Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2016 – 06:01 PM EDT

PDB ID	:	4ZIV
Title	:	Crystal structure of AcrB triple mutant in P21 space group
Authors	:	Ababou, A.; Koronakis, V.
Deposited on	:	2015-04-28
Resolution	:	3.16 Å(reported)

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

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

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

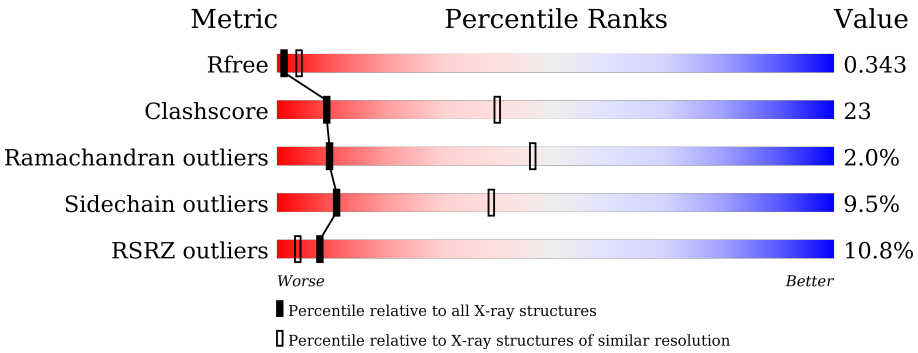
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.16 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	1049	8% 52% 43%
1	B	1049	7% 53% 39% 6%
1	C	1049	11% 53% 41% 6%
1	D	1049	11% 53% 41%
1	E	1049	13% 48% 43% 7%
1	F	1049	15% 52% 43%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	B	1101	X	-	-	-
2	LMT	C	1101	X	-	-	-
2	LMT	E	1101	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47736 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	B	1046	Total	C	N	O	S	0	0	0
			7939	5099	1314	1483	43			
1	C	1044	Total	C	N	O	S	0	0	0
			7924	5090	1312	1479	43			
1	D	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	F	1046	Total	C	N	O	S	0	0	0
			7939	5099	1314	1483	43			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	615	ALA	PHE	engineered mutation	UNP P31224
A	617	ALA	PHE	engineered mutation	UNP P31224
A	620	ALA	ARG	engineered mutation	UNP P31224
B	615	ALA	PHE	engineered mutation	UNP P31224
B	617	ALA	PHE	engineered mutation	UNP P31224
B	620	ALA	ARG	engineered mutation	UNP P31224
C	615	ALA	PHE	engineered mutation	UNP P31224
C	617	ALA	PHE	engineered mutation	UNP P31224
C	620	ALA	ARG	engineered mutation	UNP P31224
D	615	ALA	PHE	engineered mutation	UNP P31224
D	617	ALA	PHE	engineered mutation	UNP P31224
D	620	ALA	ARG	engineered mutation	UNP P31224
E	615	ALA	PHE	engineered mutation	UNP P31224
E	617	ALA	PHE	engineered mutation	UNP P31224
E	620	ALA	ARG	engineered mutation	UNP P31224
F	615	ALA	PHE	engineered mutation	UNP P31224
F	617	ALA	PHE	engineered mutation	UNP P31224

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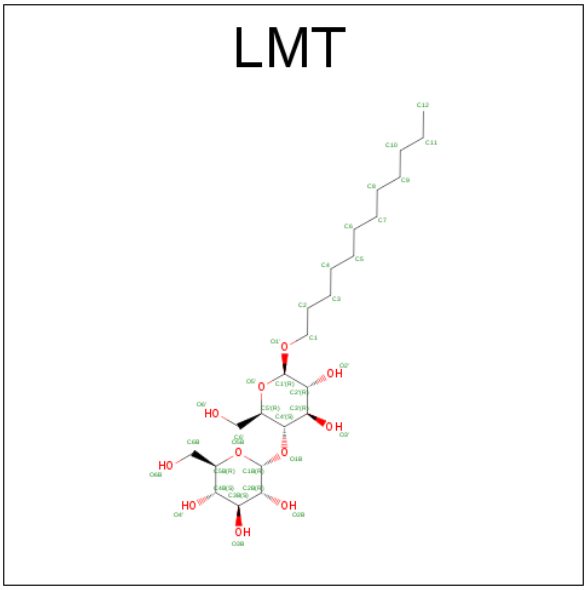
Chain	Residue	Modelled	Actual	Comment	Reference
F	620	ALA	ARG	engineered mutation	UNP P31224

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0

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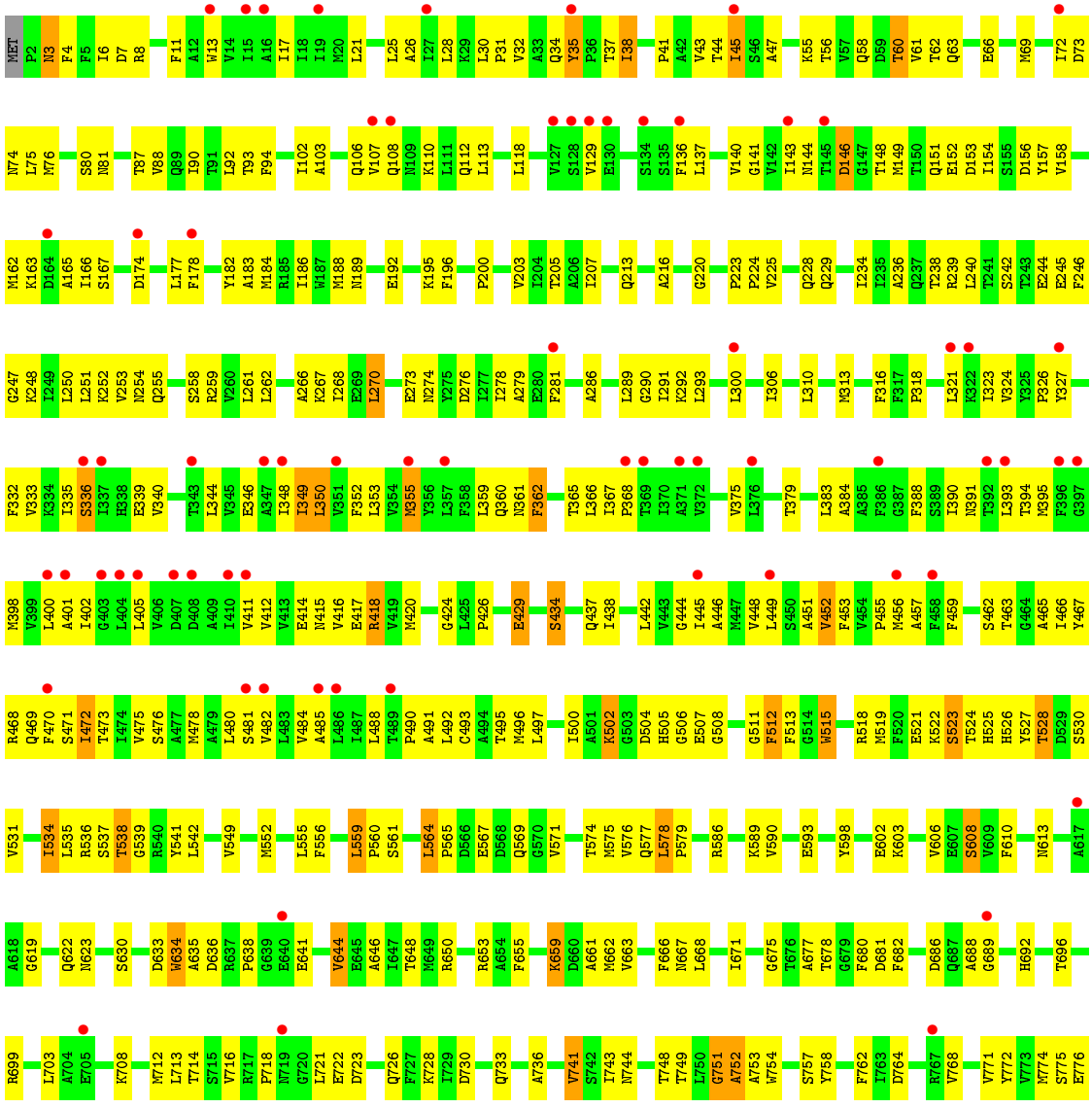
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Ni 1 1	0	0

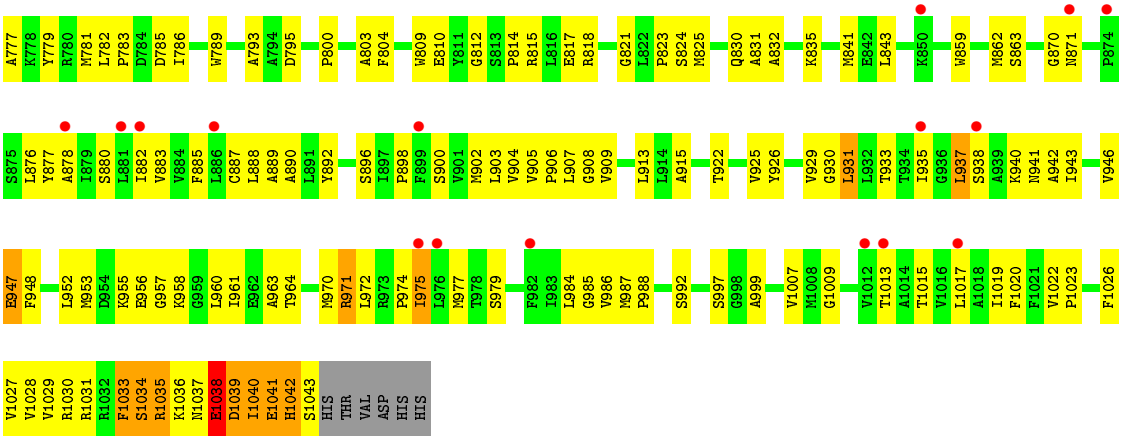
3 Residue-property plots (i)

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

- Molecule 1: Multidrug efflux pump subunit AcrB

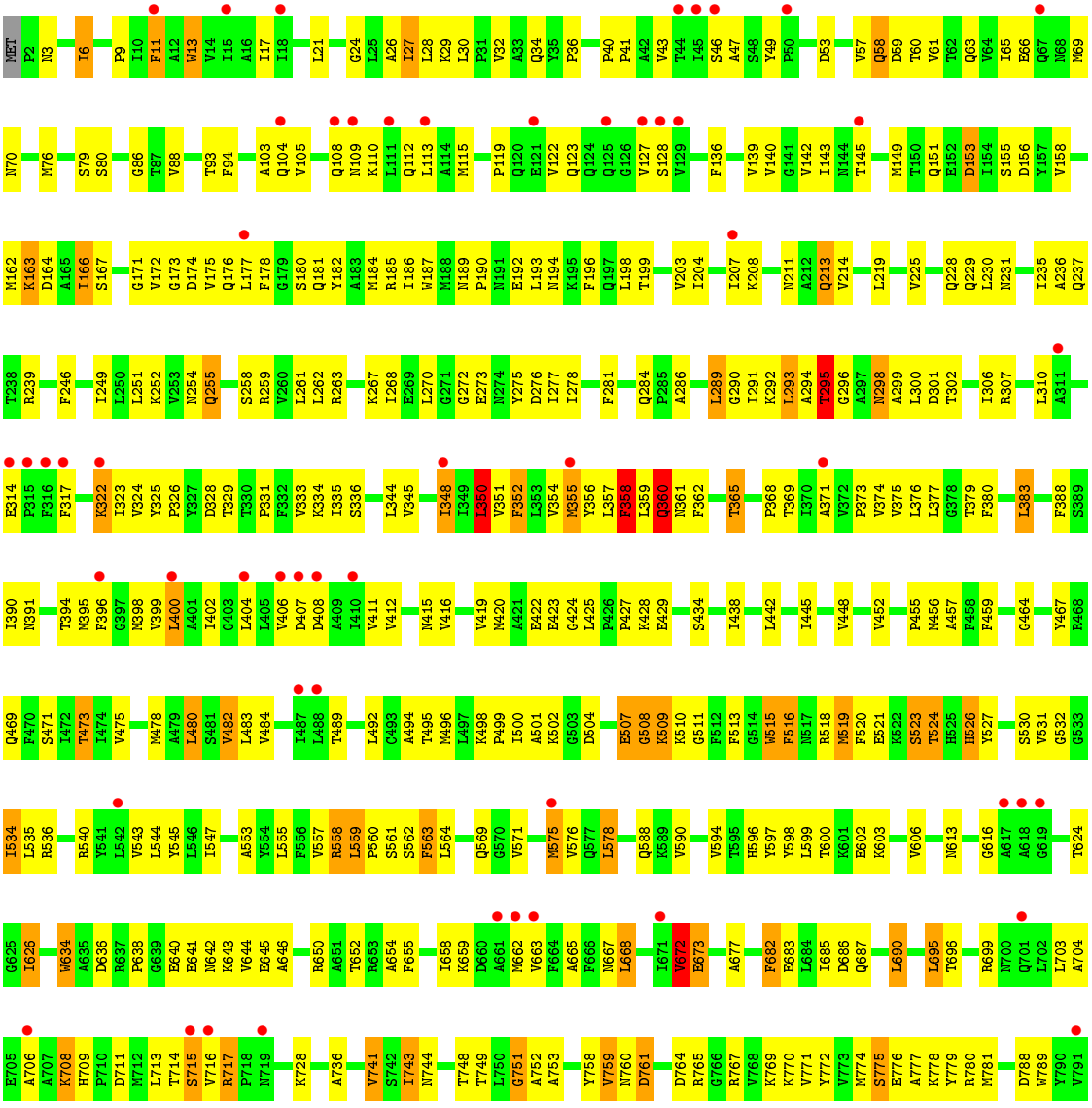
Chain A:

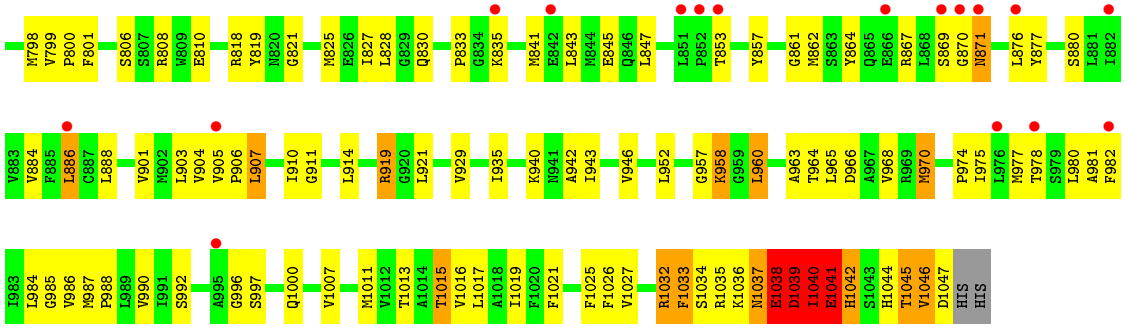




- Molecule 1: Multidrug efflux pump subunit AcrB

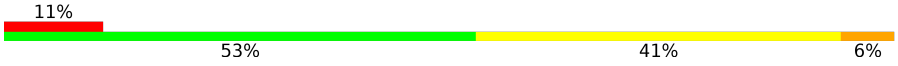
Chain B:

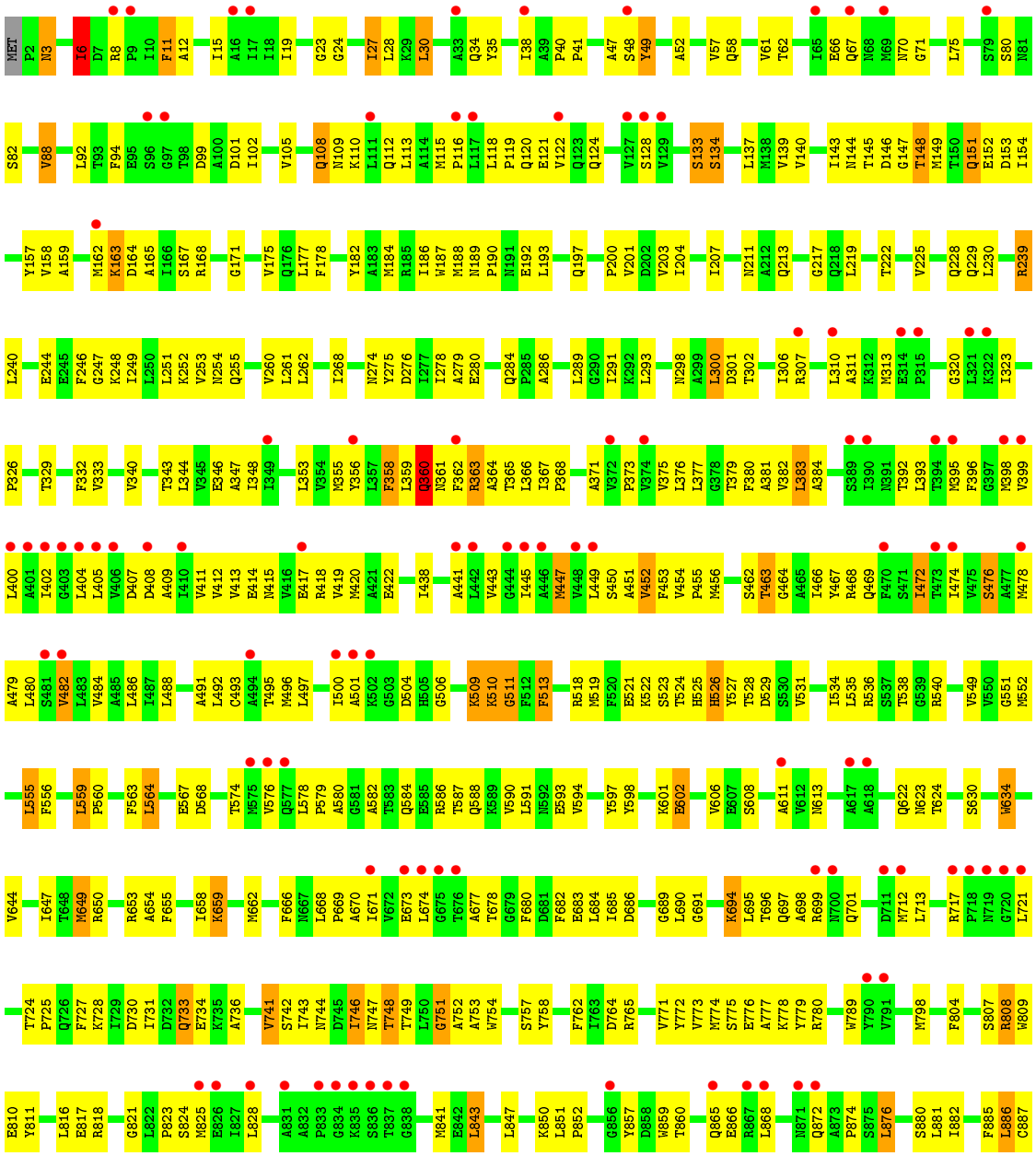


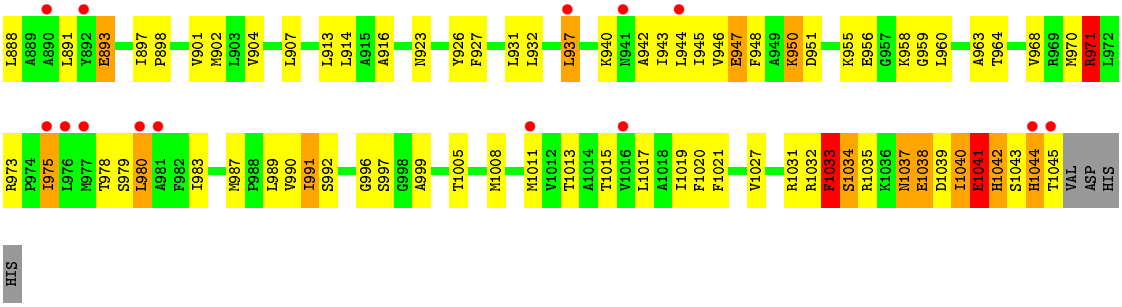


- Molecule 1: Multidrug efflux pump subunit AcrB

Chain C:

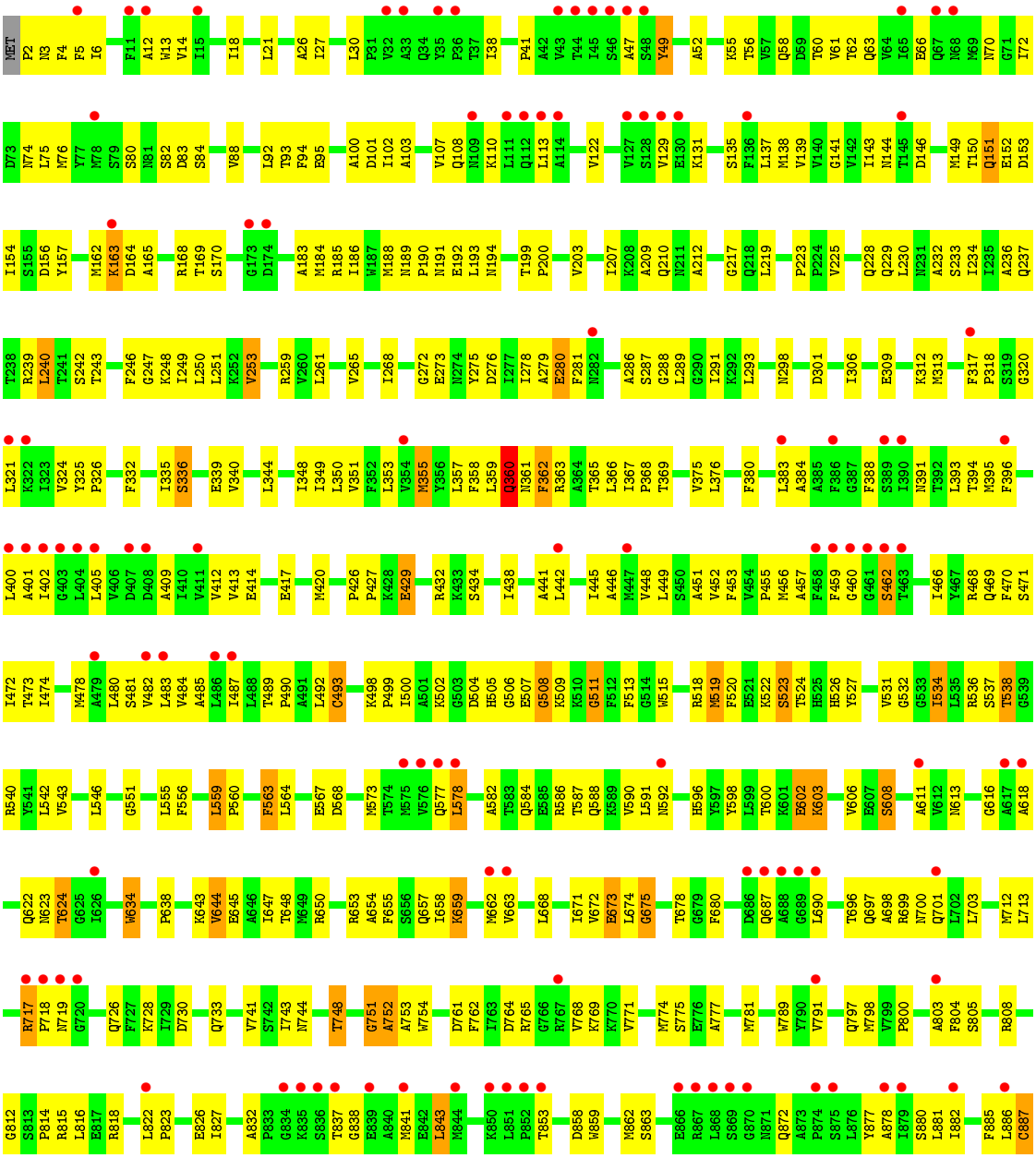


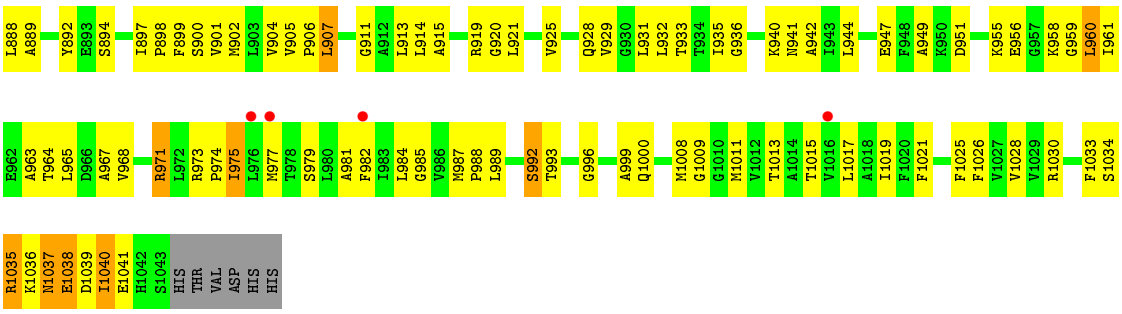




• Molecule 1: Multidrug efflux pump subunit AcrB

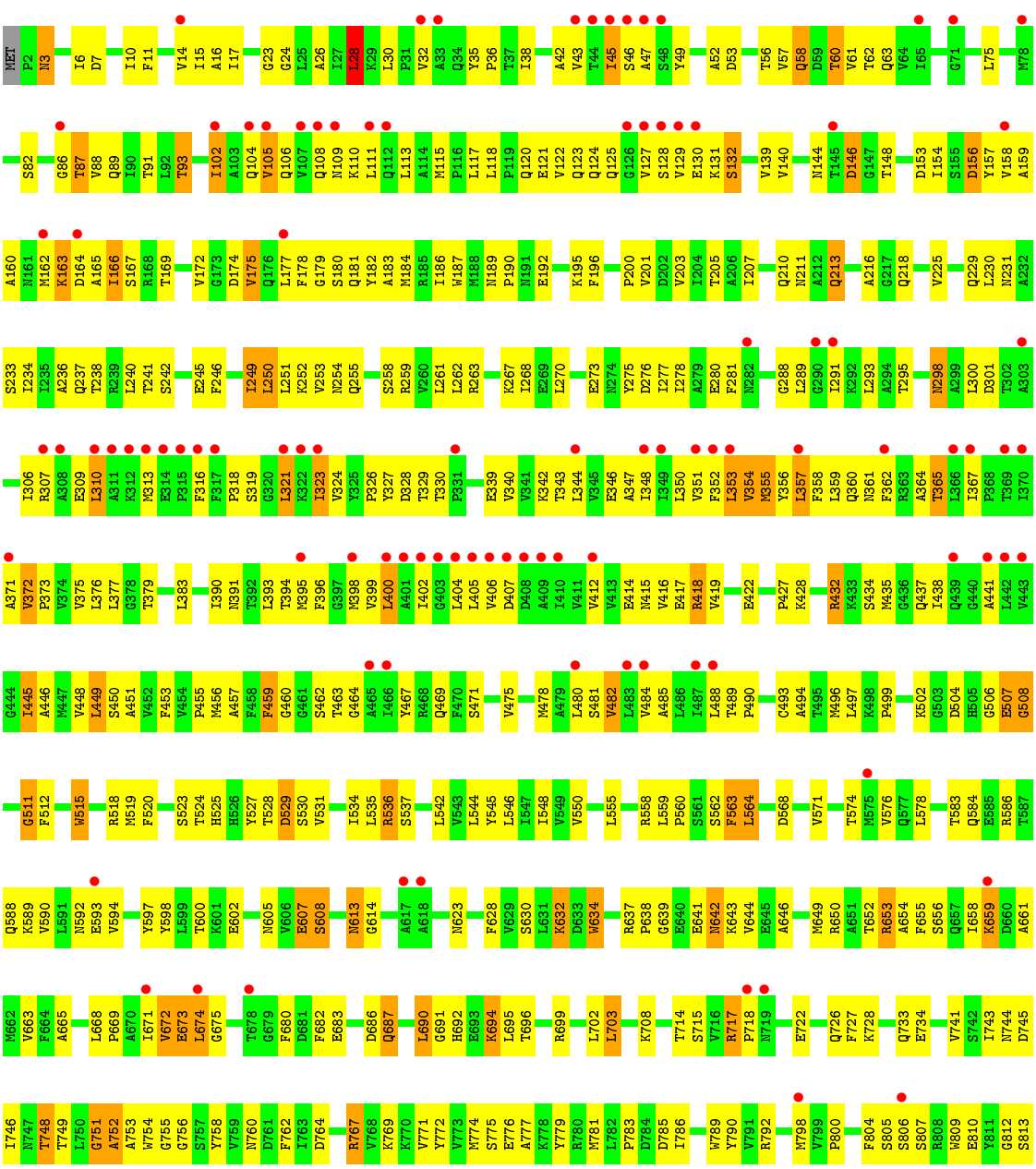
Chain D:

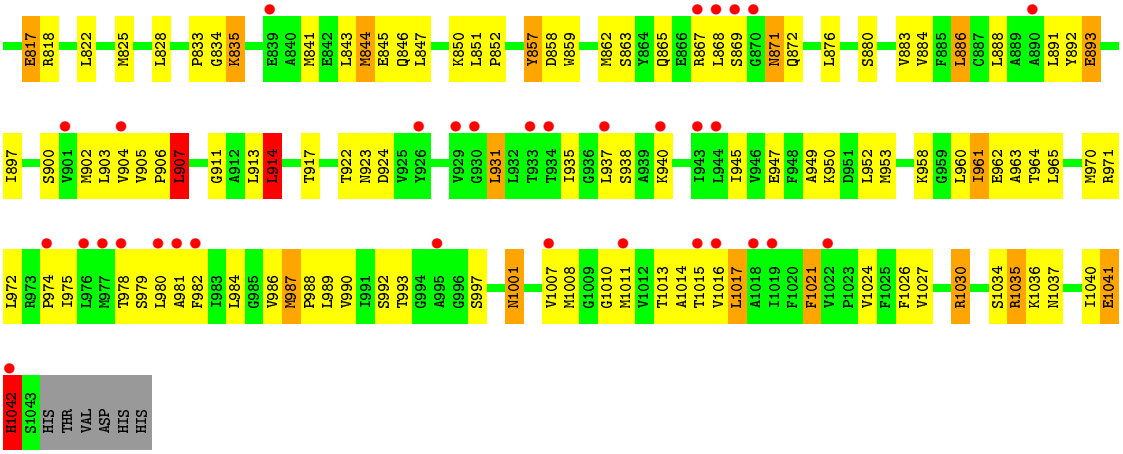




- Molecule 1: Multidrug efflux pump subunit AcrB

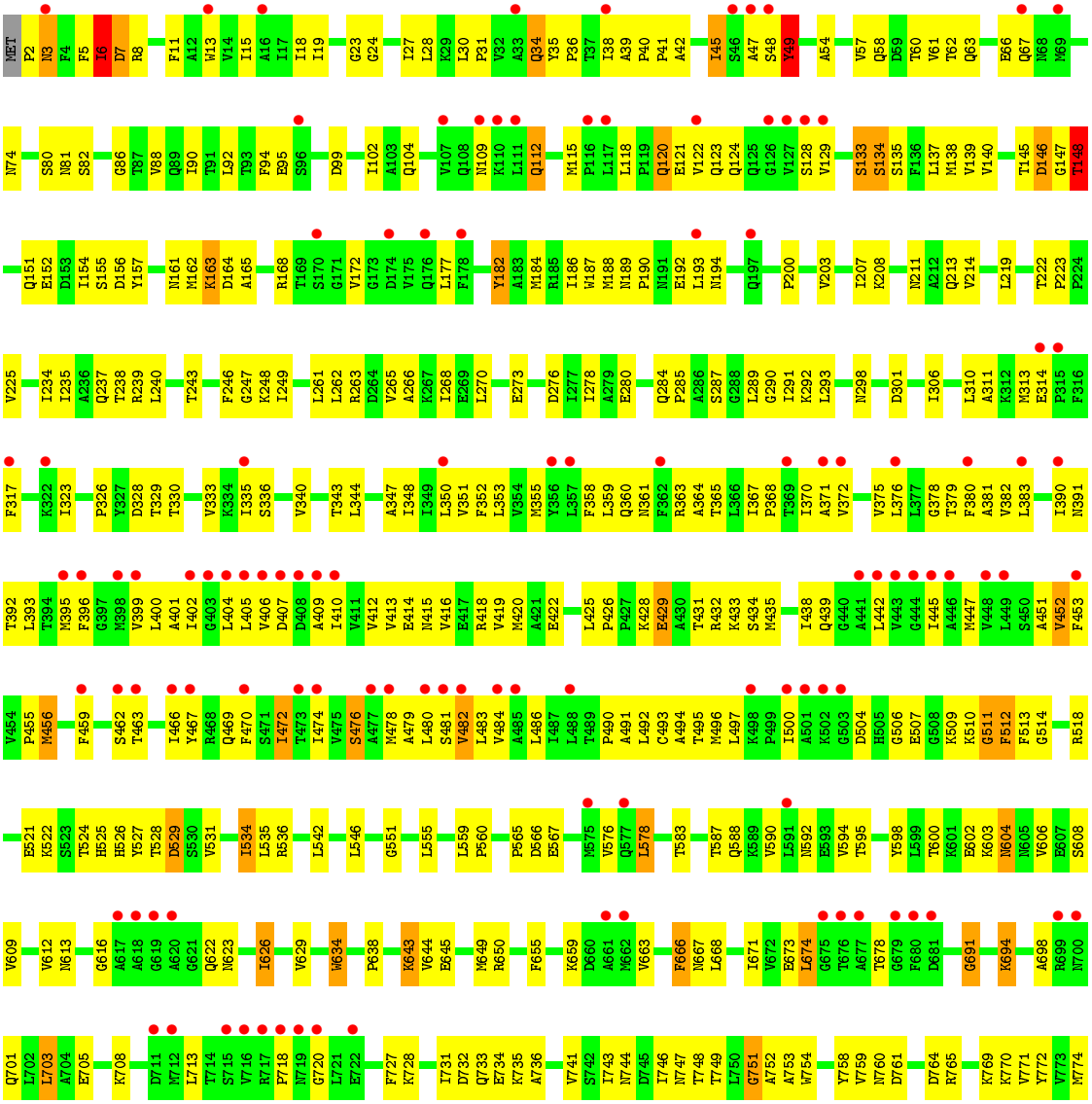
Chain E:

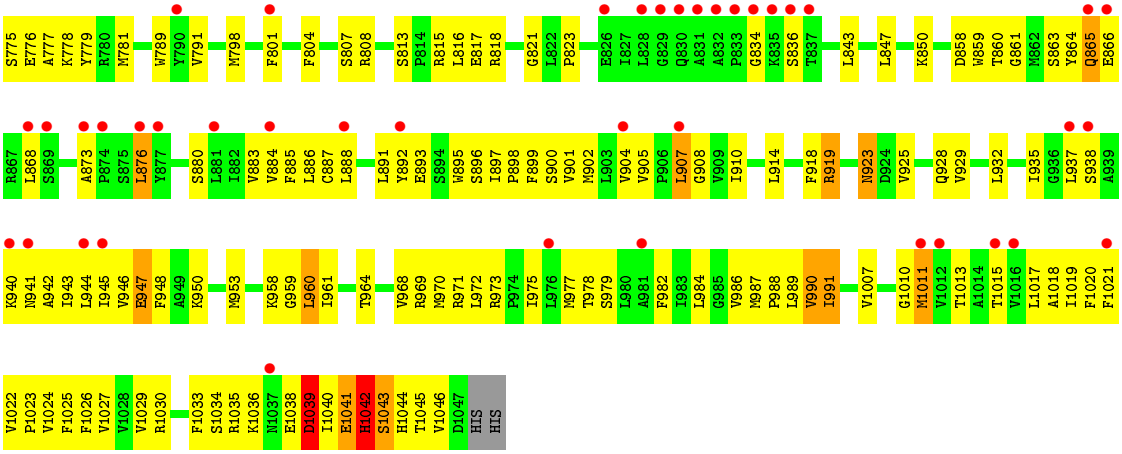




• Molecule 1: Multidrug efflux pump subunit AcrB

Chain F:




S775 E776 A777 K778 Y779 R780 M781 W789 Y790 V791 M798 F801 F804 S807 R808 S813 P814 R815 L816 E817 R818 G821 L822 P823 E826 I827 L828 G829 Q830 A831 A832 P833 G834 K835 S836 T837 L843 L847 K850 D858 W859 T860 G861 M862 S863 Y864 Q865 E866
R867 L868 S869 A873 P874 S875 L876 Y877 S880 L881 I882 V883 V884 F885 L886 C887 L888 L891 Y892 E893 S894 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 V905 P906 L907 G908 V909 I910 L914 F918 R919 N923 D924 V925 Q928 V929 L932 I935 G936 L937 S938 A939
K940 N941 A942 I943 L944 I945 V946 E947 F948 A949 K950 M953 K958 G959 L960 I961 T964 V968 R969 M970 R971 L972 R973 P974 I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 M987 P988 L989 V990 I991 V1007 G1010 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021
V1022 P1023 V1024 F1025 F1026 V1027 V1028 V1029 R1030 F1033 S1034 R1035 K1036 H1037 E1038 D1039 I1040 E1041 H1042 S1043 H1044 T1045 V1046 D1047 HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	152.28Å 157.49Å 219.16Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	19.98 – 3.16 109.45 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-3.16) 97.7 (109.45-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.270 , 0.335 0.280 , 0.343	Depositor DCC
R_{free} test set	8594 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	95.0	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 63.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.076 for -k,-h,-l 0.095 for k,h,-l 0.089 for h,-k,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	47736	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.23 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.6624e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] 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

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

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	0.61	1/8056 (0.0%)	0.83	5/10940 (0.0%)
1	B	0.63	1/8089 (0.0%)	0.86	6/10986 (0.1%)
1	C	0.63	0/8074	0.89	16/10965 (0.1%)
1	D	0.56	2/8056 (0.0%)	0.82	8/10940 (0.1%)
1	E	0.57	2/8056 (0.0%)	0.83	9/10940 (0.1%)
1	F	0.58	0/8089	0.85	7/10986 (0.1%)
All	All	0.60	6/48420 (0.0%)	0.85	51/65757 (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	C	0	1
1	D	0	2
1	F	0	2
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	TRP	CB-CG	7.82	1.64	1.50
1	E	515	TRP	CB-CG	6.85	1.62	1.50
1	D	515	TRP	CB-CG	6.71	1.62	1.50
1	B	515	TRP	CB-CG	6.47	1.61	1.50
1	E	493	CYS	CB-SG	-6.06	1.72	1.82
1	D	887	CYS	CB-SG	-5.98	1.72	1.81

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	529	ASP	CB-CG-OD1	9.33	126.69	118.30
1	E	914	LEU	CA-CB-CG	7.93	133.55	115.30
1	A	972	LEU	CA-CB-CG	7.92	133.50	115.30
1	E	529	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	357	LEU	CA-CB-CG	7.55	132.67	115.30
1	D	914	LEU	CA-CB-CG	7.17	131.80	115.30
1	B	350	LEU	CA-CB-CG	-7.07	99.04	115.30
1	C	529	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	483	LEU	CA-CB-CG	7.05	131.51	115.30
1	C	383	LEU	CA-CB-CG	6.78	130.90	115.30
1	E	357	LEU	CA-CB-CG	6.60	130.49	115.30
1	E	843	LEU	CA-CB-CG	6.46	130.17	115.30
1	C	1033	PHE	C-N-CA	6.43	137.77	121.70
1	A	937	LEU	CA-CB-CG	-6.41	100.55	115.30
1	E	293	LEU	CA-CB-CG	6.23	129.62	115.30
1	D	944	LEU	CA-CB-CG	-6.16	101.13	115.30
1	F	1041	GLU	C-N-CA	6.13	137.03	121.70
1	E	250	LEU	CA-CB-CG	6.09	129.31	115.30
1	C	971	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	1034	SER	C-N-CA	5.72	136.00	121.70
1	C	366	LEU	CA-CB-CG	5.69	128.39	115.30
1	C	937	LEU	CA-CB-CG	-5.59	102.43	115.30
1	F	691	GLY	N-CA-C	5.59	127.07	113.10
1	C	30	LEU	CA-CB-CG	5.58	128.12	115.30
1	B	1039	ASP	N-CA-C	5.55	125.98	111.00
1	C	113	LEU	CA-CB-CG	5.51	127.98	115.30
1	C	1041	GLU	N-CA-C	-5.38	96.46	111.00
1	C	529	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	21	LEU	CA-CB-CG	5.35	127.61	115.30
1	E	511	GLY	N-CA-C	5.34	126.45	113.10
1	E	28	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	300	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	1041	GLU	C-N-CA	5.27	134.88	121.70
1	F	834	GLY	N-CA-C	-5.27	99.92	113.10
1	B	519	MET	CB-CG-SD	5.27	128.20	112.40
1	D	21	LEU	CA-CB-CG	-5.26	103.20	115.30
1	A	534	ILE	CG1-CB-CG2	-5.22	99.91	111.40
1	C	1041	GLU	CA-C-N	5.22	128.68	117.20
1	F	49	TYR	CA-CB-CG	5.21	123.31	113.40
1	E	1041	GLU	C-N-CA	5.20	134.69	121.70
1	C	1033	PHE	CA-C-N	5.19	128.62	117.20
1	D	673	GLU	N-CA-C	5.19	125.00	111.00
1	D	511	GLY	N-CA-C	5.18	126.06	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	529	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	240	LEU	CA-CB-CG	5.16	127.16	115.30
1	C	8	ARG	N-CA-C	-5.15	97.09	111.00
1	F	919	ARG	N-CA-C	-5.11	97.19	111.00
1	D	534	ILE	CG1-CB-CG2	-5.09	100.21	111.40
1	A	35	TYR	C-N-CD	5.08	139.06	128.40
1	C	980	LEU	CA-CB-CG	-5.08	103.62	115.30
1	D	519	MET	CB-CG-SD	5.01	127.43	112.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	6	ILE	Peptide
1	D	1034	SER	Peptide
1	D	992	SER	Peptide
1	F	1036	LYS	Peptide
1	F	1039	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7907	0	8050	393	0
1	B	7939	0	8077	355	0
1	C	7924	0	8064	396	0
1	D	7907	0	8050	369	0
1	E	7907	0	8050	414	1
1	F	7939	0	8077	397	1
2	A	35	0	46	4	0
2	B	35	0	46	3	0
2	C	35	0	46	4	0
2	D	35	0	46	1	0
2	E	35	0	46	4	0
2	F	35	0	46	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
All	All	47736	0	48644	2245	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (2245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.39	0.99
1:A:957:GLY:HA2	1:A:1042:HIS:HB2	1.41	0.99
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.46	0.98
1:D:536:ARG:NH2	2:D:1101:LMT:O3B	1.97	0.97
1:F:578:LEU:HG	1:F:587:THR:HG22	1.46	0.95
1:F:135:SER:HB3	1:F:673:GLU:HB3	1.49	0.94
1:E:196:PHE:O	1:E:252:LYS:NZ	2.04	0.91
1:D:457:ALA:O	1:D:468:ARG:NE	2.03	0.90
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.54	0.90
1:F:35:TYR:HB3	1:F:38:ILE:HD12	1.54	0.89
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.54	0.89
1:E:159:ALA:O	1:E:767:ARG:NH2	2.07	0.88
1:E:354:VAL:HG11	1:E:980:LEU:HB3	1.55	0.88
1:C:1041:GLU:HB3	1:C:1042:HIS:HB2	1.53	0.88
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.54	0.88
1:F:1041:GLU:HB3	1:F:1042:HIS:HB3	1.56	0.88
1:F:452:VAL:HG12	1:F:880:SER:HB3	1.56	0.88
1:D:578:LEU:HD21	1:D:590:VAL:HG21	1.56	0.87
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.56	0.87
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.57	0.87
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.09	0.86
1:B:919:ARG:NH2	1:B:990:VAL:O	2.09	0.86
1:B:399:VAL:O	1:B:402:ILE:HG13	1.76	0.86
1:F:616:GLY:HA2	1:F:626:ILE:HD13	1.57	0.85
1:A:350:LEU:HD22	1:A:984:LEU:HB3	1.58	0.85
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.58	0.85
1:C:38:ILE:HG23	1:C:462:SER:HB2	1.57	0.85
1:A:400:LEU:HD23	1:A:929:VAL:HG12	1.59	0.84
1:E:56:THR:O	1:E:60:THR:OG1	1.95	0.84
1:A:619:GLY:HA3	1:A:815:ARG:HH22	1.40	0.84
1:F:559:LEU:HD22	1:F:560:PRO:HD2	1.60	0.84
1:C:112:GLN:HA	1:C:115:MET:HB2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:992:SER:O	1:B:997:SER:OG	1.96	0.83
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.59	0.83
1:C:940:LYS:HZ1	1:C:978:THR:HG21	1.44	0.83
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.14	0.82
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.59	0.82
1:E:58:GLN:OE1	1:E:818:ARG:NH1	2.12	0.82
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.11	0.82
1:A:38:ILE:HG12	1:A:462:SER:HB2	1.62	0.81
1:E:692:HIS:NE2	1:E:813:SER:OG	2.13	0.81
1:D:170:SER:HB2	1:E:75:LEU:H	1.42	0.81
1:D:219:LEU:HD23	1:E:754:TRP:HZ3	1.45	0.81
1:E:702:LEU:HD11	1:E:847:LEU:HB3	1.60	0.81
1:E:508:GLY:HA3	1:E:518:ARG:HE	1.46	0.81
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.13	0.80
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.63	0.80
1:A:196:PHE:O	1:A:252:LYS:NZ	2.14	0.80
1:C:536:ARG:NH2	2:C:1101:LMT:O3B	2.13	0.80
1:B:186:ILE:HG12	1:B:268:ILE:HG12	1.63	0.80
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.62	0.80
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.62	0.80
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.64	0.80
1:C:3:ASN:N	1:C:3:ASN:OD1	2.13	0.80
1:E:156:ASP:OD1	1:E:769:LYS:NZ	2.15	0.80
1:E:261:LEU:HD12	1:E:263:ARG:HH12	1.46	0.79
1:E:236:ALA:O	1:F:728:LYS:NZ	2.15	0.79
1:A:146:ASP:OD2	1:A:146:ASP:N	2.16	0.79
1:A:248:LYS:HA	1:A:261:LEU:HD13	1.64	0.79
1:B:508:GLY:HA2	1:B:518:ARG:HH21	1.47	0.79
1:F:510:LYS:HA	1:F:518:ARG:HH12	1.45	0.79
1:A:564:LEU:HD13	1:A:671:ILE:HD11	1.64	0.79
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.63	0.79
1:A:56:THR:O	1:A:60:THR:OG1	1.98	0.79
1:B:1013:THR:O	1:B:1017:LEU:HB2	1.83	0.79
1:F:986:VAL:HG21	1:F:1007:VAL:HG11	1.63	0.78
1:C:452:VAL:HG12	1:C:880:SER:HB3	1.65	0.78
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.64	0.78
1:F:509:LYS:O	1:F:518:ARG:NH1	2.16	0.78
1:E:555:LEU:HD22	1:E:913:LEU:HB3	1.64	0.78
1:F:944:LEU:HB3	1:F:971:ARG:HE	1.49	0.78
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.66	0.78
1:C:356:TYR:HA	1:C:365:THR:HG21	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ARG:HH12	1:A:823:PRO:HG3	1.46	0.78
1:A:885:PHE:HD1	1:A:902:MET:HE1	1.48	0.78
1:B:350:LEU:HD22	1:B:984:LEU:HB3	1.64	0.78
1:C:940:LYS:NZ	1:C:978:THR:HG21	1.98	0.78
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.66	0.77
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.66	0.77
1:E:559:LEU:HD22	1:E:560:PRO:HD2	1.65	0.77
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.64	0.77
1:D:58:GLN:O	1:D:63:GLN:HG3	1.85	0.77
1:E:326:PRO:O	1:E:630:SER:OG	2.01	0.77
1:F:536:ARG:NH1	2:F:1101:LMT:O4'	2.16	0.77
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.66	0.77
1:B:602:GLU:OE2	1:B:650:ARG:NH1	2.17	0.77
1:B:957:GLY:O	1:B:1041:GLU:HA	1.83	0.77
1:B:6:ILE:O	1:B:428:LYS:NZ	2.17	0.77
1:D:426:PRO:HD2	1:D:429:GLU:HG3	1.67	0.77
1:A:108:GLN:NE2	1:B:109:ASN:O	2.17	0.77
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.67	0.77
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.66	0.77
1:B:196:PHE:O	1:B:252:LYS:NZ	2.17	0.77
1:F:298:ASN:ND2	1:F:301:ASP:OD2	2.17	0.77
1:B:362:PHE:O	1:B:365:THR:HG22	1.84	0.77
1:C:602:GLU:OE2	1:C:650:ARG:NH1	2.18	0.77
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.68	0.76
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.51	0.76
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.67	0.76
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.68	0.76
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.66	0.75
1:D:507:GLU:O	1:D:509:LYS:N	2.19	0.75
1:D:61:VAL:HG21	1:D:122:VAL:HG21	1.68	0.75
1:E:907:LEU:HG	1:E:1017:LEU:HB3	1.68	0.75
1:F:705:GLU:HA	1:F:708:LYS:HE3	1.68	0.75
1:C:527:TYR:OH	1:C:1019:ILE:O	2.03	0.75
1:A:236:ALA:O	1:B:728:LYS:NZ	2.18	0.74
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.69	0.74
1:C:671:ILE:HD13	1:C:674:LEU:HD12	1.68	0.74
1:F:525:HIS:HA	1:F:528:THR:HG22	1.69	0.74
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.67	0.74
1:E:1026:PHE:O	1:E:1030:ARG:HB2	1.88	0.74
1:F:23:GLY:HA2	1:F:381:ALA:HB2	1.69	0.74
1:B:108:GLN:HE22	1:C:112:GLN:HB3	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:LEU:HD13	1:C:611:ALA:HB1	1.69	0.74
1:F:588:GLN:O	1:F:592:ASN:ND2	2.18	0.74
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.68	0.74
1:F:944:LEU:HB3	1:F:971:ARG:NE	2.03	0.74
1:A:1039:ASP:OD1	1:A:1039:ASP:N	2.20	0.74
1:B:163:LYS:HA	1:B:289:LEU:HD11	1.70	0.74
1:E:637:ARG:HB3	1:E:642:ASN:HB3	1.68	0.74
1:A:712:MET:HB3	1:A:713:LEU:HD22	1.69	0.73
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.69	0.73
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.51	0.73
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.70	0.73
1:D:248:LYS:HA	1:D:261:LEU:HD13	1.70	0.73
1:E:146:ASP:N	1:E:146:ASP:OD2	2.19	0.73
1:A:362:PHE:O	1:A:365:THR:HG22	1.88	0.73
1:E:61:VAL:HA	1:E:118:LEU:HD22	1.70	0.73
1:F:344:LEU:HD22	1:F:402:ILE:HD11	1.69	0.73
1:E:602:GLU:OE2	1:E:650:ARG:NH1	2.21	0.73
1:B:139:VAL:O	1:B:326:PRO:HD2	1.87	0.73
1:B:345:VAL:O	1:B:348:ILE:HG22	1.89	0.73
1:C:1043:SER:OG	1:C:1044:HIS:N	2.21	0.73
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.69	0.73
1:D:144:ASN:HA	1:D:320:GLY:O	1.89	0.73
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.71	0.73
1:E:986:VAL:HG21	1:E:1007:VAL:HG11	1.69	0.73
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.71	0.72
1:E:157:TYR:OH	1:E:316:PHE:O	2.05	0.72
1:F:733:GLN:HE22	1:F:743:ILE:HG21	1.55	0.72
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.70	0.72
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.54	0.72
1:A:26:ALA:O	1:A:30:LEU:HB2	1.90	0.72
1:B:58:GLN:O	1:B:63:GLN:HG3	1.88	0.72
1:E:162:MET:O	1:E:164:ASP:N	2.17	0.72
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.72	0.72
1:B:508:GLY:O	1:B:510:LYS:N	2.22	0.72
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.71	0.72
1:D:455:PRO:HG2	1:D:880:SER:HB2	1.70	0.72
1:E:520:PHE:O	1:E:523:SER:OG	2.05	0.72
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.71	0.72
1:B:236:ALA:O	1:C:728:LYS:NZ	2.19	0.72
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.72	0.72
1:C:240:LEU:HB2	1:C:246:PHE:HE1	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:971:ARG:HH21	1:F:975:ILE:HD11	1.55	0.72
1:F:972:LEU:HA	1:F:975:ILE:HD12	1.71	0.71
1:A:417:GLU:O	1:A:420:MET:N	2.24	0.71
1:B:26:ALA:O	1:B:30:LEU:HB2	1.89	0.71
1:B:871:ASN:N	1:B:871:ASN:OD1	2.23	0.71
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.72	0.71
1:D:375:VAL:HG22	1:D:484:VAL:HG21	1.72	0.71
1:E:353:LEU:O	1:E:355:MET:N	2.21	0.71
1:B:428:LYS:HD3	1:B:494:ALA:HB1	1.70	0.71
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.72	0.71
1:A:25:LEU:HA	1:A:28:LEU:HD12	1.72	0.71
1:D:971:ARG:NH1	1:D:971:ARG:H	1.88	0.71
1:F:1041:GLU:CB	1:F:1042:HIS:HB3	2.21	0.71
1:D:555:LEU:HD22	1:D:913:LEU:HB3	1.73	0.71
1:E:658:ILE:O	1:E:659:LYS:NZ	2.22	0.71
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.55	0.70
1:A:555:LEU:HD22	1:A:913:LEU:HB3	1.74	0.70
1:E:508:GLY:HA3	1:E:518:ARG:NE	2.06	0.70
1:B:1037:ASN:H	1:B:1038:GLU:HB3	1.55	0.70
1:B:527:TYR:O	1:B:531:VAL:HG23	1.90	0.70
1:C:193:LEU:HD13	1:C:200:PRO:HD3	1.73	0.70
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.27	0.70
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.73	0.70
1:C:578:LEU:HD13	1:C:579:PRO:HD2	1.73	0.70
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.73	0.70
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.26	0.70
1:D:18:ILE:HG13	1:E:886:LEU:HD23	1.74	0.70
1:A:186:ILE:HG12	1:A:268:ILE:HG12	1.74	0.70
1:B:60:THR:HG22	1:B:119:PRO:HD3	1.74	0.70
1:C:1033:PHE:H	1:C:1034:SER:CB	2.03	0.70
1:E:45:ILE:HG23	1:E:129:VAL:HG22	1.73	0.70
1:F:211:ASN:O	1:F:760:ASN:ND2	2.24	0.70
1:F:317:PHE:HE2	1:F:323:ILE:HD11	1.57	0.70
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.73	0.70
1:F:668:LEU:H	1:F:668:LEU:HD23	1.56	0.70
1:B:383:LEU:HD13	1:B:388:PHE:HD1	1.57	0.69
1:B:845:GLU:OE2	1:B:867:ARG:NH1	2.24	0.69
1:D:318:PRO:HD2	1:D:321:LEU:HD12	1.71	0.69
1:E:422:GLU:O	1:E:502:LYS:NZ	2.25	0.69
1:E:463:THR:O	1:E:467:TYR:HD1	1.75	0.69
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:971:ARG:NH2	1:F:975:ILE:HD11	2.07	0.69
1:A:519:MET:O	1:A:523:SER:OG	2.09	0.69
1:E:203:VAL:O	1:E:207:ILE:HG13	1.92	0.69
1:A:35:TYR:CE2	1:A:564:LEU:HD21	2.27	0.69
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.73	0.69
1:E:211:ASN:OD1	1:E:760:ASN:ND2	2.26	0.69
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.74	0.69
1:E:971:ARG:O	1:E:975:ILE:HG12	1.91	0.69
1:A:721:LEU:HB3	1:A:814:PRO:HG2	1.75	0.69
1:A:129:VAL:O	1:B:110:LYS:NZ	2.22	0.69
1:F:383:LEU:HD23	1:F:472:ILE:HD13	1.75	0.69
1:F:731:ILE:HD13	1:F:746:ILE:HD11	1.74	0.69
1:E:534:ILE:HG22	2:E:1101:LMT:H1'	1.74	0.68
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.08	0.68
1:C:556:PHE:HD1	1:C:913:LEU:HD21	1.59	0.68
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.73	0.68
1:F:420:MET:HB3	1:F:500:ILE:HB	1.74	0.68
1:F:604:ASN:OD1	1:F:604:ASN:N	2.26	0.68
1:D:298:ASN:HB3	1:D:301:ASP:HB2	1.74	0.68
1:D:564:LEU:HD13	1:D:671:ILE:HD13	1.76	0.68
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.75	0.68
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.75	0.68
1:C:201:VAL:HA	1:C:204:ILE:HD12	1.74	0.68
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.29	0.67
1:A:411:VAL:HG22	1:A:971:ARG:HH22	1.60	0.67
1:D:151:GLN:H	1:D:151:GLN:CD	1.97	0.67
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.76	0.67
1:E:613:ASN:HD22	1:E:614:GLY:N	1.92	0.67
1:A:1034:SER:OG	1:A:1035:ARG:O	2.12	0.67
1:B:225:VAL:HG12	1:C:777:ALA:HB1	1.75	0.67
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.75	0.67
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.76	0.67
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.75	0.67
1:C:298:ASN:ND2	1:C:301:ASP:OD2	2.23	0.67
1:D:967:ALA:O	1:D:971:ARG:NH1	2.27	0.67
1:A:696:THR:HG23	1:A:699:ARG:HH12	1.57	0.67
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.77	0.67
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.76	0.67
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.77	0.67
1:A:203:VAL:O	1:A:207:ILE:HG13	1.95	0.67
1:D:979:SER:OG	1:D:1015:THR:HG21	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.77	0.67
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.75	0.67
1:D:191:ASN:O	1:D:194:ASN:N	2.27	0.67
1:D:393:LEU:HD11	1:D:466:ILE:HD13	1.75	0.67
1:E:445:ILE:HG12	1:E:940:LYS:HE3	1.76	0.67
1:F:146:ASP:O	1:F:148:THR:N	2.27	0.67
1:A:564:LEU:HD23	1:A:565:PRO:HD2	1.75	0.67
1:C:987:MET:O	1:C:990:VAL:N	2.26	0.67
1:E:166:ILE:HD11	1:E:310:LEU:HD13	1.76	0.67
1:E:451:ALA:HB1	1:E:883:VAL:HG13	1.75	0.67
1:E:546:LEU:O	1:E:550:VAL:HG23	1.94	0.67
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.77	0.67
1:C:587:THR:HG21	1:C:622:GLN:O	1.93	0.67
1:D:344:LEU:HD13	1:D:376:LEU:HD13	1.77	0.66
1:D:982:PHE:O	1:D:985:GLY:N	2.28	0.66
1:B:142:VAL:HG21	1:B:162:MET:HE1	1.78	0.66
1:F:34:GLN:HG2	1:F:333:VAL:HG22	1.76	0.66
1:B:469:GLN:O	1:B:473:THR:OG1	2.14	0.66
1:F:139:VAL:HG22	1:F:290:GLY:HA2	1.78	0.66
1:B:249:ILE:HD11	1:B:262:LEU:HD22	1.78	0.66
1:B:396:PHE:O	1:B:400:LEU:HB2	1.95	0.66
1:B:108:GLN:OE1	1:C:112:GLN:HG3	1.96	0.66
1:D:190:PRO:HB3	1:D:789:TRP:CE2	2.30	0.66
1:C:531:VAL:O	1:C:534:ILE:HG13	1.95	0.66
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.78	0.66
1:E:525:HIS:HA	1:E:528:THR:HG22	1.77	0.66
1:A:1030:ARG:HH12	1:A:1033:PHE:HB3	1.61	0.66
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.76	0.66
1:E:653:ARG:O	1:E:656:SER:OG	2.14	0.66
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.78	0.65
1:B:176:GLN:O	1:B:289:LEU:HD23	1.95	0.65
1:D:82:SER:HB2	1:D:816:LEU:HB2	1.77	0.65
1:F:329:THR:O	1:F:333:VAL:HG23	1.96	0.65
1:F:401:ALA:HB2	1:F:474:ILE:HG12	1.78	0.65
1:F:38:ILE:HG23	1:F:462:SER:HB2	1.78	0.65
1:C:11:PHE:O	1:C:11:PHE:HD2	1.78	0.65
1:F:1040:ILE:HA	1:F:1041:GLU:HB2	1.77	0.65
1:F:400:LEU:HB3	1:F:474:ILE:HD11	1.79	0.65
1:A:527:TYR:OH	1:A:1019:ILE:O	2.09	0.65
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.78	0.65
1:B:558:ARG:HA	1:B:558:ARG:HE	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:GLY:O	1:F:27:ILE:HG12	1.96	0.65
1:F:534:ILE:HD11	1:F:1024:VAL:HG22	1.77	0.65
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.27	0.65
1:C:947:GLU:HG3	1:C:948:PHE:HD1	1.61	0.65
1:A:455:PRO:HG2	1:A:880:SER:HB2	1.79	0.65
1:A:979:SER:OG	1:A:1015:THR:HG21	1.96	0.65
1:B:578:LEU:HD21	1:B:590:VAL:HG21	1.78	0.65
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.78	0.65
1:D:584:GLN:HB2	1:D:622:GLN:HG2	1.78	0.65
1:E:641:GLU:HA	1:E:646:ALA:HB3	1.80	0.65
1:F:58:GLN:HA	1:F:62:THR:HB	1.79	0.65
1:E:120:GLN:OE1	1:E:123:GLN:NE2	2.30	0.64
1:C:146:ASP:O	1:C:148:THR:N	2.30	0.64
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.79	0.64
1:B:901:VAL:HG12	1:B:946:VAL:HG21	1.78	0.64
1:C:66:GLU:OE1	1:C:821:GLY:HA2	1.97	0.64
1:D:332:PHE:O	1:D:336:SER:HB3	1.98	0.64
1:B:576:VAL:HG22	1:B:663:VAL:HG22	1.79	0.64
1:E:1013:THR:O	1:E:1017:LEU:HB2	1.97	0.64
1:E:703:LEU:HD11	1:E:718:PRO:HG3	1.78	0.64
1:C:248:LYS:HA	1:C:261:LEU:HD13	1.79	0.64
1:E:733:GLN:NE2	1:E:743:ILE:HG21	2.13	0.64
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.80	0.64
1:C:420:MET:HB3	1:C:500:ILE:HB	1.80	0.64
1:D:699:ARG:HG3	1:D:827:ILE:HD11	1.79	0.64
1:C:23:GLY:HA2	1:C:381:ALA:HB2	1.80	0.64
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.80	0.63
1:C:555:LEU:HD22	1:C:913:LEU:HB3	1.79	0.63
1:D:388:PHE:HE2	1:D:472:ILE:HG21	1.64	0.63
1:F:509:LYS:HG2	1:F:513:PHE:HB2	1.79	0.63
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.81	0.63
1:B:272:GLY:N	1:B:275:TYR:OH	2.30	0.63
1:E:184:MET:HB3	1:E:771:VAL:HG13	1.81	0.63
1:F:291:ILE:HD13	1:F:306:ILE:HD13	1.79	0.63
1:B:171:GLY:O	1:B:294:ALA:N	2.30	0.63
1:F:935:ILE:O	1:F:938:SER:OG	2.16	0.63
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.27	0.63
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.82	0.63
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.32	0.63
1:A:400:LEU:HD21	1:A:930:GLY:HA2	1.78	0.63
1:A:941:ASN:HB3	1:A:975:ILE:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:LEU:HB3	1:C:478:MET:SD	2.39	0.63
1:D:452:VAL:HA	1:D:880:SER:OG	1.99	0.63
1:A:183:ALA:HB2	1:A:273:GLU:HG3	1.81	0.63
1:B:13:TRP:CH2	1:B:492:LEU:HD21	2.33	0.63
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.81	0.63
1:B:459:PHE:CE1	1:B:876:LEU:HD12	2.34	0.63
1:C:746:ILE:HG13	1:C:747:ASN:N	2.14	0.63
1:D:567:GLU:OE1	1:D:996:GLY:HA2	1.99	0.63
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.81	0.62
1:E:144:ASN:ND2	1:E:319:SER:O	2.30	0.62
1:D:591:LEU:HD13	1:D:611:ALA:HB1	1.81	0.62
1:E:949:ALA:HB3	1:E:1026:PHE:HE2	1.64	0.62
1:E:945:ILE:HD12	1:E:971:ARG:HD3	1.81	0.62
1:A:445:ILE:HD13	1:A:940:LYS:HE2	1.82	0.62
1:A:531:VAL:O	1:A:535:LEU:HG	1.99	0.62
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.80	0.62
1:C:535:LEU:HD13	1:C:1027:VAL:HG21	1.81	0.62
1:D:358:PHE:CD1	1:D:977:MET:HG2	2.35	0.62
1:F:187:TRP:HA	1:F:774:MET:O	1.99	0.62
1:F:203:VAL:O	1:F:207:ILE:HG13	1.99	0.62
1:A:449:LEU:HD22	1:A:453:PHE:HE1	1.64	0.62
1:E:471:SER:O	1:E:475:VAL:HG23	2.00	0.62
1:F:120:GLN:HG3	1:F:123:GLN:HB2	1.81	0.62
1:C:536:ARG:HH21	2:C:1101:LMT:H3O1	1.43	0.62
1:D:280:GLU:OE2	1:D:588:GLN:NE2	2.32	0.62
1:D:360:GLN:NE2	1:D:513:PHE:O	2.31	0.62
1:A:246:PHE:HB3	1:A:268:ILE:HD13	1.80	0.62
1:A:359:LEU:O	1:A:361:ASN:N	2.32	0.62
1:A:492:LEU:O	1:A:496:MET:HG2	1.99	0.62
1:C:450:SER:O	1:C:454:VAL:HG23	2.00	0.62
1:D:445:ILE:O	1:D:449:LEU:HB2	1.98	0.62
1:F:1043:SER:OG	1:F:1044:HIS:N	2.32	0.62
1:F:602:GLU:OE2	1:F:650:ARG:NH1	2.32	0.62
1:B:298:ASN:HB3	1:B:301:ASP:HB2	1.81	0.62
1:B:442:LEU:O	1:B:445:ILE:HG13	2.00	0.62
1:C:950:LYS:HG3	1:C:951:ASP:N	2.14	0.62
1:B:531:VAL:HA	1:B:534:ILE:HG23	1.82	0.62
1:C:712:MET:HB3	1:C:713:LEU:HD12	1.82	0.62
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.82	0.62
1:F:698:ALA:O	1:F:701:GLN:HB3	1.99	0.62
1:C:162:MET:O	1:C:164:ASP:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASN:HA	1:C:320:GLY:O	1.99	0.62
1:E:751:GLY:O	1:E:753:ALA:N	2.33	0.62
1:F:733:GLN:NE2	1:F:743:ILE:HG21	2.14	0.62
1:A:216:ALA:HB1	1:A:234:ILE:HG22	1.82	0.61
1:C:380:PHE:HD2	1:C:383:LEU:HD12	1.64	0.61
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.35	0.61
1:F:5:PHE:O	1:F:7:ASP:N	2.25	0.61
1:A:445:ILE:HD13	1:A:940:LYS:CE	2.30	0.61
1:B:219:LEU:HD23	1:C:754:TRP:HZ3	1.64	0.61
1:B:658:ILE:O	1:B:659:LYS:HD2	1.99	0.61
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.80	0.61
1:E:717:ARG:HH21	1:E:828:LEU:HB3	1.63	0.61
1:F:365:THR:O	1:F:368:PRO:HD2	1.98	0.61
1:A:375:VAL:HG11	1:A:481:SER:HB2	1.82	0.61
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.82	0.61
1:C:584:GLN:HB2	1:C:622:GLN:HG2	1.82	0.61
1:C:960:LEU:O	1:C:964:THR:HG23	2.00	0.61
1:F:1039:ASP:HB3	1:F:1040:ILE:HA	1.83	0.61
1:F:919:ARG:NH2	1:F:990:VAL:O	2.33	0.61
1:D:281:PHE:CZ	1:D:608:SER:HB2	2.34	0.61
1:E:441:ALA:O	1:E:445:ILE:HG23	1.99	0.61
1:E:960:LEU:HD13	1:E:1030:ARG:HG2	1.81	0.61
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.81	0.61
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.82	0.61
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.81	0.61
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.31	0.61
1:C:252:LYS:NZ	1:C:254:ASN:OD1	2.33	0.61
1:D:388:PHE:CE2	1:D:472:ILE:HG21	2.34	0.61
1:E:692:HIS:CD2	1:E:813:SER:HG	2.16	0.61
1:A:703:LEU:HD21	1:A:718:PRO:HD3	1.83	0.61
1:C:897:ILE:HD12	1:C:946:VAL:CG1	2.31	0.61
1:C:731:ILE:HD13	1:C:746:ILE:HD11	1.81	0.61
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.82	0.61
1:F:66:GLU:OE2	1:F:80:SER:OG	2.13	0.61
1:F:470:PHE:CD1	1:F:929:VAL:HG11	2.36	0.61
1:C:482:VAL:O	1:C:486:LEU:HG	2.01	0.61
1:F:559:LEU:HD12	1:F:923:ASN:HB2	1.83	0.61
1:B:706:ALA:HB3	1:B:716:VAL:HG11	1.81	0.60
1:C:115:MET:HB3	1:C:116:PRO:HD3	1.81	0.60
1:E:354:VAL:HG12	1:E:354:VAL:O	2.00	0.60
1:A:154:ILE:O	1:A:157:TYR:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:HE21	1:A:63:GLN:HE21	1.49	0.60
1:C:578:LEU:HG	1:C:587:THR:HG22	1.83	0.60
1:C:623:ASN:N	1:C:623:ASN:OD1	2.34	0.60
1:C:668:LEU:H	1:C:668:LEU:HD23	1.65	0.60
1:A:157:TYR:OH	1:A:316:PHE:O	2.20	0.60
1:A:326:PRO:HA	1:A:630:SER:OG	2.01	0.60
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.82	0.60
1:C:817:GLU:HB2	1:C:824:SER:O	2.01	0.60
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.83	0.60
1:F:350:LEU:HD23	1:F:984:LEU:HB3	1.84	0.60
1:A:681:ASP:HB2	1:A:862:MET:HE3	1.82	0.60
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.83	0.60
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.02	0.60
1:D:519:MET:O	1:D:523:SER:OG	2.17	0.60
1:F:248:LYS:HA	1:F:261:LEU:HD13	1.84	0.60
1:B:171:GLY:HA3	1:B:302:THR:OG1	2.00	0.60
1:D:278:ILE:HG13	1:D:613:ASN:HB3	1.83	0.60
1:D:904:VAL:HG21	1:D:942:ALA:HB2	1.83	0.60
1:D:228:GLN:HB3	1:E:583:THR:HG21	1.83	0.60
1:F:527:TYR:O	1:F:531:VAL:HG23	2.02	0.60
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.84	0.60
1:C:559:LEU:HD23	1:C:560:PRO:HD2	1.84	0.60
1:C:563:PHE:CE2	1:C:564:LEU:HD22	2.36	0.60
1:E:140:VAL:N	1:E:289:LEU:O	2.35	0.60
1:F:542:LEU:O	1:F:546:LEU:HG	2.02	0.60
1:C:1040:ILE:HG12	1:C:1041:GLU:N	2.16	0.59
1:C:38:ILE:CG2	1:C:462:SER:HB2	2.29	0.59
1:D:70:ASN:O	1:D:110:LYS:NZ	2.36	0.59
1:E:111:LEU:HD11	1:E:127:VAL:HB	1.84	0.59
1:A:379:THR:HG23	1:A:476:SER:OG	2.02	0.59
1:A:943:ILE:O	1:A:947:GLU:HB3	2.02	0.59
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.84	0.59
1:D:958:LYS:HB3	1:D:963:ALA:HB2	1.83	0.59
1:F:45:ILE:HG23	1:F:129:VAL:HG22	1.82	0.59
1:F:429:GLU:O	1:F:433:LYS:HB2	2.02	0.59
1:A:906:PRO:O	1:A:908:GLY:N	2.35	0.59
1:B:203:VAL:O	1:B:207:ILE:HG13	2.02	0.59
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.33	0.59
1:A:518:ARG:O	1:A:522:LYS:HG3	2.03	0.59
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.84	0.59
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.83	0.59
1:B:682:PHE:O	1:B:827:ILE:N	2.22	0.59
1:E:211:ASN:ND2	1:E:240:LEU:H	2.00	0.59
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.85	0.59
1:F:455:PRO:HG2	1:F:880:SER:HA	1.83	0.59
1:A:960:LEU:O	1:A:964:THR:HG23	2.02	0.59
1:B:369:THR:O	1:B:373:PRO:HG2	2.03	0.59
1:C:959:GLY:HA2	1:C:1041:GLU:O	2.03	0.59
1:E:353:LEU:C	1:E:355:MET:H	2.06	0.59
1:F:462:SER:OG	1:F:865:GLN:HG2	2.03	0.59
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.67	0.59
1:B:354:VAL:O	1:B:358:PHE:HB2	2.03	0.59
1:D:699:ARG:NE	1:D:718:PRO:HB3	2.18	0.59
1:C:634:TRP:N	1:C:634:TRP:CD1	2.71	0.59
1:E:979:SER:HB3	1:E:1015:THR:HG21	1.85	0.59
1:E:562:SER:OG	1:E:563:PHE:N	2.33	0.59
1:F:587:THR:HG21	1:F:622:GLN:O	2.03	0.59
1:A:577:GLN:O	1:A:661:ALA:HB1	2.03	0.59
1:A:696:THR:HG23	1:A:699:ARG:NH1	2.18	0.59
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.84	0.59
1:C:443:VAL:O	1:C:447:MET:HB3	2.02	0.59
1:A:394:THR:HG23	1:A:469:GLN:HB3	1.84	0.58
1:B:162:MET:O	1:B:164:ASP:N	2.36	0.58
1:B:213:GLN:HE22	1:C:52:ALA:HA	1.68	0.58
1:C:518:ARG:O	1:C:522:LYS:HG3	2.02	0.58
1:C:66:GLU:OE2	1:C:80:SER:OG	2.15	0.58
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.85	0.58
1:B:744:ASN:O	1:B:748:THR:HG23	2.03	0.58
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.34	0.58
1:E:703:LEU:HD21	1:E:718:PRO:HD3	1.85	0.58
1:E:752:ALA:O	1:E:774:MET:HA	2.04	0.58
1:F:982:PHE:HD2	1:F:1011:MET:HG2	1.67	0.58
1:A:904:VAL:HG12	1:A:938:SER:HB2	1.84	0.58
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.03	0.58
1:B:351:VAL:HG22	1:B:981:ALA:HB1	1.85	0.58
1:B:104:GLN:HG2	1:C:109:ASN:ND2	2.18	0.58
1:B:173:GLY:HA2	1:C:71:GLY:HA3	1.85	0.58
1:C:751:GLY:O	1:C:753:ALA:N	2.35	0.58
1:D:751:GLY:O	1:D:753:ALA:N	2.36	0.58
1:E:166:ILE:HG13	1:E:309:GLU:HB3	1.86	0.58
1:E:394:THR:HG23	1:E:469:GLN:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.69	0.58
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.85	0.58
1:F:492:LEU:HA	1:F:495:THR:OG1	2.03	0.58
1:F:551:GLY:O	1:F:555:LEU:HB2	2.03	0.58
1:A:459:PHE:CZ	1:A:876:LEU:HD12	2.39	0.58
1:A:733:GLN:NE2	1:A:743:ILE:HG21	2.18	0.58
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.69	0.58
1:C:371:ALA:O	1:C:375:VAL:HG23	2.04	0.58
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.85	0.58
1:D:696:THR:HG23	1:D:699:ARG:HH12	1.68	0.58
1:B:685:ILE:HD11	1:B:819:TYR:HD2	1.68	0.58
1:E:14:VAL:HG22	1:F:886:LEU:HD12	1.84	0.58
1:E:871:ASN:N	1:E:871:ASN:OD1	2.37	0.58
1:F:351:VAL:HG11	1:F:406:VAL:HG11	1.85	0.58
1:A:906:PRO:O	1:A:909:VAL:N	2.37	0.58
1:F:380:PHE:HA	1:F:383:LEU:HD12	1.85	0.58
1:A:960:LEU:HD23	1:A:1031:ARG:CZ	2.34	0.58
1:A:146:ASP:HB2	1:A:148:THR:HG23	1.85	0.58
1:A:140:VAL:HG11	1:A:310:LEU:HD21	1.86	0.58
1:B:189:ASN:HB3	1:B:192:GLU:HB2	1.86	0.58
1:D:897:ILE:HG12	1:D:1030:ARG:HD2	1.85	0.58
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.84	0.58
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.67	0.58
1:D:230:LEU:HD21	1:E:809:TRP:HH2	1.68	0.58
1:F:1040:ILE:CA	1:F:1041:GLU:HB2	2.33	0.58
1:A:137:LEU:HB2	1:A:293:LEU:HB2	1.85	0.58
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.39	0.58
1:F:164:ASP:O	1:F:168:ARG:NH1	2.36	0.58
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.85	0.58
1:A:400:LEU:CD2	1:A:929:VAL:HG12	2.33	0.57
1:C:1039:ASP:HB3	1:C:1040:ILE:HA	1.85	0.57
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.85	0.57
1:C:414:GLU:OE1	1:C:973:ARG:NH1	2.36	0.57
1:B:167:SER:OG	1:C:70:ASN:ND2	2.37	0.57
1:D:383:LEU:HD22	1:D:388:PHE:HD2	1.69	0.57
1:D:674:LEU:HD23	1:D:675:GLY:N	2.19	0.57
1:D:971:ARG:C	1:D:974:PRO:HD2	2.23	0.57
1:C:578:LEU:CD1	1:C:579:PRO:HD2	2.33	0.57
1:D:420:MET:HB3	1:D:500:ILE:HB	1.85	0.57
1:E:166:ILE:HG23	1:E:306:ILE:HG12	1.87	0.57
1:E:869:SER:O	1:E:869:SER:OG	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.38	0.57
1:F:66:GLU:OE1	1:F:821:GLY:HA2	2.04	0.57
1:F:81:ASN:HD21	1:F:815:ARG:HH22	1.52	0.57
1:A:590:VAL:O	1:A:593:GLU:HB2	2.04	0.57
1:D:448:VAL:HG22	1:D:887:CYS:CB	2.34	0.57
1:E:162:MET:C	1:E:164:ASP:H	2.04	0.57
1:A:13:TRP:O	1:A:17:ILE:HG13	2.04	0.57
1:C:326:PRO:O	1:C:630:SER:HB2	2.04	0.57
1:C:521:GLU:O	1:C:524:THR:HG22	2.03	0.57
1:C:525:HIS:HA	1:C:528:THR:HG22	1.87	0.57
1:D:989:LEU:HB3	1:D:1000:GLN:O	2.04	0.57
1:E:931:LEU:O	1:E:935:ILE:HG13	2.03	0.57
1:F:426:PRO:HD2	1:F:429:GLU:HG2	1.85	0.57
1:A:165:ALA:HB3	1:A:313:MET:HE1	1.85	0.57
1:A:832:ALA:O	1:A:835:LYS:HB2	2.05	0.57
1:A:947:GLU:HG3	1:A:948:PHE:HD1	1.69	0.57
1:D:154:ILE:O	1:D:157:TYR:N	2.37	0.57
1:D:52:ALA:HB1	1:D:56:THR:HB	1.86	0.57
1:D:728:LYS:HG2	1:D:808:ARG:NH1	2.19	0.57
1:F:612:VAL:HB	1:F:626:ILE:HG22	1.85	0.57
1:E:535:LEU:O	1:E:537:SER:N	2.38	0.57
1:A:465:ALA:O	1:A:469:GLN:HG2	2.04	0.57
1:A:971:ARG:C	1:A:974:PRO:HD2	2.25	0.57
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.86	0.57
1:E:359:LEU:O	1:E:361:ASN:N	2.37	0.57
1:E:911:GLY:HA3	1:E:1013:THR:OG1	2.05	0.57
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.87	0.57
1:F:744:ASN:O	1:F:748:THR:HG23	2.04	0.57
1:A:254:ASN:HB2	1:A:258:SER:O	2.05	0.57
1:A:515:TRP:O	1:A:519:MET:HG3	2.05	0.57
1:A:744:ASN:O	1:A:748:THR:HG23	2.04	0.57
1:C:418:ARG:O	1:C:422:GLU:HB2	2.05	0.57
1:E:987:MET:O	1:E:990:VAL:N	2.35	0.57
1:A:344:LEU:HD11	1:A:398:MET:HB3	1.85	0.57
1:A:414:GLU:HG3	1:A:977:MET:HE1	1.87	0.57
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.04	0.57
1:D:344:LEU:CD2	1:D:402:ILE:HD11	2.34	0.57
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.86	0.57
1:E:634:TRP:N	1:E:634:TRP:CD1	2.71	0.57
1:E:699:ARG:NH2	1:E:722:GLU:OE2	2.38	0.57
1:D:781:MET:HE2	1:F:225:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:PHE:O	1:A:8:ARG:HD2	2.04	0.56
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.87	0.56
1:A:411:VAL:HG22	1:A:971:ARG:NH2	2.20	0.56
1:B:540:ARG:O	1:B:543:VAL:HB	2.05	0.56
1:C:6:ILE:CG2	1:C:12:ALA:HB2	2.35	0.56
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.87	0.56
1:E:841:MET:HE1	1:E:867:ARG:HB2	1.87	0.56
1:F:694:LYS:H	1:F:694:LYS:HD2	1.70	0.56
1:B:535:LEU:HD13	1:B:1027:VAL:HG21	1.86	0.56
1:B:181:GLN:NE2	1:B:769:LYS:HG2	2.19	0.56
1:B:686:ASP:HB2	1:B:695:LEU:HD23	1.88	0.56
1:D:350:LEU:HD13	1:D:984:LEU:O	2.05	0.56
1:E:399:VAL:O	1:E:402:ILE:HG13	2.05	0.56
1:F:336:SER:O	1:F:340:VAL:HG23	2.04	0.56
1:A:69:MET:SD	1:A:72:ILE:HD11	2.45	0.56
1:D:485:ALA:O	1:D:490:PRO:HD3	2.04	0.56
1:D:527:TYR:O	1:D:531:VAL:HG23	2.05	0.56
1:E:355:MET:SD	1:E:365:THR:HA	2.44	0.56
1:F:1039:ASP:OD2	1:F:1041:GLU:HG3	2.05	0.56
1:F:713:LEU:HD11	1:F:843:LEU:HD12	1.87	0.56
1:A:947:GLU:HG3	1:A:948:PHE:N	2.19	0.56
1:B:400:LEU:HG	1:B:929:VAL:HG12	1.87	0.56
1:D:350:LEU:HD22	1:D:984:LEU:HB3	1.88	0.56
1:E:542:LEU:O	1:E:546:LEU:HG	2.05	0.56
1:B:713:LEU:HD11	1:B:843:LEU:HD12	1.86	0.56
1:C:958:LYS:HB3	1:C:963:ALA:HB2	1.88	0.56
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.05	0.56
1:F:420:MET:HG2	1:F:425:LEU:O	2.06	0.56
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.87	0.56
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.40	0.56
1:A:395:MET:O	1:A:398:MET:HB2	2.06	0.56
1:A:564:LEU:HD22	1:A:671:ILE:HG13	1.87	0.56
1:B:194:ASN:HA	1:B:798:MET:HE1	1.88	0.56
1:D:184:MET:HB3	1:D:771:VAL:HG13	1.87	0.56
1:D:932:LEU:HD23	1:D:935:ILE:HD12	1.87	0.56
1:F:137:LEU:HB2	1:F:293:LEU:HB2	1.87	0.56
1:F:156:ASP:OD1	1:F:765:ARG:NH2	2.38	0.56
1:F:414:GLU:OE1	1:F:973:ARG:HD3	2.06	0.56
1:F:455:PRO:HG3	1:F:883:VAL:HG21	1.87	0.56
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.86	0.56
1:A:512:PHE:HB3	1:A:513:PHE:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:TYR:HE1	1:C:362:PHE:HA	1.70	0.56
1:C:979:SER:HB3	1:C:1015:THR:HG21	1.87	0.56
1:D:391:ASN:O	1:D:395:MET:HG2	2.05	0.56
1:D:393:LEU:HD13	1:D:466:ILE:HA	1.88	0.56
1:D:507:GLU:C	1:D:509:LYS:H	2.09	0.56
1:F:99:ASP:O	1:F:102:ILE:HB	2.05	0.56
1:A:332:PHE:O	1:A:336:SER:HB3	2.05	0.56
1:A:549:VAL:O	1:A:552:MET:HB3	2.04	0.56
1:A:623:ASN:OD1	1:A:623:ASN:N	2.36	0.56
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.88	0.56
1:E:347:ALA:HB1	1:E:402:ILE:HG21	1.88	0.56
1:E:367:ILE:HG12	1:E:496:MET:SD	2.45	0.56
1:A:751:GLY:O	1:A:753:ALA:N	2.39	0.56
1:B:652:THR:CG2	1:B:665:ALA:H	2.19	0.56
1:C:968:VAL:HA	1:C:971:ARG:HH12	1.71	0.56
1:C:40:PRO:HD2	1:C:674:LEU:HD11	1.88	0.56
1:C:6:ILE:HG21	1:C:12:ALA:HB2	1.87	0.56
1:D:955:LYS:O	1:D:956:GLU:HG2	2.06	0.56
1:E:459:PHE:CB	1:E:464:GLY:HA2	2.36	0.56
1:E:589:LYS:HA	1:E:592:ASN:HD22	1.70	0.56
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.71	0.56
1:E:699:ARG:O	1:E:703:LEU:HB2	2.05	0.56
1:F:743:ILE:O	1:F:746:ILE:HG13	2.06	0.56
1:D:251:LEU:HD11	1:D:265:VAL:HG21	1.88	0.56
1:D:66:GLU:OE2	1:D:80:SER:OG	2.14	0.56
1:D:643:LYS:NZ	1:D:993:THR:HG23	2.21	0.56
1:E:42:ALA:HB3	1:E:132:SER:HB3	1.87	0.56
1:E:524:THR:O	1:E:527:TYR:HB3	2.06	0.56
1:F:409:ALA:O	1:F:413:VAL:HG23	2.06	0.56
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.41	0.55
1:B:399:VAL:HG13	1:B:402:ILE:HD11	1.88	0.55
1:B:456:MET:HG3	1:B:471:SER:OG	2.06	0.55
1:C:947:GLU:HG3	1:C:948:PHE:CD1	2.41	0.55
1:D:699:ARG:HE	1:D:703:LEU:HD11	1.70	0.55
1:E:751:GLY:O	1:E:754:TRP:N	2.39	0.55
1:F:671:ILE:HG21	1:F:674:LEU:HB2	1.87	0.55
1:F:350:LEU:HD23	1:F:984:LEU:HD22	1.88	0.55
1:C:187:TRP:HA	1:C:774:MET:O	2.05	0.55
1:D:38:ILE:HG23	1:D:462:SER:OG	2.06	0.55
1:A:220:GLY:HA2	1:B:781:MET:HE3	1.86	0.55
1:A:736:ALA:HB1	1:A:741:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:O	1:C:112:GLN:HG2	2.06	0.55
1:C:121:GLU:O	1:C:124:GLN:HG2	2.06	0.55
1:D:185:ARG:NE	1:D:272:GLY:O	2.39	0.55
1:D:366:LEU:HA	1:D:369:THR:HB	1.87	0.55
1:B:1011:MET:O	1:B:1015:THR:HG23	2.05	0.55
1:B:861:GLY:O	1:B:864:TYR:HB3	2.07	0.55
1:F:359:LEU:O	1:F:361:ASN:N	2.39	0.55
1:A:166:ILE:HD12	1:A:306:ILE:HG12	1.87	0.55
1:C:775:SER:HB2	1:C:789:TRP:CZ2	2.42	0.55
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.72	0.55
1:C:441:ALA:HB2	1:C:948:PHE:HE1	1.72	0.55
1:D:456:MET:HG3	1:D:471:SER:HB2	1.89	0.55
1:E:534:ILE:CG2	2:E:1101:LMT:H1'	2.36	0.55
1:E:668:LEU:HD23	1:E:668:LEU:H	1.71	0.55
1:E:692:HIS:CE1	1:E:813:SER:HG	2.15	0.55
1:F:135:SER:HB3	1:F:673:GLU:CB	2.31	0.55
1:C:363:ARG:HB3	1:C:363:ARG:HH11	1.71	0.55
1:C:355:MET:SD	1:C:368:PRO:HB2	2.46	0.55
1:C:654:ALA:O	1:C:658:ILE:HG12	2.07	0.55
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.71	0.55
1:D:449:LEU:HB3	1:D:478:MET:SD	2.47	0.55
1:F:703:LEU:HD11	1:F:718:PRO:HD3	1.87	0.55
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.42	0.55
1:B:377:LEU:O	1:B:380:PHE:HB2	2.06	0.55
1:C:375:VAL:HA	1:C:480:LEU:HD13	1.89	0.55
1:C:568:ASP:O	1:C:634:TRP:HZ3	1.89	0.55
1:C:758:TYR:HB2	1:C:772:TYR:CZ	2.41	0.55
1:D:75:LEU:HD11	1:D:92:LEU:HD23	1.88	0.55
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.89	0.55
1:B:375:VAL:O	1:B:379:THR:OG1	2.23	0.55
1:E:775:SER:HB2	1:E:789:TRP:CZ2	2.42	0.55
1:A:453:PHE:O	1:A:471:SER:OG	2.13	0.55
1:C:279:ALA:HB3	1:C:286:ALA:O	2.07	0.55
1:C:464:GLY:O	1:C:468:ARG:HB2	2.06	0.55
1:C:590:VAL:HA	1:C:593:GLU:OE1	2.07	0.55
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.88	0.55
1:D:4:PHE:HB2	1:D:5:PHE:CD1	2.42	0.55
1:D:668:LEU:H	1:D:668:LEU:HD23	1.70	0.55
1:A:318:PRO:HD2	1:A:321:LEU:HD12	1.89	0.55
1:B:456:MET:O	1:B:467:TYR:HB3	2.07	0.55
1:D:480:LEU:O	1:D:484:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:987:MET:HB3	1:D:988:PRO:HD3	1.89	0.55
1:E:254:ASN:HB2	1:E:258:SER:O	2.06	0.55
1:A:136:PHE:HE2	1:A:290:GLY:HA3	1.72	0.54
1:A:144:ASN:OD1	1:A:148:THR:OG1	2.25	0.54
1:A:244:GLU:O	1:A:247:GLY:N	2.36	0.54
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.88	0.54
1:A:521:GLU:O	1:A:524:THR:HG22	2.07	0.54
1:A:327:TYR:HA	1:A:571:VAL:HG11	1.89	0.54
1:B:616:GLY:HA3	1:B:624:THR:HB	1.87	0.54
1:E:140:VAL:O	1:E:289:LEU:N	2.39	0.54
1:E:669:PRO:HB3	1:E:674:LEU:HD12	1.89	0.54
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.88	0.54
1:F:623:ASN:OD1	1:F:623:ASN:N	2.40	0.54
1:B:1037:ASN:N	1:B:1038:GLU:HB3	2.23	0.54
1:D:169:THR:HG21	1:D:306:ILE:HG13	1.90	0.54
1:D:647:ILE:HG12	1:D:650:ARG:HH12	1.72	0.54
1:E:376:LEU:O	1:E:379:THR:N	2.39	0.54
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.90	0.54
1:B:317:PHE:CE2	1:B:323:ILE:HD11	2.43	0.54
1:E:139:VAL:O	1:E:326:PRO:HD2	2.06	0.54
1:E:459:PHE:HB2	1:E:464:GLY:HA2	1.89	0.54
1:E:950:LYS:HA	1:E:953:MET:HE3	1.89	0.54
1:F:145:THR:HA	1:F:284:GLN:HE22	1.73	0.54
1:A:531:VAL:O	1:A:534:ILE:HG13	2.07	0.54
1:B:685:ILE:HD11	1:B:819:TYR:CD2	2.41	0.54
1:D:394:THR:HG22	1:D:473:THR:OG1	2.07	0.54
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.88	0.54
1:F:940:LYS:NZ	1:F:978:THR:HG21	2.23	0.54
1:B:545:TYR:CE2	1:B:1025:PHE:HZ	2.26	0.54
1:E:104:GLN:HB2	1:E:131:LYS:HD2	1.90	0.54
1:E:181:GLN:HG2	1:E:182:TYR:N	2.23	0.54
1:E:201:VAL:HG21	1:E:745:ASP:HB3	1.90	0.54
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.90	0.54
1:F:184:MET:HB3	1:F:771:VAL:HG13	1.88	0.54
1:C:412:VAL:HG22	1:C:438:ILE:HD12	1.89	0.54
1:C:504:ASP:OD1	1:C:506:GLY:N	2.35	0.54
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.41	0.54
1:D:1017:LEU:O	1:D:1021:PHE:HB2	2.08	0.54
1:F:139:VAL:O	1:F:326:PRO:HD2	2.08	0.54
1:D:728:LYS:HA	1:F:235:ILE:HB	1.89	0.54
1:A:34:GLN:HA	1:A:333:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:MET:HE1	1:C:225:VAL:H	1.72	0.54
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.90	0.54
1:B:294:ALA:O	1:B:296:GLY:N	2.40	0.54
1:B:600:THR:O	1:B:603:LYS:HB2	2.08	0.54
1:B:66:GLU:OE2	1:B:818:ARG:HD3	2.08	0.54
1:C:668:LEU:HB2	1:C:669:PRO:HD2	1.90	0.54
1:C:187:TRP:HB3	1:C:776:GLU:HG2	1.90	0.54
1:A:641:GLU:HB2	1:A:650:ARG:HH22	1.72	0.54
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.89	0.54
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.89	0.54
1:C:598:TYR:HB3	1:C:606:VAL:HG21	1.88	0.54
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.43	0.54
1:C:61:VAL:HG11	1:C:88:VAL:HG11	1.89	0.54
1:C:971:ARG:HH11	1:C:971:ARG:HB3	1.72	0.54
1:E:213:GLN:HA	1:E:237:GLN:O	2.08	0.54
1:E:179:GLY:HA2	1:E:277:ILE:HD11	1.90	0.54
1:E:776:GLU:HB3	1:E:779:TYR:CD1	2.42	0.54
1:F:249:ILE:HB	1:F:262:LEU:HB2	1.90	0.54
1:B:530:SER:OG	2:B:1101:LMT:H12	2.07	0.54
1:C:393:LEU:HD13	1:C:466:ILE:HA	1.88	0.54
1:C:669:PRO:HD3	1:C:677:ALA:C	2.28	0.54
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.42	0.54
1:E:165:ALA:HB3	1:E:313:MET:CE	2.38	0.54
1:A:401:ALA:O	1:A:405:LEU:HG	2.08	0.54
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.37	0.54
1:B:553:ALA:O	1:B:557:VAL:HG23	2.08	0.54
1:B:596:HIS:O	1:B:600:THR:OG1	2.18	0.54
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.43	0.54
1:E:121:GLU:O	1:E:125:GLN:HB2	2.08	0.54
1:E:351:VAL:HG22	1:E:981:ALA:HB1	1.90	0.54
1:F:428:LYS:O	1:F:432:ARG:HG3	2.08	0.54
1:A:434:SER:O	1:A:438:ILE:HG12	2.08	0.53
1:B:448:VAL:O	1:B:452:VAL:HG13	2.08	0.53
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.37	0.53
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.90	0.53
1:D:889:ALA:HA	1:D:894:SER:O	2.09	0.53
1:E:1041:GLU:HB3	1:E:1042:HIS:CB	2.39	0.53
1:F:145:THR:HA	1:F:284:GLN:NE2	2.22	0.53
1:B:174:ASP:HB3	1:B:292:LYS:HD2	1.90	0.53
1:C:587:THR:HA	1:C:590:VAL:HG23	1.91	0.53
1:D:225:VAL:O	1:D:228:GLN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:LEU:O	1:D:361:ASN:N	2.41	0.53
1:E:165:ALA:HB3	1:E:313:MET:HE3	1.90	0.53
1:F:527:TYR:OH	1:F:1019:ILE:O	2.21	0.53
1:F:960:LEU:HD21	1:F:1027:VAL:HA	1.91	0.53
1:B:239:ARG:NH1	1:B:761:ASP:HB3	2.23	0.53
1:D:1038:GLU:OE1	1:D:1038:GLU:HA	2.09	0.53
1:D:459:PHE:O	1:D:468:ARG:NH2	2.41	0.53
1:E:7:ASP:OD2	1:E:432:ARG:NH2	2.41	0.53
1:F:355:MET:HB3	1:F:365:THR:HG23	1.90	0.53
1:A:225:VAL:HG22	1:B:781:MET:HE2	1.91	0.53
1:A:888:LEU:HD22	1:A:892:TYR:CE2	2.43	0.53
1:D:885:PHE:CE1	1:D:898:PRO:HB2	2.43	0.53
1:E:669:PRO:CB	1:E:674:LEU:HD12	2.38	0.53
1:F:368:PRO:O	1:F:371:ALA:HB3	2.08	0.53
1:A:186:ILE:HD13	1:A:262:LEU:HD21	1.91	0.53
1:B:398:MET:HG3	1:B:473:THR:HG22	1.91	0.53
1:B:652:THR:HG22	1:B:665:ALA:H	1.73	0.53
1:D:414:GLU:HG3	1:D:974:PRO:HG3	1.90	0.53
1:E:158:VAL:HG13	1:E:162:MET:HB2	1.91	0.53
1:E:559:LEU:HD12	1:E:923:ASN:HB2	1.90	0.53
1:F:187:TRP:CB	1:F:776:GLU:HG2	2.38	0.53
1:A:200:PRO:HA	1:A:203:VAL:HG23	1.91	0.53
1:B:307:ARG:HG2	1:B:325:TYR:OH	2.08	0.53
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.43	0.53
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.43	0.53
1:E:1041:GLU:HB3	1:E:1042:HIS:HB3	1.90	0.53
1:D:234:ILE:HD11	1:E:754:TRP:CE3	2.44	0.53
1:F:758:TYR:HB2	1:F:772:TYR:CZ	2.43	0.53
1:C:376:LEU:HD22	1:C:398:MET:SD	2.49	0.53
1:C:594:VAL:HG22	1:C:655:PHE:CE2	2.44	0.53
1:D:726:GLN:CD	1:D:812:GLY:HA3	2.29	0.53
1:E:157:TYR:CE1	1:E:318:PRO:HD3	2.44	0.53
1:E:675:GLY:HA3	1:E:862:MET:SD	2.49	0.53
1:A:598:TYR:HB3	1:A:606:VAL:HG21	1.89	0.53
1:B:34:GLN:HG3	1:B:333:VAL:HG22	1.90	0.53
1:D:335:ILE:O	1:D:339:GLU:HG2	2.09	0.53
1:E:639:GLY:O	1:E:643:LYS:HG3	2.09	0.53
1:F:27:ILE:HA	1:F:30:LEU:HD22	1.91	0.53
1:A:43:VAL:HG23	1:A:94:PHE:HE1	1.74	0.53
1:B:751:GLY:O	1:B:753:ALA:N	2.42	0.53
1:C:3:ASN:O	1:C:6:ILE:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.44	0.53
1:D:556:PHE:HD1	1:D:913:LEU:HD21	1.72	0.53
1:E:1035:ARG:HB3	1:E:1035:ARG:CZ	2.39	0.53
1:E:445:ILE:HD12	1:E:449:LEU:HG	1.91	0.53
1:D:754:TRP:HZ3	1:F:219:LEU:HD23	1.73	0.53
1:F:186:ILE:HD13	1:F:262:LEU:HD21	1.90	0.53
1:F:378:GLY:HA3	1:F:480:LEU:HD11	1.91	0.53
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.91	0.53
1:D:396:PHE:HE1	1:D:999:ALA:HB1	1.74	0.53
1:D:602:GLU:HB3	1:D:606:VAL:HG23	1.90	0.53
1:E:343:THR:HG21	1:E:399:VAL:HG13	1.91	0.53
1:E:190:PRO:HB3	1:E:789:TRP:CE2	2.43	0.53
1:F:152:GLU:HA	1:F:155:SER:HB2	1.90	0.53
1:F:352:PHE:HD2	1:F:353:LEU:HD23	1.73	0.53
1:F:378:GLY:O	1:F:382:VAL:HG23	2.08	0.53
1:F:643:LYS:HE2	1:F:645:GLU:CG	2.39	0.53
1:C:743:ILE:HD12	1:C:743:ILE:H	1.74	0.52
1:E:38:ILE:HG22	1:E:462:SER:HB3	1.92	0.52
1:D:886:LEU:HD13	1:F:18:ILE:HG13	1.91	0.52
1:A:1034:SER:HA	1:A:1035:ARG:HB2	1.91	0.52
1:A:952:LEU:O	1:A:956:GLU:HB2	2.09	0.52
1:B:36:PRO:HD3	1:B:391:ASN:OD1	2.09	0.52
1:B:516:PHE:HA	1:B:519:MET:HB2	1.91	0.52
1:B:594:VAL:HG22	1:B:655:PHE:CE2	2.44	0.52
1:D:412:VAL:HG22	1:D:438:ILE:CD1	2.39	0.52
1:D:442:LEU:O	1:D:445:ILE:HG13	2.10	0.52
1:D:744:ASN:O	1:D:748:THR:HG23	2.09	0.52
1:E:237:GLN:OE1	1:F:747:ASN:ND2	2.39	0.52
1:E:124:GLN:HE21	1:E:758:TYR:HD2	1.56	0.52
1:A:712:MET:HG2	1:A:843:LEU:HG	1.91	0.52
1:A:955:LYS:O	1:A:956:GLU:HG2	2.10	0.52
1:C:396:PHE:O	1:C:400:LEU:HB2	2.08	0.52
1:C:694:LYS:HE3	1:C:694:LYS:H	1.74	0.52
1:C:449:LEU:HD11	1:C:937:LEU:HD21	1.91	0.52
1:C:968:VAL:HA	1:C:971:ARG:NH1	2.24	0.52
1:D:577:GLN:OE1	1:D:624:THR:HG23	2.09	0.52
1:E:111:LEU:O	1:E:115:MET:HG2	2.10	0.52
1:E:415:ASN:O	1:E:419:VAL:HG23	2.09	0.52
1:E:418:ARG:HD2	1:E:422:GLU:OE1	2.09	0.52
1:E:817:GLU:OE1	1:E:825:MET:HA	2.09	0.52
1:C:310:LEU:HD23	1:C:323:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:VAL:O	1:C:417:GLU:HG2	2.10	0.52
1:C:818:ARG:NH2	1:C:821:GLY:O	2.43	0.52
1:D:58:GLN:HA	1:D:62:THR:HB	1.92	0.52
1:E:960:LEU:HD21	1:E:1027:VAL:HA	1.90	0.52
1:A:1020:PHE:CE2	2:A:1101:LMT:H22	2.44	0.52
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.92	0.52
1:C:456:MET:HB3	1:C:876:LEU:HD21	1.90	0.52
1:D:230:LEU:HD21	1:E:809:TRP:CH2	2.43	0.52
1:E:35:TYR:HD2	1:E:393:LEU:HG	1.74	0.52
1:F:764:ASP:OD1	1:F:765:ARG:HG3	2.09	0.52
1:F:947:GLU:HG3	1:F:948:PHE:N	2.24	0.52
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.92	0.52
1:A:781:MET:CE	1:C:225:VAL:H	2.23	0.52
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.44	0.52
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.89	0.52
1:E:987:MET:HB3	1:E:988:PRO:HD3	1.91	0.52
1:F:165:ALA:HB3	1:F:313:MET:HE1	1.91	0.52
1:F:412:VAL:HG22	1:F:438:ILE:HD12	1.92	0.52
1:F:447:MET:SD	1:F:891:LEU:HD22	2.50	0.52
1:B:415:ASN:O	1:B:419:VAL:HG23	2.09	0.52
1:E:949:ALA:HB3	1:E:1026:PHE:CE2	2.45	0.52
1:E:536:ARG:CZ	2:E:1101:LMT:H4B	2.39	0.52
1:F:379:THR:HG23	1:F:476:SER:OG	2.09	0.52
1:A:350:LEU:CD2	1:A:984:LEU:HB3	2.36	0.52
1:C:682:PHE:HE1	1:C:857:TYR:HB2	1.73	0.52
1:C:898:PRO:O	1:C:901:VAL:HG12	2.10	0.52
1:E:371:ALA:O	1:E:375:VAL:HG23	2.09	0.52
1:D:14:VAL:HG13	1:E:886:LEU:HG	1.91	0.52
1:B:149:MET:HB3	1:B:153:ASP:HB3	1.92	0.52
1:B:516:PHE:O	1:B:520:PHE:N	2.43	0.52
1:A:768:VAL:HG12	1:B:63:GLN:NE2	2.24	0.52
1:C:551:GLY:O	1:C:555:LEU:HB2	2.10	0.52
1:C:893:GLU:HG3	1:C:893:GLU:O	2.09	0.52
1:E:783:PRO:HA	1:E:786:ILE:HG12	1.91	0.52
1:F:743:ILE:H	1:F:743:ILE:HD12	1.74	0.52
1:A:375:VAL:HG21	1:A:481:SER:HA	1.92	0.52
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.44	0.52
1:A:743:ILE:HD12	1:A:743:ILE:H	1.75	0.52
1:B:641:GLU:O	1:B:650:ARG:NH2	2.24	0.52
1:D:355:MET:HB3	1:D:365:THR:OG1	2.10	0.52
1:D:540:ARG:O	1:D:543:VAL:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:435:MET:SD	1:E:490:PRO:HB3	2.50	0.52
1:E:588:GLN:O	1:E:592:ASN:ND2	2.42	0.52
1:E:576:VAL:HG22	1:E:663:VAL:HG22	1.91	0.52
1:E:846:GLN:O	1:E:850:LYS:HG2	2.11	0.52
1:E:57:VAL:HG11	1:E:86:GLY:HA2	1.92	0.52
1:E:445:ILE:HB	1:E:940:LYS:HG3	1.92	0.52
1:F:407:ASP:OD1	1:F:978:THR:HG23	2.09	0.52
1:F:491:ALA:O	1:F:495:THR:HG23	2.10	0.52
1:F:63:GLN:OE1	1:F:67:GLN:NE2	2.43	0.52
1:F:925:VAL:HA	1:F:928:GLN:OE1	2.09	0.52
1:A:586:ARG:O	1:A:589:LYS:HB3	2.10	0.51
1:A:817:GLU:HB2	1:A:824:SER:O	2.10	0.51
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.92	0.51
1:D:394:THR:HG23	1:D:469:GLN:HB3	1.92	0.51
1:D:13:TRP:CZ2	1:D:492:LEU:HD21	2.45	0.51
1:D:445:ILE:HG12	1:D:940:LYS:HE3	1.92	0.51
1:E:347:ALA:CB	1:E:402:ILE:HG21	2.40	0.51
1:F:463:THR:HG23	1:F:925:VAL:HG22	1.92	0.51
1:F:531:VAL:O	1:F:535:LEU:HG	2.10	0.51
1:A:508:GLY:O	1:A:511:GLY:N	2.42	0.51
1:A:957:GLY:HA2	1:A:1042:HIS:CB	2.28	0.51
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.91	0.51
1:B:654:ALA:O	1:B:658:ILE:HG12	2.10	0.51
1:D:587:THR:HB	1:D:613:ASN:HD21	1.74	0.51
1:E:691:GLY:N	1:E:694:LYS:HD3	2.25	0.51
1:E:743:ILE:H	1:E:743:ILE:HD12	1.75	0.51
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.45	0.51
1:F:1035:ARG:HB2	1:F:1038:GLU:HB2	1.92	0.51
1:F:456:MET:HE3	1:F:932:LEU:HD12	1.93	0.51
1:F:888:LEU:HD11	1:F:943:ILE:HD11	1.91	0.51
1:A:58:GLN:NE2	1:A:63:GLN:HE21	2.08	0.51
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.91	0.51
1:A:47:ALA:O	1:A:87:THR:HA	2.11	0.51
1:B:356:TYR:C	1:B:358:PHE:H	2.13	0.51
1:D:360:GLN:NE2	1:D:513:PHE:HB3	2.25	0.51
1:F:412:VAL:CG2	1:F:442:LEU:HD11	2.41	0.51
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.44	0.51
1:A:888:LEU:HD22	1:A:892:TYR:HE2	1.75	0.51
1:A:238:THR:HG23	1:B:728:LYS:NZ	2.26	0.51
1:C:742:SER:O	1:C:746:ILE:HG23	2.10	0.51
1:D:219:LEU:HD23	1:E:754:TRP:CZ3	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:TYR:O	1:E:530:SER:HB3	2.10	0.51
1:E:527:TYR:CE2	1:E:972:LEU:HG	2.46	0.51
1:F:192:GLU:HB3	1:F:265:VAL:HA	1.92	0.51
1:F:504:ASP:C	1:F:506:GLY:H	2.12	0.51
1:F:525:HIS:HA	1:F:528:THR:CG2	2.40	0.51
1:A:958:LYS:HB3	1:A:963:ALA:HB2	1.92	0.51
1:B:143:ILE:HG21	1:B:281:PHE:CD2	2.46	0.51
1:B:231:ASN:HD22	1:C:622:GLN:CD	2.13	0.51
1:B:65:ILE:O	1:B:69:MET:HG2	2.11	0.51
1:D:2:PRO:O	1:D:6:ILE:HG23	2.10	0.51
1:D:717:ARG:O	1:D:827:ILE:HG23	2.10	0.51
1:E:457:ALA:HB2	1:E:471:SER:CB	2.40	0.51
1:F:594:VAL:HG22	1:F:655:PHE:CE2	2.45	0.51
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.92	0.51
1:C:736:ALA:HB1	1:C:741:VAL:HG23	1.92	0.51
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.92	0.51
1:F:1034:SER:OG	1:F:1035:ARG:N	2.43	0.51
1:F:162:MET:O	1:F:164:ASP:N	2.43	0.51
1:F:479:ALA:O	1:F:483:LEU:HD23	2.10	0.51
1:F:566:ASP:CG	1:F:678:THR:HG23	2.31	0.51
1:F:945:ILE:HA	1:F:971:ARG:NH1	2.25	0.51
1:F:973:ARG:HG2	1:F:977:MET:HE3	1.91	0.51
1:B:575:MET:HB3	1:B:626:ILE:HG13	1.92	0.51
1:B:715:SER:O	1:B:715:SER:OG	2.29	0.51
1:D:393:LEU:HD12	1:D:469:GLN:HG3	1.92	0.51
1:E:776:GLU:HB3	1:E:779:TYR:CE1	2.44	0.51
1:D:777:ALA:HB1	1:F:225:VAL:HG12	1.91	0.51
1:F:873:ALA:HB2	1:F:928:GLN:NE2	2.25	0.51
1:F:947:GLU:HG3	1:F:948:PHE:HD1	1.75	0.51
1:A:904:VAL:CG1	1:A:938:SER:HB2	2.40	0.51
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.92	0.51
1:D:616:GLY:HA3	1:D:624:THR:HG22	1.93	0.51
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.25	0.51
1:F:376:LEU:O	1:F:379:THR:N	2.44	0.51
1:F:400:LEU:HD11	1:F:1007:VAL:HG21	1.93	0.51
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.92	0.51
1:F:720:GLY:HA3	1:F:817:GLU:OE1	2.11	0.51
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.93	0.51
1:A:355:MET:HB3	1:A:365:THR:OG1	2.10	0.51
1:A:775:SER:HB2	1:A:789:TRP:CZ2	2.46	0.51
1:A:726:GLN:OE1	1:A:812:GLY:HA3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:GLU:O	1:B:502:LYS:NZ	2.44	0.51
1:B:267:LYS:HD3	1:B:776:GLU:OE2	2.11	0.51
1:C:408:ASP:O	1:C:412:VAL:HG23	2.11	0.51
1:C:40:PRO:HG2	1:C:674:LEU:HD21	1.91	0.51
1:D:1026:PHE:CE2	1:D:1030:ARG:HG3	2.46	0.51
1:D:941:ASN:HB3	1:D:975:ILE:HD13	1.93	0.51
1:E:203:VAL:HG12	1:E:207:ILE:HD11	1.93	0.51
1:E:46:SER:OG	1:E:89:GLN:HG2	2.10	0.51
1:B:295:THR:O	1:B:295:THR:OG1	2.25	0.51
1:C:149:MET:HB2	1:C:153:ASP:HB3	1.91	0.51
1:F:27:ILE:HG22	1:F:380:PHE:HB3	1.93	0.51
1:C:576:VAL:HG21	1:C:591:LEU:HD23	1.93	0.50
1:C:751:GLY:O	1:C:754:TRP:N	2.44	0.50
1:C:888:LEU:HD11	1:C:943:ILE:HD11	1.93	0.50
1:D:532:GLY:O	1:D:536:ARG:HG3	2.11	0.50
1:E:167:SER:HB2	1:E:175:VAL:HG11	1.93	0.50
1:E:183:ALA:HB2	1:E:273:GLU:HG3	1.93	0.50
1:F:344:LEU:HA	1:F:399:VAL:HG22	1.93	0.50
1:C:139:VAL:O	1:C:326:PRO:HD2	2.11	0.50
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.94	0.50
1:C:683:GLU:HB3	1:C:685:ILE:HD11	1.94	0.50
1:D:775:SER:HB2	1:D:789:TRP:HZ2	1.76	0.50
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.93	0.50
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.93	0.50
1:A:144:ASN:HD22	1:A:321:LEU:HD23	1.76	0.50
1:A:467:TYR:HE2	1:A:925:VAL:HG13	1.76	0.50
1:B:352:PHE:CD2	1:B:352:PHE:C	2.85	0.50
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.93	0.50
1:B:877:TYR:HA	1:B:880:SER:HB3	1.93	0.50
1:B:966:ASP:O	1:B:970:MET:HG2	2.10	0.50
1:F:182:TYR:O	1:F:769:LYS:HD3	2.11	0.50
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.93	0.50
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.93	0.50
1:A:391:ASN:O	1:A:395:MET:HG2	2.10	0.50
1:B:267:LYS:N	1:B:267:LYS:HD2	2.25	0.50
1:D:401:ALA:O	1:D:405:LEU:HG	2.12	0.50
1:D:892:TYR:CD2	1:D:897:ILE:HG22	2.47	0.50
1:E:102:ILE:O	1:E:106:GLN:HG3	2.11	0.50
1:E:190:PRO:HB3	1:E:789:TRP:CD2	2.46	0.50
1:F:431:THR:HG21	1:F:490:PRO:O	2.12	0.50
1:C:112:GLN:OE1	1:C:115:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:VAL:O	1:C:207:ILE:HG13	2.12	0.50
1:C:744:ASN:O	1:C:748:THR:HG23	2.12	0.50
1:D:634:TRP:CD1	1:D:634:TRP:N	2.80	0.50
1:E:362:PHE:O	1:E:365:THR:HG22	2.11	0.50
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.94	0.50
1:B:412:VAL:HG22	1:B:438:ILE:HD11	1.93	0.50
1:E:16:ALA:HB2	1:E:488:LEU:HD13	1.94	0.50
1:E:298:ASN:HB3	1:E:301:ASP:HB2	1.92	0.50
1:E:339:GLU:HA	1:E:342:LYS:HB2	1.93	0.50
1:F:896:SER:HB3	1:F:1033:PHE:CE1	2.47	0.50
1:F:404:LEU:HB3	1:F:478:MET:SD	2.51	0.50
1:F:987:MET:HB3	1:F:988:PRO:HD3	1.93	0.50
1:A:896:SER:HB3	1:A:1033:PHE:CD1	2.47	0.50
1:A:878:ALA:O	1:A:882:ILE:HG12	2.12	0.50
1:B:531:VAL:O	1:B:534:ILE:HG23	2.12	0.50
1:C:359:LEU:O	1:C:361:ASN:N	2.43	0.50
1:D:191:ASN:O	1:D:193:LEU:N	2.44	0.50
1:E:1016:VAL:HG12	1:E:1016:VAL:O	2.11	0.50
1:F:959:GLY:HA3	1:F:1042:HIS:O	2.12	0.50
1:F:372:VAL:HA	1:F:405:LEU:HD13	1.93	0.50
1:F:5:PHE:CE2	1:F:8:ARG:HD2	2.46	0.50
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.46	0.50
1:D:563:PHE:C	1:D:564:LEU:HD12	2.32	0.50
1:D:563:PHE:O	1:D:564:LEU:HD12	2.11	0.50
1:D:598:TYR:HB3	1:D:606:VAL:HG11	1.93	0.50
1:A:985:GLY:O	1:A:988:PRO:HD2	2.12	0.50
1:C:343:THR:HA	1:C:346:GLU:OE1	2.12	0.50
1:C:597:TYR:CD1	1:C:601:LYS:HD2	2.47	0.50
1:D:907:LEU:HD21	1:D:1021:PHE:CB	2.41	0.50
1:E:163:LYS:O	1:E:163:LYS:HG2	2.12	0.50
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.47	0.50
1:E:668:LEU:HD12	1:E:672:VAL:HG12	1.94	0.50
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.12	0.50
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.12	0.49
1:A:692:HIS:HE2	1:A:723:ASP:CG	2.15	0.49
1:B:383:LEU:HD11	1:B:473:THR:HG23	1.94	0.49
1:C:1020:PHE:CD1	2:C:1101:LMT:H41	2.47	0.49
1:C:730:ASP:CG	1:C:808:ARG:HH21	2.15	0.49
1:D:162:MET:HA	1:D:313:MET:SD	2.52	0.49
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.42	0.49
1:F:194:ASN:OD1	1:F:798:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:SER:OG	1:F:293:LEU:O	2.28	0.49
1:B:478:MET:O	1:B:482:VAL:HG12	2.12	0.49
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.27	0.49
1:C:979:SER:CB	1:C:1015:THR:HG21	2.43	0.49
1:D:362:PHE:O	1:D:365:THR:HG22	2.11	0.49
1:E:3:ASN:HA	1:E:6:ILE:HD12	1.93	0.49
1:E:46:SER:HA	1:E:88:VAL:O	2.12	0.49
1:F:969:ARG:HH11	1:F:970:MET:HB3	1.77	0.49
1:A:17:ILE:CG2	1:B:886:LEU:HD21	2.42	0.49
1:A:452:VAL:HA	1:A:880:SER:OG	2.13	0.49
1:B:151:GLN:OE1	1:B:278:ILE:HA	2.12	0.49
1:B:425:LEU:HD13	1:B:429:GLU:HG3	1.93	0.49
1:B:544:LEU:O	1:B:547:ILE:HB	2.12	0.49
1:B:184:MET:HB3	1:B:771:VAL:HA	1.94	0.49
1:B:185:ARG:HH22	1:B:774:MET:HE3	1.76	0.49
1:E:484:VAL:HG13	1:E:488:LEU:HB3	1.93	0.49
1:E:987:MET:HA	1:E:1008:MET:HE3	1.94	0.49
1:F:139:VAL:HA	1:F:289:LEU:O	2.12	0.49
1:F:435:MET:CE	1:F:490:PRO:HB3	2.43	0.49
1:A:228:GLN:HG3	1:A:229:GLN:N	2.27	0.49
1:B:527:TYR:OH	1:B:1019:ILE:O	2.19	0.49
1:B:155:SER:O	1:B:158:VAL:HB	2.12	0.49
1:B:47:ALA:HB2	1:B:127:VAL:HG13	1.94	0.49
1:C:144:ASN:HB3	1:C:148:THR:HG23	1.95	0.49
1:D:623:ASN:OD1	1:D:623:ASN:N	2.45	0.49
1:D:83:ASP:OD1	1:D:815:ARG:HD3	2.13	0.49
1:E:654:ALA:O	1:E:658:ILE:HG12	2.11	0.49
1:F:344:LEU:CD2	1:F:402:ILE:HD11	2.42	0.49
1:A:1037:ASN:HA	1:A:1038:GLU:O	2.12	0.49
1:A:1040:ILE:HG12	1:A:1041:GLU:H	1.77	0.49
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.95	0.49
1:B:905:VAL:HG13	1:B:935:ILE:HG23	1.94	0.49
1:C:35:TYR:HB3	1:C:38:ILE:HD12	1.94	0.49
1:C:968:VAL:CA	1:C:971:ARG:HH12	2.26	0.49
1:E:343:THR:OG1	1:E:989:LEU:HD21	2.13	0.49
1:F:480:LEU:O	1:F:484:VAL:HG23	2.13	0.49
1:A:348:ILE:HG22	1:A:349:ILE:HD13	1.94	0.49
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.94	0.49
1:C:534:ILE:HD12	1:C:535:LEU:HD23	1.94	0.49
1:D:156:ASP:OD1	1:D:765:ARG:NH2	2.45	0.49
1:D:236:ALA:O	1:E:728:LYS:NZ	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.93	0.49
1:E:42:ALA:O	1:E:132:SER:N	2.27	0.49
1:E:904:VAL:HG12	1:E:938:SER:OG	2.11	0.49
1:B:394:THR:O	1:B:473:THR:HG21	2.12	0.49
1:B:508:GLY:C	1:B:510:LYS:H	2.14	0.49
1:B:668:LEU:HD23	1:B:668:LEU:H	1.77	0.49
1:C:1033:PHE:N	1:C:1034:SER:OG	2.27	0.49
1:F:940:LYS:HZ1	1:F:978:THR:HG21	1.78	0.49
1:A:17:ILE:HG22	1:B:886:LEU:HD21	1.95	0.49
1:A:484:VAL:HG13	1:A:488:LEU:HB3	1.93	0.49
1:B:562:SER:OG	1:B:563:PHE:N	2.46	0.49
1:B:736:ALA:HB1	1:B:741:VAL:HG23	1.94	0.49
1:C:154:ILE:O	1:C:157:TYR:N	2.45	0.49
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.94	0.49
1:C:945:ILE:HG12	1:C:971:ARG:CZ	2.43	0.49
1:D:445:ILE:HD13	1:D:940:LYS:HE3	1.95	0.49
1:E:32:VAL:HA	1:E:390:ILE:O	2.13	0.49
1:E:979:SER:CB	1:E:1015:THR:HG21	2.42	0.49
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.94	0.49
1:A:534:ILE:HG22	1:A:541:TYR:OH	2.13	0.49
1:A:776:GLU:HG2	1:A:777:ALA:H	1.77	0.49
1:C:244:GLU:O	1:C:247:GLY:N	2.46	0.49
1:D:163:LYS:O	1:D:163:LYS:HG2	2.12	0.49
1:D:696:THR:HG23	1:D:699:ARG:NH1	2.28	0.49
1:E:507:GLU:OE1	1:E:518:ARG:HG2	2.13	0.49
1:C:904:VAL:O	1:C:907:LEU:HB2	2.12	0.49
1:D:859:TRP:HE3	1:D:863:SER:HG	1.59	0.49
1:F:163:LYS:O	1:F:163:LYS:HG2	2.13	0.49
1:F:968:VAL:O	1:F:972:LEU:HB2	2.13	0.49
1:B:76:MET:HB2	1:B:93:THR:O	2.13	0.48
1:D:531:VAL:O	1:D:534:ILE:HG13	2.13	0.48
1:D:643:LYS:HZ2	1:D:993:THR:HG23	1.77	0.48
1:F:112:GLN:HA	1:F:115:MET:HB2	1.94	0.48
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.94	0.48
1:D:754:TRP:CZ3	1:F:219:LEU:HD23	2.48	0.48
1:F:459:PHE:CE1	1:F:876:LEU:HG	2.48	0.48
1:F:941:ASN:CG	1:F:975:ILE:HG23	2.34	0.48
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.43	0.48
1:A:76:MET:HB2	1:A:93:THR:O	2.13	0.48
1:B:307:ARG:HG2	1:B:325:TYR:CZ	2.49	0.48
1:B:672:VAL:O	1:B:673:GLU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:THR:HB	1:B:749:THR:HG21	1.95	0.48
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.77	0.48
1:C:885:PHE:HD2	1:C:886:LEU:HD13	1.78	0.48
1:D:445:ILE:CD1	1:D:940:LYS:HE3	2.43	0.48
1:A:393:LEU:CD1	1:A:466:ILE:HA	2.43	0.48
1:A:752:ALA:O	1:A:774:MET:HA	2.13	0.48
1:B:532:GLY:O	1:B:536:ARG:N	2.46	0.48
1:B:758:TYR:HB2	1:B:772:TYR:CZ	2.48	0.48
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.78	0.48
1:E:744:ASN:O	1:E:748:THR:HG23	2.13	0.48
1:E:922:THR:O	1:E:924:ASP:N	2.43	0.48
1:F:358:PHE:O	1:F:973:ARG:NH2	2.45	0.48
1:A:751:GLY:O	1:A:754:TRP:N	2.45	0.48
1:B:383:LEU:HD13	1:B:388:PHE:CD1	2.44	0.48
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.48	0.48
1:C:504:ASP:C	1:C:506:GLY:H	2.17	0.48
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.95	0.48
1:D:445:ILE:CG1	1:D:940:LYS:HE3	2.44	0.48
1:E:982:PHE:CD2	1:E:1011:MET:HG3	2.49	0.48
1:E:261:LEU:HD12	1:E:263:ARG:NH1	2.24	0.48
1:E:776:GLU:HG2	1:E:777:ALA:H	1.78	0.48
1:A:536:ARG:HD2	2:A:1101:LMT:O4'	2.13	0.48
1:B:110:LYS:HD3	1:B:113:LEU:HD12	1.96	0.48
1:B:158:VAL:HA	1:B:162:MET:HE2	1.95	0.48
1:B:24:GLY:O	1:B:27:ILE:HG22	2.14	0.48
1:D:911:GLY:HA3	1:D:1013:THR:OG1	2.13	0.48
1:D:470:PHE:CD2	1:D:929:VAL:HG21	2.48	0.48
1:F:733:GLN:OE1	1:F:743:ILE:HG12	2.14	0.48
1:A:141:GLY:O	1:A:323:ILE:HA	2.14	0.48
1:A:412:VAL:O	1:A:416:VAL:HG23	2.13	0.48
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.95	0.48
1:B:423:GLU:O	1:B:502:LYS:HD2	2.14	0.48
1:B:76:MET:SD	1:B:864:TYR:HE2	2.37	0.48
1:C:58:GLN:HA	1:C:62:THR:HB	1.96	0.48
1:C:197:GLN:HA	1:C:798:MET:SD	2.53	0.48
1:D:279:ALA:HB3	1:D:286:ALA:O	2.14	0.48
1:D:348:ILE:HG22	1:D:349:ILE:HD12	1.94	0.48
1:E:902:MET:O	1:E:905:VAL:HG23	2.14	0.48
1:F:456:MET:HB3	1:F:876:LEU:HD21	1.96	0.48
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.49	0.48
1:A:279:ALA:HB3	1:A:286:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLN:HG3	1:C:82:SER:OG	2.14	0.48
1:D:647:ILE:HG12	1:D:650:ARG:NH1	2.29	0.48
1:E:26:ALA:O	1:E:30:LEU:HB2	2.13	0.48
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.95	0.48
1:A:887:CYS:O	1:A:890:ALA:HB3	2.14	0.48
1:B:11:PHE:O	1:B:11:PHE:HD2	1.97	0.48
1:B:136:PHE:CD2	1:B:290:GLY:HA3	2.49	0.48
1:B:527:TYR:O	1:B:530:SER:HB3	2.14	0.48
1:C:182:TYR:HD2	1:C:765:ARG:NH2	2.12	0.48
1:D:141:GLY:HA3	1:D:324:VAL:HG12	1.95	0.48
1:D:137:LEU:HB2	1:D:293:LEU:HB2	1.96	0.48
1:D:453:PHE:O	1:D:471:SER:OG	2.21	0.48
1:E:527:TYR:O	1:E:531:VAL:HG23	2.14	0.48
1:E:586:ARG:O	1:E:589:LYS:HB3	2.14	0.48
1:A:902:MET:O	1:A:905:VAL:HG23	2.13	0.48
1:B:501:ALA:O	1:B:504:ASP:HB2	2.14	0.48
1:B:208:LYS:HE3	1:B:759:VAL:HG22	1.95	0.48
1:B:985:GLY:O	1:B:988:PRO:HD2	2.14	0.48
1:C:901:VAL:HG23	1:C:942:ALA:CB	2.44	0.48
1:E:210:GLN:O	1:E:237:GLN:NE2	2.44	0.48
1:E:844:MET:HA	1:E:844:MET:CE	2.44	0.48
1:F:351:VAL:O	1:F:355:MET:HE2	2.14	0.48
1:F:941:ASN:HA	1:F:944:LEU:HD12	1.94	0.48
1:A:110:LYS:HA	1:A:110:LYS:HD3	1.59	0.48
1:A:216:ALA:HB1	1:A:234:ILE:CG2	2.44	0.48
1:B:153:ASP:OD2	1:B:182:TYR:OH	2.26	0.48
1:B:888:LEU:HD21	1:B:943:ILE:HD11	1.95	0.48
1:C:375:VAL:HB	1:C:405:LEU:HD22	1.96	0.48
1:D:191:ASN:C	1:D:193:LEU:H	2.17	0.48
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.96	0.48
1:E:504:ASP:C	1:E:506:GLY:H	2.16	0.48
1:F:380:PHE:O	1:F:383:LEU:HB2	2.14	0.48
1:F:452:VAL:O	1:F:455:PRO:HD2	2.14	0.48
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.36	0.47
1:B:845:GLU:HG2	1:B:857:TYR:CE1	2.48	0.47
1:C:1032:ARG:O	1:C:1033:PHE:HD1	1.97	0.47
1:C:479:ALA:O	1:C:482:VAL:HG23	2.14	0.47
1:E:414:GLU:HG3	1:E:974:PRO:HB3	1.96	0.47
1:D:233:SER:O	1:E:726:GLN:HB2	2.14	0.47
1:F:47:ALA:HB1	1:F:122:VAL:HG13	1.96	0.47
1:F:600:THR:C	1:F:602:GLU:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:TYR:HB2	1:A:772:TYR:CZ	2.49	0.47
1:C:960:LEU:HB2	1:C:1040:ILE:HG13	1.95	0.47
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.97	0.47
1:C:649:MET:SD	1:C:653:ARG:NH2	2.87	0.47
1:D:49:TYR:CE1	1:D:60:THR:HG21	2.48	0.47
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.96	0.47
1:F:987:MET:O	1:F:990:VAL:HG23	2.14	0.47
1:C:400:LEU:HD23	1:C:474:ILE:HD11	1.95	0.47
1:C:992:SER:HB3	1:C:997:SER:HB2	1.96	0.47
1:D:542:LEU:O	1:D:546:LEU:HG	2.14	0.47
1:D:644:VAL:HG12	1:D:645:GLU:N	2.30	0.47
1:F:659:LYS:HD3	1:F:659:LYS:HA	1.63	0.47
1:A:420:MET:HB3	1:A:500:ILE:HB	1.96	0.47
1:A:444:GLY:O	1:A:448:VAL:HG23	2.13	0.47
1:A:641:GLU:HB2	1:A:650:ARG:NH2	2.29	0.47
1:A:841:MET:HG2	1:A:859:TRP:CH2	2.49	0.47
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.14	0.47
1:B:600:THR:C	1:B:602:GLU:H	2.17	0.47
1:B:789:TRP:O	1:B:801:PHE:HD2	1.97	0.47
1:B:960:LEU:O	1:B:964:THR:HG23	2.14	0.47
1:C:186:ILE:HG22	1:C:773:VAL:HG23	1.96	0.47
1:C:409:ALA:O	1:C:413:VAL:HG23	2.14	0.47
1:D:586:ARG:O	1:D:590:VAL:HG23	2.14	0.47
1:E:11:PHE:HE2	1:E:15:ILE:HD11	1.78	0.47
1:E:535:LEU:O	1:E:536:ARG:C	2.51	0.47
1:E:597:TYR:OH	1:E:650:ARG:HG3	2.14	0.47
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.44	0.47
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.97	0.47
1:A:276:ASP:HA	1:C:222:THR:HG21	1.96	0.47
1:B:270:LEU:HA	1:B:270:LEU:HD12	1.67	0.47
1:B:521:GLU:HA	1:B:524:THR:HG23	1.97	0.47
1:B:767:ARG:HH11	1:B:767:ARG:HG2	1.79	0.47
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.43	0.47
1:C:447:MET:SD	1:C:891:LEU:HD22	2.54	0.47
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.96	0.47
1:D:355:MET:HG3	1:D:359:LEU:HD12	1.96	0.47
1:E:542:LEU:O	1:E:545:TYR:HB3	2.15	0.47
1:E:961:ILE:HG13	1:E:962:GLU:N	2.28	0.47
1:F:727:PHE:CZ	1:F:807:SER:HB2	2.49	0.47
1:A:567:GLU:O	1:A:569:GLN:HG3	2.14	0.47
1:A:728:LYS:HB2	1:A:810:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:PHE:N	1:B:827:ILE:O	2.47	0.47
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.45	0.47
1:C:382:VAL:HG12	1:C:472:ILE:HD11	1.95	0.47
1:C:944:LEU:C	1:C:971:ARG:HD2	2.34	0.47
1:D:987:MET:HA	1:D:1008:MET:HE1	1.96	0.47
1:D:100:ALA:HB1	1:D:131:LYS:HD2	1.96	0.47
1:D:508:GLY:H	1:D:518:ARG:HG3	1.79	0.47
1:D:984:LEU:HD23	1:D:984:LEU:HA	1.71	0.47
1:E:544:LEU:O	1:E:548:ILE:HG13	2.15	0.47
1:F:901:VAL:HG22	1:F:942:ALA:HB1	1.96	0.47
1:B:728:LYS:HB2	1:B:810:GLU:OE1	2.15	0.47
1:C:177:LEU:HD23	1:C:178:PHE:N	2.29	0.47
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.97	0.47
1:C:329:THR:O	1:C:332:PHE:HB3	2.14	0.47
1:C:340:VAL:HG12	1:C:395:MET:HE3	1.96	0.47
1:C:881:LEU:HD22	1:C:902:MET:HE1	1.97	0.47
1:D:137:LEU:HD13	1:D:293:LEU:HB2	1.97	0.47
1:D:933:THR:O	1:D:936:GLY:N	2.47	0.47
1:E:104:GLN:OE1	1:E:131:LYS:HD3	2.14	0.47
1:E:376:LEU:HD22	1:E:398:MET:HE3	1.96	0.47
1:E:858:ASP:OD1	1:E:859:TRP:N	2.48	0.47
1:E:911:GLY:HA2	1:E:914:LEU:HD22	1.96	0.47
1:F:904:VAL:HG21	1:F:1022:VAL:HG22	1.96	0.47
1:A:818:ARG:HH22	1:A:823:PRO:HD3	1.79	0.47
1:B:459:PHE:O	1:B:464:GLY:HA3	2.13	0.47
1:B:428:LYS:HE2	1:B:494:ALA:O	2.14	0.47
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.62	0.47
1:B:588:GLN:HB2	1:B:613:ASN:HD22	1.79	0.47
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.80	0.47
1:C:647:ILE:HG12	1:C:650:ARG:HH12	1.80	0.47
1:D:1040:ILE:HG23	1:D:1041:GLU:N	2.30	0.47
1:D:137:LEU:HG	1:D:138:MET:HE3	1.96	0.47
1:D:582:ALA:HA	1:D:586:ARG:HH21	1.79	0.47
1:E:350:LEU:HD21	1:E:984:LEU:HB2	1.95	0.47
1:E:478:MET:O	1:E:482:VAL:HG12	2.14	0.47
1:E:886:LEU:HA	1:E:886:LEU:HD12	1.72	0.47
1:F:509:LYS:HB3	1:F:514:GLY:HA3	1.96	0.47
1:A:783:PRO:HA	1:A:786:ILE:HG12	1.97	0.47
1:B:317:PHE:HE2	1:B:323:ILE:HD11	1.79	0.47
1:B:520:PHE:O	1:B:524:THR:HG22	2.14	0.47
1:B:910:ILE:HG23	1:B:911:GLY:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1037:ASN:O	1:C:1038:GLU:HB2	2.15	0.47
1:C:61:VAL:HG13	1:C:118:LEU:HD13	1.96	0.47
1:F:937:LEU:HD13	1:F:1011:MET:SD	2.54	0.47
1:F:776:GLU:HB2	1:F:779:TYR:CD1	2.50	0.47
1:A:394:THR:HG22	1:A:473:THR:OG1	2.15	0.47
1:A:47:ALA:HB3	1:A:88:VAL:CG1	2.44	0.47
1:B:46:SER:HA	1:B:88:VAL:O	2.15	0.47
1:C:990:VAL:HG13	1:C:1005:THR:OG1	2.14	0.47
1:D:250:LEU:HD13	1:D:261:LEU:HD23	1.95	0.47
1:D:728:LYS:HG2	1:D:808:ARG:CZ	2.45	0.47
1:E:588:GLN:NE2	1:E:592:ASN:OD1	2.47	0.47
1:F:858:ASP:OD2	1:F:859:TRP:N	2.48	0.47
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.97	0.47
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.50	0.47
1:C:407:ASP:OD2	1:C:940:LYS:HD2	2.15	0.47
1:D:317:PHE:HA	1:D:318:PRO:HD3	1.60	0.47
1:D:518:ARG:O	1:D:522:LYS:HG3	2.15	0.47
1:F:451:ALA:HB3	1:F:884:VAL:HG22	1.97	0.47
1:A:383:LEU:HD11	1:A:473:THR:HG23	1.97	0.46
1:A:892:TYR:OH	1:A:943:ILE:HA	2.15	0.46
1:C:363:ARG:O	1:C:367:ILE:HG13	2.14	0.46
1:C:907:LEU:HD21	1:C:1021:PHE:CB	2.44	0.46
1:D:162:MET:O	1:D:164:ASP:N	2.48	0.46
1:D:199:THR:CG2	1:D:791:VAL:HA	2.45	0.46
1:D:645:GLU:O	1:D:648:THR:OG1	2.30	0.46
1:D:719:ASN:HB3	1:D:826:GLU:HG2	1.97	0.46
1:E:1001:ASN:HD22	1:E:1001:ASN:N	2.12	0.46
1:F:986:VAL:HG11	1:F:1007:VAL:HG12	1.97	0.46
1:F:214:VAL:HG23	1:F:237:GLN:HB2	1.97	0.46
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.48	0.46
1:F:425:LEU:HD13	1:F:429:GLU:HG3	1.96	0.46
1:F:898:PRO:O	1:F:902:MET:HG2	2.15	0.46
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.96	0.46
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.48	0.46
1:B:164:ASP:HA	1:B:167:SER:HB3	1.96	0.46
1:B:182:TYR:O	1:B:769:LYS:HD3	2.14	0.46
1:B:254:ASN:HB2	1:B:258:SER:O	2.15	0.46
1:B:402:ILE:O	1:B:406:VAL:HG23	2.15	0.46
1:D:587:THR:OG1	1:D:622:GLN:O	2.14	0.46
1:D:168:ARG:HB3	1:E:75:LEU:HD22	1.97	0.46
1:A:457:ALA:HB2	1:A:471:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HD12	1:A:90:ILE:HD12	1.96	0.46
1:A:648:THR:HG21	1:A:666:PHE:HA	1.97	0.46
1:B:235:ILE:HB	1:C:728:LYS:HA	1.98	0.46
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.97	0.46
1:C:364:ALA:O	1:C:368:PRO:HD3	2.15	0.46
1:C:527:TYR:O	1:C:531:VAL:HG23	2.15	0.46
1:D:841:MET:HG2	1:D:859:TRP:CH2	2.50	0.46
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.15	0.46
1:A:445:ILE:HD12	1:A:446:ALA:N	2.30	0.46
1:B:571:VAL:HG12	1:B:668:LEU:HD21	1.98	0.46
1:C:480:LEU:O	1:C:484:VAL:HG23	2.15	0.46
1:D:900:SER:HA	1:D:1025:PHE:HB3	1.97	0.46
1:D:108:GLN:OE1	1:D:129:VAL:HB	2.15	0.46
1:D:26:ALA:O	1:D:30:LEU:HB2	2.15	0.46
1:E:715:SER:O	1:E:715:SER:OG	2.31	0.46
1:F:156:ASP:OD2	1:F:769:LYS:NZ	2.47	0.46
1:F:576:VAL:HG22	1:F:663:VAL:HG22	1.97	0.46
1:F:736:ALA:HB1	1:F:741:VAL:HG23	1.97	0.46
1:A:335:ILE:O	1:A:339:GLU:HG2	2.16	0.46
1:A:524:THR:O	1:A:527:TYR:HB3	2.16	0.46
1:A:525:HIS:HA	1:A:528:THR:HG22	1.96	0.46
1:B:536:ARG:NH1	2:B:1101:LMT:O4'	2.48	0.46
1:B:140:VAL:HG11	1:B:310:LEU:HD21	1.96	0.46
1:B:261:LEU:HD12	1:B:263:ARG:NH1	2.31	0.46
1:B:776:GLU:O	1:B:780:ARG:HG2	2.16	0.46
1:B:57:VAL:HG11	1:B:86:GLY:O	2.15	0.46
1:C:61:VAL:HG21	1:C:122:VAL:HG21	1.98	0.46
1:D:979:SER:CB	1:D:1015:THR:HG21	2.46	0.46
1:E:160:ALA:HA	1:E:767:ARG:NH2	2.31	0.46
1:E:987:MET:O	1:E:990:VAL:HG23	2.16	0.46
1:F:818:ARG:HH12	1:F:823:PRO:HG3	1.80	0.46
1:F:897:ILE:HG23	1:F:946:VAL:CG1	2.44	0.46
1:A:162:MET:HA	1:A:313:MET:SD	2.56	0.46
1:A:538:THR:O	1:A:542:LEU:HD13	2.15	0.46
1:B:753:ALA:O	1:B:775:SER:HB3	2.16	0.46
1:E:418:ARG:HD3	1:E:970:MET:HB2	1.98	0.46
1:D:225:VAL:HG13	1:E:781:MET:SD	2.56	0.46
1:F:751:GLY:O	1:F:753:ALA:N	2.49	0.46
1:A:906:PRO:HA	1:A:909:VAL:HB	1.96	0.46
1:B:1032:ARG:O	1:B:1033:PHE:HB2	2.15	0.46
1:B:597:TYR:OH	1:B:650:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.50	0.46
1:C:668:LEU:HA	1:C:677:ALA:HA	1.97	0.46
1:D:135:SER:HB3	1:D:672:VAL:HG11	1.98	0.46
1:D:965:LEU:HA	1:D:965:LEU:HD23	1.63	0.46
1:E:1041:GLU:HB3	1:E:1042:HIS:C	2.36	0.46
1:E:291:ILE:HG21	1:E:306:ILE:CD1	2.45	0.46
1:E:903:LEU:O	1:E:906:PRO:HD2	2.15	0.46
1:A:539:GLY:O	1:A:542:LEU:HB2	2.15	0.46
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.96	0.46
1:B:261:LEU:HD12	1:B:263:ARG:HH12	1.81	0.46
1:B:767:ARG:HG2	1:B:767:ARG:NH1	2.31	0.46
1:B:459:PHE:CD1	1:B:876:LEU:HD12	2.50	0.46
1:C:167:SER:HA	1:C:175:VAL:HG21	1.98	0.46
1:C:415:ASN:O	1:C:419:VAL:HG23	2.15	0.46
1:C:35:TYR:HE1	1:C:670:ALA:HB1	1.80	0.46
1:D:194:ASN:HA	1:D:798:MET:HE1	1.97	0.46
1:E:356:TYR:HE1	1:E:362:PHE:N	2.13	0.46
1:E:520:PHE:O	1:E:524:THR:HG23	2.16	0.46
1:E:978:THR:O	1:E:982:PHE:N	2.47	0.46
1:F:1020:PHE:CZ	2:F:1101:LMT:H31	2.51	0.46
1:F:361:ASN:HB3	1:F:364:ALA:CB	2.46	0.46
1:F:415:ASN:O	1:F:419:VAL:HG23	2.16	0.46
1:F:452:VAL:HG13	1:F:884:VAL:HG23	1.98	0.46
1:E:225:VAL:HG13	1:F:781:MET:SD	2.55	0.46
1:A:504:ASP:O	1:A:506:GLY:N	2.49	0.46
1:B:412:VAL:O	1:B:416:VAL:HG23	2.15	0.46
1:B:415:ASN:HB3	1:B:434:SER:OG	2.16	0.46
1:C:144:ASN:O	1:C:148:THR:HG23	2.16	0.46
1:C:937:LEU:HD23	1:C:937:LEU:HA	1.50	0.46
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.97	0.46
1:E:200:PRO:HB2	1:E:749:THR:HG22	1.97	0.46
1:B:27:ILE:HD12	1:B:27:ILE:HA	1.66	0.46
1:B:509:LYS:HE2	1:B:509:LYS:HB3	1.63	0.46
1:C:898:PRO:HA	1:C:901:VAL:HG12	1.98	0.46
1:E:589:LYS:O	1:E:592:ASN:HB2	2.15	0.46
1:F:959:GLY:HA3	1:F:1043:SER:HA	1.98	0.46
1:F:80:SER:HB3	1:F:90:ILE:HG23	1.97	0.46
1:F:940:LYS:HZ1	1:F:978:THR:CG2	2.29	0.46
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.46	0.45
1:A:523:SER:O	1:A:526:HIS:HB2	2.16	0.45
1:B:1026:PHE:CD2	1:B:1026:PHE:C	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:MET:O	1:C:523:SER:OG	2.26	0.45
1:C:778:LYS:HG3	1:C:779:TYR:CE1	2.51	0.45
1:D:592:ASN:O	1:D:596:HIS:HB2	2.15	0.45
1:D:58:GLN:OE1	1:D:63:GLN:NE2	2.49	0.45
1:E:231:ASN:HB2	1:F:583:THR:HG22	1.97	0.45
1:E:348:ILE:HG12	1:E:372:VAL:HG21	1.97	0.45
1:E:594:VAL:HG22	1:E:655:PHE:CE2	2.52	0.45
1:F:445:ILE:HG23	1:F:940:LYS:HG3	1.98	0.45
1:A:174:ASP:HB3	1:A:292:LYS:HB2	1.99	0.45
1:B:1038:GLU:CG	1:B:1039:ASP:H	2.29	0.45
1:C:158:VAL:HG22	1:C:162:MET:HE2	1.98	0.45
1:C:730:ASP:OD2	1:C:808:ARG:NH2	2.49	0.45
1:C:947:GLU:HG3	1:C:948:PHE:N	2.30	0.45
1:D:596:HIS:O	1:D:600:THR:OG1	2.25	0.45
1:D:602:GLU:OE2	1:D:650:ARG:NH1	2.50	0.45
1:D:680:PHE:HB2	1:D:859:TRP:HZ3	1.82	0.45
1:E:162:MET:C	1:E:164:ASP:N	2.67	0.45
1:A:244:GLU:O	1:A:246:PHE:N	2.49	0.45
1:A:30:LEU:HD11	1:A:384:ALA:HA	1.97	0.45
1:A:491:ALA:O	1:A:495:THR:OG1	2.22	0.45
1:B:139:VAL:HG13	1:B:178:PHE:CE1	2.52	0.45
1:C:493:CYS:O	1:C:497:LEU:HB2	2.17	0.45
1:D:74:ASN:HB3	1:D:95:GLU:CG	2.46	0.45
1:D:899:PHE:HA	1:D:902:MET:HE2	1.98	0.45
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.98	0.45
1:F:410:ILE:HD13	1:F:977:MET:HG2	1.99	0.45
1:A:281:PHE:HD1	1:A:610:PHE:HD1	1.63	0.45
1:A:650:ARG:O	1:A:653:ARG:HB3	2.16	0.45
1:B:181:GLN:HG2	1:B:182:TYR:N	2.30	0.45
1:B:277:ILE:HG13	1:B:277:ILE:H	1.68	0.45
1:B:273:GLU:CD	1:B:770:LYS:HD2	2.36	0.45
1:B:903:LEU:O	1:B:906:PRO:HD2	2.16	0.45
1:D:412:VAL:HG22	1:D:438:ILE:HD12	1.97	0.45
1:D:414:GLU:CD	1:D:974:PRO:HG3	2.36	0.45
1:D:960:LEU:O	1:D:964:THR:HG23	2.16	0.45
1:D:520:PHE:HE2	1:D:973:ARG:HG3	1.80	0.45
1:E:412:VAL:O	1:E:416:VAL:HG23	2.16	0.45
1:E:613:ASN:HD22	1:E:614:GLY:H	1.64	0.45
1:F:1022:VAL:HA	1:F:1025:PHE:HD1	1.82	0.45
1:F:1025:PHE:O	1:F:1029:VAL:HG23	2.16	0.45
1:E:105:VAL:HG23	1:F:109:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:PHE:CD2	1:F:383:LEU:HD12	2.42	0.45
1:F:2:PRO:HB2	1:F:3:ASN:H	1.59	0.45
1:A:459:PHE:CE2	1:A:876:LEU:HD12	2.52	0.45
1:B:198:LEU:HA	1:B:198:LEU:HD23	1.79	0.45
1:B:758:TYR:OH	1:B:761:ASP:OD1	2.35	0.45
1:C:1011:MET:O	1:C:1015:THR:HG23	2.17	0.45
1:C:368:PRO:HA	1:C:409:ALA:HB1	1.98	0.45
1:C:699:ARG:HD3	1:C:825:MET:SD	2.56	0.45
1:D:527:TYR:OH	1:D:1019:ILE:O	2.19	0.45
1:D:538:THR:HG21	1:D:1028:VAL:HG22	1.98	0.45
1:D:752:ALA:O	1:D:774:MET:HA	2.16	0.45
1:E:230:LEU:HG	1:E:231:ASN:N	2.30	0.45
1:F:1018:ALA:O	1:F:1022:VAL:HG23	2.16	0.45
1:F:1030:ARG:HH11	1:F:1033:PHE:HD2	1.64	0.45
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.88	0.45
1:F:363:ARG:O	1:F:367:ILE:HG13	2.17	0.45
1:A:692:HIS:NE2	1:A:723:ASP:OD1	2.50	0.45
1:B:457:ALA:HB2	1:B:471:SER:CB	2.46	0.45
1:B:743:ILE:HG13	1:B:743:ILE:H	1.65	0.45
1:B:919:ARG:HB3	1:B:921:LEU:CD2	2.46	0.45
1:C:1034:SER:O	1:C:1035:ARG:HG2	2.16	0.45
1:C:149:MET:HB2	1:C:153:ASP:CB	2.47	0.45
1:D:13:TRP:CE2	1:D:492:LEU:HD21	2.51	0.45
1:D:344:LEU:HD23	1:D:402:ILE:HD11	1.97	0.45
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.99	0.45
1:D:959:GLY:CA	1:D:1039:ASP:HA	2.47	0.45
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.98	0.45
1:E:574:THR:HG21	1:E:598:TYR:HE2	1.81	0.45
1:F:11:PHE:HE2	1:F:15:ILE:HD11	1.81	0.45
1:F:34:GLN:CG	1:F:333:VAL:HG22	2.47	0.45
1:F:38:ILE:CG2	1:F:462:SER:HB2	2.43	0.45
1:F:497:LEU:HD12	1:F:497:LEU:HA	1.50	0.45
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.99	0.45
1:F:893:GLU:O	1:F:893:GLU:HG3	2.16	0.45
1:B:519:MET:O	1:B:523:SER:OG	2.33	0.45
1:B:764:ASP:OD1	1:B:765:ARG:HG3	2.17	0.45
1:B:799:VAL:HG12	1:B:800:PRO:O	2.16	0.45
1:B:974:PRO:HA	1:B:977:MET:HE2	1.99	0.45
1:C:1044:HIS:HB2	1:C:1045:THR:H	1.45	0.45
1:C:733:GLN:OE1	1:C:743:ILE:HG21	2.16	0.45
1:D:191:ASN:C	1:D:193:LEU:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:ALA:HB2	1:E:471:SER:OG	2.17	0.45
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.51	0.45
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.52	0.45
1:F:595:THR:HG23	1:F:609:VAL:HB	1.98	0.45
1:A:393:LEU:HD13	1:A:466:ILE:HA	1.99	0.45
1:A:424:GLY:HA3	1:A:502:LYS:CG	2.37	0.45
1:A:449:LEU:HB3	1:A:478:MET:SD	2.57	0.45
1:A:75:LEU:HD11	1:A:92:LEU:HB3	1.99	0.45
1:B:13:TRP:CE3	1:B:13:TRP:HA	2.52	0.45
1:B:300:LEU:CD2	1:B:334:LYS:HG3	2.47	0.45
1:C:189:ASN:O	1:C:193:LEU:N	2.49	0.45
1:D:441:ALA:HB2	1:D:947:GLU:CD	2.37	0.45
1:F:375:VAL:HG11	1:F:405:LEU:HB3	1.99	0.45
1:F:850:LYS:O	1:F:850:LYS:HG3	2.17	0.45
1:A:542:LEU:HD11	1:A:1028:VAL:HG21	1.98	0.45
1:A:1034:SER:HA	1:A:1035:ARG:CB	2.46	0.45
1:A:200:PRO:HB2	1:A:749:THR:HG22	1.99	0.45
1:B:344:LEU:HD11	1:B:398:MET:CE	2.47	0.45
1:B:767:ARG:NH2	1:C:67:GLN:HE22	2.14	0.45
1:E:1021:PHE:HA	1:E:1024:VAL:HG23	1.98	0.45
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.99	0.45
1:E:361:ASN:O	1:E:365:THR:HB	2.17	0.45
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.52	0.45
1:F:789:TRP:O	1:F:801:PHE:HD2	2.00	0.45
1:F:885:PHE:HE1	1:F:899:PHE:CE2	2.35	0.45
1:F:910:ILE:O	1:F:914:LEU:HB2	2.17	0.45
1:A:108:GLN:O	1:A:112:GLN:HG2	2.17	0.45
1:A:497:LEU:HA	1:A:497:LEU:HD12	1.83	0.45
1:A:703:LEU:CD2	1:A:718:PRO:HD3	2.46	0.45
1:B:682:PHE:CD2	1:B:827:ILE:HD12	2.52	0.45
1:C:684:LEU:HD11	1:C:851:LEU:HD11	1.99	0.45
1:C:717:ARG:NH2	1:C:828:LEU:HD13	2.32	0.45
1:C:686:ASP:HB3	1:C:823:PRO:O	2.17	0.45
1:D:223:PRO:HD3	1:E:275:TYR:CD1	2.52	0.45
1:E:310:LEU:CD1	1:E:323:ILE:HG12	2.46	0.45
1:E:687:GLN:HG3	1:E:822:LEU:HD13	1.99	0.45
1:F:371:ALA:O	1:F:375:VAL:HG23	2.17	0.45
1:F:486:LEU:O	1:F:490:PRO:HG2	2.17	0.45
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.53	0.44
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.99	0.44
1:B:145:THR:HA	1:B:284:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HD3	1:B:772:TYR:HB2	1.98	0.44
1:C:11:PHE:CD2	1:C:11:PHE:C	2.91	0.44
1:D:239:ARG:HD2	1:D:761:ASP:O	2.16	0.44
1:E:115:MET:HE3	1:E:123:GLN:HG2	1.98	0.44
1:E:47:ALA:O	1:E:87:THR:HA	2.18	0.44
1:F:746:ILE:HG22	1:F:791:VAL:HG21	1.99	0.44
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.21	0.44
1:A:785:ASP:O	1:A:789:TRP:HD1	2.00	0.44
1:A:793:ALA:HB3	1:A:795:ASP:OD2	2.17	0.44
1:B:507:GLU:O	1:B:509:LYS:N	2.50	0.44
1:C:200:PRO:CG	1:C:749:THR:HG22	2.47	0.44
1:D:460:GLY:H	1:D:872:GLN:HE22	1.65	0.44
1:D:498:LYS:HG3	1:D:499:PRO:HD2	1.99	0.44
1:F:121:GLU:O	1:F:124:GLN:HG2	2.17	0.44
1:B:843:LEU:HD13	1:B:847:LEU:HG	2.00	0.44
1:B:904:VAL:O	1:B:907:LEU:HB2	2.18	0.44
1:C:1041:GLU:HB3	1:C:1042:HIS:CB	2.36	0.44
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.51	0.44
1:D:212:ALA:HA	1:D:239:ARG:HD3	1.99	0.44
1:E:417:GLU:HG2	1:E:497:LEU:HD21	2.00	0.44
1:E:542:LEU:HD23	1:E:542:LEU:HA	1.68	0.44
1:E:659:LYS:HE3	1:E:659:LYS:HB3	1.60	0.44
1:F:587:THR:HG21	1:F:623:ASN:HA	1.98	0.44
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.98	0.44
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.74	0.44
1:A:442:LEU:O	1:A:445:ILE:HG13	2.17	0.44
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.53	0.44
1:A:66:GLU:OE1	1:A:821:GLY:HA2	2.18	0.44
1:A:400:LEU:HG	1:A:933:THR:OG1	2.18	0.44
1:A:971:ARG:O	1:A:975:ILE:HG13	2.17	0.44
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.00	0.44
1:B:228:GLN:HG3	1:B:229:GLN:H	1.82	0.44
1:B:398:MET:HE3	1:B:398:MET:HB3	1.60	0.44
1:B:686:ASP:OD1	1:B:690:LEU:HG	2.17	0.44
1:B:996:GLY:O	1:B:1000:GLN:HG3	2.17	0.44
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	1.99	0.44
1:D:982:PHE:HD2	1:D:1011:MET:HG3	1.82	0.44
1:E:607:GLU:HG3	1:E:607:GLU:O	2.17	0.44
1:E:327:TYR:HB2	1:E:628:PHE:CE2	2.53	0.44
1:E:892:TYR:O	1:E:893:GLU:HB2	2.16	0.44
1:F:479:ALA:O	1:F:482:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:OD1	1:A:276:ASP:HB2	2.17	0.44
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.98	0.44
1:A:352:PHE:HD2	1:A:353:LEU:HD23	1.82	0.44
1:A:579:PRO:HD3	1:A:661:ALA:HB2	2.00	0.44
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.52	0.44
1:B:1045:THR:HB	1:B:1047:ASP:H	1.82	0.44
1:B:228:GLN:HG3	1:B:229:GLN:N	2.32	0.44
1:B:211:ASN:ND2	1:B:760:ASN:HD22	2.16	0.44
1:D:165:ALA:HB3	1:D:313:MET:HE3	1.99	0.44
1:D:242:SER:O	1:D:246:PHE:HD1	2.00	0.44
1:E:1034:SER:HB3	1:E:1035:ARG:H	1.59	0.44
1:E:600:THR:C	1:E:602:GLU:H	2.21	0.44
1:E:674:LEU:HB3	1:E:675:GLY:H	1.40	0.44
1:F:892:TYR:CD1	1:F:897:ILE:HG21	2.53	0.44
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.99	0.44
1:A:366:LEU:HA	1:A:366:LEU:HD23	1.63	0.44
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.82	0.44
1:B:119:PRO:O	1:B:123:GLN:HG3	2.18	0.44
1:B:211:ASN:O	1:B:760:ASN:ND2	2.44	0.44
1:B:293:LEU:HG	1:B:299:ALA:HA	1.99	0.44
1:B:545:TYR:HB2	1:B:1021:PHE:CE2	2.53	0.44
1:B:982:PHE:O	1:B:985:GLY:N	2.50	0.44
1:C:152:GLU:H	1:C:152:GLU:CD	2.20	0.44
1:C:188:MET:SD	1:C:200:PRO:HG3	2.58	0.44
1:C:713:LEU:HD11	1:C:843:LEU:HD12	1.99	0.44
1:E:448:VAL:HG13	1:E:884:VAL:HG13	2.00	0.44
1:E:762:PHE:HD2	1:E:771:VAL:HG22	1.83	0.44
1:D:55:LYS:NZ	1:F:238:THR:OG1	2.23	0.44
1:F:54:ALA:HB1	1:F:816:LEU:HG	2.00	0.44
1:F:908:GLY:O	1:F:1010:GLY:HA2	2.18	0.44
1:A:536:ARG:NH1	2:A:1101:LMT:O3B	2.51	0.44
1:A:158:VAL:HA	1:A:162:MET:HE2	1.99	0.44
1:A:177:LEU:HD23	1:A:178:PHE:N	2.32	0.44
1:A:216:ALA:HB3	1:A:234:ILE:O	2.17	0.44
1:A:818:ARG:NH1	1:A:823:PRO:HG3	2.25	0.44
1:A:47:ALA:HB3	1:A:88:VAL:HG13	1.99	0.44
1:D:193:LEU:HD13	1:D:200:PRO:HD3	2.00	0.44
1:D:438:ILE:O	1:D:441:ALA:HB3	2.17	0.44
1:D:877:TYR:O	1:D:881:LEU:HB2	2.17	0.44
1:E:246:PHE:O	1:E:249:ILE:HG23	2.18	0.44
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:428:LYS:HG2	1:E:494:ALA:HB1	1.99	0.44
1:E:727:PHE:CZ	1:E:807:SER:HB2	2.53	0.44
2:F:1101:LMT:H72	2:F:1101:LMT:H101	1.40	0.44
1:F:964:THR:O	1:F:968:VAL:HB	2.17	0.44
1:A:708:LYS:HE3	1:A:708:LYS:HB3	1.73	0.44
1:B:204:ILE:HG23	1:B:759:VAL:HG21	2.00	0.44
1:B:300:LEU:HD23	1:B:334:LYS:HG3	2.00	0.44
1:B:643:LYS:O	1:B:645:GLU:N	2.51	0.44
1:C:307:ARG:NH2	1:C:311:ALA:HB2	2.32	0.44
1:C:344:LEU:HD11	1:C:376:LEU:HD11	1.98	0.44
1:C:647:ILE:HG12	1:C:650:ARG:NH1	2.33	0.44
1:C:746:ILE:HG13	1:C:747:ASN:H	1.81	0.44
1:D:60:THR:HG23	1:D:61:VAL:HG23	2.00	0.44
1:E:115:MET:HE1	1:E:123:GLN:HA	1.99	0.44
1:E:166:ILE:HG12	1:E:306:ILE:HG23	1.99	0.44
1:E:515:TRP:O	1:E:519:MET:HG3	2.17	0.44
1:E:327:TYR:HB2	1:E:628:PHE:CZ	2.53	0.44
1:E:637:ARG:HD2	1:E:642:ASN:O	2.18	0.44
1:E:952:LEU:HB2	1:E:963:ALA:HB1	2.00	0.44
1:F:200:PRO:HB2	1:F:749:THR:HG22	2.00	0.44
1:F:492:LEU:O	1:F:496:MET:HG2	2.18	0.44
1:F:521:GLU:O	1:F:524:THR:HG22	2.17	0.44
1:F:603:LYS:HB2	1:F:603:LYS:HE3	1.80	0.44
2:A:1101:LMT:H21	2:A:1101:LMT:H51	1.66	0.44
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.71	0.44
1:B:143:ILE:HG12	1:B:322:LYS:O	2.18	0.44
1:B:190:PRO:HG3	1:B:779:TYR:HB3	2.00	0.44
1:B:952:LEU:HD13	1:B:966:ASP:HB3	2.00	0.44
1:C:472:ILE:O	1:C:476:SER:HB3	2.18	0.44
1:D:139:VAL:HA	1:D:289:LEU:O	2.18	0.44
1:D:188:MET:HB2	1:D:188:MET:HE2	1.82	0.44
1:D:504:ASP:C	1:D:506:GLY:H	2.22	0.44
1:D:805:SER:OG	1:D:805:SER:O	2.35	0.44
1:E:343:THR:HA	1:E:346:GLU:OE1	2.18	0.44
1:A:184:MET:HB3	1:A:771:VAL:HG13	2.00	0.43
1:A:659:LYS:HD3	1:A:659:LYS:HA	1.48	0.43
1:B:1040:ILE:HG23	1:B:1041:GLU:H	1.83	0.43
1:B:361:ASN:OD1	1:B:498:LYS:HD2	2.17	0.43
1:B:958:LYS:HB3	1:B:963:ALA:HB2	2.00	0.43
1:C:983:ILE:HG23	1:C:1008:MET:HE2	2.00	0.43
1:C:144:ASN:O	1:C:284:GLN:NE2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:GLN:NE2	1:C:222:THR:HG22	2.33	0.43
1:C:524:THR:O	1:C:527:TYR:HB3	2.18	0.43
1:C:580:ALA:HB1	1:C:724:THR:HG22	2.00	0.43
1:D:228:GLN:HG3	1:D:229:GLN:N	2.33	0.43
1:D:413:VAL:O	1:D:417:GLU:HG2	2.18	0.43
1:E:61:VAL:HG21	1:E:122:VAL:HG21	2.00	0.43
1:E:178:PHE:HD1	1:E:288:GLY:HA3	1.82	0.43
1:E:459:PHE:HD1	1:E:467:TYR:CG	2.36	0.43
1:E:47:ALA:HB3	1:E:88:VAL:HB	1.98	0.43
1:E:182:TYR:O	1:E:769:LYS:HD3	2.17	0.43
1:F:504:ASP:C	1:F:506:GLY:N	2.71	0.43
1:A:166:ILE:HD13	1:A:166:ILE:HA	1.65	0.43
1:A:346:GLU:O	1:A:349:ILE:N	2.51	0.43
1:A:7:ASP:O	1:A:8:ARG:HG3	2.18	0.43
1:A:870:GLY:O	1:A:871:ASN:HB2	2.18	0.43
1:B:344:LEU:HD11	1:B:398:MET:HE3	1.99	0.43
1:C:694:LYS:HA	1:C:697:GLN:OE1	2.18	0.43
1:D:108:GLN:NE2	1:E:109:ASN:HB3	2.32	0.43
1:D:460:GLY:N	1:D:872:GLN:HE22	2.15	0.43
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.47	0.43
1:E:578:LEU:HB2	1:E:623:ASN:O	2.18	0.43
1:D:259:ARG:NH1	1:E:734:GLU:OE2	2.51	0.43
1:F:452:VAL:C	1:F:455:PRO:HD2	2.38	0.43
1:F:667:ASN:O	1:F:678:THR:OG1	2.22	0.43
1:A:225:VAL:H	1:B:781:MET:CE	2.31	0.43
1:A:270:LEU:HA	1:A:270:LEU:HD12	1.72	0.43
1:A:534:ILE:HG22	1:A:541:TYR:CZ	2.53	0.43
1:A:66:GLU:OE2	1:A:80:SER:OG	2.30	0.43
1:B:112:GLN:HA	1:B:115:MET:HG2	2.00	0.43
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.46	0.43
1:B:76:MET:HG2	1:B:864:TYR:OH	2.18	0.43
1:C:1034:SER:OG	1:C:1035:ARG:N	2.48	0.43
1:C:492:LEU:HA	1:C:495:THR:HG1	1.83	0.43
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.70	0.43
1:C:690:LEU:O	1:C:694:LYS:HB2	2.19	0.43
1:C:698:ALA:O	1:C:701:GLN:HB3	2.18	0.43
1:C:888:LEU:HA	1:C:888:LEU:HD23	1.75	0.43
1:C:944:LEU:HB3	1:C:971:ARG:CD	2.45	0.43
1:D:449:LEU:O	1:D:453:PHE:HD1	2.02	0.43
1:E:986:VAL:HG12	1:E:1008:MET:HE3	2.00	0.43
1:E:132:SER:O	1:E:132:SER:OG	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:THR:N	1:E:245:GLU:OE1	2.52	0.43
1:F:2:PRO:O	1:F:5:PHE:HB3	2.18	0.43
1:F:42:ALA:HA	1:F:92:LEU:O	2.17	0.43
1:C:163:LYS:O	1:C:163:LYS:HG2	2.17	0.43
1:C:492:LEU:HA	1:C:495:THR:OG1	2.18	0.43
1:C:757:SER:O	1:C:772:TYR:HA	2.17	0.43
1:C:559:LEU:HD11	1:C:916:ALA:HB1	1.99	0.43
1:D:247:GLY:O	1:D:261:LEU:HB3	2.19	0.43
1:D:904:VAL:HG21	1:D:942:ALA:CB	2.47	0.43
1:E:690:LEU:HB2	1:E:694:LYS:HB2	2.00	0.43
1:A:448:VAL:O	1:A:451:ALA:HB3	2.19	0.43
1:A:459:PHE:CE1	1:A:876:LEU:HD12	2.53	0.43
1:A:818:ARG:NH2	1:A:823:PRO:HD3	2.33	0.43
1:B:1033:PHE:HA	1:B:1034:SER:HA	1.78	0.43
1:B:211:ASN:ND2	1:B:246:PHE:HZ	2.17	0.43
1:B:424:GLY:HA3	1:B:502:LYS:HB2	2.01	0.43
1:B:520:PHE:O	1:B:523:SER:OG	2.36	0.43
1:D:272:GLY:N	1:D:275:TYR:OH	2.50	0.43
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.84	0.43
1:D:698:ALA:O	1:D:701:GLN:HB3	2.18	0.43
1:D:743:ILE:HD12	1:D:743:ILE:H	1.83	0.43
1:E:166:ILE:O	1:E:169:THR:HB	2.19	0.43
1:E:686:ASP:HB2	1:E:695:LEU:HD21	1.99	0.43
1:D:217:GLY:HA2	1:E:755:GLY:CA	2.48	0.43
1:F:379:THR:O	1:F:382:VAL:HB	2.18	0.43
1:F:671:ILE:CG2	1:F:674:LEU:HB2	2.48	0.43
1:F:135:SER:CB	1:F:673:GLU:HB3	2.35	0.43
1:F:560:PRO:HB2	1:F:836:SER:OG	2.18	0.43
1:A:250:LEU:HD11	1:A:259:ARG:HD2	2.00	0.43
1:A:485:ALA:O	1:A:490:PRO:HD3	2.18	0.43
1:A:75:LEU:CD1	1:A:92:LEU:HB3	2.49	0.43
1:A:900:SER:HB3	1:A:1029:VAL:HG21	2.01	0.43
1:A:903:LEU:HD23	1:A:903:LEU:HA	1.65	0.43
1:A:926:TYR:HE1	1:A:999:ALA:HB1	1.83	0.43
1:B:480:LEU:O	1:B:484:VAL:HG23	2.18	0.43
1:C:1032:ARG:O	1:C:1033:PHE:CD1	2.71	0.43
1:D:904:VAL:O	1:D:907:LEU:HB2	2.18	0.43
1:D:925:VAL:HA	1:D:928:GLN:OE1	2.17	0.43
1:E:52:ALA:HB3	1:E:57:VAL:HG12	2.01	0.43
1:F:565:PRO:O	1:F:567:GLU:HG2	2.19	0.43
1:A:634:TRP:CD1	1:A:634:TRP:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:SER:O	1:A:772:TYR:HA	2.19	0.43
1:A:862:MET:HG3	1:A:863:SER:H	1.84	0.43
1:B:136:PHE:HD2	1:B:290:GLY:HA3	1.82	0.43
1:C:1027:VAL:O	1:C:1031:ARG:HG3	2.19	0.43
1:C:363:ARG:CZ	1:C:363:ARG:H	2.32	0.43
1:C:523:SER:HA	1:C:526:HIS:HB2	2.00	0.43
1:C:549:VAL:O	1:C:552:MET:HB3	2.18	0.43
1:C:955:LYS:O	1:C:956:GLU:HG2	2.18	0.43
1:D:971:ARG:NH1	1:D:971:ARG:N	2.64	0.43
1:E:455:PRO:O	1:E:876:LEU:HD13	2.18	0.43
1:E:743:ILE:O	1:E:746:ILE:HB	2.19	0.43
1:F:140:VAL:HG11	1:F:310:LEU:CD2	2.49	0.43
1:F:405:LEU:HD12	1:F:406:VAL:N	2.34	0.43
1:F:54:ALA:HB3	1:F:813:SER:O	2.18	0.43
1:A:1040:ILE:HG23	1:A:1041:GLU:N	2.33	0.43
1:A:668:LEU:H	1:A:668:LEU:HD23	1.84	0.43
1:A:686:ASP:OD1	1:A:689:GLY:N	2.48	0.43
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.71	0.43
1:B:350:LEU:HD13	1:B:984:LEU:O	2.18	0.43
1:B:709:HIS:CE1	1:B:847:LEU:HD21	2.54	0.43
1:C:881:LEU:HD22	1:C:902:MET:CE	2.48	0.43
1:D:203:VAL:O	1:D:207:ILE:HG13	2.19	0.43
1:D:678:THR:HA	1:D:837:THR:OG1	2.19	0.43
1:E:177:LEU:HA	1:E:289:LEU:HD23	2.00	0.43
1:E:702:LEU:HA	1:E:702:LEU:HD12	1.81	0.43
1:E:888:LEU:HD23	1:E:888:LEU:HA	1.70	0.43
1:F:270:LEU:HA	1:F:270:LEU:HD12	1.89	0.43
1:F:396:PHE:O	1:F:400:LEU:HB2	2.19	0.43
1:A:156:ASP:OD2	1:A:182:TYR:HB2	2.19	0.43
1:A:359:LEU:C	1:A:361:ASN:H	2.21	0.43
1:A:641:GLU:HA	1:A:646:ALA:HB3	1.99	0.43
1:B:214:VAL:HG23	1:B:237:GLN:HB3	2.00	0.43
1:B:331:PRO:O	1:B:335:ILE:HD13	2.19	0.43
1:B:641:GLU:HA	1:B:646:ALA:HB3	2.01	0.43
1:B:704:ALA:O	1:B:708:LYS:HE3	2.19	0.43
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.89	0.43
1:E:571:VAL:HG13	1:E:628:PHE:HE1	1.83	0.43
1:E:583:THR:HG22	1:E:584:GLN:N	2.33	0.43
1:E:880:SER:O	1:E:884:VAL:HG23	2.19	0.43
1:F:157:TYR:O	1:F:161:ASN:HB2	2.18	0.43
1:F:3:ASN:ND2	1:F:486:LEU:HD22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:598:TYR:CE2	1:F:629:VAL:HG21	2.53	0.43
1:F:239:ARG:CZ	1:F:761:ASP:HB2	2.49	0.43
1:F:343:THR:HG21	1:F:989:LEU:HD23	2.00	0.43
1:A:259:ARG:NH2	1:A:261:LEU:HD11	2.34	0.43
1:A:394:THR:HG22	1:A:473:THR:HG1	1.82	0.43
1:B:187:TRP:HA	1:B:774:MET:O	2.19	0.43
1:B:523:SER:O	1:B:526:HIS:HB2	2.19	0.43
1:C:907:LEU:HD21	1:C:1021:PHE:HB3	2.01	0.43
1:D:1040:ILE:HG12	1:D:1041:GLU:H	1.84	0.43
1:D:49:TYR:HE1	1:D:60:THR:HG21	1.84	0.43
1:D:973:ARG:HB3	1:D:974:PRO:HD3	2.01	0.43
1:E:180:SER:OG	1:E:273:GLU:N	2.52	0.43
1:F:188:MET:HA	1:F:266:ALA:HB2	1.99	0.43
1:F:361:ASN:HB3	1:F:364:ALA:HB3	2.00	0.43
1:F:511:GLY:O	1:F:512:PHE:CD2	2.72	0.43
1:F:534:ILE:HG22	2:F:1101:LMT:H5'	1.99	0.43
1:F:583:THR:O	1:F:587:THR:HG23	2.19	0.43
1:F:752:ALA:O	1:F:774:MET:HA	2.19	0.43
1:A:167:SER:O	1:B:70:ASN:HB2	2.19	0.42
1:A:225:VAL:HG11	1:B:778:LYS:HA	2.01	0.42
1:C:110:LYS:HA	1:C:110:LYS:HD3	1.86	0.42
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.39	0.42
1:C:943:ILE:O	1:C:947:GLU:HB3	2.19	0.42
1:D:654:ALA:O	1:D:658:ILE:HG12	2.18	0.42
1:D:351:VAL:HG22	1:D:981:ALA:HB1	2.01	0.42
1:E:43:VAL:HA	1:E:130:GLU:O	2.19	0.42
1:E:652:THR:OG1	1:E:665:ALA:HB3	2.18	0.42
1:E:869:SER:HB2	1:E:872:GLN:NE2	2.33	0.42
1:F:979:SER:HA	1:F:1011:MET:HE3	2.01	0.42
1:F:15:ILE:O	1:F:19:ILE:HG13	2.19	0.42
1:D:75:LEU:HD23	1:F:168:ARG:HB3	2.01	0.42
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.55	0.42
1:F:751:GLY:O	1:F:754:TRP:N	2.52	0.42
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.59	0.42
1:A:58:GLN:O	1:A:63:GLN:HG3	2.19	0.42
1:A:712:MET:O	1:A:832:ALA:N	2.50	0.42
1:A:699:ARG:NH1	1:A:825:MET:SD	2.91	0.42
1:A:885:PHE:CD1	1:A:902:MET:HE1	2.40	0.42
1:B:277:ILE:HD12	1:B:277:ILE:O	2.18	0.42
1:B:668:LEU:CD2	1:B:668:LEU:H	2.33	0.42
1:C:851:LEU:HB3	1:C:852:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:904:VAL:HG12	1:C:904:VAL:O	2.18	0.42
1:D:655:PHE:HB3	1:D:663:VAL:HB	2.01	0.42
1:D:919:ARG:HG2	1:D:920:GLY:H	1.83	0.42
1:D:949:ALA:HA	1:D:967:ALA:HB2	2.01	0.42
1:E:187:TRP:HA	1:E:774:MET:O	2.19	0.42
1:E:53:ASP:O	1:E:57:VAL:HG13	2.18	0.42
1:D:768:VAL:HG12	1:E:63:GLN:OE1	2.19	0.42
1:E:965:LEU:HD23	1:E:965:LEU:HA	1.86	0.42
1:F:311:ALA:HA	1:F:314:GLU:HG3	2.01	0.42
1:F:39:ALA:HA	1:F:40:PRO:HD2	1.87	0.42
1:A:633:ASP:OD1	1:A:635:ALA:HB3	2.19	0.42
1:B:1016:VAL:HG13	2:B:1101:LMT:H102	2.01	0.42
1:B:13:TRP:HE3	1:B:13:TRP:HA	1.83	0.42
1:B:455:PRO:HG2	1:B:880:SER:HB2	2.01	0.42
1:C:101:ASP:O	1:C:105:VAL:HG23	2.19	0.42
1:C:133:SER:O	1:C:134:SER:HB2	2.19	0.42
1:C:213:GLN:HG2	1:C:239:ARG:HG3	2.02	0.42
1:C:274:ASN:OD1	1:C:276:ASP:HB2	2.20	0.42
1:C:182:TYR:HD2	1:C:765:ARG:HH22	1.67	0.42
1:C:897:ILE:HB	1:C:898:PRO:HD3	2.01	0.42
1:D:367:ILE:HD13	1:D:493:CYS:HA	2.01	0.42
1:D:690:LEU:HD11	1:D:853:THR:O	2.18	0.42
1:D:858:ASP:OD2	1:D:859:TRP:N	2.50	0.42
1:E:102:ILE:HD12	1:E:102:ILE:HA	1.73	0.42
1:E:30:LEU:HA	1:E:30:LEU:HD12	1.83	0.42
1:E:728:LYS:HB2	1:E:810:GLU:OE1	2.19	0.42
1:E:897:ILE:O	1:E:900:SER:OG	2.27	0.42
1:F:1022:VAL:N	1:F:1023:PRO:HD2	2.34	0.42
1:F:247:GLY:O	1:F:261:LEU:HB3	2.19	0.42
1:F:261:LEU:HD12	1:F:263:ARG:NH1	2.33	0.42
1:F:588:GLN:OE1	1:F:592:ASN:ND2	2.42	0.42
1:F:634:TRP:CD1	1:F:634:TRP:N	2.82	0.42
1:F:731:ILE:HG13	1:F:731:ILE:O	2.19	0.42
1:F:991:ILE:O	1:F:991:ILE:HG23	2.19	0.42
1:A:242:SER:OG	1:A:245:GLU:HG2	2.19	0.42
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.84	0.42
1:B:368:PRO:HA	1:B:371:ALA:HB3	2.00	0.42
1:B:448:VAL:HG13	1:B:884:VAL:HG22	2.01	0.42
1:C:356:TYR:C	1:C:358:PHE:H	2.23	0.42
1:E:1010:GLY:O	1:E:1014:ALA:HB2	2.20	0.42
1:E:1034:SER:O	1:E:1035:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:434:SER:O	1:E:438:ILE:HG12	2.20	0.42
1:E:61:VAL:CG2	1:E:122:VAL:HG21	2.49	0.42
1:F:189:ASN:OD1	1:F:190:PRO:HD2	2.20	0.42
1:A:41:PRO:HG2	1:A:94:PHE:CB	2.41	0.42
1:A:889:ALA:N	1:A:898:PRO:HG3	2.34	0.42
1:B:575:MET:HB3	1:B:626:ILE:CG1	2.49	0.42
1:B:576:VAL:HG22	1:B:663:VAL:CG2	2.49	0.42
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.76	0.42
1:C:364:ALA:HA	1:C:367:ILE:CD1	2.49	0.42
1:C:492:LEU:O	1:C:496:MET:HG2	2.19	0.42
1:C:536:ARG:NH2	2:C:1101:LMT:H3O1	2.09	0.42
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.54	0.42
1:C:923:ASN:HA	1:C:927:PHE:CD2	2.55	0.42
1:D:151:GLN:H	1:D:151:GLN:NE2	2.17	0.42
1:D:186:ILE:HG12	1:D:268:ILE:HG12	2.02	0.42
1:D:751:GLY:O	1:D:754:TRP:N	2.53	0.42
1:D:838:GLY:O	1:D:841:MET:HB2	2.20	0.42
1:F:348:ILE:HG13	1:F:402:ILE:HD13	2.01	0.42
1:F:355:MET:SD	1:F:368:PRO:HB2	2.60	0.42
1:F:863:SER:HA	1:F:866:GLU:HB3	2.01	0.42
1:F:905:VAL:HG13	1:F:935:ILE:HG12	2.01	0.42
1:A:151:GLN:HG2	1:A:152:GLU:N	2.34	0.42
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.50	0.42
1:B:66:GLU:OE1	1:B:821:GLY:HA2	2.18	0.42
1:C:11:PHE:C	1:C:11:PHE:HD2	2.23	0.42
1:E:460:GLY:O	1:E:463:THR:OG1	2.38	0.42
1:D:225:VAL:HG12	1:E:777:ALA:HB1	2.01	0.42
1:E:448:VAL:HG13	1:E:884:VAL:HG22	2.01	0.42
1:F:134:SER:H	1:F:292:LYS:HD3	1.84	0.42
1:F:753:ALA:HA	1:F:775:SER:HB3	2.02	0.42
1:A:537:SER:O	1:A:537:SER:OG	2.23	0.42
1:A:75:LEU:CD2	1:C:168:ARG:HD3	2.50	0.42
1:A:831:ALA:HB1	1:A:835:LYS:HB3	2.02	0.42
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.50	0.42
1:B:139:VAL:HG13	1:B:178:PHE:HE1	1.85	0.42
1:B:281:PHE:O	1:B:284:GLN:HB2	2.20	0.42
1:C:958:LYS:CB	1:C:963:ALA:HB2	2.50	0.42
1:D:344:LEU:HD13	1:D:376:LEU:CD1	2.46	0.42
1:D:563:PHE:CE2	1:D:674:LEU:HD22	2.55	0.42
1:D:76:MET:HB2	1:D:93:THR:O	2.20	0.42
1:E:189:ASN:ND2	1:E:192:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:649:MET:O	1:E:653:ARG:HB2	2.20	0.42
1:E:758:TYR:HB2	1:E:772:TYR:CZ	2.54	0.42
1:F:163:LYS:HD2	1:F:177:LEU:HD12	2.02	0.42
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.89	0.42
1:A:457:ALA:HB1	1:A:468:ARG:HG3	2.00	0.42
1:A:809:TRP:HH2	1:C:230:LEU:HD21	1.85	0.42
1:B:300:LEU:HD11	1:B:333:VAL:HG12	2.01	0.42
1:B:355:MET:HG3	1:B:359:LEU:HD12	2.01	0.42
1:C:252:LYS:O	1:C:260:VAL:HG23	2.20	0.42
1:C:356:TYR:HD1	1:C:365:THR:HG21	1.85	0.42
1:C:379:THR:HG23	1:C:476:SER:OG	2.19	0.42
1:E:324:VAL:HG12	1:E:326:PRO:HD3	2.01	0.42
1:F:249:ILE:O	1:F:262:LEU:N	2.52	0.42
1:F:588:GLN:HB2	1:F:613:ASN:HD22	1.85	0.42
1:F:892:TYR:HD1	1:F:897:ILE:HG21	1.84	0.42
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.96	0.42
1:B:911:GLY:O	1:B:914:LEU:HB3	2.20	0.42
1:C:447:MET:O	1:C:451:ALA:HB2	2.20	0.42
1:C:587:THR:HG21	1:C:623:ASN:HA	2.02	0.42
1:C:567:GLU:OE1	1:C:996:GLY:HA2	2.19	0.42
1:D:138:MET:HG2	1:D:291:ILE:HB	2.01	0.42
1:D:489:THR:O	1:D:493:CYS:HB2	2.19	0.42
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.61	0.42
1:E:536:ARG:NH1	2:E:1101:LMT:H4B	2.35	0.42
1:E:960:LEU:O	1:E:964:THR:HG23	2.19	0.42
1:F:138:MET:HE3	1:F:328:ASP:OD1	2.20	0.42
1:F:778:LYS:HG3	1:F:779:TYR:CE1	2.55	0.42
1:F:953:MET:HE3	1:F:953:MET:HB2	1.90	0.42
1:A:937:LEU:HA	1:A:937:LEU:HD23	1.53	0.42
1:B:634:TRP:N	1:B:634:TRP:CD1	2.79	0.42
1:A:781:MET:HE2	1:C:225:VAL:HG22	2.02	0.42
1:C:445:ILE:HG23	1:C:940:LYS:HG3	2.01	0.42
1:C:940:LYS:O	1:C:943:ILE:HB	2.19	0.42
1:D:453:PHE:CE2	1:D:474:ILE:HG21	2.54	0.42
1:D:534:ILE:HG13	1:D:534:ILE:H	1.66	0.42
1:D:818:ARG:HH12	1:D:823:PRO:HG3	1.85	0.42
1:D:971:ARG:C	1:D:971:ARG:CZ	2.88	0.42
1:E:270:LEU:HA	1:E:270:LEU:HD12	1.87	0.42
1:E:508:GLY:N	1:E:518:ARG:HG3	2.35	0.42
1:E:834:GLY:O	1:E:835:LYS:HE2	2.20	0.42
1:E:851:LEU:HB3	1:E:852:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:PRO:HD3	1:F:391:ASN:ND2	2.35	0.42
1:F:273:GLU:CD	1:F:770:LYS:HD2	2.39	0.42
1:A:300:LEU:HD11	1:A:333:VAL:HG11	2.02	0.41
1:A:471:SER:O	1:A:475:VAL:HG23	2.20	0.41
1:B:445:ILE:HG21	1:B:940:LYS:HG3	2.02	0.41
1:C:885:PHE:CD1	1:C:898:PRO:HB3	2.55	0.41
1:D:520:PHE:O	1:D:524:THR:HG22	2.20	0.41
1:D:764:ASP:HB3	1:D:769:LYS:HD2	2.02	0.41
1:D:862:MET:HG3	1:D:863:SER:H	1.85	0.41
1:D:556:PHE:CD1	1:D:913:LEU:HD21	2.54	0.41
1:E:1041:GLU:HB3	1:E:1042:HIS:CA	2.50	0.41
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.54	0.41
1:E:564:LEU:CD1	1:E:671:ILE:HD12	2.50	0.41
1:E:267:LYS:HD3	1:E:776:GLU:OE2	2.20	0.41
1:E:790:TYR:CE1	1:E:800:PRO:HB3	2.55	0.41
1:E:726:GLN:CD	1:E:812:GLY:HA3	2.40	0.41
1:E:892:TYR:CD2	1:E:897:ILE:HG22	2.55	0.41
1:F:182:TYR:HD1	1:F:182:TYR:HA	1.73	0.41
1:F:777:ALA:O	1:F:781:MET:HG2	2.20	0.41
1:F:49:TYR:N	1:F:86:GLY:O	2.41	0.41
1:A:102:ILE:HD12	1:C:101:ASP:HB3	2.02	0.41
1:A:1035:ARG:C	1:A:1037:ASN:H	2.23	0.41
1:B:177:LEU:HD23	1:B:178:PHE:N	2.36	0.41
1:B:36:PRO:HD3	1:B:391:ASN:CG	2.39	0.41
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.51	0.41
1:B:420:MET:HB3	1:B:500:ILE:HB	2.02	0.41
1:C:159:ALA:HB2	1:C:177:LEU:HD11	2.02	0.41
1:C:15:ILE:O	1:C:19:ILE:HG13	2.20	0.41
1:C:228:GLN:HG3	1:C:229:GLN:N	2.36	0.41
1:C:211:ASN:ND2	1:C:246:PHE:HZ	2.18	0.41
1:C:280:GLU:OE2	1:C:588:GLN:NE2	2.49	0.41
1:C:30:LEU:HD13	1:C:384:ALA:HB2	2.02	0.41
1:C:360:GLN:HB3	1:C:513:PHE:CE2	2.55	0.41
1:C:75:LEU:HA	1:C:94:PHE:HD2	1.85	0.41
1:D:219:LEU:HD12	1:D:232:ALA:HB3	2.02	0.41
1:E:58:GLN:O	1:E:62:THR:HB	2.19	0.41
1:F:193:LEU:HD23	1:F:193:LEU:HA	1.76	0.41
1:F:23:GLY:O	1:F:27:ILE:HG23	2.19	0.41
1:A:244:GLU:C	1:A:246:PHE:N	2.73	0.41
1:A:141:GLY:O	1:A:323:ILE:HG23	2.20	0.41
1:A:456:MET:HB3	1:A:877:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:SER:O	1:A:997:SER:HB2	2.20	0.41
1:B:251:LEU:HD21	1:B:262:LEU:HD13	2.02	0.41
1:B:420:MET:HG2	1:B:425:LEU:O	2.21	0.41
1:B:888:LEU:HA	1:B:888:LEU:HD23	1.71	0.41
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.68	0.41
1:D:1008:MET:HB2	1:D:1008:MET:HE3	1.90	0.41
1:D:163:LYS:HG3	1:D:289:LEU:HD21	2.01	0.41
1:D:700:ASN:HA	1:D:703:LEU:HD12	2.02	0.41
1:D:775:SER:HB2	1:D:789:TRP:CZ2	2.54	0.41
1:E:785:ASP:OD1	1:E:785:ASP:N	2.54	0.41
1:F:208:LYS:HE3	1:F:759:VAL:HG13	2.02	0.41
1:F:311:ALA:HA	1:F:314:GLU:CD	2.41	0.41
1:A:946:VAL:HG22	1:A:1026:PHE:HB2	2.03	0.41
1:A:149:MET:CE	1:A:153:ASP:HB3	2.50	0.41
1:A:149:MET:HE2	1:A:153:ASP:HB3	2.03	0.41
1:A:457:ALA:O	1:A:468:ARG:NE	2.28	0.41
1:A:782:LEU:HA	1:A:783:PRO:HD3	1.85	0.41
1:A:905:VAL:HG13	1:A:935:ILE:HD13	2.01	0.41
1:B:1038:GLU:HG3	1:B:1039:ASP:H	1.85	0.41
1:B:249:ILE:HD13	1:B:249:ILE:HG21	1.83	0.41
1:B:390:ILE:HG23	1:B:395:MET:CG	2.51	0.41
1:C:151:GLN:N	1:C:151:GLN:OE1	2.54	0.41
1:C:189:ASN:O	1:C:193:LEU:HG	2.21	0.41
1:D:602:GLU:OE1	1:D:647:ILE:HG23	2.20	0.41
1:D:190:PRO:HB3	1:D:789:TRP:CZ2	2.54	0.41
1:D:618:ALA:O	1:D:815:ARG:NH2	2.54	0.41
1:E:907:LEU:HD21	1:E:1021:PHE:HB3	2.02	0.41
1:E:148:THR:HG21	1:E:319:SER:OG	2.20	0.41
1:E:402:ILE:HG22	1:E:406:VAL:HG23	2.01	0.41
1:E:482:VAL:O	1:E:485:ALA:HB3	2.20	0.41
1:D:781:MET:CE	1:F:225:VAL:H	2.33	0.41
1:F:418:ARG:O	1:F:422:GLU:HB2	2.20	0.41
1:A:3:ASN:O	1:A:6:ILE:HG13	2.20	0.41
1:A:463:THR:O	1:A:466:ILE:HB	2.20	0.41
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.73	0.41
1:A:575:MET:O	1:A:575:MET:HG3	2.18	0.41
1:A:678:THR:OG1	1:A:678:THR:O	2.36	0.41
1:B:407:ASP:O	1:B:411:VAL:HG23	2.20	0.41
1:C:121:GLU:N	1:C:121:GLU:OE1	2.49	0.41
1:D:26:ALA:HB1	1:D:384:ALA:CB	2.50	0.41
1:D:5:PHE:HD2	1:D:12:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ASN:HB3	1:D:95:GLU:HG3	2.03	0.41
1:E:364:ALA:HB2	1:E:497:LEU:HD11	2.01	0.41
1:E:578:LEU:HD13	1:E:661:ALA:HB2	2.03	0.41
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.56	0.41
1:E:783:PRO:O	1:E:786:ILE:HB	2.20	0.41
1:E:841:MET:O	1:E:845:GLU:HG3	2.20	0.41
1:F:900:SER:OG	1:F:1026:PHE:HD1	2.04	0.41
1:F:352:PHE:CD2	1:F:353:LEU:HD23	2.53	0.41
1:F:602:GLU:OE2	1:F:650:ARG:HD2	2.20	0.41
1:F:666:PHE:CD1	1:F:666:PHE:N	2.88	0.41
1:F:953:MET:HE1	1:F:960:LEU:HA	2.02	0.41
1:A:576:VAL:HG22	1:A:663:VAL:HG22	2.02	0.41
1:A:58:GLN:NE2	1:A:818:ARG:NH1	2.69	0.41
1:B:255:GLN:HG3	1:B:255:GLN:H	1.29	0.41
1:D:27:ILE:HD11	1:D:380:PHE:CD1	2.56	0.41
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.55	0.41
1:D:603:LYS:HB3	1:D:603:LYS:HE2	1.91	0.41
1:D:921:LEU:HA	1:D:921:LEU:HD13	1.84	0.41
1:F:982:PHE:CD2	1:F:1011:MET:HG2	2.52	0.41
1:A:182:TYR:HA	1:A:182:TYR:HD1	1.66	0.41
1:A:143:ILE:HG22	1:A:286:ALA:HB2	2.02	0.41
1:A:714:THR:HB	1:A:830:GLN:HB2	2.03	0.41
1:B:373:PRO:O	1:B:376:LEU:HB2	2.20	0.41
1:B:524:THR:O	1:B:527:TYR:HB3	2.20	0.41
1:C:725:PRO:HG3	1:C:811:TYR:HE1	1.85	0.41
1:D:61:VAL:CG2	1:D:122:VAL:HG21	2.42	0.41
1:D:822:LEU:HA	1:D:823:PRO:HD3	1.95	0.41
1:D:932:LEU:HD23	1:D:932:LEU:HA	1.75	0.41
1:E:108:GLN:HA	1:E:129:VAL:HG21	2.03	0.41
1:E:357:LEU:O	1:E:358:PHE:HD1	2.04	0.41
1:E:868:LEU:HD23	1:E:868:LEU:HA	1.73	0.41
1:F:45:ILE:H	1:F:45:ILE:HG13	1.54	0.41
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	2.03	0.41
1:A:158:VAL:HG22	1:A:162:MET:HE1	2.02	0.41
1:A:475:VAL:HA	1:A:478:MET:CE	2.51	0.41
1:B:1038:GLU:HG3	1:B:1040:ILE:HB	2.01	0.41
1:B:166:ILE:CD1	1:B:310:LEU:HD13	2.51	0.41
1:B:80:SER:HB3	1:B:818:ARG:HB2	2.03	0.41
1:B:682:PHE:HB3	1:B:827:ILE:HB	2.02	0.41
1:C:453:PHE:CD2	1:C:456:MET:HE2	2.56	0.41
1:C:504:ASP:C	1:C:506:GLY:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:THR:H	1:C:587:THR:HG23	1.62	0.41
1:C:944:LEU:HD13	1:C:975:ILE:HG12	2.03	0.41
1:D:959:GLY:HA2	1:D:1039:ASP:HA	2.02	0.41
1:D:531:VAL:HB	1:D:965:LEU:HD21	2.02	0.41
1:D:659:LYS:HD3	1:D:659:LYS:HA	1.76	0.41
1:D:888:LEU:HD13	1:D:898:PRO:O	2.21	0.41
1:E:353:LEU:C	1:E:355:MET:N	2.72	0.41
1:E:6:ILE:HG23	1:E:494:ALA:HB2	2.03	0.41
1:D:225:VAL:H	1:E:781:MET:CE	2.34	0.41
1:F:1041:GLU:OE1	1:F:1044:HIS:ND1	2.54	0.41
1:D:754:TRP:CE3	1:F:234:ILE:HD11	2.56	0.41
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.80	0.41
1:A:375:VAL:CG2	1:A:481:SER:HA	2.51	0.41
1:A:728:LYS:HE3	1:A:730:ASP:HB2	2.03	0.41
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.53	0.41
1:A:957:GLY:O	1:A:1041:GLU:HA	2.21	0.41
1:B:3:ASN:O	1:B:6:ILE:HB	2.21	0.41
1:C:563:PHE:HB2	1:C:866:GLU:CG	2.50	0.41
1:C:882:ILE:HG22	1:C:886:LEU:HD22	2.02	0.41
1:D:185:ARG:HA	1:D:185:ARG:HD3	1.95	0.41
1:D:189:ASN:OD1	1:D:190:PRO:HD2	2.21	0.41
1:D:209:ALA:O	1:D:237:GLN:NE2	2.53	0.41
1:D:340:VAL:HG22	1:D:396:PHE:CE2	2.56	0.41
1:E:949:ALA:CB	1:E:1026:PHE:HE2	2.32	0.41
1:E:43:VAL:HG13	1:E:130:GLU:O	2.21	0.41
1:E:407:ASP:OD2	1:E:940:LYS:HD3	2.20	0.41
1:F:393:LEU:HD12	1:F:469:GLN:HG3	2.02	0.41
1:F:6:ILE:C	1:F:8:ARG:H	2.23	0.41
1:F:905:VAL:CG1	1:F:935:ILE:HG12	2.50	0.41
1:A:81:ASN:O	1:A:88:VAL:HA	2.21	0.41
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	2.02	0.41
1:B:1041:GLU:HB2	1:B:1042:HIS:H	1.71	0.41
1:B:108:GLN:HE22	1:C:112:GLN:CB	2.29	0.41
1:B:448:VAL:HG13	1:B:884:VAL:HG13	2.03	0.41
1:B:375:VAL:HG22	1:B:484:VAL:HG21	2.02	0.41
1:C:373:PRO:O	1:C:377:LEU:N	2.49	0.41
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.55	0.41
1:C:850:LYS:O	1:C:850:LYS:HG3	2.21	0.41
1:D:405:LEU:HD22	1:D:481:SER:HB2	2.02	0.41
1:D:800:PRO:HG2	1:D:803:ALA:HB2	2.02	0.41
1:D:84:SER:HB3	1:D:814:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:878:ALA:O	1:D:882:ILE:HG12	2.19	0.41
1:E:249:ILE:HD13	1:E:262:LEU:HD22	2.03	0.41
1:E:162:MET:CE	1:E:323:ILE:HD11	2.51	0.41
1:E:682:PHE:CE1	1:E:857:TYR:HB2	2.56	0.41
1:F:462:SER:O	1:F:466:ILE:HG12	2.21	0.41
1:F:463:THR:HG23	1:F:925:VAL:CG2	2.50	0.41
1:F:746:ILE:HG13	1:F:747:ASN:H	1.86	0.41
1:A:1042:HIS:HB3	1:A:1043:SER:H	1.75	0.41
1:A:188:MET:HA	1:A:266:ALA:HB2	2.03	0.41
1:A:393:LEU:HB3	1:A:470:PHE:CE1	2.56	0.41
1:B:415:ASN:HD22	1:B:434:SER:CB	2.33	0.41
1:B:695:LEU:HD12	1:B:825:MET:HG3	2.02	0.41
1:C:188:MET:HB3	1:C:193:LEU:HD11	2.02	0.41
1:C:449:LEU:HD11	1:C:937:LEU:CD2	2.50	0.41
1:D:188:MET:HE3	1:D:789:TRP:CH2	2.56	0.41
1:D:325:TYR:HA	1:D:326:PRO:HD2	1.88	0.41
1:D:361:ASN:HD21	1:D:363:ARG:HG2	1.85	0.41
1:D:451:ALA:O	1:D:880:SER:OG	2.32	0.41
1:D:455:PRO:HG2	1:D:880:SER:CB	2.47	0.41
1:D:687:GLN:HA	1:D:822:LEU:HD13	2.03	0.41
1:E:445:ILE:HG13	1:E:446:ALA:N	2.35	0.41
1:E:605:ASN:O	1:E:632:LYS:HG3	2.21	0.41
1:F:1041:GLU:HB3	1:F:1042:HIS:CB	2.39	0.41
1:F:732:ASP:HB3	1:F:735:LYS:HG3	2.02	0.41
1:F:776:GLU:HB2	1:F:779:TYR:HD1	1.84	0.41
1:A:525:HIS:CD2	1:A:525:HIS:O	2.74	0.40
1:B:166:ILE:HA	1:B:166:ILE:HD12	1.71	0.40
1:B:207:ILE:HG12	1:B:249:ILE:CD1	2.50	0.40
1:B:682:PHE:C	1:B:682:PHE:CD2	2.95	0.40
1:B:905:VAL:HB	1:B:906:PRO:HD3	2.03	0.40
1:C:407:ASP:O	1:C:411:VAL:HG23	2.21	0.40
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.03	0.40
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.87	0.40
1:D:150:THR:HB	1:D:151:GLN:NE2	2.36	0.40
1:D:309:GLU:O	1:D:312:LYS:HB2	2.21	0.40
1:E:242:SER:O	1:E:246:PHE:HD1	2.04	0.40
1:E:252:LYS:HE2	1:E:252:LYS:HB3	1.83	0.40
1:E:47:ALA:N	1:E:88:VAL:O	2.46	0.40
1:F:172:VAL:HG13	1:F:291:ILE:HG23	2.03	0.40
1:F:445:ILE:HG12	1:F:940:LYS:HG3	2.03	0.40
1:A:244:GLU:C	1:A:246:PHE:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:CD2	1:A:565:PRO:HD2	2.47	0.40
1:A:781:MET:SD	1:C:225:VAL:HG13	2.61	0.40
1:B:360:GLN:HB3	1:B:513:PHE:CZ	2.56	0.40
1:B:108:GLN:CD	1:C:112:GLN:HG3	2.42	0.40
1:C:344:LEU:HA	1:C:399:VAL:HG22	2.02	0.40
1:C:61:VAL:HG22	1:C:119:PRO:HD2	2.01	0.40
1:C:872:GLN:C	1:C:874:PRO:HD2	2.41	0.40
1:C:932:LEU:HA	1:C:932:LEU:HD23	1.81	0.40
1:D:149:MET:HB2	1:D:153:ASP:HB3	2.04	0.40
1:D:210:GLN:OE1	1:D:249:ILE:HG23	2.20	0.40
1:D:6:ILE:CD1	1:D:432:ARG:HE	2.34	0.40
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.56	0.40
1:D:913:LEU:HA	1:D:913:LEU:HD23	1.96	0.40
1:E:756:GLY:HA2	1:E:774:MET:HG3	2.03	0.40
1:F:120:GLN:HA	1:F:123:GLN:HB2	2.03	0.40
1:F:412:VAL:O	1:F:416:VAL:HG23	2.21	0.40
1:F:453:PHE:CD1	1:F:453:PHE:N	2.89	0.40
1:F:453:PHE:HD1	1:F:453:PHE:N	2.19	0.40
1:A:1040:ILE:HG23	1:A:1041:GLU:H	1.86	0.40
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.53	0.40
1:A:538:THR:HG23	1:A:542:LEU:HD13	2.03	0.40
1:B:307:ARG:NH1	1:B:328:ASP:OD2	2.50	0.40
1:B:58:GLN:HG2	1:B:59:ASP:OD1	2.21	0.40
1:B:717:ARG:HD2	1:B:828:LEU:HB2	2.04	0.40
1:B:699:ARG:HH11	1:B:825:MET:HE1	1.86	0.40
1:B:841:MET:O	1:B:845:GLU:HG3	2.21	0.40
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.21	0.40
1:C:201:VAL:O	1:C:204:ILE:HB	2.21	0.40
1:C:488:LEU:O	1:C:491:ALA:HB3	2.21	0.40
1:C:671:ILE:HG21	1:C:674:LEU:HD12	2.03	0.40
1:D:409:ALA:O	1:D:413:VAL:HG23	2.22	0.40
1:D:429:GLU:HG2	1:D:429:GLU:H	1.44	0.40
1:D:47:ALA:HB3	1:D:88:VAL:CG1	2.52	0.40
1:D:551:GLY:O	1:D:555:LEU:HB2	2.21	0.40
1:D:650:ARG:O	1:D:653:ARG:HB3	2.21	0.40
1:D:888:LEU:CB	1:D:898:PRO:HB3	2.51	0.40
1:E:167:SER:OG	1:E:175:VAL:HG21	2.22	0.40
1:E:189:ASN:HB3	1:E:192:GLU:CB	2.47	0.40
1:E:24:GLY:O	1:E:28:LEU:HB2	2.20	0.40
1:E:680:PHE:HB2	1:E:863:SER:OG	2.21	0.40
1:E:992:SER:O	1:E:997:SER:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:746:ILE:HG22	1:F:791:VAL:HG11	2.03	0.40
1:A:492:LEU:HD22	1:A:496:MET:SD	2.62	0.40
1:A:74:ASN:O	1:A:94:PHE:HD2	2.04	0.40
1:B:492:LEU:O	1:B:496:MET:HG2	2.21	0.40
1:C:725:PRO:HG3	1:C:811:TYR:CE1	2.57	0.40
1:D:199:THR:HG21	1:D:791:VAL:HA	2.03	0.40
1:E:383:LEU:HA	1:E:383:LEU:HD23	1.83	0.40
1:E:588:GLN:HG3	1:E:592:ASN:HD21	1.86	0.40
1:E:602:GLU:OE1	1:E:650:ARG:HD2	2.22	0.40
1:E:805:SER:OG	1:E:805:SER:O	2.37	0.40
1:F:58:GLN:HG3	1:F:82:SER:OG	2.21	0.40
1:F:674:LEU:CD2	1:F:861:GLY:HA2	2.51	0.40
1:A:909:VAL:HG22	1:A:931:LEU:HD21	2.04	0.40
1:B:427:PRO:CD	1:B:499:PRO:HB3	2.52	0.40
1:C:165:ALA:HB3	1:C:313:MET:CE	2.50	0.40
1:C:246:PHE:O	1:C:249:ILE:HG13	2.22	0.40
1:C:501:ALA:O	1:C:504:ASP:HB2	2.20	0.40
1:C:510:LYS:HG2	1:C:511:GLY:N	2.37	0.40
1:C:948:PHE:HB3	1:C:970:MET:CE	2.52	0.40
1:C:991:ILE:O	1:C:991:ILE:HD13	2.21	0.40
1:C:926:TYR:HE1	1:C:999:ALA:HA	1.87	0.40
1:D:287:SER:OG	1:D:288:GLY:N	2.50	0.40
1:D:537:SER:O	1:D:537:SER:OG	2.38	0.40
1:D:712:MET:O	1:D:832:ALA:N	2.46	0.40
1:D:730:ASP:HB2	1:D:808:ARG:NH2	2.37	0.40
1:D:964:THR:O	1:D:967:ALA:HB3	2.22	0.40
1:E:1017:LEU:HD12	1:E:1017:LEU:HA	1.70	0.40
1:E:154:ILE:O	1:E:157:TYR:N	2.55	0.40
1:E:162:MET:HA	1:E:313:MET:HE1	2.03	0.40
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.42	0.40
1:E:396:PHE:O	1:E:400:LEU:HB2	2.20	0.40
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.47	0.40
1:E:453:PHE:HB3	1:E:475:VAL:HG22	2.02	0.40
1:E:792:ARG:HB2	1:E:798:MET:SD	2.61	0.40
1:E:834:GLY:C	1:E:835:LYS:HE2	2.42	0.40
1:E:445:ILE:CG1	1:E:940:LYS:HE3	2.48	0.40
1:F:222:THR:HA	1:F:223:PRO:HA	1.90	0.40
1:F:435:MET:HE1	1:F:490:PRO:HB3	2.04	0.40
1:F:522:LYS:O	1:F:525:HIS:N	2.54	0.40
1:F:535:LEU:HA	1:F:535:LEU:HD23	1.72	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:529:ASP:OD1	1:F:529:ASP:OD2[2_555]	2.08	0.12

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	1040/1049 (99%)	939 (90%)	82 (8%)	19 (2%)	11	49
1	B	1044/1049 (100%)	925 (89%)	92 (9%)	27 (3%)	7	38
1	C	1042/1049 (99%)	931 (89%)	91 (9%)	20 (2%)	10	48
1	D	1040/1049 (99%)	941 (90%)	83 (8%)	16 (2%)	13	53
1	E	1040/1049 (99%)	919 (88%)	97 (9%)	24 (2%)	8	42
1	F	1044/1049 (100%)	936 (90%)	87 (8%)	21 (2%)	9	46
All	All	6250/6294 (99%)	5591 (90%)	532 (8%)	127 (2%)	9	46

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	675	GLY
1	A	1038	GLU
1	B	163	LYS
1	B	360	GLN
1	B	509	LYS
1	B	516	PHE
1	B	644	VAL
1	B	673	GLU
1	B	677	ALA
1	B	1033	PHE
1	B	1038	GLU
1	B	1040	ILE

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Mol	Chain	Res	Type
1	B	1041	GLU
1	B	1046	VAL
1	C	134	SER
1	C	147	GLY
1	C	163	LYS
1	C	360	GLN
1	C	509	LYS
1	C	691	GLY
1	C	1034	SER
1	C	1038	GLU
1	D	163	LYS
1	D	360	GLN
1	D	508	GLY
1	D	511	GLY
1	D	644	VAL
1	D	1035	ARG
1	D	1037	ASN
1	E	163	LYS
1	E	354	VAL
1	E	360	GLN
1	E	536	ARG
1	E	632	LYS
1	E	644	VAL
1	E	673	GLU
1	E	674	LEU
1	E	893	GLU
1	E	1035	ARG
1	F	134	SER
1	F	147	GLY
1	F	360	GLN
1	F	644	VAL
1	F	691	GLY
1	F	1039	ASP
1	F	1042	HIS
1	F	1045	THR
1	F	1046	VAL
1	A	507	GLU
1	A	644	VAL
1	A	677	ALA
1	A	751	GLY
1	A	1040	ILE
1	B	295	THR

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Mol	Chain	Res	Type
1	B	508	GLY
1	B	751	GLY
1	B	1037	ASN
1	C	133	SER
1	C	644	VAL
1	C	689	GLY
1	C	751	GLY
1	C	752	ALA
1	C	893	GLU
1	C	1042	HIS
1	D	675	GLY
1	D	751	GLY
1	D	752	ALA
1	D	992	SER
1	D	1033	PHE
1	D	1040	ILE
1	E	132	SER
1	E	508	GLY
1	E	672	VAL
1	E	751	GLY
1	E	1040	ILE
1	F	6	ILE
1	F	163	LYS
1	F	751	GLY
1	F	1043	SER
1	A	37	THR
1	A	752	ALA
1	A	907	LEU
1	A	1035	ARG
1	B	41	PRO
1	B	358	PHE
1	B	638	PRO
1	B	672	VAL
1	B	833	PRO
1	B	960	LEU
1	C	1033	PHE
1	C	1037	ASN
1	C	1041	GLU
1	D	960	LEU
1	E	752	ALA
1	E	907	LEU
1	E	993	THR

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Mol	Chain	Res	Type
1	F	133	SER
1	F	146	ASP
1	F	148	THR
1	A	163	LYS
1	A	505	HIS
1	A	688	ALA
1	A	1033	PHE
1	B	1044	HIS
1	D	907	LEU
1	E	195	LYS
1	E	1042	HIS
1	F	638	PRO
1	F	907	LEU
1	B	40	PRO
1	B	752	ALA
1	E	638	PRO
1	E	1037	ASN
1	F	960	LEU
1	A	195	LYS
1	A	418	ARG
1	A	638	PRO
1	B	907	LEU
1	E	353	LEU
1	F	923	ASN
1	B	870	GLY
1	C	511	GLY
1	E	833	PRO
1	C	217	GLY
1	D	638	PRO
1	F	511	GLY

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	845/852 (99%)	789 (93%)	56 (7%)	21 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	849/852 (100%)	735 (87%)	114 (13%)	5 22
1	C	847/852 (99%)	769 (91%)	78 (9%)	11 40
1	D	845/852 (99%)	786 (93%)	59 (7%)	19 57
1	E	845/852 (99%)	735 (87%)	110 (13%)	5 23
1	F	849/852 (100%)	783 (92%)	66 (8%)	16 51
All	All	5080/5112 (99%)	4597 (90%)	483 (10%)	11 38

All (483) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	11	PHE
1	A	38	ILE
1	A	44	THR
1	A	45	ILE
1	A	60	THR
1	A	146	ASP
1	A	205	THR
1	A	253	VAL
1	A	255	GLN
1	A	267	LYS
1	A	270	LEU
1	A	336	SER
1	A	349	ILE
1	A	350	LEU
1	A	355	MET
1	A	362	PHE
1	A	429	GLU
1	A	434	SER
1	A	437	GLN
1	A	452	VAL
1	A	472	ILE
1	A	493	CYS
1	A	502	LYS
1	A	512	PHE
1	A	523	SER
1	A	528	THR
1	A	530	SER
1	A	538	THR
1	A	559	LEU

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Mol	Chain	Res	Type
1	A	561	SER
1	A	564	LEU
1	A	578	LEU
1	A	602	GLU
1	A	603	LYS
1	A	608	SER
1	A	634	TRP
1	A	636	ASP
1	A	659	LYS
1	A	662	MET
1	A	682	PHE
1	A	716	VAL
1	A	741	VAL
1	A	804	PHE
1	A	922	THR
1	A	931	LEU
1	A	947	GLU
1	A	961	ILE
1	A	970	MET
1	A	971	ARG
1	A	975	ILE
1	A	1036	LYS
1	A	1038	GLU
1	A	1039	ASP
1	A	1041	GLU
1	A	1042	HIS
1	B	6	ILE
1	B	11	PHE
1	B	13	TRP
1	B	17	ILE
1	B	27	ILE
1	B	28	LEU
1	B	29	LYS
1	B	32	VAL
1	B	43	VAL
1	B	49	TYR
1	B	53	ASP
1	B	58	GLN
1	B	79	SER
1	B	105	VAL
1	B	128	SER
1	B	153	ASP

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Mol	Chain	Res	Type
1	B	166	ILE
1	B	175	VAL
1	B	180	SER
1	B	213	GLN
1	B	255	GLN
1	B	259	ARG
1	B	276	ASP
1	B	289	LEU
1	B	293	LEU
1	B	295	THR
1	B	298	ASN
1	B	314	GLU
1	B	322	LYS
1	B	329	THR
1	B	336	SER
1	B	348	ILE
1	B	350	LEU
1	B	352	PHE
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	365	THR
1	B	374	VAL
1	B	383	LEU
1	B	400	LEU
1	B	404	LEU
1	B	473	THR
1	B	475	VAL
1	B	480	LEU
1	B	482	VAL
1	B	489	THR
1	B	507	GLU
1	B	523	SER
1	B	524	THR
1	B	526	HIS
1	B	534	ILE
1	B	555	LEU
1	B	558	ARG
1	B	559	LEU
1	B	561	SER
1	B	563	PHE
1	B	564	LEU

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Mol	Chain	Res	Type
1	B	569	GLN
1	B	575	MET
1	B	578	LEU
1	B	599	LEU
1	B	626	ILE
1	B	634	TRP
1	B	636	ASP
1	B	640	GLU
1	B	642	ASN
1	B	662	MET
1	B	667	ASN
1	B	668	LEU
1	B	672	VAL
1	B	682	PHE
1	B	683	GLU
1	B	687	GLN
1	B	690	LEU
1	B	695	LEU
1	B	703	LEU
1	B	708	LYS
1	B	711	ASP
1	B	715	SER
1	B	717	ARG
1	B	741	VAL
1	B	743	ILE
1	B	759	VAL
1	B	761	ASP
1	B	775	SER
1	B	788	ASP
1	B	806	SER
1	B	808	ARG
1	B	835	LYS
1	B	853	THR
1	B	862	MET
1	B	869	SER
1	B	871	ASN
1	B	886	LEU
1	B	919	ARG
1	B	958	LYS
1	B	965	LEU
1	B	968	VAL
1	B	970	MET

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Mol	Chain	Res	Type
1	B	975	ILE
1	B	978	THR
1	B	980	LEU
1	B	1015	THR
1	B	1032	ARG
1	B	1035	ARG
1	B	1036	LYS
1	B	1038	GLU
1	B	1039	ASP
1	B	1040	ILE
1	B	1041	GLU
1	B	1042	HIS
1	B	1045	THR
1	B	1046	VAL
1	C	3	ASN
1	C	6	ILE
1	C	11	PHE
1	C	27	ILE
1	C	28	LEU
1	C	48	SER
1	C	49	TYR
1	C	88	VAL
1	C	92	LEU
1	C	108	GLN
1	C	120	GLN
1	C	145	THR
1	C	148	THR
1	C	151	GLN
1	C	239	ARG
1	C	253	VAL
1	C	255	GLN
1	C	275	TYR
1	C	300	LEU
1	C	353	LEU
1	C	358	PHE
1	C	360	GLN
1	C	363	ARG
1	C	392	THR
1	C	447	MET
1	C	452	VAL
1	C	463	THR
1	C	472	ILE

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Mol	Chain	Res	Type
1	C	476	SER
1	C	482	VAL
1	C	510	LYS
1	C	513	PHE
1	C	526	HIS
1	C	538	THR
1	C	540	ARG
1	C	555	LEU
1	C	559	LEU
1	C	564	LEU
1	C	602	GLU
1	C	608	SER
1	C	624	THR
1	C	634	TRP
1	C	649	MET
1	C	659	LYS
1	C	662	MET
1	C	666	PHE
1	C	673	GLU
1	C	678	THR
1	C	694	LYS
1	C	695	LEU
1	C	696	THR
1	C	721	LEU
1	C	733	GLN
1	C	734	GLU
1	C	741	VAL
1	C	746	ILE
1	C	748	THR
1	C	804	PHE
1	C	808	ARG
1	C	843	LEU
1	C	847	LEU
1	C	860	THR
1	C	865	GLN
1	C	868	LEU
1	C	876	LEU
1	C	886	LEU
1	C	887	CYS
1	C	914	LEU
1	C	947	GLU
1	C	950	LYS

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Mol	Chain	Res	Type
1	C	971	ARG
1	C	975	ILE
1	C	980	LEU
1	C	991	ILE
1	C	1033	PHE
1	C	1040	ILE
1	C	1041	GLU
1	C	1044	HIS
1	D	3	ASN
1	D	49	TYR
1	D	101	ASP
1	D	102	ILE
1	D	146	ASP
1	D	151	GLN
1	D	152	GLU
1	D	253	VAL
1	D	276	ASP
1	D	280	GLU
1	D	336	SER
1	D	353	LEU
1	D	355	MET
1	D	357	LEU
1	D	360	GLN
1	D	362	PHE
1	D	400	LEU
1	D	429	GLU
1	D	434	SER
1	D	462	SER
1	D	483	LEU
1	D	493	CYS
1	D	502	LYS
1	D	505	HIS
1	D	523	SER
1	D	526	HIS
1	D	538	THR
1	D	559	LEU
1	D	563	PHE
1	D	573	MET
1	D	578	LEU
1	D	602	GLU
1	D	603	LYS
1	D	608	SER

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Mol	Chain	Res	Type
1	D	624	THR
1	D	634	TRP
1	D	657	GLN
1	D	659	LYS
1	D	662	MET
1	D	673	GLU
1	D	697	GLN
1	D	717	ARG
1	D	733	GLN
1	D	741	VAL
1	D	748	THR
1	D	797	GLN
1	D	804	PHE
1	D	843	LEU
1	D	901	VAL
1	D	931	LEU
1	D	951	ASP
1	D	961	ILE
1	D	968	VAL
1	D	971	ARG
1	D	975	ILE
1	D	1035	ARG
1	D	1036	LYS
1	D	1037	ASN
1	D	1038	GLU
1	E	3	ASN
1	E	10	ILE
1	E	17	ILE
1	E	28	LEU
1	E	45	ILE
1	E	49	TYR
1	E	58	GLN
1	E	60	THR
1	E	82	SER
1	E	87	THR
1	E	91	THR
1	E	93	THR
1	E	102	ILE
1	E	105	VAL
1	E	110	LYS
1	E	113	LEU
1	E	117	LEU

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Mol	Chain	Res	Type
1	E	128	SER
1	E	146	ASP
1	E	153	ASP
1	E	156	ASP
1	E	166	ILE
1	E	174	ASP
1	E	175	VAL
1	E	205	THR
1	E	213	GLN
1	E	218	GLN
1	E	229	GLN
1	E	233	SER
1	E	238	THR
1	E	249	ILE
1	E	250	LEU
1	E	253	VAL
1	E	255	GLN
1	E	259	ARG
1	E	268	ILE
1	E	276	ASP
1	E	280	GLU
1	E	295	THR
1	E	298	ASN
1	E	300	LEU
1	E	310	LEU
1	E	321	LEU
1	E	323	ILE
1	E	329	THR
1	E	330	THR
1	E	352	PHE
1	E	355	MET
1	E	365	THR
1	E	372	VAL
1	E	400	LEU
1	E	404	LEU
1	E	418	ARG
1	E	432	ARG
1	E	445	ILE
1	E	449	LEU
1	E	450	SER
1	E	456	MET
1	E	459	PHE

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Mol	Chain	Res	Type
1	E	480	LEU
1	E	482	VAL
1	E	507	GLU
1	E	512	PHE
1	E	558	ARG
1	E	563	PHE
1	E	564	LEU
1	E	593	GLU
1	E	607	GLU
1	E	608	SER
1	E	613	ASN
1	E	634	TRP
1	E	642	ASN
1	E	653	ARG
1	E	659	LYS
1	E	673	GLU
1	E	683	GLU
1	E	687	GLN
1	E	690	LEU
1	E	694	LYS
1	E	703	LEU
1	E	708	LYS
1	E	714	THR
1	E	717	ARG
1	E	741	VAL
1	E	748	THR
1	E	767	ARG
1	E	804	PHE
1	E	806	SER
1	E	817	GLU
1	E	835	LYS
1	E	844	MET
1	E	857	TYR
1	E	865	GLN
1	E	871	ASN
1	E	886	LEU
1	E	907	LEU
1	E	914	LEU
1	E	917	THR
1	E	931	LEU
1	E	937	LEU
1	E	947	GLU

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Mol	Chain	Res	Type
1	E	958	LYS
1	E	961	ILE
1	E	987	MET
1	E	1001	ASN
1	E	1017	LEU
1	E	1021	PHE
1	E	1030	ARG
1	E	1036	LYS
1	E	1042	HIS
1	F	3	ASN
1	F	6	ILE
1	F	7	ASP
1	F	28	LEU
1	F	34	GLN
1	F	45	ILE
1	F	48	SER
1	F	49	TYR
1	F	60	THR
1	F	104	GLN
1	F	112	GLN
1	F	120	GLN
1	F	148	THR
1	F	151	GLN
1	F	182	TYR
1	F	243	THR
1	F	276	ASP
1	F	280	GLU
1	F	330	THR
1	F	335	ILE
1	F	392	THR
1	F	429	GLU
1	F	434	SER
1	F	439	GLN
1	F	452	VAL
1	F	456	MET
1	F	472	ILE
1	F	476	SER
1	F	481	SER
1	F	482	VAL
1	F	493	CYS
1	F	512	PHE
1	F	526	HIS

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Mol	Chain	Res	Type
1	F	534	ILE
1	F	578	LEU
1	F	604	ASN
1	F	608	SER
1	F	626	ILE
1	F	634	TRP
1	F	643	LYS
1	F	649	MET
1	F	666	PHE
1	F	674	LEU
1	F	694	LYS
1	F	703	LEU
1	F	734	GLU
1	F	804	PHE
1	F	808	ARG
1	F	847	LEU
1	F	860	THR
1	F	864	TYR
1	F	865	GLN
1	F	868	LEU
1	F	876	LEU
1	F	887	CYS
1	F	895	TRP
1	F	918	PHE
1	F	947	GLU
1	F	950	LYS
1	F	958	LYS
1	F	961	ILE
1	F	990	VAL
1	F	991	ILE
1	F	1011	MET
1	F	1015	THR
1	F	1042	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	231	ASN
1	A	584	GLN
1	B	63	GLN
1	B	108	GLN

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Mol	Chain	Res	Type
1	B	189	ASN
1	B	213	GLN
1	B	584	GLN
1	B	709	HIS
1	B	760	ASN
1	B	865	GLN
1	B	1037	ASN
1	C	67	GLN
1	C	70	ASN
1	C	928	GLN
1	D	151	GLN
1	D	505	HIS
1	E	34	GLN
1	E	112	GLN
1	E	123	GLN
1	E	125	GLN
1	E	189	ASN
1	E	211	ASN
1	E	588	GLN
1	E	592	ASN
1	E	613	ASN
1	E	760	ASN
1	F	63	GLN
1	F	67	GLN
1	F	70	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LMT	A	1101	-	36,36,36	1.82	10 (27%)	47,47,47	1.27	6 (12%)
2	LMT	B	1101	-	36,36,36	1.78	9 (25%)	47,47,47	1.34	8 (17%)
2	LMT	C	1101	-	36,36,36	1.71	7 (19%)	47,47,47	1.61	10 (21%)
2	LMT	D	1101	-	36,36,36	1.74	9 (25%)	47,47,47	1.37	7 (14%)
2	LMT	E	1101	-	36,36,36	1.81	11 (30%)	47,47,47	1.45	7 (14%)
2	LMT	F	1101	-	36,36,36	1.93	10 (27%)	47,47,47	1.45	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	A	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	B	1101	-	1/1/10/10	0/21/61/61	0/2/2/2
2	LMT	C	1101	-	1/1/10/10	0/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	E	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	F	1101	-	-	0/21/61/61	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	LMT	C6'-C5'	-3.46	1.39	1.51
2	C	1101	LMT	C6'-C5'	-3.35	1.40	1.51
2	B	1101	LMT	C6'-C5'	-3.19	1.40	1.51
2	F	1101	LMT	C6'-C5'	-3.11	1.40	1.51
2	A	1101	LMT	C6'-C5'	-3.04	1.41	1.51
2	A	1101	LMT	C3'-C2'	-3.00	1.44	1.52
2	C	1101	LMT	C3'-C2'	-2.99	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	C6'-C5'	-2.89	1.41	1.51
2	D	1101	LMT	C3B-C2B	-2.75	1.45	1.52
2	E	1101	LMT	C3B-C2B	-2.54	1.45	1.52
2	D	1101	LMT	C3'-C2'	-2.45	1.45	1.52
2	E	1101	LMT	C3'-C2'	-2.37	1.46	1.52
2	F	1101	LMT	C3'-C2'	-2.33	1.46	1.52
2	F	1101	LMT	C3B-C2B	-2.32	1.46	1.52
2	B	1101	LMT	C3'-C2'	-2.26	1.46	1.52
2	D	1101	LMT	O2'-C2'	2.01	1.47	1.43
2	B	1101	LMT	O3'-C3'	2.02	1.47	1.43
2	A	1101	LMT	O2'-C2'	2.02	1.47	1.43
2	E	1101	LMT	C5-C4	2.06	1.63	1.51
2	F	1101	LMT	C5-C4	2.07	1.63	1.51
2	A	1101	LMT	C5-C4	2.07	1.63	1.51
2	E	1101	LMT	O2'-C2'	2.09	1.47	1.43
2	A	1101	LMT	O3'-C3'	2.15	1.48	1.43
2	B	1101	LMT	O2'-C2'	2.16	1.48	1.43
2	E	1101	LMT	O3'-C3'	2.20	1.48	1.43
2	F	1101	LMT	O2'-C2'	2.29	1.48	1.43
2	D	1101	LMT	O3B-C3B	2.65	1.49	1.43
2	E	1101	LMT	O3B-C3B	2.66	1.49	1.43
2	C	1101	LMT	O3B-C3B	2.66	1.49	1.43
2	A	1101	LMT	O3B-C3B	2.67	1.49	1.43
2	A	1101	LMT	O1'-C1'	2.71	1.45	1.40
2	D	1101	LMT	O1'-C1'	2.71	1.45	1.40
2	F	1101	LMT	O3B-C3B	2.79	1.49	1.43
2	D	1101	LMT	O5'-C1'	3.02	1.49	1.41
2	B	1101	LMT	O5'-C1'	3.05	1.49	1.41
2	C	1101	LMT	O5'-C1'	3.11	1.49	1.41
2	A	1101	LMT	O5'-C1'	3.13	1.49	1.41
2	B	1101	LMT	O3B-C3B	3.28	1.50	1.43
2	E	1101	LMT	O5'-C1'	3.28	1.50	1.41
2	D	1101	LMT	O5B-C1B	3.37	1.50	1.41
2	C	1101	LMT	O1'-C1'	3.38	1.46	1.40
2	E	1101	LMT	O5B-C1B	3.44	1.50	1.41
2	D	1101	LMT	O5'-C5'	3.56	1.53	1.44
2	A	1101	LMT	O5B-C1B	3.57	1.51	1.41
2	B	1101	LMT	O1'-C1'	3.61	1.46	1.40
2	B	1101	LMT	O5'-C5'	3.66	1.53	1.44
2	C	1101	LMT	O5'-C5'	3.69	1.53	1.44
2	C	1101	LMT	O5B-C1B	3.75	1.51	1.41
2	B	1101	LMT	O5B-C1B	3.78	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	LMT	O5'-C1'	3.81	1.51	1.41
2	E	1101	LMT	O1'-C1'	3.82	1.47	1.40
2	E	1101	LMT	O5'-C5'	3.96	1.54	1.44
2	F	1101	LMT	O5B-C1B	3.97	1.52	1.41
2	A	1101	LMT	O5'-C5'	4.27	1.55	1.44
2	F	1101	LMT	O1'-C1'	4.33	1.48	1.40
2	F	1101	LMT	O5'-C5'	4.58	1.55	1.44

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1101	LMT	O3B-C3B-C2B	-4.15	101.01	110.36
2	A	1101	LMT	C1B-O1B-C4'	-3.76	107.99	118.00
2	D	1101	LMT	C1B-O1B-C4'	-3.59	108.46	118.00
2	C	1101	LMT	O5B-C5B-C4B	-3.47	103.05	109.67
2	A	1101	LMT	C1'-C2'-C3'	-2.97	104.09	109.98
2	C	1101	LMT	O3'-C3'-C2'	-2.80	104.04	110.36
2	F	1101	LMT	C1B-O1B-C4'	-2.59	111.13	118.00
2	E	1101	LMT	C1B-O1B-C4'	-2.49	111.37	118.00
2	D	1101	LMT	O2B-C2B-C3B	-2.42	104.90	110.36
2	E	1101	LMT	C6B-C5B-C4B	-2.23	107.39	112.99
2	C	1101	LMT	O4'-C4B-C3B	-2.14	105.54	110.36
2	B	1101	LMT	O2'-C2'-C3'	-2.12	105.58	110.36
2	C	1101	LMT	O6'-C6'-C5'	-2.07	104.38	111.30
2	B	1101	LMT	C6B-C5B-C4B	-2.06	107.83	112.99
2	C	1101	LMT	O1B-C1B-C2B	2.03	113.15	108.12
2	D	1101	LMT	C3B-C4B-C5B	2.05	113.89	110.23
2	F	1101	LMT	O5'-C5'-C4'	2.09	114.23	109.78
2	A	1101	LMT	C4B-C3B-C2B	2.11	114.67	110.79
2	A	1101	LMT	C1B-C2B-C3B	2.13	114.20	109.98
2	D	1101	LMT	O1'-C1'-C2'	2.13	110.63	108.00
2	E	1101	LMT	O1'-C1'-C2'	2.27	110.80	108.00
2	D	1101	LMT	C4B-C3B-C2B	2.30	115.02	110.79
2	E	1101	LMT	C1-O1'-C1'	2.31	118.03	114.00
2	B	1101	LMT	C3B-C4B-C5B	2.35	114.42	110.23
2	A	1101	LMT	O5B-C1B-C2B	2.37	115.21	110.28
2	A	1101	LMT	O1'-C1'-C2'	2.44	111.00	108.00
2	B	1101	LMT	C2'-C3'-C4'	2.45	115.04	109.63
2	B	1101	LMT	C1'-C2'-C3'	2.46	114.87	109.98
2	E	1101	LMT	C1'-C2'-C3'	2.57	115.08	109.98
2	F	1101	LMT	C1-O1'-C1'	2.71	118.73	114.00
2	D	1101	LMT	O5B-C5B-C4B	2.76	114.93	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1101	LMT	O5B-C5B-C6B	2.88	113.85	106.38
2	C	1101	LMT	O1'-C1'-C2'	2.91	111.58	108.00
2	F	1101	LMT	C1'-O5'-C5'	2.95	119.52	113.74
2	B	1101	LMT	O5B-C5B-C6B	2.97	114.07	106.38
2	B	1101	LMT	O1'-C1'-C2'	3.18	111.91	108.00
2	C	1101	LMT	C1B-C2B-C3B	3.23	116.38	109.98
2	B	1101	LMT	C1-O1'-C1'	3.24	119.67	114.00
2	C	1101	LMT	C3B-C4B-C5B	3.27	116.07	110.23
2	F	1101	LMT	C1B-O5B-C5B	3.57	120.76	113.74
2	F	1101	LMT	O1'-C1'-C2'	3.79	112.66	108.00
2	F	1101	LMT	O5B-C5B-C4B	3.84	116.99	109.67
2	E	1101	LMT	C3B-C4B-C5B	3.85	117.10	110.23
2	E	1101	LMT	O5B-C5B-C4B	4.30	117.86	109.67
2	C	1101	LMT	C4B-C3B-C2B	4.67	119.39	110.79

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1101	LMT	C3B
2	C	1101	LMT	C3B

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	LMT	4	0
2	B	1101	LMT	3	0
2	C	1101	LMT	4	0
2	D	1101	LMT	1	0
2	E	1101	LMT	4	0
2	F	1101	LMT	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1042/1049 (99%)	0.32	85 (8%) 14 7	28, 63, 113, 139	0
1	B	1046/1049 (99%)	0.18	71 (6%) 20 10	26, 57, 100, 161	0
1	C	1044/1049 (99%)	0.46	117 (11%) 7 3	17, 56, 98, 173	0
1	D	1042/1049 (99%)	0.46	115 (11%) 7 3	21, 81, 133, 168	0
1	E	1042/1049 (99%)	0.53	132 (12%) 5 2	38, 77, 119, 154	0
1	F	1046/1049 (99%)	0.63	154 (14%) 3 2	29, 73, 120, 143	0
All	All	6262/6294 (99%)	0.43	674 (10%) 8 4	17, 68, 116, 173	0

All (674) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	314	GLU	16.2
1	E	315	PRO	15.9
1	D	869	SER	14.3
1	F	481	SER	12.4
1	E	128	SER	12.3
1	C	720	GLY	11.9
1	B	315	PRO	11.2
1	C	719	ASN	10.8
1	F	676	THR	10.8
1	F	442	LEU	10.7
1	F	941	ASN	10.3
1	F	719	ASN	10.3
1	B	314	GLU	10.2
1	F	836	SER	9.9
1	E	129	VAL	9.2
1	F	406	VAL	9.1
1	F	127	VAL	9.0
1	F	128	SER	8.9
1	B	869	SER	8.7

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Mol	Chain	Res	Type	RSRZ
1	D	461	GLY	8.6
1	F	829	GLY	8.6
1	D	322	LYS	8.5
1	D	689	GLY	8.5
1	E	311	ALA	8.4
1	F	403	GLY	7.8
1	C	402	ILE	7.7
1	E	44	THR	7.5
1	E	408	ASP	7.5
1	E	348	ILE	7.5
1	F	441	ALA	7.5
1	D	719	ASN	7.3
1	D	459	PHE	7.3
1	F	407	ASP	7.1
1	C	403	GLY	7.1
1	F	618	ALA	7.1
1	F	46	SER	7.1
1	F	828	LEU	7.1
1	F	402	ILE	7.1
1	A	369	THR	7.1
1	E	405	LEU	7.0
1	C	837	THR	6.9
1	D	720	GLY	6.9
1	E	310	LEU	6.8
1	F	720	GLY	6.8
1	F	445	ILE	6.8
1	A	404	LEU	6.7
1	E	978	THR	6.6
1	E	307	ARG	6.6
1	A	396	PHE	6.5
1	F	617	ALA	6.5
1	F	410	ILE	6.4
1	C	314	GLU	6.4
1	A	35	TYR	6.3
1	C	826	GLU	6.3
1	E	409	ALA	6.3
1	F	675	GLY	6.2
1	E	487	ILE	6.2
1	A	408	ASP	6.1
1	B	617	ALA	6.1
1	C	481	SER	6.0
1	E	164	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	482	VAL	6.0
1	A	372	VAL	6.0
1	C	445	ILE	6.0
1	E	406	VAL	5.9
1	E	443	VAL	5.9
1	E	105	VAL	5.9
1	E	322	LYS	5.8
1	D	460	GLY	5.8
1	F	700	ASN	5.8
1	E	977	MET	5.7
1	A	174	ASP	5.7
1	C	406	VAL	5.7
1	E	869	SER	5.6
1	F	111	LEU	5.6
1	D	690	LEU	5.6
1	D	617	ALA	5.6
1	D	868	LEU	5.5
1	F	405	LEU	5.5
1	F	449	LEU	5.5
1	F	937	LEU	5.5
1	C	618	ALA	5.4
1	E	308	ALA	5.4
1	F	446	ALA	5.4
1	D	851	LEU	5.4
1	D	128	SER	5.4
1	F	448	VAL	5.3
1	A	371	ALA	5.3
1	C	501	ALA	5.3
1	C	721	LEU	5.3
1	D	282	ASN	5.3
1	E	46	SER	5.3
1	F	837	THR	5.2
1	C	835	LYS	5.2
1	F	362	PHE	5.2
1	F	834	GLY	5.2
1	E	981	ALA	5.2
1	E	317	PHE	5.2
1	C	676	THR	5.2
1	F	711	ASP	5.2
1	F	718	PRO	5.1
1	C	322	LYS	5.0
1	C	838	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	486	LEU	5.0
1	C	48	SER	5.0
1	A	368	PRO	5.0
1	C	449	LEU	5.0
1	E	108	GLN	5.0
1	F	835	LYS	5.0
1	F	474	ILE	5.0
1	C	127	VAL	4.9
1	E	442	LEU	4.9
1	D	486	LEU	4.9
1	A	400	LEU	4.9
1	C	448	VAL	4.9
1	E	933	THR	4.9
1	F	47	ALA	4.9
1	C	856	GLY	4.9
1	F	873	ALA	4.9
1	E	352	PHE	4.8
1	A	376	LEU	4.8
1	E	410	ILE	4.8
1	D	174	ASP	4.8
1	F	48	SER	4.8
1	E	47	ALA	4.8
1	A	321	LEU	4.8
1	C	446	ALA	4.8
1	F	826	GLU	4.8
1	F	315	PRO	4.7
1	D	400	LEU	4.7
1	A	935	ILE	4.7
1	F	944	LEU	4.7
1	C	129	VAL	4.7
1	E	398	MET	4.7
1	E	316	PHE	4.7
1	F	408	ASP	4.7
1	A	976	LEU	4.7
1	E	370	ILE	4.6
1	D	688	ALA	4.6
1	C	442	LEU	4.6
1	C	405	LEU	4.6
1	F	717	ARG	4.6
1	D	145	THR	4.6
1	E	33	ALA	4.6
1	E	944	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	982	PHE	4.6
1	D	839	GLU	4.6
1	C	717	ARG	4.6
1	A	405	LEU	4.6
1	F	699	ARG	4.6
1	D	401	ALA	4.5
1	E	929	VAL	4.5
1	B	322	LYS	4.5
1	C	674	LEU	4.5
1	E	349	ILE	4.5
1	D	408	ASP	4.5
1	A	881	LEU	4.5
1	D	575	MET	4.5
1	E	127	VAL	4.5
1	F	109	ASN	4.5
1	E	488	LEU	4.5
1	E	362	PHE	4.5
1	C	836	SER	4.4
1	D	853	THR	4.4
1	F	372	VAL	4.4
1	E	104	GLN	4.4
1	C	394	THR	4.4
1	A	128	SER	4.4
1	A	899	PHE	4.4
1	C	500	ILE	4.4
1	F	404	LEU	4.4
1	F	502	LYS	4.4
1	E	130	GLU	4.3
1	C	831	ALA	4.3
1	C	398	MET	4.3
1	E	402	ILE	4.3
1	E	1019	ILE	4.3
1	E	404	LEU	4.3
1	F	874	PRO	4.3
1	F	500	ILE	4.3
1	E	369	THR	4.3
1	F	444	GLY	4.3
1	E	111	LEU	4.2
1	F	110	LYS	4.2
1	B	316	PHE	4.2
1	F	938	SER	4.2
1	D	687	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	129	VAL	4.2
1	A	15	ILE	4.2
1	E	483	LEU	4.1
1	A	411	VAL	4.1
1	F	888	LEU	4.1
1	D	836	SER	4.1
1	C	718	PRO	4.1
1	D	576	VAL	4.1
1	E	367	ILE	4.1
1	D	404	LEU	4.1
1	F	662	MET	4.1
1	A	640	GLU	4.1
1	D	458	PHE	4.0
1	A	485	ALA	4.0
1	E	366	LEU	4.0
1	C	502	LYS	4.0
1	D	411	VAL	4.0
1	D	852	PRO	4.0
1	A	355	MET	4.0
1	D	136	PHE	4.0
1	E	109	ASN	4.0
1	F	712	MET	4.0
1	D	487	ILE	4.0
1	F	482	VAL	4.0
1	F	904	VAL	4.0
1	C	128	SER	4.0
1	D	15	ILE	4.0
1	A	1017	LEU	4.0
1	F	33	ALA	4.0
1	A	322	LYS	4.0
1	A	882	ILE	4.0
1	F	322	LYS	4.0
1	C	390	ILE	3.9
1	F	1016	VAL	3.9
1	E	678	THR	3.9
1	A	407	ASP	3.9
1	C	441	ALA	3.9
1	D	482	VAL	3.9
1	E	400	LEU	3.9
1	D	386	PHE	3.9
1	C	372	VAL	3.9
1	D	791	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	79	SER	3.9
1	D	866	GLU	3.8
1	B	129	VAL	3.8
1	C	408	ASP	3.8
1	A	719	ASN	3.8
1	F	501	ALA	3.8
1	C	410	ILE	3.8
1	D	870	GLY	3.8
1	B	348	ILE	3.8
1	F	443	VAL	3.8
1	E	395	MET	3.8
1	A	16	ALA	3.8
1	D	875	SER	3.8
1	A	410	ILE	3.8
1	A	878	ALA	3.8
1	F	117	LEU	3.8
1	F	976	LEU	3.8
1	E	466	ILE	3.8
1	F	484	VAL	3.8
1	E	282	ASN	3.7
1	C	33	ALA	3.7
1	A	470	PHE	3.7
1	F	398	MET	3.7
1	E	617	ALA	3.7
1	D	462	SER	3.7
1	C	315	PRO	3.7
1	C	712	MET	3.7
1	B	406	VAL	3.7
1	D	611	ALA	3.6
1	E	904	VAL	3.6
1	A	129	VAL	3.6
1	A	392	THR	3.6
1	B	111	LEU	3.6
1	A	456	MET	3.6
1	E	868	LEU	3.6
1	E	407	ASP	3.6
1	F	376	LEU	3.6
1	C	941	ASN	3.6
1	D	835	LYS	3.6
1	E	974	PRO	3.6
1	E	43	VAL	3.5
1	D	321	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	715	SER	3.5
1	C	404	LEU	3.5
1	D	867	ARG	3.5
1	A	871	ASN	3.5
1	E	291	ILE	3.5
1	B	317	PHE	3.5
1	F	16	ALA	3.5
1	E	980	LEU	3.5
1	F	865	GLN	3.5
1	C	474	ILE	3.4
1	C	307	ARG	3.4
1	E	484	VAL	3.4
1	F	409	ALA	3.4
1	F	399	VAL	3.4
1	D	396	PHE	3.4
1	D	44	THR	3.4
1	D	113	LEU	3.4
1	E	321	LEU	3.4
1	C	494	ALA	3.4
1	C	1044	HIS	3.4
1	A	403	GLY	3.4
1	F	1015	THR	3.4
1	D	383	LEU	3.4
1	D	718	PRO	3.4
1	E	937	LEU	3.4
1	A	1013	THR	3.4
1	B	842	GLU	3.4
1	A	351	VAL	3.4
1	B	177	LEU	3.3
1	D	111	LEU	3.3
1	F	591	LEU	3.3
1	A	136	PHE	3.3
1	B	371	ALA	3.3
1	B	663	VAL	3.3
1	F	356	TYR	3.3
1	B	542	LEU	3.3
1	D	618	ALA	3.3
1	E	126	GLY	3.3
1	B	113	LEU	3.3
1	D	112	GLN	3.2
1	B	671	ILE	3.2
1	F	477	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	833	PRO	3.2
1	F	945	ILE	3.2
1	F	470	PHE	3.2
1	C	69	MET	3.2
1	A	481	SER	3.2
1	C	711	ASP	3.2
1	F	395	MET	3.2
1	B	871	ASN	3.2
1	E	940	LYS	3.2
1	F	69	MET	3.2
1	D	850	LYS	3.2
1	C	868	LEU	3.2
1	F	193	LEU	3.2
1	D	11	PHE	3.2
1	E	107	VAL	3.2
1	C	38	ILE	3.2
1	A	982	PHE	3.2
1	B	128	SER	3.2
1	B	408	ASP	3.2
1	C	473	THR	3.2
1	A	617	ALA	3.1
1	E	618	ALA	3.1
1	C	401	ALA	3.1
1	A	938	SER	3.1
1	E	303	ALA	3.1
1	C	400	LEU	3.1
1	D	483	LEU	3.1
1	F	473	THR	3.1
1	D	463	THR	3.1
1	C	321	LEU	3.1
1	D	886	LEU	3.1
1	E	86	GLY	3.1
1	E	351	VAL	3.1
1	E	718	PRO	3.1
1	A	445	ILE	3.1
1	F	877	TYR	3.1
1	C	478	MET	3.1
1	E	177	LEU	3.1
1	C	444	GLY	3.0
1	D	67	GLN	3.0
1	E	401	ALA	3.0
1	F	881	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	311	ALA	3.0
1	D	129	VAL	3.0
1	C	9	PRO	3.0
1	C	576	VAL	3.0
1	A	348	ILE	3.0
1	C	611	ALA	3.0
1	D	35	TYR	3.0
1	C	981	ALA	3.0
1	F	940	LYS	3.0
1	E	313	MET	3.0
1	E	1018	ALA	3.0
1	C	791	VAL	3.0
1	E	290	GLY	3.0
1	A	336	SER	3.0
1	A	178	PHE	3.0
1	A	19	ILE	3.0
1	C	699	ARG	2.9
1	F	892	TYR	2.9
1	D	701	GLN	2.9
1	D	577	GLN	2.9
1	E	465	ALA	2.9
1	F	369	THR	2.9
1	F	981	ALA	2.9
1	C	828	LEU	2.9
1	E	312	LYS	2.9
1	E	403	GLY	2.9
1	F	197	GLN	2.9
1	E	995	ALA	2.9
1	C	675	GLY	2.9
1	C	17	ILE	2.9
1	C	1011	MET	2.9
1	D	32	VAL	2.9
1	F	831	ALA	2.9
1	F	396	PHE	2.9
1	B	109	ASN	2.9
1	C	65	ILE	2.9
1	C	162	MET	2.9
1	B	876	LEU	2.9
1	F	869	SER	2.9
1	B	905	VAL	2.9
1	E	162	MET	2.9
1	F	833	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	362	PHE	2.8
1	E	719	ASN	2.8
1	F	1012	VAL	2.8
1	F	178	PHE	2.8
1	A	145	THR	2.8
1	C	122	VAL	2.8
1	B	661	ALA	2.8
1	D	803	ALA	2.8
1	F	3	ASN	2.8
1	F	1037	ASN	2.8
1	C	834	GLY	2.8
1	F	619	GLY	2.8
1	E	65	ILE	2.8
1	F	126	GLY	2.8
1	B	487	ILE	2.8
1	B	870	GLY	2.8
1	C	310	LEU	2.8
1	D	46	SER	2.8
1	E	870	GLY	2.8
1	B	853	THR	2.8
1	C	617	ALA	2.8
1	E	930	GLY	2.8
1	C	577	GLN	2.8
1	E	1022	VAL	2.8
1	D	407	ASP	2.8
1	F	96	SER	2.8
1	B	791	VAL	2.8
1	B	835	LYS	2.8
1	B	852	PRO	2.8
1	E	45	ILE	2.7
1	D	977	MET	2.7
1	F	680	PHE	2.7
1	E	943	ILE	2.7
1	A	397	GLY	2.7
1	C	97	GLY	2.7
1	C	865	GLN	2.7
1	D	114	ALA	2.7
1	E	1015	THR	2.7
1	E	32	VAL	2.7
1	F	335	ILE	2.7
1	F	907	LEU	2.7
1	E	71	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	2.7
1	F	357	LEU	2.7
1	B	18	ILE	2.7
1	D	65	ILE	2.7
1	B	44	THR	2.7
1	C	872	GLN	2.7
1	A	108	GLN	2.7
1	D	767	ARG	2.7
1	D	173	GLY	2.7
1	F	67	GLN	2.7
1	F	462	SER	2.7
1	A	164	ASP	2.7
1	F	116	PRO	2.7
1	D	390	ILE	2.7
1	B	400	LEU	2.6
1	D	976	LEU	2.6
1	F	13	TRP	2.6
1	E	1042	HIS	2.6
1	A	13	TRP	2.6
1	F	478	MET	2.6
1	C	8	ARG	2.6
1	C	395	MET	2.6
1	E	839	GLU	2.6
1	F	122	VAL	2.6
1	A	347	ALA	2.6
1	A	886	LEU	2.6
1	C	111	LEU	2.6
1	D	36	PRO	2.6
1	D	663	VAL	2.6
1	F	176	GLN	2.6
1	F	314	GLU	2.6
1	B	355	MET	2.6
1	F	876	LEU	2.6
1	F	453	PHE	2.6
1	B	866	GLU	2.6
1	C	575	MET	2.6
1	C	389	SER	2.6
1	D	109	ASN	2.6
1	B	662	MET	2.6
1	F	480	LEU	2.6
1	A	401	ALA	2.6
1	E	48	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	463	THR	2.6
1	E	441	ALA	2.6
1	F	830	GLN	2.6
1	D	717	ARG	2.6
1	C	944	LEU	2.6
1	C	417	GLU	2.5
1	A	449	LEU	2.5
1	C	976	LEU	2.5
1	C	937	LEU	2.5
1	D	45	ILE	2.5
1	C	890	ALA	2.5
1	D	837	THR	2.5
1	C	399	VAL	2.5
1	A	1012	VAL	2.5
1	D	447	MET	2.5
1	D	47	ALA	2.5
1	E	480	LEU	2.5
1	B	575	MET	2.5
1	F	38	ILE	2.5
1	B	995	ALA	2.5
1	C	671	ILE	2.5
1	D	43	VAL	2.5
1	A	134	SER	2.5
1	D	48	SER	2.5
1	A	767	ARG	2.5
1	E	926	TYR	2.5
1	E	102	ILE	2.5
1	E	934	THR	2.5
1	F	716	VAL	2.5
1	F	677	ALA	2.5
1	B	67	GLN	2.5
1	D	822	LEU	2.4
1	D	1016	VAL	2.4
1	D	479	ALA	2.4
1	D	982	PHE	2.4
1	D	68	ASN	2.4
1	B	15	ILE	2.4
1	E	323	ILE	2.4
1	F	107	VAL	2.4
1	D	389	SER	2.4
1	A	975	ILE	2.4
1	E	1011	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	143	ILE	2.4
1	F	350	LEU	2.4
1	E	867	ARG	2.4
1	C	977	MET	2.4
1	E	357	LEU	2.4
1	E	145	THR	2.4
1	A	458	PHE	2.4
1	B	851	LEU	2.4
1	F	380	PHE	2.4
1	A	705	GLU	2.4
1	F	371	ALA	2.4
1	F	488	LEU	2.4
1	D	834	GLY	2.4
1	C	356	TYR	2.4
1	F	866	GLU	2.4
1	A	357	LEU	2.4
1	E	798	MET	2.4
1	F	1021	PHE	2.4
1	D	841	MET	2.4
1	A	850	LYS	2.4
1	C	1045	THR	2.4
1	E	353	LEU	2.4
1	E	1007	VAL	2.3
1	D	405	LEU	2.3
1	C	700	ASN	2.3
1	C	1016	VAL	2.3
1	F	459	PHE	2.3
1	D	626	ILE	2.3
1	F	466	ILE	2.3
1	B	50	PRO	2.3
1	C	482	VAL	2.3
1	A	300	LEU	2.3
1	B	618	ALA	2.3
1	C	980	LEU	2.3
1	E	14	VAL	2.3
1	F	170	SER	2.3
1	D	130	GLU	2.3
1	A	337	ILE	2.3
1	B	46	SER	2.3
1	E	806	SER	2.3
1	C	374	VAL	2.3
1	D	686	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	715	SER	2.3
1	D	578	LEU	2.3
1	C	16	ALA	2.3
1	D	878	ALA	2.3
1	E	890	ALA	2.3
1	B	404	LEU	2.3
1	B	886	LEU	2.3
1	F	620	ALA	2.3
1	B	145	THR	2.3
1	E	593	GLU	2.3
1	F	681	ASP	2.3
1	D	882	ILE	2.3
1	A	343	THR	2.3
1	C	871	ASN	2.3
1	F	174	ASP	2.3
1	B	976	LEU	2.3
1	C	117	LEU	2.3
1	A	281	PHE	2.3
1	E	659	LYS	2.3
1	E	158	VAL	2.3
1	F	485	ALA	2.3
1	F	661	ALA	2.3
1	F	790	TYR	2.3
1	F	884	VAL	2.3
1	C	673	GLU	2.2
1	B	410	ILE	2.2
1	C	790	TYR	2.2
1	D	662	MET	2.2
1	C	96	SER	2.2
1	D	163	LYS	2.2
1	F	1011	MET	2.2
1	A	107	VAL	2.2
1	B	706	ALA	2.2
1	B	716	VAL	2.2
1	B	978	THR	2.2
1	F	722	GLU	2.2
1	A	45	ILE	2.2
1	E	901	VAL	2.2
1	F	832	ALA	2.2
1	C	975	ILE	2.2
1	D	354	VAL	2.2
1	D	33	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	467	TYR	2.2
1	C	349	ILE	2.2
1	E	575	MET	2.2
1	A	327	TYR	2.2
1	E	344	LEU	2.2
1	F	868	LEU	2.2
1	A	489	THR	2.2
1	D	403	GLY	2.2
1	B	882	ILE	2.2
1	F	498	LYS	2.2
1	A	27	ILE	2.2
1	B	407	ASP	2.2
1	D	78	MET	2.2
1	B	719	ASN	2.2
1	D	442	LEU	2.1
1	E	976	LEU	2.1
1	B	207	ILE	2.1
1	B	104	GLN	2.1
1	A	874	PRO	2.1
1	E	331	PRO	2.1
1	A	127	VAL	2.1
1	B	108	GLN	2.1
1	A	689	GLY	2.1
1	B	619	GLY	2.1
1	C	116	PRO	2.1
1	D	402	ILE	2.1
1	C	825	MET	2.1
1	E	674	LEU	2.1
1	A	386	PHE	2.1
1	D	12	ALA	2.1
1	B	127	VAL	2.1
1	F	390	ILE	2.1
1	E	78	MET	2.1
1	A	72	ILE	2.1
1	B	45	ILE	2.1
1	D	127	VAL	2.1
1	F	577	GLN	2.1
1	F	801	PHE	2.1
1	E	371	ALA	2.1
1	D	879	ILE	2.1
1	B	125	GLN	2.1
1	C	67	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	503	GLY	2.1
1	F	679	GLY	2.1
1	C	470	PHE	2.1
1	A	130	GLU	2.1
1	B	11	PHE	2.1
1	C	867	ARG	2.1
1	E	412	VAL	2.0
1	B	396	PHE	2.0
1	D	5	PHE	2.0
1	D	317	PHE	2.0
1	E	112	GLN	2.0
1	E	439	GLN	2.0
1	F	575	MET	2.0
1	E	671	ILE	2.0
1	F	383	LEU	2.0
1	B	701	GLN	2.0
1	B	982	PHE	2.0
1	D	592	ASN	2.0
1	F	317	PHE	2.0
1	E	1016	VAL	2.0
1	D	874	PRO	2.0
1	B	121	GLU	2.0
1	D	844	MET	2.0
1	A	393	LEU	2.0
1	C	892	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	LMT	F	1101	35/35	0.81	0.37	1.33	19,65,82,87	0
2	LMT	B	1101	35/35	0.82	0.37	0.90	40,61,68,70	0
2	LMT	A	1101	35/35	0.88	0.32	0.83	40,56,74,75	0
2	LMT	D	1101	35/35	0.86	0.31	0.75	35,48,67,83	0
2	LMT	C	1101	35/35	0.84	0.33	0.72	29,44,62,65	0
2	LMT	E	1101	35/35	0.73	0.40	0.69	43,83,98,109	0
3	NI	A	1102	1/1	0.97	0.08	-	31,31,31,31	0
3	NI	E	1102	1/1	0.99	0.08	-	64,64,64,64	0
3	NI	C	1102	1/1	0.99	0.12	-	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.