:A:2060:GLN:NE2	1:A:2092:GLN:O	2.39	0.56
1:A:4618:ILE:HD12	1:A:4667:ILE:HD12	1.88	0.56
1:B:986:ILE:HD12	1:B:1059:GLY:HA2	1.88	0.56
1:C:4161:TRP:HD1	1:C:4201:MET:HE1	1.71	0.56
1:C:4618:ILE:HD12	1:C:4667:ILE:HD12	1.88	0.56
1:C:4791:ARG:NE	1:D:4523:VAL:HG11	2.20	0.56
1:B:1124:PRO:HB2	1:B:1252:SER:HB3	1.86	0.55
1:D:2060:GLN:NE2	1:D:2092:GLN:O	2.39	0.55
1:B:1433:PHE:HD2	1:B:1551:ASN:HB3	1.70	0.55
1:B:2060:GLN:NE2	1:B:2092:GLN:O	2.39	0.55
1:D:1272:ARG:NH2	1:D:1590:PHE:O	2.39	0.55
1:A:1272:ARG:NH2	1:A:1590:PHE:O	2.39	0.55
1:A:4523:VAL:HG11	1:D:4791:ARG:NE	2.20	0.55
1:B:375:GLN:HE21	1:B:392:ILE:HD13	1.72	0.55
1:B:473:GLU:OE2	1:B:477:ASN:ND2	2.39	0.55
1:C:1726:ILE:HD11	1:C:2121:LEU:HD11	1.89	0.55
1:D:1726:ILE:HD11	1:D:2121:LEU:HD11	1.89	0.55
1:A:2463:PRO:HB3	1:A:2516:ALA:HA	1.88	0.55
1:A:618:CYS:SG	1:A:629:GLN:NE2	2.80	0.55
1:A:986:ILE:HD12	1:A:1059:GLY:HA2	1.88	0.55
1:B:4618:ILE:HD12	1:B:4667:ILE:HD12	1.88	0.55
1:B:4819:TYR:O	1:B:4823:ARG:NH2	2.33	0.55
1:C:1272:ARG:NH2	1:C:1590:PHE:O	2.39	0.55
1:D:58:VAL:HG22	1:D:320:GLU:HA	1.87	0.55
1:A:1699:ARG:NH1	1:A:1816:PHE:O	2.39	0.55
1:A:375:GLN:HE21	1:A:392:ILE:HD13	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4618:ILE:HD12	1:D:4667:ILE:HD12	1.88	0.55
1:B:2843:GLU:OE1	1:B:2887:ARG:NH2	2.40	0.55
1:C:2843:GLU:OE1	1:C:2887:ARG:NH2	2.40	0.55
1:C:4840:TYR:O	1:C:4844:ARG:N	2.40	0.55
1:B:1272:ARG:NH2	1:B:1590:PHE:O	2.39	0.55
1:C:2463:PRO:HB3	1:C:2516:ALA:HA	1.88	0.55
1:C:247:VAL:O	1:C:272:ARG:NH1	2.36	0.55
1:B:1442:TRP:HD1	1:B:1488:VAL:HG13	1.71	0.55
1:B:618:CYS:SG	1:B:629:GLN:NE2	2.80	0.55
1:C:797:GLY:HA2	1:C:1622:LEU:HA	1.89	0.55
1:D:1699:ARG:NH1	1:D:1816:PHE:O	2.39	0.55
1:D:375:GLN:HE21	1:D:392:ILE:HD13	1.72	0.55
1:C:618:CYS:SG	1:C:629:GLN:NE2	2.80	0.55
1:D:2463:PRO:HB3	1:D:2516:ALA:HA	1.88	0.55
1:D:797:GLY:HA2	1:D:1622:LEU:HA	1.89	0.55
1:A:4514:ILE:HG21	1:A:4740:PHE:HE2	1.72	0.55
1:B:1726:ILE:HD11	1:B:2121:LEU:HD11	1.89	0.55
1:B:4514:ILE:HG21	1:B:4740:PHE:HE2	1.72	0.55
1:C:986:ILE:HD12	1:C:1059:GLY:HA2	1.88	0.55
1:C:4514:ILE:HG21	1:C:4740:PHE:HE2	1.72	0.55
1:A:1510:VAL:HG12	1:A:1511:VAL:HG23	1.89	0.54
1:A:473:GLU:OE2	1:A:477:ASN:ND2	2.39	0.54
1:B:3960:SER:HG	1:B:4070:CYS:HG	1.53	0.54
1:D:2158:GLN:O	1:D:3616:ARG:NH1	2.40	0.54
1:A:1156:TRP:HB3	1:A:1177:LEU:HD11	1.90	0.54
1:B:4840:TYR:O	1:B:4844:ARG:N	2.40	0.54
1:C:258:ARG:NH1	1:C:317:MET:SD	2.80	0.54
1:A:1726:ILE:HD11	1:A:2121:LEU:HD11	1.89	0.54
1:A:258:ARG:NH1	1:A:317:MET:SD	2.80	0.54
1:B:258:ARG:NH1	1:B:317:MET:SD	2.80	0.54
1:B:2158:GLN:O	1:B:3616:ARG:NH1	2.40	0.54
1:D:258:ARG:NH1	1:D:317:MET:SD	2.80	0.54
1:D:2843:GLU:OE1	1:D:2887:ARG:NH2	2.40	0.54
1:D:986:ILE:HD12	1:D:1059:GLY:HA2	1.88	0.54
1:A:2158:GLN:O	1:A:3616:ARG:NH1	2.40	0.54
1:C:2158:GLN:O	1:C:3616:ARG:NH1	2.40	0.54
1:C:375:GLN:HE21	1:C:392:ILE:HD13	1.72	0.54
1:D:4514:ILE:HG21	1:D:4740:PHE:HE2	1.72	0.54
1:D:618:CYS:SG	1:D:629:GLN:NE2	2.80	0.54
1:A:797:GLY:HA2	1:A:1622:LEU:HA	1.89	0.54
1:B:4046:LYS:HG3	1:B:4068:LEU:HD22	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1601:ASN:ND2	1:C:1643:GLU:OE2	2.41	0.54
1:A:2843:GLU:OE1	1:A:2887:ARG:NH2	2.40	0.54
1:B:1156:TRP:HB3	1:B:1177:LEU:HD11	1.90	0.54
1:B:1601:ASN:ND2	1:B:1643:GLU:OE2	2.41	0.54
1:B:247:VAL:O	1:B:272:ARG:NH1	2.36	0.54
1:C:1156:TRP:HB3	1:C:1177:LEU:HD11	1.90	0.54
1:C:4046:LYS:HG3	1:C:4068:LEU:HD22	1.90	0.54
1:D:1510:VAL:HG12	1:D:1511:VAL:HG23	1.89	0.54
1:A:1607:ASP:HB3	1:A:1608:VAL:HG23	1.90	0.54
1:B:1510:VAL:HG12	1:B:1511:VAL:HG23	1.89	0.54
1:B:228:LEU:HB3	1:B:289:ILE:HB	1.90	0.54
1:C:1607:ASP:HB3	1:C:1608:VAL:HG23	1.90	0.54
1:D:1156:TRP:HB3	1:D:1177:LEU:HD11	1.90	0.54
1:A:1601:ASN:ND2	1:A:1643:GLU:OE2	2.41	0.54
1:A:4161:TRP:HD1	1:A:4201:MET:HE1	1.71	0.54
1:C:228:LEU:HB3	1:C:289:ILE:HB	1.90	0.54
1:D:598:ILE:HG23	1:D:636:LEU:HD12	1.90	0.54
1:B:2463:PRO:HB3	1:B:2516:ALA:HA	1.88	0.54
1:B:797:GLY:HA2	1:B:1622:LEU:HA	1.89	0.54
1:B:1121:GLY:O	1:B:1133:ARG:NH1	2.38	0.54
1:B:1607:ASP:HB3	1:B:1608:VAL:HG23	1.90	0.54
1:D:1601:ASN:ND2	1:D:1643:GLU:OE2	2.41	0.54
1:A:4840:TYR:O	1:A:4844:ARG:N	2.40	0.53
1:C:1911:LEU:HD11	1:C:2063:ILE:HG12	1.90	0.53
1:C:26:ALA:HB3	1:C:33:GLN:HB3	1.90	0.53
1:D:4819:TYR:O	1:D:4823:ARG:NH2	2.33	0.53
1:C:3926:GLN:HE21	1:C:4936:GLY:H	1.56	0.53
1:C:4660:GLU:HG3	1:C:4664:ARG:HH21	1.73	0.53
1:B:598:ILE:HG23	1:B:636:LEU:HD12	1.90	0.53
1:D:4161:TRP:HD1	1:D:4201:MET:HE1	1.71	0.53
1:A:3926:GLN:HE21	1:A:4936:GLY:H	1.56	0.53
1:C:1121:GLY:O	1:C:1133:ARG:NH1	2.38	0.53
1:D:1607:ASP:HB3	1:D:1608:VAL:HG23	1.90	0.53
1:D:1726:ILE:HB	1:D:2109:ILE:HD11	1.91	0.53
1:D:4840:TYR:O	1:D:4844:ARG:N	2.40	0.53
1:D:636:LEU:HD21	1:D:643:LEU:HD21	1.90	0.53
1:C:3730:ALA:HA	1:C:3733:HIS:CE1	2.44	0.53
1:D:1911:LEU:HD11	1:D:2063:ILE:HG12	1.90	0.53
1:D:2488:LEU:O	1:D:2492:GLY:N	2.42	0.53
1:B:3730:ALA:HA	1:B:3733:HIS:CE1	2.44	0.53
1:C:61:ASP:OD2	1:C:417:ARG:NH2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:ILE:HG23	1:C:636:LEU:HD12	1.90	0.53
1:D:26:ALA:HB3	1:D:33:GLN:HB3	1.90	0.53
1:D:4046:LYS:HG3	1:D:4068:LEU:HD22	1.90	0.53
1:A:1726:ILE:HB	1:A:2109:ILE:HD11	1.91	0.53
1:A:3730:ALA:HA	1:A:3733:HIS:CE1	2.44	0.53
1:A:3798:MET:HE1	1:A:3875:THR:HB	1.91	0.53
1:A:598:ILE:HG23	1:A:636:LEU:HD12	1.90	0.53
1:B:1726:ILE:HB	1:B:2109:ILE:HD11	1.91	0.53
1:B:61:ASP:OD2	1:B:417:ARG:NH2	2.42	0.53
1:C:1510:VAL:HG12	1:C:1511:VAL:HG23	1.89	0.53
1:D:4660:GLU:HG3	1:D:4664:ARG:HH21	1.73	0.53
1:B:677:LEU:HD11	1:B:792:VAL:HG21	1.91	0.53
1:B:4660:GLU:HG3	1:B:4664:ARG:HH21	1.73	0.53
1:C:4889:CYS:HB3	1:C:4892:CYS:SG	2.49	0.53
1:D:3798:MET:HE1	1:D:3875:THR:HB	1.91	0.53
1:D:4889:CYS:HB3	1:D:4892:CYS:SG	2.49	0.53
1:A:228:LEU:HB3	1:A:289:ILE:HB	1.90	0.52
1:A:2488:LEU:O	1:A:2492:GLY:N	2.42	0.52
1:A:2793:THR:OG1	1:A:2901:GLY:O	2.25	0.52
1:B:4889:CYS:HB3	1:B:4892:CYS:SG	2.49	0.52
1:D:228:LEU:HB3	1:D:289:ILE:HB	1.90	0.52
1:D:3729:GLN:O	1:D:3733:HIS:ND1	2.41	0.52
1:D:4108:GLU:HG3	1:D:4136:ARG:HH22	1.74	0.52
1:D:61:ASP:OD2	1:D:417:ARG:NH2	2.42	0.52
1:B:1094:TYR:OH	1:B:1808:ASP:OD1	2.28	0.52
1:B:4050:HIS:HB2	1:B:4068:LEU:HD11	1.91	0.52
1:B:636:LEU:HD21	1:B:643:LEU:HD21	1.90	0.52
1:C:677:LEU:HD11	1:C:792:VAL:HG21	1.91	0.52
1:B:1911:LEU:HD11	1:B:2063:ILE:HG12	1.90	0.52
1:B:3798:MET:HE1	1:B:3875:THR:HB	1.91	0.52
1:C:1094:TYR:OH	1:C:1808:ASP:OD1	2.28	0.52
1:C:3798:MET:HE1	1:C:3875:THR:HB	1.92	0.52
1:A:1911:LEU:HD11	1:A:2063:ILE:HG12	1.90	0.52
1:B:2488:LEU:O	1:B:2492:GLY:N	2.42	0.52
1:B:4791:ARG:CZ	1:C:4523:VAL:HG11	2.39	0.52
1:A:26:ALA:HB3	1:A:33:GLN:HB3	1.90	0.52
1:A:364:GLN:HE21	1:A:369:GLY:HA2	1.75	0.52
1:A:4889:CYS:HB3	1:A:4892:CYS:SG	2.49	0.52
1:C:2488:LEU:O	1:C:2492:GLY:N	2.42	0.52
1:A:4660:GLU:HG3	1:A:4664:ARG:HH21	1.73	0.52
1:A:4819:TYR:O	1:A:4823:ARG:NH2	2.33	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1487:MET:HB3	1:B:1520:PHE:HZ	1.75	0.52
1:B:26:ALA:HB3	1:B:33:GLN:HB3	1.90	0.52
1:B:3926:GLN:HE21	1:B:4936:GLY:H	1.56	0.52
1:C:4108:GLU:HG3	1:C:4136:ARG:HH22	1.74	0.52
1:A:1487:MET:HB3	1:A:1520:PHE:HZ	1.75	0.52
1:A:192:LEU:O	1:A:212:TRP:NE1	2.42	0.52
1:A:4046:LYS:HG3	1:A:4068:LEU:HD22	1.90	0.52
1:A:4791:ARG:CZ	1:B:4523:VAL:HG11	2.39	0.52
1:C:1726:ILE:HB	1:C:2109:ILE:HD11	1.91	0.52
1:C:636:LEU:HD21	1:C:643:LEU:HD21	1.90	0.52
1:D:3730:ALA:HA	1:D:3733:HIS:CE1	2.44	0.52
1:A:61:ASP:OD2	1:A:417:ARG:NH2	2.42	0.52
1:C:1938:GLN:HE22	1:C:3614:ARG:HA	1.75	0.52
1:A:1252:SER:HB2	1:A:1598:ARG:HB2	1.92	0.52
1:A:4108:GLU:HG3	1:A:4136:ARG:HH22	1.74	0.52
1:A:4523:VAL:HG11	1:D:4791:ARG:CZ	2.39	0.52
1:D:1094:TYR:OH	1:D:1808:ASP:OD1	2.28	0.52
1:D:1632:ILE:HD11	1:D:1637:ARG:HG2	1.92	0.52
1:C:4791:ARG:CZ	1:D:4523:VAL:HG11	2.39	0.52
1:A:1703:TYR:HD2	1:A:1820:PRO:HB2	1.75	0.52
1:A:476:GLN:NE2	1:A:3679:GLU:OE1	2.43	0.52
1:A:636:LEU:HD21	1:A:643:LEU:HD21	1.90	0.52
1:A:677:LEU:HD11	1:A:792:VAL:HG21	1.91	0.52
1:B:2192:LYS:O	1:B:2196:ASN:ND2	2.43	0.52
1:B:4108:GLU:HG3	1:B:4136:ARG:HH22	1.74	0.52
1:C:1632:ILE:HD11	1:C:1637:ARG:HG2	1.92	0.52
1:C:4050:HIS:HB2	1:C:4068:LEU:HD11	1.91	0.52
1:C:4873:GLU:HA	1:D:4875:ARG:HH11	1.68	0.52
1:D:3926:GLN:HE21	1:D:4936:GLY:H	1.56	0.52
1:A:4873:GLU:HA	1:B:4875:ARG:HH11	1.68	0.51
1:B:1252:SER:HB2	1:B:1598:ARG:HB2	1.92	0.51
1:D:1487:MET:HB3	1:D:1520:PHE:HZ	1.75	0.51
1:A:1938:GLN:HE22	1:A:3614:ARG:HA	1.75	0.51
1:B:1629:SER:HA	1:B:1640:ASP:HA	1.93	0.51
1:B:2103:LEU:HA	1:B:2106:THR:HG22	1.93	0.51
1:C:1487:MET:HB3	1:C:1520:PHE:HZ	1.75	0.51
1:C:2103:LEU:HA	1:C:2106:THR:HG22	1.93	0.51
1:C:2192:LYS:O	1:C:2196:ASN:ND2	2.43	0.51
1:D:4809:ASP:O	1:D:4813:CYS:N	2.39	0.51
1:A:1613:GLU:HB2	1:A:1618:LEU:H	1.76	0.51
1:B:1613:GLU:HB2	1:B:1618:LEU:H	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:GLN:NE2	1:B:3679:GLU:OE1	2.43	0.51
1:D:1613:GLU:HB2	1:D:1618:LEU:H	1.76	0.51
1:D:1629:SER:HA	1:D:1640:ASP:HA	1.93	0.51
1:D:677:LEU:HD11	1:D:792:VAL:HG21	1.91	0.51
1:C:1629:SER:HA	1:C:1640:ASP:HA	1.93	0.51
1:C:1703:TYR:HD2	1:C:1820:PRO:HB2	1.75	0.51
1:C:4809:ASP:O	1:C:4813:CYS:N	2.39	0.51
1:D:476:GLN:NE2	1:D:3679:GLU:OE1	2.43	0.51
1:B:364:GLN:HE21	1:B:369:GLY:HA2	1.75	0.51
1:C:1613:GLU:HB2	1:C:1618:LEU:H	1.76	0.51
1:C:476:GLN:NE2	1:C:3679:GLU:OE1	2.43	0.51
1:C:3980:VAL:HA	1:C:3983:LEU:HD23	1.92	0.51
1:D:1703:TYR:HD2	1:D:1820:PRO:HB2	1.75	0.51
1:D:364:GLN:HE21	1:D:369:GLY:HA2	1.75	0.51
1:A:4050:HIS:HB2	1:A:4068:LEU:HD11	1.91	0.51
1:B:1654:HIS:O	1:B:1657:THR:OG1	2.26	0.51
1:B:23:GLN:HA	1:B:36:CYS:HA	1.92	0.51
1:B:4163:LYS:HB2	1:B:4164:PRO:HD3	1.92	0.51
1:C:4636:ILE:O	1:C:4651:LYS:NZ	2.44	0.51
1:D:1252:SER:HB2	1:D:1598:ARG:HB2	1.92	0.51
1:D:192:LEU:O	1:D:212:TRP:NE1	2.42	0.51
1:D:2192:LYS:O	1:D:2196:ASN:ND2	2.43	0.51
1:D:1938:GLN:HE22	1:D:3614:ARG:HA	1.75	0.51
1:D:4636:ILE:O	1:D:4651:LYS:NZ	2.44	0.51
1:A:1094:TYR:OH	1:A:1808:ASP:OD1	2.28	0.51
1:A:4163:LYS:HB2	1:A:4164:PRO:HD3	1.92	0.51
1:B:1576:LYS:NZ	1:B:1589:GLN:OE1	2.44	0.51
1:B:4636:ILE:O	1:B:4651:LYS:NZ	2.44	0.51
1:C:1252:SER:HB2	1:C:1598:ARG:HB2	1.92	0.51
1:C:364:GLN:HE21	1:C:369:GLY:HA2	1.75	0.51
1:B:1703:TYR:HD2	1:B:1820:PRO:HB2	1.75	0.51
1:A:4875:ARG:CZ	1:D:4872:GLY:O	2.59	0.51
1:A:1576:LYS:NZ	1:A:1589:GLN:OE1	2.44	0.51
1:A:2103:LEU:HA	1:A:2106:THR:HG22	1.93	0.51
1:A:4636:ILE:O	1:A:4651:LYS:NZ	2.44	0.51
1:C:4872:GLY:O	1:D:4875:ARG:CZ	2.59	0.51
1:A:2192:LYS:O	1:A:2196:ASN:ND2	2.43	0.51
1:B:4872:GLY:O	1:C:4875:ARG:CZ	2.59	0.51
1:C:4819:TYR:O	1:C:4823:ARG:NH2	2.33	0.51
1:D:2103:LEU:HA	1:D:2106:THR:HG22	1.93	0.51
1:D:4050:HIS:HB2	1:D:4068:LEU:HD11	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1632:ILE:HD11	1:B:1637:ARG:HG2	1.92	0.50
1:B:4052:ALA:O	1:B:4056:HIS:ND1	2.44	0.50
1:C:150:GLN:NE2	1:C:158:CYS:SG	2.80	0.50
1:C:4052:ALA:O	1:C:4056:HIS:ND1	2.44	0.50
1:D:1726:ILE:HG13	1:D:1757:LEU:HD23	1.93	0.50
1:D:4174:ILE:HG21	1:D:4885:MET:HE2	1.93	0.50
1:A:1629:SER:HA	1:A:1640:ASP:HA	1.93	0.50
1:A:2857:LYS:HE3	1:A:2861:LEU:HD11	1.93	0.50
1:B:260:VAL:HG12	1:B:391:ALA:HB3	1.92	0.50
1:B:3980:VAL:HA	1:B:3983:LEU:HD23	1.92	0.50
1:C:419:ILE:HD13	1:C:492:GLU:HG3	1.93	0.50
1:A:3980:VAL:HA	1:A:3983:LEU:HD23	1.92	0.50
1:A:1911:LEU:HD22	1:A:2088:LEU:HD13	1.94	0.50
1:A:260:VAL:HG12	1:A:391:ALA:HB3	1.92	0.50
1:C:1128:LEU:HD13	1:C:1206:SER:HB2	1.94	0.50
1:C:1654:HIS:O	1:C:1657:THR:OG1	2.26	0.50
1:C:23:GLN:HA	1:C:36:CYS:HA	1.92	0.50
1:C:4647:ASP:O	1:C:4650:VAL:HG23	2.12	0.50
1:A:1632:ILE:HD11	1:A:1637:ARG:HG2	1.92	0.50
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.41	0.50
1:A:812:LYS:HD3	1:A:813:PHE:HB2	1.93	0.50
1:B:1431:ARG:HB3	1:B:1554:GLN:HB2	1.94	0.50
1:B:150:GLN:NE2	1:B:158:CYS:SG	2.80	0.50
1:B:1726:ILE:HG13	1:B:1757:LEU:HD23	1.93	0.50
1:B:2857:LYS:HE3	1:B:2861:LEU:HD11	1.93	0.50
1:B:1938:GLN:HE22	1:B:3614:ARG:HA	1.75	0.50
1:D:1128:LEU:HD13	1:D:1206:SER:HB2	1.94	0.50
1:D:1911:LEU:HD22	1:D:2088:LEU:HD13	1.94	0.50
1:C:1576:LYS:NZ	1:C:1589:GLN:OE1	2.44	0.50
1:C:260:VAL:HG12	1:C:391:ALA:HB3	1.92	0.50
1:C:812:LYS:HD3	1:C:813:PHE:HB2	1.93	0.50
1:D:1228:THR:HA	1:D:1232:LEU:HD12	1.94	0.50
1:A:1726:ILE:HG13	1:A:1757:LEU:HD23	1.93	0.50
1:A:2783:MET:HG2	1:A:2788:TRP:HE3	1.77	0.50
1:D:23:GLN:HA	1:D:36:CYS:HA	1.92	0.50
1:A:2439:ILE:HD13	1:A:2465:HIS:HB3	1.94	0.50
1:B:1444:GLY:HA2	1:B:1487:MET:HB2	1.94	0.50
1:C:1228:THR:HA	1:C:1232:LEU:HD12	1.94	0.50
1:C:1726:ILE:HG13	1:C:1757:LEU:HD23	1.93	0.50
1:C:565:LEU:HG	1:C:604:HIS:CE1	2.47	0.50
1:A:23:GLN:HA	1:A:36:CYS:HA	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4780:TYR:HA	1:A:4783:THR:HG22	1.94	0.50
1:B:419:ILE:HD13	1:B:492:GLU:HG3	1.93	0.50
1:C:4861:ALA:HA	1:C:4864:GLN:HB2	1.94	0.50
1:D:260:VAL:HG12	1:D:391:ALA:HB3	1.92	0.50
1:D:4163:LYS:HB2	1:D:4164:PRO:HD3	1.92	0.50
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.44	0.49
1:A:3961:GLN:NE2	1:A:4069:SER:OG	2.45	0.49
1:B:2439:ILE:HD13	1:B:2465:HIS:HB3	1.94	0.49
1:B:4647:ASP:O	1:B:4650:VAL:HG23	2.12	0.49
1:B:565:LEU:HG	1:B:604:HIS:CE1	2.47	0.49
1:C:1444:GLY:HA2	1:C:1487:MET:HB2	1.94	0.49
1:D:1576:LYS:NZ	1:D:1589:GLN:OE1	2.44	0.49
1:A:4811:LEU:HD23	1:B:4519:LEU:HG	1.94	0.49
1:A:4872:GLY:O	1:B:4875:ARG:CZ	2.59	0.49
1:B:4784:VAL:HG13	1:C:4738:PHE:CE2	2.47	0.49
1:B:4861:ALA:HA	1:B:4864:GLN:HB2	1.94	0.49
1:C:1911:LEU:HD22	1:C:2088:LEU:HD13	1.94	0.49
1:D:1654:HIS:O	1:D:1657:THR:OG1	2.26	0.49
1:D:2857:LYS:HE3	1:D:2861:LEU:HD11	1.93	0.49
1:D:719:GLY:H	1:D:722:LEU:HD12	1.77	0.49
1:A:4632:ASP:OD1	1:A:4709:TRP:NE1	2.42	0.49
1:A:4784:VAL:HG13	1:B:4738:PHE:CE2	2.47	0.49
1:B:2783:MET:HG2	1:B:2788:TRP:HE3	1.77	0.49
1:B:4811:LEU:HD23	1:C:4519:LEU:HG	1.94	0.49
1:C:4784:VAL:HG13	1:D:4738:PHE:CE2	2.47	0.49
1:D:3961:GLN:NE2	1:D:4069:SER:OG	2.45	0.49
1:D:4610:LYS:HB3	1:D:4616:LEU:HD22	1.94	0.49
1:A:1444:GLY:HA2	1:A:1487:MET:HB2	1.94	0.49
1:A:2521:LEU:HD22	1:A:2565:ALA:HB2	1.94	0.49
1:A:477:ASN:OD1	1:A:480:ARG:NH1	2.46	0.49
1:B:3961:GLN:NE2	1:B:4069:SER:OG	2.45	0.49
1:B:4780:TYR:HA	1:B:4783:THR:HG22	1.94	0.49
1:D:3980:VAL:HA	1:D:3983:LEU:HD23	1.92	0.49
1:A:4519:LEU:HG	1:D:4811:LEU:HD23	1.94	0.49
1:D:812:LYS:HD3	1:D:813:PHE:HB2	1.93	0.49
1:A:1228:THR:HA	1:A:1232:LEU:HD12	1.94	0.49
1:A:1431:ARG:HB3	1:A:1554:GLN:HB2	1.94	0.49
1:D:1444:GLY:HA2	1:D:1487:MET:HB2	1.94	0.49
1:D:2521:LEU:HD22	1:D:2565:ALA:HB2	1.94	0.49
1:A:288:HIS:ND1	1:A:349:MET:O	2.43	0.49
1:B:1911:LEU:HD22	1:B:2088:LEU:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2783:MET:HG2	1:C:2788:TRP:HE3	1.77	0.49
1:C:4163:LYS:HB2	1:C:4164:PRO:HD3	1.92	0.49
1:D:4003:MET:HG3	1:D:4004:LEU:HG	1.95	0.49
1:A:4647:ASP:O	1:A:4650:VAL:HG23	2.12	0.49
1:A:419:ILE:HD13	1:A:492:GLU:HG3	1.93	0.49
1:B:1184:ASP:HB3	1:B:1186:SER:H	1.78	0.49
1:B:1228:THR:HA	1:B:1232:LEU:HD12	1.94	0.49
1:C:2857:LYS:HE3	1:C:2861:LEU:HD11	1.93	0.49
1:D:227:TYR:CE1	1:D:355:LYS:HG2	2.47	0.49
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.44	0.49
1:D:477:ASN:OD1	1:D:480:ARG:NH1	2.46	0.49
1:A:1128:LEU:HD13	1:A:1206:SER:HB2	1.94	0.49
1:A:4610:LYS:HB3	1:A:4616:LEU:HD22	1.94	0.49
1:B:2521:LEU:HD22	1:B:2565:ALA:HB2	1.94	0.49
1:B:3729:GLN:O	1:B:3733:HIS:ND1	2.41	0.49
1:B:335:LYS:NZ	1:B:398:HIS:O	2.44	0.49
1:B:812:LYS:HD3	1:B:813:PHE:HB2	1.93	0.49
1:C:227:TYR:CE1	1:C:355:LYS:HG2	2.47	0.49
1:C:335:LYS:NZ	1:C:398:HIS:O	2.44	0.49
1:D:4647:ASP:O	1:D:4650:VAL:HG23	2.12	0.49
1:B:1473:LYS:HE2	1:B:1475:LYS:HE3	1.95	0.49
1:C:2439:ILE:HD13	1:C:2465:HIS:HB3	1.94	0.49
1:C:4610:LYS:HB3	1:C:4616:LEU:HD22	1.94	0.49
1:D:1086:ARG:HH22	1:D:1254:ARG:HB2	1.78	0.49
1:D:419:ILE:HD13	1:D:492:GLU:HG3	1.93	0.49
1:D:4780:TYR:HA	1:D:4783:THR:HG22	1.94	0.49
1:D:565:LEU:HG	1:D:604:HIS:CE1	2.47	0.49
1:A:1184:ASP:HB3	1:A:1186:SER:H	1.78	0.49
1:A:565:LEU:HG	1:A:604:HIS:CE1	2.47	0.49
1:B:2421:ARG:HH21	1:B:2425:ARG:HH21	1.61	0.49
1:B:719:GLY:H	1:B:722:LEU:HD12	1.77	0.49
1:C:1431:ARG:HB3	1:C:1554:GLN:HB2	1.94	0.49
1:C:2521:LEU:HD22	1:C:2565:ALA:HB2	1.94	0.49
1:C:4003:MET:HG3	1:C:4004:LEU:HG	1.95	0.49
1:D:1184:ASP:HB3	1:D:1186:SER:H	1.78	0.49
1:D:1431:ARG:HB3	1:D:1554:GLN:HB2	1.94	0.49
1:A:3663:ASP:OD2	1:A:3735:ARG:NH2	2.46	0.48
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.80	0.48
1:A:4774:LEU:HD13	1:B:4754:LEU:HD21	1.95	0.48
1:B:1086:ARG:HB2	1:B:1207:LEU:HB2	1.95	0.48
1:B:1220:ASP:O	1:B:1223:THR:N	2.35	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ASN:OD1	1:C:480:ARG:NH1	2.46	0.48
1:C:4174:ILE:HD13	1:C:4885:MET:HE1	1.96	0.48
1:D:2783:MET:HG2	1:D:2788:TRP:HE3	1.77	0.48
1:A:4191:VAL:HA	1:A:4194:CYS:HB2	1.96	0.48
1:A:4732:LEU:O	1:A:4736:ASN:N	2.44	0.48
1:A:4861:ALA:HA	1:A:4864:GLN:HB2	1.94	0.48
1:B:1128:LEU:HD13	1:B:1206:SER:HB2	1.94	0.48
1:B:2345:LEU:HD21	1:B:2434:VAL:HB	1.96	0.48
1:C:3663:ASP:OD2	1:C:3735:ARG:NH2	2.46	0.48
1:C:4780:TYR:HA	1:C:4783:THR:HG22	1.94	0.48
1:C:4764:ASN:ND2	1:C:4866:LEU:O	2.47	0.48
1:D:3663:ASP:OD2	1:D:3735:ARG:NH2	2.46	0.48
1:D:4861:ALA:HA	1:D:4864:GLN:HB2	1.94	0.48
1:A:1934:VAL:O	1:A:1938:GLN:N	2.43	0.48
1:A:2345:LEU:HD21	1:A:2434:VAL:HB	1.96	0.48
1:A:719:GLY:H	1:A:722:LEU:HD12	1.77	0.48
1:B:1184:ASP:OD2	1:B:1188:SER:OG	2.31	0.48
1:B:3663:ASP:OD2	1:B:3735:ARG:NH2	2.46	0.48
1:B:477:ASN:OD1	1:B:480:ARG:NH1	2.46	0.48
1:B:653:SER:OG	1:B:794:PHE:O	2.31	0.48
1:C:192:LEU:O	1:C:212:TRP:NE1	2.42	0.48
1:C:2723:ASN:OD1	1:C:2773:ARG:NH2	2.47	0.48
1:C:4774:LEU:HD13	1:D:4754:LEU:HD21	1.95	0.48
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.80	0.48
1:D:2209:ARG:HG3	1:D:2251:ASN:HD21	1.79	0.48
1:D:2345:LEU:HD21	1:D:2434:VAL:HB	1.96	0.48
1:A:4003:MET:HG3	1:A:4004:LEU:HG	1.95	0.48
1:B:1086:ARG:HH22	1:B:1254:ARG:HB2	1.78	0.48
1:C:2421:ARG:HH21	1:C:2425:ARG:HH21	1.61	0.48
1:C:4811:LEU:HD23	1:D:4519:LEU:HG	1.94	0.48
1:D:1184:ASP:OD2	1:D:1188:SER:OG	2.31	0.48
1:A:4013:MET:O	1:A:4017:PHE:N	2.46	0.48
1:C:2345:LEU:HD21	1:C:2434:VAL:HB	1.96	0.48
1:D:1473:LYS:HE2	1:D:1475:LYS:HE3	1.95	0.48
1:C:4780:TYR:OH	1:D:4515:ASN:ND2	2.46	0.48
1:A:1220:ASP:O	1:A:1223:THR:N	2.35	0.48
1:A:1473:LYS:HE2	1:A:1475:LYS:HE3	1.95	0.48
1:A:2421:ARG:HH21	1:A:2425:ARG:HH21	1.61	0.48
1:C:374:TYR:HA	1:C:391:ALA:HA	1.96	0.48
1:C:3961:GLN:NE2	1:C:4069:SER:OG	2.45	0.48
1:C:719:GLY:H	1:C:722:LEU:HD12	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:852:GLY:HA2	1:C:853:PRO:HA	1.69	0.48
1:D:2723:ASN:OD1	1:D:2773:ARG:NH2	2.47	0.48
1:A:1833:ILE:HG22	1:A:1834:PHE:H	1.79	0.48
1:A:428:ARG:O	1:A:432:GLY:N	2.46	0.48
1:A:4515:ASN:ND2	1:D:4780:TYR:OH	2.46	0.48
1:A:4780:TYR:OH	1:B:4515:ASN:ND2	2.46	0.48
1:C:2717:LYS:HB2	1:C:2792:ARG:HH22	1.79	0.48
1:D:4764:ASN:ND2	1:D:4866:LEU:O	2.47	0.48
1:A:4738:PHE:CE2	1:D:4784:VAL:HG13	2.47	0.48
1:A:4130:PHE:O	1:A:4134:LEU:N	2.45	0.48
1:B:2723:ASN:OD1	1:B:2773:ARG:NH2	2.47	0.48
1:B:4771:THR:OG1	1:C:4757:ILE:HD13	2.14	0.48
1:B:4780:TYR:OH	1:C:4515:ASN:ND2	2.46	0.48
1:D:2439:ILE:HD13	1:D:2465:HIS:HB3	1.94	0.48
1:B:1833:ILE:HG22	1:B:1834:PHE:H	1.79	0.48
1:B:192:LEU:O	1:B:212:TRP:NE1	2.42	0.48
1:B:3911:ILE:HG21	1:B:3971:GLU:HB3	1.96	0.48
1:B:4610:LYS:HB3	1:B:4616:LEU:HD22	1.94	0.48
1:C:1184:ASP:HB3	1:C:1186:SER:H	1.78	0.48
1:D:1086:ARG:HB2	1:D:1207:LEU:HB2	1.95	0.48
1:D:1626:GLN:O	1:D:1687:TYR:OH	2.32	0.48
1:B:4191:VAL:HA	1:B:4194:CYS:HB2	1.96	0.47
1:C:1473:LYS:HE2	1:C:1475:LYS:HE3	1.95	0.47
1:D:2717:LYS:HB2	1:D:2792:ARG:HH22	1.79	0.47
1:D:4013:MET:O	1:D:4017:PHE:N	2.46	0.47
1:D:4191:VAL:HA	1:D:4194:CYS:HB2	1.96	0.47
1:B:115:TYR:HB3	1:B:164:PRO:HD3	1.97	0.47
1:C:3729:GLN:O	1:C:3733:HIS:ND1	2.41	0.47
1:C:3911:ILE:HG21	1:C:3971:GLU:HB3	1.96	0.47
1:D:2421:ARG:HH21	1:D:2425:ARG:HH21	1.61	0.47
1:D:374:TYR:HA	1:D:391:ALA:HA	1.96	0.47
1:D:3911:ILE:HG21	1:D:3971:GLU:HB3	1.96	0.47
1:A:1086:ARG:HH22	1:A:1254:ARG:HB2	1.78	0.47
1:A:2723:ASN:OD1	1:A:2773:ARG:NH2	2.47	0.47
1:A:4764:ASN:ND2	1:A:4866:LEU:O	2.47	0.47
1:A:4771:THR:OG1	1:B:4757:ILE:HD13	2.14	0.47
1:D:2076:ILE:HG21	1:D:2081:LEU:HD22	1.97	0.47
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	1.96	0.47
1:A:115:TYR:HB3	1:A:164:PRO:HD3	1.97	0.47
1:A:3911:ILE:HG21	1:A:3971:GLU:HB3	1.96	0.47
1:B:4774:LEU:HD13	1:C:4754:LEU:HD21	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4764:ASN:ND2	1:B:4866:LEU:O	2.47	0.47
1:C:1086:ARG:HH22	1:C:1254:ARG:HB2	1.78	0.47
1:D:115:TYR:HB3	1:D:164:PRO:HD3	1.97	0.47
1:D:2793:THR:OG1	1:D:2901:GLY:O	2.25	0.47
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.31	0.47
1:A:2076:ILE:HG21	1:A:2081:LEU:HD22	1.97	0.47
1:A:374:TYR:HA	1:A:391:ALA:HA	1.96	0.47
1:B:4003:MET:HG3	1:B:4004:LEU:HG	1.95	0.47
1:C:590:LYS:HB2	1:C:593:HIS:HD2	1.80	0.47
1:C:718:VAL:HA	1:C:736:CYS:HB2	1.96	0.47
1:A:2717:LYS:HB2	1:A:2792:ARG:HH22	1.79	0.47
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.96	0.47
1:A:572:LEU:O	1:A:576:HIS:N	2.47	0.47
1:B:300:VAL:O	1:B:420:ARG:NH2	2.48	0.47
1:B:3800:SER:OG	1:B:3801:CYS:N	2.47	0.47
1:B:4191:VAL:HB	1:B:4950:TRP:HH2	1.79	0.47
1:B:572:LEU:O	1:B:576:HIS:N	2.47	0.47
1:C:1184:ASP:OD2	1:C:1188:SER:OG	2.31	0.47
1:C:1086:ARG:HB2	1:C:1207:LEU:HB2	1.95	0.47
1:C:115:TYR:HB3	1:C:164:PRO:HD3	1.97	0.47
1:C:2737:LYS:HB3	1:C:2742:TRP:HB2	1.96	0.47
1:A:4757:ILE:HD13	1:D:4771:THR:OG1	2.14	0.47
1:D:4191:VAL:HB	1:D:4950:TRP:HH2	1.79	0.47
1:A:1707:ILE:HA	1:A:1711:LEU:HB2	1.97	0.47
1:A:2209:ARG:HG3	1:A:2251:ASN:HD21	1.79	0.47
1:B:2076:ILE:HG21	1:B:2081:LEU:HD22	1.97	0.47
1:B:2717:LYS:HB2	1:B:2792:ARG:HH22	1.79	0.47
1:B:374:TYR:HA	1:B:391:ALA:HA	1.96	0.47
1:C:2121:LEU:O	1:C:2125:GLY:N	2.47	0.47
1:C:2793:THR:OG1	1:C:2901:GLY:O	2.25	0.47
1:C:4752:LYS:HA	1:C:4755:ARG:HE	1.80	0.47
1:A:1086:ARG:HB2	1:A:1207:LEU:HB2	1.95	0.47
1:C:2076:ILE:HG21	1:C:2081:LEU:HD22	1.97	0.47
1:C:4771:THR:OG1	1:D:4757:ILE:HD13	2.14	0.47
1:D:335:LYS:NZ	1:D:398:HIS:O	2.44	0.47
1:D:125:TYR:CZ	1:D:417:ARG:HB3	2.50	0.47
1:D:718:VAL:HA	1:D:736:CYS:HB2	1.96	0.47
1:B:2209:ARG:HG3	1:B:2251:ASN:HD21	1.79	0.47
1:B:2424:LEU:HD23	1:B:2476:VAL:HG22	1.97	0.47
1:B:2737:LYS:HB3	1:B:2742:TRP:HB2	1.96	0.47
1:B:4207:ILE:HG22	1:B:4498:ARG:HE	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4174:ILE:HG21	1:B:4885:MET:HE2	1.96	0.47
1:C:4191:VAL:HA	1:C:4194:CYS:HB2	1.96	0.47
1:D:300:VAL:O	1:D:420:ARG:NH2	2.48	0.47
1:D:4732:LEU:O	1:D:4736:ASN:N	2.44	0.47
1:D:590:LYS:HB2	1:D:593:HIS:HD2	1.80	0.47
1:A:4207:ILE:HG22	1:A:4498:ARG:HE	1.80	0.47
1:C:125:TYR:CZ	1:C:417:ARG:HB3	2.50	0.47
1:B:2301:ASP:OD1	1:B:2304:ARG:NH2	2.48	0.47
1:B:3696:MET:O	1:B:3699:SER:OG	2.26	0.47
1:B:4130:PHE:O	1:B:4134:LEU:N	2.45	0.47
1:B:4752:LYS:HA	1:B:4755:ARG:HE	1.80	0.47
1:A:1172:THR:HG21	1:A:1190:LEU:HD13	1.97	0.46
1:A:2301:ASP:OD1	1:A:2304:ARG:NH2	2.48	0.46
1:A:2737:LYS:HB3	1:A:2742:TRP:HB2	1.96	0.46
1:A:300:VAL:O	1:A:420:ARG:NH2	2.48	0.46
1:A:298:ARG:HE	1:A:303:GLY:HA2	1.81	0.46
1:A:125:TYR:CZ	1:A:417:ARG:HB3	2.50	0.46
1:B:125:TYR:CZ	1:B:417:ARG:HB3	2.50	0.46
1:C:1833:ILE:HG22	1:C:1834:PHE:H	1.79	0.46
1:C:2424:LEU:HD23	1:C:2476:VAL:HG22	1.97	0.46
1:D:1172:THR:HG21	1:D:1190:LEU:HD13	1.97	0.46
1:A:1174:MET:SD	1:A:1236:TYR:OH	2.73	0.46
1:B:1445:TRP:H	1:B:1487:MET:HB2	1.81	0.46
1:B:590:LYS:HB2	1:B:593:HIS:HD2	1.80	0.46
1:C:1172:THR:HG21	1:C:1190:LEU:HD13	1.97	0.46
1:C:2209:ARG:HG3	1:C:2251:ASN:HD21	1.79	0.46
1:C:300:VAL:O	1:C:420:ARG:NH2	2.48	0.46
1:D:1833:ILE:HG22	1:D:1834:PHE:H	1.79	0.46
1:D:2301:ASP:OD1	1:D:2304:ARG:NH2	2.48	0.46
1:D:2737:LYS:HB3	1:D:2742:TRP:HB2	1.96	0.46
1:D:4565:SER:OG	1:D:4566:SER:N	2.49	0.46
1:A:2858:LYS:HG2	1:A:2872:LEU:HD13	1.96	0.46
1:A:4565:SER:OG	1:A:4566:SER:N	2.49	0.46
1:A:590:LYS:HB2	1:A:593:HIS:HD2	1.80	0.46
1:B:1172:THR:HG21	1:B:1190:LEU:HD13	1.97	0.46
1:B:1763:PHE:HB3	1:B:1781:GLU:HB3	1.98	0.46
1:B:3804:LEU:HD13	1:B:3910:ALA:HB2	1.96	0.46
1:B:4627:ILE:O	1:B:4631:TRP:N	2.48	0.46
1:B:657:PRO:HA	1:B:834:VAL:HA	1.97	0.46
1:C:1626:GLN:O	1:C:1687:TYR:OH	2.32	0.46
1:C:4191:VAL:HB	1:C:4950:TRP:HH2	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4752:LYS:HA	1:D:4755:ARG:HE	1.80	0.46
1:A:4754:LEU:HD21	1:D:4774:LEU:HD13	1.95	0.46
1:A:1445:TRP:H	1:A:1487:MET:HB2	1.81	0.46
1:A:4752:LYS:HA	1:A:4755:ARG:HE	1.80	0.46
1:A:718:VAL:HA	1:A:736:CYS:HB2	1.96	0.46
1:B:1707:ILE:HA	1:B:1711:LEU:HB2	1.97	0.46
1:B:2121:LEU:O	1:B:2125:GLY:N	2.47	0.46
1:B:428:ARG:O	1:B:432:GLY:N	2.46	0.46
1:C:648:LEU:HD23	1:C:1684:GLN:HA	1.98	0.46
1:A:648:LEU:HD23	1:A:1684:GLN:HA	1.98	0.46
1:B:4201:MET:O	1:B:4205:ALA:N	2.49	0.46
1:B:648:LEU:HD23	1:B:1684:GLN:HA	1.98	0.46
1:B:718:VAL:HA	1:B:736:CYS:HB2	1.96	0.46
1:C:180:ASP:HB3	1:C:211:LEU:HD22	1.97	0.46
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.96	0.46
1:D:2858:LYS:HG2	1:D:2872:LEU:HD13	1.96	0.46
1:A:1763:PHE:HB3	1:A:1781:GLU:HB3	1.98	0.46
1:A:2326:ILE:HA	1:A:2326:ILE:HD13	1.83	0.46
1:A:2424:LEU:HD23	1:A:2476:VAL:HG22	1.97	0.46
1:A:4191:VAL:HB	1:A:4950:TRP:HH2	1.79	0.46
1:B:852:GLY:HA2	1:B:853:PRO:HA	1.69	0.46
1:D:2424:LEU:HD23	1:D:2476:VAL:HG22	1.97	0.46
1:A:4174:ILE:HG21	1:A:4885:MET:HE2	1.97	0.46
1:A:657:PRO:HA	1:A:834:VAL:HA	1.97	0.46
1:B:2858:LYS:HG2	1:B:2872:LEU:HD13	1.96	0.46
1:B:436:LEU:HD13	1:B:518:ALA:HA	1.98	0.46
1:C:1174:MET:SD	1:C:1236:TYR:OH	2.73	0.46
1:C:2301:ASP:OD1	1:C:2304:ARG:NH2	2.48	0.46
1:C:298:ARG:HA	1:C:305:TYR:HA	1.97	0.46
1:C:4632:ASP:OD1	1:C:4709:TRP:NE1	2.42	0.46
1:C:698:ALA:HB2	1:C:722:LEU:HD23	1.98	0.46
1:D:298:ARG:HA	1:D:305:TYR:HA	1.97	0.46
1:D:698:ALA:HB2	1:D:722:LEU:HD23	1.98	0.46
1:A:298:ARG:HA	1:A:305:TYR:HA	1.97	0.46
1:A:436:LEU:HD13	1:A:518:ALA:HA	1.98	0.46
1:B:180:ASP:HB3	1:B:211:LEU:HD22	1.97	0.46
1:C:1707:ILE:HA	1:C:1711:LEU:HB2	1.97	0.46
1:C:170:SER:OG	1:C:171:GLU:N	2.49	0.46
1:C:4627:ILE:O	1:C:4631:TRP:N	2.48	0.46
1:C:572:LEU:O	1:C:576:HIS:N	2.47	0.46
1:D:298:ARG:HE	1:D:303:GLY:HA2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4201:MET:O	1:D:4205:ALA:N	2.49	0.46
1:A:4875:ARG:HH11	1:D:4873:GLU:HA	1.68	0.46
1:D:657:PRO:HA	1:D:834:VAL:HA	1.97	0.46
1:B:1174:MET:SD	1:B:1236:TYR:OH	2.73	0.46
1:A:189:GLU:CG	1:B:2419:ARG:NH2	2.79	0.46
1:B:298:ARG:HA	1:B:305:TYR:HA	1.97	0.46
1:B:4565:SER:OG	1:B:4566:SER:N	2.49	0.46
1:B:189:GLU:CG	1:C:2419:ARG:NH2	2.79	0.46
1:C:2858:LYS:HG2	1:C:2872:LEU:HD13	1.96	0.46
1:D:1174:MET:SD	1:D:1236:TYR:OH	2.73	0.46
1:C:189:GLU:OE1	1:D:2419:ARG:CZ	2.64	0.46
1:D:537:LEU:HD11	1:D:551:PHE:HZ	1.81	0.46
1:A:695:VAL:O	1:A:725:TYR:N	2.49	0.46
1:B:537:LEU:HD11	1:B:551:PHE:HZ	1.81	0.46
1:C:288:HIS:ND1	1:C:349:MET:O	2.43	0.46
1:C:478:ARG:HE	1:C:485:ARG:HH22	1.64	0.46
1:D:648:LEU:HD23	1:D:1684:GLN:HA	1.98	0.46
1:D:1707:ILE:HA	1:D:1711:LEU:HB2	1.97	0.46
1:C:189:GLU:CG	1:D:2419:ARG:NH2	2.79	0.46
1:D:478:ARG:HE	1:D:485:ARG:HH22	1.64	0.46
1:A:537:LEU:HD11	1:A:551:PHE:HZ	1.81	0.45
1:C:298:ARG:HE	1:C:303:GLY:HA2	1.81	0.45
1:C:4565:SER:OG	1:C:4566:SER:N	2.49	0.45
1:D:4207:ILE:HG22	1:D:4498:ARG:HE	1.80	0.45
1:D:428:ARG:O	1:D:432:GLY:N	2.46	0.45
1:D:4627:ILE:O	1:D:4631:TRP:N	2.48	0.45
1:A:170:SER:OG	1:A:171:GLU:N	2.49	0.45
1:B:237:LEU:N	1:B:404:ASN:O	2.49	0.45
1:B:4869:ASP:O	1:B:4873:GLU:N	2.49	0.45
1:C:237:LEU:N	1:C:404:ASN:O	2.49	0.45
1:C:646:THR:OG1	1:C:1684:GLN:NE2	2.49	0.45
1:C:657:PRO:HA	1:C:834:VAL:HA	1.97	0.45
1:D:1763:PHE:HB3	1:D:1781:GLU:HB3	1.98	0.45
1:A:2419:ARG:CZ	1:D:189:GLU:OE1	2.64	0.45
1:A:848:ARG:HB2	1:A:1603:PHE:HZ	1.81	0.45
1:A:180:ASP:HB3	1:A:211:LEU:HD22	1.97	0.45
1:C:1445:TRP:H	1:C:1487:MET:HB2	1.81	0.45
1:C:1763:PHE:HB3	1:C:1781:GLU:HB3	1.98	0.45
1:D:848:ARG:HB2	1:D:1603:PHE:HZ	1.81	0.45
1:A:646:THR:OG1	1:A:1684:GLN:NE2	2.49	0.45
1:A:698:ALA:HB2	1:A:722:LEU:HD23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLU:OE1	1:C:2419:ARG:CZ	2.64	0.45
1:B:698:ALA:HB2	1:B:722:LEU:HD23	1.98	0.45
1:C:4207:ILE:HG22	1:C:4498:ARG:HE	1.80	0.45
1:A:2419:ARG:NH2	1:D:189:GLU:CG	2.79	0.45
1:D:180:ASP:HB3	1:D:211:LEU:HD22	1.97	0.45
1:D:4869:ASP:O	1:D:4873:GLU:N	2.49	0.45
1:A:189:GLU:OE1	1:B:2419:ARG:CZ	2.64	0.45
1:A:4201:MET:O	1:A:4205:ALA:N	2.49	0.45
1:B:298:ARG:HE	1:B:303:GLY:HA2	1.81	0.45
1:C:4013:MET:O	1:C:4017:PHE:N	2.46	0.45
1:D:3859:LEU:HD22	1:D:3871:ILE:HG21	1.98	0.45
1:D:843:GLU:HA	1:D:848:ARG:HG2	1.98	0.45
1:A:227:TYR:CE1	1:A:355:LYS:HG2	2.47	0.45
1:A:4588:ILE:HG22	1:A:4723:LEU:HD23	1.99	0.45
1:B:1602:GLN:HB3	1:B:1604:LEU:HD12	1.99	0.45
1:B:4142:SER:HB3	1:B:4940:TYR:CE1	2.52	0.45
1:D:436:LEU:HD13	1:D:518:ALA:HA	1.98	0.45
1:D:4588:ILE:HG22	1:D:4723:LEU:HD23	1.99	0.45
1:D:766:ILE:HB	1:D:779:PHE:HB2	1.99	0.45
1:A:4142:SER:HB3	1:A:4940:TYR:CE1	2.52	0.45
1:A:478:ARG:HE	1:A:485:ARG:HH22	1.64	0.45
1:B:478:ARG:HE	1:B:485:ARG:HH22	1.64	0.45
1:C:1220:ASP:O	1:C:1223:THR:N	2.35	0.45
1:C:4201:MET:O	1:C:4205:ALA:N	2.49	0.45
1:C:4142:SER:HB3	1:C:4940:TYR:CE1	2.52	0.45
1:C:537:LEU:HD11	1:C:551:PHE:HZ	1.81	0.45
1:C:766:ILE:HB	1:C:779:PHE:HB2	1.99	0.45
1:D:1445:TRP:H	1:D:1487:MET:HB2	1.81	0.45
1:D:3800:SER:OG	1:D:3801:CYS:N	2.47	0.45
1:A:843:GLU:HA	1:A:848:ARG:HG2	1.98	0.45
1:B:1934:VAL:O	1:B:1938:GLN:N	2.43	0.45
1:C:419:ILE:HG12	1:C:489:PHE:CE1	2.52	0.45
1:C:4588:ILE:HG22	1:C:4723:LEU:HD23	1.99	0.45
1:D:289:ILE:HG22	1:D:354:ILE:HD12	1.99	0.45
1:A:2525:VAL:HG13	1:A:2528:LEU:HD12	1.99	0.45
1:B:695:VAL:O	1:B:725:TYR:N	2.49	0.45
1:C:3743:GLN:NE2	1:C:3781:TYR:OH	2.43	0.45
1:C:3952:PHE:HB3	1:C:3976:GLN:HE22	1.82	0.45
1:D:3737:ALA:O	1:D:3740:MET:HG2	2.17	0.45
1:A:3952:PHE:HB3	1:A:3976:GLN:HE22	1.82	0.45
1:B:308:LEU:HD22	1:B:370:LEU:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3737:ALA:O	1:B:3740:MET:HG2	2.17	0.45
1:C:4203:LEU:O	1:C:4207:ILE:HG12	2.17	0.45
1:C:428:ARG:O	1:C:432:GLY:N	2.46	0.45
1:C:436:LEU:HD13	1:C:518:ALA:HA	1.98	0.45
1:A:766:ILE:HB	1:A:779:PHE:HB2	1.99	0.44
1:B:4036:TYR:HE2	1:B:4048:ASP:HB3	1.82	0.44
1:B:419:ILE:HG12	1:B:489:PHE:CE1	2.52	0.44
1:C:143:LEU:CD2	1:D:2426:SER:HB3	2.47	0.44
1:C:1602:GLN:HB3	1:C:1604:LEU:HD12	1.99	0.44
1:C:4747:ILE:HG13	1:C:4754:LEU:HD22	1.99	0.44
1:C:843:GLU:HA	1:C:848:ARG:HG2	1.98	0.44
1:D:4844:ARG:HH12	1:D:4848:ASP:HB2	1.83	0.44
1:D:419:ILE:HG12	1:D:489:PHE:CE1	2.52	0.44
1:D:745:ASN:ND2	1:D:773:GLN:OE1	2.48	0.44
1:A:1626:GLN:O	1:A:1687:TYR:OH	2.32	0.44
1:A:4627:ILE:O	1:A:4631:TRP:N	2.48	0.44
1:A:4844:ARG:HH12	1:A:4848:ASP:HB2	1.83	0.44
1:A:4869:ASP:O	1:A:4873:GLU:N	2.49	0.44
1:A:419:ILE:HG12	1:A:489:PHE:CE1	2.52	0.44
1:B:848:ARG:HB2	1:B:1603:PHE:HZ	1.81	0.44
1:B:4747:ILE:HG13	1:B:4754:LEU:HD22	1.99	0.44
1:B:4845:ILE:O	1:B:4849:ILE:N	2.44	0.44
1:B:4844:ARG:HH12	1:B:4848:ASP:HB2	1.83	0.44
1:C:3737:ALA:O	1:C:3740:MET:HG2	2.17	0.44
1:D:1170:GLU:O	1:D:1172:THR:N	2.50	0.44
1:D:2121:LEU:O	1:D:2125:GLY:N	2.47	0.44
1:D:4203:LEU:O	1:D:4207:ILE:HG12	2.17	0.44
1:D:4632:ASP:OD1	1:D:4709:TRP:NE1	2.42	0.44
1:A:308:LEU:HD22	1:A:370:LEU:HD12	1.98	0.44
1:A:3859:LEU:HD22	1:A:3871:ILE:HG21	1.98	0.44
1:B:1799:VAL:O	1:B:1803:SER:N	2.46	0.44
1:B:2525:VAL:HG13	1:B:2528:LEU:HD12	1.99	0.44
1:B:3859:LEU:HD22	1:B:3871:ILE:HG21	1.98	0.44
1:B:3925:ILE:HG21	1:B:3925:ILE:HD13	1.70	0.44
1:B:4013:MET:O	1:B:4017:PHE:N	2.46	0.44
1:B:4588:ILE:HG22	1:B:4723:LEU:HD23	1.99	0.44
1:B:766:ILE:HB	1:B:779:PHE:HB2	1.99	0.44
1:C:1087:ILE:HG23	1:C:1128:LEU:HD12	2.00	0.44
1:C:289:ILE:HG22	1:C:354:ILE:HD12	1.99	0.44
1:C:695:VAL:O	1:C:725:TYR:N	2.49	0.44
1:D:466:PRO:HB3	1:D:478:ARG:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4747:ILE:HG13	1:A:4754:LEU:HD22	1.99	0.44
1:A:745:ASN:ND2	1:A:773:GLN:OE1	2.48	0.44
1:B:4203:LEU:O	1:B:4207:ILE:HG12	2.17	0.44
1:B:466:PRO:HB3	1:B:478:ARG:HG2	1.99	0.44
1:D:308:LEU:HD22	1:D:370:LEU:HD12	1.98	0.44
1:D:695:VAL:O	1:D:725:TYR:N	2.49	0.44
1:A:2390:MET:HG3	1:A:2465:HIS:CE1	2.53	0.44
1:A:3767:LEU:O	1:A:3770:GLY:N	2.51	0.44
1:A:4203:LEU:O	1:A:4207:ILE:HG12	2.17	0.44
1:B:646:THR:OG1	1:B:1684:GLN:NE2	2.49	0.44
1:C:848:ARG:HB2	1:C:1603:PHE:HZ	1.81	0.44
1:C:2390:MET:HG3	1:C:2465:HIS:CE1	2.53	0.44
1:C:4130:PHE:O	1:C:4134:LEU:N	2.45	0.44
1:D:1011:ARG:HB3	1:D:1032:LEU:HD21	2.00	0.44
1:D:1934:VAL:O	1:D:1938:GLN:N	2.43	0.44
1:D:4747:ILE:HG13	1:D:4754:LEU:HD22	1.99	0.44
1:A:1136:ALA:HB3	1:A:1145:TRP:HB2	2.00	0.44
1:A:1602:GLN:HB3	1:A:1604:LEU:HD12	1.99	0.44
1:A:2121:LEU:O	1:A:2125:GLY:N	2.47	0.44
1:A:2832:VAL:O	1:A:2895:LYS:NZ	2.45	0.44
1:A:466:PRO:HB3	1:A:478:ARG:HG2	1.99	0.44
1:B:843:GLU:HA	1:B:848:ARG:HG2	1.98	0.44
1:C:2525:VAL:HG13	1:C:2528:LEU:HD12	1.99	0.44
1:C:299:HIS:NE2	1:C:301:THR:OG1	2.46	0.44
1:C:308:LEU:HD22	1:C:370:LEU:HD12	1.98	0.44
1:D:1087:ILE:HG23	1:D:1128:LEU:HD12	2.00	0.44
1:D:2390:MET:HG3	1:D:2465:HIS:CE1	2.53	0.44
1:D:3952:PHE:HB3	1:D:3976:GLN:HE22	1.82	0.44
1:D:237:LEU:N	1:D:404:ASN:O	2.49	0.44
1:D:4142:SER:HB3	1:D:4940:TYR:CE1	2.52	0.44
1:A:1664:VAL:HG12	1:A:1672:VAL:HG11	2.00	0.44
1:A:1799:VAL:O	1:A:1803:SER:N	2.46	0.44
1:A:4867:ILE:HG23	1:A:4867:ILE:HD12	1.80	0.44
1:B:1092:LYS:H	1:B:1250:TRP:HZ3	1.66	0.44
1:B:123:HIS:CD2	1:B:126:SER:H	2.34	0.44
1:B:4632:ASP:OD1	1:B:4709:TRP:NE1	2.42	0.44
1:B:655:MET:HG2	1:B:836:HIS:HA	2.00	0.44
1:C:123:HIS:CD2	1:C:126:SER:H	2.34	0.44
1:C:4732:LEU:O	1:C:4736:ASN:N	2.44	0.44
1:C:655:MET:HG2	1:C:836:HIS:HA	2.00	0.44
1:B:1626:GLN:O	1:B:1687:TYR:OH	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:TYR:O	1:B:201:LEU:N	2.51	0.44
1:B:2390:MET:HG3	1:B:2465:HIS:CE1	2.53	0.44
1:B:2732:LYS:HA	1:B:2732:LYS:HD2	1.82	0.44
1:B:4500:PHE:HA	1:B:4503:MET:HB2	2.00	0.44
1:B:4732:LEU:O	1:B:4736:ASN:N	2.44	0.44
1:C:4500:PHE:HA	1:C:4503:MET:HB2	2.00	0.44
1:D:1664:VAL:HG12	1:D:1672:VAL:HG11	2.00	0.44
1:D:1720:MET:HE2	1:D:2128:ARG:HD2	2.00	0.44
1:D:4036:TYR:HE2	1:D:4048:ASP:HB3	1.82	0.44
1:A:289:ILE:HG22	1:A:354:ILE:HD12	1.99	0.44
1:A:655:MET:HG2	1:A:836:HIS:HA	2.00	0.44
1:B:4610:LYS:O	1:B:4615:GLY:N	2.51	0.44
1:D:196:TYR:O	1:D:201:LEU:N	2.51	0.44
1:D:3767:LEU:O	1:D:3770:GLY:N	2.51	0.44
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.51	0.43
1:A:196:TYR:O	1:A:201:LEU:N	2.51	0.43
1:A:4610:LYS:O	1:A:4615:GLY:N	2.51	0.43
1:A:4178:VAL:HG11	1:A:4881:VAL:HA	1.99	0.43
1:B:3743:GLN:NE2	1:B:3781:TYR:OH	2.43	0.43
1:B:4739:PHE:HA	1:B:4739:PHE:HD1	1.76	0.43
1:C:1011:ARG:HB3	1:C:1032:LEU:HD21	2.00	0.43
1:D:4610:LYS:O	1:D:4615:GLY:N	2.51	0.43
1:D:646:THR:OG1	1:D:1684:GLN:NE2	2.49	0.43
1:D:655:MET:HG2	1:D:836:HIS:HA	2.00	0.43
1:A:2426:SER:HB3	1:D:143:LEU:CD2	2.47	0.43
1:A:908:ARG:HA	1:A:916:PRO:HD3	2.00	0.43
1:B:289:ILE:HG22	1:B:354:ILE:HD12	1.99	0.43
1:B:288:HIS:ND1	1:B:349:MET:O	2.43	0.43
1:B:227:TYR:CE1	1:B:355:LYS:HG2	2.47	0.43
1:C:3859:LEU:HD22	1:C:3871:ILE:HG21	1.98	0.43
1:C:4759:SER:O	1:C:4763:HIS:ND1	2.30	0.43
1:C:4869:ASP:O	1:C:4873:GLU:N	2.49	0.43
1:C:4763:HIS:CE1	1:C:4870:ALA:HB1	2.53	0.43
1:C:758:CYS:SG	1:C:759:LEU:N	2.91	0.43
1:D:1602:GLN:HB3	1:D:1604:LEU:HD12	1.99	0.43
1:D:170:SER:OG	1:D:171:GLU:N	2.49	0.43
1:D:2525:VAL:HG13	1:D:2528:LEU:HD12	1.99	0.43
1:D:4763:HIS:CE1	1:D:4870:ALA:HB1	2.53	0.43
1:D:758:CYS:SG	1:D:759:LEU:N	2.91	0.43
1:D:908:ARG:HA	1:D:916:PRO:HD3	2.00	0.43
1:A:143:LEU:CD2	1:B:2426:SER:HB3	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1720:MET:HE2	1:A:2128:ARG:HD2	2.00	0.43
1:A:4763:HIS:CE1	1:A:4870:ALA:HB1	2.53	0.43
1:B:1664:VAL:HG12	1:B:1672:VAL:HG11	2.00	0.43
1:A:189:GLU:HB2	1:B:2419:ARG:HH22	1.84	0.43
1:B:908:ARG:HA	1:B:916:PRO:HD3	2.00	0.43
1:C:466:PRO:HB3	1:C:478:ARG:HG2	1.99	0.43
1:C:4178:VAL:HG11	1:C:4881:VAL:HA	1.99	0.43
1:A:2419:ARG:HH22	1:D:189:GLU:HB2	1.84	0.43
1:A:1092:LYS:H	1:A:1250:TRP:HZ3	1.66	0.43
1:A:1654:HIS:O	1:A:1657:THR:OG1	2.26	0.43
1:A:4036:TYR:HE2	1:A:4048:ASP:HB3	1.82	0.43
1:A:4523:VAL:HG22	1:D:4808:ASP:OD2	2.19	0.43
1:A:4514:ILE:HG21	1:A:4740:PHE:CE2	2.52	0.43
1:A:462:TYR:O	1:A:485:ARG:NH1	2.51	0.43
1:A:758:CYS:SG	1:A:759:LEU:N	2.91	0.43
1:B:170:SER:OG	1:B:171:GLU:N	2.49	0.43
1:B:189:GLU:HB2	1:C:2419:ARG:HH22	1.84	0.43
1:C:1090:ALA:HB3	1:C:1203:PRO:HD2	2.00	0.43
1:C:462:TYR:O	1:C:485:ARG:NH1	2.51	0.43
1:D:1136:ALA:HB3	1:D:1145:TRP:HB2	2.00	0.43
1:A:3737:ALA:O	1:A:3740:MET:HG2	2.17	0.43
1:A:237:LEU:N	1:A:404:ASN:O	2.49	0.43
1:A:4791:ARG:HD2	1:A:4808:ASP:HB2	2.00	0.43
1:A:4924:MET:O	1:A:4928:ASN:HB2	2.18	0.43
1:B:1449:ASP:N	1:B:1449:ASP:OD1	2.51	0.43
1:B:4763:HIS:CE1	1:B:4870:ALA:HB1	2.53	0.43
1:B:4809:ASP:O	1:B:4813:CYS:N	2.39	0.43
1:B:758:CYS:SG	1:B:759:LEU:N	2.91	0.43
1:B:745:ASN:ND2	1:B:773:GLN:OE1	2.48	0.43
1:C:4036:TYR:HE2	1:C:4048:ASP:HB3	1.82	0.43
1:D:1220:ASP:O	1:D:1223:THR:N	2.35	0.43
1:C:189:GLU:HB2	1:D:2419:ARG:HH22	1.84	0.43
1:A:1165:MET:HB2	1:A:1174:MET:HB2	2.01	0.43
1:A:2440:ALA:HB2	1:A:2466:LYS:HD2	2.01	0.43
1:A:335:LYS:NZ	1:A:398:HIS:O	2.44	0.43
1:A:4500:PHE:HA	1:A:4503:MET:HB2	2.00	0.43
1:A:4808:ASP:OD2	1:B:4523:VAL:HG22	2.19	0.43
1:B:1011:ARG:HB3	1:B:1032:LEU:HD21	2.00	0.43
1:B:1087:ILE:HG23	1:B:1128:LEU:HD12	2.00	0.43
1:C:1092:LYS:H	1:C:1250:TRP:HZ3	1.66	0.43
1:C:4739:PHE:HA	1:C:4739:PHE:HD1	1.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4844:ARG:HH12	1:C:4848:ASP:HB2	1.83	0.43
1:C:604:HIS:HA	1:C:1588:VAL:HB	2.01	0.43
1:C:691:THR:HB	1:C:796:ALA:HB2	2.01	0.43
1:C:832:LEU:O	1:C:1614:ARG:NH1	2.51	0.43
1:D:1719:LEU:HD21	1:D:1830:ILE:HD13	2.01	0.43
1:D:691:THR:HB	1:D:796:ALA:HB2	2.01	0.43
1:A:1011:ARG:HB3	1:A:1032:LEU:HD21	2.00	0.43
1:A:532:SER:HA	1:A:535:GLU:HB3	2.01	0.43
1:B:1136:ALA:HB3	1:B:1145:TRP:HB2	2.00	0.43
1:B:1790:LYS:O	1:B:1794:MET:N	2.44	0.43
1:B:3952:PHE:HB3	1:B:3976:GLN:HE22	1.82	0.43
1:B:4178:VAL:HG11	1:B:4881:VAL:HA	1.99	0.43
1:C:1719:LEU:HD21	1:C:1830:ILE:HD13	2.01	0.43
1:C:196:TYR:O	1:C:201:LEU:N	2.51	0.43
1:C:2832:VAL:O	1:C:2895:LYS:NZ	2.45	0.43
1:C:4610:LYS:O	1:C:4615:GLY:N	2.51	0.43
1:C:4791:ARG:HD2	1:C:4808:ASP:HB2	2.00	0.43
1:C:4845:ILE:O	1:C:4849:ILE:N	2.44	0.43
1:D:4725:TRP:O	1:D:4729:MET:HG2	2.19	0.43
1:A:1090:ALA:HB3	1:A:1203:PRO:HD2	2.00	0.43
1:A:1719:LEU:HD21	1:A:1830:ILE:HD13	2.01	0.43
1:B:1090:ALA:HB3	1:B:1203:PRO:HD2	2.00	0.43
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.84	0.43
1:C:1449:ASP:OD1	1:C:1449:ASP:N	2.51	0.43
1:C:1664:VAL:HG12	1:C:1672:VAL:HG11	2.00	0.43
1:C:1733:THR:HG22	1:C:1755:THR:HB	2.00	0.43
1:C:2102:ALA:O	1:C:2106:THR:N	2.47	0.43
1:C:4514:ILE:HG21	1:C:4740:PHE:CE2	2.52	0.43
1:C:4571:PRO:O	1:C:4575:ILE:N	2.49	0.43
1:C:745:ASN:ND2	1:C:773:GLN:OE1	2.48	0.43
1:D:1165:MET:HB2	1:D:1174:MET:HB2	2.01	0.43
1:D:4178:VAL:HG11	1:D:4881:VAL:HA	1.99	0.43
1:D:4791:ARG:HD2	1:D:4808:ASP:HB2	2.00	0.43
1:D:462:TYR:O	1:D:485:ARG:NH1	2.51	0.43
1:A:1170:GLU:O	1:A:1172:THR:N	2.50	0.43
1:A:1733:THR:HG22	1:A:1755:THR:HB	2.00	0.43
1:A:4725:TRP:O	1:A:4729:MET:HG2	2.19	0.43
1:A:629:GLN:OE1	1:A:1669:ASN:ND2	2.52	0.43
1:B:4808:ASP:OD2	1:C:4523:VAL:HG22	2.19	0.43
1:C:1119:ARG:NH2	1:C:1196:ASP:O	2.48	0.43
1:C:1799:VAL:O	1:C:1803:SER:N	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3800:SER:OG	1:C:3801:CYS:N	2.47	0.43
1:A:1087:ILE:HG23	1:A:1128:LEU:HD12	2.00	0.43
1:A:832:LEU:O	1:A:1614:ARG:NH1	2.51	0.43
1:A:4809:ASP:O	1:A:4813:CYS:N	2.39	0.43
1:B:1172:THR:HG22	1:B:1193:LYS:HG3	2.01	0.43
1:B:1719:LEU:HD21	1:B:1830:ILE:HD13	2.01	0.43
1:B:3767:LEU:O	1:B:3770:GLY:N	2.51	0.43
1:B:4791:ARG:HD2	1:B:4808:ASP:HB2	2.00	0.43
1:B:629:GLN:OE1	1:B:1669:ASN:ND2	2.52	0.43
1:C:1032:LEU:HD23	1:C:1032:LEU:HA	1.82	0.43
1:C:1790:LYS:O	1:C:1794:MET:N	2.44	0.43
1:C:2196:ASN:OD1	1:C:2199:ARG:NH1	2.52	0.43
1:C:411:GLU:HA	1:C:414:ARG:HB2	2.01	0.43
1:C:4924:MET:O	1:C:4928:ASN:HB2	2.18	0.43
1:D:1090:ALA:HB3	1:D:1203:PRO:HD2	2.00	0.43
1:D:1733:THR:HG22	1:D:1755:THR:HB	2.00	0.43
1:D:2196:ASN:OD1	1:D:2199:ARG:NH1	2.52	0.43
1:D:4130:PHE:O	1:D:4134:LEU:N	2.45	0.43
1:D:4500:PHE:HA	1:D:4503:MET:HB2	2.00	0.43
1:D:4514:ILE:HG21	1:D:4740:PHE:CE2	2.52	0.43
1:D:4867:ILE:HD12	1:D:4867:ILE:HG23	1.80	0.43
1:D:4924:MET:O	1:D:4928:ASN:HB2	2.18	0.43
1:A:691:THR:HB	1:A:796:ALA:HB2	2.01	0.42
1:B:832:LEU:O	1:B:1614:ARG:NH1	2.51	0.42
1:B:2102:ALA:O	1:B:2106:THR:N	2.47	0.42
1:B:258:ARG:HA	1:B:316:LEU:HB2	2.01	0.42
1:B:3919:ASN:O	1:B:3922:THR:OG1	2.35	0.42
1:B:565:LEU:HD11	1:B:603:LYS:HG2	2.01	0.42
1:C:258:ARG:HA	1:C:316:LEU:HB2	2.01	0.42
1:C:565:LEU:HD11	1:C:603:LYS:HG2	2.01	0.42
1:D:2834:LEU:HG	1:D:2895:LYS:HZ3	1.84	0.42
1:A:1156:TRP:HB2	1:A:1160:ASP:HB2	2.01	0.42
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.84	0.42
1:B:4514:ILE:HG21	1:B:4740:PHE:CE2	2.52	0.42
1:B:462:TYR:O	1:B:485:ARG:NH1	2.51	0.42
1:B:604:HIS:HA	1:B:1588:VAL:HB	2.01	0.42
1:B:703:TYR:CZ	1:B:722:LEU:HD21	2.54	0.42
1:C:1136:ALA:HB3	1:C:1145:TRP:HB2	2.00	0.42
1:C:4808:ASP:OD2	1:D:4523:VAL:HG22	2.19	0.42
1:C:908:ARG:HA	1:C:916:PRO:HD3	2.00	0.42
1:D:604:HIS:HA	1:D:1588:VAL:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:GLN:OE1	1:D:1669:ASN:ND2	2.52	0.42
1:A:1172:THR:HG22	1:A:1193:LYS:HG3	2.01	0.42
1:A:4161:TRP:CD1	1:A:4201:MET:HE1	2.53	0.42
1:B:1165:MET:HB2	1:B:1174:MET:HB2	2.01	0.42
1:B:1119:ARG:NH2	1:B:1196:ASP:O	2.48	0.42
1:B:694:ARG:N	1:B:793:SER:O	2.45	0.42
1:C:703:TYR:CZ	1:C:722:LEU:HD21	2.54	0.42
1:D:1449:ASP:N	1:D:1449:ASP:OD1	2.51	0.42
1:D:3696:MET:O	1:D:3699:SER:OG	2.26	0.42
1:D:4161:TRP:CD1	1:D:4201:MET:HE1	2.53	0.42
1:D:532:SER:HA	1:D:535:GLU:HB3	2.01	0.42
1:A:355:LYS:HE3	1:A:355:LYS:HB3	1.94	0.42
1:A:585:ALA:HA	1:A:588:ILE:HD12	2.02	0.42
1:B:1733:THR:HG22	1:B:1755:THR:HB	2.00	0.42
1:B:4166:VAL:O	1:B:4170:LYS:N	2.52	0.42
1:B:613:VAL:O	1:B:617:LEU:N	2.46	0.42
1:C:3759:THR:O	1:C:3763:GLY:N	2.51	0.42
1:C:4725:TRP:O	1:C:4729:MET:HG2	2.19	0.42
1:C:629:GLN:OE1	1:C:1669:ASN:ND2	2.52	0.42
1:D:1092:LYS:H	1:D:1250:TRP:HZ3	1.66	0.42
1:C:189:GLU:HG3	1:D:2419:ARG:NH2	2.35	0.42
1:D:585:ALA:HA	1:D:588:ILE:HD12	2.02	0.42
1:B:1570:LEU:O	1:B:1573:SER:OG	2.36	0.42
1:B:4924:MET:O	1:B:4928:ASN:HB2	2.18	0.42
1:C:243:GLU:OE2	1:C:389:ARG:NH1	2.53	0.42
1:C:4636:ILE:HG22	1:C:4671:LEU:HD22	2.02	0.42
1:C:565:LEU:HA	1:C:568:SER:HB2	2.02	0.42
1:D:1029:ASN:HA	1:D:1030:PRO:HD3	1.82	0.42
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.84	0.42
1:D:123:HIS:CD2	1:D:126:SER:H	2.34	0.42
1:D:832:LEU:O	1:D:1614:ARG:NH1	2.51	0.42
1:D:116:GLY:N	1:D:162:ILE:O	2.45	0.42
1:D:1682:GLU:HA	1:D:1685:LEU:HD13	2.02	0.42
1:A:2419:ARG:NH2	1:D:189:GLU:HG3	2.35	0.42
1:D:243:GLU:OE2	1:D:389:ARG:NH1	2.53	0.42
1:D:572:LEU:O	1:D:576:HIS:N	2.47	0.42
1:A:190:ARG:HG2	1:A:207:PHE:CE1	2.55	0.42
1:A:2196:ASN:OD1	1:A:2199:ARG:NH1	2.52	0.42
1:B:1170:GLU:O	1:B:1172:THR:N	2.50	0.42
1:B:4725:TRP:O	1:B:4729:MET:HG2	2.19	0.42
1:C:1692:LYS:HA	1:C:1810:VAL:HG13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3921:LEU:HD23	1:C:3921:LEU:HA	1.84	0.42
1:D:852:GLY:HA3	1:D:1086:ARG:HG3	2.01	0.42
1:D:1799:VAL:O	1:D:1803:SER:N	2.46	0.42
1:D:2326:ILE:HD13	1:D:2326:ILE:HA	1.83	0.42
1:A:123:HIS:CD2	1:A:126:SER:H	2.34	0.42
1:A:1730:THR:O	1:A:1733:THR:OG1	2.31	0.42
1:A:565:LEU:HA	1:A:568:SER:HB2	2.02	0.42
1:B:2440:ALA:HB2	1:B:2466:LYS:HD2	2.01	0.42
1:B:2834:LEU:HG	1:B:2895:LYS:HZ3	1.84	0.42
1:B:532:SER:HA	1:B:535:GLU:HB3	2.01	0.42
1:B:691:THR:HB	1:B:796:ALA:HB2	2.01	0.42
1:C:2440:ALA:HB2	1:C:2466:LYS:HD2	2.01	0.42
1:C:3767:LEU:O	1:C:3770:GLY:N	2.51	0.42
1:C:3925:ILE:HD13	1:C:3925:ILE:HG21	1.70	0.42
1:C:585:ALA:HA	1:C:588:ILE:HD12	2.02	0.42
1:D:1172:THR:HG22	1:D:1193:LYS:HG3	2.01	0.42
1:D:2440:ALA:HB2	1:D:2466:LYS:HD2	2.01	0.42
1:D:3759:THR:O	1:D:3763:GLY:N	2.51	0.42
1:D:3797:LEU:HD13	1:D:3840:LEU:HD11	2.02	0.42
1:D:3914:ALA:HB3	1:D:3975:LEU:HD11	2.02	0.42
1:D:565:LEU:HA	1:D:568:SER:HB2	2.02	0.42
1:A:189:GLU:HG3	1:B:2419:ARG:NH2	2.35	0.42
1:A:258:ARG:HA	1:A:316:LEU:HB2	2.01	0.42
1:A:4636:ILE:HG22	1:A:4671:LEU:HD22	2.02	0.42
1:B:1091:GLU:HA	1:B:1250:TRP:CZ3	2.55	0.42
1:B:1692:LYS:HA	1:B:1810:VAL:HG13	2.02	0.42
1:B:2326:ILE:HA	1:B:2326:ILE:HD13	1.83	0.42
1:C:776:GLN:HG2	1:C:1472:GLU:HA	2.01	0.42
1:D:190:ARG:HG2	1:D:207:PHE:CE1	2.55	0.42
1:D:258:ARG:HA	1:D:316:LEU:HB2	2.01	0.42
1:D:4636:ILE:HG22	1:D:4671:LEU:HD22	2.02	0.42
1:A:1682:GLU:HA	1:A:1685:LEU:HD13	2.02	0.42
1:A:2102:ALA:O	1:A:2106:THR:N	2.47	0.42
1:A:4931:GLU:OE2	1:A:4942:TRP:NE1	2.53	0.42
1:A:604:HIS:HA	1:A:1588:VAL:HB	2.01	0.42
1:B:243:GLU:OE2	1:B:389:ARG:NH1	2.53	0.42
1:B:4621:GLN:HE22	1:B:4633:ARG:HH12	1.68	0.42
1:B:565:LEU:HA	1:B:568:SER:HB2	2.02	0.42
1:C:1172:THR:HG22	1:C:1193:LYS:HG3	2.01	0.42
1:C:1090:ALA:HA	1:C:1249:MET:HG2	2.02	0.42
1:C:3797:LEU:HD13	1:C:3840:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:GLU:HA	1:D:414:ARG:HB2	2.01	0.42
1:D:4515:ASN:HD22	1:D:4518:LEU:HB2	1.85	0.42
1:D:674:TYR:OH	1:D:676:GLU:OE2	2.27	0.42
1:D:852:GLY:HA2	1:D:853:PRO:HA	1.69	0.42
1:A:1091:GLU:HA	1:A:1250:TRP:CZ3	2.55	0.42
1:A:4621:GLN:HE22	1:A:4633:ARG:HH12	1.68	0.42
1:A:4739:PHE:HD1	1:A:4739:PHE:HA	1.76	0.42
1:A:565:LEU:HD11	1:A:603:LYS:HG2	2.01	0.42
1:A:852:GLY:HA3	1:A:1086:ARG:HG3	2.01	0.42
1:B:1682:GLU:HA	1:B:1685:LEU:HD13	2.02	0.42
1:B:2196:ASN:OD1	1:B:2199:ARG:NH1	2.52	0.42
1:B:2858:LYS:HG3	1:B:2872:LEU:HD22	2.02	0.42
1:B:4636:ILE:HG22	1:B:4671:LEU:HD22	2.02	0.42
1:B:614:LEU:HD23	1:B:617:LEU:HD12	2.01	0.42
1:C:1156:TRP:HB2	1:C:1160:ASP:HB2	2.01	0.42
1:C:1165:MET:HB2	1:C:1174:MET:HB2	2.01	0.42
1:C:3914:ALA:HB3	1:C:3975:LEU:HD11	2.02	0.42
1:C:3919:ASN:O	1:C:3922:THR:OG1	2.35	0.42
1:C:534:TYR:O	1:C:538:ALA:N	2.51	0.42
1:C:796:ALA:HB3	1:C:798:ILE:HG13	2.02	0.42
1:D:2421:ARG:HA	1:D:2424:LEU:HB2	2.01	0.42
1:D:796:ALA:HB3	1:D:798:ILE:HG13	2.02	0.42
1:A:1029:ASN:HA	1:A:1030:PRO:HD3	1.82	0.41
1:A:3743:GLN:NE2	1:A:3781:TYR:OH	2.43	0.41
1:B:190:ARG:HG2	1:B:207:PHE:CE1	2.55	0.41
1:B:712:GLU:OE2	1:B:1636:ASN:ND2	2.46	0.41
1:B:189:GLU:HG3	1:C:2419:ARG:NH2	2.35	0.41
1:B:4852:PHE:CG	1:C:4823:ARG:HG2	2.55	0.41
1:C:4931:GLU:OE2	1:C:4942:TRP:NE1	2.53	0.41
1:D:1156:TRP:HB2	1:D:1160:ASP:HB2	2.01	0.41
1:D:565:LEU:HD11	1:D:603:LYS:HG2	2.01	0.41
1:D:614:LEU:HD23	1:D:617:LEU:HD12	2.01	0.41
1:A:4515:ASN:HD22	1:A:4518:LEU:HB2	1.85	0.41
1:A:703:TYR:CZ	1:A:722:LEU:HD21	2.54	0.41
1:B:776:GLN:HG2	1:B:1472:GLU:HA	2.01	0.41
1:B:2421:ARG:HA	1:B:2424:LEU:HB2	2.01	0.41
1:B:3911:ILE:HD13	1:B:3911:ILE:HA	1.91	0.41
1:B:585:ALA:HA	1:B:588:ILE:HD12	2.02	0.41
1:C:1682:GLU:HA	1:C:1685:LEU:HD13	2.02	0.41
1:D:1090:ALA:HA	1:D:1249:MET:HG2	2.02	0.41
1:D:1146:HIS:HB2	1:D:1192:PHE:HE1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.48	0.41
1:D:182:ILE:HD12	1:D:209:GLN:HB3	2.02	0.41
1:D:4739:PHE:HD1	1:D:4739:PHE:HA	1.76	0.41
1:C:4852:PHE:CG	1:D:4823:ARG:HG2	2.55	0.41
1:D:703:TYR:CZ	1:D:722:LEU:HD21	2.54	0.41
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.84	0.41
1:A:243:GLU:OE2	1:A:389:ARG:NH1	2.53	0.41
1:A:411:GLU:HA	1:A:414:ARG:HB2	2.01	0.41
1:A:725:TYR:OH	1:A:775:VAL:HG11	2.21	0.41
1:B:833:LYS:HA	1:B:1614:ARG:HH12	1.86	0.41
1:C:1905:LEU:HD23	1:C:2081:LEU:HA	2.03	0.41
1:B:143:LEU:CD2	1:C:2426:SER:HB3	2.47	0.41
1:C:2858:LYS:HG3	1:C:2872:LEU:HD22	2.02	0.41
1:C:836:HIS:HB2	1:C:839:GLU:HG2	2.03	0.41
1:C:852:GLY:HA3	1:C:1086:ARG:HG3	2.01	0.41
1:D:1692:LYS:HA	1:D:1810:VAL:HG13	2.02	0.41
1:A:1146:HIS:HB2	1:A:1192:PHE:HE1	1.85	0.41
1:A:1256:PRO:HB3	1:A:1597:SER:HA	2.02	0.41
1:A:3914:ALA:HB3	1:A:3975:LEU:HD11	2.02	0.41
1:A:796:ALA:HB3	1:A:798:ILE:HG13	2.02	0.41
1:B:2160:PRO:HB3	1:B:2207:ILE:HD12	2.02	0.41
1:B:796:ALA:HB3	1:B:798:ILE:HG13	2.02	0.41
1:B:836:HIS:HB2	1:B:839:GLU:HG2	2.03	0.41
1:C:1256:PRO:HB3	1:C:1597:SER:HA	2.02	0.41
1:C:1934:VAL:O	1:C:1938:GLN:N	2.43	0.41
1:C:2884:ALA:HA	1:C:2887:ARG:HB3	2.03	0.41
1:C:3779:LEU:HD11	1:C:3783:LYS:HE2	2.03	0.41
1:C:532:SER:HA	1:C:535:GLU:HB3	2.01	0.41
1:D:244:CYS:SG	1:D:245:LEU:N	2.93	0.41
1:A:4823:ARG:HG2	1:D:4852:PHE:CG	2.55	0.41
1:A:1090:ALA:HA	1:A:1249:MET:HG2	2.02	0.41
1:A:833:LYS:HA	1:A:1614:ARG:HH12	1.86	0.41
1:A:2421:ARG:HA	1:A:2424:LEU:HB2	2.01	0.41
1:A:2858:LYS:HG3	1:A:2872:LEU:HD22	2.02	0.41
1:A:3800:SER:OG	1:A:3801:CYS:N	2.47	0.41
1:A:614:LEU:HD23	1:A:617:LEU:HD12	2.01	0.41
1:B:852:GLY:HA3	1:B:1086:ARG:HG3	2.01	0.41
1:B:1137:PHE:HD1	1:B:1144:ARG:HB3	1.86	0.41
1:B:1090:ALA:HA	1:B:1249:MET:HG2	2.02	0.41
1:B:1905:LEU:HD23	1:B:2081:LEU:HA	2.03	0.41
1:B:2127:ILE:HD12	1:B:2127:ILE:HA	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2541:HIS:O	1:B:2545:LEU:N	2.49	0.41
1:C:244:CYS:SG	1:C:245:LEU:N	2.93	0.41
1:C:4161:TRP:CD1	1:C:4201:MET:HE1	2.53	0.41
1:C:653:SER:OG	1:C:794:PHE:O	2.31	0.41
1:D:3743:GLN:NE2	1:D:3781:TYR:OH	2.43	0.41
1:D:725:TYR:OH	1:D:775:VAL:HG11	2.21	0.41
1:D:833:LYS:HA	1:D:1614:ARG:HH12	1.86	0.41
1:A:1905:LEU:HD23	1:A:2081:LEU:HA	2.03	0.41
1:A:2732:LYS:HA	1:A:2732:LYS:HD2	1.82	0.41
1:A:3925:ILE:HG21	1:A:3925:ILE:HD13	1.70	0.41
1:A:4045:SER:HA	1:A:4078:THR:HG22	2.03	0.41
1:B:1156:TRP:HB2	1:B:1160:ASP:HB2	2.01	0.41
1:B:2884:ALA:HA	1:B:2887:ARG:HB3	2.03	0.41
1:C:182:ILE:HD12	1:C:209:GLN:HB3	2.02	0.41
1:C:3743:GLN:O	1:C:3746:SER:OG	2.32	0.41
1:D:1091:GLU:HA	1:D:1250:TRP:CZ3	2.55	0.41
1:D:288:HIS:ND1	1:D:349:MET:O	2.43	0.41
1:D:4621:GLN:HE22	1:D:4633:ARG:HH12	1.68	0.41
1:A:1137:PHE:HD1	1:A:1144:ARG:HB3	1.86	0.41
1:A:1692:LYS:HA	1:A:1810:VAL:HG13	2.02	0.41
1:A:2154:LYS:HA	1:A:2154:LYS:HD3	1.90	0.41
1:A:244:CYS:SG	1:A:245:LEU:N	2.93	0.41
1:A:3797:LEU:HD13	1:A:3840:LEU:HD11	2.02	0.41
1:B:3921:LEU:HA	1:B:3921:LEU:HD23	1.84	0.41
1:C:1132:GLU:HG2	1:C:1133:ARG:HG3	2.03	0.41
1:C:1170:GLU:O	1:C:1172:THR:N	2.50	0.41
1:C:2463:PRO:HD3	1:C:2516:ALA:HB2	2.02	0.41
1:C:614:LEU:HD23	1:C:617:LEU:HD12	2.01	0.41
1:D:3779:LEU:HD11	1:D:3783:LYS:HE2	2.03	0.41
1:D:3996:ILE:H	1:D:3996:ILE:HG22	1.64	0.41
1:D:534:TYR:CZ	1:D:571:ILE:HG13	2.56	0.41
1:D:613:VAL:O	1:D:617:LEU:N	2.46	0.41
1:A:182:ILE:HD12	1:A:209:GLN:HB3	2.02	0.41
1:A:534:TYR:CZ	1:A:571:ILE:HG13	2.56	0.41
1:A:650:ASN:HA	1:A:1626:GLN:HA	2.03	0.41
1:A:836:HIS:HB2	1:A:839:GLU:HG2	2.03	0.41
1:A:935:MET:O	1:A:939:THR:OG1	2.36	0.41
1:B:3914:ALA:HB3	1:B:3975:LEU:HD11	2.02	0.41
1:A:4852:PHE:CG	1:B:4823:ARG:HG2	2.55	0.41
1:B:534:TYR:CZ	1:B:571:ILE:HG13	2.56	0.41
1:C:1029:ASN:HA	1:C:1030:PRO:HD3	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1137:PHE:HD1	1:C:1144:ARG:HB3	1.86	0.41
1:C:2421:ARG:HA	1:C:2424:LEU:HB2	2.01	0.41
1:C:299:HIS:N	1:C:304:LYS:O	2.54	0.41
1:C:4872:GLY:C	1:D:4875:ARG:CZ	2.89	0.41
1:C:4894:ILE:HD12	1:C:4961:LYS:HE3	2.03	0.41
1:D:1256:PRO:HB3	1:D:1597:SER:HA	2.02	0.41
1:D:776:GLN:HG2	1:D:1472:GLU:HA	2.01	0.41
1:D:4045:SER:HA	1:D:4078:THR:HG22	2.03	0.41
1:D:836:HIS:HB2	1:D:839:GLU:HG2	2.03	0.41
1:A:881:ILE:HG21	1:A:1062:TYR:CZ	2.56	0.41
1:A:551:PHE:HA	1:A:551:PHE:HD1	1.74	0.41
1:A:776:GLN:HG2	1:A:1472:GLU:HA	2.01	0.41
1:B:1146:HIS:HB2	1:B:1192:PHE:HE1	1.85	0.41
1:B:1699:ARG:HH22	1:B:1821:LEU:HD11	1.86	0.41
1:B:182:ILE:HD12	1:B:209:GLN:HB3	2.02	0.41
1:B:3779:LEU:HD11	1:B:3783:LYS:HE2	2.03	0.41
1:B:4022:LEU:HD23	1:B:4022:LEU:HA	1.85	0.41
1:B:4872:GLY:C	1:C:4875:ARG:CZ	2.89	0.41
1:C:1091:GLU:HA	1:C:1250:TRP:CZ3	2.55	0.41
1:C:706:TYR:CD1	1:C:1253:LYS:HD2	2.56	0.41
1:C:190:ARG:HG2	1:C:207:PHE:CE1	2.55	0.41
1:C:4621:GLN:HE22	1:C:4633:ARG:HH12	1.68	0.41
1:C:534:TYR:CZ	1:C:571:ILE:HG13	2.56	0.41
1:D:1652:LYS:HB3	1:D:1652:LYS:HE2	1.90	0.41
1:D:1716:THR:HA	1:D:1719:LEU:HD12	2.03	0.41
1:D:1905:LEU:HD23	1:D:2081:LEU:HA	2.03	0.41
1:D:650:ASN:HA	1:D:1626:GLN:HA	2.03	0.41
1:A:2160:PRO:HB3	1:A:2207:ILE:HD12	2.02	0.41
1:B:1132:GLU:HG2	1:B:1133:ARG:HG3	2.03	0.41
1:B:244:CYS:SG	1:B:245:LEU:N	2.93	0.41
1:B:2829:MET:HE1	1:B:2896:PHE:HB2	2.03	0.41
1:B:411:GLU:HA	1:B:414:ARG:HB2	2.01	0.41
1:B:4161:TRP:CD1	1:B:4201:MET:HE1	2.53	0.41
1:B:725:TYR:OH	1:B:775:VAL:HG11	2.21	0.41
1:C:650:ASN:HA	1:C:1626:GLN:HA	2.03	0.41
1:C:3911:ILE:HA	1:C:3911:ILE:HD13	1.91	0.41
1:C:4515:ASN:HD22	1:C:4518:LEU:HB2	1.85	0.41
1:D:881:ILE:HG21	1:D:1062:TYR:CZ	2.56	0.41
1:D:1132:GLU:HG2	1:D:1133:ARG:HG3	2.03	0.41
1:D:2160:PRO:HB3	1:D:2207:ILE:HD12	2.02	0.41
1:D:4853:PHE:HA	1:D:4857:VAL:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ALA:HA	1:A:161:THR:HA	2.03	0.41
1:A:1255:LEU:HA	1:A:1256:PRO:HD3	1.92	0.41
1:A:1716:THR:HA	1:A:1719:LEU:HD12	2.03	0.41
1:A:2463:PRO:HD3	1:A:2516:ALA:HB2	2.02	0.41
1:A:4823:ARG:HA	1:D:4852:PHE:CE1	2.53	0.41
1:A:681:HIS:HA	1:A:751:THR:HG22	2.03	0.41
1:A:852:GLY:HA2	1:A:853:PRO:HA	1.69	0.41
1:B:1505:LEU:H	1:B:1523:ASN:HA	1.86	0.41
1:B:2463:PRO:HD3	1:B:2516:ALA:HB2	2.02	0.41
1:C:1177:LEU:HA	1:C:1177:LEU:HD12	1.92	0.41
1:C:833:LYS:HA	1:C:1614:ARG:HH12	1.86	0.41
1:C:217:ILE:HG23	1:C:285:SER:HB3	2.03	0.41
1:C:3808:ALA:HA	1:C:3811:ARG:HD2	2.03	0.41
1:C:4045:SER:HA	1:C:4078:THR:HG22	2.03	0.41
1:C:506:HIS:HB2	1:C:561:ARG:NH1	2.36	0.41
1:C:64:ILE:HG12	1:C:417:ARG:HH21	1.86	0.41
1:D:2884:ALA:HA	1:D:2887:ARG:HB3	2.03	0.41
1:A:1132:GLU:HG2	1:A:1133:ARG:HG3	2.03	0.40
1:A:1783:PRO:HB3	1:A:1786:ILE:HD12	2.02	0.40
1:B:3797:LEU:HD13	1:B:3840:LEU:HD11	2.02	0.40
1:B:4045:SER:HA	1:B:4078:THR:HG22	2.03	0.40
1:B:4515:ASN:HD22	1:B:4518:LEU:HB2	1.85	0.40
1:B:534:TYR:O	1:B:538:ALA:N	2.51	0.40
1:B:681:HIS:HA	1:B:751:THR:HG22	2.03	0.40
1:C:3642:ILE:HD12	1:C:3642:ILE:HG23	1.91	0.40
1:D:1137:PHE:HD1	1:D:1144:ARG:HB3	1.86	0.40
1:D:217:ILE:HG23	1:D:285:SER:HB3	2.03	0.40
1:D:2858:LYS:HG3	1:D:2872:LEU:HD22	2.02	0.40
1:D:4640:SER:HB3	1:D:4643:ASN:ND2	2.37	0.40
1:A:4875:ARG:CZ	1:D:4872:GLY:C	2.89	0.40
1:D:4931:GLU:OE2	1:D:4942:TRP:NE1	2.53	0.40
1:A:1699:ARG:HH22	1:A:1821:LEU:HD11	1.86	0.40
1:A:2270:LEU:HD21	1:A:2299:TYR:HB2	2.04	0.40
1:A:4166:VAL:O	1:A:4170:LYS:N	2.52	0.40
1:A:731:HIS:HE1	1:A:738:ALA:HB1	1.87	0.40
1:B:1032:LEU:HD23	1:B:1032:LEU:HA	1.82	0.40
1:B:706:TYR:CD1	1:B:1253:LYS:HD2	2.56	0.40
1:B:3808:ALA:HA	1:B:3811:ARG:HD2	2.03	0.40
1:B:4591:TYR:CE1	1:B:4595:LYS:HB2	2.57	0.40
1:B:4722:TYR:OH	1:B:4745:LEU:O	2.40	0.40
1:B:4770:LEU:HA	1:B:4770:LEU:HD23	1.98	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4853:PHE:HA	1:B:4857:VAL:HB	2.03	0.40
1:B:64:ILE:H	1:B:64:ILE:HG13	1.79	0.40
1:A:116:GLY:N	1:A:162:ILE:O	2.45	0.40
1:A:2069:ARG:HD3	1:A:2069:ARG:HA	1.92	0.40
1:A:3779:LEU:HD11	1:A:3783:LYS:HE2	2.03	0.40
1:A:534:TYR:O	1:A:538:ALA:N	2.51	0.40
1:B:2270:LEU:HD21	1:B:2299:TYR:HB2	2.04	0.40
1:B:217:ILE:HG23	1:B:285:SER:HB3	2.03	0.40
1:B:415:THR:O	1:B:419:ILE:HG13	2.22	0.40
1:B:4873:GLU:HA	1:C:4875:ARG:HH11	1.68	0.40
1:C:3777:LYS:HE3	1:C:3777:LYS:HB2	1.94	0.40
1:C:4640:SER:HB3	1:C:4643:ASN:ND2	2.37	0.40
1:C:725:TYR:OH	1:C:775:VAL:HG11	2.21	0.40
1:C:681:HIS:HA	1:C:751:THR:HG22	2.03	0.40
1:D:2775:PRO:HB2	1:D:2889:LYS:NZ	2.36	0.40
1:D:506:HIS:HB2	1:D:561:ARG:NH1	2.36	0.40
1:A:2834:LEU:HG	1:A:2895:LYS:HZ3	1.87	0.40
1:A:628:ASN:O	1:A:632:ILE:HG12	2.22	0.40
1:B:1256:PRO:HB3	1:B:1597:SER:HA	2.02	0.40
1:B:1716:THR:HA	1:B:1719:LEU:HD12	2.03	0.40
1:B:1729:MET:HG2	1:B:2110:ASN:HA	2.03	0.40
1:B:2775:PRO:HB2	1:B:2889:LYS:NZ	2.36	0.40
1:B:3747:ALA:O	1:B:3749:LYS:HD2	2.22	0.40
1:A:4852:PHE:CE1	1:B:4823:ARG:HA	2.53	0.40
1:B:551:PHE:HD1	1:B:551:PHE:HA	1.74	0.40
1:B:650:ASN:HA	1:B:1626:GLN:HA	2.03	0.40
1:C:881:ILE:HG21	1:C:1062:TYR:CZ	2.56	0.40
1:C:1146:HIS:HB2	1:C:1192:PHE:HE1	1.85	0.40
1:C:1783:PRO:HB3	1:C:1786:ILE:HD12	2.02	0.40
1:C:2270:LEU:HD21	1:C:2299:TYR:HB2	2.04	0.40
1:C:3886:ILE:HG23	1:C:3886:ILE:HD12	1.92	0.40
1:D:706:TYR:CD1	1:D:1253:LYS:HD2	2.56	0.40
1:D:3756:VAL:O	1:D:3759:THR:OG1	2.31	0.40
1:D:628:ASN:O	1:D:632:ILE:HG12	2.22	0.40
1:D:731:HIS:HE1	1:D:738:ALA:HB1	1.87	0.40
1:D:694:ARG:N	1:D:793:SER:O	2.45	0.40
1:A:3747:ALA:O	1:A:3749:LYS:HD2	2.22	0.40
1:A:3808:ALA:HA	1:A:3811:ARG:HD2	2.03	0.40
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.35	0.40
1:A:3921:LEU:HD23	1:A:3921:LEU:HA	1.84	0.40
1:A:3988:GLU:HB2	1:A:4937:GLN:NE2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4640:SER:HB3	1:A:4643:ASN:ND2	2.37	0.40
1:A:4804:ASP:N	1:A:4804:ASP:OD1	2.54	0.40
1:A:506:HIS:HB2	1:A:561:ARG:NH1	2.36	0.40
1:B:116:GLY:N	1:B:162:ILE:O	2.45	0.40
1:B:2788:TRP:HH2	1:B:2844:MET:HB2	1.87	0.40
1:B:3993:ASN:HD22	1:B:4110:MET:HG3	1.87	0.40
1:B:628:ASN:O	1:B:632:ILE:HG12	2.22	0.40
1:B:64:ILE:HG12	1:B:417:ARG:HH21	1.86	0.40
1:B:894:VAL:HG11	1:B:976:TYR:HD2	1.87	0.40
1:C:1255:LEU:HA	1:C:1256:PRO:HD3	1.92	0.40
1:C:118:ALA:HA	1:C:161:THR:HA	2.03	0.40
1:C:49:LEU:HD21	1:C:203:VAL:HG23	2.04	0.40
1:C:2160:PRO:HB3	1:C:2207:ILE:HD12	2.02	0.40
1:B:189:GLU:CD	1:C:2419:ARG:CZ	2.90	0.40
1:C:3993:ASN:HD22	1:C:4110:MET:HG3	1.87	0.40
1:C:4722:TYR:OH	1:C:4745:LEU:O	2.40	0.40
1:C:894:VAL:HG11	1:C:976:TYR:HD2	1.87	0.40
1:D:1783:PRO:HB3	1:D:1786:ILE:HD12	2.02	0.40
1:D:3808:ALA:HA	1:D:3811:ARG:HD2	2.03	0.40
1:D:4894:ILE:HD12	1:D:4961:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	B	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	C	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	D	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
All	All	13156/19872 (66%)	11932 (91%)	1140 (9%)	84 (1%)	34	74

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4071	ALA
1	B	4071	ALA
1	C	4071	ALA
1	D	4071	ALA
1	A	730	LEU
1	A	1580	PRO
1	A	3802	SER
1	A	4164	PRO
1	A	4916	LEU
1	B	730	LEU
1	B	1580	PRO
1	B	3802	SER
1	B	4164	PRO
1	B	4916	LEU
1	C	730	LEU
1	C	1580	PRO
1	C	3802	SER
1	C	4164	PRO
1	C	4916	LEU
1	D	730	LEU
1	D	1580	PRO
1	D	3802	SER
1	D	4164	PRO
1	D	4916	LEU
1	A	1581	GLN
1	A	1809	PRO
1	A	2075	VAL
1	A	3805	ASP
1	A	4030	SER
1	A	4646	TRP
1	B	1581	GLN
1	B	1809	PRO
1	B	2075	VAL
1	B	3805	ASP
1	B	4030	SER
1	B	4646	TRP
1	C	1581	GLN
1	C	1809	PRO
1	C	2075	VAL
1	C	3805	ASP
1	C	4030	SER
1	C	4646	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1581	GLN
1	D	1809	PRO
1	D	2075	VAL
1	D	3805	ASP
1	D	4030	SER
1	D	4646	TRP
1	A	819	TYR
1	A	980	PRO
1	A	3804	LEU
1	B	819	TYR
1	B	980	PRO
1	B	3804	LEU
1	C	819	TYR
1	C	980	PRO
1	C	3804	LEU
1	D	819	TYR
1	D	980	PRO
1	D	3804	LEU
1	A	792	VAL
1	B	792	VAL
1	C	792	VAL
1	D	792	VAL
1	A	853	PRO
1	A	1848	PRO
1	B	853	PRO
1	B	1848	PRO
1	C	853	PRO
1	C	1848	PRO
1	D	853	PRO
1	D	1848	PRO
1	A	1476	VAL
1	A	2329	PRO
1	A	4163	LYS
1	B	1476	VAL
1	B	2329	PRO
1	B	4163	LYS
1	C	1476	VAL
1	C	2329	PRO
1	C	4163	LYS
1	D	1476	VAL
1	D	2329	PRO
1	D	4163	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2659/4355 (61%)	2628 (99%)	31 (1%)	78 90
1	B	2658/4355 (61%)	2627 (99%)	31 (1%)	78 90
1	C	2659/4355 (61%)	2627 (99%)	32 (1%)	78 90
1	D	2660/4355 (61%)	2628 (99%)	32 (1%)	78 90
All	All	10636/17420 (61%)	10510 (99%)	126 (1%)	79 90

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	84	ASN
1	A	298	ARG
1	A	420	ARG
1	A	439	LYS
1	A	527	LYS
1	A	531	ASN
1	A	628	ASN
1	A	658	ASN
1	A	841	LYS
1	A	854	THR
1	A	925	PRO
1	A	990	PRO
1	A	1054	VAL
1	A	1089	ARG
1	A	1761	MET
1	A	2211	ASN
1	A	3722	LYS
1	A	3813	ASN
1	A	3906	ASN
1	A	4131	GLN
1	A	4136	ARG
1	A	4170	LYS
1	A	4171	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4179	ASN
1	A	4499	ASN
1	A	4515	ASN
1	A	4652	ARG
1	A	4781	LEU
1	A	4875	ARG
1	A	4879	GLU
1	B	44	ASN
1	B	84	ASN
1	B	298	ARG
1	B	420	ARG
1	B	439	LYS
1	B	527	LYS
1	B	531	ASN
1	B	628	ASN
1	B	658	ASN
1	B	841	LYS
1	B	854	THR
1	B	925	PRO
1	B	990	PRO
1	B	1054	VAL
1	B	1089	ARG
1	B	1761	MET
1	B	2211	ASN
1	B	3722	LYS
1	B	3813	ASN
1	B	3906	ASN
1	B	4131	GLN
1	B	4136	ARG
1	B	4170	LYS
1	B	4171	ARG
1	B	4179	ASN
1	B	4499	ASN
1	B	4515	ASN
1	B	4652	ARG
1	B	4781	LEU
1	B	4875	ARG
1	B	4879	GLU
1	C	44	ASN
1	C	84	ASN
1	C	298	ARG
1	C	420	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	439	LYS
1	C	527	LYS
1	C	531	ASN
1	C	628	ASN
1	C	658	ASN
1	C	841	LYS
1	C	854	THR
1	C	925	PRO
1	C	950	VAL
1	C	990	PRO
1	C	1054	VAL
1	C	1089	ARG
1	C	1761	MET
1	C	2211	ASN
1	C	3722	LYS
1	C	3813	ASN
1	C	3906	ASN
1	C	4131	GLN
1	C	4136	ARG
1	C	4170	LYS
1	C	4171	ARG
1	C	4179	ASN
1	C	4499	ASN
1	C	4515	ASN
1	C	4652	ARG
1	C	4781	LEU
1	C	4875	ARG
1	C	4879	GLU
1	D	44	ASN
1	D	84	ASN
1	D	298	ARG
1	D	420	ARG
1	D	439	LYS
1	D	527	LYS
1	D	531	ASN
1	D	628	ASN
1	D	658	ASN
1	D	841	LYS
1	D	854	THR
1	D	925	PRO
1	D	950	VAL
1	D	990	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1054	VAL
1	D	1089	ARG
1	D	1761	MET
1	D	2211	ASN
1	D	3722	LYS
1	D	3813	ASN
1	D	3906	ASN
1	D	4131	GLN
1	D	4136	ARG
1	D	4170	LYS
1	D	4171	ARG
1	D	4179	ASN
1	D	4499	ASN
1	D	4515	ASN
1	D	4652	ARG
1	D	4781	LEU
1	D	4875	ARG
1	D	4879	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	84	ASN
1	A	123	HIS
1	A	293	GLN
1	A	364	GLN
1	A	375	GLN
1	A	476	GLN
1	A	531	ASN
1	A	593	HIS
1	A	604	HIS
1	A	628	ASN
1	A	1267	HIS
1	A	1294	ASN
1	A	1602	GLN
1	A	1631	HIS
1	A	1684	GLN
1	A	1722	ASN
1	A	1835	HIS
1	A	2090	HIS
1	A	2212	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2225	ASN
1	A	2251	ASN
1	A	2310	ASN
1	A	3856	GLN
1	A	3906	ASN
1	A	3916	GLN
1	A	3926	GLN
1	A	3950	HIS
1	A	3956	GLN
1	A	3961	GLN
1	A	3976	GLN
1	A	3993	ASN
1	A	4179	ASN
1	A	4499	ASN
1	A	4515	ASN
1	A	4621	GLN
1	A	4914	HIS
1	A	4962	GLN
1	B	23	GLN
1	B	44	ASN
1	B	84	ASN
1	B	123	HIS
1	B	293	GLN
1	B	364	GLN
1	B	375	GLN
1	B	476	GLN
1	B	531	ASN
1	B	593	HIS
1	B	604	HIS
1	B	628	ASN
1	B	1267	HIS
1	B	1294	ASN
1	B	1440	ASN
1	B	1602	GLN
1	B	1631	HIS
1	B	1684	GLN
1	B	1722	ASN
1	B	1835	HIS
1	B	2090	HIS
1	B	2212	GLN
1	B	2225	ASN
1	B	2251	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2310	ASN
1	B	2730	HIS
1	B	3856	GLN
1	B	3906	ASN
1	B	3916	GLN
1	B	3926	GLN
1	B	3956	GLN
1	B	3961	GLN
1	B	3976	GLN
1	B	3993	ASN
1	B	4179	ASN
1	B	4499	ASN
1	B	4515	ASN
1	B	4621	GLN
1	B	4914	HIS
1	B	4962	GLN
1	C	23	GLN
1	C	44	ASN
1	C	84	ASN
1	C	123	HIS
1	C	293	GLN
1	C	364	GLN
1	C	375	GLN
1	C	476	GLN
1	C	531	ASN
1	C	593	HIS
1	C	604	HIS
1	C	628	ASN
1	C	1267	HIS
1	C	1294	ASN
1	C	1440	ASN
1	C	1602	GLN
1	C	1631	HIS
1	C	1684	GLN
1	C	1691	ASN
1	C	1722	ASN
1	C	1835	HIS
1	C	2090	HIS
1	C	2212	GLN
1	C	2225	ASN
1	C	2251	ASN
1	C	2310	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2730	HIS
1	C	3856	GLN
1	C	3906	ASN
1	C	3916	GLN
1	C	3926	GLN
1	C	3956	GLN
1	C	3961	GLN
1	C	3976	GLN
1	C	3993	ASN
1	C	4179	ASN
1	C	4499	ASN
1	C	4515	ASN
1	C	4621	GLN
1	C	4914	HIS
1	C	4962	GLN
1	D	44	ASN
1	D	84	ASN
1	D	123	HIS
1	D	293	GLN
1	D	364	GLN
1	D	375	GLN
1	D	476	GLN
1	D	531	ASN
1	D	593	HIS
1	D	604	HIS
1	D	628	ASN
1	D	1267	HIS
1	D	1294	ASN
1	D	1602	GLN
1	D	1631	HIS
1	D	1684	GLN
1	D	1722	ASN
1	D	1835	HIS
1	D	2090	HIS
1	D	2212	GLN
1	D	2225	ASN
1	D	2251	ASN
1	D	2730	HIS
1	D	3856	GLN
1	D	3906	ASN
1	D	3916	GLN
1	D	3926	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3956	GLN
1	D	3961	GLN
1	D	3976	GLN
1	D	3993	ASN
1	D	4179	ASN
1	D	4499	ASN
1	D	4515	ASN
1	D	4621	GLN
1	D	4914	HIS
1	D	4962	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.