Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 10:25 am BST

PDB ID	:	5L5G
Title	:	Plexin A2 full extracellular region, domains 1 to 8 modeled, data to 10 angstrom
Authors	:	Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.
Deposited on	:	2016-05-28
Resolution	:	10.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

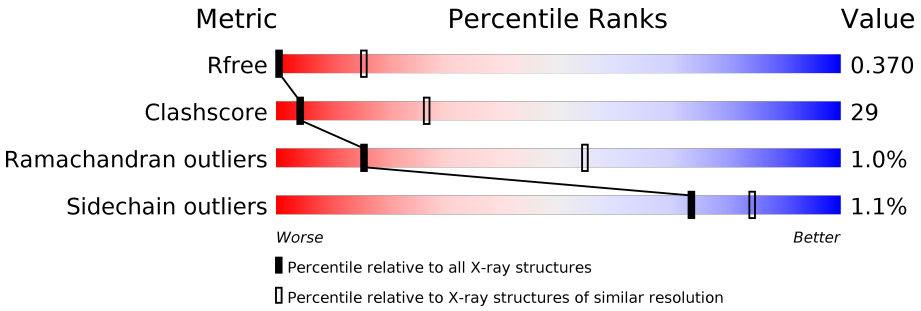
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 10.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1071 (15.00-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1212	51% 23% • 25%
1	B	1212	47% 19% • 33%
1	C	1212	53% 27% • 18%
1	D	1212	54% 27% • 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28787 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Plexin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	906	Total	C	N	O	S	0	0	0
			7060	4461	1214	1333	52			
1	B	809	Total	C	N	O	S	0	0	0
			6337	4004	1092	1195	46			
1	C	993	Total	C	N	O	S	0	0	0
			7695	4856	1321	1462	56			
1	D	993	Total	C	N	O	S	0	0	0
			7695	4856	1321	1462	56			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	-	expression tag	UNP P70207
A	1232	GLY	-	expression tag	UNP P70207
A	1233	GLY	-	expression tag	UNP P70207
A	1234	SER	-	expression tag	UNP P70207
A	1235	ARG	-	expression tag	UNP P70207
A	1236	THR	-	expression tag	UNP P70207
A	1237	LYS	-	expression tag	UNP P70207
A	1238	HIS	-	expression tag	UNP P70207
A	1239	HIS	-	expression tag	UNP P70207
A	1240	HIS	-	expression tag	UNP P70207
A	1241	HIS	-	expression tag	UNP P70207
A	1242	HIS	-	expression tag	UNP P70207
A	1243	HIS	-	expression tag	UNP P70207
B	32	GLU	-	expression tag	UNP P70207
B	1232	GLY	-	expression tag	UNP P70207
B	1233	GLY	-	expression tag	UNP P70207
B	1234	SER	-	expression tag	UNP P70207
B	1235	ARG	-	expression tag	UNP P70207
B	1236	THR	-	expression tag	UNP P70207
B	1237	LYS	-	expression tag	UNP P70207
B	1238	HIS	-	expression tag	UNP P70207

Continued on next page...

Continued from previous page...

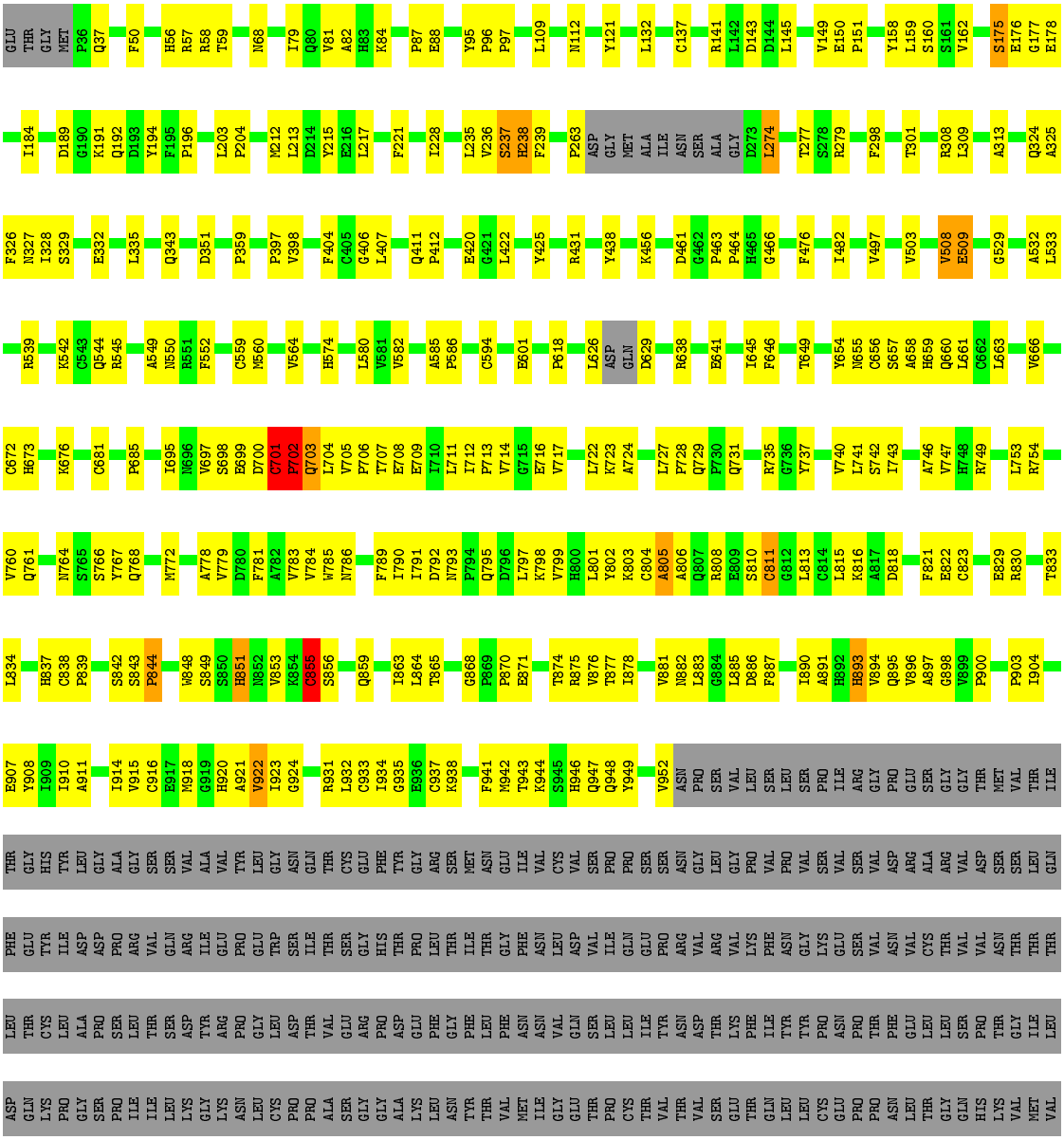
Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	HIS	-	expression tag	UNP P70207
B	1240	HIS	-	expression tag	UNP P70207
B	1241	HIS	-	expression tag	UNP P70207
B	1242	HIS	-	expression tag	UNP P70207
B	1243	HIS	-	expression tag	UNP P70207
C	32	GLU	-	expression tag	UNP P70207
C	1232	GLY	-	expression tag	UNP P70207
C	1233	GLY	-	expression tag	UNP P70207
C	1234	SER	-	expression tag	UNP P70207
C	1235	ARG	-	expression tag	UNP P70207
C	1236	THR	-	expression tag	UNP P70207
C	1237	LYS	-	expression tag	UNP P70207
C	1238	HIS	-	expression tag	UNP P70207
C	1239	HIS	-	expression tag	UNP P70207
C	1240	HIS	-	expression tag	UNP P70207
C	1241	HIS	-	expression tag	UNP P70207
C	1242	HIS	-	expression tag	UNP P70207
C	1243	HIS	-	expression tag	UNP P70207
D	32	GLU	-	expression tag	UNP P70207
D	1232	GLY	-	expression tag	UNP P70207
D	1233	GLY	-	expression tag	UNP P70207
D	1234	SER	-	expression tag	UNP P70207
D	1235	ARG	-	expression tag	UNP P70207
D	1236	THR	-	expression tag	UNP P70207
D	1237	LYS	-	expression tag	UNP P70207
D	1238	HIS	-	expression tag	UNP P70207
D	1239	HIS	-	expression tag	UNP P70207
D	1240	HIS	-	expression tag	UNP P70207
D	1241	HIS	-	expression tag	UNP P70207
D	1242	HIS	-	expression tag	UNP P70207
D	1243	HIS	-	expression tag	UNP P70207

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

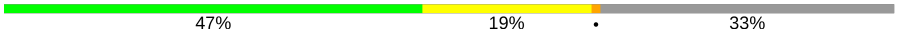
- Molecule 1: Plexin-A2

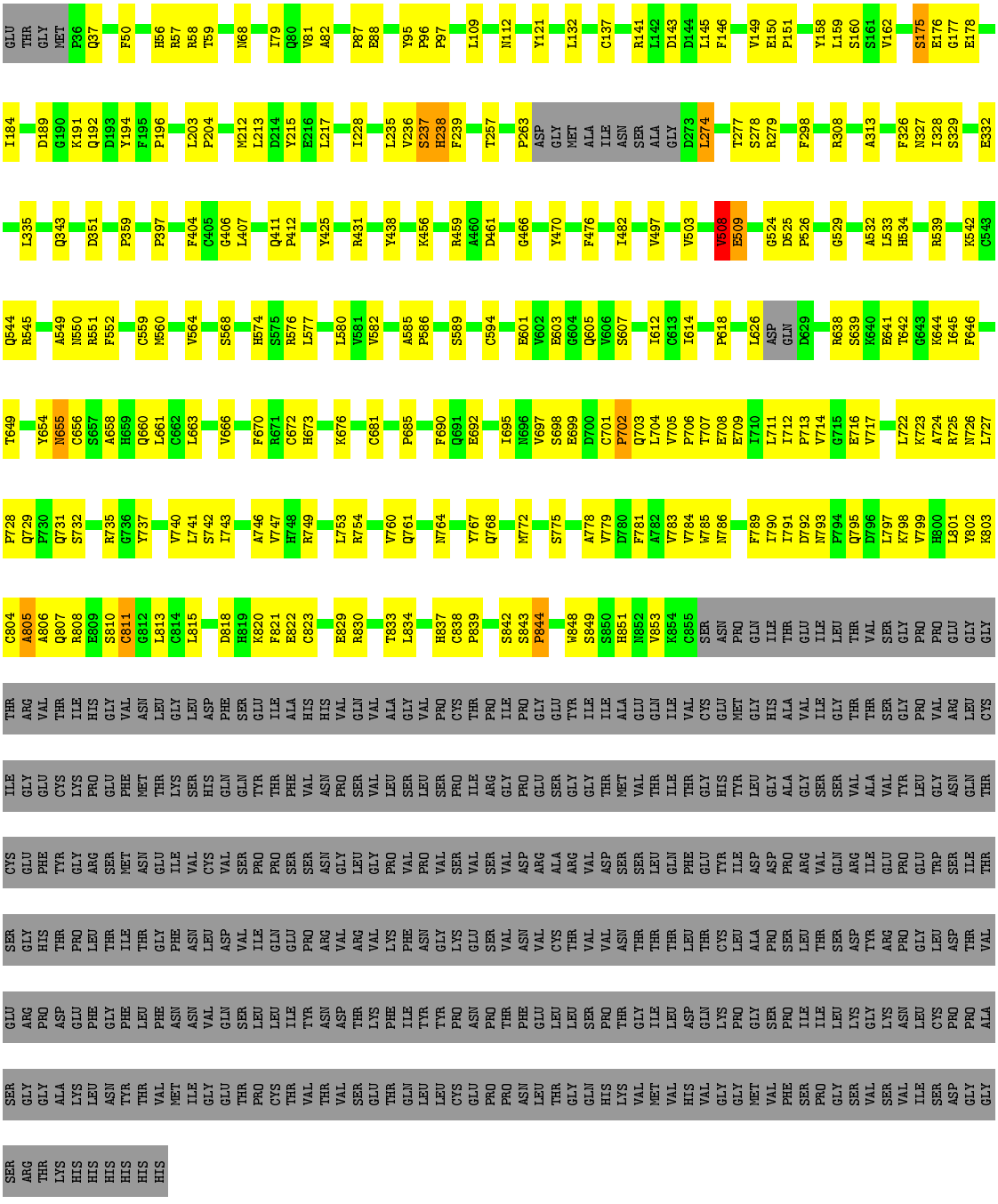
Chain A:



- Molecule 1: Plexin-A2

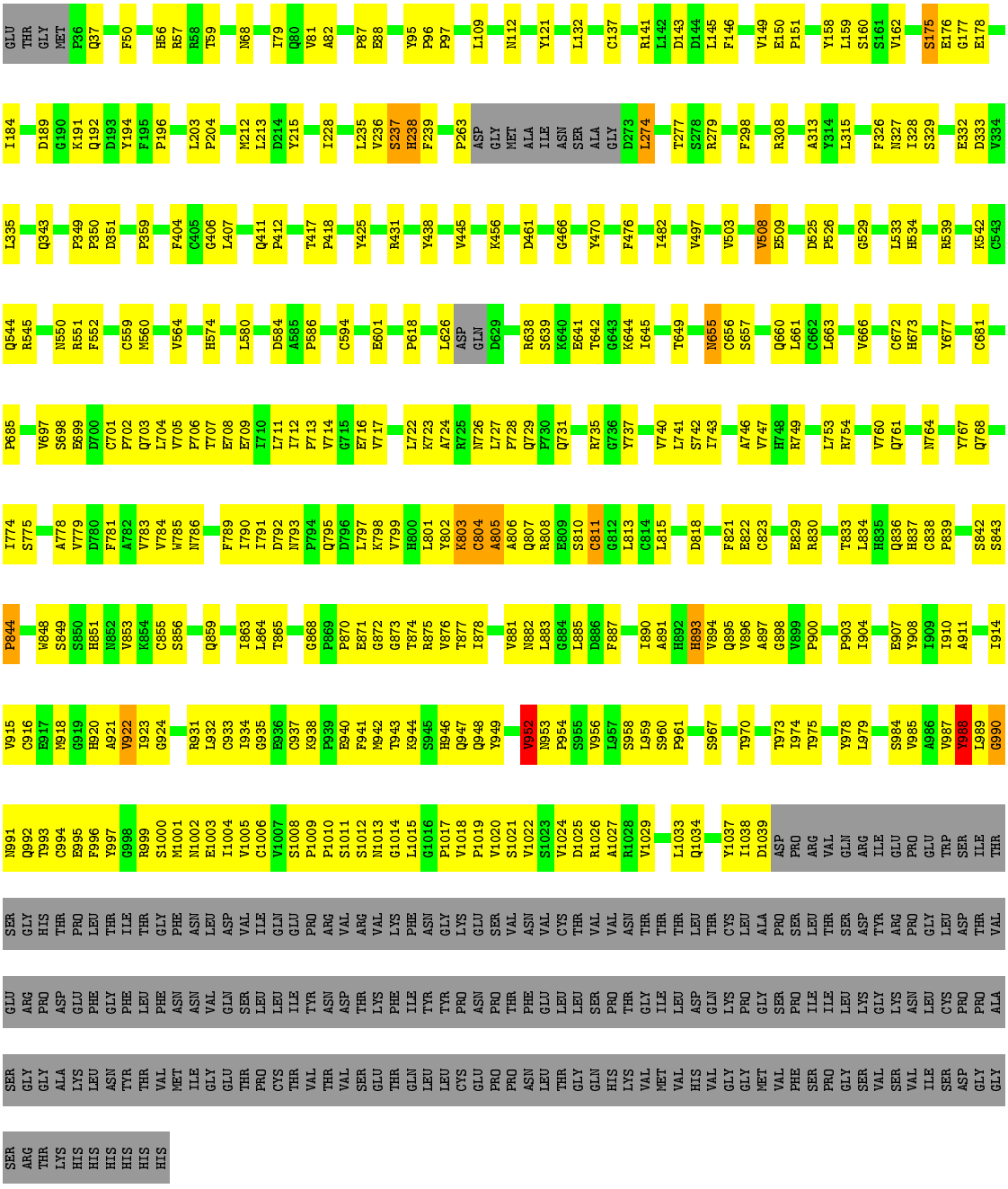
Chain B:





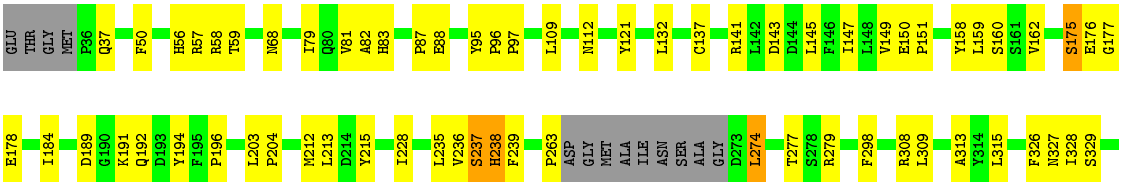
- Molecule 1: Plexin-A2

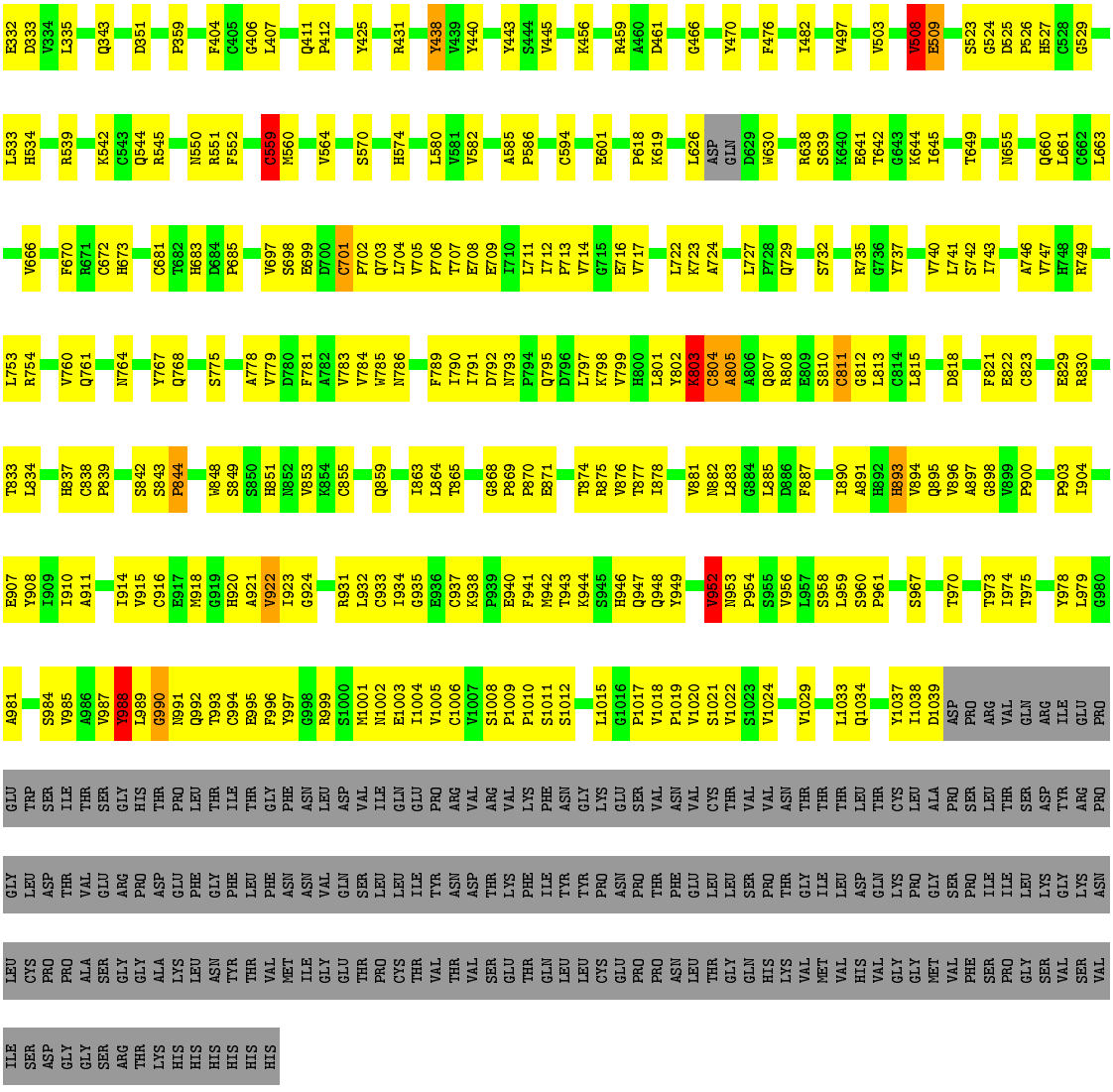
Chain C:



- Molecule 1: Plexin-A2

Chain D:




E332 D333 V334 L335 Q343 D351 P359 F404 C405 G406 L407 Q411 P412 Y425 R431 Y438 V439 Y440 Y443 S444 V445 K456 R459 A460 D461 G466 Y470 F476 I482 V497 V503 V508 E509 S523 G524 D525 P526 H527 C528 G529
L533 H534 R539 K542 C543 Q544 R545 N550 R551 F552 C559 M560 V564 S570 H574 L580 V581 V582 A585 P586 C594 E601 P618 K619 L626 ASP GLN D629 W630 R638 S639 K640 E641 T642 G643 K644 I645 T649 N655 Q660 L661 C662 L663
V666 F670 R671 C672 H673 C681 T682 H683 D684 P685 V697 S698 E699 D700 C701 P702 Q703 L704 V705 P706 T707 E708 E709 I710 L711 I712 P713 V714 G715 E716 V717 L722 K723 A724 L727 F728 Q729 S732 R735 G736 Y737 V740 L741 S742 I743 A746 V747 H748 R749
L753 R754 V760 Q761 N764 Y767 Q768 S775 A778 V779 D780 F781 A782 V783 V784 W785 N786 F789 I790 I791 D792 N793 P794 Q795 D796 L797 K798 V799 H800 L801 Y802 K803 C804 A805 A806 Q807 R808 E809 S810 C811 G812 L813 C814 L815 D818 F821 E822 C823 E829 R830
T833 L834 H837 C838 P839 S842 S843 P844 W848 S849 S850 H851 N852 V853 K854 C855 Q859 I863 L864 T865 G868 P869 P870 E871 T874 R875 V876 T877 I878 V881 N882 L883 G884 L885 D886 F887 I890 A891 H892 H893 V894 Q895 V896 A897 G898 V899 P900 P903 I904
E907 Y908 I909 I910 A911 I914 V915 C916 E917 M918 G919 H920 A921 V922 I923 G924 R931 L932 C933 I934 G935 E936 C937 K938 P939 E940 F941 M942 T943 K944 S945 H946 Q947 Q948 Y949 V952 N953 P954 S955 V956 L957 S958 L959 S960 P961 S967 T970 T973 I974 T975 Y978 L979 G980
A981 S984 V985 A986 V987 Y988 L989 G990 N991 Q992 T993 C994 E995 F996 Y997 G998 R999 S1000 M1001 N1002 E1003 I1004 V1005 C1006 V1007 S1008 P1009 P1010 S1011 S1012 L1015 G1016 P1017 V1018 P1019 V1020 S1021 V1022 S1023 V1024 V1029 L1033 Q1034 Y1037 I1038 D1039 ASP PRO ARG VAL GLN ARG ILE GLU PRO
GLU TRP SER ILE THR SER GLY HIS THR PRO LEU THR ILE THR GLY PHE ASN LEU ASP VAL SER LEU ILE GLN GLU ILE PRO ARG VAL ARG VAL LYS PHE ASN GLY LYS GLU SER VAL ASN VAL CYS THR VAL VAL ASN THR THR THR LEU LEU THR CYS LEU ALA PRO SER LEU THR SER ASP TYR ARG PRO
GLY LEU ASP THR VAL GLU ARG PRO ASP GLU PHE GLY PHE LEU PHE ASN ASN VAL GLN SER LEU LEU ILE TYR ASN ASP THR LYS PHE ILE TYR ASN GLY PRO ASN PRO THR PHE ASP VAL GLU LEU LEU PRO SER PRO ILE ILE LEU LYS GLY PRO VAL HIS VAL GLY GLY MET VAL PHE SER PRO ILE LEU LEU LYS GLY LYS ASN
LEU CYS PRO PRO ALA SER GLY GLY ALA LYS LEU ASN TYR THR VAL MET ILE GLY GLU THR PRO CYS THR VAL THR VAL SER GLU THR GLN LEU LEU LEU LEU LEU LEU ILE GLY GLN HIS LYS VAL MET VAL HIS VAL GLY GLY MET VAL PHE SER PRO GLY SER VAL SER VAL
ILE SER ASP GLY GLY SER ARG THR LYS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	238.40Å 238.40Å 642.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.05 – 10.00 63.05 – 10.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (63.05-10.00) 92.6 (63.05-10.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.335 , 0.370 0.336 , 0.370	Depositor DCC
R_{free} test set	529 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 306.7	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	28787	wwPDB-VP
Average B, all atoms (Å^2)	236.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.68	4/7230 (0.1%)	0.74	8/9821 (0.1%)
1	B	0.64	3/6488 (0.0%)	0.89	7/8804 (0.1%)
1	C	0.65	7/7878 (0.1%)	0.94	13/10705 (0.1%)
1	D	0.68	8/7879 (0.1%)	1.02	23/10708 (0.2%)
All	All	0.66	22/29475 (0.1%)	0.91	51/40038 (0.1%)

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	2
1	B	0	1
1	C	0	4
1	D	0	4
All	All	0	11

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	702	PRO	C-N	26.25	1.94	1.34
1	A	508	VAL	C-N	-24.18	0.78	1.34
1	A	702	PRO	C-N	24.13	1.89	1.34
1	D	655	ASN	C-N	-16.53	0.96	1.34
1	B	655	ASN	C-N	16.05	1.71	1.34
1	D	508	VAL	C-N	-15.27	0.98	1.34
1	B	508	VAL	C-N	-15.08	0.99	1.34
1	D	952	VAL	C-N	14.06	1.66	1.34
1	C	701	CYS	C-N	13.82	1.60	1.34
1	C	508	VAL	C-N	-11.74	1.07	1.34
1	D	988	TYR	CB-CG	-11.45	1.34	1.51
1	C	988	TYR	CB-CG	-11.43	1.34	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	701	CYS	C-N	-7.54	1.20	1.34
1	A	803	LYS	C-N	-6.78	1.18	1.34
1	D	559	CYS	C-N	6.25	1.48	1.34
1	C	803	LYS	C-N	-6.09	1.20	1.34
1	C	988	TYR	CD1-CE1	-5.94	1.30	1.39
1	D	988	TYR	CD1-CE1	-5.92	1.30	1.39
1	C	952	VAL	C-N	-5.51	1.21	1.34
1	D	803	LYS	C-N	5.43	1.46	1.34
1	D	988	TYR	CA-CB	5.16	1.65	1.53
1	C	988	TYR	CA-CB	5.09	1.65	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	702	PRO	O-C-N	-44.19	51.99	122.70
1	C	988	TYR	CB-CG-CD1	-34.32	100.41	121.00
1	D	988	TYR	CB-CG-CD1	-34.12	100.53	121.00
1	B	508	VAL	O-C-N	-33.23	69.54	122.70
1	C	803	LYS	O-C-N	-31.50	72.31	122.70
1	D	559	CYS	O-C-N	-30.43	74.01	122.70
1	C	988	TYR	CG-CD2-CE2	-20.96	104.53	121.30
1	D	988	TYR	CG-CD2-CE2	-20.93	104.56	121.30
1	D	988	TYR	CA-CB-CG	-19.39	76.55	113.40
1	C	988	TYR	CA-CB-CG	-19.37	76.60	113.40
1	C	988	TYR	CD1-CG-CD2	16.26	135.78	117.90
1	D	988	TYR	CD1-CG-CD2	16.17	135.69	117.90
1	D	701	CYS	O-C-N	15.93	151.37	121.10
1	D	952	VAL	O-C-N	-14.95	98.79	122.70
1	D	508	VAL	CA-C-N	-14.47	85.36	117.20
1	D	508	VAL	O-C-N	13.46	144.24	122.70
1	D	559	CYS	CA-C-N	12.75	145.25	117.20
1	B	508	VAL	CA-C-N	12.52	144.74	117.20
1	D	508	VAL	C-N-CA	-11.89	91.97	121.70
1	D	701	CYS	CA-C-N	-11.40	85.18	117.10
1	D	701	CYS	C-N-CD	11.34	152.21	128.40
1	A	702	PRO	O-C-N	-11.10	104.94	122.70
1	A	508	VAL	O-C-N	-10.48	105.93	122.70
1	B	702	PRO	C-N-CA	10.32	147.50	121.70
1	D	559	CYS	C-N-CA	9.34	145.06	121.70
1	C	988	TYR	CG-CD1-CE1	-9.29	113.86	121.30
1	D	988	TYR	CG-CD1-CE1	-9.26	113.89	121.30
1	A	701	CYS	CA-C-N	-9.25	91.19	117.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	702	PRO	CA-C-N	9.15	137.34	117.20
1	D	803	LYS	C-N-CA	-8.45	100.58	121.70
1	D	701	CYS	C-N-CA	-8.42	86.63	122.00
1	C	844	PRO	N-CA-C	8.24	133.52	112.10
1	B	844	PRO	N-CA-C	8.23	133.50	112.10
1	A	844	PRO	N-CA-C	8.23	133.50	112.10
1	D	844	PRO	N-CA-C	8.23	133.50	112.10
1	A	508	VAL	C-N-CA	8.20	142.21	121.70
1	A	855	CYS	O-C-N	-8.11	109.73	122.70
1	D	952	VAL	CA-C-N	7.39	133.45	117.20
1	D	952	VAL	C-N-CA	7.36	140.10	121.70
1	A	508	VAL	CA-C-N	7.04	132.68	117.20
1	D	803	LYS	CA-C-N	-6.78	102.29	117.20
1	A	701	CYS	C-N-CA	-6.45	94.92	122.00
1	B	508	VAL	C-N-CA	6.45	137.82	121.70
1	C	803	LYS	C-N-CA	-5.97	106.78	121.70
1	C	655	ASN	C-N-CA	-5.81	107.17	121.70
1	D	988	TYR	CD1-CE1-CZ	-5.79	114.59	119.80
1	C	988	TYR	CD1-CE1-CZ	-5.74	114.64	119.80
1	C	655	ASN	CA-C-N	-5.61	104.87	117.20
1	D	990	GLY	C-N-CA	5.51	135.47	121.70
1	C	990	GLY	C-N-CA	5.50	135.45	121.70
1	C	655	ASN	O-C-N	5.17	130.98	122.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	701	CYS	Mainchain
1	A	855	CYS	Mainchain
1	B	508	VAL	Mainchain
1	C	508	VAL	Mainchain
1	C	803	LYS	Mainchain
1	C	952	VAL	Mainchain
1	C	988	TYR	Sidechain
1	D	508	VAL	Mainchain
1	D	559	CYS	Mainchain
1	D	803	LYS	Mainchain
1	D	988	TYR	Sidechain

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	7060	0	6854	430	9
1	B	6337	0	6141	353	8
1	C	7695	0	7466	460	5
1	D	7695	0	7468	492	4
All	All	28787	0	27929	1661	13

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 29.

All (1661) 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:463:PRO:HG2	1:B:612:ILE:CG2	1.25	1.55
1:A:407:LEU:CD2	1:C:944:LYS:HD2	1.03	1.48
1:D:533:LEU:CD1	1:D:642:THR:HG23	1.41	1.48
1:A:407:LEU:CD2	1:C:944:LYS:CD	1.93	1.43
1:A:702:PRO:O	1:A:703:GLN:CG	1.65	1.41
1:B:655:ASN:C	1:B:656:CYS:N	1.71	1.40
1:B:533:LEU:CD2	1:B:646:PHE:CG	2.09	1.36
1:C:551:ARG:NH1	1:C:641:GLU:OE2	1.60	1.34
1:B:663:LEU:HD11	1:B:703:GLN:NE2	1.41	1.33
1:B:549:ALA:O	1:B:586:PRO:CB	1.75	1.32
1:D:533:LEU:CB	1:D:642:THR:HG21	1.59	1.30
1:D:533:LEU:O	1:D:644:LYS:HB2	1.32	1.30
1:A:508:VAL:O	1:A:509:GLU:N	1.63	1.28
1:C:663:LEU:HD11	1:C:792:ASP:OD2	1.32	1.27
1:A:407:LEU:HD21	1:C:944:LYS:CD	1.56	1.27
1:B:533:LEU:HD23	1:B:646:PHE:CG	1.67	1.25
1:D:550:ASN:HB2	1:D:586:PRO:CB	1.65	1.25
1:B:775:SER:N	1:B:807:GLN:OE1	1.67	1.25
1:A:702:PRO:C	1:A:703:GLN:N	1.89	1.25
1:B:550:ASN:ND2	1:B:585:ALA:O	1.70	1.24
1:D:550:ASN:CB	1:D:586:PRO:HB3	1.66	1.24
1:A:422:LEU:CD1	1:B:605:GLN:HG2	1.68	1.23
1:A:463:PRO:CG	1:B:612:ILE:CG2	2.18	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:LEU:CD1	1:C:792:ASP:OD2	1.90	1.20
1:D:533:LEU:CD1	1:D:642:THR:CG2	2.21	1.19
1:B:549:ALA:O	1:B:586:PRO:HB3	1.02	1.17
1:D:663:LEU:HD12	1:D:792:ASP:CB	1.73	1.17
1:D:775:SER:CB	1:D:807:GLN:HG3	1.72	1.17
1:B:533:LEU:CD2	1:B:646:PHE:CD1	2.28	1.17
1:C:533:LEU:HB3	1:C:642:THR:HG21	1.24	1.17
1:A:508:VAL:C	1:A:509:GLU:CA	2.13	1.16
1:B:778:ALA:HB1	1:B:798:LYS:HD2	1.15	1.14
1:D:533:LEU:HB3	1:D:642:THR:CG2	1.76	1.14
1:D:778:ALA:HB1	1:D:798:LYS:HD2	1.15	1.13
1:A:655:ASN:HB3	1:A:658:ALA:HB2	1.15	1.13
1:B:663:LEU:CD1	1:B:703:GLN:NE2	2.12	1.13
1:B:545:ARG:NH1	1:B:641:GLU:OE2	1.80	1.13
1:B:533:LEU:HD22	1:B:646:PHE:CD1	1.82	1.13
1:A:810:SER:HB2	1:A:882:ASN:OD1	1.49	1.12
1:C:702:PRO:HB3	1:C:728:PRO:HD3	1.18	1.11
1:A:655:ASN:C	1:A:656:CYS:N	2.03	1.11
1:D:932:LEU:HB3	1:D:943:THR:HG22	1.32	1.11
1:C:932:LEU:HB3	1:C:943:THR:HG22	1.33	1.11
1:D:534:HIS:HA	1:D:644:LYS:HG3	1.32	1.11
1:A:932:LEU:HB3	1:A:943:THR:HG22	1.33	1.10
1:D:533:LEU:HD12	1:D:642:THR:HG23	1.16	1.10
1:A:325:ALA:HB2	1:B:577:LEU:HD13	1.12	1.10
1:C:778:ALA:HB1	1:C:798:LYS:HD2	1.15	1.10
1:A:778:ALA:HB1	1:A:798:LYS:HD2	1.15	1.10
1:A:532:ALA:HB1	1:A:560:MET:HE3	1.23	1.10
1:A:407:LEU:HD22	1:C:944:LYS:HD2	1.24	1.10
1:A:508:VAL:CA	1:A:509:GLU:N	2.14	1.10
1:C:677:TYR:CD1	1:C:731:GLN:HG3	1.86	1.09
1:D:533:LEU:HB3	1:D:642:THR:HG21	1.20	1.09
1:A:325:ALA:HB2	1:B:577:LEU:CD1	1.82	1.09
1:D:533:LEU:HD13	1:D:642:THR:HG23	1.19	1.09
1:A:532:ALA:HB1	1:A:560:MET:CE	1.83	1.09
1:A:463:PRO:HG2	1:B:612:ILE:HG22	1.10	1.08
1:B:532:ALA:HB1	1:B:560:MET:HE3	1.29	1.08
1:D:815:LEU:HD23	1:D:853:VAL:HG11	1.33	1.08
1:A:463:PRO:HG2	1:B:612:ILE:CB	1.83	1.07
1:D:958:SER:HA	1:D:1033:LEU:HD22	1.34	1.07
1:B:815:LEU:HD23	1:B:853:VAL:HG11	1.33	1.07
1:C:815:LEU:HD23	1:C:853:VAL:HG11	1.33	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:LEU:HD22	1:D:639:SER:CB	1.84	1.06
1:B:692:GLU:CD	1:D:141:ARG:HH22	1.57	1.06
1:C:958:SER:HA	1:C:1033:LEU:HD22	1.34	1.06
1:D:775:SER:HB2	1:D:807:GLN:HG3	1.37	1.06
1:D:533:LEU:CD2	1:D:639:SER:CB	2.34	1.06
1:A:702:PRO:C	1:A:703:GLN:HG3	1.76	1.05
1:A:463:PRO:CG	1:B:612:ILE:HG22	1.83	1.05
1:A:463:PRO:HG2	1:B:612:ILE:HG21	1.33	1.05
1:A:325:ALA:CB	1:B:577:LEU:HD13	1.87	1.04
1:D:550:ASN:HD22	1:D:586:PRO:HA	1.14	1.04
1:A:655:ASN:O	1:A:658:ALA:HB3	1.57	1.04
1:A:815:LEU:HD23	1:A:853:VAL:HG11	1.33	1.04
1:B:533:LEU:HD23	1:B:646:PHE:CD2	1.92	1.03
1:A:464:PRO:HB3	1:B:603:GLU:O	1.56	1.03
1:A:559:CYS:C	1:A:560:MET:N	2.11	1.03
1:B:803:LYS:C	1:B:804:CYS:N	2.12	1.01
1:C:959:LEU:HG	1:C:974:ILE:HG22	1.41	1.01
1:D:533:LEU:HD22	1:D:639:SER:HB3	1.41	1.01
1:D:661:LEU:HD21	1:D:790:ILE:HD11	1.40	1.00
1:D:959:LEU:HG	1:D:974:ILE:HG22	1.41	1.00
1:B:692:GLU:OE2	1:D:141:ARG:NH2	1.94	1.00
1:C:551:ARG:NH1	1:C:641:GLU:CD	2.15	1.00
1:A:676:LYS:HE2	1:A:728:PRO:HB3	1.43	1.00
1:B:676:LYS:HE2	1:B:728:PRO:HB3	1.42	1.00
1:A:407:LEU:HD23	1:C:944:LYS:HD2	1.43	0.99
1:B:663:LEU:HD11	1:B:703:GLN:HE22	0.85	0.99
1:C:775:SER:N	1:C:806:ALA:HB3	1.78	0.99
1:D:533:LEU:HD21	1:D:639:SER:HB2	1.42	0.98
1:D:534:HIS:CD2	1:D:644:LYS:HZ3	1.81	0.98
1:C:533:LEU:HB3	1:C:642:THR:CG2	1.93	0.98
1:D:959:LEU:HD13	1:D:1033:LEU:HD23	1.44	0.98
1:C:959:LEU:HD13	1:C:1033:LEU:HD23	1.44	0.98
1:D:533:LEU:CD2	1:D:639:SER:HB2	1.91	0.98
1:A:655:ASN:CB	1:A:658:ALA:HB2	1.94	0.98
1:D:533:LEU:CB	1:D:642:THR:CG2	2.37	0.98
1:B:532:ALA:HB1	1:B:560:MET:CE	1.93	0.97
1:A:863:ILE:HD12	1:A:878:ILE:HG12	1.46	0.97
1:A:810:SER:HB2	1:A:882:ASN:CG	1.85	0.97
1:C:663:LEU:HD11	1:C:792:ASP:CG	1.85	0.97
1:D:729:GLN:HG3	1:D:754:ARG:HH12	1.26	0.97
1:A:397:PRO:HB2	1:C:947:GLN:HE22	1.25	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:GLN:HG3	1:A:754:ARG:HH12	1.26	0.97
1:C:805:ALA:HB1	1:C:808:ARG:H	1.30	0.97
1:D:663:LEU:CD1	1:D:792:ASP:OD2	2.12	0.97
1:D:863:ILE:HD12	1:D:878:ILE:HG12	1.45	0.97
1:A:407:LEU:HD23	1:C:944:LYS:CE	1.95	0.96
1:A:702:PRO:O	1:A:703:GLN:HG3	0.79	0.96
1:B:729:GLN:HG3	1:B:754:ARG:HH12	1.26	0.96
1:D:805:ALA:HB1	1:D:808:ARG:H	1.30	0.96
1:A:422:LEU:HD11	1:B:605:GLN:HG2	1.46	0.96
1:D:551:ARG:NH1	1:D:641:GLU:OE2	1.99	0.95
1:B:805:ALA:HB1	1:B:808:ARG:H	1.30	0.95
1:A:407:LEU:HD23	1:C:944:LYS:NZ	1.80	0.95
1:D:661:LEU:HD21	1:D:790:ILE:CD1	1.95	0.95
1:B:732:SER:HB2	1:D:83:HIS:CD2	2.01	0.95
1:C:729:GLN:HG3	1:C:754:ARG:HH12	1.26	0.95
1:C:863:ILE:HD12	1:C:878:ILE:HG12	1.45	0.95
1:D:663:LEU:CD1	1:D:792:ASP:CG	2.35	0.94
1:C:533:LEU:CB	1:C:642:THR:HG21	1.97	0.94
1:B:237:SER:HA	1:B:239:PHE:H	1.33	0.94
1:B:735:ARG:HG2	1:B:786:ASN:HA	1.50	0.94
1:C:735:ARG:HG2	1:C:786:ASN:HA	1.50	0.94
1:D:533:LEU:HB2	1:D:642:THR:HG21	1.45	0.94
1:D:735:ARG:HG2	1:D:786:ASN:HA	1.50	0.94
1:B:663:LEU:CD1	1:B:703:GLN:HE22	1.74	0.93
1:C:237:SER:HA	1:C:239:PHE:H	1.33	0.93
1:C:533:LEU:HD13	1:C:642:THR:HG23	1.48	0.93
1:D:533:LEU:O	1:D:644:LYS:CB	2.16	0.93
1:A:805:ALA:HB1	1:A:808:ARG:H	1.30	0.93
1:A:816:LYS:HE3	1:A:910:ILE:CG2	1.98	0.93
1:D:534:HIS:HD2	1:D:644:LYS:NZ	1.66	0.93
1:A:237:SER:HA	1:A:239:PHE:H	1.33	0.92
1:D:663:LEU:HD12	1:D:792:ASP:HB2	1.50	0.92
1:C:702:PRO:CB	1:C:728:PRO:HD3	1.99	0.92
1:B:795:GLN:HB2	1:B:797:LEU:CD1	1.99	0.92
1:B:778:ALA:CB	1:B:798:LYS:HD2	2.00	0.92
1:D:237:SER:HA	1:D:239:PHE:H	1.33	0.92
1:C:778:ALA:CB	1:C:798:LYS:HD2	2.00	0.92
1:A:735:ARG:HG2	1:A:786:ASN:HA	1.50	0.92
1:A:795:GLN:HB2	1:A:797:LEU:CD1	1.99	0.92
1:D:533:LEU:HD13	1:D:642:THR:CG2	1.92	0.92
1:C:795:GLN:HB2	1:C:797:LEU:CD1	1.99	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ALA:O	1:B:586:PRO:CA	2.18	0.91
1:D:533:LEU:HB3	1:D:642:THR:CB	2.00	0.91
1:D:795:GLN:HB2	1:D:797:LEU:CD1	1.99	0.91
1:A:655:ASN:OD1	1:A:657:SER:HB2	1.71	0.91
1:A:778:ALA:CB	1:A:798:LYS:HD2	2.00	0.91
1:D:534:HIS:HD2	1:D:644:LYS:HZ3	0.94	0.91
1:C:702:PRO:HB3	1:C:728:PRO:CD	2.01	0.90
1:D:737:TYR:CE1	1:D:754:ARG:HD2	2.06	0.90
1:B:692:GLU:OE2	1:D:141:ARG:NH1	2.05	0.90
1:C:737:TYR:CE1	1:C:754:ARG:HD2	2.06	0.90
1:A:737:TYR:CE1	1:A:754:ARG:HD2	2.06	0.90
1:B:707:THR:HG21	1:B:723:LYS:HD3	1.54	0.90
1:B:737:TYR:CE1	1:B:754:ARG:HD2	2.06	0.90
1:A:422:LEU:CD1	1:B:605:GLN:CG	2.49	0.90
1:A:655:ASN:HB3	1:A:658:ALA:CB	2.02	0.90
1:A:816:LYS:CE	1:A:910:ILE:HG23	2.02	0.89
1:C:533:LEU:CD1	1:C:642:THR:HG23	2.01	0.89
1:D:778:ALA:CB	1:D:798:LYS:HD2	2.00	0.89
1:A:707:THR:HG21	1:A:723:LYS:HD3	1.54	0.89
1:B:533:LEU:HA	1:B:646:PHE:HB2	1.54	0.89
1:B:706:PRO:HA	1:B:797:LEU:HD21	1.55	0.89
1:C:707:THR:HG21	1:C:723:LYS:HD3	1.54	0.89
1:A:810:SER:CB	1:A:882:ASN:OD1	2.22	0.88
1:A:810:SER:HB2	1:A:882:ASN:ND2	1.89	0.88
1:C:533:LEU:HD22	1:C:639:SER:CB	2.04	0.88
1:A:932:LEU:HB3	1:A:943:THR:CG2	2.04	0.88
1:C:663:LEU:HD12	1:C:792:ASP:CB	2.04	0.87
1:C:893:HIS:HB2	1:C:933:CYS:O	1.75	0.87
1:A:655:ASN:O	1:A:658:ALA:CB	2.21	0.87
1:C:959:LEU:CD1	1:C:1033:LEU:HD23	2.04	0.87
1:D:533:LEU:HD12	1:D:642:THR:CG2	1.91	0.87
1:D:550:ASN:HB2	1:D:586:PRO:HB3	0.89	0.87
1:D:707:THR:HG21	1:D:723:LYS:HD3	1.54	0.87
1:D:959:LEU:CD1	1:D:1033:LEU:HD23	2.04	0.87
1:B:533:LEU:HA	1:B:646:PHE:CB	2.04	0.87
1:A:549:ALA:O	1:A:586:PRO:HB3	1.74	0.87
1:D:893:HIS:HB2	1:D:933:CYS:O	1.75	0.87
1:D:551:ARG:NH2	1:D:642:THR:HG22	1.89	0.87
1:D:932:LEU:HB3	1:D:943:THR:CG2	2.04	0.86
1:A:706:PRO:HA	1:A:797:LEU:HD21	1.55	0.86
1:C:706:PRO:HA	1:C:797:LEU:HD21	1.55	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:706:PRO:HA	1:D:797:LEU:HD21	1.55	0.86
1:D:711:LEU:HD23	1:D:821:PHE:CD1	2.10	0.86
1:C:934:ILE:HD12	1:C:941:PHE:HD1	1.40	0.86
1:D:550:ASN:CB	1:D:586:PRO:CB	2.39	0.86
1:C:932:LEU:HB3	1:C:943:THR:CG2	2.04	0.86
1:D:663:LEU:HD11	1:D:792:ASP:CG	1.94	0.86
1:B:533:LEU:CD2	1:B:646:PHE:CD2	2.55	0.85
1:B:775:SER:H	1:B:807:GLN:CD	1.79	0.85
1:D:934:ILE:HD12	1:D:941:PHE:HD1	1.40	0.85
1:D:550:ASN:ND2	1:D:586:PRO:HA	1.91	0.85
1:D:775:SER:HB3	1:D:807:GLN:HG3	1.59	0.85
1:A:655:ASN:C	1:A:656:CYS:CA	2.44	0.85
1:A:893:HIS:HB2	1:A:933:CYS:O	1.75	0.85
1:A:934:ILE:HD12	1:A:941:PHE:HD1	1.40	0.85
1:C:533:LEU:HD22	1:C:639:SER:HB2	1.57	0.84
1:D:775:SER:CB	1:D:807:GLN:CG	2.55	0.84
1:C:663:LEU:CD1	1:C:792:ASP:CG	2.44	0.84
1:B:743:ILE:HB	1:B:746:ALA:O	1.78	0.84
1:A:655:ASN:C	1:A:658:ALA:H	1.80	0.84
1:C:743:ILE:HB	1:C:746:ALA:O	1.78	0.84
1:B:702:PRO:HB3	1:B:726:ASN:O	1.76	0.83
1:C:795:GLN:HB2	1:C:797:LEU:HD12	1.60	0.83
1:D:743:ILE:HB	1:D:746:ALA:O	1.78	0.83
1:A:508:VAL:C	1:A:509:GLU:N	0.78	0.83
1:A:407:LEU:CD2	1:C:944:LYS:CE	2.56	0.83
1:C:818:ASP:HB2	1:C:821:PHE:CD2	2.14	0.83
1:B:818:ASP:HB2	1:B:821:PHE:CD2	2.14	0.83
1:A:743:ILE:HB	1:A:746:ALA:O	1.78	0.83
1:A:301:THR:HG21	1:B:589:SER:HB2	1.60	0.83
1:C:893:HIS:CE1	1:C:894:VAL:HG22	2.14	0.83
1:D:663:LEU:HD12	1:D:792:ASP:CG	1.99	0.83
1:A:818:ASP:HB2	1:A:821:PHE:CD2	2.14	0.82
1:B:795:GLN:HB2	1:B:797:LEU:HD12	1.60	0.82
1:A:893:HIS:CE1	1:A:894:VAL:HG22	2.14	0.82
1:D:663:LEU:HD11	1:D:792:ASP:OD2	1.78	0.82
1:D:893:HIS:CE1	1:D:894:VAL:HG22	2.14	0.82
1:D:550:ASN:HD22	1:D:586:PRO:CA	1.93	0.82
1:D:534:HIS:CD2	1:D:644:LYS:NZ	2.43	0.82
1:D:818:ASP:HB2	1:D:821:PHE:CD2	2.14	0.82
1:A:893:HIS:HD1	1:A:932:LEU:HA	1.44	0.81
1:D:795:GLN:HB2	1:D:797:LEU:HD12	1.60	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:GLN:HB2	1:A:797:LEU:HD12	1.60	0.81
1:A:816:LYS:HE3	1:A:910:ILE:HG23	1.61	0.81
1:C:907:GLU:OE1	1:C:915:VAL:HG11	1.81	0.81
1:B:741:LEU:O	1:B:747:VAL:HG23	1.81	0.81
1:A:407:LEU:HD23	1:C:944:LYS:CD	1.96	0.81
1:B:711:LEU:HD21	1:B:820:LYS:HB3	1.62	0.81
1:C:893:HIS:HD1	1:C:932:LEU:HA	1.44	0.81
1:A:907:GLU:OE1	1:A:915:VAL:HG11	1.81	0.81
1:C:735:ARG:CG	1:C:786:ASN:HA	2.11	0.81
1:D:893:HIS:HD1	1:D:932:LEU:HA	1.44	0.81
1:D:741:LEU:O	1:D:747:VAL:HG23	1.81	0.81
1:D:907:GLU:OE1	1:D:915:VAL:HG11	1.81	0.81
1:B:802:TYR:CG	1:B:821:PHE:CD1	2.69	0.80
1:C:741:LEU:O	1:C:747:VAL:HG23	1.81	0.80
1:C:883:LEU:HB2	1:C:911:ALA:HA	1.63	0.80
1:D:735:ARG:CG	1:D:786:ASN:HA	2.11	0.80
1:A:784:VAL:HG22	1:A:790:ILE:HG22	1.63	0.80
1:A:422:LEU:HD12	1:B:605:GLN:CD	2.01	0.80
1:B:701:CYS:C	1:B:702:PRO:N	2.35	0.80
1:C:677:TYR:CD1	1:C:731:GLN:CG	2.63	0.80
1:D:883:LEU:HB2	1:D:911:ALA:HA	1.63	0.80
1:B:735:ARG:CG	1:B:786:ASN:HA	2.11	0.80
1:D:904:ILE:CG2	1:D:907:GLU:HB2	2.12	0.80
1:A:904:ILE:CG2	1:A:907:GLU:HB2	2.12	0.80
1:B:784:VAL:HG22	1:B:790:ILE:HG22	1.63	0.80
1:B:692:GLU:OE2	1:D:141:ARG:CZ	2.29	0.80
1:D:551:ARG:NH1	1:D:641:GLU:CD	2.35	0.80
1:D:803:LYS:C	1:D:804:CYS:O	2.17	0.80
1:D:775:SER:HB2	1:D:807:GLN:CG	2.12	0.80
1:A:735:ARG:CG	1:A:786:ASN:HA	2.11	0.80
1:C:904:ILE:CG2	1:C:907:GLU:HB2	2.12	0.80
1:C:893:HIS:CE1	1:C:932:LEU:HG	2.18	0.79
1:D:812:GLY:HA3	1:D:885:LEU:CD2	2.11	0.79
1:A:217:LEU:HD11	1:C:940:GLU:OE1	1.83	0.79
1:A:397:PRO:HB2	1:C:947:GLN:NE2	1.95	0.79
1:D:784:VAL:HG22	1:D:790:ILE:HG22	1.63	0.79
1:A:407:LEU:HD21	1:C:944:LYS:HD2	0.79	0.79
1:A:741:LEU:O	1:A:747:VAL:HG23	1.81	0.79
1:B:690:PHE:HE2	1:B:731:GLN:HB3	1.47	0.79
1:B:775:SER:CB	1:B:807:GLN:OE1	2.30	0.79
1:B:663:LEU:CD1	1:B:703:GLN:HE21	1.96	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:VAL:HG22	1:C:790:ILE:HG22	1.63	0.79
1:D:533:LEU:CD1	1:D:639:SER:OG	2.31	0.79
1:D:893:HIS:CE1	1:D:932:LEU:HG	2.18	0.78
1:A:463:PRO:HD2	1:B:577:LEU:HD22	1.65	0.78
1:D:663:LEU:CD1	1:D:792:ASP:CB	2.56	0.78
1:D:823:CYS:HA	1:D:834:LEU:HD23	1.65	0.78
1:A:422:LEU:HD12	1:B:605:GLN:CG	2.14	0.78
1:C:823:CYS:HA	1:C:834:LEU:HD23	1.65	0.78
1:D:958:SER:HA	1:D:1033:LEU:CD2	2.13	0.78
1:A:463:PRO:HG2	1:B:612:ILE:HB	1.66	0.78
1:D:812:GLY:CA	1:D:885:LEU:CD2	2.62	0.78
1:A:893:HIS:CE1	1:A:932:LEU:HG	2.18	0.78
1:A:883:LEU:HB2	1:A:911:ALA:HA	1.63	0.77
1:A:737:TYR:HE1	1:A:754:ARG:HD2	1.50	0.77
1:A:508:VAL:O	1:A:509:GLU:CA	2.29	0.77
1:B:550:ASN:HB2	1:B:586:PRO:CA	2.13	0.77
1:A:890:ILE:HD13	1:A:908:TYR:CE1	2.20	0.77
1:D:786:ASN:HB3	1:D:789:PHE:HD2	1.50	0.77
1:A:655:ASN:C	1:A:656:CYS:C	2.43	0.77
1:D:795:GLN:HB2	1:D:797:LEU:HD11	1.67	0.77
1:B:533:LEU:HD22	1:B:646:PHE:CG	2.00	0.77
1:B:823:CYS:HA	1:B:834:LEU:HD23	1.65	0.77
1:D:890:ILE:HD13	1:D:908:TYR:CE1	2.20	0.77
1:D:729:GLN:HG3	1:D:754:ARG:NH1	2.00	0.76
1:A:795:GLN:HB2	1:A:797:LEU:HD11	1.67	0.76
1:A:823:CYS:HA	1:A:834:LEU:HD23	1.65	0.76
1:C:795:GLN:HB2	1:C:797:LEU:HD11	1.67	0.76
1:D:533:LEU:HB3	1:D:642:THR:OG1	1.86	0.76
1:A:786:ASN:HB3	1:A:789:PHE:HD2	1.50	0.76
1:C:729:GLN:HG3	1:C:754:ARG:NH1	2.00	0.76
1:B:550:ASN:HB2	1:B:586:PRO:N	1.99	0.76
1:D:812:GLY:CA	1:D:885:LEU:HD21	2.16	0.76
1:A:815:LEU:HD23	1:A:853:VAL:CG1	2.15	0.76
1:C:958:SER:HA	1:C:1033:LEU:CD2	2.13	0.76
1:C:786:ASN:HB3	1:C:789:PHE:HD2	1.50	0.76
1:B:729:GLN:HG3	1:B:754:ARG:NH1	2.00	0.76
1:C:890:ILE:HD13	1:C:908:TYR:CE1	2.20	0.76
1:A:463:PRO:CG	1:B:612:ILE:HG21	2.00	0.76
1:D:440:TYR:CE2	1:D:527:HIS:HA	2.21	0.75
1:D:737:TYR:HE1	1:D:754:ARG:HD2	1.50	0.75
1:D:803:LYS:O	1:D:804:CYS:C	2.16	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:GLN:HG3	1:A:754:ARG:NH1	2.00	0.75
1:B:559:CYS:C	1:B:560:MET:N	2.40	0.75
1:B:795:GLN:HB2	1:B:797:LEU:HD11	1.67	0.75
1:D:996:PHE:HZ	1:D:999:ARG:HB2	1.51	0.75
1:C:996:PHE:HZ	1:C:999:ARG:HB2	1.51	0.75
1:C:960:SER:OG	1:C:973:THR:HB	1.86	0.75
1:C:707:THR:CG2	1:C:723:LYS:HD3	2.17	0.75
1:B:786:ASN:HB3	1:B:789:PHE:HD2	1.50	0.75
1:B:802:TYR:CD2	1:B:821:PHE:CD1	2.75	0.75
1:C:737:TYR:HE1	1:C:754:ARG:HD2	1.50	0.75
1:A:870:PRO:O	1:A:921:ALA:HB3	1.87	0.75
1:D:870:PRO:O	1:D:921:ALA:HB3	1.87	0.75
1:D:815:LEU:HD23	1:D:853:VAL:CG1	2.15	0.74
1:D:960:SER:OG	1:D:973:THR:HB	1.86	0.74
1:B:459:ARG:NH1	1:B:524:GLY:O	2.20	0.74
1:D:707:THR:CG2	1:D:723:LYS:HD3	2.17	0.74
1:B:775:SER:CA	1:B:807:GLN:OE1	2.36	0.74
1:A:815:LEU:CB	1:A:885:LEU:HD11	2.17	0.74
1:B:550:ASN:HB2	1:B:585:ALA:C	2.08	0.74
1:D:714:VAL:HG13	1:D:767:TYR:O	1.88	0.74
1:A:714:VAL:HG13	1:A:767:TYR:O	1.88	0.73
1:B:714:VAL:HG13	1:B:767:TYR:O	1.88	0.73
1:B:707:THR:CG2	1:B:723:LYS:HD3	2.17	0.73
1:C:873:GLY:HA3	1:C:1026:ARG:HG3	1.70	0.73
1:C:870:PRO:O	1:C:921:ALA:HB3	1.87	0.73
1:A:893:HIS:ND1	1:A:932:LEU:HA	2.02	0.73
1:C:714:VAL:HG13	1:C:767:TYR:O	1.88	0.73
1:C:445:VAL:HG22	1:C:526:PRO:HG2	1.70	0.73
1:A:707:THR:CG2	1:A:723:LYS:HD3	2.17	0.73
1:D:533:LEU:HD21	1:D:639:SER:CB	2.07	0.73
1:B:533:LEU:HD23	1:B:646:PHE:CB	2.19	0.73
1:D:997:TYR:HB3	1:D:1005:VAL:HG23	1.70	0.73
1:D:893:HIS:ND1	1:D:932:LEU:HA	2.02	0.73
1:C:893:HIS:ND1	1:C:932:LEU:HA	2.02	0.73
1:C:997:TYR:HB3	1:C:1005:VAL:HG23	1.70	0.73
1:D:550:ASN:HB2	1:D:586:PRO:CA	2.18	0.73
1:D:786:ASN:HB3	1:D:789:PHE:CD2	2.24	0.72
1:A:702:PRO:O	1:A:703:GLN:CB	2.35	0.72
1:B:775:SER:HB2	1:B:807:GLN:CD	2.08	0.72
1:B:786:ASN:HB3	1:B:789:PHE:CD2	2.24	0.72
1:B:544:GLN:HG2	1:B:545:ARG:HG2	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1018:VAL:O	1:C:1034:GLN:HG3	1.88	0.72
1:D:1018:VAL:O	1:D:1034:GLN:HG3	1.88	0.72
1:B:533:LEU:HD21	1:B:646:PHE:CD1	2.24	0.72
1:C:663:LEU:HD12	1:C:792:ASP:HB3	1.72	0.72
1:D:988:TYR:HB3	1:D:1021:SER:HB3	1.70	0.72
1:A:863:ILE:CD1	1:A:878:ILE:HG12	2.20	0.72
1:D:775:SER:HB3	1:D:807:GLN:CG	2.18	0.72
1:A:655:ASN:O	1:A:658:ALA:N	2.22	0.71
1:C:872:GLY:O	1:C:1026:ARG:HB2	1.89	0.71
1:A:422:LEU:HD12	1:B:605:GLN:HG2	1.66	0.71
1:C:988:TYR:HB3	1:C:1021:SER:HB3	1.71	0.71
1:D:893:HIS:NE2	1:D:914:ILE:HD13	2.05	0.71
1:A:786:ASN:HB3	1:A:789:PHE:CD2	2.24	0.71
1:A:883:LEU:HD23	1:A:914:ILE:HD11	1.72	0.71
1:C:863:ILE:CD1	1:C:878:ILE:HG12	2.20	0.71
1:C:893:HIS:NE2	1:C:914:ILE:HD13	2.05	0.71
1:D:883:LEU:HD23	1:D:914:ILE:HD11	1.72	0.71
1:B:732:SER:HB2	1:D:83:HIS:NE2	2.04	0.71
1:B:711:LEU:CD2	1:B:820:LYS:HB3	2.20	0.71
1:C:815:LEU:HD23	1:C:853:VAL:CG1	2.15	0.71
1:A:810:SER:HB2	1:A:882:ASN:HD21	1.53	0.71
1:C:786:ASN:HB3	1:C:789:PHE:CD2	2.24	0.71
1:A:893:HIS:NE2	1:A:914:ILE:HD13	2.05	0.71
1:D:855:CYS:SG	1:D:885:LEU:HD21	2.30	0.71
1:A:221:PHE:CZ	1:C:830:ARG:HB2	2.25	0.71
1:B:549:ALA:O	1:B:586:PRO:HA	1.91	0.71
1:B:532:ALA:CB	1:B:560:MET:HE3	2.16	0.71
1:B:737:TYR:HE1	1:B:754:ARG:HD2	1.50	0.71
1:B:775:SER:CB	1:B:807:GLN:CD	2.59	0.71
1:A:655:ASN:CG	1:A:658:ALA:N	2.45	0.70
1:A:655:ASN:CA	1:A:656:CYS:N	2.54	0.70
1:C:544:GLN:HG2	1:C:545:ARG:HG2	1.71	0.70
1:D:544:GLN:HG2	1:D:545:ARG:HG2	1.71	0.70
1:A:544:GLN:HG2	1:A:545:ARG:HG2	1.71	0.70
1:A:920:HIS:NE2	1:A:922:VAL:HG23	2.06	0.70
1:D:863:ILE:CD1	1:D:878:ILE:HG12	2.20	0.70
1:D:920:HIS:NE2	1:D:922:VAL:HG23	2.06	0.70
1:B:690:PHE:HE2	1:B:731:GLN:CB	2.03	0.70
1:B:697:VAL:HG12	1:B:699:GLU:H	1.57	0.70
1:C:920:HIS:NE2	1:C:922:VAL:HG23	2.06	0.70
1:A:811:CYS:O	1:A:815:LEU:HD13	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:CYS:SG	1:A:839:PRO:HD2	2.32	0.70
1:B:815:LEU:HD23	1:B:853:VAL:CG1	2.15	0.70
1:C:697:VAL:HG12	1:C:699:GLU:H	1.57	0.70
1:C:811:CYS:O	1:C:815:LEU:HD13	1.92	0.70
1:C:883:LEU:HD23	1:C:914:ILE:HD11	1.72	0.70
1:D:838:CYS:SG	1:D:839:PRO:HD2	2.32	0.70
1:B:833:THR:CG2	1:B:837:HIS:HB2	2.22	0.70
1:D:811:CYS:O	1:D:815:LEU:HD13	1.92	0.70
1:A:697:VAL:HG12	1:A:699:GLU:H	1.56	0.70
1:D:938:LYS:HB2	1:D:941:PHE:HD2	1.57	0.70
1:B:838:CYS:SG	1:B:839:PRO:HD2	2.32	0.69
1:C:938:LYS:HB2	1:C:941:PHE:HD2	1.57	0.69
1:A:868:GLY:HA3	1:A:949:TYR:OH	1.92	0.69
1:B:811:CYS:O	1:B:815:LEU:HD13	1.92	0.69
1:C:818:ASP:HB2	1:C:821:PHE:CE2	2.28	0.69
1:D:697:VAL:HG12	1:D:699:GLU:H	1.57	0.69
1:A:810:SER:CB	1:A:882:ASN:HD21	2.06	0.69
1:A:870:PRO:HD3	1:A:952:VAL:O	1.92	0.69
1:D:533:LEU:HD11	1:D:639:SER:OG	1.91	0.69
1:A:818:ASP:HB2	1:A:821:PHE:CE2	2.28	0.69
1:B:470:TYR:CE1	1:B:525:ASP:CG	2.66	0.69
1:A:833:THR:CG2	1:A:837:HIS:HB2	2.22	0.69
1:A:938:LYS:HB2	1:A:941:PHE:HD2	1.57	0.69
1:C:663:LEU:CD1	1:C:792:ASP:CB	2.69	0.69
1:C:838:CYS:SG	1:C:839:PRO:HD2	2.32	0.69
1:C:868:GLY:HA3	1:C:949:TYR:OH	1.92	0.69
1:D:818:ASP:HB2	1:D:821:PHE:CE2	2.28	0.69
1:B:818:ASP:HB2	1:B:821:PHE:CE2	2.28	0.69
1:D:550:ASN:HB3	1:D:586:PRO:HG3	1.73	0.69
1:A:463:PRO:CG	1:B:612:ILE:HB	2.23	0.69
1:C:833:THR:CG2	1:C:837:HIS:HB2	2.22	0.69
1:C:870:PRO:HD3	1:C:952:VAL:O	1.92	0.69
1:D:868:GLY:HA3	1:D:949:TYR:OH	1.92	0.69
1:A:893:HIS:NE2	1:A:894:VAL:HG22	2.08	0.69
1:D:870:PRO:HD3	1:D:952:VAL:O	1.93	0.69
1:A:815:LEU:HB3	1:A:885:LEU:HD11	1.74	0.69
1:D:833:THR:CG2	1:D:837:HIS:HB2	2.22	0.69
1:D:663:LEU:CD1	1:D:792:ASP:HB2	2.23	0.68
1:D:893:HIS:NE2	1:D:894:VAL:HG22	2.08	0.68
1:A:740:VAL:HG22	1:A:749:ARG:HD2	1.76	0.68
1:A:815:LEU:HA	1:A:848:TRP:CD1	2.29	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:ILE:HB	1:A:893:HIS:HD2	1.58	0.68
1:D:890:ILE:HB	1:D:893:HIS:HD2	1.59	0.68
1:A:79:ILE:HD11	1:A:82:ALA:HB2	1.75	0.68
1:C:550:ASN:CB	1:C:586:PRO:HB3	2.24	0.68
1:D:79:ILE:HD11	1:D:82:ALA:HB2	1.75	0.68
1:B:815:LEU:HA	1:B:848:TRP:CD1	2.29	0.68
1:C:79:ILE:HD11	1:C:82:ALA:HB2	1.75	0.68
1:C:890:ILE:HB	1:C:893:HIS:HD2	1.59	0.68
1:B:737:TYR:CD2	1:B:785:TRP:HB3	2.29	0.68
1:C:737:TYR:CD2	1:C:785:TRP:HB3	2.29	0.68
1:D:564:VAL:HG22	1:D:580:LEU:HD13	1.76	0.68
1:D:815:LEU:HA	1:D:848:TRP:CD1	2.29	0.68
1:D:737:TYR:CD2	1:D:785:TRP:HB3	2.29	0.68
1:A:704:LEU:HD11	1:A:783:VAL:CG2	2.24	0.68
1:A:706:PRO:CA	1:A:797:LEU:HD21	2.24	0.68
1:B:79:ILE:HD11	1:B:82:ALA:HB2	1.75	0.68
1:B:810:SER:OG	1:B:813:LEU:HD13	1.94	0.68
1:C:810:SER:OG	1:C:813:LEU:HD13	1.94	0.68
1:B:740:VAL:HG22	1:B:749:ARG:HD2	1.75	0.67
1:D:704:LEU:HD11	1:D:783:VAL:CG2	2.24	0.67
1:B:550:ASN:CB	1:B:585:ALA:C	2.63	0.67
1:C:704:LEU:HD11	1:C:783:VAL:CG2	2.24	0.67
1:C:713:PRO:HG3	1:C:802:TYR:OH	1.95	0.67
1:B:704:LEU:HD11	1:B:783:VAL:CG2	2.24	0.67
1:B:713:PRO:HG3	1:B:802:TYR:OH	1.95	0.67
1:C:564:VAL:HG22	1:C:580:LEU:HD13	1.76	0.67
1:C:863:ILE:HG13	1:C:877:THR:O	1.94	0.67
1:A:863:ILE:HG13	1:A:877:THR:O	1.95	0.67
1:D:713:PRO:HG3	1:D:802:TYR:OH	1.95	0.67
1:C:815:LEU:HA	1:C:848:TRP:CD1	2.29	0.67
1:D:1015:LEU:HD12	1:D:1015:LEU:H	1.59	0.67
1:D:810:SER:OG	1:D:813:LEU:HD13	1.94	0.67
1:A:737:TYR:CD2	1:A:785:TRP:HB3	2.29	0.67
1:A:810:SER:OG	1:A:813:LEU:HD13	1.94	0.67
1:B:568:SER:HG	1:B:670:PHE:HD1	1.41	0.67
1:A:463:PRO:CD	1:B:612:ILE:HG21	2.24	0.67
1:C:893:HIS:NE2	1:C:894:VAL:HG22	2.08	0.67
1:D:740:VAL:HG22	1:D:749:ARG:HD2	1.76	0.67
1:B:564:VAL:HG22	1:B:580:LEU:HD13	1.76	0.67
1:B:703:GLN:HA	1:B:792:ASP:OD1	1.95	0.67
1:C:1015:LEU:H	1:C:1015:LEU:HD12	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:ASN:OD1	1:C:657:SER:HB2	1.94	0.67
1:B:666:VAL:HG11	1:B:698:SER:N	2.10	0.67
1:B:805:ALA:HB1	1:B:808:ARG:N	2.08	0.67
1:B:237:SER:HA	1:B:239:PHE:N	2.07	0.66
1:B:690:PHE:CD2	1:B:731:GLN:HG3	2.30	0.66
1:C:740:VAL:HG22	1:C:749:ARG:HD2	1.75	0.66
1:A:564:VAL:HG22	1:A:580:LEU:HD13	1.76	0.66
1:B:706:PRO:CA	1:B:797:LEU:HD21	2.24	0.66
1:C:559:CYS:O	1:C:584:ASP:CB	2.43	0.66
1:C:702:PRO:HA	1:C:726:ASN:O	1.95	0.66
1:C:533:LEU:CD2	1:C:639:SER:HB2	2.23	0.66
1:C:956:VAL:HG23	1:C:975:THR:O	1.95	0.66
1:D:666:VAL:HG11	1:D:698:SER:N	2.10	0.66
1:D:956:VAL:HG23	1:D:975:THR:O	1.95	0.66
1:B:714:VAL:HG13	1:B:768:GLN:HA	1.77	0.66
1:D:703:GLN:HA	1:D:792:ASP:OD1	1.95	0.66
1:D:863:ILE:HG13	1:D:877:THR:O	1.94	0.66
1:A:706:PRO:HG3	1:A:795:GLN:HG3	1.78	0.66
1:B:533:LEU:HD21	1:B:646:PHE:CE1	2.31	0.66
1:C:677:TYR:HD1	1:C:731:GLN:HG3	1.55	0.66
1:C:706:PRO:CA	1:C:797:LEU:HD21	2.24	0.66
1:A:713:PRO:HG3	1:A:802:TYR:OH	1.95	0.66
1:A:324:GLN:HE21	1:B:577:LEU:H	1.42	0.66
1:C:237:SER:HA	1:C:239:PHE:N	2.08	0.66
1:D:717:VAL:CG1	1:D:764:ASN:HB3	2.26	0.66
1:A:714:VAL:HG13	1:A:768:GLN:HA	1.78	0.66
1:B:717:VAL:CG1	1:B:764:ASN:HB3	2.26	0.66
1:B:732:SER:CB	1:D:83:HIS:CD2	2.78	0.66
1:C:714:VAL:HG13	1:C:768:GLN:HA	1.77	0.66
1:B:802:TYR:CD1	1:B:821:PHE:CD1	2.84	0.66
1:C:855:CYS:C	1:C:856:SER:N	2.48	0.66
1:D:793:ASN:OD1	1:D:797:LEU:HD13	1.96	0.66
1:A:237:SER:HA	1:A:239:PHE:N	2.08	0.66
1:C:1015:LEU:HD21	1:C:1039:ASP:HB2	1.78	0.65
1:A:666:VAL:HG11	1:A:698:SER:N	2.10	0.65
1:A:703:GLN:HA	1:A:792:ASP:OD1	1.95	0.65
1:B:551:ARG:NH2	1:B:642:THR:HG21	2.11	0.65
1:C:666:VAL:HG11	1:C:698:SER:N	2.10	0.65
1:C:717:VAL:CG1	1:C:764:ASN:HB3	2.26	0.65
1:C:703:GLN:HA	1:C:792:ASP:OD1	1.95	0.65
1:C:793:ASN:OD1	1:C:797:LEU:HD13	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:SER:HA	1:D:239:PHE:N	2.08	0.65
1:A:701:CYS:O	1:A:703:GLN:HG3	1.95	0.65
1:D:706:PRO:CA	1:D:797:LEU:HD21	2.24	0.65
1:D:1015:LEU:HD21	1:D:1039:ASP:HB2	1.78	0.65
1:B:711:LEU:HD21	1:B:820:LYS:CB	2.25	0.65
1:C:774:ILE:C	1:C:806:ALA:HB3	2.15	0.65
1:A:717:VAL:CG1	1:A:764:ASN:HB3	2.26	0.65
1:B:793:ASN:OD1	1:B:797:LEU:HD13	1.96	0.65
1:B:803:LYS:C	1:B:804:CYS:CA	2.65	0.65
1:D:864:LEU:HG	1:D:865:THR:N	2.12	0.65
1:D:812:GLY:CA	1:D:885:LEU:HD22	2.26	0.65
1:D:714:VAL:HG13	1:D:768:GLN:HA	1.78	0.65
1:A:742:SER:O	1:A:779:VAL:HG13	1.97	0.65
1:C:864:LEU:HG	1:C:865:THR:N	2.12	0.65
1:A:772:MET:O	1:A:806:ALA:HB1	1.97	0.65
1:A:864:LEU:HG	1:A:865:THR:N	2.12	0.65
1:C:742:SER:O	1:C:779:VAL:HG13	1.97	0.65
1:C:88:GLU:HB2	1:C:132:LEU:HD21	1.79	0.65
1:A:793:ASN:OD1	1:A:797:LEU:HD13	1.96	0.64
1:A:88:GLU:HB2	1:A:132:LEU:HD21	1.79	0.64
1:D:706:PRO:HG3	1:D:795:GLN:HG3	1.78	0.64
1:A:655:ASN:OD1	1:A:658:ALA:N	2.30	0.64
1:D:88:GLU:HB2	1:D:132:LEU:HD21	1.79	0.64
1:D:742:SER:O	1:D:779:VAL:HG13	1.97	0.64
1:A:704:LEU:HD11	1:A:783:VAL:HG21	1.80	0.64
1:A:842:SER:OG	1:A:844:PRO:HD2	1.97	0.64
1:B:695:ILE:CD1	1:B:702:PRO:HD3	2.28	0.64
1:A:805:ALA:HB1	1:A:808:ARG:N	2.08	0.64
1:C:842:SER:OG	1:C:844:PRO:HD2	1.97	0.64
1:D:812:GLY:HA3	1:D:885:LEU:HD22	1.78	0.64
1:B:550:ASN:HB2	1:B:586:PRO:HA	1.80	0.64
1:C:706:PRO:HG3	1:C:795:GLN:HG3	1.78	0.64
1:A:549:ALA:O	1:A:586:PRO:CB	2.45	0.64
1:B:706:PRO:HG3	1:B:795:GLN:HG3	1.78	0.64
1:C:533:LEU:HD13	1:C:639:SER:OG	1.98	0.64
1:A:810:SER:CB	1:A:882:ASN:ND2	2.61	0.63
1:B:742:SER:O	1:B:779:VAL:HG13	1.97	0.63
1:D:931:ARG:HD2	1:D:942:MET:HE3	1.79	0.63
1:B:533:LEU:CD2	1:B:646:PHE:CB	2.76	0.63
1:B:842:SER:OG	1:B:844:PRO:HD2	1.97	0.63
1:C:704:LEU:HD11	1:C:783:VAL:HG21	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:775:SER:HB2	1:C:807:GLN:H	1.62	0.63
1:D:959:LEU:HG	1:D:974:ILE:CG2	2.25	0.63
1:B:704:LEU:HD11	1:B:783:VAL:HG21	1.80	0.63
1:C:855:CYS:O	1:C:856:SER:N	2.32	0.63
1:D:1001:MET:HG3	1:D:1002:ASN:N	2.13	0.63
1:D:842:SER:OG	1:D:844:PRO:HD2	1.97	0.63
1:B:706:PRO:HA	1:B:797:LEU:CD2	2.29	0.63
1:A:407:LEU:HD23	1:C:944:LYS:HZ2	1.61	0.63
1:C:1001:MET:HG3	1:C:1002:ASN:N	2.13	0.63
1:C:959:LEU:HG	1:C:974:ILE:CG2	2.25	0.63
1:D:470:TYR:HB2	1:D:523:SER:O	1.98	0.63
1:D:704:LEU:HD11	1:D:783:VAL:HG21	1.80	0.63
1:D:988:TYR:HE1	1:D:992:GLN:C	2.02	0.63
1:B:88:GLU:HB2	1:B:132:LEU:HD21	1.79	0.63
1:C:931:ARG:HD2	1:C:942:MET:HE3	1.79	0.63
1:C:988:TYR:HE1	1:C:992:GLN:C	2.02	0.63
1:D:630:TRP:HB3	1:D:670:PHE:CE2	2.34	0.63
1:C:994:CYS:HA	1:C:1009:PRO:HD3	1.81	0.63
1:C:274:LEU:H	1:C:274:LEU:HD12	1.64	0.63
1:C:904:ILE:HG23	1:C:907:GLU:HB2	1.79	0.63
1:D:994:CYS:HA	1:D:1009:PRO:HD3	1.81	0.63
1:D:904:ILE:HG23	1:D:907:GLU:HB2	1.79	0.63
1:C:989:LEU:HG	1:C:1020:VAL:HG12	1.81	0.62
1:D:661:LEU:HD21	1:D:790:ILE:CG1	2.28	0.62
1:A:274:LEU:H	1:A:274:LEU:HD12	1.64	0.62
1:A:834:LEU:HB2	1:A:837:HIS:HD2	1.64	0.62
1:B:834:LEU:HB2	1:B:837:HIS:HD2	1.64	0.62
1:D:989:LEU:HG	1:D:1020:VAL:HG12	1.81	0.62
1:B:663:LEU:HD12	1:B:703:GLN:HE21	1.63	0.62
1:D:274:LEU:H	1:D:274:LEU:HD12	1.64	0.62
1:A:934:ILE:HD12	1:A:941:PHE:CD1	2.30	0.62
1:A:895:GLN:HG2	1:A:931:ARG:HB3	1.82	0.62
1:C:790:ILE:HG13	1:C:790:ILE:O	2.00	0.62
1:C:885:LEU:HD22	1:C:910:ILE:HD11	1.81	0.62
1:D:885:LEU:CD2	1:D:910:ILE:HD11	2.30	0.62
1:B:274:LEU:H	1:B:274:LEU:HD12	1.64	0.62
1:A:463:PRO:CB	1:B:612:ILE:HG22	2.29	0.62
1:C:805:ALA:HB1	1:C:808:ARG:N	2.08	0.61
1:A:881:VAL:HG13	1:A:882:ASN:N	2.16	0.61
1:A:885:LEU:CD2	1:A:910:ILE:HD11	2.30	0.61
1:A:904:ILE:HG23	1:A:907:GLU:HB2	1.79	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:LEU:HD22	1:A:910:ILE:HD11	1.81	0.61
1:B:702:PRO:CB	1:B:726:ASN:O	2.47	0.61
1:D:834:LEU:HB2	1:D:837:HIS:HD2	1.64	0.61
1:C:874:THR:HA	1:C:1025:ASP:OD2	2.00	0.61
1:C:885:LEU:CD2	1:C:910:ILE:HD11	2.30	0.61
1:D:881:VAL:HG13	1:D:882:ASN:N	2.16	0.61
1:B:550:ASN:O	1:B:586:PRO:HG3	2.00	0.61
1:C:834:LEU:HB2	1:C:837:HIS:HD2	1.64	0.61
1:D:706:PRO:HA	1:D:797:LEU:CD2	2.29	0.61
1:C:706:PRO:HA	1:C:797:LEU:CD2	2.29	0.61
1:C:895:GLN:HG2	1:C:931:ARG:HB3	1.82	0.61
1:B:532:ALA:CB	1:B:560:MET:CE	2.75	0.61
1:C:881:VAL:HG13	1:C:882:ASN:N	2.16	0.61
1:A:864:LEU:HG	1:A:865:THR:H	1.66	0.61
1:B:802:TYR:CZ	1:B:821:PHE:HD1	2.19	0.61
1:D:885:LEU:HD22	1:D:910:ILE:HD11	1.81	0.61
1:D:989:LEU:HD12	1:D:989:LEU:N	2.15	0.61
1:B:655:ASN:C	1:B:656:CYS:CA	2.66	0.61
1:B:790:ILE:O	1:B:790:ILE:HG13	2.00	0.61
1:B:786:ASN:HD22	1:B:789:PHE:HE2	1.48	0.60
1:D:551:ARG:NH2	1:D:642:THR:CG2	2.62	0.60
1:A:842:SER:CB	1:A:844:PRO:HD2	2.31	0.60
1:B:508:VAL:CG1	1:B:539:ARG:NH2	2.64	0.60
1:B:802:TYR:CG	1:B:821:PHE:CE1	2.89	0.60
1:D:1015:LEU:HD12	1:D:1015:LEU:N	2.16	0.60
1:D:760:VAL:HG12	1:D:761:GLN:N	2.16	0.60
1:A:815:LEU:HB2	1:A:885:LEU:HD11	1.81	0.60
1:C:661:LEU:HD21	1:C:790:ILE:HD11	1.83	0.60
1:C:842:SER:CB	1:C:844:PRO:HD2	2.31	0.60
1:A:324:GLN:NE2	1:B:577:LEU:H	2.00	0.60
1:A:532:ALA:HB1	1:A:560:MET:HE2	1.78	0.60
1:A:533:LEU:HD23	1:A:646:PHE:CG	2.36	0.60
1:A:760:VAL:HG12	1:A:761:GLN:N	2.16	0.60
1:C:1015:LEU:HD12	1:C:1015:LEU:N	2.16	0.60
1:C:191:LYS:HB3	1:C:194:TYR:HB2	1.83	0.60
1:C:989:LEU:N	1:C:989:LEU:HD12	2.15	0.60
1:D:790:ILE:HG13	1:D:790:ILE:O	2.00	0.60
1:D:842:SER:CB	1:D:844:PRO:HD2	2.31	0.60
1:A:549:ALA:O	1:A:586:PRO:HA	2.02	0.60
1:B:815:LEU:HA	1:B:848:TRP:HD1	1.66	0.60
1:D:786:ASN:HD22	1:D:789:PHE:HE2	1.48	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:895:GLN:HG2	1:D:931:ARG:HB3	1.82	0.60
1:C:934:ILE:HD12	1:C:941:PHE:CD1	2.30	0.60
1:B:786:ASN:ND2	1:B:789:PHE:HE2	2.00	0.60
1:B:842:SER:CB	1:B:844:PRO:HD2	2.31	0.60
1:C:663:LEU:HD23	1:C:698:SER:HB2	1.84	0.60
1:A:931:ARG:HH11	1:A:942:MET:HE3	1.66	0.60
1:A:706:PRO:HA	1:A:797:LEU:CD2	2.29	0.60
1:A:790:ILE:O	1:A:790:ILE:HG13	2.00	0.60
1:B:760:VAL:HG12	1:B:761:GLN:N	2.16	0.60
1:B:815:LEU:HB3	1:B:848:TRP:HB3	1.84	0.60
1:C:786:ASN:HD22	1:C:789:PHE:HE2	1.48	0.60
1:D:191:LYS:HB3	1:D:194:TYR:HB2	1.83	0.60
1:A:550:ASN:ND2	1:A:585:ALA:O	2.29	0.59
1:C:864:LEU:HG	1:C:865:THR:H	1.66	0.59
1:D:533:LEU:CG	1:D:642:THR:CG2	2.80	0.59
1:A:786:ASN:HD22	1:A:789:PHE:HE2	1.48	0.59
1:D:550:ASN:HB3	1:D:586:PRO:CG	2.32	0.59
1:D:805:ALA:HB1	1:D:808:ARG:N	2.08	0.59
1:B:191:LYS:HB3	1:B:194:TYR:HB2	1.83	0.59
1:D:663:LEU:HD23	1:D:698:SER:HB2	1.84	0.59
1:D:786:ASN:ND2	1:D:789:PHE:HE2	2.00	0.59
1:A:191:LYS:HB3	1:A:194:TYR:HB2	1.83	0.59
1:C:760:VAL:HG12	1:C:761:GLN:N	2.16	0.59
1:A:786:ASN:ND2	1:A:789:PHE:HE2	2.00	0.59
1:A:855:CYS:SG	1:A:856:SER:N	2.75	0.59
1:C:815:LEU:HA	1:C:848:TRP:HD1	1.66	0.59
1:A:655:ASN:OD1	1:A:657:SER:CB	2.45	0.59
1:A:931:ARG:HD2	1:A:942:MET:HE3	1.84	0.59
1:B:802:TYR:CE2	1:B:821:PHE:HD1	2.19	0.59
1:C:663:LEU:HD12	1:C:792:ASP:OD2	1.95	0.59
1:D:815:LEU:HB3	1:D:848:TRP:HB3	1.84	0.59
1:A:97:PRO:HG2	1:A:158:TYR:CE1	2.38	0.59
1:B:663:LEU:HD23	1:B:698:SER:HB2	1.84	0.59
1:B:802:TYR:CD1	1:B:821:PHE:CE1	2.90	0.59
1:D:97:PRO:HG2	1:D:158:TYR:CE1	2.38	0.59
1:D:864:LEU:HG	1:D:865:THR:H	1.66	0.59
1:C:959:LEU:HD13	1:C:1033:LEU:CD2	2.26	0.59
1:D:887:PHE:O	1:D:890:ILE:HG12	2.02	0.59
1:C:97:PRO:HG2	1:C:158:TYR:CE1	2.38	0.58
1:C:703:GLN:HG2	1:C:792:ASP:OD1	2.03	0.58
1:C:887:PHE:O	1:C:890:ILE:HG12	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:VAL:HG22	1:D:526:PRO:HG2	1.85	0.58
1:B:459:ARG:CD	1:B:526:PRO:HG3	2.33	0.58
1:B:803:LYS:CA	1:B:804:CYS:N	2.65	0.58
1:D:443:TYR:HB2	1:D:526:PRO:HB3	1.85	0.58
1:A:703:GLN:HG2	1:A:792:ASP:OD1	2.03	0.58
1:C:815:LEU:HB3	1:C:848:TRP:HB3	1.84	0.58
1:C:853:VAL:HG13	1:C:853:VAL:O	2.04	0.58
1:A:663:LEU:HD23	1:A:698:SER:HB2	1.84	0.58
1:A:815:LEU:HB3	1:A:848:TRP:HB3	1.84	0.58
1:A:887:PHE:O	1:A:890:ILE:HG12	2.02	0.58
1:A:938:LYS:HE3	1:A:941:PHE:CD2	2.38	0.58
1:C:895:GLN:CG	1:C:931:ARG:HB3	2.33	0.58
1:A:815:LEU:HA	1:A:848:TRP:HD1	1.66	0.58
1:B:802:TYR:CE1	1:B:821:PHE:HD1	2.21	0.58
1:C:876:VAL:HG22	1:C:916:CYS:O	2.03	0.58
1:A:853:VAL:HG13	1:A:853:VAL:O	2.04	0.58
1:A:895:GLN:CG	1:A:931:ARG:HB3	2.33	0.58
1:A:876:VAL:HG22	1:A:916:CYS:O	2.03	0.58
1:B:97:PRO:HG2	1:B:158:TYR:CE1	2.38	0.58
1:A:422:LEU:HD13	1:B:605:GLN:HG2	1.78	0.58
1:B:533:LEU:HD13	1:B:639:SER:CB	2.33	0.58
1:D:1015:LEU:HD23	1:D:1039:ASP:N	2.18	0.58
1:D:876:VAL:HG22	1:D:916:CYS:O	2.04	0.58
1:D:550:ASN:HB3	1:D:586:PRO:CB	2.33	0.58
1:D:895:GLN:CG	1:D:931:ARG:HB3	2.34	0.58
1:D:938:LYS:HE3	1:D:941:PHE:CD2	2.39	0.58
1:D:988:TYR:C	1:D:989:LEU:HD12	2.24	0.58
1:C:1017:PRO:HB3	1:C:1034:GLN:NE2	2.19	0.58
1:C:988:TYR:C	1:C:989:LEU:HD12	2.24	0.58
1:D:703:GLN:HG2	1:D:792:ASP:OD1	2.03	0.58
1:D:815:LEU:CD2	1:D:853:VAL:HG11	2.23	0.58
1:D:959:LEU:HD13	1:D:1033:LEU:CD2	2.26	0.58
1:A:815:LEU:N	1:A:815:LEU:HD12	2.19	0.58
1:A:931:ARG:HD3	1:A:943:THR:O	2.04	0.58
1:C:1015:LEU:HD23	1:C:1039:ASP:N	2.18	0.58
1:D:1017:PRO:HB3	1:D:1034:GLN:NE2	2.19	0.58
1:D:815:LEU:HA	1:D:848:TRP:HD1	1.66	0.58
1:D:931:ARG:HD3	1:D:943:THR:O	2.04	0.58
1:A:700:ASP:O	1:A:702:PRO:HD3	2.04	0.57
1:B:703:GLN:HG2	1:B:792:ASP:OD1	2.03	0.57
1:C:786:ASN:ND2	1:C:789:PHE:HE2	2.00	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:988:TYR:CE2	1:C:991:ASN:N	2.71	0.57
1:D:815:LEU:N	1:D:815:LEU:HD12	2.19	0.57
1:C:938:LYS:HE3	1:C:941:PHE:CD2	2.38	0.57
1:D:459:ARG:HD3	1:D:524:GLY:O	2.04	0.57
1:B:690:PHE:HD2	1:B:731:GLN:HG3	1.68	0.57
1:B:843:SER:OG	1:B:844:PRO:HD3	2.05	0.57
1:C:910:ILE:HG23	1:C:910:ILE:O	2.04	0.57
1:A:815:LEU:CD2	1:A:853:VAL:HG11	2.23	0.57
1:B:815:LEU:HD12	1:B:815:LEU:N	2.19	0.57
1:D:853:VAL:HG13	1:D:853:VAL:O	2.04	0.57
1:B:533:LEU:O	1:B:646:PHE:HB3	2.04	0.57
1:B:775:SER:HB3	1:B:807:GLN:OE1	2.04	0.57
1:C:815:LEU:N	1:C:815:LEU:HD12	2.20	0.57
1:D:910:ILE:HG23	1:D:910:ILE:O	2.04	0.57
1:D:934:ILE:HD12	1:D:941:PHE:CD1	2.30	0.57
1:D:988:TYR:CE2	1:D:991:ASN:N	2.71	0.57
1:A:175:SER:OG	1:A:178:GLU:HG2	2.04	0.57
1:C:931:ARG:HD3	1:C:943:THR:O	2.04	0.57
1:C:988:TYR:CZ	1:C:989:LEU:N	2.73	0.57
1:A:910:ILE:HG23	1:A:910:ILE:O	2.04	0.57
1:C:175:SER:OG	1:C:178:GLU:HG2	2.04	0.57
1:C:843:SER:OG	1:C:844:PRO:HD3	2.05	0.57
1:D:988:TYR:CZ	1:D:989:LEU:N	2.73	0.57
1:B:425:TYR:OH	1:B:456:LYS:HE2	2.05	0.57
1:C:550:ASN:HB2	1:C:586:PRO:HB3	1.86	0.57
1:D:175:SER:OG	1:D:178:GLU:HG2	2.04	0.57
1:B:802:TYR:CD2	1:B:821:PHE:HD1	2.23	0.56
1:D:533:LEU:HD13	1:D:642:THR:CB	2.35	0.56
1:B:853:VAL:O	1:B:853:VAL:HG13	2.04	0.56
1:C:775:SER:HB2	1:C:806:ALA:H	1.69	0.56
1:D:407:LEU:O	1:D:411:GLN:HG2	2.05	0.56
1:D:529:GLY:HA3	1:D:552:PHE:CZ	2.40	0.56
1:A:532:ALA:CB	1:A:560:MET:CE	2.73	0.56
1:B:533:LEU:CD2	1:B:646:PHE:CE1	2.85	0.56
1:B:663:LEU:HD12	1:B:703:GLN:NE2	2.12	0.56
1:D:663:LEU:CG	1:D:792:ASP:OD2	2.53	0.56
1:A:529:GLY:HA3	1:A:552:PHE:CZ	2.40	0.56
1:C:425:TYR:OH	1:C:456:LYS:HE2	2.05	0.56
1:C:529:GLY:HA3	1:C:552:PHE:CZ	2.41	0.56
1:D:830:ARG:HG2	1:D:830:ARG:O	2.06	0.56
1:B:175:SER:OG	1:B:178:GLU:HG2	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:974:ILE:HD11	1:C:1004:ILE:HB	1.88	0.56
1:D:663:LEU:HD12	1:D:792:ASP:OD2	2.02	0.56
1:D:843:SER:OG	1:D:844:PRO:HD3	2.05	0.56
1:A:420:GLU:HB3	1:B:607:SER:HB3	1.87	0.56
1:B:407:LEU:O	1:B:411:GLN:HG2	2.05	0.56
1:C:407:LEU:O	1:C:411:GLN:HG2	2.05	0.56
1:A:324:GLN:NE2	1:B:576:ARG:HD2	2.20	0.56
1:A:533:LEU:HD23	1:A:646:PHE:CD2	2.41	0.56
1:B:529:GLY:HA3	1:B:552:PHE:CZ	2.40	0.56
1:B:676:LYS:HG3	1:B:702:PRO:HG2	1.86	0.56
1:D:974:ILE:HD11	1:D:1004:ILE:HB	1.88	0.56
1:B:551:ARG:HH22	1:B:642:THR:CG2	2.19	0.56
1:C:985:VAL:HG11	1:C:999:ARG:HD3	1.88	0.56
1:C:815:LEU:CD2	1:C:853:VAL:HG11	2.23	0.56
1:D:508:VAL:HG12	1:D:509:GLU:N	2.20	0.56
1:A:753:LEU:N	1:A:753:LEU:HD12	2.21	0.56
1:C:830:ARG:O	1:C:830:ARG:HG2	2.06	0.56
1:D:985:VAL:HG11	1:D:999:ARG:HD3	1.88	0.56
1:B:551:ARG:HH22	1:B:642:THR:HG21	1.71	0.55
1:A:407:LEU:O	1:A:411:GLN:HG2	2.05	0.55
1:A:425:TYR:OH	1:A:456:LYS:HE2	2.05	0.55
1:A:843:SER:OG	1:A:844:PRO:HD3	2.05	0.55
1:C:235:LEU:HG	1:C:236:VAL:HG23	1.88	0.55
1:D:425:TYR:OH	1:D:456:LYS:HE2	2.05	0.55
1:D:938:LYS:HE3	1:D:941:PHE:CE2	2.41	0.55
1:A:235:LEU:HG	1:A:236:VAL:HG23	1.88	0.55
1:A:830:ARG:HG2	1:A:830:ARG:O	2.06	0.55
1:C:923:ILE:HG12	1:C:924:GLY:H	1.72	0.55
1:D:533:LEU:HD13	1:D:639:SER:OG	2.05	0.55
1:D:663:LEU:HD12	1:D:792:ASP:HB3	1.75	0.55
1:D:904:ILE:HG21	1:D:907:GLU:HB2	1.88	0.55
1:A:508:VAL:O	1:A:509:GLU:HA	2.06	0.55
1:B:753:LEU:HD12	1:B:753:LEU:N	2.21	0.55
1:C:727:LEU:HD11	1:C:760:VAL:CG2	2.37	0.55
1:C:904:ILE:HG21	1:C:907:GLU:HB2	1.88	0.55
1:C:938:LYS:HE3	1:C:941:PHE:CE2	2.41	0.55
1:D:235:LEU:HG	1:D:236:VAL:HG23	1.88	0.55
1:B:830:ARG:HG2	1:B:830:ARG:O	2.06	0.55
1:C:1015:LEU:HD21	1:C:1039:ASP:CA	2.37	0.55
1:A:727:LEU:HD11	1:A:760:VAL:CG2	2.37	0.55
1:A:938:LYS:HE3	1:A:941:PHE:CE2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:LEU:HD11	1:B:760:VAL:CG2	2.37	0.55
1:C:747:VAL:HG13	1:C:747:VAL:O	2.07	0.55
1:C:753:LEU:N	1:C:753:LEU:HD12	2.21	0.55
1:D:923:ILE:HG12	1:D:924:GLY:H	1.72	0.55
1:C:894:VAL:HG21	1:C:903:PRO:HG3	1.89	0.55
1:D:1015:LEU:HD21	1:D:1039:ASP:CA	2.37	0.55
1:A:883:LEU:N	1:A:883:LEU:HD12	2.21	0.55
1:B:235:LEU:HG	1:B:236:VAL:HG23	1.88	0.55
1:B:747:VAL:O	1:B:747:VAL:HG13	2.07	0.55
1:C:1024:VAL:O	1:C:1024:VAL:HG13	2.06	0.55
1:C:873:GLY:CA	1:C:1026:ARG:HG3	2.35	0.55
1:C:883:LEU:N	1:C:883:LEU:HD12	2.22	0.55
1:B:775:SER:HB2	1:B:807:GLN:CG	2.37	0.54
1:D:1024:VAL:HG13	1:D:1024:VAL:O	2.06	0.54
1:D:747:VAL:HG13	1:D:747:VAL:O	2.07	0.54
1:A:747:VAL:O	1:A:747:VAL:HG13	2.07	0.54
1:B:87:PRO:HB2	1:B:109:LEU:HD11	1.90	0.54
1:D:663:LEU:HG	1:D:792:ASP:OD2	2.08	0.54
1:D:894:VAL:HG21	1:D:903:PRO:HG3	1.89	0.54
1:A:904:ILE:HG21	1:A:907:GLU:HB2	1.88	0.54
1:B:802:TYR:CD1	1:B:821:PHE:HD1	2.24	0.54
1:C:574:HIS:ND1	1:C:618:PRO:HD3	2.22	0.54
1:D:883:LEU:N	1:D:883:LEU:HD12	2.22	0.54
1:B:550:ASN:CB	1:B:585:ALA:O	2.56	0.54
1:C:887:PHE:CD1	1:C:890:ILE:HD11	2.43	0.54
1:D:1020:VAL:O	1:D:1020:VAL:HG23	2.07	0.54
1:A:890:ILE:HB	1:A:893:HIS:CD2	2.42	0.54
1:B:784:VAL:HG12	1:B:785:TRP:N	2.23	0.54
1:C:1020:VAL:O	1:C:1020:VAL:HG23	2.07	0.54
1:C:1015:LEU:HD21	1:C:1039:ASP:CB	2.38	0.54
1:D:1015:LEU:HD21	1:D:1039:ASP:CB	2.38	0.54
1:D:551:ARG:HH12	1:D:641:GLU:CD	2.06	0.54
1:D:887:PHE:CD1	1:D:890:ILE:HD11	2.43	0.54
1:A:894:VAL:HG21	1:A:903:PRO:HG3	1.89	0.54
1:C:551:ARG:NH2	1:C:642:THR:HG22	2.22	0.54
1:D:574:HIS:ND1	1:D:618:PRO:HD3	2.22	0.54
1:D:775:SER:H	1:D:807:GLN:HG3	1.72	0.54
1:B:574:HIS:ND1	1:B:618:PRO:HD3	2.22	0.54
1:D:775:SER:HB3	1:D:807:GLN:CD	2.28	0.54
1:D:812:GLY:HA2	1:D:885:LEU:CD2	2.36	0.54
1:A:887:PHE:CD1	1:A:890:ILE:HD11	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:ASN:O	1:B:658:ALA:CB	2.56	0.54
1:D:1015:LEU:CD1	1:D:1015:LEU:H	2.21	0.54
1:D:727:LEU:HD11	1:D:760:VAL:CG2	2.37	0.54
1:D:753:LEU:N	1:D:753:LEU:HD12	2.21	0.54
1:D:784:VAL:HG12	1:D:785:TRP:N	2.23	0.54
1:A:574:HIS:ND1	1:A:618:PRO:HD3	2.22	0.54
1:C:1015:LEU:H	1:C:1015:LEU:CD1	2.21	0.54
1:A:87:PRO:HB2	1:A:109:LEU:HD11	1.90	0.53
1:A:907:GLU:HB3	1:A:915:VAL:HG21	1.91	0.53
1:C:1038:ILE:HG22	1:C:1039:ASP:N	2.23	0.53
1:C:784:VAL:HG12	1:C:785:TRP:N	2.23	0.53
1:D:812:GLY:HA3	1:D:885:LEU:HD21	1.84	0.53
1:D:885:LEU:HA	1:D:910:ILE:HD11	1.90	0.53
1:A:883:LEU:HD23	1:A:914:ILE:CD1	2.39	0.53
1:D:1038:ILE:HG22	1:D:1039:ASP:N	2.23	0.53
1:D:87:PRO:HB2	1:D:109:LEU:HD11	1.90	0.53
1:D:438:TYR:HH	1:D:527:HIS:CD2	2.23	0.53
1:D:883:LEU:HD23	1:D:914:ILE:CD1	2.39	0.53
1:A:923:ILE:HG12	1:A:924:GLY:H	1.72	0.53
1:B:550:ASN:HB2	1:B:585:ALA:O	2.09	0.53
1:B:723:LYS:HD2	1:B:723:LYS:N	2.24	0.53
1:B:533:LEU:HA	1:B:646:PHE:HB3	1.88	0.53
1:A:705:VAL:HG12	1:A:706:PRO:N	2.24	0.53
1:A:754:ARG:O	1:A:754:ARG:HG3	2.09	0.53
1:C:470:TYR:CE1	1:C:525:ASP:CG	2.82	0.53
1:C:87:PRO:HB2	1:C:109:LEU:HD11	1.90	0.53
1:A:885:LEU:HA	1:A:910:ILE:HD11	1.90	0.53
1:C:876:VAL:CG2	1:C:916:CYS:HB3	2.39	0.53
1:C:883:LEU:HD23	1:C:914:ILE:CD1	2.39	0.53
1:C:988:TYR:OH	1:C:992:GLN:N	2.42	0.53
1:D:907:GLU:HB3	1:D:915:VAL:HG21	1.90	0.53
1:A:723:LYS:N	1:A:723:LYS:HD2	2.24	0.53
1:B:802:TYR:CE2	1:B:821:PHE:CD1	2.97	0.53
1:C:712:ILE:HB	1:C:801:LEU:HD23	1.91	0.53
1:D:876:VAL:CG2	1:D:916:CYS:HB3	2.39	0.53
1:B:712:ILE:HB	1:B:801:LEU:HD23	1.91	0.53
1:C:550:ASN:HB3	1:C:586:PRO:HB3	1.91	0.53
1:D:988:TYR:OH	1:D:992:GLN:N	2.42	0.53
1:A:463:PRO:CD	1:B:612:ILE:CG2	2.84	0.52
1:B:702:PRO:HA	1:B:726:ASN:HB2	1.91	0.52
1:C:907:GLU:HB3	1:C:915:VAL:HG21	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:958:SER:C	1:C:959:LEU:HD12	2.30	0.52
1:B:550:ASN:C	1:B:586:PRO:HG3	2.29	0.52
1:C:1015:LEU:CD2	1:C:1039:ASP:HB2	2.39	0.52
1:C:885:LEU:HA	1:C:910:ILE:HD11	1.90	0.52
1:D:443:TYR:CB	1:D:526:PRO:HB3	2.39	0.52
1:D:938:LYS:HB2	1:D:941:PHE:CD2	2.42	0.52
1:A:784:VAL:HG12	1:A:785:TRP:N	2.23	0.52
1:D:1015:LEU:CD2	1:D:1039:ASP:HB2	2.39	0.52
1:D:723:LYS:N	1:D:723:LYS:HD2	2.24	0.52
1:D:958:SER:C	1:D:959:LEU:HD12	2.30	0.52
1:A:549:ALA:O	1:A:586:PRO:CA	2.57	0.52
1:A:816:LYS:NZ	1:A:910:ILE:HG23	2.24	0.52
1:B:533:LEU:HD21	1:B:646:PHE:CG	2.34	0.52
1:C:785:TRP:CE3	1:C:786:ASN:HB2	2.45	0.52
1:C:797:LEU:N	1:C:797:LEU:HD12	2.25	0.52
1:A:785:TRP:CE3	1:A:786:ASN:HB2	2.45	0.52
1:A:797:LEU:HD12	1:A:797:LEU:N	2.25	0.52
1:B:754:ARG:HG3	1:B:754:ARG:O	2.09	0.52
1:A:221:PHE:CZ	1:C:830:ARG:CB	2.92	0.52
1:D:712:ILE:HB	1:D:801:LEU:HD23	1.91	0.52
1:A:533:LEU:CD2	1:A:646:PHE:CG	2.93	0.52
1:A:876:VAL:CG2	1:A:916:CYS:HB3	2.39	0.52
1:C:1005:VAL:O	1:C:1005:VAL:HG23	2.09	0.52
1:C:723:LYS:N	1:C:723:LYS:HD2	2.24	0.52
1:C:967:SER:O	1:C:1010:PRO:HG3	2.09	0.52
1:D:785:TRP:CE3	1:D:786:ASN:HB2	2.45	0.52
1:D:996:PHE:CZ	1:D:999:ARG:HB2	2.39	0.52
1:A:702:PRO:C	1:A:703:GLN:CA	2.77	0.52
1:A:890:ILE:O	1:A:893:HIS:HB3	2.09	0.52
1:B:711:LEU:HD12	1:B:711:LEU:N	2.25	0.52
1:B:797:LEU:N	1:B:797:LEU:HD12	2.25	0.52
1:B:815:LEU:CD2	1:B:853:VAL:HG11	2.23	0.52
1:C:533:LEU:HD12	1:C:642:THR:HG23	1.89	0.52
1:D:822:GLU:HG2	1:D:822:GLU:O	2.10	0.52
1:C:533:LEU:CD1	1:C:642:THR:CG2	2.83	0.52
1:C:822:GLU:HG2	1:C:822:GLU:O	2.10	0.52
1:D:967:SER:O	1:D:1010:PRO:HG3	2.09	0.52
1:B:470:TYR:CE1	1:B:525:ASP:OD2	2.63	0.52
1:C:996:PHE:CZ	1:C:999:ARG:HB2	2.39	0.52
1:A:422:LEU:HD12	1:B:605:GLN:NE2	2.25	0.52
1:B:702:PRO:O	1:B:703:GLN:HG3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:988:TYR:HB3	1:C:1021:SER:O	2.09	0.52
1:C:711:LEU:HD12	1:C:711:LEU:N	2.25	0.51
1:C:754:ARG:HG3	1:C:754:ARG:O	2.09	0.51
1:D:1005:VAL:O	1:D:1005:VAL:HG23	2.09	0.51
1:D:705:VAL:HG12	1:D:706:PRO:N	2.24	0.51
1:D:711:LEU:HD12	1:D:711:LEU:N	2.25	0.51
1:D:797:LEU:N	1:D:797:LEU:HD12	2.25	0.51
1:D:890:ILE:O	1:D:893:HIS:HB3	2.10	0.51
1:A:712:ILE:HB	1:A:801:LEU:HD23	1.91	0.51
1:A:822:GLU:HG2	1:A:822:GLU:O	2.10	0.51
1:B:274:LEU:N	1:B:274:LEU:HD12	2.25	0.51
1:B:655:ASN:O	1:B:658:ALA:HB3	2.10	0.51
1:B:705:VAL:HG12	1:B:706:PRO:N	2.24	0.51
1:C:655:ASN:C	1:C:657:SER:N	2.62	0.51
1:C:993:THR:HG22	1:C:994:CYS:N	2.25	0.51
1:D:956:VAL:O	1:D:956:VAL:HG13	2.10	0.51
1:B:308:ARG:HB2	1:B:343:GLN:HG2	1.92	0.51
1:D:988:TYR:HB3	1:D:1021:SER:O	2.09	0.51
1:D:923:ILE:HG12	1:D:924:GLY:N	2.26	0.51
1:A:716:GLU:HA	1:A:716:GLU:OE1	2.10	0.51
1:C:533:LEU:CD1	1:C:641:GLU:HB3	2.40	0.51
1:C:890:ILE:HB	1:C:893:HIS:CD2	2.42	0.51
1:C:956:VAL:O	1:C:956:VAL:HG13	2.10	0.51
1:D:754:ARG:HG3	1:D:754:ARG:O	2.09	0.51
1:D:993:THR:HG22	1:D:994:CYS:N	2.25	0.51
1:A:923:ILE:HG12	1:A:924:GLY:N	2.26	0.51
1:C:445:VAL:CG2	1:C:526:PRO:HG2	2.39	0.51
1:C:705:VAL:HG12	1:C:706:PRO:N	2.24	0.51
1:D:896:VAL:O	1:D:897:ALA:HB3	2.10	0.51
1:A:655:ASN:O	1:A:658:ALA:CA	2.58	0.51
1:B:785:TRP:CE3	1:B:786:ASN:HB2	2.45	0.51
1:C:533:LEU:O	1:C:644:LYS:HB2	2.10	0.51
1:D:574:HIS:CE1	1:D:618:PRO:HD3	2.46	0.51
1:D:713:PRO:HG3	1:D:802:TYR:CZ	2.45	0.51
1:D:931:ARG:HH11	1:D:942:MET:HE3	1.75	0.51
1:A:176:GLU:HG3	1:A:177:GLY:N	2.26	0.51
1:A:711:LEU:N	1:A:711:LEU:HD12	2.25	0.51
1:B:235:LEU:HD21	1:B:263:PRO:HG2	1.92	0.51
1:B:676:LYS:HE2	1:B:728:PRO:CB	2.28	0.51
1:B:692:GLU:CD	1:D:141:ARG:NH2	2.42	0.51
1:C:716:GLU:OE1	1:C:716:GLU:HA	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:PRO:HG3	1:C:978:TYR:O	2.10	0.51
1:D:308:ARG:HB2	1:D:343:GLN:HG2	1.92	0.51
1:D:954:PRO:HG3	1:D:978:TYR:O	2.10	0.51
1:A:274:LEU:HD12	1:A:274:LEU:N	2.25	0.51
1:A:574:HIS:CE1	1:A:618:PRO:HD3	2.46	0.51
1:A:816:LYS:CE	1:A:910:ILE:CG2	2.70	0.51
1:A:896:VAL:O	1:A:897:ALA:HB3	2.10	0.51
1:A:938:LYS:HB2	1:A:941:PHE:CD2	2.42	0.51
1:B:822:GLU:HG2	1:B:822:GLU:O	2.10	0.51
1:C:871:GLU:OE1	1:C:1027:ALA:HB2	2.11	0.51
1:C:574:HIS:CE1	1:C:618:PRO:HD3	2.46	0.51
1:D:716:GLU:HA	1:D:716:GLU:OE1	2.10	0.51
1:D:799:VAL:HG23	1:D:799:VAL:O	2.11	0.51
1:C:988:TYR:O	1:C:1020:VAL:HA	2.11	0.51
1:C:890:ILE:O	1:C:893:HIS:HB3	2.10	0.51
1:C:923:ILE:HG12	1:C:924:GLY:N	2.26	0.51
1:C:713:PRO:HG3	1:C:802:TYR:CZ	2.45	0.51
1:C:938:LYS:HB2	1:C:941:PHE:CD2	2.42	0.51
1:D:461:ASP:O	1:D:466:GLY:O	2.29	0.51
1:A:533:LEU:HD22	1:A:646:PHE:CD1	2.46	0.50
1:A:890:ILE:HG13	1:A:891:ALA:N	2.26	0.50
1:B:532:ALA:HB1	1:B:560:MET:HE2	1.89	0.50
1:B:833:THR:HG23	1:B:837:HIS:HB2	1.92	0.50
1:C:461:ASP:O	1:C:466:GLY:O	2.29	0.50
1:A:713:PRO:HG3	1:A:802:TYR:CZ	2.45	0.50
1:A:833:THR:HG23	1:A:837:HIS:HB2	1.91	0.50
1:A:870:PRO:HG2	1:A:871:GLU:OE1	2.11	0.50
1:B:176:GLU:HG3	1:B:177:GLY:N	2.26	0.50
1:B:461:ASP:O	1:B:466:GLY:O	2.29	0.50
1:B:699:GLU:O	1:B:725:ARG:NH2	2.45	0.50
1:B:713:PRO:HG3	1:B:802:TYR:CZ	2.46	0.50
1:C:235:LEU:HD21	1:C:263:PRO:HG2	1.93	0.50
1:C:896:VAL:O	1:C:897:ALA:HB3	2.10	0.50
1:C:988:TYR:HE2	1:C:991:ASN:H	1.55	0.50
1:D:988:TYR:O	1:D:1020:VAL:HA	2.11	0.50
1:D:176:GLU:HG3	1:D:177:GLY:N	2.26	0.50
1:D:274:LEU:N	1:D:274:LEU:HD12	2.25	0.50
1:B:533:LEU:HD21	1:B:646:PHE:CZ	2.45	0.50
1:C:308:ARG:HB2	1:C:343:GLN:HG2	1.92	0.50
1:C:533:LEU:CD1	1:C:639:SER:OG	2.59	0.50
1:C:775:SER:CA	1:C:806:ALA:HB3	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:833:THR:HG23	1:C:837:HIS:HB2	1.92	0.50
1:D:833:THR:HG23	1:D:837:HIS:HB2	1.91	0.50
1:D:848:TRP:HA	1:D:853:VAL:HG11	1.94	0.50
1:C:848:TRP:HA	1:C:853:VAL:HG11	1.94	0.50
1:D:870:PRO:HG2	1:D:871:GLU:OE1	2.11	0.50
1:D:863:ILE:HD11	1:D:876:VAL:HB	1.94	0.50
1:A:461:ASP:O	1:A:466:GLY:O	2.29	0.50
1:A:808:ARG:HD2	1:A:813:LEU:C	2.32	0.50
1:B:799:VAL:HG23	1:B:799:VAL:O	2.11	0.50
1:B:808:ARG:HD2	1:B:813:LEU:C	2.32	0.50
1:C:808:ARG:HD2	1:C:813:LEU:C	2.32	0.50
1:C:988:TYR:CE2	1:C:990:GLY:N	2.80	0.50
1:D:988:TYR:CE2	1:D:990:GLY:N	2.80	0.50
1:A:308:ARG:HB2	1:A:343:GLN:HG2	1.92	0.50
1:B:574:HIS:CE1	1:B:618:PRO:HD3	2.46	0.50
1:B:716:GLU:OE1	1:B:716:GLU:HA	2.10	0.50
1:C:931:ARG:CG	1:C:942:MET:HE3	2.41	0.50
1:D:890:ILE:HB	1:D:893:HIS:CD2	2.42	0.50
1:A:863:ILE:HD11	1:A:876:VAL:HB	1.94	0.50
1:D:550:ASN:CB	1:D:586:PRO:CA	2.85	0.50
1:A:815:LEU:CA	1:A:848:TRP:CD1	2.94	0.50
1:C:274:LEU:HD12	1:C:274:LEU:N	2.25	0.50
1:C:815:LEU:CA	1:C:848:TRP:CD1	2.94	0.50
1:D:235:LEU:HD21	1:D:263:PRO:HG2	1.93	0.50
1:A:539:ARG:HD2	1:A:542:LYS:NZ	2.27	0.50
1:C:1017:PRO:HB3	1:C:1034:GLN:CD	2.31	0.50
1:C:539:ARG:HD2	1:C:542:LYS:NZ	2.27	0.50
1:D:508:VAL:CG1	1:D:509:GLU:N	2.67	0.50
1:D:815:LEU:CA	1:D:848:TRP:CD1	2.94	0.50
1:A:235:LEU:HD21	1:A:263:PRO:HG2	1.92	0.49
1:B:815:LEU:CA	1:B:848:TRP:CD1	2.94	0.49
1:C:931:ARG:HH11	1:C:942:MET:HE3	1.77	0.49
1:D:1017:PRO:HB3	1:D:1034:GLN:CD	2.31	0.49
1:A:655:ASN:CG	1:A:658:ALA:HB2	2.32	0.49
1:C:559:CYS:O	1:C:584:ASP:HB3	2.10	0.49
1:C:863:ILE:HD11	1:C:876:VAL:HB	1.93	0.49
1:C:933:CYS:HA	1:C:942:MET:SD	2.53	0.49
1:D:539:ARG:HD2	1:D:542:LYS:NZ	2.27	0.49
1:A:799:VAL:O	1:A:799:VAL:HG23	2.11	0.49
1:A:848:TRP:HA	1:A:853:VAL:HG11	1.94	0.49
1:A:933:CYS:HA	1:A:942:MET:SD	2.53	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:893:HIS:CE1	1:C:932:LEU:HA	2.47	0.49
1:D:775:SER:HB2	1:D:807:GLN:CB	2.42	0.49
1:D:808:ARG:HD2	1:D:813:LEU:C	2.32	0.49
1:A:324:GLN:NE2	1:B:576:ARG:HE	2.11	0.49
1:D:974:ILE:CG1	1:D:1004:ILE:HB	2.43	0.49
1:D:533:LEU:O	1:D:644:LYS:CG	2.61	0.49
1:D:988:TYR:HE2	1:D:991:ASN:H	1.55	0.49
1:A:673:HIS:CD2	1:A:685:PRO:HG3	2.48	0.49
1:D:984:SER:O	1:D:1024:VAL:HG23	2.13	0.49
1:B:539:ARG:HD2	1:B:542:LYS:NZ	2.27	0.49
1:C:974:ILE:CG1	1:C:1004:ILE:HB	2.43	0.49
1:C:176:GLU:HG3	1:C:177:GLY:N	2.26	0.49
1:C:673:HIS:CD2	1:C:685:PRO:HG3	2.48	0.49
1:C:799:VAL:O	1:C:799:VAL:HG23	2.11	0.49
1:C:774:ILE:C	1:C:806:ALA:CB	2.81	0.49
1:D:1022:VAL:O	1:D:1022:VAL:HG13	2.12	0.49
1:D:673:HIS:CD2	1:D:685:PRO:HG3	2.48	0.49
1:D:898:GLY:O	1:D:900:PRO:HD3	2.12	0.49
1:D:931:ARG:CG	1:D:942:MET:HE3	2.42	0.49
1:B:560:MET:CE	1:B:586:PRO:HD3	2.43	0.49
1:B:705:VAL:HG13	1:B:706:PRO:HD2	1.95	0.49
1:B:775:SER:N	1:B:807:GLN:CD	2.50	0.49
1:C:1022:VAL:HG13	1:C:1022:VAL:O	2.12	0.49
1:C:677:TYR:HD1	1:C:731:GLN:CG	2.17	0.49
1:C:890:ILE:HG13	1:C:891:ALA:N	2.26	0.49
1:A:217:LEU:CD1	1:C:940:GLU:OE1	2.55	0.49
1:D:893:HIS:CE1	1:D:932:LEU:HA	2.48	0.49
1:D:970:THR:HG22	1:D:1008:SER:OG	2.13	0.49
1:A:864:LEU:HB3	1:A:877:THR:HB	1.95	0.49
1:B:237:SER:OG	1:B:238:HIS:HA	2.13	0.49
1:B:848:TRP:HA	1:B:853:VAL:HG11	1.94	0.49
1:C:137:CYS:SG	1:C:159:LEU:HD11	2.53	0.49
1:C:560:MET:CE	1:C:586:PRO:HD3	2.43	0.49
1:C:870:PRO:HG2	1:C:871:GLU:OE1	2.11	0.49
1:D:959:LEU:CG	1:D:974:ILE:HG22	2.28	0.49
1:A:898:GLY:O	1:A:900:PRO:HD3	2.12	0.49
1:C:970:THR:HG22	1:C:1008:SER:OG	2.13	0.49
1:D:890:ILE:HG13	1:D:891:ALA:N	2.26	0.49
1:A:237:SER:OG	1:A:238:HIS:HA	2.13	0.49
1:A:533:LEU:CD2	1:A:646:PHE:CD1	2.96	0.49
1:A:560:MET:CE	1:A:586:PRO:HD3	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:GLN:O	1:B:724:ALA:HB1	2.13	0.49
1:C:984:SER:O	1:C:1024:VAL:HG23	2.13	0.49
1:C:988:TYR:CZ	1:C:991:ASN:N	2.80	0.49
1:D:988:TYR:CZ	1:D:991:ASN:N	2.80	0.49
1:C:859:GLN:HA	1:C:859:GLN:OE1	2.13	0.48
1:C:898:GLY:O	1:C:900:PRO:HD3	2.12	0.48
1:C:938:LYS:CE	1:C:941:PHE:CE2	2.96	0.48
1:A:398:VAL:HG22	1:C:946:HIS:O	2.13	0.48
1:C:959:LEU:CG	1:C:974:ILE:HG22	2.28	0.48
1:D:50:PHE:CE2	1:D:503:VAL:HG23	2.48	0.48
1:D:859:GLN:OE1	1:D:859:GLN:HA	2.13	0.48
1:D:864:LEU:HB3	1:D:877:THR:HB	1.95	0.48
1:D:933:CYS:HA	1:D:942:MET:SD	2.53	0.48
1:A:893:HIS:CE1	1:A:932:LEU:HA	2.48	0.48
1:B:459:ARG:HG3	1:B:526:PRO:HG3	1.94	0.48
1:C:533:LEU:CD2	1:C:639:SER:CB	2.84	0.48
1:A:705:VAL:HG13	1:A:706:PRO:HD2	1.95	0.48
1:C:703:GLN:O	1:C:724:ALA:HB1	2.14	0.48
1:C:804:CYS:SG	1:C:833:THR:HA	2.54	0.48
1:C:864:LEU:HB3	1:C:877:THR:HB	1.95	0.48
1:D:137:CYS:SG	1:D:159:LEU:HD11	2.53	0.48
1:D:711:LEU:HD23	1:D:821:PHE:CE1	2.48	0.48
1:D:661:LEU:HD21	1:D:790:ILE:HG13	1.94	0.48
1:D:829:GLU:O	1:D:830:ARG:HB3	2.14	0.48
1:B:137:CYS:SG	1:B:159:LEU:HD11	2.53	0.48
1:B:804:CYS:SG	1:B:833:THR:HA	2.54	0.48
1:D:703:GLN:O	1:D:724:ALA:HB1	2.14	0.48
1:D:804:CYS:SG	1:D:833:THR:HA	2.53	0.48
1:A:50:PHE:CE2	1:A:503:VAL:HG23	2.48	0.48
1:A:859:GLN:OE1	1:A:859:GLN:HA	2.13	0.48
1:B:50:PHE:CE2	1:B:503:VAL:HG23	2.48	0.48
1:B:732:SER:CB	1:D:83:HIS:NE2	2.75	0.48
1:D:440:TYR:CG	1:D:527:HIS:CD2	3.01	0.48
1:D:705:VAL:HG13	1:D:706:PRO:HD2	1.95	0.48
1:B:829:GLU:O	1:B:830:ARG:HB3	2.14	0.48
1:C:959:LEU:HD12	1:C:1033:LEU:HD23	1.94	0.48
1:C:237:SER:OG	1:C:238:HIS:HA	2.13	0.48
1:C:50:PHE:CE2	1:C:503:VAL:HG23	2.48	0.48
1:D:351:ASP:HA	1:D:431:ARG:HB2	1.96	0.48
1:D:660:GLN:C	1:D:661:LEU:HD12	2.34	0.48
1:D:848:TRP:HA	1:D:853:VAL:CG1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:938:LYS:CE	1:D:941:PHE:CE2	2.97	0.48
1:A:221:PHE:CE1	1:C:830:ARG:HB2	2.49	0.48
1:A:938:LYS:CE	1:A:941:PHE:CE2	2.97	0.48
1:B:550:ASN:CG	1:B:585:ALA:O	2.46	0.48
1:B:95:TYR:HA	1:B:96:PRO:C	2.33	0.48
1:C:351:ASP:HA	1:C:431:ARG:HB2	1.96	0.48
1:C:559:CYS:O	1:C:584:ASP:HB2	2.14	0.48
1:C:705:VAL:HG13	1:C:706:PRO:HD2	1.95	0.48
1:C:932:LEU:HD23	1:C:933:CYS:N	2.28	0.48
1:A:594:CYS:O	1:A:601:GLU:HA	2.14	0.48
1:A:660:GLN:C	1:A:661:LEU:HD12	2.34	0.48
1:A:816:LYS:CD	1:A:910:ILE:HG23	2.44	0.48
1:A:95:TYR:HA	1:A:96:PRO:C	2.33	0.48
1:C:848:TRP:HA	1:C:853:VAL:CG1	2.44	0.48
1:D:594:CYS:O	1:D:601:GLU:HA	2.14	0.48
1:D:842:SER:HB2	1:D:844:PRO:HD2	1.96	0.48
1:D:933:CYS:SG	1:D:937:CYS:N	2.87	0.48
1:D:931:ARG:CD	1:D:942:MET:HE3	2.42	0.48
1:A:932:LEU:HD23	1:A:933:CYS:N	2.28	0.48
1:B:594:CYS:O	1:B:601:GLU:HA	2.14	0.48
1:B:660:GLN:C	1:B:661:LEU:HD12	2.34	0.48
1:B:673:HIS:CD2	1:B:685:PRO:HG3	2.48	0.48
1:C:960:SER:CB	1:C:973:THR:HB	2.43	0.48
1:D:237:SER:OG	1:D:238:HIS:HA	2.13	0.48
1:D:875:ARG:HG2	1:D:915:VAL:CG1	2.44	0.48
1:D:95:TYR:HA	1:D:96:PRO:C	2.33	0.48
1:A:137:CYS:SG	1:A:159:LEU:HD11	2.53	0.48
1:A:848:TRP:HA	1:A:853:VAL:CG1	2.44	0.48
1:A:851:HIS:ND1	1:A:886:ASP:OD2	2.47	0.48
1:B:690:PHE:CE2	1:B:731:GLN:HG3	2.49	0.48
1:B:842:SER:HB2	1:B:844:PRO:HD2	1.96	0.48
1:B:848:TRP:HA	1:B:853:VAL:CG1	2.44	0.48
1:C:326:PHE:CG	1:C:359:PRO:HG3	2.49	0.48
1:C:933:CYS:SG	1:C:937:CYS:N	2.87	0.48
1:D:960:SER:CB	1:D:973:THR:HB	2.43	0.48
1:A:695:ILE:CD1	1:A:702:PRO:HD3	2.44	0.47
1:A:797:LEU:HD12	1:A:797:LEU:H	1.79	0.47
1:A:829:GLU:O	1:A:830:ARG:HB3	2.14	0.47
1:A:842:SER:HB2	1:A:844:PRO:HD2	1.96	0.47
1:B:327:ASN:CG	1:B:327:ASN:O	2.52	0.47
1:B:797:LEU:HD12	1:B:797:LEU:H	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:829:GLU:O	1:C:830:ARG:HB3	2.14	0.47
1:D:812:GLY:HA2	1:D:885:LEU:HD22	1.93	0.47
1:D:833:THR:HG21	1:D:837:HIS:CB	2.44	0.47
1:A:141:ARG:HD2	1:A:143:ASP:OD1	2.14	0.47
1:A:804:CYS:SG	1:A:833:THR:HA	2.54	0.47
1:B:326:PHE:CG	1:B:359:PRO:HG3	2.49	0.47
1:C:931:ARG:CD	1:C:942:MET:HE3	2.42	0.47
1:D:932:LEU:HD23	1:D:933:CYS:N	2.28	0.47
1:A:326:PHE:CG	1:A:359:PRO:HG3	2.50	0.47
1:B:470:TYR:HE1	1:B:525:ASP:OD2	1.98	0.47
1:C:327:ASN:CG	1:C:327:ASN:O	2.52	0.47
1:C:594:CYS:O	1:C:601:GLU:HA	2.14	0.47
1:C:660:GLN:C	1:C:661:LEU:HD12	2.34	0.47
1:C:932:LEU:HD23	1:C:932:LEU:C	2.34	0.47
1:D:1022:VAL:HG13	1:D:1029:VAL:HG12	1.94	0.47
1:D:560:MET:CE	1:D:586:PRO:HD3	2.43	0.47
1:A:932:LEU:C	1:A:932:LEU:HD23	2.34	0.47
1:B:141:ARG:HD2	1:B:143:ASP:OD1	2.14	0.47
1:C:833:THR:HG21	1:C:837:HIS:CB	2.44	0.47
1:C:876:VAL:HG23	1:C:876:VAL:O	2.14	0.47
1:D:874:THR:HG22	1:D:875:ARG:N	2.30	0.47
1:D:932:LEU:HD23	1:D:932:LEU:C	2.34	0.47
1:A:351:ASP:HA	1:A:431:ARG:HB2	1.96	0.47
1:A:695:ILE:HD13	1:A:702:PRO:HD3	1.97	0.47
1:A:903:PRO:HA	1:A:916:CYS:HA	1.96	0.47
1:C:1022:VAL:HG13	1:C:1029:VAL:HG12	1.94	0.47
1:C:141:ARG:HD2	1:C:143:ASP:OD1	2.14	0.47
1:D:959:LEU:HD12	1:D:1033:LEU:HD23	1.94	0.47
1:A:703:GLN:O	1:A:724:ALA:HB1	2.13	0.47
1:A:833:THR:HG21	1:A:837:HIS:CB	2.44	0.47
1:A:876:VAL:HG23	1:A:876:VAL:O	2.14	0.47
1:A:933:CYS:SG	1:A:937:CYS:N	2.87	0.47
1:B:712:ILE:HD12	1:B:799:VAL:HB	1.97	0.47
1:D:534:HIS:CD2	1:D:644:LYS:HZ2	2.32	0.47
1:D:551:ARG:HH11	1:D:641:GLU:CD	2.16	0.47
1:A:655:ASN:OD1	1:A:657:SER:CA	2.63	0.47
1:A:874:THR:HG22	1:A:875:ARG:N	2.30	0.47
1:B:655:ASN:CA	1:B:656:CYS:N	2.69	0.47
1:C:95:TYR:HA	1:C:96:PRO:C	2.33	0.47
1:D:326:PHE:CG	1:D:359:PRO:HG3	2.49	0.47
1:A:463:PRO:O	1:B:577:LEU:HD21	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LEU:HD11	1:A:703:GLN:HE21	1.80	0.47
1:C:797:LEU:H	1:C:797:LEU:HD12	1.79	0.47
1:C:875:ARG:HG2	1:C:915:VAL:CG1	2.44	0.47
1:C:874:THR:HG22	1:C:875:ARG:N	2.30	0.47
1:D:701:CYS:HA	1:D:702:PRO:HD3	1.75	0.47
1:A:722:LEU:C	1:A:723:LYS:HD2	2.36	0.47
1:A:896:VAL:HG21	1:A:918:MET:CE	2.45	0.47
1:B:833:THR:HG21	1:B:837:HIS:CB	2.44	0.47
1:C:737:TYR:HE1	1:C:754:ARG:CD	2.25	0.47
1:C:896:VAL:HG21	1:C:918:MET:CE	2.45	0.47
1:C:960:SER:HB2	1:C:961:PRO:CD	2.45	0.47
1:D:141:ARG:HD2	1:D:143:ASP:OD1	2.14	0.47
1:D:550:ASN:ND2	1:D:585:ALA:O	2.48	0.47
1:D:638:ARG:HB2	1:D:645:ILE:HD13	1.97	0.47
1:D:960:SER:HB2	1:D:961:PRO:CD	2.45	0.47
1:A:327:ASN:O	1:A:327:ASN:CG	2.52	0.47
1:A:875:ARG:HG2	1:A:915:VAL:CG1	2.44	0.47
1:B:351:ASP:HA	1:B:431:ARG:HB2	1.96	0.47
1:D:327:ASN:CG	1:D:327:ASN:O	2.52	0.47
1:D:869:PRO:HD3	1:D:981:ALA:HB1	1.97	0.47
1:B:722:LEU:C	1:B:723:LYS:HD2	2.35	0.46
1:C:842:SER:HB2	1:C:844:PRO:HD2	1.96	0.46
1:A:655:ASN:CB	1:A:658:ALA:CB	2.77	0.46
1:D:159:LEU:HD13	1:D:184:ILE:HD13	1.98	0.46
1:D:896:VAL:HG21	1:D:918:MET:CE	2.45	0.46
1:A:476:PHE:CE2	1:A:482:ILE:HD13	2.51	0.46
1:A:663:LEU:HD11	1:A:703:GLN:NE2	2.30	0.46
1:A:712:ILE:HD12	1:A:799:VAL:HB	1.97	0.46
1:B:277:THR:HG22	1:B:279:ARG:HG3	1.98	0.46
1:C:328:ILE:HB	1:C:332:GLU:OE1	2.16	0.46
1:C:712:ILE:HD12	1:C:799:VAL:HB	1.97	0.46
1:C:988:TYR:C	1:C:988:TYR:CD2	2.84	0.46
1:D:775:SER:N	1:D:807:GLN:HG3	2.30	0.46
1:D:893:HIS:CG	1:D:894:VAL:N	2.83	0.46
1:A:539:ARG:HB2	1:A:542:LYS:HD3	1.97	0.46
1:B:638:ARG:HB2	1:B:645:ILE:HD13	1.97	0.46
1:C:159:LEU:HD13	1:C:184:ILE:HD13	1.98	0.46
1:C:875:ARG:HD3	1:C:907:GLU:OE1	2.16	0.46
1:D:445:VAL:CG2	1:D:526:PRO:HG2	2.44	0.46
1:D:712:ILE:HD12	1:D:799:VAL:HB	1.97	0.46
1:D:876:VAL:HG23	1:D:876:VAL:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD13	1:A:184:ILE:HD13	1.98	0.46
1:A:893:HIS:CG	1:A:894:VAL:N	2.83	0.46
1:B:654:TYR:CD2	1:B:670:PHE:CG	3.04	0.46
1:D:988:TYR:HE1	1:D:992:GLN:O	1.97	0.46
1:A:277:THR:HG22	1:A:279:ARG:HG3	1.98	0.46
1:A:81:VAL:HG11	1:A:145:LEU:HB2	1.98	0.46
1:A:875:ARG:HD3	1:A:907:GLU:OE1	2.16	0.46
1:B:328:ILE:HB	1:B:332:GLU:OE1	2.16	0.46
1:C:903:PRO:HA	1:C:916:CYS:HA	1.96	0.46
1:D:328:ILE:HB	1:D:332:GLU:OE1	2.16	0.46
1:A:328:ILE:HB	1:A:332:GLU:OE1	2.16	0.46
1:C:638:ARG:HB2	1:C:645:ILE:HD13	1.97	0.46
1:C:722:LEU:C	1:C:723:LYS:HD2	2.35	0.46
1:C:893:HIS:CG	1:C:894:VAL:N	2.83	0.46
1:C:896:VAL:HG21	1:C:918:MET:HE3	1.98	0.46
1:B:508:VAL:HG12	1:B:539:ARG:NH2	2.30	0.46
1:C:476:PHE:CE2	1:C:482:ILE:HD13	2.51	0.46
1:C:663:LEU:CG	1:C:792:ASP:OD2	2.59	0.46
1:C:988:TYR:HE1	1:C:992:GLN:O	1.97	0.46
1:D:476:PHE:CE2	1:D:482:ILE:HD13	2.51	0.46
1:D:903:PRO:HA	1:D:916:CYS:HA	1.96	0.46
1:D:988:TYR:CE1	1:D:992:GLN:O	2.68	0.46
1:A:654:TYR:HE1	1:A:656:CYS:SG	2.39	0.46
1:A:655:ASN:C	1:A:657:SER:N	2.68	0.46
1:A:672:CYS:HB3	1:A:681:CYS:SG	2.56	0.46
1:A:737:TYR:CE2	1:A:785:TRP:HB3	2.51	0.46
1:C:988:TYR:CE1	1:C:992:GLN:O	2.68	0.46
1:D:979:LEU:HD12	1:D:1003:GLU:HA	1.97	0.46
1:D:875:ARG:HD3	1:D:907:GLU:OE1	2.16	0.46
1:A:112:ASN:HB2	1:A:132:LEU:HD22	1.98	0.46
1:A:550:ASN:HB2	1:A:585:ALA:O	2.16	0.46
1:B:329:SER:HB3	1:B:332:GLU:HG3	1.98	0.46
1:D:539:ARG:HB2	1:D:542:LYS:HD3	1.97	0.46
1:D:722:LEU:C	1:D:723:LYS:HD2	2.35	0.46
1:D:797:LEU:H	1:D:797:LEU:HD12	1.79	0.46
1:D:904:ILE:HG23	1:D:904:ILE:O	2.15	0.46
1:A:545:ARG:NH1	1:A:641:GLU:OE2	2.49	0.45
1:B:476:PHE:CE2	1:B:482:ILE:HD13	2.51	0.45
1:C:533:LEU:CB	1:C:642:THR:CG2	2.73	0.45
1:C:672:CYS:HB3	1:C:681:CYS:SG	2.56	0.45
1:C:785:TRP:CD1	1:C:791:ILE:HD11	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:TYR:CE1	1:D:525:ASP:CG	2.90	0.45
1:A:463:PRO:O	1:B:614:ILE:HG12	2.14	0.45
1:A:904:ILE:HG23	1:A:904:ILE:O	2.15	0.45
1:B:539:ARG:HB2	1:B:542:LYS:HD3	1.97	0.45
1:B:737:TYR:CE2	1:B:785:TRP:HB3	2.51	0.45
1:C:979:LEU:HD12	1:C:1003:GLU:HA	1.98	0.45
1:B:112:ASN:HB2	1:B:132:LEU:HD22	1.98	0.45
1:C:112:ASN:HB2	1:C:132:LEU:HD22	1.98	0.45
1:C:539:ARG:HB2	1:C:542:LYS:HD3	1.97	0.45
1:C:737:TYR:CE2	1:C:785:TRP:HB3	2.51	0.45
1:B:159:LEU:HD13	1:B:184:ILE:HD13	1.98	0.45
1:B:732:SER:HA	1:D:147:ILE:HD11	1.98	0.45
1:D:277:THR:HG22	1:D:279:ARG:HG3	1.98	0.45
1:D:672:CYS:HB3	1:D:681:CYS:SG	2.56	0.45
1:D:988:TYR:CD2	1:D:988:TYR:C	2.84	0.45
1:B:81:VAL:HG11	1:B:145:LEU:HB2	1.98	0.45
1:B:672:CYS:HB3	1:B:681:CYS:SG	2.56	0.45
1:D:735:ARG:HG3	1:D:786:ASN:HA	1.96	0.45
1:B:534:HIS:CD2	1:B:644:LYS:HG3	2.51	0.45
1:B:690:PHE:CE2	1:B:731:GLN:HB3	2.38	0.45
1:D:785:TRP:CD1	1:D:791:ILE:HD11	2.51	0.45
1:B:785:TRP:CD1	1:B:791:ILE:HD11	2.51	0.45
1:A:559:CYS:C	1:A:560:MET:CA	2.83	0.45
1:A:324:GLN:HE22	1:B:576:ARG:HA	1.82	0.45
1:B:802:TYR:CE2	1:B:821:PHE:HB3	2.51	0.45
1:D:112:ASN:HB2	1:D:132:LEU:HD22	1.98	0.45
1:D:551:ARG:HH12	1:D:641:GLU:CG	2.30	0.45
1:A:638:ARG:HB2	1:A:645:ILE:HD13	1.97	0.45
1:C:1022:VAL:CG1	1:C:1029:VAL:CG1	2.94	0.45
1:C:329:SER:HB3	1:C:332:GLU:HG3	1.98	0.45
1:C:808:ARG:HD2	1:C:813:LEU:O	2.17	0.45
1:C:954:PRO:HA	1:C:978:TYR:HB2	1.99	0.45
1:D:1022:VAL:CG1	1:D:1029:VAL:CG1	2.94	0.45
1:A:162:VAL:CG2	1:A:189:ASP:HB2	2.47	0.45
1:A:407:LEU:HD22	1:C:944:LYS:CD	2.04	0.45
1:A:705:VAL:CG1	1:A:706:PRO:N	2.80	0.45
1:B:533:LEU:HA	1:B:533:LEU:HD23	1.84	0.45
1:B:560:MET:HE1	1:B:586:PRO:HD3	1.98	0.45
1:C:162:VAL:CG2	1:C:189:ASP:HB2	2.47	0.45
1:C:533:LEU:HD23	1:C:533:LEU:HA	1.84	0.45
1:D:162:VAL:CG2	1:D:189:ASP:HB2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:HG11	1:D:145:LEU:HB2	1.98	0.45
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.84	0.44
1:D:920:HIS:CD2	1:D:922:VAL:H	2.35	0.44
1:D:954:PRO:HA	1:D:978:TYR:HB2	1.99	0.44
1:A:785:TRP:CD1	1:A:791:ILE:HD11	2.52	0.44
1:B:203:LEU:HA	1:B:203:LEU:HD23	1.84	0.44
1:C:985:VAL:HG23	1:C:985:VAL:O	2.16	0.44
1:D:737:TYR:CE2	1:D:785:TRP:HB3	2.51	0.44
1:D:985:VAL:O	1:D:985:VAL:HG23	2.16	0.44
1:A:329:SER:HB3	1:A:332:GLU:HG3	1.98	0.44
1:C:277:THR:HG22	1:C:279:ARG:HG3	1.98	0.44
1:C:904:ILE:O	1:C:904:ILE:HG23	2.15	0.44
1:C:920:HIS:CD2	1:C:922:VAL:H	2.35	0.44
1:C:992:GLN:OE1	1:C:1012:SER:HB2	2.17	0.44
1:A:655:ASN:CG	1:A:658:ALA:H	2.20	0.44
1:A:920:HIS:CD2	1:A:922:VAL:H	2.35	0.44
1:B:482:ILE:HG23	1:B:497:VAL:HG13	2.00	0.44
1:B:705:VAL:CG1	1:B:706:PRO:N	2.80	0.44
1:C:81:VAL:HG11	1:C:145:LEU:HB2	1.98	0.44
1:D:661:LEU:CD2	1:D:790:ILE:HG13	2.46	0.44
1:D:705:VAL:H	1:D:724:ALA:HA	1.83	0.44
1:D:855:CYS:SG	1:D:885:LEU:CD2	2.96	0.44
1:A:325:ALA:CA	1:B:577:LEU:HD13	2.46	0.44
1:B:808:ARG:HD2	1:B:813:LEU:O	2.17	0.44
1:C:149:VAL:HG22	1:C:150:GLU:N	2.33	0.44
1:C:705:VAL:CG1	1:C:706:PRO:N	2.80	0.44
1:D:992:GLN:OE1	1:D:1012:SER:HB2	2.17	0.44
1:D:808:ARG:HD2	1:D:813:LEU:O	2.17	0.44
1:D:974:ILE:HG13	1:D:974:ILE:O	2.18	0.44
1:B:772:MET:HB3	1:B:806:ALA:HB1	1.98	0.44
1:C:775:SER:CB	1:C:806:ALA:H	2.30	0.44
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.83	0.44
1:D:705:VAL:CG1	1:D:706:PRO:N	2.80	0.44
1:A:559:CYS:CA	1:A:560:MET:N	2.80	0.44
1:A:808:ARG:HD2	1:A:813:LEU:O	2.17	0.44
1:A:890:ILE:HD13	1:A:908:TYR:CZ	2.53	0.44
1:D:1015:LEU:HD21	1:D:1039:ASP:HA	2.00	0.44
1:B:191:LYS:HD2	1:B:191:LYS:N	2.33	0.44
1:C:191:LYS:N	1:C:191:LYS:HD2	2.33	0.44
1:C:482:ILE:HG23	1:C:497:VAL:HG13	2.00	0.44
1:C:525:ASP:HA	1:C:526:PRO:HD3	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:HIS:HD2	1:C:644:LYS:NZ	2.15	0.44
1:C:890:ILE:CB	1:C:893:HIS:HD2	2.30	0.44
1:C:974:ILE:O	1:C:974:ILE:HG13	2.18	0.44
1:D:329:SER:HB3	1:D:332:GLU:HG3	1.98	0.44
1:A:760:VAL:CG1	1:A:761:GLN:N	2.81	0.44
1:A:944:LYS:O	1:A:944:LYS:HG3	2.18	0.44
1:B:162:VAL:CG2	1:B:189:ASP:HB2	2.48	0.44
1:B:705:VAL:H	1:B:724:ALA:HA	1.83	0.44
1:C:655:ASN:OD1	1:C:657:SER:CB	2.64	0.44
1:D:149:VAL:HG22	1:D:150:GLU:N	2.33	0.44
1:D:411:GLN:HA	1:D:412:PRO:C	2.38	0.44
1:D:890:ILE:HD13	1:D:908:TYR:CZ	2.53	0.44
1:B:459:ARG:HG3	1:B:526:PRO:CG	2.48	0.43
1:A:463:PRO:HB2	1:B:612:ILE:HG22	2.00	0.43
1:C:959:LEU:H	1:C:1033:LEU:HD21	1.83	0.43
1:D:313:ALA:HB1	1:D:335:LEU:HD11	2.00	0.43
1:D:533:LEU:CD2	1:D:639:SER:OG	2.65	0.43
1:D:959:LEU:H	1:D:1033:LEU:HD21	1.83	0.43
1:A:931:ARG:CG	1:A:942:MET:CE	2.96	0.43
1:C:1015:LEU:CD2	1:C:1039:ASP:N	2.81	0.43
1:C:1015:LEU:HD21	1:C:1039:ASP:HA	2.00	0.43
1:C:775:SER:HB2	1:C:806:ALA:N	2.33	0.43
1:C:995:GLU:O	1:C:1006:CYS:HB2	2.18	0.43
1:D:931:ARG:CG	1:D:942:MET:CE	2.96	0.43
1:A:57:ARG:HG2	1:A:121:TYR:CE1	2.53	0.43
1:C:313:ALA:HB1	1:C:335:LEU:HD11	2.00	0.43
1:C:947:GLN:HG3	1:C:948:GLN:N	2.34	0.43
1:D:1015:LEU:CD2	1:D:1039:ASP:N	2.81	0.43
1:A:313:ALA:HB1	1:A:335:LEU:HD11	2.00	0.43
1:B:533:LEU:HD21	1:B:646:PHE:CD2	2.47	0.43
1:D:482:ILE:HG23	1:D:497:VAL:HG13	2.00	0.43
1:B:735:ARG:HG3	1:B:786:ASN:HA	1.95	0.43
1:C:411:GLN:HA	1:C:412:PRO:C	2.38	0.43
1:C:57:ARG:HG2	1:C:121:TYR:CE1	2.53	0.43
1:C:890:ILE:HD13	1:C:908:TYR:CZ	2.53	0.43
1:C:944:LYS:O	1:C:944:LYS:HG3	2.18	0.43
1:B:741:LEU:HD12	1:B:767:TYR:CD1	2.54	0.43
1:B:802:TYR:CE1	1:B:821:PHE:CD1	3.05	0.43
1:C:56:HIS:HB3	1:C:59:THR:OG1	2.19	0.43
1:D:191:LYS:HD2	1:D:191:LYS:N	2.33	0.43
1:D:890:ILE:CB	1:D:893:HIS:HD2	2.30	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLN:HA	1:A:412:PRO:C	2.38	0.43
1:B:533:LEU:HD21	1:B:646:PHE:CE2	2.53	0.43
1:B:568:SER:CB	1:B:670:PHE:CE1	3.02	0.43
1:B:833:THR:CG2	1:B:837:HIS:CB	2.95	0.43
1:C:996:PHE:HE1	1:C:1004:ILE:HG23	1.83	0.43
1:C:931:ARG:CG	1:C:942:MET:CE	2.96	0.43
1:D:996:PHE:HE1	1:D:1004:ILE:HG23	1.83	0.43
1:A:149:VAL:HG22	1:A:150:GLU:N	2.33	0.43
1:A:191:LYS:HD2	1:A:191:LYS:N	2.33	0.43
1:B:411:GLN:HA	1:B:412:PRO:C	2.38	0.43
1:D:947:GLN:HG3	1:D:948:GLN:N	2.34	0.43
1:D:995:GLU:O	1:D:1006:CYS:HB2	2.18	0.43
1:A:741:LEU:HD12	1:A:767:TYR:CD1	2.54	0.43
1:A:324:GLN:HE22	1:B:576:ARG:HD2	1.84	0.43
1:B:57:ARG:HG2	1:B:121:TYR:CE1	2.54	0.43
1:B:784:VAL:CG1	1:B:785:TRP:N	2.82	0.43
1:C:1011:SER:HB2	1:C:1037:TYR:CD1	2.54	0.43
1:C:539:ARG:HD2	1:C:542:LYS:HZ2	1.84	0.43
1:C:885:LEU:O	1:C:910:ILE:HD12	2.19	0.43
1:D:57:ARG:HG2	1:D:121:TYR:CE1	2.54	0.43
1:D:775:SER:CA	1:D:807:GLN:HG3	2.42	0.43
1:A:908:TYR:CE1	1:A:914:ILE:HG12	2.54	0.43
1:B:690:PHE:CE2	1:B:731:GLN:CG	3.01	0.43
1:C:705:VAL:H	1:C:724:ALA:HA	1.82	0.43
1:C:741:LEU:HD12	1:C:767:TYR:CD1	2.54	0.43
1:C:908:TYR:CE1	1:C:914:ILE:HG12	2.54	0.43
1:C:987:VAL:HB	1:C:994:CYS:HB3	2.00	0.43
1:D:533:LEU:HD23	1:D:533:LEU:HA	1.84	0.43
1:D:56:HIS:HB3	1:D:59:THR:OG1	2.19	0.43
1:D:970:THR:HG22	1:D:1008:SER:CB	2.49	0.43
1:A:463:PRO:O	1:B:614:ILE:CG1	2.66	0.42
1:A:705:VAL:H	1:A:724:ALA:HA	1.83	0.42
1:A:947:GLN:HG3	1:A:948:GLN:N	2.34	0.42
1:D:1011:SER:HB2	1:D:1037:TYR:CD1	2.54	0.42
1:D:741:LEU:HD12	1:D:767:TYR:CD1	2.54	0.42
1:A:407:LEU:HD21	1:C:944:LYS:HD3	1.77	0.42
1:A:482:ILE:HG23	1:A:497:VAL:HG13	2.00	0.42
1:A:864:LEU:CG	1:A:865:THR:N	2.82	0.42
1:B:196:PRO:HG3	1:B:215:TYR:OH	2.20	0.42
1:C:677:TYR:CE1	1:C:731:GLN:CG	3.02	0.42
1:C:848:TRP:CG	1:C:848:TRP:O	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:946:HIS:CG	1:C:947:GLN:N	2.87	0.42
1:C:993:THR:CG2	1:C:994:CYS:N	2.82	0.42
1:D:944:LYS:HG3	1:D:944:LYS:O	2.18	0.42
1:D:987:VAL:HB	1:D:994:CYS:HB3	2.00	0.42
1:D:993:THR:CG2	1:D:994:CYS:N	2.82	0.42
1:A:37:GLN:OE1	1:A:37:GLN:HA	2.20	0.42
1:A:655:ASN:HA	1:A:656:CYS:N	2.33	0.42
1:A:784:VAL:CG1	1:A:785:TRP:N	2.82	0.42
1:A:885:LEU:O	1:A:910:ILE:HD12	2.19	0.42
1:B:149:VAL:HG22	1:B:150:GLU:N	2.33	0.42
1:C:192:GLN:HG3	1:C:228:ILE:O	2.20	0.42
1:C:970:THR:HG22	1:C:1008:SER:CB	2.49	0.42
1:D:1001:MET:CG	1:D:1002:ASN:N	2.83	0.42
1:D:881:VAL:CG1	1:D:882:ASN:N	2.82	0.42
1:D:896:VAL:HG21	1:D:918:MET:HE3	2.01	0.42
1:A:192:GLN:HG3	1:A:228:ILE:O	2.20	0.42
1:A:810:SER:OG	1:A:882:ASN:OD1	2.37	0.42
1:B:708:GLU:HG2	1:B:709:GLU:N	2.35	0.42
1:B:760:VAL:CG1	1:B:761:GLN:N	2.81	0.42
1:C:37:GLN:HA	1:C:37:GLN:OE1	2.20	0.42
1:C:735:ARG:HG3	1:C:786:ASN:HA	1.96	0.42
1:D:192:GLN:HG3	1:D:228:ILE:O	2.20	0.42
1:D:482:ILE:HD12	1:D:497:VAL:HG11	2.02	0.42
1:D:440:TYR:CD2	1:D:527:HIS:HA	2.55	0.42
1:D:706:PRO:CG	1:D:795:GLN:HG3	2.49	0.42
1:D:863:ILE:HG13	1:D:877:THR:C	2.40	0.42
1:D:885:LEU:O	1:D:910:ILE:HD12	2.19	0.42
1:A:56:HIS:HB3	1:A:59:THR:OG1	2.19	0.42
1:A:704:LEU:CD1	1:A:783:VAL:HG21	2.49	0.42
1:C:482:ILE:HD12	1:C:497:VAL:HG11	2.02	0.42
1:C:881:VAL:CG1	1:C:882:ASN:N	2.82	0.42
1:D:151:PRO:HG2	1:D:213:LEU:HD12	2.02	0.42
1:D:37:GLN:HA	1:D:37:GLN:OE1	2.20	0.42
1:D:470:TYR:CD1	1:D:525:ASP:HB2	2.55	0.42
1:A:818:ASP:HB2	1:A:821:PHE:HD2	1.79	0.42
1:A:810:SER:CB	1:A:882:ASN:CG	2.71	0.42
1:A:881:VAL:CG1	1:A:882:ASN:N	2.82	0.42
1:C:1001:MET:CG	1:C:1002:ASN:N	2.83	0.42
1:C:151:PRO:HG2	1:C:213:LEU:HD12	2.02	0.42
1:C:863:ILE:HG13	1:C:877:THR:C	2.40	0.42
1:C:988:TYR:OH	1:C:991:ASN:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1038:ILE:CG2	1:D:1039:ASP:N	2.82	0.42
1:A:324:GLN:NE2	1:B:576:ARG:NE	2.68	0.42
1:B:37:GLN:OE1	1:B:37:GLN:HA	2.20	0.42
1:B:56:HIS:HB3	1:B:59:THR:OG1	2.19	0.42
1:C:775:SER:H	1:C:807:GLN:HG3	1.85	0.42
1:C:872:GLY:O	1:C:1026:ARG:CB	2.63	0.42
1:D:708:GLU:HG2	1:D:709:GLU:N	2.35	0.42
1:D:908:TYR:CE1	1:D:914:ILE:HG12	2.54	0.42
1:A:708:GLU:HG2	1:A:709:GLU:N	2.35	0.42
1:A:815:LEU:N	1:A:815:LEU:CD1	2.83	0.42
1:C:655:ASN:O	1:C:656:CYS:C	2.54	0.42
1:C:708:GLU:HG2	1:C:709:GLU:N	2.35	0.42
1:C:883:LEU:HG	1:C:932:LEU:HD11	2.02	0.42
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.89	0.42
1:B:151:PRO:HG2	1:B:213:LEU:HD12	2.01	0.42
1:B:508:VAL:HG11	1:B:539:ARG:HH22	1.85	0.42
1:B:549:ALA:C	1:B:586:PRO:HA	2.40	0.42
1:C:1038:ILE:CG2	1:C:1039:ASP:N	2.82	0.42
1:C:933:CYS:SG	1:C:942:MET:SD	3.18	0.42
1:D:815:LEU:CD1	1:D:815:LEU:N	2.83	0.42
1:D:933:CYS:SG	1:D:942:MET:SD	3.18	0.42
1:D:988:TYR:OH	1:D:991:ASN:N	2.53	0.42
1:A:149:VAL:HG22	1:A:151:PRO:HD3	2.02	0.42
1:A:204:PRO:HD2	1:A:212:MET:SD	2.60	0.42
1:A:848:TRP:CG	1:A:848:TRP:O	2.73	0.42
1:C:784:VAL:CG1	1:C:785:TRP:N	2.82	0.42
1:D:791:ILE:HG22	1:D:792:ASP:N	2.35	0.42
1:A:196:PRO:HG3	1:A:215:TYR:OH	2.19	0.41
1:B:313:ALA:HB1	1:B:335:LEU:HD11	2.00	0.41
1:B:57:ARG:HG3	1:B:58:ARG:HG3	2.02	0.41
1:C:938:LYS:CE	1:C:941:PHE:HE2	2.33	0.41
1:D:784:VAL:CG1	1:D:785:TRP:N	2.82	0.41
1:D:864:LEU:CG	1:D:865:THR:N	2.82	0.41
1:D:883:LEU:HG	1:D:932:LEU:HD11	2.02	0.41
1:A:655:ASN:OD1	1:A:657:SER:C	2.58	0.41
1:B:192:GLN:HG3	1:B:228:ILE:O	2.20	0.41
1:B:476:PHE:HE2	1:B:482:ILE:HD13	1.85	0.41
1:B:482:ILE:HD12	1:B:497:VAL:HG11	2.02	0.41
1:C:716:GLU:OE2	1:C:836:GLN:HG2	2.20	0.41
1:C:833:THR:HG21	1:C:837:HIS:HB2	1.99	0.41
1:D:149:VAL:HG22	1:D:151:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:863:ILE:O	1:D:863:ILE:HG23	2.20	0.41
1:D:946:HIS:CG	1:D:947:GLN:N	2.87	0.41
1:A:324:GLN:NE2	1:B:576:ARG:CD	2.84	0.41
1:A:482:ILE:HD12	1:A:497:VAL:HG11	2.02	0.41
1:A:737:TYR:HE1	1:A:754:ARG:CD	2.25	0.41
1:A:791:ILE:HG22	1:A:792:ASP:N	2.36	0.41
1:C:760:VAL:CG1	1:C:761:GLN:N	2.81	0.41
1:D:760:VAL:CG1	1:D:761:GLN:N	2.81	0.41
1:D:848:TRP:CG	1:D:848:TRP:O	2.73	0.41
1:D:931:ARG:HG2	1:D:942:MET:CE	2.50	0.41
1:A:629:ASP:OD1	1:A:659:HIS:CE1	2.72	0.41
1:A:931:ARG:HG2	1:A:942:MET:CE	2.50	0.41
1:C:1015:LEU:CD1	1:C:1015:LEU:N	2.83	0.41
1:C:204:PRO:HD2	1:C:212:MET:SD	2.60	0.41
1:C:843:SER:N	1:C:844:PRO:CD	2.84	0.41
1:C:863:ILE:O	1:C:863:ILE:HG23	2.20	0.41
1:D:815:LEU:O	1:D:848:TRP:CD1	2.74	0.41
1:A:815:LEU:HB3	1:A:885:LEU:CD1	2.46	0.41
1:A:883:LEU:HG	1:A:932:LEU:HD11	2.02	0.41
1:C:203:LEU:HA	1:C:203:LEU:HD23	1.83	0.41
1:C:417:THR:HA	1:C:418:PRO:HD3	1.74	0.41
1:C:560:MET:HE2	1:C:586:PRO:HD3	2.03	0.41
1:C:781:PHE:C	1:C:781:PHE:CD1	2.94	0.41
1:C:815:LEU:CD1	1:C:815:LEU:N	2.83	0.41
1:D:1015:LEU:CD1	1:D:1015:LEU:N	2.83	0.41
1:A:564:VAL:HG23	1:A:649:THR:HG21	2.03	0.41
1:A:781:PHE:CD1	1:A:781:PHE:C	2.94	0.41
1:A:863:ILE:HG13	1:A:877:THR:C	2.40	0.41
1:B:508:VAL:CG1	1:B:539:ARG:HH22	2.33	0.41
1:B:564:VAL:HG23	1:B:649:THR:HG21	2.03	0.41
1:B:815:LEU:O	1:B:848:TRP:CD1	2.74	0.41
1:C:1018:VAL:HG12	1:C:1019:PRO:N	2.35	0.41
1:C:476:PHE:HE2	1:C:482:ILE:HD13	1.85	0.41
1:D:204:PRO:HD2	1:D:212:MET:SD	2.60	0.41
1:D:570:SER:CB	1:D:683:HIS:CG	3.03	0.41
1:D:938:LYS:CE	1:D:941:PHE:HE2	2.34	0.41
1:A:815:LEU:O	1:A:848:TRP:CD1	2.74	0.41
1:A:946:HIS:CG	1:A:947:GLN:N	2.87	0.41
1:B:204:PRO:HD2	1:B:212:MET:SD	2.60	0.41
1:B:582:VAL:CG1	1:B:585:ALA:HB2	2.51	0.41
1:B:848:TRP:CG	1:B:848:TRP:O	2.72	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:VAL:HG23	1:C:649:THR:HG21	2.03	0.41
1:C:68:ASN:ND2	1:C:87:PRO:HG3	2.36	0.41
1:D:533:LEU:CD1	1:D:641:GLU:HB3	2.51	0.41
1:D:864:LEU:CG	1:D:865:THR:H	2.32	0.41
1:A:843:SER:N	1:A:844:PRO:CD	2.84	0.41
1:A:87:PRO:HB2	1:A:109:LEU:CD1	2.51	0.41
1:B:843:SER:N	1:B:844:PRO:CD	2.84	0.41
1:C:864:LEU:CG	1:C:865:THR:H	2.32	0.41
1:D:196:PRO:HG3	1:D:215:TYR:OH	2.19	0.41
1:D:843:SER:N	1:D:844:PRO:CD	2.84	0.41
1:D:68:ASN:ND2	1:D:87:PRO:HG3	2.36	0.41
1:A:781:PHE:CE2	1:A:797:LEU:O	2.74	0.41
1:A:933:CYS:SG	1:A:942:MET:SD	3.18	0.41
1:C:149:VAL:HG22	1:C:151:PRO:HD3	2.03	0.41
1:D:1018:VAL:HG12	1:D:1019:PRO:N	2.35	0.41
1:D:404:PHE:CE2	1:D:406:GLY:HA2	2.56	0.41
1:D:533:LEU:HD11	1:D:641:GLU:HB3	2.03	0.41
1:D:709:GLU:O	1:D:711:LEU:HD12	2.21	0.41
1:A:532:ALA:O	1:A:646:PHE:HB2	2.20	0.41
1:A:68:ASN:ND2	1:A:87:PRO:HG3	2.36	0.41
1:A:714:VAL:CG1	1:A:768:GLN:HA	2.49	0.41
1:B:404:PHE:CE2	1:B:406:GLY:HA2	2.56	0.41
1:A:463:PRO:CG	1:B:612:ILE:CB	2.68	0.41
1:C:196:PRO:HG3	1:C:215:TYR:OH	2.20	0.41
1:C:315:LEU:HD11	1:C:333:ASP:HB3	2.03	0.41
1:C:709:GLU:OE1	1:C:709:GLU:HA	2.21	0.41
1:C:791:ILE:HG22	1:C:792:ASP:N	2.36	0.41
1:D:476:PHE:HE2	1:D:482:ILE:HD13	1.85	0.41
1:D:781:PHE:CE2	1:D:797:LEU:O	2.74	0.41
1:A:582:VAL:CG1	1:A:585:ALA:HB2	2.51	0.41
1:A:57:ARG:HG3	1:A:58:ARG:HG3	2.02	0.41
1:A:709:GLU:O	1:A:711:LEU:HD12	2.21	0.41
1:A:883:LEU:HD13	1:A:911:ALA:O	2.21	0.41
1:B:781:PHE:CE2	1:B:797:LEU:O	2.74	0.41
1:B:68:ASN:ND2	1:B:87:PRO:HG3	2.36	0.41
1:C:815:LEU:O	1:C:848:TRP:CD1	2.74	0.41
1:C:931:ARG:HG2	1:C:942:MET:CE	2.50	0.41
1:D:309:LEU:HA	1:D:309:LEU:HD23	1.89	0.41
1:D:807:GLN:HE21	1:D:807:GLN:HB3	1.65	0.41
1:A:151:PRO:HG2	1:A:213:LEU:HD12	2.02	0.40
1:A:709:GLU:HA	1:A:709:GLU:OE1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:GLU:O	1:B:711:LEU:HD12	2.21	0.40
1:B:815:LEU:CD1	1:B:815:LEU:N	2.83	0.40
1:B:815:LEU:HD23	1:B:848:TRP:HB3	2.04	0.40
1:C:709:GLU:O	1:C:711:LEU:HD12	2.21	0.40
1:C:864:LEU:CG	1:C:865:THR:N	2.82	0.40
1:C:979:LEU:HD12	1:C:1002:ASN:C	2.41	0.40
1:D:539:ARG:HD2	1:D:542:LYS:HZ2	1.86	0.40
1:D:564:VAL:HG23	1:D:649:THR:HG21	2.03	0.40
1:D:582:VAL:CG1	1:D:585:ALA:HB2	2.51	0.40
1:D:619:LYS:HA	1:D:619:LYS:HD3	1.91	0.40
1:D:979:LEU:HD12	1:D:1002:ASN:C	2.41	0.40
1:A:404:PHE:CE2	1:A:406:GLY:HA2	2.56	0.40
1:A:407:LEU:HD22	1:C:944:LYS:CG	2.48	0.40
1:A:863:ILE:HG23	1:A:863:ILE:O	2.20	0.40
1:A:931:ARG:HG2	1:A:942:MET:HE1	2.03	0.40
1:B:257:THR:O	1:B:278:SER:HA	2.22	0.40
1:A:463:PRO:HD2	1:B:612:ILE:HG21	2.03	0.40
1:B:781:PHE:CD1	1:B:781:PHE:C	2.94	0.40
1:C:404:PHE:CE2	1:C:406:GLY:HA2	2.56	0.40
1:C:883:LEU:HD13	1:C:911:ALA:O	2.21	0.40
1:A:550:ASN:O	1:A:586:PRO:HG3	2.21	0.40
1:A:815:LEU:HD23	1:A:848:TRP:HB3	2.04	0.40
1:A:864:LEU:CG	1:A:865:THR:H	2.32	0.40
1:A:923:ILE:CG1	1:A:924:GLY:H	2.35	0.40
1:C:702:PRO:HB3	1:C:728:PRO:CG	2.52	0.40
1:C:781:PHE:CE2	1:C:797:LEU:O	2.74	0.40
1:C:952:VAL:HG23	1:C:954:PRO:HD3	2.03	0.40
1:D:315:LEU:HD11	1:D:333:ASP:HB3	2.03	0.40
1:A:931:ARG:CG	1:A:942:MET:HE1	2.52	0.40
1:B:149:VAL:HG22	1:B:151:PRO:HD3	2.02	0.40
1:D:57:ARG:HG3	1:D:58:ARG:HG3	2.02	0.40
1:D:781:PHE:CD1	1:D:781:PHE:C	2.94	0.40
1:D:87:PRO:HB2	1:D:109:LEU:CD1	2.51	0.40
1:D:993:THR:HG22	1:D:994:CYS:O	2.22	0.40
1:A:810:SER:HB3	1:A:882:ASN:HD21	1.83	0.40
1:C:1013:ASN:HB3	1:C:1014:GLY:H	1.68	0.40
1:C:349:PRO:HA	1:C:350:PRO:HD3	1.96	0.40
1:C:979:LEU:HB2	1:C:1000:SER:O	2.21	0.40
1:D:883:LEU:HD13	1:D:911:ALA:O	2.21	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:PRO:CB	1:B:768:GLN:OE1[5_665]	1.27	0.93
1:B:397:PRO:CG	1:D:947:GLN:OE1[2_564]	1.51	0.69
1:A:731:GLN:OE1	1:C:146:PHE:CD1[3_455]	1.56	0.64
1:B:407:LEU:CD2	1:D:944:LYS:CD[2_564]	1.79	0.41
1:A:731:GLN:NE2	1:C:146:PHE:CE1[3_455]	1.87	0.33
1:A:766:SER:OG	1:B:839:PRO:CA[5_665]	1.98	0.22
1:A:839:PRO:CG	1:B:768:GLN:OE1[5_665]	2.02	0.18
1:B:146:PHE:CE1	1:C:677:TYR:OH[4_565]	2.03	0.17
1:A:731:GLN:CD	1:C:146:PHE:CD1[3_455]	2.08	0.12
1:A:766:SER:OG	1:B:839:PRO:CB[5_665]	2.12	0.08
1:A:731:GLN:CD	1:C:146:PHE:CE1[3_455]	2.15	0.05
1:A:84:LYS:CB	1:D:732:SER:OG[5_555]	2.15	0.05
1:B:217:LEU:CD1	1:D:940:GLU:OE1[2_564]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	896/1212 (74%)	861 (96%)	26 (3%)	9 (1%)	15	55
1	B	797/1212 (66%)	771 (97%)	19 (2%)	7 (1%)	17	57
1	C	981/1212 (81%)	937 (96%)	35 (4%)	9 (1%)	17	57
1	D	983/1212 (81%)	942 (96%)	31 (3%)	10 (1%)	15	55
All	All	3657/4848 (75%)	3511 (96%)	111 (3%)	35 (1%)	15	55

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	702	PRO
1	A	851	HIS
1	B	508	VAL
1	B	509	GLU
1	B	851	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	804	CYS
1	C	851	HIS
1	D	804	CYS
1	D	851	HIS
1	A	703	GLN
1	A	160	SER
1	A	175	SER
1	A	805	ALA
1	B	160	SER
1	B	175	SER
1	B	805	ALA
1	C	160	SER
1	C	175	SER
1	C	805	ALA
1	D	160	SER
1	D	175	SER
1	D	805	ALA
1	A	849	SER
1	B	849	SER
1	C	849	SER
1	D	559	CYS
1	D	849	SER
1	A	935	GLY
1	C	935	GLY
1	C	952	VAL
1	D	935	GLY
1	D	952	VAL
1	A	922	VAL
1	C	922	VAL
1	D	922	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	796/1064 (75%)	787 (99%)	9 (1%)	73 84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	714/1064 (67%)	706 (99%)	8 (1%)	73 84
1	C	870/1064 (82%)	860 (99%)	10 (1%)	73 84
1	D	870/1064 (82%)	860 (99%)	10 (1%)	73 84
All	All	3250/4256 (76%)	3213 (99%)	37 (1%)	73 84

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	A	238	HIS
1	A	274	LEU
1	A	298	PHE
1	A	438	TYR
1	A	509	GLU
1	A	626	LEU
1	A	811	CYS
1	A	893	HIS
1	B	237	SER
1	B	238	HIS
1	B	274	LEU
1	B	298	PHE
1	B	438	TYR
1	B	509	GLU
1	B	626	LEU
1	B	811	CYS
1	C	237	SER
1	C	238	HIS
1	C	274	LEU
1	C	298	PHE
1	C	438	TYR
1	C	509	GLU
1	C	626	LEU
1	C	811	CYS
1	C	893	HIS
1	C	953	ASN
1	D	237	SER
1	D	238	HIS
1	D	274	LEU
1	D	298	PHE
1	D	438	TYR
1	D	509	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	626	LEU
1	D	811	CYS
1	D	893	HIS
1	D	953	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	726	ASN
1	A	731	GLN
1	A	761	GLN
1	A	837	HIS
1	B	513	GLN
1	B	534	HIS
1	B	703	GLN
1	B	761	GLN
1	B	837	HIS
1	C	534	HIS
1	C	726	ASN
1	C	761	GLN
1	C	807	GLN
1	C	837	HIS
1	C	953	ASN
1	C	1034	GLN
1	D	513	GLN
1	D	534	HIS
1	D	550	ASN
1	D	726	ASN
1	D	761	GLN
1	D	807	GLN
1	D	837	HIS
1	D	953	ASN
1	D	1034	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	6
1	A	6
1	C	6
1	D	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	855:CYS	C	856:SER	N	5.61
1	C	702:PRO	C	703:GLN	N	3.75
1	D	702:PRO	C	703:GLN	N	3.35
1	C	559:CYS	C	560:MET	N	2.82
1	C	855:CYS	C	856:SER	N	2.48
1	B	559:CYS	C	560:MET	N	2.40
1	B	701:CYS	C	702:PRO	N	2.35
1	B	803:LYS	C	804:CYS	N	2.12
1	A	559:CYS	C	560:MET	N	2.11
1	A	655:ASN	C	656:CYS	N	2.03
1	B	702:PRO	C	703:GLN	N	1.94
1	A	702:PRO	C	703:GLN	N	1.89
1	B	655:ASN	C	656:CYS	N	1.71

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	952:VAL	C	953:ASN	N	1.66
1	C	701:CYS	C	702:PRO	N	1.60
1	C	803:LYS	C	804:CYS	N	1.20
1	A	701:CYS	C	702:PRO	N	1.19
1	A	803:LYS	C	804:CYS	N	1.18
1	C	508:VAL	C	509:GLU	N	1.07
1	B	508:VAL	C	509:GLU	N	0.99
1	D	508:VAL	C	509:GLU	N	0.98
1	D	655:ASN	C	656:CYS	N	0.96
1	A	508:VAL	C	509:GLU	N	0.78

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.