Full wwPDB X-ray Structure Validation Report (i)

Jul 19, 2016 – 04:02 AM EDT

PDB ID	:	4ZJL
Title	:	Crystal structure of AcrB in complex with antibiotic in P21 space group
Authors	:	Ababou, A.; Koronakis, V.
Deposited on	:	2015-04-29
Resolution	:	3.47 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 (i) symbol.

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

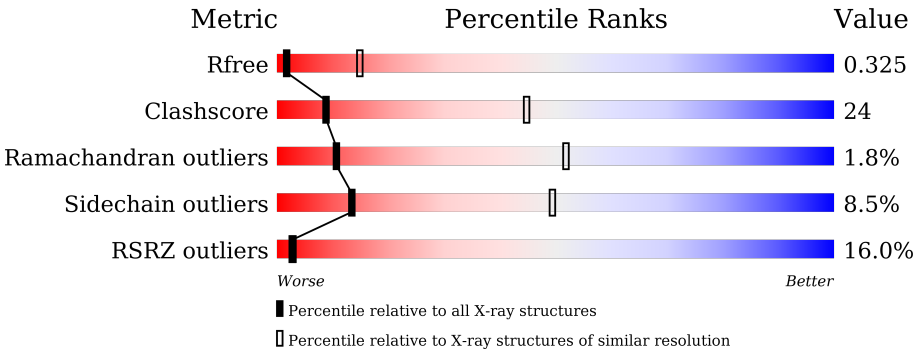
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 3.47 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	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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	13% 52% 43% 5%
1	B	1049	13% 56% 38% 5% •
1	C	1049	16% 50% 45% 5% •
1	D	1049	15% 52% 43% 5% •
1	E	1049	17% 52% 41% 6% •
1	F	1049	20% 50% 43% 6% ••

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	ERY	A	1101	-	-	-	X
2	ERY	D	1101	-	-	-	X
3	LMT	A	1102	-	-	-	X
3	LMT	A	1103	-	-	-	X
3	LMT	B	1101	-	-	-	X
3	LMT	C	1101	-	-	-	X
3	LMT	D	1102	-	-	-	X
3	LMT	D	1103	-	-	-	X
3	LMT	E	1101	-	-	-	X
3	LMT	F	1101	-	-	-	X

2 Entry composition

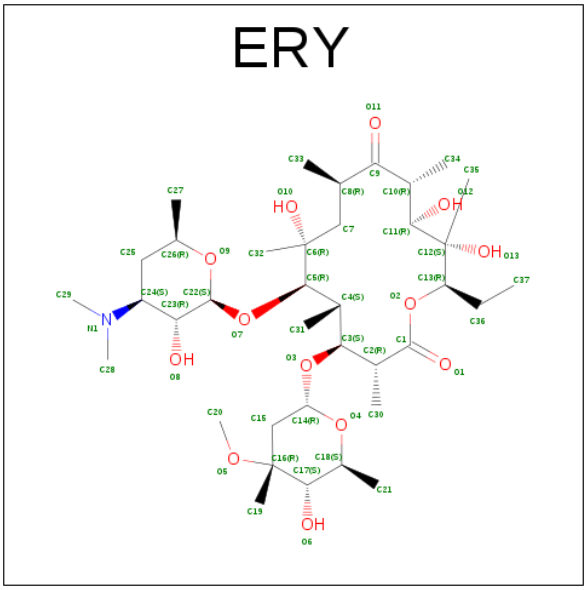
There are 4 unique types of molecules in this entry. The entry contains 47962 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

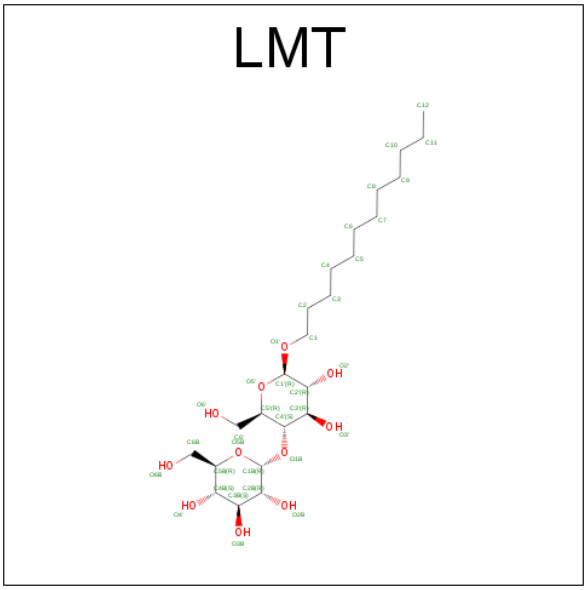
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7942	5105	1315	1479	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	C	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	D	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	F	1043	Total	C	N	O	S	0	0	0
			7935	5101	1314	1477	43			

- Molecule 2 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			51	37	1	13		
2	D	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

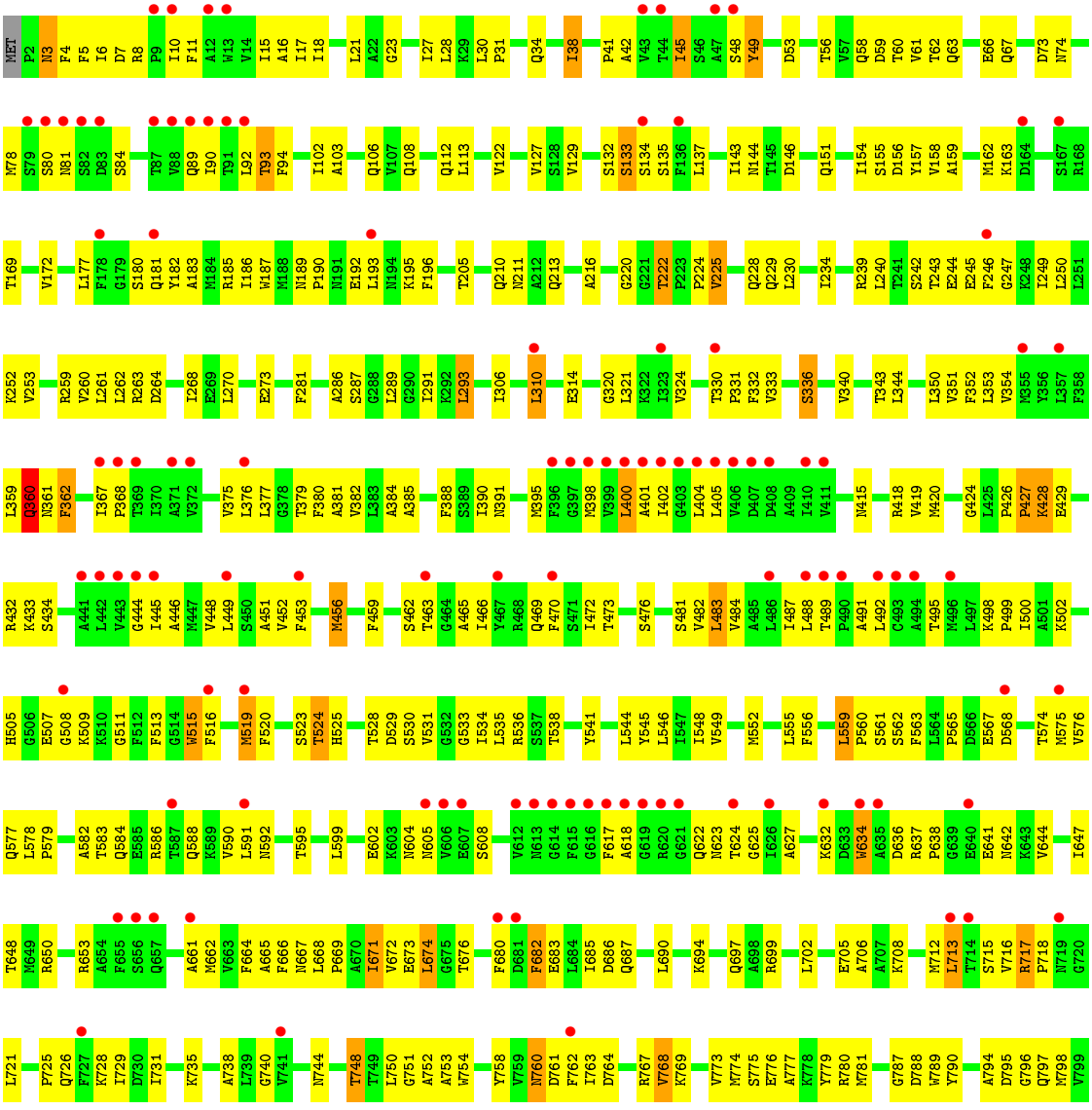
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ni 1 1	0	0
4	C	1	Total Ni 1 1	0	0
4	E	1	Total Ni 1 1	0	0

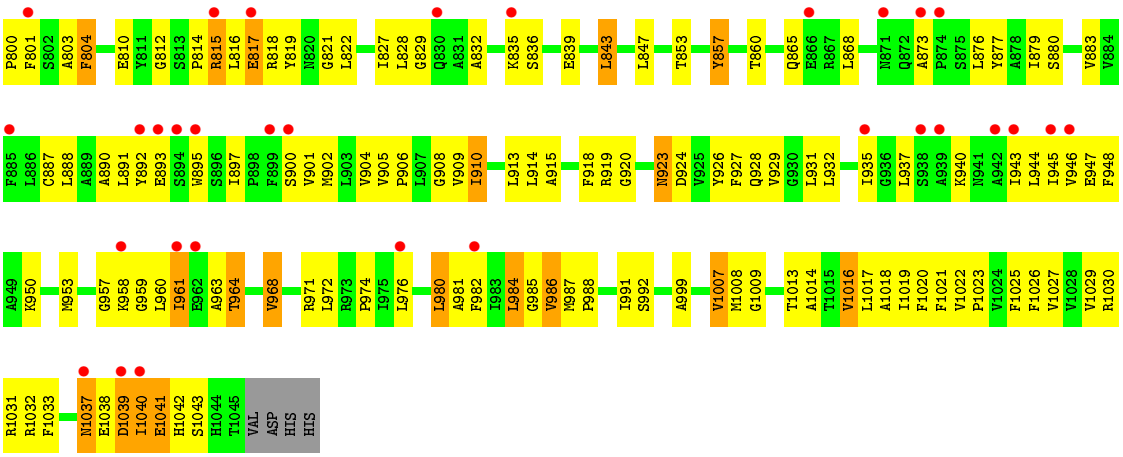
3 Residue-property plots (i)

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

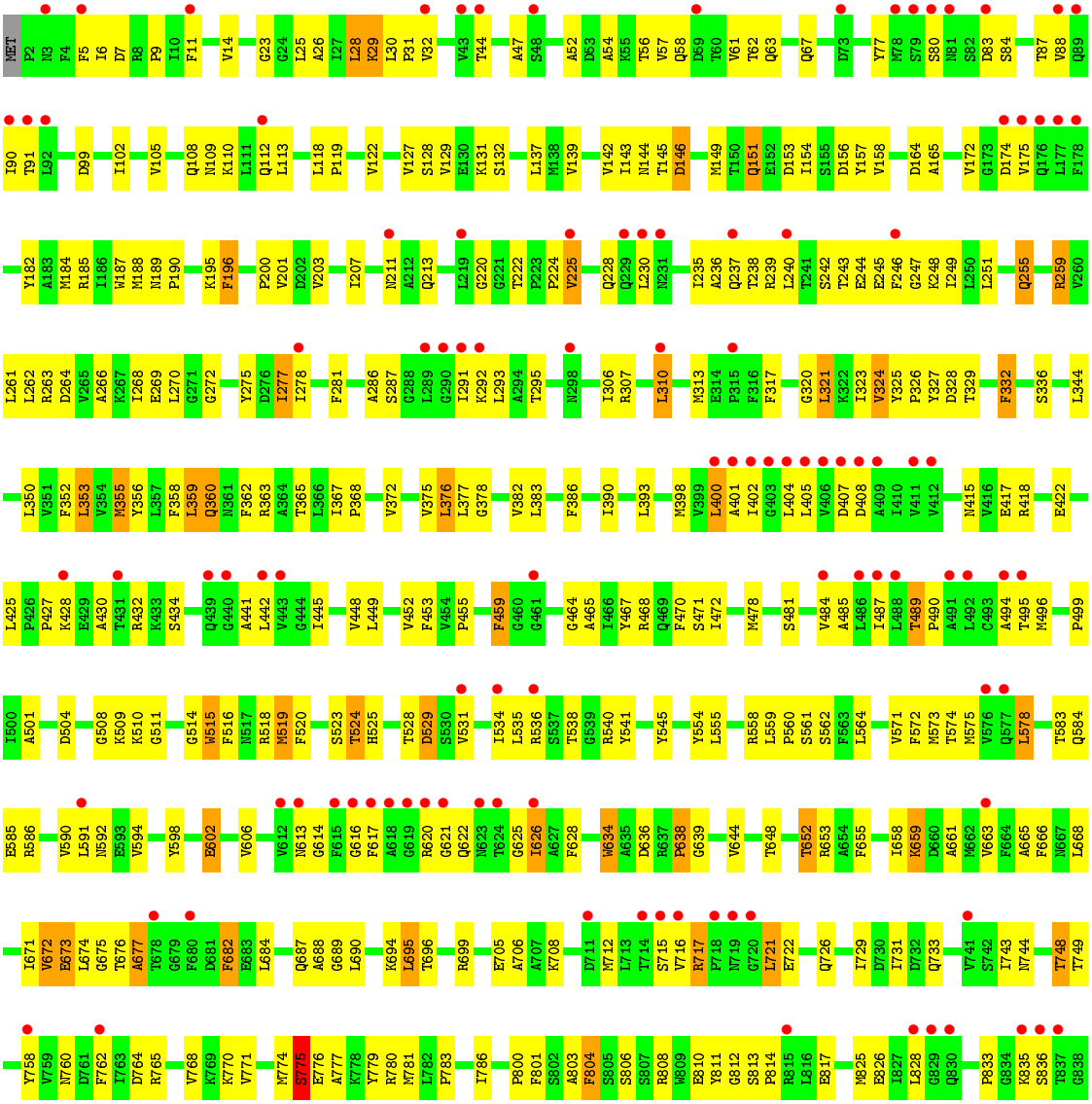
Chain A:

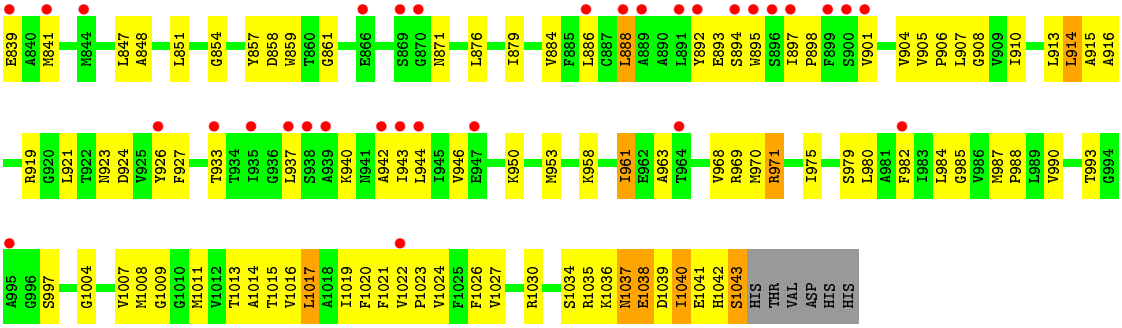




- Molecule 1: Multidrug efflux pump subunit AcrB

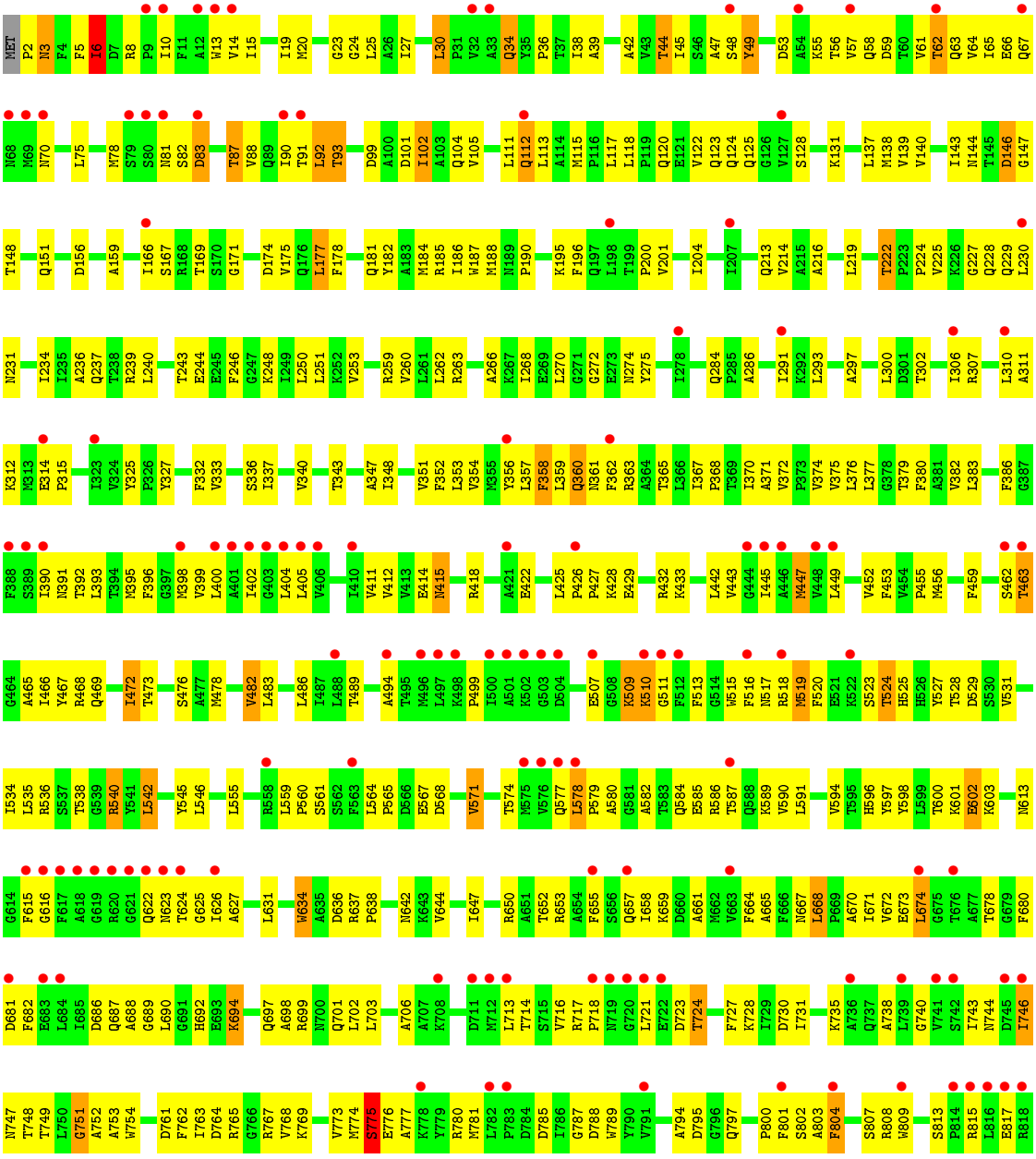
Chain B:

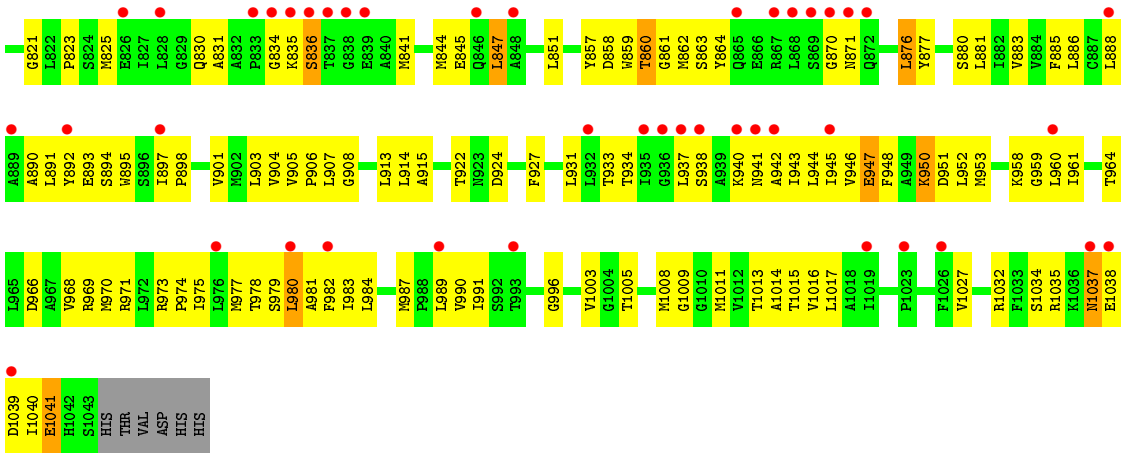




• Molecule 1: Multidrug efflux pump subunit AcrB

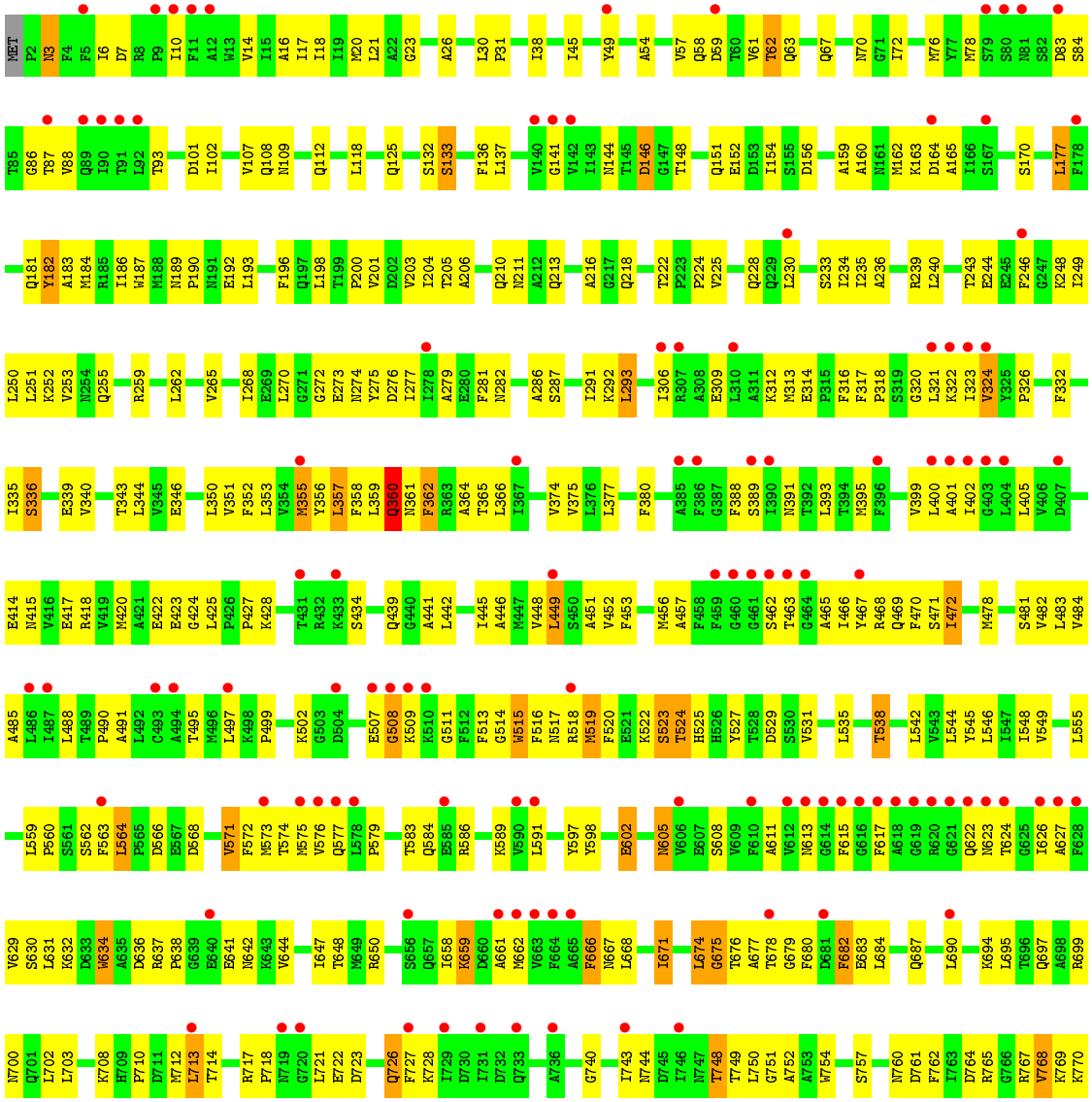
Chain C:

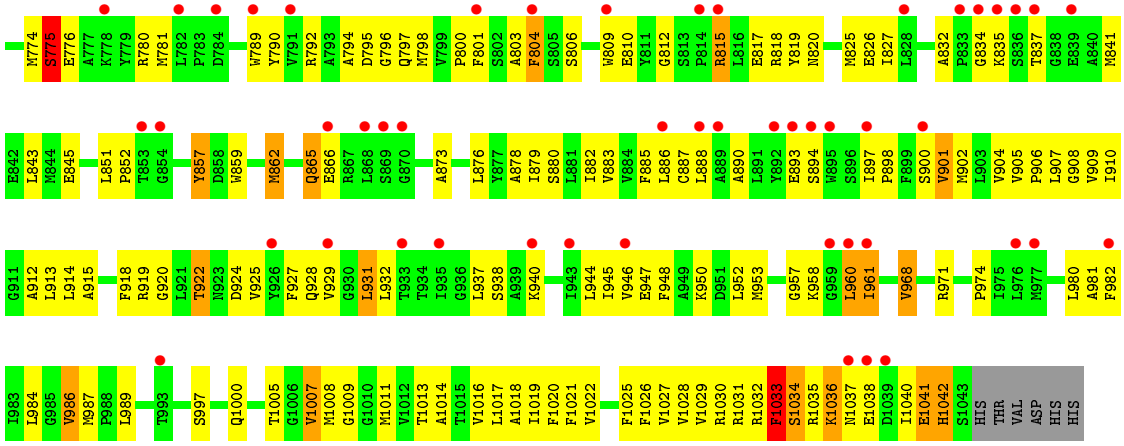




- Molecule 1: Multidrug efflux pump subunit AcrB

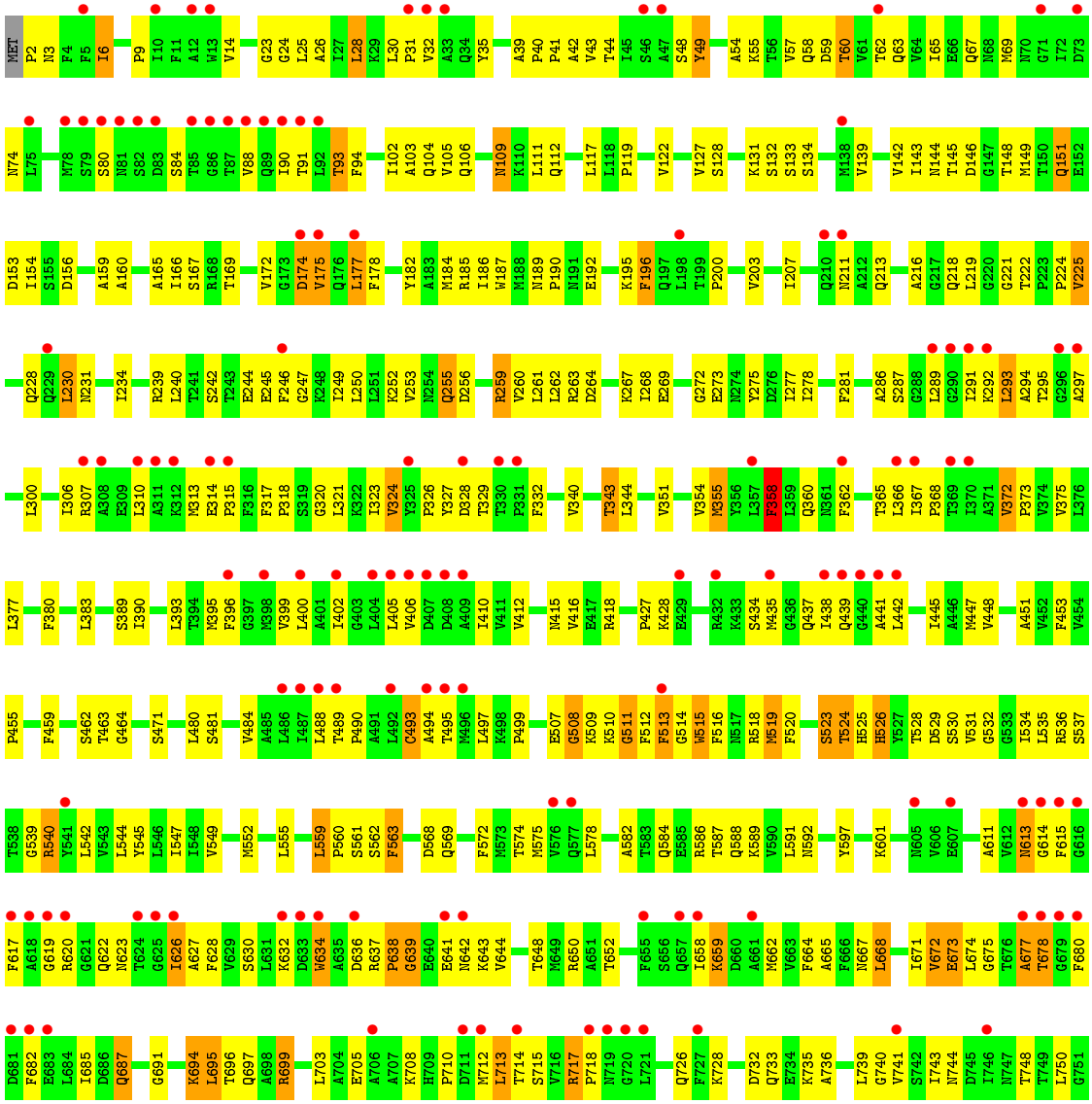
Chain D:

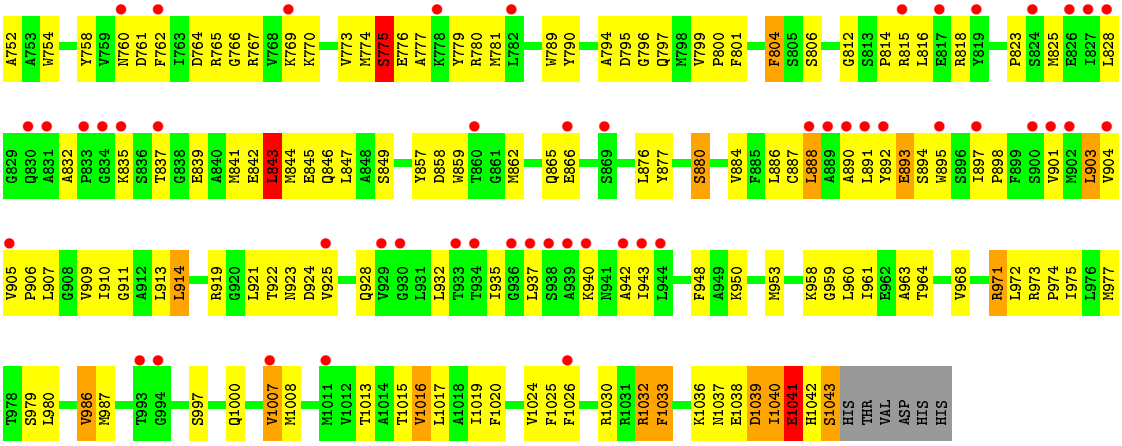




• Molecule 1: Multidrug efflux pump subunit AcrB

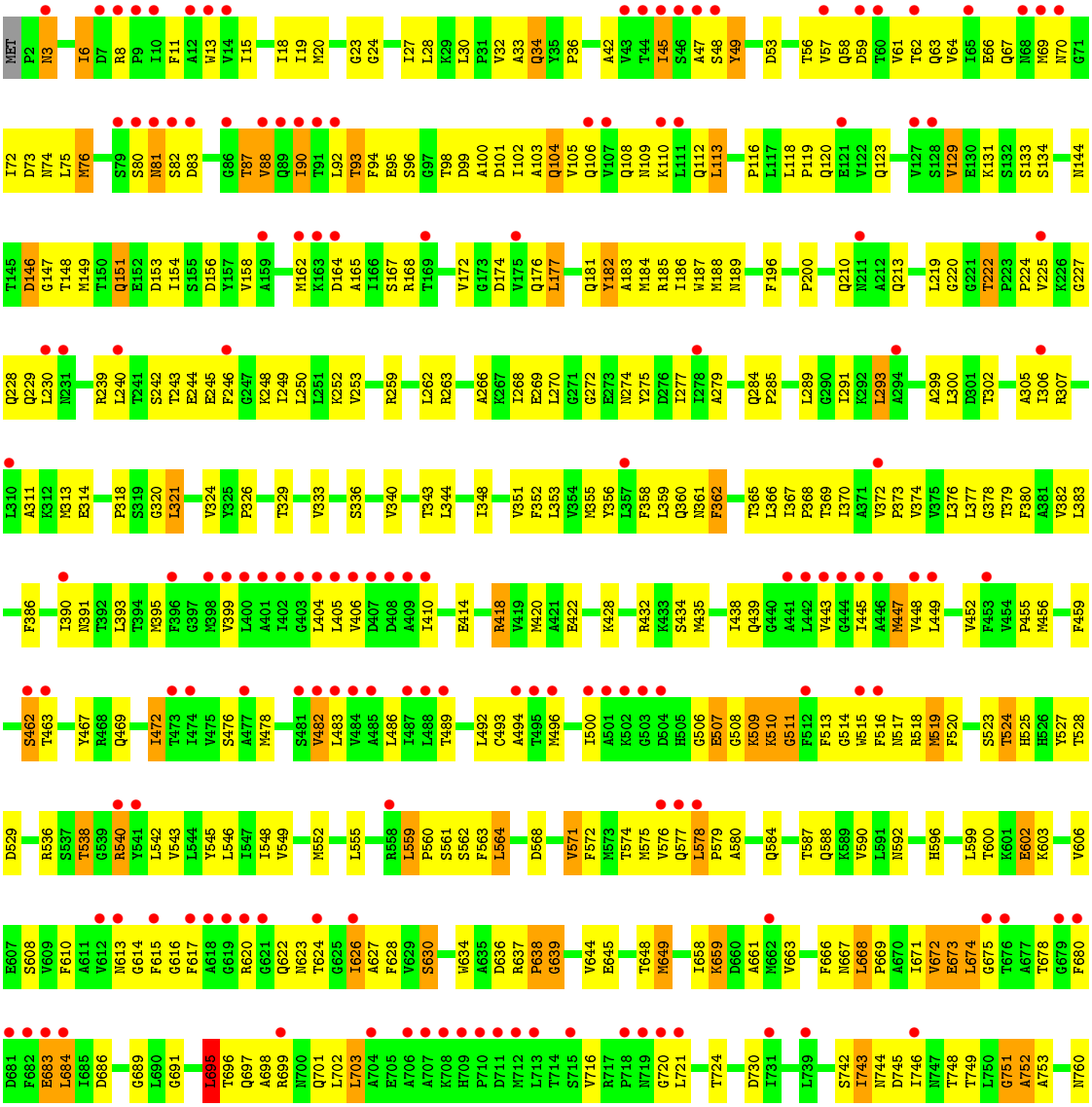
Chain E:

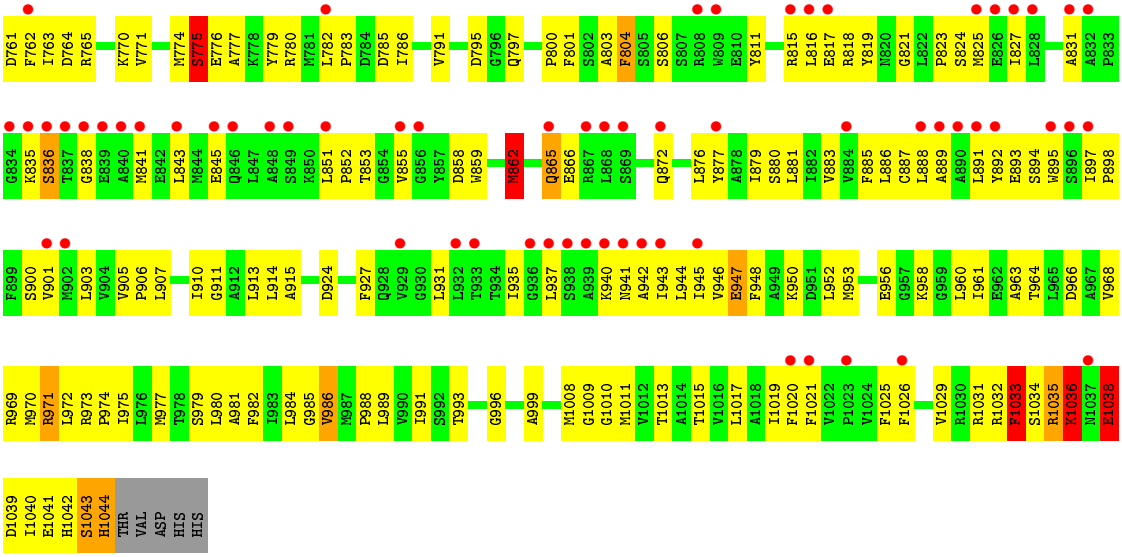




- Molecule 1: Multidrug efflux pump subunit AcrB

Chain F:




D761 F762 I763 D764 R765 K770 V771 W774 S775 E776 A777 K778 Y779 R780 M781 L782 P783 D784 D785 I786 V791 D795 G796 Q797 P800 F801 S802 A803 F804 S805 S806 S807 R808 W809 E810 Y811 R815 L816 E817 R818 Y819 N820 G821 L822 P823 S824 N825 E826 I827 L828 A831 A832 P833
G834 K835 S836 T837 G838 E839 A840 M841 E842 L843 M844 E845 Q846 L847 A848 S849 K850 L851 P852 T853 G854 V855 G856 Y857 D858 W859 N862 Q865 E866 R867 L868 S869 Q872 L876 Y877 A878 I879 S880 L881 I882 V883 V884 F885 L886 C887 L888 A889 A890 L891 Y892 E893 S894 W895 S896 I897 P898
F899 S900 V901 M902 L903 V904 V905 P906 L907 I910 G911 A912 L913 L914 A915 D924 F927 Q928 V929 G930 L931 L932 T933 T934 I935 G936 L937 S938 A939 K940 N941 A942 I943 L944 I945 V946 E947 F948 A949 K950 D951 L952 M953 E956 G957 K958 G959 L960 I961 E962 A963 T964 L965 D966 A967 V968
R969 M970 R971 L972 R973 P974 I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 N987 P988 L989 V990 I991 S992 T993 G996 A999 M1008 G1009 G1010 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1022 P1023 V1024 F1025 F1026 V1029 R1030 R1031 R1032 F1033 S1034 R1035 K1036 N1037 E1038
D1039 I1040 E1041 H1042 S1043 H1044 THR VAL ASP 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	150.95Å 155.66Å 217.01Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	19.97 – 3.47 108.39 – 3.47	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.97-3.47) 92.9 (108.39-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.251 , 0.321 0.256 , 0.325	Depositor DCC
R_{free} test set	6046 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	92.6	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.057 for -k,-h,-l 0.074 for k,h,-l 0.065 for h,-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	47962	wwPDB-VP
Average B, all atoms (Å^2)	82.0	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 44.42 % 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 1.5309e-04.*

[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, ERY

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	0.59	1/8094 (0.0%)	0.83	6/10990 (0.1%)
1	B	0.59	1/8076 (0.0%)	0.83	7/10965 (0.1%)
1	C	0.59	0/8076	0.85	8/10965 (0.1%)
1	D	0.55	1/8076 (0.0%)	0.81	3/10965 (0.0%)
1	E	0.57	2/8076 (0.0%)	0.83	7/10965 (0.1%)
1	F	0.57	0/8087	0.86	7/10980 (0.1%)
All	All	0.58	5/48485 (0.0%)	0.84	38/65830 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	515	TRP	CB-CG	7.95	1.64	1.50
1	A	515	TRP	CB-CG	7.35	1.63	1.50
1	E	493	CYS	CB-SG	-7.17	1.70	1.82
1	E	515	TRP	CB-CG	6.61	1.62	1.50
1	B	515	TRP	CB-CG	5.40	1.59	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	529	ASP	CB-CG-OD1	12.19	129.28	118.30
1	C	540	ARG	NE-CZ-NH2	9.67	125.14	120.30
1	B	529	ASP	CB-CG-OD1	9.03	126.42	118.30
1	D	529	ASP	CB-CG-OD1	8.46	125.91	118.30
1	E	529	ASP	CB-CG-OD1	7.85	125.36	118.30
1	F	529	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	C	92	LEU	CA-CB-CG	6.82	130.99	115.30
1	B	888	LEU	CA-CB-CG	-6.55	100.23	115.30
1	B	359	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	293	LEU	CA-CB-CG	6.22	129.62	115.30
1	E	293	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	1017	LEU	CA-CB-CG	6.12	129.38	115.30
1	C	540	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	A	449	LEU	CA-CB-CG	6.09	129.31	115.30
1	C	30	LEU	CA-CB-CG	6.06	129.23	115.30
1	F	972	LEU	CA-CB-CG	6.01	129.13	115.30
1	F	684	LEU	CA-CB-CG	5.99	129.09	115.30
1	C	515	TRP	CA-CB-CG	5.72	124.58	113.70
1	A	456	MET	CB-CG-SD	-5.68	95.35	112.40
1	C	616	GLY	N-CA-C	-5.63	99.03	113.10
1	B	1037	ASN	C-N-CA	5.62	135.75	121.70
1	D	449	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	972	LEU	CA-CB-CG	5.61	128.20	115.30
1	E	972	LEU	CA-CB-CG	5.49	127.92	115.30
1	C	83	ASP	N-CA-C	5.49	125.81	111.00
1	C	529	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	376	LEU	CA-CB-CG	-5.28	103.15	115.30
1	E	843	LEU	CA-CB-CG	5.24	127.34	115.30
1	E	117	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	357	LEU	CA-CB-CG	5.16	127.17	115.30
1	E	914	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	888	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	F	695	LEU	CA-CB-CG	5.14	127.13	115.30
1	F	113	LEU	CA-CB-CG	5.13	127.11	115.30
1	F	1036	LYS	N-CA-C	5.10	124.77	111.00
1	A	38	ILE	CG1-CB-CG2	-5.10	100.18	111.40
1	E	888	LEU	CA-CB-CG	-5.06	103.65	115.30
1	A	529	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1039	ASP	Peptide
1	B	1039	ASP	Peptide
1	B	132	SER	Peptide
1	C	834	GLY	Peptide
1	D	1033	PHE	Peptide
1	E	1039	ASP	Peptide
1	F	1036	LYS	Peptide
1	F	1041	GLU	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	7942	0	8080	420	0
1	B	7925	0	8066	330	0
1	C	7925	0	8066	424	0
1	D	7925	0	8066	414	0
1	E	7925	0	8066	394	0
1	F	7935	0	8073	390	0
2	A	51	0	67	6	0
2	D	51	0	67	12	0
3	A	70	0	92	14	0
3	B	35	0	46	5	0
3	C	35	0	46	2	0
3	D	70	0	92	6	0
3	E	35	0	46	5	0
3	F	35	0	46	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47962	0	48919	2279	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2279) 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:225:VAL:H	1:E:781:MET:HE1	1.13	1.09
1:A:225:VAL:H	1:B:781:MET:HE1	1.15	1.06
1:F:941:ASN:HD21	1:F:1015:THR:HG22	1.18	1.04
1:D:210:GLN:HE22	1:D:250:LEU:HB3	1.27	0.99
1:E:691:GLY:H	1:E:694:LYS:HE3	1.27	0.98
1:A:781:MET:HE1	1:C:225:VAL:H	1.28	0.96
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.48	0.96
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.49	0.94
1:A:134:SER:OG	2:A:1101:ERY:H323	1.67	0.93
1:D:228:GLN:NE2	1:D:230:LEU:O	2.01	0.93
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.51	0.91
1:D:415:ASN:HD22	1:D:434:SER:HB2	1.34	0.91
1:B:775:SER:OG	1:B:776:GLU:O	1.88	0.91
1:D:225:VAL:HG12	1:E:777:ALA:HB1	1.50	0.90
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.53	0.89
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.54	0.88
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.56	0.87
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.57	0.87
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.54	0.87
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.56	0.87
1:C:894:SER:HB3	1:C:897:ILE:HG12	1.57	0.87
1:F:559:LEU:HD23	1:F:560:PRO:HD2	1.55	0.87
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.56	0.86
1:C:892:TYR:O	1:C:894:SER:N	2.07	0.86
1:F:937:LEU:HD13	1:F:1011:MET:HE2	1.56	0.86
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.58	0.86
1:E:516:PHE:HA	1:E:519:MET:HG3	1.57	0.86
1:B:696:THR:HG23	1:B:699:ARG:HH12	1.38	0.86
1:A:38:ILE:HD11	1:A:466:ILE:HD11	1.57	0.86
1:A:877:TYR:OH	1:A:928:GLN:NE2	2.09	0.85
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.58	0.85
1:B:350:LEU:HD13	1:B:984:LEU:HB3	1.58	0.85
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.59	0.85
1:B:525:HIS:CD2	1:B:529:ASP:OD2	2.31	0.84
1:F:3:ASN:HD22	1:F:435:MET:HG3	1.42	0.84
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.11	0.83
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.60	0.83
1:D:38:ILE:HG23	1:D:462:SER:HB2	1.60	0.83
1:F:356:TYR:HA	1:F:365:THR:HG21	1.60	0.83
1:C:740:GLY:O	1:C:794:ALA:N	2.12	0.83
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.58	0.83
1:C:465:ALA:HA	1:C:468:ARG:HH12	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:THR:HA	1:E:224:PRO:HD3	1.61	0.82
1:A:935:ILE:HD12	3:A:1103:LMT:H72	1.62	0.82
1:B:971:ARG:O	1:B:975:ILE:HG12	1.78	0.82
1:C:356:TYR:HA	1:C:365:THR:HG21	1.60	0.82
1:D:445:ILE:HD13	1:D:940:LYS:HE3	1.60	0.82
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.61	0.82
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.60	0.81
1:A:530:SER:HG	3:A:1102:LMT:H2O2	1.02	0.81
1:B:525:HIS:NE2	1:B:529:ASP:OD2	2.12	0.81
1:C:579:PRO:HD3	1:C:661:ALA:HB2	1.63	0.81
1:D:187:TRP:HB3	1:D:776:GLU:HA	1.63	0.81
1:A:137:LEU:HD22	1:A:293:LEU:HG	1.60	0.81
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.63	0.81
1:E:559:LEU:HD22	1:E:560:PRO:HD2	1.63	0.81
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.63	0.80
1:D:1034:SER:OG	1:D:1035:ARG:N	2.14	0.80
1:C:3:ASN:OD1	1:C:3:ASN:N	2.14	0.80
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.63	0.80
1:D:244:GLU:HG2	1:D:248:LYS:HE2	1.63	0.80
1:A:445:ILE:HD13	1:A:940:LYS:HE3	1.63	0.80
1:C:240:LEU:HB2	1:C:246:PHE:HE1	1.47	0.80
1:A:690:LEU:HB3	1:A:694:LYS:HD3	1.64	0.79
1:D:181:GLN:OE1	1:D:767:ARG:NH2	2.15	0.79
1:D:740:GLY:O	1:D:794:ALA:N	2.14	0.79
1:E:530:SER:OG	3:E:1101:LMT:O2'	1.66	0.79
1:A:67:GLN:OE1	1:C:767:ARG:NH1	2.15	0.79
1:D:700:ASN:HA	1:D:703:LEU:HD12	1.63	0.79
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.65	0.79
1:D:690:LEU:HB3	1:D:694:LYS:HD3	1.65	0.79
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.65	0.79
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.16	0.78
1:D:137:LEU:HD22	1:D:293:LEU:HG	1.65	0.78
1:A:181:GLN:OE1	1:A:767:ARG:NH2	2.16	0.78
1:B:516:PHE:HA	1:B:519:MET:HG3	1.65	0.78
1:E:959:GLY:HA2	1:E:1040:ILE:HB	1.65	0.78
1:A:222:THR:HA	1:A:224:PRO:HD3	1.64	0.77
1:B:508:GLY:O	1:B:510:LYS:N	2.16	0.77
1:A:1037:ASN:HA	1:A:1038:GLU:HB2	1.63	0.77
1:E:979:SER:OG	1:E:1015:THR:HG21	1.84	0.77
1:D:507:GLU:O	1:D:509:LYS:N	2.17	0.77
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:PHE:HA	1:F:355:MET:HE2	1.67	0.77
1:D:196:PHE:O	1:D:252:LYS:NZ	2.18	0.77
1:A:579:PRO:HD3	1:A:661:ALA:HB2	1.66	0.77
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.66	0.77
1:C:664:PHE:HD2	1:C:717:ARG:HD2	1.50	0.77
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.67	0.77
1:E:832:ALA:HB3	1:E:835:LYS:HD3	1.67	0.77
1:D:775:SER:OG	1:D:776:GLU:O	2.02	0.76
1:B:228:GLN:NE2	1:C:781:MET:SD	2.59	0.76
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.17	0.76
1:B:14:VAL:HG22	1:C:886:LEU:HD12	1.64	0.76
1:E:196:PHE:O	1:E:252:LYS:NZ	2.17	0.76
1:C:971:ARG:HB3	1:C:971:ARG:CZ	2.15	0.76
1:B:668:LEU:HD23	1:B:668:LEU:H	1.50	0.76
1:E:971:ARG:O	1:E:975:ILE:HG12	1.85	0.76
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.68	0.76
1:E:652:THR:HG23	1:E:665:ALA:HB3	1.67	0.75
1:C:34:GLN:HE21	1:C:333:VAL:HG22	1.50	0.75
1:D:453:PHE:O	1:D:471:SER:OG	2.04	0.75
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.68	0.75
1:A:1039:ASP:HA	1:A:1040:ILE:HB	1.68	0.75
1:C:944:LEU:HB3	1:C:971:ARG:NE	2.01	0.75
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.67	0.75
1:C:382:VAL:HG21	1:C:476:SER:HB2	1.69	0.75
1:C:228:GLN:NE2	1:C:230:LEU:O	2.19	0.74
1:F:775:SER:OG	1:F:776:GLU:O	2.04	0.74
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.69	0.74
1:A:758:TYR:OH	1:A:761:ASP:OD1	2.05	0.74
1:E:340:VAL:HG21	1:E:395:MET:HB3	1.69	0.74
1:D:491:ALA:O	1:D:495:THR:OG1	2.04	0.74
1:B:228:GLN:HE22	1:C:781:MET:HB3	1.52	0.74
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.69	0.74
1:A:350:LEU:HD22	1:A:984:LEU:HB3	1.69	0.74
1:C:307:ARG:NH2	1:C:314:GLU:OE2	2.21	0.74
1:D:586:ARG:O	1:D:589:LYS:HB3	1.88	0.74
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.71	0.73
1:B:26:ALA:O	1:B:30:LEU:HB2	1.89	0.73
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.23	0.73
1:E:588:GLN:O	1:E:592:ASN:ND2	2.22	0.73
1:A:360:GLN:NE2	1:A:513:PHE:HB3	2.03	0.73
1:B:1035:ARG:HG3	1:B:1036:LYS:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:PHE:HA	1:D:519:MET:SD	2.29	0.73
1:E:775:SER:OG	1:E:776:GLU:O	2.06	0.73
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.17	0.73
1:B:1037:ASN:HA	1:B:1038:GLU:HB2	1.71	0.72
1:D:579:PRO:HD3	1:D:661:ALA:HB2	1.70	0.72
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.71	0.72
1:C:699:ARG:NH1	1:C:825:MET:SD	2.62	0.72
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.71	0.72
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.70	0.72
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.23	0.72
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.72	0.72
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.22	0.72
1:D:236:ALA:O	1:E:728:LYS:NZ	2.19	0.72
1:B:187:TRP:NE1	1:B:269:GLU:OE2	2.23	0.71
1:F:156:ASP:OD1	1:F:765:ARG:NH2	2.23	0.71
1:B:6:ILE:O	1:B:428:LYS:NZ	2.23	0.71
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.04	0.71
1:B:1036:LYS:HA	1:B:1038:GLU:HG2	1.72	0.71
1:D:343:THR:HG21	1:D:989:LEU:HD21	1.71	0.71
1:E:428:LYS:HG2	1:E:494:ALA:HB1	1.72	0.71
1:F:83:ASP:HB2	1:F:87:THR:O	1.89	0.71
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.56	0.71
1:A:225:VAL:N	1:B:781:MET:HE1	2.00	0.71
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.23	0.71
1:F:892:TYR:O	1:F:894:SER:N	2.24	0.71
1:A:637:ARG:NH1	1:A:642:ASN:O	2.23	0.71
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.73	0.71
1:D:781:MET:HE1	1:F:225:VAL:HG13	1.73	0.71
1:A:740:GLY:O	1:A:794:ALA:N	2.22	0.71
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.72	0.70
1:D:888:LEU:HD13	1:D:901:VAL:HG13	1.70	0.70
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.73	0.70
1:F:667:ASN:O	1:F:678:THR:OG1	2.07	0.70
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.08	0.70
1:A:210:GLN:NE2	1:A:250:LEU:O	2.24	0.70
1:B:236:ALA:O	1:C:728:LYS:NZ	2.16	0.70
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.71	0.70
1:B:508:GLY:HA2	1:B:518:ARG:HH21	1.55	0.70
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.07	0.70
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.73	0.70
1:B:901:VAL:HG23	1:B:942:ALA:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:GLU:HG2	1:C:518:ARG:HG3	1.73	0.70
1:D:699:ARG:NH1	1:D:825:MET:SD	2.64	0.70
1:D:317:PHE:CD2	1:D:321:LEU:HD12	2.26	0.70
1:D:583:THR:HG21	1:F:229:GLN:HA	1.74	0.70
1:F:525:HIS:HA	1:F:528:THR:HG22	1.74	0.70
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.72	0.70
1:A:452:VAL:HG11	3:A:1103:LMT:H111	1.74	0.70
1:F:452:VAL:O	1:F:455:PRO:HD2	1.91	0.70
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.74	0.69
1:E:562:SER:HB3	1:E:924:ASP:HB3	1.74	0.69
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.27	0.69
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.74	0.69
1:B:404:LEU:HD23	1:B:478:MET:HG3	1.73	0.69
1:A:605:ASN:HD22	1:A:647:ILE:HD11	1.56	0.69
1:A:775:SER:OG	1:A:776:GLU:O	2.10	0.69
1:A:945:ILE:HG13	1:A:971:ARG:HH22	1.56	0.69
1:D:519:MET:O	1:D:523:SER:OG	2.10	0.69
1:F:941:ASN:ND2	1:F:1015:THR:HG22	2.01	0.69
1:F:153:ASP:OD2	1:F:182:TYR:OH	2.09	0.69
1:F:746:ILE:HG22	1:F:791:VAL:HG21	1.75	0.69
1:C:568:ASP:OD1	1:C:637:ARG:NH1	2.20	0.69
1:D:326:PRO:O	1:D:630:SER:OG	2.11	0.69
1:D:18:ILE:HG13	1:E:886:LEU:HD23	1.75	0.69
1:A:879:ILE:HD13	1:C:25:LEU:HD21	1.74	0.69
1:D:781:MET:HE1	1:F:225:VAL:H	1.57	0.69
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.73	0.69
1:A:426:PRO:HB2	1:A:429:GLU:OE2	1.93	0.69
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.74	0.69
1:C:580:ALA:HB1	1:C:724:THR:HG23	1.74	0.69
1:D:1037:ASN:HA	1:D:1038:GLU:HB2	1.75	0.69
1:B:531:VAL:O	1:B:534:ILE:HG13	1.93	0.69
1:D:355:MET:HB3	1:D:365:THR:OG1	1.92	0.69
1:C:519:MET:O	1:C:523:SER:OG	2.06	0.68
1:D:535:LEU:HD21	1:D:1027:VAL:HG21	1.75	0.68
1:C:520:PHE:O	1:C:524:THR:HG22	1.92	0.68
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.74	0.68
1:D:109:ASN:HD21	1:F:129:VAL:HG23	1.58	0.68
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.28	0.68
1:C:831:ALA:HB3	1:C:835:LYS:HG3	1.74	0.68
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.27	0.68
1:D:971:ARG:HG2	1:D:974:PRO:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:762:PHE:CE1	1:F:764:ASP:HB2	2.29	0.68
1:C:841:MET:O	1:C:845:GLU:HG2	1.94	0.68
1:E:986:VAL:HG21	1:E:1007:VAL:HG11	1.74	0.68
1:A:957:GLY:O	1:A:1042:HIS:N	2.27	0.68
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.75	0.68
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.75	0.68
1:D:442:LEU:O	1:D:445:ILE:HG13	1.94	0.68
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.76	0.67
1:F:222:THR:HA	1:F:224:PRO:HD3	1.75	0.67
1:A:80:SER:HB3	1:A:90:ILE:HG12	1.76	0.67
1:D:350:LEU:HD13	1:D:984:LEU:HB3	1.77	0.67
1:E:242:SER:HB2	1:E:245:GLU:H	1.58	0.67
1:F:577:GLN:HG3	1:F:624:THR:HG22	1.76	0.67
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.77	0.67
1:D:516:PHE:O	1:D:519:MET:HG2	1.94	0.67
1:E:159:ALA:O	1:E:767:ARG:NH2	2.28	0.67
1:F:937:LEU:HD11	1:F:982:PHE:CE2	2.30	0.67
1:B:559:LEU:HD23	1:B:560:PRO:HD2	1.76	0.67
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.29	0.67
1:E:680:PHE:CZ	1:E:844:MET:HG3	2.29	0.67
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.77	0.67
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.76	0.67
1:B:146:ASP:N	1:B:146:ASP:OD2	2.23	0.67
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.77	0.67
1:A:332:PHE:O	1:A:336:SER:HB3	1.94	0.67
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.76	0.67
1:C:775:SER:OG	1:C:776:GLU:O	2.12	0.67
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.77	0.67
1:E:441:ALA:O	1:E:445:ILE:HG23	1.95	0.67
1:F:404:LEU:HG	1:F:449:LEU:HD13	1.77	0.67
1:F:885:PHE:HD2	1:F:886:LEU:HD22	1.60	0.67
1:C:907:LEU:HG	1:C:1017:LEU:HD23	1.76	0.66
1:A:931:LEU:HB3	3:A:1103:LMT:H51	1.77	0.66
1:A:971:ARG:HB3	1:A:971:ARG:CZ	2.24	0.66
1:B:448:VAL:HG13	1:B:884:VAL:HG22	1.77	0.66
1:D:213:GLN:HG2	1:D:239:ARG:HG2	1.75	0.66
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.77	0.66
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.76	0.66
1:A:932:LEU:HA	3:A:1103:LMT:H71	1.78	0.66
1:A:465:ALA:O	1:A:469:GLN:HG2	1.96	0.66
1:C:578:LEU:HG	1:C:587:THR:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.78	0.66
1:F:894:SER:HB3	1:F:897:ILE:HG12	1.77	0.66
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.77	0.66
1:E:986:VAL:HG11	1:E:1007:VAL:HG12	1.77	0.66
1:D:902:MET:O	1:D:905:VAL:HG23	1.96	0.66
1:E:901:VAL:HG21	1:E:943:ILE:HG13	1.77	0.66
1:F:966:ASP:OD1	1:F:969:ARG:NH1	2.29	0.66
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.75	0.66
1:D:1035:ARG:HH22	1:D:1036:LYS:HE3	1.61	0.66
1:D:415:ASN:HD22	1:D:434:SER:CB	2.07	0.66
1:F:610:PHE:HB3	1:F:628:PHE:HB2	1.78	0.66
1:B:555:LEU:HB3	1:B:913:LEU:HB3	1.78	0.66
1:B:971:ARG:HB3	1:B:971:ARG:CZ	2.24	0.66
1:C:668:LEU:H	1:C:668:LEU:HD23	1.61	0.65
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.79	0.65
1:F:324:VAL:HG23	1:F:326:PRO:HD3	1.76	0.65
1:F:817:GLU:OE2	1:F:825:MET:HA	1.96	0.65
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.78	0.65
1:B:688:ALA:O	1:B:690:LEU:N	2.29	0.65
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.79	0.65
1:E:801:PHE:HA	1:E:804:PHE:CE2	2.31	0.65
1:F:562:SER:HB2	1:F:924:ASP:HB3	1.77	0.65
1:A:781:MET:HE3	1:C:228:GLN:HB2	1.78	0.65
1:D:465:ALA:O	1:D:469:GLN:HG2	1.97	0.65
1:E:324:VAL:HG13	1:E:326:PRO:HD3	1.79	0.65
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.12	0.65
1:C:1038:GLU:HA	1:C:1039:ASP:HB2	1.77	0.65
1:C:940:LYS:NZ	1:C:978:THR:HG21	2.11	0.65
1:E:588:GLN:HE21	1:E:592:ASN:HD21	1.44	0.65
2:D:1101:ERY:H18	2:D:1101:ERY:H5	1.77	0.65
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.78	0.65
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.61	0.65
1:F:831:ALA:HB3	1:F:835:LYS:HG3	1.78	0.65
1:F:943:ILE:O	1:F:947:GLU:HB3	1.96	0.65
1:B:540:ARG:NH2	3:B:1101:LMT:O6B	2.30	0.65
1:F:434:SER:O	1:F:438:ILE:HG12	1.97	0.65
1:F:587:THR:OG1	1:F:613:ASN:ND2	2.26	0.65
1:D:211:ASN:O	1:D:760:ASN:ND2	2.30	0.65
1:D:418:ARG:O	1:D:422:GLU:HB2	1.97	0.64
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.79	0.64
1:A:155:SER:HB3	1:A:180:SER:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:O	1:C:361:ASN:N	2.31	0.64
1:F:482:VAL:O	1:F:486:LEU:HG	1.97	0.64
1:A:491:ALA:O	1:A:495:THR:OG1	2.13	0.64
1:A:563:PHE:HE2	1:A:671:ILE:HD13	1.62	0.64
1:E:508:GLY:O	1:E:510:LYS:N	2.30	0.64
1:F:695:LEU:HD22	1:F:855:VAL:HG22	1.79	0.64
1:E:907:LEU:HG	1:E:1017:LEU:HD23	1.78	0.64
1:A:18:ILE:HG13	1:B:886:LEU:HD23	1.80	0.64
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.63	0.64
1:B:578:LEU:HD21	1:B:590:VAL:HG21	1.80	0.64
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.79	0.64
1:E:14:VAL:HG22	1:F:886:LEU:HD12	1.79	0.64
1:A:565:PRO:HG2	1:A:567:GLU:OE2	1.98	0.64
1:F:399:VAL:HG11	1:F:989:LEU:HD21	1.80	0.64
1:D:470:PHE:CD2	1:D:929:VAL:HG11	2.33	0.64
1:A:507:GLU:O	1:A:509:LYS:N	2.30	0.64
1:B:445:ILE:HG21	1:B:940:LYS:HD2	1.79	0.64
1:A:516:PHE:HA	1:A:519:MET:HG3	1.78	0.63
1:C:482:VAL:O	1:C:486:LEU:HG	1.97	0.63
1:B:1037:ASN:HA	1:B:1038:GLU:CB	2.29	0.63
1:A:728:LYS:NZ	1:C:236:ALA:O	2.16	0.63
1:D:418:ARG:NH2	1:D:948:PHE:HE2	1.95	0.63
1:B:536:ARG:NH1	3:B:1101:LMT:O3B	2.31	0.63
1:B:146:ASP:OD2	1:B:320:GLY:HA3	1.98	0.63
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.29	0.63
1:C:272:GLY:N	1:C:275:TYR:OH	2.26	0.63
1:C:356:TYR:C	1:C:358:PHE:H	2.01	0.63
1:D:146:ASP:OD2	1:D:146:ASP:N	2.19	0.63
1:D:222:THR:OG1	1:E:275:TYR:O	2.16	0.63
1:E:80:SER:HB3	1:E:90:ILE:HG12	1.80	0.63
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.79	0.63
1:D:360:GLN:OE1	1:D:513:PHE:HB3	1.98	0.63
1:E:49:TYR:HE1	1:E:60:THR:HG21	1.62	0.63
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.64	0.63
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.63	0.63
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.79	0.63
1:A:588:GLN:NE2	1:A:592:ASN:OD1	2.31	0.63
1:C:634:TRP:N	1:C:634:TRP:CD1	2.63	0.62
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.79	0.62
1:A:928:GLN:OE1	3:A:1103:LMT:O6'	2.10	0.62
1:B:658:ILE:O	1:B:659:LYS:HD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:726:GLN:NE2	1:D:812:GLY:HA3	2.14	0.62
1:E:139:VAL:O	1:E:326:PRO:HD2	1.99	0.62
1:E:415:ASN:CG	1:E:418:ARG:HH12	2.02	0.62
1:E:559:LEU:HD11	1:E:922:THR:HA	1.82	0.62
1:F:456:MET:HA	1:F:876:LEU:HD21	1.80	0.62
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.63	0.62
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.81	0.62
1:B:87:THR:HG21	1:B:620:ARG:HH12	1.65	0.62
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.81	0.62
1:E:153:ASP:OD2	1:E:182:TYR:OH	2.18	0.62
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.34	0.62
1:F:636:ASP:O	1:F:638:PRO:HD3	1.99	0.62
1:A:359:LEU:O	1:A:361:ASN:N	2.33	0.62
1:B:1013:THR:O	1:B:1017:LEU:HB2	1.98	0.62
1:C:352:PHE:HD2	1:C:353:LEU:HD23	1.63	0.62
1:B:362:PHE:HA	1:B:365:THR:HG22	1.81	0.62
1:B:717:ARG:HD2	1:B:828:LEU:HB2	1.81	0.62
1:C:907:LEU:HD23	1:C:1017:LEU:HB3	1.81	0.62
1:D:617:PHE:HD2	2:D:1101:ERY:H361	1.63	0.62
1:B:764:ASP:OD1	1:B:765:ARG:HG3	2.00	0.62
1:E:272:GLY:N	1:E:275:TYR:OH	2.25	0.62
1:E:634:TRP:N	1:E:634:TRP:CD1	2.68	0.62
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.83	0.62
1:E:919:ARG:HB3	1:E:921:LEU:HD23	1.80	0.62
1:D:225:VAL:N	1:E:781:MET:HE1	1.99	0.62
1:B:1034:SER:OG	1:B:1035:ARG:N	2.28	0.61
1:E:534:ILE:HG22	3:E:1101:LMT:H5'	1.81	0.61
2:D:1101:ERY:H323	2:D:1101:ERY:H211	1.82	0.61
1:D:318:PRO:HD2	1:D:321:LEU:HG	1.81	0.61
1:A:744:ASN:O	1:A:748:THR:HG23	2.00	0.61
1:C:185:ARG:HB3	1:C:187:TRP:NE1	2.15	0.61
1:D:945:ILE:HG13	1:D:971:ARG:HH22	1.65	0.61
1:E:43:VAL:HG22	1:E:131:LYS:HG3	1.80	0.61
1:F:753:ALA:O	1:F:775:SER:HB3	1.99	0.61
1:A:350:LEU:HD13	1:A:984:LEU:O	1.99	0.61
1:C:452:VAL:O	1:C:455:PRO:HD2	2.00	0.61
1:D:712:MET:SD	1:D:835:LYS:HE2	2.40	0.61
1:E:259:ARG:H	1:E:259:ARG:HD3	1.65	0.61
1:C:201:VAL:HG23	1:C:749:THR:HG23	1.82	0.61
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.83	0.61
1:E:435:MET:SD	1:E:490:PRO:HB3	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:PHE:HD2	1:F:353:LEU:HD23	1.64	0.61
1:A:452:VAL:HA	1:A:880:SER:OG	2.00	0.61
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.83	0.61
1:E:572:PHE:HA	1:E:668:LEU:HD21	1.83	0.61
1:F:600:THR:O	1:F:603:LYS:HG3	2.01	0.61
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.01	0.61
1:E:219:LEU:HD13	1:F:783:PRO:HG3	1.82	0.61
1:B:327:TYR:HB2	1:B:628:PHE:CZ	2.35	0.61
1:E:327:TYR:HB2	1:E:628:PHE:CZ	2.36	0.61
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.82	0.60
1:A:108:GLN:NE2	1:B:109:ASN:O	2.34	0.60
1:A:134:SER:OG	2:A:1101:ERY:C32	2.48	0.60
1:B:744:ASN:O	1:B:748:THR:HG23	2.01	0.60
1:B:225:VAL:HG12	1:C:777:ALA:HB1	1.84	0.60
1:C:351:VAL:HG22	1:C:981:ALA:HB1	1.82	0.60
1:D:907:LEU:HD23	1:D:1017:LEU:HB3	1.83	0.60
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.16	0.60
1:F:672:VAL:O	1:F:674:LEU:N	2.32	0.60
1:F:961:ILE:HD12	1:F:961:ILE:H	1.65	0.60
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.82	0.60
1:B:452:VAL:HG23	1:B:453:PHE:HD2	1.65	0.60
1:C:222:THR:HA	1:C:224:PRO:HD3	1.83	0.60
1:F:291:ILE:HG21	1:F:306:ILE:HD11	1.81	0.60
1:F:576:VAL:HG22	1:F:663:VAL:HG13	1.82	0.60
1:F:744:ASN:O	1:F:748:THR:HG23	2.01	0.60
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.83	0.60
1:A:253:VAL:HG12	1:A:259:ARG:HG2	1.84	0.60
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.00	0.60
1:A:112:GLN:HG3	1:B:112:GLN:OE1	2.01	0.60
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.84	0.60
1:B:979:SER:OG	1:B:1015:THR:HG21	2.02	0.60
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.65	0.60
1:A:1019:ILE:HG13	1:A:1020:PHE:CD1	2.37	0.60
1:B:1016:VAL:HG22	3:B:1101:LMT:H112	1.83	0.60
1:C:1038:GLU:HA	1:C:1039:ASP:CB	2.31	0.60
1:C:789:TRP:HB2	1:C:801:PHE:CD2	2.37	0.60
1:F:580:ALA:HB1	1:F:724:THR:HG22	1.83	0.60
1:D:61:VAL:HG22	1:D:118:LEU:HD22	1.82	0.60
1:E:531:VAL:O	1:E:534:ILE:HG13	2.02	0.60
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.83	0.60
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:HB2	1:B:246:PHE:CE1	2.37	0.60
1:D:58:GLN:HE21	1:D:63:GLN:HE21	1.48	0.60
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.36	0.60
1:A:211:ASN:O	1:A:760:ASN:ND2	2.35	0.60
1:D:272:GLY:N	1:D:275:TYR:OH	2.29	0.60
1:E:695:LEU:HD22	1:E:825:MET:SD	2.41	0.60
1:F:462:SER:HB3	1:F:865:GLN:HG2	1.84	0.60
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.84	0.60
1:A:1030:ARG:HH12	1:A:1033:PHE:HB2	1.67	0.59
1:A:196:PHE:O	1:A:252:LYS:NZ	2.35	0.59
1:B:200:PRO:HB2	1:B:749:THR:HG22	1.82	0.59
1:B:277:ILE:HA	1:B:613:ASN:O	2.01	0.59
1:E:717:ARG:HD2	1:E:828:LEU:HB2	1.83	0.59
1:F:242:SER:HB2	1:F:245:GLU:HG3	1.84	0.59
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.84	0.59
1:C:465:ALA:HA	1:C:468:ARG:NH1	2.13	0.59
1:C:744:ASN:O	1:C:748:THR:HG23	2.02	0.59
1:D:699:ARG:NH2	1:D:722:GLU:OE1	2.35	0.59
1:E:26:ALA:O	1:E:30:LEU:HB2	2.02	0.59
1:A:360:GLN:HE22	1:A:513:PHE:HB3	1.67	0.59
1:E:971:ARG:CZ	1:E:971:ARG:HB3	2.32	0.59
1:F:104:GLN:NE2	1:F:108:GLN:OE1	2.35	0.59
1:A:388:PHE:CZ	1:A:472:ILE:HG12	2.37	0.59
1:B:1037:ASN:HB3	1:B:1040:ILE:HG12	1.84	0.59
1:D:239:ARG:NH1	1:D:761:ASP:O	2.36	0.59
1:E:1013:THR:O	1:E:1017:LEU:HB2	2.02	0.59
1:E:399:VAL:O	1:E:402:ILE:HG12	2.01	0.59
1:F:684:LEU:HD22	1:F:827:ILE:HD11	1.84	0.59
1:B:652:THR:HG23	1:B:665:ALA:H	1.68	0.59
1:C:623:ASN:N	1:C:623:ASN:OD1	2.27	0.59
1:B:11:PHE:CE1	1:C:890:ALA:HB1	2.38	0.59
1:C:948:PHE:HD2	1:C:970:MET:HE3	1.66	0.59
1:D:873:ALA:HB2	3:D:1103:LMT:H51	1.84	0.59
1:C:789:TRP:HB2	1:C:801:PHE:HD2	1.67	0.59
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.85	0.59
1:A:1037:ASN:CA	1:A:1038:GLU:HB2	2.30	0.59
1:A:781:MET:CE	1:C:225:VAL:H	2.10	0.59
1:C:156:ASP:OD1	1:C:765:ARG:NH2	2.35	0.59
1:D:897:ILE:HD13	1:D:950:LYS:HE3	1.85	0.59
1:E:250:LEU:HD21	1:E:253:VAL:HG23	1.84	0.59
1:E:261:LEU:N	1:E:264:ASP:OD2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:PHE:HD1	1:E:634:TRP:HH2	1.50	0.59
1:E:9:PRO:HB3	1:E:495:THR:HG21	1.84	0.59
1:F:196:PHE:O	1:F:252:LYS:NZ	2.25	0.59
1:A:62:THR:HG21	1:A:818:ARG:HD3	1.83	0.59
1:D:309:GLU:O	1:D:312:LYS:HB2	2.02	0.59
1:D:457:ALA:O	1:D:468:ARG:NE	2.35	0.59
1:D:781:MET:HB3	1:F:228:GLN:HE22	1.68	0.59
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.85	0.59
1:D:344:LEU:HD21	1:D:399:VAL:HG22	1.83	0.59
1:C:200:PRO:HB2	1:C:749:THR:HG22	1.85	0.59
1:D:344:LEU:HD22	1:D:402:ILE:HD12	1.83	0.59
1:B:237:GLN:HG3	1:C:731:ILE:HD11	1.85	0.58
1:B:235:ILE:O	1:C:728:LYS:HD2	2.03	0.58
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.38	0.58
1:D:971:ARG:CZ	1:D:971:ARG:HB3	2.33	0.58
1:F:1038:GLU:HB2	1:F:1039:ASP:CG	2.23	0.58
1:F:58:GLN:HA	1:F:62:THR:HB	1.85	0.58
1:F:698:ALA:O	1:F:701:GLN:HB3	2.03	0.58
1:B:441:ALA:O	1:B:445:ILE:HG23	2.02	0.58
1:B:455:PRO:O	1:B:876:LEU:HD13	2.02	0.58
1:C:310:LEU:O	1:C:314:GLU:HG3	2.03	0.58
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.84	0.58
1:A:928:GLN:OE1	3:A:1103:LMT:C6'	2.51	0.58
1:D:1031:ARG:HH12	1:D:1038:GLU:HG3	1.68	0.58
1:D:108:GLN:HE21	1:D:112:GLN:HE21	1.50	0.58
1:D:637:ARG:HD2	1:D:642:ASN:O	2.03	0.58
1:D:919:ARG:NH1	1:D:1005:THR:OG1	2.35	0.58
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.85	0.58
1:E:675:GLY:HA2	1:E:862:MET:HG3	1.84	0.58
1:A:1030:ARG:HH12	1:A:1033:PHE:CB	2.16	0.58
1:A:456:MET:SD	1:A:932:LEU:HD11	2.44	0.58
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.85	0.58
1:F:379:THR:HG23	1:F:476:SER:OG	2.03	0.58
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.19	0.58
1:D:909:VAL:HG22	1:D:931:LEU:HD21	1.85	0.58
1:E:195:LYS:HZ1	1:E:196:PHE:HE1	1.52	0.58
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.38	0.58
1:E:703:LEU:HD21	1:E:718:PRO:HD3	1.86	0.58
1:F:538:THR:HG23	1:F:542:LEU:HD13	1.86	0.58
1:F:910:ILE:O	1:F:914:LEU:HB2	2.03	0.58
1:F:947:GLU:HG3	1:F:948:PHE:HD1	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:SER:HB3	1:B:90:ILE:HG12	1.85	0.58
1:C:83:ASP:HB2	1:C:87:THR:O	2.03	0.58
1:D:617:PHE:HA	2:D:1101:ERY:H351	1.85	0.58
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.34	0.58
1:C:36:PRO:O	1:C:38:ILE:HG13	2.03	0.58
1:E:151:GLN:HE22	1:E:278:ILE:HA	1.68	0.58
1:A:584:GLN:HB2	1:A:622:GLN:HG2	1.84	0.58
1:C:81:ASN:OD1	1:C:815:ARG:NH1	2.37	0.58
1:E:165:ALA:HB3	1:E:313:MET:CE	2.33	0.58
1:E:671:ILE:HB	1:E:674:LEU:HG	1.86	0.58
1:F:578:LEU:HG	1:F:587:THR:HG22	1.86	0.58
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.39	0.58
1:B:188:MET:HA	1:B:266:ALA:HB2	1.84	0.58
1:B:99:ASP:HB3	1:B:102:ILE:HB	1.86	0.58
1:D:222:THR:HA	1:D:224:PRO:HD3	1.86	0.58
1:D:768:VAL:HG12	1:E:63:GLN:OE1	2.03	0.58
1:A:945:ILE:CG1	1:A:971:ARG:HH22	2.15	0.57
1:B:261:LEU:N	1:B:264:ASP:OD2	2.33	0.57
1:E:44:THR:HG1	1:E:91:THR:HG1	1.26	0.57
1:E:182:TYR:HB2	1:E:769:LYS:HZ2	1.69	0.57
1:C:190:PRO:HB3	1:C:789:TRP:CZ3	2.39	0.57
1:C:58:GLN:O	1:C:62:THR:HB	2.03	0.57
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.87	0.57
1:C:915:ALA:HB2	1:C:1009:GLY:HA3	1.86	0.57
1:D:344:LEU:HD21	1:D:399:VAL:HA	1.86	0.57
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.39	0.57
1:F:1043:SER:OG	1:F:1044:HIS:N	2.37	0.57
1:F:520:PHE:O	1:F:524:THR:HG22	2.02	0.57
1:C:463:THR:HG23	1:C:467:TYR:CE1	2.40	0.57
1:E:396:PHE:O	1:E:400:LEU:HB2	2.04	0.57
1:E:442:LEU:O	1:E:445:ILE:HG13	2.03	0.57
1:E:713:LEU:HD21	1:E:843:LEU:HD12	1.86	0.57
1:F:1034:SER:OG	1:F:1035:ARG:HA	2.04	0.57
1:A:544:LEU:O	1:A:548:ILE:HG13	2.04	0.57
1:B:559:LEU:HD23	1:B:560:PRO:CD	2.34	0.57
1:C:426:PRO:HD2	1:C:429:GLU:HB3	1.86	0.57
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.70	0.57
1:E:678:THR:HA	1:E:837:THR:OG1	2.03	0.57
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.86	0.57
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.85	0.57
1:A:242:SER:OG	1:A:245:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	1.87	0.57
1:C:201:VAL:HG22	1:C:748:THR:OG1	2.05	0.57
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.39	0.57
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.87	0.57
1:B:916:ALA:O	1:B:919:ARG:N	2.36	0.57
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.87	0.57
1:C:404:LEU:HB3	1:C:478:MET:SD	2.45	0.57
1:C:688:ALA:O	1:C:690:LEU:N	2.38	0.57
1:C:698:ALA:O	1:C:701:GLN:HB3	2.04	0.57
1:D:78:MET:O	1:D:820:ASN:N	2.26	0.57
1:D:17:ILE:HG22	1:E:886:LEU:HD21	1.86	0.57
1:F:358:PHE:CD2	1:F:977:MET:HG3	2.40	0.57
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.85	0.57
1:B:985:GLY:O	1:B:988:PRO:HD2	2.04	0.57
1:D:919:ARG:HG2	1:D:920:GLY:H	1.69	0.57
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.87	0.57
1:F:3:ASN:HD22	1:F:435:MET:CG	2.16	0.57
1:A:577:GLN:OE1	1:A:624:THR:HG22	2.05	0.57
1:B:28:LEU:HB3	1:B:29:LYS:HD2	1.87	0.57
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.40	0.57
1:B:668:LEU:CD2	1:B:668:LEU:H	2.14	0.57
1:D:928:GLN:HG2	3:D:1103:LMT:H82	1.86	0.57
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.87	0.57
1:C:795:ASP:OD2	1:C:797:GLN:HG2	2.05	0.57
1:E:591:LEU:HD13	1:E:611:ALA:HB1	1.86	0.57
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.86	0.57
1:B:652:THR:CG2	1:B:665:ALA:H	2.18	0.57
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.05	0.57
1:C:650:ARG:O	1:C:653:ARG:HB3	2.05	0.57
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.87	0.57
1:D:986:VAL:HG21	1:D:1007:VAL:HG11	1.86	0.57
1:D:876:LEU:HD23	1:D:879:ILE:HD12	1.86	0.57
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.87	0.57
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.40	0.56
1:B:142:VAL:HG21	1:B:158:VAL:HG22	1.87	0.56
1:E:532:GLY:O	1:E:535:LEU:N	2.37	0.56
1:A:717:ARG:HE	1:A:828:LEU:HB2	1.69	0.56
1:B:695:LEU:HD22	1:B:825:MET:SD	2.45	0.56
1:A:777:ALA:HB1	1:C:225:VAL:HG12	1.86	0.56
1:C:228:GLN:NE2	1:C:230:LEU:H	2.02	0.56
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:815:ARG:HH21	2:D:1101:ERY:H291	1.70	0.56
1:F:113:LEU:O	1:F:116:PRO:HD2	2.05	0.56
1:A:154:ILE:O	1:A:157:TYR:N	2.38	0.56
1:A:644:VAL:CG1	1:A:667:ASN:HB2	2.32	0.56
1:C:990:VAL:HG13	1:C:1005:THR:OG1	2.05	0.56
1:D:59:ASP:HB3	1:F:763:ILE:HD11	1.87	0.56
1:F:555:LEU:HB3	1:F:913:LEU:HB3	1.87	0.56
1:F:64:VAL:HA	1:F:67:GLN:OE1	2.06	0.56
1:A:728:LYS:HB2	1:A:810:GLU:OE1	2.05	0.56
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.69	0.56
1:F:455:PRO:HG2	1:F:880:SER:HA	1.88	0.56
1:F:351:VAL:HG22	1:F:981:ALA:HB1	1.87	0.56
1:C:427:PRO:HD3	1:C:499:PRO:HB3	1.88	0.56
1:D:210:GLN:NE2	1:D:250:LEU:HB3	2.10	0.56
1:E:58:GLN:OE1	1:E:816:LEU:HD13	2.04	0.56
1:F:945:ILE:HA	1:F:971:ARG:NH1	2.20	0.56
1:A:563:PHE:CE2	1:A:671:ILE:HD13	2.40	0.56
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.70	0.56
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.33	0.56
1:D:201:VAL:HA	1:D:204:ILE:HD12	1.86	0.56
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.88	0.56
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.86	0.56
1:B:545:TYR:HE2	1:B:907:LEU:HD11	1.70	0.56
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.71	0.56
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.88	0.56
1:C:959:GLY:HA2	1:C:1041:GLU:HA	1.87	0.56
1:D:317:PHE:HB3	1:D:321:LEU:HB3	1.87	0.56
1:E:901:VAL:HG23	1:E:942:ALA:HB3	1.87	0.56
1:F:587:THR:HG21	1:F:622:GLN:O	2.06	0.56
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.88	0.56
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.70	0.56
1:B:153:ASP:OD2	1:B:182:TYR:OH	2.23	0.56
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.40	0.56
1:D:3:ASN:HA	1:D:6:ILE:HG12	1.88	0.56
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.21	0.56
1:E:575:MET:HA	1:E:626:ILE:HG13	1.87	0.56
1:D:235:ILE:O	1:E:728:LYS:HD2	2.06	0.56
1:D:276:ASP:OD1	1:F:222:THR:HG21	2.05	0.56
1:E:758:TYR:HE1	1:E:770:LYS:HG2	1.71	0.56
1:F:53:ASP:OD1	1:F:56:THR:OG1	2.17	0.56
1:A:530:SER:CB	3:A:1102:LMT:H2O2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.31	0.56
1:D:644:VAL:HG11	1:D:667:ASN:HB2	1.87	0.56
1:D:682:PHE:HD2	1:D:683:GLU:N	2.04	0.56
1:E:380:PHE:HA	1:E:383:LEU:HD12	1.88	0.56
1:F:1035:ARG:NH1	1:F:1038:GLU:OE1	2.39	0.56
1:A:186:ILE:HB	1:A:773:VAL:HG22	1.88	0.55
1:C:746:ILE:HG13	1:C:747:ASN:N	2.21	0.55
1:C:966:ASP:OD1	1:C:969:ARG:NH2	2.39	0.55
1:F:187:TRP:HA	1:F:774:MET:O	2.06	0.55
1:F:579:PRO:HD3	1:F:661:ALA:HB2	1.87	0.55
1:C:898:PRO:HA	1:C:901:VAL:HG12	1.89	0.55
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.89	0.55
1:E:582:ALA:HA	1:E:586:ARG:HH21	1.71	0.55
1:E:710:PRO:HA	1:E:713:LEU:O	2.06	0.55
1:F:101:ASP:OD1	1:F:131:LYS:NZ	2.27	0.55
1:F:343:THR:HG21	1:F:989:LEU:HD21	1.87	0.55
1:C:585:GLU:O	1:C:589:LYS:HG3	2.07	0.55
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.41	0.55
1:C:945:ILE:HG12	1:C:971:ARG:HH22	1.70	0.55
1:E:156:ASP:OD1	1:E:765:ARG:NH2	2.39	0.55
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.87	0.55
1:E:516:PHE:CA	1:E:519:MET:HG3	2.34	0.55
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.88	0.55
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.88	0.55
1:A:459:PHE:CZ	1:A:873:ALA:HA	2.40	0.55
1:B:400:LEU:HD12	1:B:933:THR:HG21	1.89	0.55
1:C:187:TRP:HA	1:C:774:MET:O	2.05	0.55
1:C:752:ALA:O	1:C:774:MET:HA	2.07	0.55
1:D:683:GLU:HG2	1:D:819:TYR:CG	2.41	0.55
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.89	0.55
1:A:935:ILE:HG21	3:A:1103:LMT:H112	1.88	0.55
1:B:616:GLY:HA2	1:B:626:ILE:HB	1.87	0.55
1:C:764:ASP:OD1	1:C:765:ARG:HG3	2.07	0.55
1:E:632:LYS:O	1:E:637:ARG:NE	2.36	0.55
1:E:987:MET:HA	1:E:1008:MET:HE3	1.89	0.55
1:A:535:LEU:HD21	1:A:1027:VAL:HG21	1.89	0.55
1:A:781:MET:HE1	1:C:225:VAL:HG13	1.88	0.55
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.88	0.55
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.87	0.55
1:E:415:ASN:HD22	1:E:434:SER:CB	2.18	0.55
1:E:613:ASN:HD22	1:E:614:GLY:N	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:SER:CB	1:E:90:ILE:HG12	2.36	0.55
1:F:1042:HIS:CG	1:F:1043:SER:N	2.75	0.55
1:F:144:ASN:OD1	1:F:148:THR:HA	2.07	0.55
1:F:944:LEU:HB3	1:F:971:ARG:NE	2.22	0.55
1:A:897:ILE:HA	1:A:1029:VAL:CG1	2.37	0.55
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.88	0.55
1:B:733:GLN:HE22	1:B:743:ILE:HG21	1.71	0.55
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.88	0.55
1:D:359:LEU:O	1:D:361:ASN:N	2.40	0.55
1:E:545:TYR:OH	1:E:903:LEU:O	2.18	0.55
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.88	0.55
1:F:947:GLU:HG3	1:F:948:PHE:N	2.21	0.55
1:A:420:MET:HB3	1:A:500:ILE:HB	1.88	0.55
1:F:877:TYR:O	1:F:881:LEU:HG	2.07	0.55
1:A:229:GLN:HE21	1:B:586:ARG:HD3	1.71	0.55
1:B:238:THR:OG1	1:C:728:LYS:NZ	2.39	0.55
1:B:415:ASN:OD1	1:B:418:ARG:NH1	2.36	0.55
1:C:187:TRP:HE3	1:C:775:SER:O	1.90	0.55
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.89	0.55
1:C:801:PHE:HA	1:C:804:PHE:CE2	2.42	0.55
1:C:961:ILE:HD12	1:C:961:ILE:H	1.72	0.55
1:D:109:ASN:ND2	1:F:129:VAL:HG23	2.22	0.55
1:D:112:GLN:HG3	1:E:112:GLN:OE1	2.07	0.55
1:D:568:ASP:OD1	1:D:637:ARG:NH1	2.26	0.55
1:F:447:MET:HG2	1:F:891:LEU:HD22	1.89	0.55
1:D:944:LEU:HB3	1:D:971:ARG:CZ	2.37	0.54
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.90	0.54
1:F:568:ASP:OD1	1:F:637:ARG:NH1	2.39	0.54
1:A:459:PHE:HZ	1:A:873:ALA:HA	1.72	0.54
1:A:535:LEU:CD2	1:A:1027:VAL:HG21	2.37	0.54
1:B:119:PRO:HG2	1:B:122:VAL:HB	1.87	0.54
1:D:658:ILE:HG13	1:D:659:LYS:NZ	2.23	0.54
1:E:343:THR:HG22	1:E:344:LEU:HD23	1.88	0.54
1:F:99:ASP:HB3	1:F:102:ILE:HB	1.89	0.54
1:F:253:VAL:HG22	1:F:259:ARG:HG2	1.90	0.54
1:F:404:LEU:HB3	1:F:478:MET:SD	2.47	0.54
1:F:45:ILE:HB	1:F:90:ILE:HG12	1.89	0.54
1:A:169:THR:HG21	1:A:306:ILE:HG13	1.89	0.54
1:A:453:PHE:CE2	1:A:932:LEU:HB3	2.42	0.54
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.72	0.54
1:A:976:LEU:O	1:A:980:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1042:HIS:CG	1:B:1043:SER:H	2.25	0.54
1:B:726:GLN:NE2	1:B:812:GLY:HA3	2.23	0.54
1:C:144:ASN:O	1:C:284:GLN:NE2	2.40	0.54
1:C:943:ILE:O	1:C:947:GLU:HB3	2.07	0.54
1:E:344:LEU:HD22	1:E:402:ILE:HG21	1.89	0.54
1:F:751:GLY:O	1:F:753:ALA:N	2.41	0.54
1:F:184:MET:HB2	1:F:762:PHE:CE2	2.42	0.54
1:C:418:ARG:O	1:C:422:GLU:HB2	2.07	0.54
1:C:586:ARG:O	1:C:589:LYS:HB2	2.08	0.54
1:D:441:ALA:O	1:D:445:ILE:HG23	2.07	0.54
1:F:277:ILE:HA	1:F:613:ASN:O	2.07	0.54
1:F:617:PHE:CE1	1:F:626:ILE:HD11	2.42	0.54
1:A:726:GLN:OE1	1:A:812:GLY:HA3	2.07	0.54
1:B:415:ASN:CG	1:B:418:ARG:HH12	2.10	0.54
1:D:744:ASN:O	1:D:748:THR:HG23	2.07	0.54
1:D:834:GLY:O	1:D:835:LYS:HD2	2.07	0.54
1:F:699:ARG:HD3	1:F:825:MET:SD	2.48	0.54
1:A:42:ALA:HB2	1:A:93:THR:HG23	1.89	0.54
1:C:703:LEU:HD11	1:C:718:PRO:HD3	1.88	0.54
1:C:674:LEU:HD22	1:C:861:GLY:HA2	1.90	0.54
1:C:941:ASN:HD21	1:C:1015:THR:HG22	1.72	0.54
1:F:519:MET:O	1:F:523:SER:OG	2.18	0.54
1:F:563:PHE:CE2	1:F:564:LEU:HD22	2.43	0.54
1:B:671:ILE:HB	1:B:674:LEU:HD12	1.89	0.54
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.33	0.54
1:D:946:VAL:HG13	1:D:1026:PHE:CE1	2.43	0.54
1:E:911:GLY:HA2	1:E:1013:THR:HG21	1.89	0.54
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.38	0.54
1:D:352:PHE:HD2	1:D:353:LEU:HD23	1.72	0.54
1:F:20:MET:HG2	1:F:374:VAL:HA	1.90	0.54
1:F:945:ILE:HA	1:F:971:ARG:HH12	1.72	0.54
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.88	0.54
1:B:575:MET:HA	1:B:626:ILE:HG13	1.89	0.54
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.89	0.54
1:C:571:VAL:N	1:C:631:LEU:HD12	2.22	0.54
1:C:579:PRO:HD3	1:C:661:ALA:CB	2.36	0.54
1:D:70:ASN:HB2	1:F:167:SER:HB2	1.90	0.54
1:E:32:VAL:HG21	1:E:300:LEU:HD13	1.89	0.54
1:E:54:ALA:HB2	1:E:84:SER:HB3	1.89	0.54
1:F:1043:SER:HB2	1:F:1044:HIS:CE1	2.43	0.54
1:F:563:PHE:HB2	1:F:866:GLU:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:VAL:HG11	1:A:433:LYS:HG2	1.90	0.54
1:A:84:SER:HB3	1:A:814:PRO:HA	1.89	0.54
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.89	0.54
1:C:559:LEU:HD23	1:C:560:PRO:HD2	1.90	0.54
1:D:10:ILE:HG13	1:E:895:TRP:CE2	2.42	0.54
1:E:519:MET:O	1:E:523:SER:OG	2.23	0.54
1:F:599:LEU:O	1:F:603:LYS:HG2	2.08	0.54
1:A:1040:ILE:HG13	1:A:1041:GLU:N	2.22	0.53
1:A:330:THR:HB	1:A:331:PRO:HD3	1.90	0.53
1:C:801:PHE:HD1	1:C:804:PHE:HE2	1.55	0.53
1:D:274:ASN:ND2	1:D:276:ASP:OD2	2.30	0.53
1:D:391:ASN:O	1:D:395:MET:HG2	2.07	0.53
1:E:790:TYR:CE1	1:E:800:PRO:HB3	2.43	0.53
1:F:376:LEU:O	1:F:379:THR:N	2.41	0.53
1:F:549:VAL:O	1:F:552:MET:HB3	2.08	0.53
1:A:591:LEU:HD11	1:A:625:GLY:HA3	1.90	0.53
1:A:960:LEU:O	1:A:964:THR:HG23	2.09	0.53
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.90	0.53
1:B:910:ILE:O	1:B:914:LEU:HB2	2.08	0.53
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.43	0.53
1:F:616:GLY:HA2	1:F:626:ILE:HD12	1.89	0.53
1:F:800:PRO:HG2	1:F:803:ALA:HB2	1.90	0.53
1:F:817:GLU:HB2	1:F:824:SER:O	2.08	0.53
1:F:915:ALA:HB2	1:F:1009:GLY:HA3	1.89	0.53
1:F:952:LEU:O	1:F:956:GLU:HB2	2.08	0.53
1:A:932:LEU:HD23	3:A:1103:LMT:H71	1.89	0.53
1:B:44:THR:OG1	1:B:91:THR:OG1	2.24	0.53
1:B:775:SER:OG	1:B:780:ARG:HG2	2.07	0.53
1:E:453:PHE:O	1:E:471:SER:OG	2.14	0.53
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.90	0.53
1:A:836:SER:HB3	1:A:839:GLU:CD	2.28	0.53
1:C:244:GLU:HG2	1:C:248:LYS:HE3	1.89	0.53
1:E:196:PHE:N	1:E:196:PHE:HD1	2.06	0.53
1:C:178:PHE:HE2	1:C:615:PHE:CD1	2.25	0.53
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.89	0.53
1:C:531:VAL:HG21	1:C:968:VAL:HG11	1.90	0.53
1:E:160:ALA:HA	1:E:767:ARG:NH2	2.23	0.53
1:F:80:SER:HB3	1:F:90:ILE:HG22	1.91	0.53
1:A:146:ASP:OD2	1:A:146:ASP:N	2.39	0.53
1:B:272:GLY:N	1:B:275:TYR:OH	2.34	0.53
1:B:362:PHE:O	1:B:365:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:PHE:HE1	1:C:857:TYR:HB2	1.70	0.53
1:D:355:MET:HA	1:D:355:MET:HE2	1.91	0.53
3:E:1101:LMT:H6D	3:E:1101:LMT:H5B	1.89	0.53
1:F:686:ASP:OD2	1:F:823:PRO:HD2	2.09	0.53
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.08	0.53
1:A:352:PHE:HD2	1:A:353:LEU:HD23	1.74	0.53
1:E:196:PHE:CD1	1:E:196:PHE:N	2.77	0.53
1:E:104:GLN:HE21	1:F:109:ASN:HD22	1.55	0.53
1:A:781:MET:HE1	1:C:225:VAL:N	2.11	0.53
1:A:453:PHE:CD2	1:A:932:LEU:HD13	2.44	0.53
1:B:415:ASN:HD22	1:B:434:SER:CB	2.19	0.53
1:B:52:ALA:HB1	1:B:56:THR:HB	1.91	0.53
1:B:644:VAL:O	1:B:648:THR:HG23	2.08	0.53
1:E:1037:ASN:H	1:E:1038:GLU:HA	1.74	0.53
1:E:511:GLY:HA2	1:E:515:TRP:HD1	1.73	0.53
1:F:548:ILE:HD13	1:F:1017:LEU:HD21	1.91	0.53
1:F:555:LEU:HD11	1:F:914:LEU:HD12	1.90	0.53
1:A:533:GLY:HA2	1:A:536:ARG:HH11	1.73	0.53
1:B:11:PHE:HE1	1:C:890:ALA:HB1	1.74	0.53
1:C:253:VAL:HG22	1:C:259:ARG:HG2	1.90	0.53
1:C:5:PHE:HD2	1:C:6:ILE:HG12	1.74	0.53
1:D:316:PHE:CD1	1:E:687:GLN:HG2	2.43	0.53
1:B:363:ARG:HD3	1:B:496:MET:O	2.09	0.53
1:B:614:GLY:HA2	1:B:621:GLY:O	2.09	0.53
1:D:14:VAL:HG11	1:E:890:ALA:HB2	1.91	0.53
1:F:897:ILE:HG23	1:F:946:VAL:CG1	2.39	0.53
1:A:520:PHE:O	1:A:524:THR:HG22	2.09	0.52
1:B:508:GLY:CA	1:B:518:ARG:HH21	2.22	0.52
1:C:356:TYR:O	1:C:358:PHE:N	2.41	0.52
1:C:178:PHE:HE2	1:C:615:PHE:HD1	1.57	0.52
1:D:727:PHE:HD1	1:D:809:TRP:CE2	2.27	0.52
1:E:42:ALA:HB3	1:E:132:SER:HB3	1.91	0.52
1:E:415:ASN:OD1	1:E:418:ARG:NH1	2.40	0.52
1:E:888:LEU:HD21	1:E:943:ILE:HD11	1.92	0.52
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.44	0.52
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.90	0.52
1:A:448:VAL:O	1:A:451:ALA:HB3	2.09	0.52
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.27	0.52
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.90	0.52
1:F:568:ASP:CG	1:F:637:ARG:HH12	2.12	0.52
1:F:720:GLY:HA2	1:F:815:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:801:PHE:HA	1:F:804:PHE:CE2	2.45	0.52
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.44	0.52
1:B:378:GLY:O	1:B:382:VAL:HG23	2.09	0.52
1:B:894:SER:HB2	1:B:897:ILE:HD12	1.91	0.52
1:C:945:ILE:HA	1:C:971:ARG:HH12	1.75	0.52
1:D:159:ALA:HB2	1:D:177:LEU:HD11	1.89	0.52
1:D:72:ILE:HD13	1:D:107:VAL:HA	1.90	0.52
1:D:957:GLY:O	1:D:1040:ILE:HB	2.09	0.52
1:C:250:LEU:HD21	1:C:253:VAL:HG23	1.91	0.52
1:C:352:PHE:CD2	1:C:353:LEU:HD23	2.44	0.52
1:C:414:GLU:OE1	1:C:973:ARG:HD3	2.09	0.52
1:C:971:ARG:NH1	1:C:971:ARG:HB3	2.24	0.52
1:E:228:GLN:NE2	1:E:230:LEU:O	2.39	0.52
1:D:17:ILE:CG2	1:E:886:LEU:HD21	2.40	0.52
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.39	0.52
1:A:715:SER:O	1:A:717:ARG:HD3	2.10	0.52
1:D:563:PHE:CD1	3:D:1103:LMT:H5B	2.45	0.52
1:E:344:LEU:HD21	1:E:399:VAL:HA	1.91	0.52
1:E:484:VAL:HG13	1:E:488:LEU:HB3	1.91	0.52
1:E:682:PHE:CZ	1:E:857:TYR:HB2	2.45	0.52
1:F:876:LEU:O	1:F:880:SER:HB2	2.08	0.52
1:A:595:THR:O	1:A:599:LEU:HG	2.10	0.52
1:A:958:LYS:C	1:A:1040:ILE:HG12	2.30	0.52
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.90	0.52
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.92	0.52
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.91	0.52
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.40	0.52
1:C:587:THR:HG21	1:C:622:GLN:O	2.09	0.52
1:D:400:LEU:HD23	1:D:929:VAL:HG12	1.91	0.52
1:D:418:ARG:HD3	1:D:422:GLU:OE1	2.10	0.52
1:D:945:ILE:HG13	1:D:971:ARG:NH2	2.24	0.52
1:E:42:ALA:O	1:E:132:SER:N	2.39	0.52
1:E:49:TYR:CE1	1:E:60:THR:HG21	2.43	0.52
1:F:352:PHE:CD2	1:F:353:LEU:HD23	2.45	0.52
1:A:361:ASN:HD21	1:A:498:LYS:HB2	1.74	0.52
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.90	0.52
1:C:455:PRO:HG2	1:C:880:SER:HA	1.92	0.52
1:C:885:PHE:HD2	1:C:886:LEU:HD22	1.75	0.52
1:F:244:GLU:HG2	1:F:248:LYS:HE3	1.92	0.52
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.38	0.52
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.92	0.52
1:D:362:PHE:O	1:D:366:LEU:HG	2.09	0.52
1:F:45:ILE:HD12	1:F:90:ILE:HG13	1.92	0.52
1:A:195:LYS:HG2	1:A:196:PHE:CE2	2.45	0.52
1:A:404:LEU:HD12	1:A:937:LEU:CD2	2.40	0.52
1:A:897:ILE:HD13	1:A:950:LYS:HE3	1.91	0.52
1:A:919:ARG:HG2	1:A:920:GLY:H	1.74	0.52
1:B:327:TYR:HD1	1:B:628:PHE:CZ	2.27	0.52
1:C:356:TYR:C	1:C:358:PHE:N	2.63	0.52
1:F:34:GLN:CB	1:F:333:VAL:HG22	2.36	0.52
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.74	0.52
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.92	0.52
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.92	0.52
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.92	0.52
1:C:443:VAL:O	1:C:447:MET:HB3	2.10	0.52
1:C:664:PHE:CD2	1:C:717:ARG:HD2	2.38	0.52
1:D:449:LEU:HB3	1:D:478:MET:SD	2.50	0.52
1:F:469:GLN:O	1:F:472:ILE:HG22	2.10	0.52
1:F:945:ILE:CG1	1:F:971:ARG:HH22	2.23	0.52
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.43	0.51
1:B:501:ALA:O	1:B:504:ASP:HB2	2.10	0.51
1:C:982:PHE:HD2	1:C:1011:MET:HG2	1.74	0.51
1:C:587:THR:HG21	1:C:623:ASN:HA	1.93	0.51
1:C:78:MET:HG3	1:C:92:LEU:HD13	1.92	0.51
1:F:911:GLY:HA3	1:F:1010:GLY:HA2	1.92	0.51
1:F:66:GLU:OE1	1:F:821:GLY:HA2	2.09	0.51
1:A:775:SER:OG	1:A:780:ARG:HG2	2.10	0.51
1:B:139:VAL:O	1:B:326:PRO:HD2	2.09	0.51
1:C:987:MET:HG3	1:C:1008:MET:HE1	1.92	0.51
1:C:23:GLY:HA3	1:C:377:LEU:O	2.10	0.51
1:D:58:GLN:HE21	1:D:63:GLN:NE2	2.07	0.51
1:D:712:MET:O	1:D:832:ALA:N	2.37	0.51
1:D:728:LYS:HB2	1:D:810:GLU:OE1	2.09	0.51
1:D:817:GLU:OE1	2:D:1101:ERY:H282	2.10	0.51
1:A:30:LEU:HD11	1:A:384:ALA:HA	1.91	0.51
1:C:727:PHE:HD1	1:C:809:TRP:CE2	2.28	0.51
1:D:31:PRO:O	1:D:389:SER:HB2	2.10	0.51
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.92	0.51
1:E:932:LEU:HD23	1:E:935:ILE:HD12	1.92	0.51
1:F:104:GLN:HG3	1:F:105:VAL:N	2.24	0.51
1:A:725:PRO:HA	1:A:810:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1026:PHE:O	1:B:1030:ARG:HB2	2.09	0.51
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.46	0.51
1:C:940:LYS:HZ1	1:C:978:THR:HG21	1.74	0.51
1:D:815:ARG:NH2	2:D:1101:ERY:H291	2.25	0.51
1:D:573:MET:HB3	1:D:666:PHE:CE1	2.44	0.51
1:E:740:GLY:O	1:E:794:ALA:N	2.43	0.51
1:F:898:PRO:HA	1:F:901:VAL:HG12	1.93	0.51
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.91	0.51
1:C:188:MET:HA	1:C:266:ALA:HB2	1.93	0.51
1:C:2:PRO:O	1:C:5:PHE:HB3	2.09	0.51
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.92	0.51
1:C:694:LYS:N	1:C:694:LYS:HD3	2.23	0.51
1:C:897:ILE:HG23	1:C:946:VAL:CG1	2.41	0.51
1:D:728:LYS:HB2	1:D:810:GLU:CD	2.31	0.51
1:D:246:PHE:HA	1:D:249:ILE:HG13	1.93	0.51
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.92	0.51
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.46	0.51
1:B:54:ALA:HB2	1:B:84:SER:HB3	1.93	0.51
1:C:1034:SER:OG	1:C:1037:ASN:HB3	2.11	0.51
1:E:715:SER:O	1:E:717:ARG:HG3	2.11	0.51
1:F:960:LEU:HD23	1:F:1031:ARG:HH21	1.76	0.51
1:F:801:PHE:CD1	1:F:804:PHE:HE2	2.29	0.51
1:A:190:PRO:HG3	1:A:779:TYR:HB3	1.92	0.51
1:B:418:ARG:O	1:B:422:GLU:HB2	2.10	0.51
1:B:534:ILE:CD1	1:B:1024:VAL:HG22	2.41	0.51
1:C:743:ILE:HD12	1:C:743:ILE:H	1.76	0.51
1:D:246:PHE:O	1:D:262:LEU:HD23	2.11	0.51
1:D:415:ASN:ND2	1:D:434:SER:HB2	2.15	0.51
1:D:617:PHE:CD2	2:D:1101:ERY:H361	2.43	0.51
1:E:584:GLN:HB2	1:E:622:GLN:HG2	1.91	0.51
1:A:935:ILE:CG2	3:A:1103:LMT:H112	2.41	0.51
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.92	0.51
1:C:841:MET:SD	1:C:863:SER:HB3	2.51	0.51
1:D:358:PHE:O	1:D:359:LEU:HD23	2.11	0.51
1:D:910:ILE:O	1:D:914:LEU:HB2	2.11	0.51
1:F:455:PRO:HB3	1:F:879:ILE:HG22	1.93	0.51
1:F:525:HIS:O	1:F:528:THR:HG22	2.11	0.51
1:C:196:PHE:HD1	1:C:260:VAL:CG1	2.24	0.51
1:C:702:LEU:HD12	1:C:851:LEU:HD11	1.92	0.51
1:C:66:GLU:OE1	1:C:821:GLY:HA2	2.11	0.51
1:C:945:ILE:CG1	1:C:971:ARG:HH22	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:VAL:HG21	1:E:406:VAL:HG11	1.94	0.51
1:E:658:ILE:HG13	1:E:659:LYS:HD2	1.93	0.51
1:E:658:ILE:O	1:E:659:LYS:HD2	2.11	0.51
1:E:858:ASP:OD1	1:E:859:TRP:N	2.39	0.51
1:E:448:VAL:HG21	1:E:888:LEU:HD21	1.93	0.51
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.46	0.51
1:F:188:MET:HA	1:F:266:ALA:HB2	1.93	0.51
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.46	0.50
1:A:959:GLY:HA2	1:A:1040:ILE:HB	1.91	0.50
1:A:61:VAL:HG21	1:A:122:VAL:HG21	1.92	0.50
1:A:225:VAL:HG12	1:B:777:ALA:CB	2.40	0.50
1:A:897:ILE:HA	1:A:1029:VAL:HG11	1.93	0.50
1:A:937:LEU:O	1:A:940:LYS:HB3	2.12	0.50
1:C:372:VAL:HG22	1:C:405:LEU:HD11	1.93	0.50
1:F:509:LYS:HE2	1:F:513:PHE:HD1	1.75	0.50
1:F:947:GLU:HG3	1:F:948:PHE:CD1	2.45	0.50
1:B:129:VAL:O	1:C:113:LEU:HD21	2.10	0.50
1:B:636:ASP:O	1:B:638:PRO:HD3	2.10	0.50
1:C:239:ARG:NH1	1:C:761:ASP:HB2	2.27	0.50
1:C:509:LYS:HE2	1:C:513:PHE:CD1	2.46	0.50
1:D:425:LEU:HD12	1:D:425:LEU:H	1.76	0.50
1:E:1019:ILE:HG13	1:E:1020:PHE:HD1	1.76	0.50
1:E:84:SER:HB3	1:E:814:PRO:HA	1.93	0.50
1:A:17:ILE:HG22	1:B:886:LEU:HD21	1.94	0.50
1:A:545:TYR:HB2	1:A:1021:PHE:CE2	2.47	0.50
1:A:865:GLN:O	1:A:868:LEU:HB2	2.11	0.50
1:A:944:LEU:O	1:A:947:GLU:HB3	2.11	0.50
1:C:979:SER:HA	1:C:1011:MET:HE3	1.93	0.50
1:C:186:ILE:HG22	1:C:773:VAL:HG23	1.93	0.50
1:C:944:LEU:HD22	1:C:971:ARG:HD2	1.93	0.50
1:D:62:THR:OG1	1:D:88:VAL:HG21	2.11	0.50
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.47	0.50
1:F:572:PHE:HD1	1:F:666:PHE:O	1.95	0.50
1:F:686:ASP:HB3	1:F:823:PRO:O	2.11	0.50
1:F:841:MET:HG2	1:F:859:TRP:CH2	2.47	0.50
1:A:1031:ARG:O	1:A:1032:ARG:HG3	2.11	0.50
1:B:583:THR:HG22	1:B:585:GLU:H	1.76	0.50
1:C:61:VAL:HA	1:C:118:LEU:CD2	2.42	0.50
1:C:990:VAL:HG21	1:C:1008:MET:SD	2.51	0.50
1:D:623:ASN:OD1	1:D:623:ASN:N	2.27	0.50
1:E:104:GLN:OE1	1:E:131:LYS:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:PHE:CE2	1:E:323:ILE:HD13	2.46	0.50
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.46	0.50
1:F:418:ARG:HD3	1:F:422:GLU:OE2	2.10	0.50
1:F:584:GLN:HB2	1:F:622:GLN:HG2	1.92	0.50
1:F:545:TYR:OH	1:F:903:LEU:O	2.22	0.50
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.27	0.50
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.92	0.50
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.47	0.50
1:D:900:SER:HB3	1:D:1029:VAL:HG21	1.94	0.50
1:E:144:ASN:HA	1:E:320:GLY:O	2.11	0.50
1:E:156:ASP:OD2	1:E:769:LYS:NZ	2.42	0.50
1:E:175:VAL:HG23	1:F:70:ASN:HD22	1.77	0.50
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.42	0.50
1:E:901:VAL:HG23	1:E:942:ALA:CB	2.41	0.50
1:A:530:SER:OG	3:A:1102:LMT:O2'	1.93	0.50
1:A:401:ALA:O	1:A:405:LEU:HG	2.12	0.50
1:A:582:ALA:HA	1:A:586:ARG:HH21	1.77	0.50
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.94	0.50
1:C:195:LYS:HG2	1:C:196:PHE:CE2	2.47	0.50
1:D:282:ASN:HD21	1:D:608:SER:HA	1.75	0.50
1:D:351:VAL:HG22	1:D:981:ALA:HB1	1.94	0.50
1:F:210:GLN:HE22	1:F:250:LEU:H	1.59	0.50
1:B:848:ALA:HA	1:B:851:LEU:HG	1.93	0.50
1:D:10:ILE:HG13	1:E:895:TRP:CZ2	2.47	0.50
1:D:31:PRO:HB2	1:D:389:SER:CB	2.40	0.50
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.76	0.50
1:D:690:LEU:O	1:D:694:LYS:HB2	2.11	0.50
1:E:537:SER:OG	1:E:540:ARG:NH2	2.43	0.50
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.46	0.50
1:E:897:ILE:N	1:E:898:PRO:HD2	2.27	0.50
1:F:362:PHE:O	1:F:366:LEU:HG	2.11	0.50
1:F:435:MET:O	1:F:439:GLN:HG2	2.11	0.50
1:A:1016:VAL:HG12	1:A:1016:VAL:O	2.12	0.50
1:A:533:GLY:HA2	1:A:536:ARG:NH1	2.27	0.50
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.77	0.50
1:B:220:GLY:HA3	1:B:230:LEU:O	2.12	0.50
1:C:376:LEU:O	1:C:379:THR:N	2.45	0.50
1:C:58:GLN:HA	1:C:62:THR:HB	1.93	0.50
1:D:170:SER:OG	1:E:74:ASN:N	2.39	0.50
1:E:795:ASP:OD2	1:E:796:GLY:N	2.45	0.50
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ALA:HB3	1:B:313:MET:CE	2.42	0.50
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.27	0.50
1:C:520:PHE:CZ	1:C:973:ARG:HG3	2.47	0.50
1:C:983:ILE:HG13	1:C:1011:MET:HG3	1.94	0.50
1:D:16:ALA:HB2	1:D:488:LEU:HD13	1.93	0.50
1:D:591:LEU:HD13	1:D:611:ALA:HB1	1.92	0.50
1:E:451:ALA:O	1:E:880:SER:OG	2.26	0.50
1:E:888:LEU:HD13	1:E:901:VAL:HG13	1.93	0.50
1:A:801:PHE:CD1	1:A:804:PHE:HE2	2.30	0.49
1:B:801:PHE:CD1	1:B:804:PHE:HE2	2.30	0.49
1:B:108:GLN:OE1	1:C:112:GLN:HB3	2.12	0.49
1:C:138:MET:HE1	1:C:325:TYR:HD2	1.77	0.49
1:C:343:THR:HG21	1:C:989:LEU:HD23	1.94	0.49
1:C:34:GLN:HG3	1:C:333:VAL:HA	1.93	0.49
1:C:678:THR:O	1:C:830:GLN:HG2	2.12	0.49
1:C:897:ILE:O	1:C:901:VAL:HG12	2.13	0.49
1:E:211:ASN:OD1	1:E:240:LEU:N	2.41	0.49
1:E:837:THR:HG22	1:E:841:MET:SD	2.52	0.49
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.77	0.49
1:A:53:ASP:OD1	1:A:56:THR:OG1	2.16	0.49
1:A:650:ARG:O	1:A:653:ARG:HB3	2.12	0.49
1:C:386:PHE:CD1	1:C:472:ILE:HD11	2.47	0.49
1:E:575:MET:HG3	1:E:664:PHE:HB2	1.93	0.49
1:F:23:GLY:HA3	1:F:377:LEU:HB3	1.95	0.49
1:A:220:GLY:HA3	1:A:230:LEU:O	2.13	0.49
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.47	0.49
1:B:244:GLU:HG2	1:B:248:LYS:HE3	1.94	0.49
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.94	0.49
1:B:520:PHE:O	1:B:524:THR:HG22	2.11	0.49
1:C:139:VAL:HB	1:C:327:TYR:HB3	1.93	0.49
1:C:668:LEU:H	1:C:668:LEU:CD2	2.23	0.49
1:C:940:LYS:HZ2	1:C:978:THR:HG21	1.77	0.49
1:D:322:LYS:HG2	1:D:323:ILE:O	2.13	0.49
1:D:31:PRO:HB2	1:D:389:SER:HB3	1.94	0.49
1:D:634:TRP:CD1	1:D:634:TRP:N	2.81	0.49
1:D:832:ALA:HB3	1:D:835:LYS:HD3	1.92	0.49
1:F:527:TYR:OH	1:F:968:VAL:HG13	2.13	0.49
1:A:568:ASP:O	1:A:634:TRP:HZ3	1.96	0.49
1:C:228:GLN:HE21	1:C:230:LEU:H	1.59	0.49
1:C:20:MET:HG2	1:C:374:VAL:HA	1.94	0.49
1:E:636:ASP:O	1:E:638:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:GLN:OE1	1:F:620:ARG:NH2	2.26	0.49
1:F:623:ASN:OD1	1:F:623:ASN:N	2.40	0.49
1:A:685:ILE:HD11	1:A:819:TYR:CD2	2.48	0.49
1:A:893:GLU:OE2	1:C:8:ARG:HB3	2.11	0.49
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.78	0.49
1:C:352:PHE:HZ	1:C:362:PHE:CE1	2.30	0.49
1:E:530:SER:O	1:E:534:ILE:HG23	2.12	0.49
1:E:790:TYR:HE1	1:E:800:PRO:HB3	1.77	0.49
1:A:190:PRO:HB2	1:A:788:ASP:O	2.13	0.49
1:A:605:ASN:ND2	1:A:647:ILE:HD11	2.25	0.49
1:A:795:ASP:OD2	1:A:796:GLY:N	2.44	0.49
1:B:327:TYR:HB2	1:B:628:PHE:CE2	2.48	0.49
1:C:1038:GLU:CA	1:C:1039:ASP:HB2	2.43	0.49
1:C:584:GLN:N	1:C:622:GLN:HB3	2.28	0.49
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.94	0.49
1:C:800:PRO:HG2	1:C:803:ALA:HB2	1.93	0.49
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.95	0.49
1:D:344:LEU:HD22	1:D:402:ILE:CD1	2.41	0.49
1:D:699:ARG:O	1:D:703:LEU:HG	2.13	0.49
1:D:713:LEU:HD21	1:D:843:LEU:CD1	2.40	0.49
1:E:190:PRO:HG3	1:E:779:TYR:HB3	1.94	0.49
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.94	0.49
1:A:668:LEU:HD23	1:A:668:LEU:H	1.76	0.49
1:B:946:VAL:HG13	1:B:1026:PHE:CE1	2.47	0.49
1:D:1030:ARG:HA	1:D:1030:ARG:NH1	2.27	0.49
1:F:3:ASN:ND2	1:F:435:MET:HG3	2.18	0.49
1:A:860:THR:HG21	2:A:1101:ERY:H281	1.95	0.49
1:D:678:THR:HA	1:D:837:THR:OG1	2.12	0.49
1:D:982:PHE:HD2	1:D:1011:MET:HG3	1.78	0.49
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.94	0.49
1:A:1038:GLU:HB3	1:A:1039:ASP:C	2.33	0.49
3:B:1101:LMT:H6E	3:B:1101:LMT:O5B	2.13	0.49
1:C:230:LEU:HG	1:C:231:ASN:N	2.28	0.49
1:C:860:THR:HA	1:C:864:TYR:HB2	1.95	0.49
1:D:309:GLU:HA	1:D:312:LYS:HD2	1.95	0.49
1:E:102:ILE:O	1:E:106:GLN:HG3	2.11	0.49
1:E:182:TYR:HB2	1:E:769:LYS:NZ	2.27	0.49
1:A:182:TYR:HB2	1:A:769:LYS:NZ	2.27	0.49
1:D:132:SER:OG	1:D:133:SER:N	2.46	0.49
1:D:141:GLY:HA3	1:D:324:VAL:HG12	1.95	0.49
1:E:375:VAL:HB	1:E:405:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:TYR:HB2	1:E:628:PHE:CE2	2.48	0.49
1:E:973:ARG:O	1:E:977:MET:HG3	2.13	0.49
1:A:444:GLY:O	1:A:448:VAL:HG23	2.13	0.48
1:A:424:GLY:CA	1:A:502:LYS:HB3	2.37	0.48
1:A:914:LEU:O	1:A:918:PHE:HB2	2.13	0.48
1:A:945:ILE:HG13	1:A:971:ARG:NH2	2.24	0.48
1:B:485:ALA:HA	1:B:489:THR:HG23	1.95	0.48
1:B:485:ALA:O	1:B:490:PRO:HD3	2.13	0.48
1:D:216:ALA:HB1	1:D:234:ILE:HG22	1.95	0.48
1:D:279:ALA:HB3	1:D:286:ALA:O	2.13	0.48
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.96	0.48
1:E:142:VAL:HG13	1:E:323:ILE:HD12	1.95	0.48
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.95	0.48
1:E:584:GLN:N	1:E:622:GLN:HB3	2.28	0.48
1:F:510:LYS:HG2	1:F:511:GLY:N	2.28	0.48
1:F:563:PHE:HE2	1:F:564:LEU:HD22	1.78	0.48
1:A:261:LEU:N	1:A:264:ASP:OD2	2.44	0.48
1:A:426:PRO:O	1:A:429:GLU:HG2	2.13	0.48
1:B:573:MET:HE3	1:B:628:PHE:HB2	1.95	0.48
1:C:55:LYS:HD2	1:C:55:LYS:O	2.13	0.48
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.48	0.48
1:C:545:TYR:OH	1:C:903:LEU:O	2.19	0.48
1:C:940:LYS:HE2	1:C:941:ASN:OD1	2.13	0.48
1:E:132:SER:O	1:E:132:SER:OG	2.24	0.48
1:E:218:GLN:HG3	1:E:221:GLY:HA2	1.95	0.48
1:E:175:VAL:HG23	1:F:70:ASN:ND2	2.28	0.48
1:A:534:ILE:HG23	3:A:1102:LMT:H1'	1.95	0.48
1:A:56:THR:O	1:A:60:THR:HG22	2.13	0.48
1:A:905:VAL:HG13	1:A:935:ILE:HD13	1.95	0.48
1:C:382:VAL:HG11	1:C:476:SER:HB3	1.95	0.48
1:E:587:THR:OG1	1:E:622:GLN:O	2.26	0.48
1:F:944:LEU:HD12	1:F:975:ILE:HG12	1.96	0.48
1:B:538:THR:O	1:B:541:TYR:HB2	2.13	0.48
1:B:774:MET:HG2	1:B:775:SER:N	2.27	0.48
1:B:80:SER:CB	1:B:90:ILE:HG12	2.44	0.48
1:B:897:ILE:N	1:B:898:PRO:HD2	2.29	0.48
1:C:34:GLN:HE21	1:C:333:VAL:CG2	2.21	0.48
1:C:414:GLU:HG2	1:C:973:ARG:NH1	2.28	0.48
1:C:636:ASP:O	1:C:638:PRO:HD3	2.12	0.48
1:C:947:GLU:HG3	1:C:948:PHE:N	2.27	0.48
1:D:146:ASP:HB2	1:D:148:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:ASN:OD1	1:D:605:ASN:N	2.46	0.48
1:E:30:LEU:HD12	1:E:31:PRO:HD2	1.95	0.48
1:F:246:PHE:O	1:F:262:LEU:HD23	2.14	0.48
1:F:669:PRO:HB2	1:F:862:MET:SD	2.54	0.48
1:F:979:SER:CB	1:F:1015:THR:HG21	2.43	0.48
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.47	0.48
1:A:576:VAL:HG21	1:A:591:LEU:CD2	2.44	0.48
1:A:712:MET:O	1:A:832:ALA:N	2.45	0.48
1:A:982:PHE:O	1:A:985:GLY:N	2.46	0.48
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.96	0.48
1:C:694:LYS:HA	1:C:697:GLN:OE1	2.13	0.48
1:D:351:VAL:O	1:D:355:MET:HB2	2.13	0.48
1:D:602:GLU:HG3	1:D:605:ASN:ND2	2.28	0.48
1:E:24:GLY:O	1:E:28:LEU:HB2	2.13	0.48
1:E:744:ASN:O	1:E:748:THR:HG23	2.13	0.48
1:E:846:GLN:O	1:E:849:SER:OG	2.22	0.48
1:F:835:LYS:HG2	1:F:836:SER:N	2.28	0.48
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.31	0.48
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.96	0.48
1:C:201:VAL:HG23	1:C:749:THR:CG2	2.44	0.48
1:C:940:LYS:O	1:C:943:ILE:HB	2.14	0.48
3:D:1102:LMT:H6E	3:D:1102:LMT:H5B	1.94	0.48
1:D:750:LEU:HD12	1:D:754:TRP:CD1	2.48	0.48
1:D:913:LEU:HD23	1:D:927:PHE:HZ	1.78	0.48
1:E:1037:ASN:HB2	1:E:1038:GLU:O	2.14	0.48
1:E:732:ASP:OD1	1:E:735:LYS:HG3	2.13	0.48
1:E:909:VAL:HG12	1:E:913:LEU:HG	1.95	0.48
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.94	0.48
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.95	0.48
1:A:172:VAL:CG2	1:A:306:ILE:HD11	2.43	0.48
1:A:80:SER:CB	1:A:90:ILE:HG12	2.42	0.48
1:B:1020:PHE:O	1:B:1023:PRO:HG2	2.13	0.48
1:C:398:MET:HG2	1:C:473:THR:HG21	1.96	0.48
1:D:762:PHE:CE1	1:D:764:ASP:HB2	2.49	0.48
1:D:894:SER:HB2	1:D:897:ILE:HD12	1.94	0.48
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.95	0.48
1:A:1040:ILE:HG13	1:A:1041:GLU:H	1.79	0.48
1:A:891:LEU:HD23	1:A:892:TYR:CE1	2.48	0.48
1:C:214:VAL:HB	1:C:236:ALA:HB3	1.95	0.48
1:E:186:ILE:HB	1:E:773:VAL:HG23	1.96	0.48
2:A:1101:ERY:H71	2:A:1101:ERY:H10	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:VAL:HG11	1:A:476:SER:HB2	1.96	0.48
1:B:459:PHE:O	1:B:464:GLY:HA3	2.14	0.48
1:C:525:HIS:HA	1:C:528:THR:HG22	1.96	0.48
1:C:531:VAL:O	1:C:534:ILE:HG13	2.13	0.48
1:C:817:GLU:OE2	1:C:825:MET:HA	2.14	0.48
1:D:726:GLN:O	1:D:810:GLU:HG2	2.14	0.48
1:D:953:MET:HE1	1:D:960:LEU:HD12	1.95	0.48
1:E:39:ALA:HA	1:E:462:SER:OG	2.14	0.48
1:D:781:MET:CE	1:F:225:VAL:H	2.26	0.48
1:F:761:ASP:OD1	1:F:770:LYS:HA	2.14	0.48
1:A:683:GLU:HG2	1:A:819:TYR:CG	2.49	0.48
1:C:156:ASP:OD2	1:C:182:TYR:HB2	2.14	0.48
1:C:358:PHE:O	1:C:359:LEU:HD23	2.14	0.48
1:C:391:ASN:OD1	1:C:393:LEU:HB2	2.14	0.48
1:C:44:THR:OG1	1:C:91:THR:OG1	2.24	0.48
1:D:352:PHE:CD2	1:D:353:LEU:HD23	2.49	0.48
1:D:571:VAL:N	1:D:631:LEU:HD12	2.29	0.48
1:D:801:PHE:HA	1:D:804:PHE:CE2	2.49	0.48
1:D:680:PHE:HD1	1:D:859:TRP:HZ3	1.61	0.48
1:E:1016:VAL:O	1:E:1016:VAL:HG12	2.14	0.48
1:E:525:HIS:HA	1:E:528:THR:HG22	1.96	0.48
1:A:376:LEU:O	1:A:379:THR:N	2.47	0.47
1:A:559:LEU:HD22	1:A:923:ASN:H	1.79	0.47
1:A:702:LEU:HD22	1:A:827:ILE:HD13	1.96	0.47
1:A:7:ASP:O	1:A:8:ARG:HG3	2.13	0.47
1:A:832:ALA:CB	1:A:835:LYS:HD3	2.38	0.47
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.49	0.47
1:D:277:ILE:HA	1:D:613:ASN:O	2.13	0.47
1:E:289:LEU:HD23	1:E:289:LEU:HA	1.66	0.47
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.95	0.47
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.96	0.47
1:F:492:LEU:O	1:F:496:MET:HG2	2.14	0.47
1:F:911:GLY:HA2	1:F:1013:THR:HG21	1.96	0.47
1:A:902:MET:O	1:A:905:VAL:HG23	2.14	0.47
1:B:188:MET:HA	1:B:266:ALA:CB	2.44	0.47
1:C:527:TYR:OH	1:C:968:VAL:HG13	2.14	0.47
1:D:1030:ARG:HA	1:D:1030:ARG:HH11	1.79	0.47
1:D:26:ALA:O	1:D:30:LEU:HB2	2.14	0.47
1:D:423:GLU:O	1:D:502:LYS:HB3	2.14	0.47
1:D:58:GLN:NE2	1:D:818:ARG:NH1	2.61	0.47
1:E:196:PHE:HD2	1:E:260:VAL:HG22	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:534:ILE:HD11	1:E:1024:VAL:HG22	1.95	0.47
1:E:462:SER:H	1:E:865:GLN:HE21	1.62	0.47
1:F:146:ASP:O	1:F:148:THR:N	2.47	0.47
1:F:158:VAL:HG22	1:F:162:MET:HE3	1.96	0.47
1:F:614:GLY:O	1:F:620:ARG:HA	2.14	0.47
1:F:775:SER:OG	1:F:780:ARG:HG2	2.14	0.47
1:F:42:ALA:HB2	1:F:93:THR:HG23	1.95	0.47
1:F:74:ASN:HB2	1:F:98:THR:HG21	1.96	0.47
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.95	0.47
1:A:63:GLN:OE1	1:C:768:VAL:HG12	2.14	0.47
1:C:348:ILE:HG13	1:C:402:ILE:CD1	2.42	0.47
1:C:586:ARG:HA	1:C:589:LYS:HD2	1.96	0.47
1:C:75:LEU:HD11	1:C:92:LEU:HB3	1.96	0.47
1:D:508:GLY:H	1:D:518:ARG:HG3	1.78	0.47
1:A:1007:VAL:HG12	1:A:1008:MET:N	2.28	0.47
1:A:648:THR:HB	1:A:665:ALA:O	2.13	0.47
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.96	0.47
1:B:904:VAL:HG13	1:B:907:LEU:HD22	1.96	0.47
1:C:382:VAL:HG11	1:C:476:SER:CB	2.44	0.47
1:C:877:TYR:O	1:C:881:LEU:HG	2.14	0.47
1:C:449:LEU:HD21	1:C:937:LEU:HD23	1.96	0.47
1:D:198:LEU:HD11	1:D:252:LYS:HB2	1.97	0.47
1:E:255:GLN:OE1	1:E:256:ASP:N	2.47	0.47
1:E:659:LYS:HE3	1:E:659:LYS:HA	1.97	0.47
1:A:172:VAL:HG22	1:A:306:ILE:HD11	1.94	0.47
1:A:210:GLN:HE22	1:A:250:LEU:N	2.13	0.47
1:B:270:LEU:HA	1:B:270:LEU:HD12	1.63	0.47
1:B:317:PHE:CE2	1:B:323:ILE:HD13	2.50	0.47
1:B:344:LEU:HD13	1:B:376:LEU:HD13	1.96	0.47
1:B:32:VAL:HG12	1:B:390:ILE:HD12	1.96	0.47
1:B:583:THR:HB	1:B:586:ARG:H	1.79	0.47
1:C:244:GLU:CG	1:C:248:LYS:HE3	2.45	0.47
1:C:637:ARG:HD2	1:C:642:ASN:O	2.13	0.47
1:C:682:PHE:HE2	1:C:702:LEU:HD11	1.80	0.47
1:D:203:VAL:O	1:D:206:ALA:HB3	2.15	0.47
1:E:2:PRO:O	1:E:6:ILE:HD12	2.14	0.47
1:D:890:ALA:HB1	1:F:11:PHE:CD1	2.50	0.47
1:F:73:ASP:OD2	1:F:106:GLN:NE2	2.33	0.47
1:A:379:THR:HA	1:A:382:VAL:HG23	1.96	0.47
1:B:442:LEU:O	1:B:445:ILE:HG13	2.14	0.47
1:B:465:ALA:HA	1:B:468:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.96	0.47
1:D:535:LEU:CD2	1:D:1027:VAL:HG21	2.45	0.47
1:D:1040:ILE:HG22	1:D:1041:GLU:N	2.29	0.47
1:D:559:LEU:HD23	1:D:560:PRO:CD	2.45	0.47
1:F:227:GLY:O	1:F:229:GLN:HG3	2.14	0.47
1:F:996:GLY:O	1:F:999:ALA:N	2.48	0.47
1:B:534:ILE:HG22	3:B:1101:LMT:H5'	1.97	0.47
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.97	0.47
1:D:1031:ARG:O	1:D:1032:ARG:HG3	2.14	0.47
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.49	0.47
1:D:417:GLU:OE1	1:D:497:LEU:HD21	2.14	0.47
1:B:836:SER:OG	1:B:839:GLU:HG3	2.14	0.47
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.96	0.47
1:D:1035:ARG:NH2	1:D:1036:LYS:HG3	2.30	0.47
1:D:58:GLN:HA	1:D:62:THR:HB	1.97	0.47
1:D:708:LYS:C	1:D:710:PRO:HD3	2.35	0.47
1:D:888:LEU:HB2	1:D:898:PRO:HB3	1.97	0.47
1:D:562:SER:HB2	1:D:924:ASP:HB3	1.97	0.47
1:E:652:THR:HG23	1:E:665:ALA:CB	2.42	0.47
1:E:904:VAL:HG21	1:E:942:ALA:CB	2.45	0.47
1:F:900:SER:HB3	1:F:1029:VAL:HG21	1.96	0.47
1:D:754:TRP:CZ3	1:F:219:LEU:HD23	2.49	0.47
1:A:367:ILE:HG12	1:A:492:LEU:HB3	1.96	0.47
1:A:751:GLY:O	1:A:753:ALA:N	2.48	0.47
1:A:690:LEU:HD11	1:A:853:THR:O	2.15	0.47
1:B:222:THR:HA	1:B:224:PRO:HD3	1.96	0.47
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.96	0.47
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.96	0.47
1:D:944:LEU:O	1:D:947:GLU:HB3	2.14	0.47
1:E:187:TRP:NE1	1:E:269:GLU:OE2	2.48	0.47
1:F:220:GLY:HA3	1:F:230:LEU:O	2.15	0.47
1:F:672:VAL:C	1:F:674:LEU:H	2.18	0.47
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.96	0.47
1:A:420:MET:HB2	1:A:500:ILE:HD12	1.96	0.47
1:A:971:ARG:C	1:A:974:PRO:HD2	2.35	0.47
1:C:1016:VAL:HG13	3:C:1101:LMT:H112	1.96	0.47
1:C:63:GLN:O	1:C:67:GLN:HG3	2.15	0.47
1:C:801:PHE:CD1	1:C:804:PHE:HE2	2.31	0.47
1:D:125:GLN:OE1	1:D:770:LYS:HE3	2.15	0.47
1:E:213:GLN:HE21	1:E:239:ARG:HG3	1.80	0.47
1:E:764:ASP:OD1	1:E:765:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ARG:HB3	1:F:187:TRP:HE1	1.79	0.47
1:F:311:ALA:O	1:F:314:GLU:HB2	2.14	0.47
1:F:514:GLY:HA2	1:F:517:ASN:OD1	2.14	0.47
1:F:696:THR:HG23	1:F:699:ARG:HH12	1.80	0.47
1:A:1039:ASP:H	1:A:1040:ILE:HD13	1.80	0.47
1:A:602:GLU:OE2	1:A:650:ARG:NH1	2.48	0.47
1:A:937:LEU:HA	1:A:937:LEU:HD23	1.74	0.47
1:A:127:VAL:HB	1:B:113:LEU:HD22	1.96	0.47
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.14	0.47
1:B:783:PRO:O	1:B:786:ILE:HG12	2.15	0.47
1:B:961:ILE:HG13	1:B:961:ILE:H	1.52	0.47
1:C:214:VAL:CG2	1:C:237:GLN:HB2	2.45	0.47
1:C:371:ALA:O	1:C:375:VAL:HG23	2.14	0.47
1:C:600:THR:O	1:C:603:LYS:HG3	2.15	0.47
1:C:922:THR:O	1:C:924:ASP:N	2.48	0.47
1:C:953:MET:HE1	1:C:960:LEU:HD12	1.97	0.47
1:D:388:PHE:CE2	1:D:472:ILE:HD12	2.50	0.47
1:D:549:VAL:HG22	1:D:906:PRO:HG2	1.97	0.47
1:E:416:VAL:HG21	1:E:493:CYS:SG	2.55	0.47
1:E:508:GLY:H	1:E:518:ARG:HE	1.63	0.47
1:E:736:ALA:HB1	1:E:741:VAL:HG23	1.96	0.47
1:A:525:HIS:HA	1:A:528:THR:HG22	1.96	0.46
1:B:244:GLU:O	1:B:247:GLY:N	2.48	0.46
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.51	0.46
1:C:196:PHE:CD2	1:C:196:PHE:N	2.83	0.46
1:C:455:PRO:HG3	1:C:883:VAL:HG21	1.97	0.46
1:C:559:LEU:HD23	1:C:560:PRO:CD	2.46	0.46
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.79	0.46
1:E:32:VAL:HA	1:E:390:ILE:O	2.15	0.46
1:E:615:PHE:HD2	1:E:620:ARG:HG2	1.81	0.46
1:E:775:SER:HB3	1:E:780:ARG:HD3	1.98	0.46
1:E:960:LEU:O	1:E:964:THR:HG23	2.15	0.46
1:F:356:TYR:CA	1:F:365:THR:HG21	2.39	0.46
1:A:574:THR:CG2	1:A:627:ALA:HB3	2.46	0.46
1:B:259:ARG:O	1:B:259:ARG:HG2	2.13	0.46
1:B:554:TYR:CZ	1:B:558:ARG:HG3	2.50	0.46
1:C:124:GLN:HG3	1:C:125:GLN:N	2.27	0.46
1:D:165:ALA:HB3	1:D:313:MET:HE1	1.96	0.46
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.96	0.46
1:D:350:LEU:HA	1:D:350:LEU:HD23	1.73	0.46
1:D:676:THR:OG1	1:D:679:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:682:PHE:CD2	1:D:683:GLU:N	2.83	0.46
1:D:83:ASP:HB2	1:D:87:THR:O	2.15	0.46
1:E:795:ASP:OD2	1:E:797:GLN:N	2.47	0.46
1:E:818:ARG:HH12	1:E:823:PRO:HG3	1.80	0.46
1:F:391:ASN:OD1	1:F:393:LEU:HB2	2.15	0.46
1:F:671:ILE:CG2	1:F:674:LEU:HB2	2.45	0.46
1:F:743:ILE:HD12	1:F:743:ILE:H	1.81	0.46
1:A:244:GLU:O	1:A:247:GLY:N	2.48	0.46
1:A:28:LEU:HA	1:A:28:LEU:HD23	1.60	0.46
1:A:34:GLN:HB2	1:A:333:VAL:CG2	2.45	0.46
1:A:531:VAL:HG12	1:A:535:LEU:HD12	1.96	0.46
1:A:929:VAL:O	1:A:932:LEU:HB2	2.15	0.46
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.98	0.46
1:B:525:HIS:HA	1:B:528:THR:HG22	1.96	0.46
1:B:184:MET:HB3	1:B:771:VAL:HG13	1.97	0.46
1:B:801:PHE:HA	1:B:804:PHE:CE2	2.51	0.46
1:C:971:ARG:C	1:C:974:PRO:HD2	2.36	0.46
1:D:198:LEU:HD23	1:D:792:ARG:HH21	1.81	0.46
1:E:623:ASN:ND2	1:E:623:ASN:O	2.48	0.46
1:E:726:GLN:NE2	1:E:812:GLY:HA3	2.30	0.46
1:F:945:ILE:HG13	1:F:971:ARG:HH22	1.80	0.46
1:B:61:VAL:HG22	1:B:118:LEU:HD22	1.96	0.46
1:C:216:ALA:HB1	1:C:234:ILE:HG22	1.97	0.46
1:C:39:ALA:CB	1:C:673:GLU:HG2	2.46	0.46
1:C:568:ASP:O	1:C:634:TRP:HZ3	1.99	0.46
1:D:520:PHE:O	1:D:524:THR:HG22	2.16	0.46
1:E:195:LYS:NZ	1:E:196:PHE:HE1	2.13	0.46
1:E:177:LEU:HG	1:E:289:LEU:HD21	1.97	0.46
1:E:367:ILE:HB	1:E:368:PRO:HD3	1.98	0.46
1:E:892:TYR:O	1:E:893:GLU:HB2	2.15	0.46
1:F:946:VAL:HG13	1:F:1026:PHE:CE1	2.51	0.46
1:F:449:LEU:HD23	1:F:449:LEU:HA	1.73	0.46
1:A:382:VAL:O	1:A:385:ALA:HB3	2.15	0.46
1:B:185:ARG:HB3	1:B:187:TRP:NE1	2.31	0.46
1:A:222:THR:HG23	1:B:275:TYR:HB2	1.97	0.46
1:B:715:SER:O	1:B:717:ARG:HG3	2.15	0.46
1:C:101:ASP:O	1:C:105:VAL:HG23	2.15	0.46
1:A:583:THR:HG21	1:C:228:GLN:HG3	1.97	0.46
1:C:45:ILE:HD12	1:C:90:ILE:HB	1.96	0.46
1:C:332:PHE:CD1	1:C:634:TRP:CH2	3.04	0.46
1:C:966:ASP:O	1:C:970:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:LEU:HD12	1:E:923:ASN:HB2	1.98	0.46
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.97	0.46
1:F:1038:GLU:HB2	1:F:1039:ASP:OD1	2.14	0.46
1:D:781:MET:HB3	1:F:228:GLN:NE2	2.30	0.46
1:F:752:ALA:O	1:F:774:MET:HA	2.16	0.46
1:A:586:ARG:O	1:A:590:VAL:HG23	2.16	0.46
1:A:641:GLU:HB2	1:A:650:ARG:NH2	2.31	0.46
1:B:535:LEU:HD22	1:B:1027:VAL:HG11	1.98	0.46
1:C:425:LEU:HD13	1:C:429:GLU:HG3	1.97	0.46
1:C:577:GLN:HG3	1:C:624:THR:HG22	1.98	0.46
1:C:671:ILE:HB	1:C:862:MET:SD	2.55	0.46
1:D:538:THR:HG21	1:D:1028:VAL:HG21	1.97	0.46
1:D:457:ALA:HB1	1:D:468:ARG:HG3	1.97	0.46
1:E:149:MET:HB2	1:E:153:ASP:CB	2.45	0.46
1:E:203:VAL:O	1:E:207:ILE:HG13	2.16	0.46
1:E:242:SER:OG	1:E:245:GLU:HG3	2.16	0.46
1:E:415:ASN:HB3	1:E:434:SER:HB2	1.97	0.46
1:F:1025:PHE:O	1:F:1029:VAL:HG23	2.15	0.46
1:E:104:GLN:NE2	1:F:109:ASN:HD22	2.14	0.46
1:F:351:VAL:HG11	1:F:406:VAL:HG11	1.96	0.46
1:A:16:ALA:HB2	1:A:488:LEU:HD13	1.98	0.46
1:A:187:TRP:HE3	1:A:775:SER:O	1.97	0.46
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.96	0.46
1:A:768:VAL:HG12	1:B:63:GLN:OE1	2.15	0.46
1:C:456:MET:HA	1:C:459:PHE:CD1	2.51	0.46
1:C:743:ILE:HA	1:C:746:ILE:HG23	1.97	0.46
1:C:354:VAL:HG23	1:C:984:LEU:HD12	1.98	0.46
1:F:352:PHE:HA	1:F:355:MET:CE	2.41	0.46
1:F:673:GLU:CD	1:F:673:GLU:H	2.19	0.46
1:C:898:PRO:O	1:C:901:VAL:N	2.49	0.46
1:E:196:PHE:CD2	1:E:260:VAL:HG22	2.51	0.46
1:E:57:VAL:HB	1:E:88:VAL:CG2	2.46	0.46
1:F:344:LEU:O	1:F:348:ILE:HG13	2.15	0.46
1:A:228:GLN:NE2	1:A:230:LEU:O	2.47	0.46
1:A:623:ASN:OD1	1:A:623:ASN:N	2.42	0.46
1:A:669:PRO:HG2	1:A:676:THR:HG22	1.97	0.46
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.45	0.46
1:B:888:LEU:HD23	1:B:888:LEU:HA	1.53	0.46
1:C:340:VAL:HG11	1:C:395:MET:CB	2.33	0.46
1:D:723:ASP:HA	1:D:812:GLY:O	2.15	0.46
1:D:76:MET:HB2	1:D:93:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.98	0.46
1:F:183:ALA:O	1:F:270:LEU:HD12	2.16	0.46
1:F:418:ARG:O	1:F:422:GLU:HB2	2.16	0.46
1:F:483:LEU:HA	1:F:483:LEU:HD23	1.77	0.46
1:F:774:MET:HG2	1:F:775:SER:N	2.31	0.46
1:A:427:PRO:CD	1:A:499:PRO:HB3	2.39	0.46
1:B:578:LEU:HD22	1:B:661:ALA:CB	2.45	0.46
1:B:774:MET:HG2	1:B:775:SER:H	1.81	0.46
1:C:555:LEU:HD11	1:C:914:LEU:HD12	1.98	0.46
1:C:973:ARG:HG2	1:C:977:MET:CE	2.46	0.46
1:E:1042:HIS:HB3	1:E:1043:SER:HB3	1.96	0.46
1:E:142:VAL:HG12	1:E:321:LEU:HD11	1.98	0.46
1:E:447:MET:HB3	1:E:887:CYS:SG	2.56	0.46
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.97	0.46
1:F:506:GLY:C	1:F:508:GLY:H	2.19	0.46
1:F:74:ASN:O	1:F:94:PHE:HD2	1.98	0.46
1:F:953:MET:HE2	1:F:963:ALA:HB3	1.97	0.46
1:A:513:PHE:O	1:A:516:PHE:HB3	2.16	0.45
1:A:987:MET:HA	1:A:1008:MET:HE3	1.98	0.45
1:B:355:MET:HG2	1:B:365:THR:HA	1.97	0.45
1:B:398:MET:HE3	1:B:398:MET:HB3	1.82	0.45
1:C:188:MET:HA	1:C:266:ALA:CB	2.47	0.45
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.46	0.45
1:D:605:ASN:HD22	1:D:647:ILE:HD11	1.81	0.45
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.51	0.45
1:D:754:TRP:CH2	1:D:780:ARG:HA	2.51	0.45
1:E:712:MET:SD	1:E:835:LYS:HG2	2.56	0.45
1:F:420:MET:HB3	1:F:500:ILE:HB	1.98	0.45
1:F:75:LEU:HD11	1:F:92:LEU:HD12	1.97	0.45
1:A:1039:ASP:N	1:A:1040:ILE:HD13	2.32	0.45
1:B:897:ILE:HD13	1:B:950:LYS:HE3	1.98	0.45
1:D:865:GLN:HA	1:D:865:GLN:HE21	1.82	0.45
1:E:455:PRO:O	1:E:876:LEU:HD13	2.15	0.45
1:E:65:ILE:O	1:E:69:MET:HG2	2.17	0.45
1:E:713:LEU:HD11	1:E:843:LEU:HD12	1.98	0.45
1:E:888:LEU:HD13	1:E:901:VAL:CG1	2.45	0.45
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.16	0.45
1:F:668:LEU:H	1:F:668:LEU:HG	1.22	0.45
1:A:577:GLN:O	1:A:661:ALA:HB1	2.16	0.45
1:A:800:PRO:O	1:A:803:ALA:HB3	2.15	0.45
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:ASP:OD1	1:B:859:TRP:N	2.48	0.45
1:D:576:VAL:HG21	1:D:591:LEU:HD23	1.98	0.45
1:D:674:LEU:HD22	1:D:675:GLY:H	1.80	0.45
1:D:953:MET:HE1	1:D:960:LEU:HA	1.98	0.45
1:E:637:ARG:HB3	1:E:642:ASN:HB3	1.99	0.45
1:E:987:MET:CA	1:E:1008:MET:HE3	2.46	0.45
1:F:164:ASP:HB3	1:F:168:ARG:HH22	1.81	0.45
1:F:24:GLY:O	1:F:27:ILE:HG13	2.16	0.45
1:F:58:GLN:HG2	1:F:63:GLN:NE2	2.30	0.45
1:F:858:ASP:OD2	1:F:859:TRP:N	2.40	0.45
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.45	0.45
1:B:453:PHE:O	1:B:471:SER:OG	2.27	0.45
1:C:429:GLU:O	1:C:433:LYS:HB2	2.16	0.45
1:D:678:THR:HG21	1:D:835:LYS:O	2.17	0.45
1:E:844:MET:HE2	1:E:847:LEU:HB2	1.99	0.45
1:F:776:GLU:HB2	1:F:779:TYR:CE1	2.52	0.45
1:F:680:PHE:CD2	1:F:859:TRP:HZ3	2.34	0.45
1:F:898:PRO:O	1:F:901:VAL:N	2.48	0.45
1:A:1039:ASP:CA	1:A:1040:ILE:HB	2.43	0.45
1:A:636:ASP:O	1:A:638:PRO:HD3	2.17	0.45
1:A:74:ASN:O	1:A:94:PHE:HD2	2.00	0.45
1:B:541:TYR:CD1	1:B:541:TYR:N	2.85	0.45
1:B:564:LEU:HD13	1:B:671:ILE:HD12	1.99	0.45
1:C:354:VAL:HG22	1:C:980:LEU:HD23	1.98	0.45
1:C:379:THR:HG23	1:C:476:SER:OG	2.16	0.45
1:D:159:ALA:HB2	1:D:177:LEU:CD1	2.47	0.45
1:D:522:LYS:O	1:D:525:HIS:HB3	2.17	0.45
1:D:876:LEU:HA	1:D:876:LEU:HD23	1.82	0.45
1:F:644:VAL:O	1:F:648:THR:HG23	2.16	0.45
1:A:418:ARG:NH2	1:A:948:PHE:HE2	2.15	0.45
1:A:511:GLY:HA2	1:A:515:TRP:CD1	2.51	0.45
1:A:80:SER:O	1:A:817:GLU:HA	2.17	0.45
1:B:946:VAL:HG13	1:B:1026:PHE:CD1	2.52	0.45
1:C:53:ASP:O	1:C:56:THR:HB	2.17	0.45
1:C:567:GLU:OE1	1:C:996:GLY:HA2	2.17	0.45
1:D:112:GLN:HA	1:D:112:GLN:OE1	2.16	0.45
1:D:400:LEU:CD2	1:D:929:VAL:HG12	2.47	0.45
1:E:166:ILE:HD11	1:E:310:LEU:CD1	2.46	0.45
1:F:948:PHE:HD2	1:F:970:MET:HE2	1.81	0.45
1:A:705:GLU:HA	1:A:708:LYS:HD3	1.99	0.45
1:A:876:LEU:HA	1:A:876:LEU:HD23	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:LEU:HD23	1:C:555:LEU:HA	1.62	0.45
1:C:730:ASP:OD1	1:C:808:ARG:NE	2.34	0.45
1:D:20:MET:HG2	1:D:374:VAL:HA	1.98	0.45
1:D:658:ILE:HG13	1:D:659:LYS:HZ1	1.80	0.45
1:D:888:LEU:HD22	1:D:901:VAL:HG11	1.99	0.45
1:D:907:LEU:O	1:D:1013:THR:OG1	2.30	0.45
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.42	0.45
1:E:775:SER:OG	1:E:776:GLU:N	2.49	0.45
1:F:293:LEU:HD11	1:F:299:ALA:HA	1.97	0.45
1:F:165:ALA:HB3	1:F:313:MET:HE1	1.98	0.45
1:F:638:PRO:HB2	1:F:639:GLY:H	1.64	0.45
1:F:578:LEU:HD22	1:F:661:ALA:CB	2.47	0.45
1:F:684:LEU:HD23	1:F:825:MET:HB2	1.98	0.45
1:F:841:MET:O	1:F:845:GLU:HG2	2.17	0.45
1:F:971:ARG:HH21	1:F:975:ILE:HD11	1.82	0.45
1:A:1030:ARG:HA	1:A:1030:ARG:NH1	2.30	0.45
1:A:541:TYR:N	1:A:541:TYR:CD1	2.82	0.45
1:A:617:PHE:CZ	2:A:1101:ERY:H312	2.52	0.45
1:A:750:LEU:HD12	1:A:754:TRP:CD1	2.52	0.45
1:B:149:MET:HG3	1:B:154:ILE:HG13	1.98	0.45
1:B:259:ARG:HG3	1:B:261:LEU:HG	1.97	0.45
1:B:407:ASP:OD2	1:B:940:LYS:NZ	2.46	0.45
1:B:584:GLN:HB2	1:B:622:GLN:HG2	1.99	0.45
1:B:634:TRP:N	1:B:634:TRP:CD1	2.72	0.45
2:D:1101:ERY:C18	2:D:1101:ERY:H5	2.44	0.45
1:D:240:LEU:HD12	1:D:246:PHE:CZ	2.52	0.45
1:D:598:TYR:CE2	1:D:629:VAL:HG21	2.52	0.45
1:D:695:LEU:HD22	1:D:825:MET:SD	2.57	0.45
1:D:674:LEU:HD22	1:D:862:MET:HB3	1.99	0.45
1:E:578:LEU:HB2	1:E:623:ASN:O	2.16	0.45
1:F:94:PHE:CE1	1:F:103:ALA:HB1	2.51	0.45
1:F:249:ILE:O	1:F:262:LEU:N	2.48	0.45
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.99	0.45
1:A:344:LEU:HD11	1:A:398:MET:CB	2.47	0.45
1:D:162:MET:O	1:D:164:ASP:N	2.50	0.45
1:D:878:ALA:O	1:D:882:ILE:HG12	2.16	0.45
1:D:925:VAL:O	1:D:928:GLN:N	2.50	0.45
1:D:987:MET:HA	1:D:1008:MET:HE3	1.99	0.45
1:E:1041:GLU:OE1	1:E:1041:GLU:N	2.50	0.45
1:E:189:ASN:OD1	1:E:190:PRO:HD2	2.16	0.45
1:F:318:PRO:HG2	1:F:321:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:VAL:HG22	1:F:390:ILE:HB	1.99	0.45
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.52	0.45
1:F:76:MET:HG3	1:F:95:GLU:CD	2.38	0.45
1:F:561:SER:O	1:F:838:GLY:HA3	2.17	0.45
1:F:937:LEU:HD11	1:F:982:PHE:HE2	1.80	0.45
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.99	0.45
1:A:584:GLN:N	1:A:622:GLN:HB3	2.32	0.45
1:B:310:LEU:HD23	1:B:325:TYR:OH	2.17	0.45
1:B:58:GLN:HA	1:B:62:THR:HB	1.98	0.45
1:C:196:PHE:HD1	1:C:260:VAL:HG13	1.82	0.45
1:C:399:VAL:HG11	1:C:989:LEU:HD21	1.98	0.45
1:C:960:LEU:HB3	1:C:1040:ILE:HG23	1.99	0.45
1:D:1019:ILE:HG13	1:D:1020:PHE:CD1	2.51	0.45
1:D:1040:ILE:HG22	1:D:1041:GLU:H	1.81	0.45
1:D:470:PHE:HD2	1:D:929:VAL:HG11	1.80	0.45
1:E:187:TRP:HE3	1:E:775:SER:O	2.00	0.45
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.99	0.45
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.99	0.45
1:E:463:THR:OG1	1:E:464:GLY:N	2.50	0.45
1:E:563:PHE:HE1	1:E:866:GLU:OE2	2.00	0.45
1:A:680:PHE:CE2	1:A:829:GLY:HA3	2.53	0.44
1:A:4:PHE:O	1:A:8:ARG:HD2	2.17	0.44
1:B:154:ILE:O	1:B:157:TYR:N	2.49	0.44
1:D:23:GLY:HA3	1:D:377:LEU:O	2.17	0.44
1:D:456:MET:SD	1:D:932:LEU:HD11	2.56	0.44
1:D:948:PHE:O	1:D:952:LEU:HG	2.17	0.44
1:E:1038:GLU:C	1:E:1040:ILE:N	2.71	0.44
1:D:886:LEU:HD13	1:F:18:ILE:HG13	1.99	0.44
1:F:219:LEU:HD13	1:F:230:LEU:HD21	1.98	0.44
1:F:888:LEU:HD13	1:F:901:VAL:HG11	1.98	0.44
1:A:158:VAL:HA	1:A:162:MET:HE3	1.99	0.44
1:A:909:VAL:HG22	1:A:935:ILE:HD11	1.98	0.44
1:B:758:TYR:HE1	1:B:770:LYS:CG	2.30	0.44
1:C:167:SER:HB3	1:C:175:VAL:HG21	1.98	0.44
1:C:240:LEU:HD12	1:C:246:PHE:CD1	2.52	0.44
1:D:270:LEU:HA	1:D:270:LEU:HD12	1.57	0.44
1:D:658:ILE:O	1:D:659:LYS:HD3	2.17	0.44
1:D:922:THR:O	1:D:924:ASP:N	2.50	0.44
1:E:30:LEU:HG	1:E:31:PRO:HD2	1.99	0.44
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.98	0.44
1:E:438:ILE:HG22	1:E:948:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:GLY:HA2	1:E:815:ARG:NH1	2.31	0.44
1:E:937:LEU:HA	1:E:937:LEU:HD23	1.69	0.44
1:F:272:GLY:N	1:F:275:TYR:OH	2.35	0.44
1:F:177:LEU:HD23	1:F:289:LEU:HD23	1.99	0.44
1:F:508:GLY:O	1:F:509:LYS:HB2	2.16	0.44
1:F:69:MET:SD	1:F:72:ILE:HD11	2.57	0.44
1:F:683:GLU:HG2	1:F:819:TYR:CG	2.53	0.44
1:A:377:LEU:HA	1:A:377:LEU:HD23	1.77	0.44
1:A:58:GLN:OE1	1:A:816:LEU:HD13	2.16	0.44
1:A:671:ILE:HD12	1:A:674:LEU:O	2.18	0.44
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.32	0.44
1:D:335:ILE:O	1:D:339:GLU:HG2	2.18	0.44
1:E:1040:ILE:O	1:E:1041:GLU:HB3	2.17	0.44
1:E:40:PRO:HD3	1:E:462:SER:OG	2.16	0.44
1:E:412:VAL:HG22	1:E:438:ILE:HD11	1.99	0.44
1:F:1034:SER:HB3	1:F:1035:ARG:HB3	1.99	0.44
1:F:302:THR:O	1:F:305:ALA:HB3	2.17	0.44
1:F:81:ASN:HD21	1:F:815:ARG:NH1	2.15	0.44
1:A:775:SER:HG	1:A:780:ARG:HG2	1.81	0.44
1:B:699:ARG:NH2	1:B:722:GLU:OE1	2.50	0.44
1:B:808:ARG:NH1	1:B:810:GLU:OE2	2.51	0.44
1:C:24:GLY:O	1:C:27:ILE:HG13	2.17	0.44
1:C:546:LEU:HD23	1:C:546:LEU:HA	1.83	0.44
1:D:900:SER:HA	1:D:1025:PHE:HB3	2.00	0.44
1:D:572:PHE:CE1	1:D:648:THR:HG22	2.52	0.44
1:D:885:PHE:CE1	1:D:898:PRO:HB2	2.53	0.44
1:D:904:VAL:CG1	1:D:938:SER:HB3	2.48	0.44
1:E:146:ASP:OD1	1:E:148:THR:OG1	2.35	0.44
1:E:525:HIS:O	1:E:526:HIS:C	2.55	0.44
1:E:950:LYS:HZ1	1:E:1030:ARG:NE	2.15	0.44
1:F:378:GLY:O	1:F:382:VAL:HG23	2.17	0.44
1:F:514:GLY:C	1:F:516:PHE:H	2.21	0.44
1:A:185:ARG:HB3	1:A:187:TRP:NE1	2.32	0.44
1:A:391:ASN:O	1:A:395:MET:HG2	2.18	0.44
1:B:758:TYR:HE1	1:B:770:LYS:HG2	1.82	0.44
1:B:800:PRO:HG2	1:B:803:ALA:HB2	2.00	0.44
1:C:1016:VAL:O	1:C:1016:VAL:HG12	2.18	0.44
1:C:182:TYR:O	1:C:769:LYS:HD3	2.18	0.44
1:C:380:PHE:HA	1:C:383:LEU:HD12	1.99	0.44
1:D:866:GLU:HB2	3:D:1103:LMT:O2B	2.17	0.44
1:D:154:ILE:CG2	1:D:287:SER:HB3	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:SER:OG	1:E:133:SER:O	2.36	0.44
1:E:375:VAL:HG13	1:E:480:LEU:HB3	1.99	0.44
1:A:158:VAL:HA	1:A:162:MET:CE	2.47	0.44
1:A:239:ARG:HB2	1:A:763:ILE:HD12	1.99	0.44
1:A:559:LEU:HD23	1:A:560:PRO:CD	2.45	0.44
1:B:190:PRO:HG3	1:B:779:TYR:HB3	1.99	0.44
1:C:293:LEU:HD11	1:C:297:ALA:O	2.17	0.44
1:C:363:ARG:H	1:C:363:ARG:HG2	1.66	0.44
1:C:636:ASP:C	1:C:638:PRO:HD3	2.38	0.44
1:C:888:LEU:HA	1:C:888:LEU:HD23	1.78	0.44
1:D:893:GLU:OE2	1:F:8:ARG:HB3	2.16	0.44
1:E:743:ILE:H	1:E:743:ILE:HD12	1.82	0.44
1:E:910:ILE:O	1:E:914:LEU:HB2	2.16	0.44
1:F:100:ALA:O	1:F:103:ALA:HB3	2.17	0.44
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.47	0.44
1:A:187:TRP:HA	1:A:774:MET:O	2.17	0.44
1:A:360:GLN:HE21	1:A:360:GLN:HB3	1.58	0.44
1:A:549:VAL:O	1:A:552:MET:HB3	2.18	0.44
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.99	0.44
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.99	0.44
1:C:597:TYR:HD2	1:C:598:TYR:CD1	2.35	0.44
1:C:568:ASP:OD1	1:C:644:VAL:HG23	2.18	0.44
1:D:357:LEU:O	1:D:357:LEU:HD23	2.16	0.44
1:D:795:ASP:OD2	1:D:796:GLY:N	2.50	0.44
1:D:938:SER:OG	1:D:1014:ALA:HB1	2.17	0.44
1:E:894:SER:HB3	1:E:897:ILE:HB	1.99	0.44
1:A:404:LEU:HD12	1:A:937:LEU:HD21	2.00	0.44
1:A:729:ILE:HG22	1:A:731:ILE:HD11	2.00	0.44
1:A:752:ALA:O	1:A:774:MET:HA	2.17	0.44
1:B:383:LEU:O	1:B:386:PHE:N	2.51	0.44
1:B:602:GLU:HB3	1:B:606:VAL:HG23	1.99	0.44
1:C:185:ARG:HD3	1:C:185:ARG:HA	1.71	0.44
1:C:785:ASP:HA	1:C:788:ASP:OD2	2.18	0.44
1:C:680:PHE:CD2	1:C:859:TRP:HZ3	2.35	0.44
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.00	0.44
1:D:1016:VAL:O	1:D:1016:VAL:HG12	2.18	0.44
1:D:218:GLN:HG2	1:D:233:SER:HA	1.98	0.44
1:D:54:ALA:HB2	1:D:84:SER:HB3	1.99	0.44
1:D:984:LEU:HD23	1:D:984:LEU:HA	1.77	0.44
1:E:459:PHE:O	1:E:464:GLY:HA3	2.18	0.44
1:E:520:PHE:O	1:E:524:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:739:LEU:HD13	1:E:799:VAL:HG11	1.99	0.44
1:D:102:ILE:HD12	1:F:101:ASP:HB3	2.00	0.44
1:D:893:GLU:OE2	1:F:11:PHE:HB2	2.18	0.44
1:F:669:PRO:HG2	1:F:675:GLY:HA3	2.00	0.44
1:F:898:PRO:O	1:F:901:VAL:HG12	2.18	0.44
1:A:30:LEU:HD12	1:A:31:PRO:HD2	2.00	0.44
1:A:672:VAL:HB	1:A:673:GLU:OE2	2.18	0.44
1:A:80:SER:HA	1:A:89:GLN:O	2.18	0.44
1:A:986:VAL:HG21	1:A:1007:VAL:CG1	2.45	0.44
1:B:249:ILE:HG12	1:B:262:LEU:HB2	1.99	0.44
1:B:484:VAL:O	1:B:489:THR:HG23	2.18	0.44
1:B:555:LEU:HA	1:B:555:LEU:HD23	1.75	0.44
1:C:542:LEU:HA	1:C:542:LEU:HD12	1.69	0.44
1:C:652:THR:OG1	1:C:665:ALA:N	2.46	0.44
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	1.99	0.44
1:E:1019:ILE:HG13	1:E:1020:PHE:CD1	2.53	0.44
1:E:314:GLU:N	1:E:315:PRO:HD2	2.32	0.44
1:E:568:ASP:O	1:E:634:TRP:CZ3	2.69	0.44
1:E:588:GLN:HE21	1:E:592:ASN:ND2	2.14	0.44
1:E:775:SER:OG	1:E:780:ARG:HG2	2.17	0.44
1:F:33:ALA:O	1:F:391:ASN:HA	2.17	0.44
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.74	0.43
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.52	0.43
1:B:894:SER:HB3	1:B:897:ILE:H	1.83	0.43
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.99	0.43
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.52	0.43
1:C:706:ALA:HB1	1:C:713:LEU:HD22	1.99	0.43
1:C:723:ASP:OD1	1:C:813:SER:HB3	2.18	0.43
1:D:393:LEU:HD12	1:D:469:GLN:HG3	2.00	0.43
1:D:644:VAL:CG1	1:D:667:ASN:HB2	2.48	0.43
1:E:1032:ARG:HA	1:E:1033:PHE:HB3	2.00	0.43
1:E:35:TYR:HE2	1:E:393:LEU:HD21	1.82	0.43
1:E:789:TRP:HB2	1:E:801:PHE:CE2	2.53	0.43
1:F:110:LYS:O	1:F:113:LEU:HB2	2.18	0.43
1:F:645:GLU:O	1:F:649:MET:HB2	2.17	0.43
1:A:225:VAL:HG13	1:B:781:MET:HE1	2.01	0.43
1:A:781:MET:CE	1:C:228:GLN:HB2	2.47	0.43
1:C:396:PHE:CD1	1:C:1003:VAL:HG21	2.53	0.43
1:C:483:LEU:HD23	1:C:483:LEU:HA	1.71	0.43
1:C:535:LEU:HD21	1:C:1027:VAL:HG21	2.00	0.43
1:D:182:TYR:HA	1:D:182:TYR:HD1	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:HD13	1:D:200:PRO:HD3	2.01	0.43
1:D:462:SER:O	1:D:466:ILE:HG12	2.18	0.43
1:D:514:GLY:HA2	1:D:517:ASN:ND2	2.33	0.43
1:D:563:PHE:O	1:D:564:LEU:HD12	2.18	0.43
1:E:55:LYS:HG2	1:E:59:ASP:OD2	2.18	0.43
1:E:588:GLN:HG3	1:E:592:ASN:HD21	1.82	0.43
1:E:644:VAL:HG11	1:E:667:ASN:ND2	2.33	0.43
1:E:717:ARG:HD2	1:E:717:ARG:O	2.18	0.43
1:E:877:TYR:HD2	1:E:877:TYR:HA	1.60	0.43
1:F:1021:PHE:HB3	1:F:1025:PHE:CZ	2.53	0.43
1:F:359:LEU:O	1:F:361:ASN:N	2.51	0.43
1:F:578:LEU:CG	1:F:587:THR:HG22	2.46	0.43
1:F:905:VAL:HB	1:F:906:PRO:HD3	1.99	0.43
1:A:216:ALA:HB1	1:A:234:ILE:HG22	1.98	0.43
1:A:27:ILE:HG12	1:A:380:PHE:CD2	2.53	0.43
1:A:699:ARG:HD2	1:A:718:PRO:HB3	2.00	0.43
1:A:857:TYR:HE2	1:C:312:LYS:NZ	2.17	0.43
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.99	0.43
1:B:520:PHE:O	1:B:523:SER:OG	2.28	0.43
1:B:682:PHE:CE2	1:B:857:TYR:HB2	2.53	0.43
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.99	0.43
1:C:201:VAL:O	1:C:204:ILE:HB	2.18	0.43
1:C:510:LYS:HG2	1:C:511:GLY:N	2.33	0.43
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.53	0.43
1:D:752:ALA:O	1:D:774:MET:HA	2.19	0.43
1:D:555:LEU:HD11	1:D:914:LEU:HD12	2.00	0.43
1:D:937:LEU:HD12	1:D:1011:MET:SD	2.58	0.43
1:E:545:TYR:CE2	1:E:1025:PHE:HZ	2.36	0.43
1:E:574:THR:CG2	1:E:627:ALA:HB3	2.47	0.43
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.53	0.43
1:F:445:ILE:HG12	1:F:940:LYS:HG3	2.00	0.43
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.52	0.43
1:A:344:LEU:HD11	1:A:398:MET:HB2	2.00	0.43
1:B:1042:HIS:CG	1:B:1043:SER:N	2.86	0.43
1:B:203:VAL:O	1:B:207:ILE:HG13	2.19	0.43
1:C:159:ALA:HB2	1:C:177:LEU:CD1	2.49	0.43
1:C:359:LEU:HB2	1:C:365:THR:HG23	2.00	0.43
1:C:3:ASN:C	1:C:5:PHE:N	2.71	0.43
1:C:602:GLU:OE2	1:C:650:ARG:NH1	2.51	0.43
1:C:931:LEU:O	1:C:934:THR:HB	2.18	0.43
1:D:332:PHE:HB2	1:D:634:TRP:HH2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:MET:HB3	1:D:713:LEU:HD22	2.00	0.43
1:D:945:ILE:CG1	1:D:971:ARG:HH22	2.31	0.43
1:E:355:MET:CE	1:E:410:ILE:HG12	2.49	0.43
1:E:572:PHE:CE1	1:E:648:THR:HG22	2.53	0.43
1:F:200:PRO:HB2	1:F:749:THR:HG22	1.99	0.43
1:F:277:ILE:CD1	1:F:620:ARG:HH11	2.32	0.43
1:F:702:LEU:HB2	1:F:851:LEU:HD11	2.00	0.43
1:F:760:ASN:O	1:F:771:VAL:HB	2.19	0.43
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.99	0.43
1:A:767:ARG:HH12	1:B:67:GLN:CD	2.22	0.43
1:B:721:LEU:HB3	1:B:814:PRO:HG2	1.99	0.43
1:B:717:ARG:CD	1:B:828:LEU:HB2	2.46	0.43
1:B:83:ASP:HB2	1:B:87:THR:O	2.17	0.43
1:C:227:GLY:O	1:C:229:GLN:HG3	2.19	0.43
1:D:422:GLU:HB3	1:D:423:GLU:HG3	2.00	0.43
1:D:182:TYR:O	1:D:769:LYS:HB3	2.17	0.43
1:D:912:ALA:O	1:D:915:ALA:N	2.51	0.43
1:E:104:GLN:HE21	1:F:109:ASN:ND2	2.15	0.43
1:D:768:VAL:HG13	1:E:67:GLN:HE22	1.84	0.43
1:F:447:MET:HE3	1:F:887:CYS:HB3	2.00	0.43
1:F:602:GLU:HB3	1:F:606:VAL:HG23	2.00	0.43
1:F:669:PRO:CG	1:F:675:GLY:HA3	2.49	0.43
1:A:376:LEU:O	1:A:377:LEU:C	2.56	0.43
1:A:429:GLU:H	1:A:429:GLU:CD	2.21	0.43
1:A:483:LEU:HD13	1:A:487:ILE:HD12	2.01	0.43
1:A:946:VAL:HG13	1:A:1026:PHE:CD1	2.53	0.43
1:B:545:TYR:HE2	1:B:907:LEU:CD1	2.30	0.43
1:B:953:MET:HE2	1:B:963:ALA:HB3	1.99	0.43
1:D:908:GLY:HA2	1:D:1014:ALA:HB2	1.98	0.43
1:D:240:LEU:HD12	1:D:246:PHE:CE1	2.54	0.43
1:D:615:PHE:CZ	2:D:1101:ERY:H343	2.53	0.43
1:E:1038:GLU:C	1:E:1040:ILE:H	2.21	0.43
1:E:512:PHE:HB3	1:E:513:PHE:CD1	2.54	0.43
1:F:49:TYR:HD1	1:F:57:VAL:HG12	1.81	0.43
1:F:782:LEU:O	1:F:785:ASP:HB2	2.18	0.43
1:F:960:LEU:O	1:F:964:THR:HG23	2.19	0.43
1:A:445:ILE:HD12	1:A:446:ALA:N	2.33	0.43
1:B:1037:ASN:HA	1:B:1038:GLU:CG	2.48	0.43
1:B:187:TRP:HE3	1:B:775:SER:O	2.02	0.43
1:B:23:GLY:HA3	1:B:377:LEU:O	2.19	0.43
1:B:675:GLY:C	1:B:677:ALA:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:PHE:HZ	1:B:926:TYR:HE2	1.67	0.43
1:C:181:GLN:OE1	1:C:767:ARG:NH2	2.49	0.43
1:D:800:PRO:O	1:D:803:ALA:HB3	2.19	0.43
1:E:178:PHE:O	1:E:287:SER:OG	2.26	0.43
1:E:959:GLY:O	1:E:963:ALA:N	2.41	0.43
1:F:284:GLN:CG	1:F:285:PRO:HD2	2.49	0.43
1:A:133:SER:OG	1:A:135:SER:O	2.36	0.43
1:A:712:MET:HG2	1:A:843:LEU:HG	2.01	0.43
1:A:961:ILE:HG13	1:A:961:ILE:H	1.38	0.43
1:B:1019:ILE:HG13	1:B:1020:PHE:CD1	2.53	0.43
1:B:196:PHE:CD1	1:B:196:PHE:N	2.87	0.43
1:B:356:TYR:HE1	1:B:362:PHE:HA	1.83	0.43
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.84	0.43
1:B:5:PHE:CE1	1:B:487:ILE:HG12	2.54	0.43
1:B:721:LEU:HA	1:B:721:LEU:HD12	1.91	0.43
1:C:938:SER:HB3	1:C:1014:ALA:HB1	2.01	0.43
1:C:146:ASP:O	1:C:148:THR:N	2.51	0.43
1:C:412:VAL:CG2	1:C:442:LEU:HD11	2.49	0.43
1:C:520:PHE:CE2	1:C:973:ARG:HG3	2.53	0.43
1:B:175:VAL:HG23	1:C:70:ASN:HD22	1.83	0.43
1:C:787:GLY:O	1:C:789:TRP:N	2.52	0.43
1:C:960:LEU:O	1:C:964:THR:HG23	2.19	0.43
1:D:63:GLN:O	1:D:67:GLN:HG3	2.17	0.43
1:E:1042:HIS:HB3	1:E:1043:SER:CB	2.49	0.43
1:E:213:GLN:HG2	1:E:239:ARG:HG3	2.00	0.43
1:E:508:GLY:HA2	1:E:518:ARG:NE	2.34	0.43
1:F:608:SER:OG	1:F:630:SER:HB3	2.18	0.43
1:A:132:SER:OG	1:A:133:SER:N	2.51	0.43
1:A:189:ASN:OD1	1:A:190:PRO:HD2	2.19	0.43
1:A:428:LYS:HG3	1:A:429:GLU:OE2	2.19	0.43
1:A:66:GLU:OE1	1:A:821:GLY:HA2	2.18	0.43
1:B:332:PHE:C	1:B:332:PHE:CD2	2.93	0.43
1:B:898:PRO:O	1:B:901:VAL:HG12	2.19	0.43
1:C:332:PHE:HD1	1:C:634:TRP:CH2	2.37	0.43
1:D:101:ASP:OD1	1:D:101:ASP:N	2.48	0.43
1:D:137:LEU:HD23	1:D:291:ILE:HG22	2.01	0.43
1:D:897:ILE:HA	1:D:1029:VAL:HG11	2.01	0.43
1:E:244:GLU:O	1:E:247:GLY:N	2.51	0.43
1:E:658:ILE:C	1:E:659:LYS:HD2	2.39	0.43
1:E:894:SER:HB2	1:E:897:ILE:HD12	2.00	0.43
1:E:905:VAL:HB	1:E:906:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:GLN:HB2	1:F:333:VAL:HG13	1.99	0.43
1:F:355:MET:HG2	1:F:410:ILE:HD11	1.99	0.43
1:F:578:LEU:HB3	1:F:579:PRO:HD2	2.01	0.43
1:F:889:ALA:HB2	1:F:898:PRO:HG2	2.00	0.43
1:A:81:ASN:OD1	2:A:1101:ERY:H272	2.19	0.43
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.69	0.43
1:A:196:PHE:CD1	1:A:260:VAL:HG13	2.53	0.43
1:A:890:ALA:HB2	1:C:14:VAL:HG11	2.01	0.43
1:A:910:ILE:HG13	1:A:910:ILE:O	2.19	0.43
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.84	0.43
1:B:356:TYR:HD1	1:B:365:THR:HG21	1.84	0.43
1:B:393:LEU:HD22	1:B:470:PHE:HE1	1.84	0.43
1:C:166:ILE:O	1:C:169:THR:HB	2.19	0.43
1:C:445:ILE:HG12	1:C:940:LYS:CG	2.49	0.43
1:D:897:ILE:HG12	1:D:1030:ARG:HD2	2.00	0.43
1:D:30:LEU:HD12	1:D:30:LEU:HA	1.80	0.43
1:D:428:LYS:HG2	1:D:428:LYS:H	1.21	0.43
1:D:38:ILE:CG2	1:D:462:SER:HB2	2.38	0.43
1:D:531:VAL:HG21	1:D:968:VAL:HG11	2.00	0.43
1:D:572:PHE:CD1	1:D:648:THR:HG22	2.53	0.43
1:E:40:PRO:HA	1:E:41:PRO:HD3	1.75	0.43
1:E:459:PHE:CD2	1:E:876:LEU:HD12	2.53	0.43
1:E:539:GLY:O	1:E:542:LEU:HB2	2.19	0.43
1:F:187:TRP:NE1	1:F:269:GLU:OE1	2.52	0.43
1:F:382:VAL:HG11	1:F:476:SER:HB2	2.00	0.43
1:F:571:VAL:HG12	1:F:668:LEU:HD11	2.01	0.43
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.19	0.42
1:A:11:PHE:HE1	1:A:15:ILE:HD11	1.84	0.42
1:A:352:PHE:CD2	1:A:353:LEU:HD23	2.53	0.42
1:A:726:GLN:O	1:A:810:GLU:HG2	2.19	0.42
1:B:211:ASN:O	1:B:760:ASN:ND2	2.52	0.42
1:B:352:PHE:CD2	1:B:353:LEU:HD23	2.49	0.42
1:C:42:ALA:HB2	1:C:93:THR:HG23	2.01	0.42
1:C:516:PHE:HA	1:C:519:MET:HE3	2.01	0.42
1:C:686:ASP:HB3	1:C:823:PRO:HB2	2.01	0.42
1:D:484:VAL:HG13	1:D:488:LEU:HB3	2.01	0.42
1:D:702:LEU:HD22	1:D:827:ILE:HD13	2.01	0.42
1:E:239:ARG:NH1	1:E:761:ASP:HB2	2.34	0.42
1:E:675:GLY:C	1:E:677:ALA:H	2.22	0.42
1:F:382:VAL:HG11	1:F:476:SER:CB	2.48	0.42
1:F:984:LEU:HA	1:F:984:LEU:HD23	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:HB3	1:A:180:SER:N	2.28	0.42
1:A:362:PHE:N	1:A:362:PHE:CD2	2.85	0.42
1:A:555:LEU:HA	1:A:555:LEU:HD23	1.57	0.42
1:B:401:ALA:O	1:B:405:LEU:HG	2.19	0.42
1:B:813:SER:HA	1:B:814:PRO:HD3	1.93	0.42
1:B:817:GLU:OE1	1:B:826:GLU:N	2.52	0.42
1:B:690:LEU:HD11	1:B:854:GLY:HA3	2.00	0.42
1:C:311:ALA:O	1:C:315:PRO:HD3	2.19	0.42
1:A:893:GLU:CD	1:C:8:ARG:HB3	2.39	0.42
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.84	0.42
1:D:156:ASP:OD1	1:D:765:ARG:NH2	2.52	0.42
1:E:174:ASP:CB	1:E:292:LYS:HB2	2.46	0.42
1:F:144:ASN:HA	1:F:320:GLY:O	2.19	0.42
1:F:659:LYS:HD3	1:F:659:LYS:HA	1.82	0.42
1:F:776:GLU:HB2	1:F:779:TYR:CD1	2.54	0.42
1:A:210:GLN:HE22	1:A:250:LEU:H	1.66	0.42
1:B:144:ASN:HA	1:B:320:GLY:O	2.20	0.42
1:C:425:LEU:HD22	1:C:429:GLU:HG2	2.00	0.42
1:C:536:ARG:HD2	3:C:1101:LMT:O4'	2.19	0.42
1:D:441:ALA:HB2	1:D:947:GLU:OE2	2.19	0.42
1:D:467:TYR:CE2	1:D:925:VAL:HG22	2.54	0.42
1:E:1007:VAL:HG12	1:E:1008:MET:N	2.35	0.42
1:E:1037:ASN:HB2	1:E:1038:GLU:CA	2.50	0.42
1:E:801:PHE:CD1	1:E:804:PHE:HE2	2.38	0.42
1:F:181:GLN:HG2	1:F:182:TYR:N	2.34	0.42
1:F:546:LEU:HD23	1:F:546:LEU:HA	1.69	0.42
1:E:766:GLY:O	1:F:59:ASP:HB2	2.20	0.42
1:F:971:ARG:C	1:F:974:PRO:HD2	2.40	0.42
1:A:1026:PHE:CE2	1:A:1030:ARG:HG3	2.55	0.42
1:B:984:LEU:HA	1:B:984:LEU:HD23	1.63	0.42
1:C:787:GLY:C	1:C:789:TRP:H	2.23	0.42
1:C:680:PHE:HA	1:C:863:SER:OG	2.20	0.42
1:C:453:PHE:HZ	1:C:933:THR:OG1	2.02	0.42
1:D:997:SER:HA	1:D:1000:GLN:HB2	2.01	0.42
1:F:73:ASP:HB2	1:F:106:GLN:OE1	2.19	0.42
1:F:356:TYR:C	1:F:358:PHE:H	2.23	0.42
1:F:455:PRO:HG3	1:F:883:VAL:HG21	2.00	0.42
1:F:913:LEU:HD23	1:F:927:PHE:HZ	1.85	0.42
1:F:985:GLY:O	1:F:988:PRO:HD2	2.19	0.42
1:B:888:LEU:HD11	1:B:943:ILE:HD11	2.02	0.42
1:C:64:VAL:CG1	1:C:117:LEU:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:PHE:O	1:C:262:LEU:HD23	2.19	0.42
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.19	0.42
1:D:108:GLN:NE2	1:E:109:ASN:O	2.53	0.42
1:D:190:PRO:HB3	1:D:789:TRP:CZ3	2.54	0.42
1:D:292:LYS:NZ	2:D:1101:ERY:O11	2.52	0.42
1:D:361:ASN:HB3	1:D:364:ALA:HB3	2.02	0.42
1:D:239:ARG:HH12	1:D:761:ASP:HB2	1.85	0.42
1:D:851:LEU:HB3	1:D:852:PRO:HD2	2.00	0.42
1:E:230:LEU:HG	1:E:231:ASN:N	2.33	0.42
1:E:355:MET:SD	1:E:365:THR:HA	2.60	0.42
1:E:519:MET:HG2	1:E:519:MET:H	1.59	0.42
1:E:549:VAL:O	1:E:552:MET:HB3	2.19	0.42
1:E:582:ALA:HA	1:E:586:ARG:NH2	2.33	0.42
1:E:971:ARG:C	1:E:974:PRO:HD2	2.40	0.42
1:F:277:ILE:HD11	1:F:620:ARG:HH11	1.84	0.42
1:F:340:VAL:HG11	1:F:395:MET:HB3	2.00	0.42
1:F:680:PHE:HB2	1:F:859:TRP:CZ3	2.54	0.42
1:A:375:VAL:HG22	1:A:484:VAL:HG21	2.02	0.42
1:A:604:ASN:O	1:A:632:LYS:HD2	2.20	0.42
1:B:47:ALA:HB2	1:B:127:VAL:HG13	2.01	0.42
1:C:647:ILE:O	1:C:650:ARG:N	2.53	0.42
1:D:577:GLN:OE1	1:D:624:THR:HG22	2.18	0.42
1:D:636:ASP:OD1	1:D:636:ASP:N	2.51	0.42
1:F:1019:ILE:HG13	1:F:1020:PHE:CD1	2.54	0.42
1:F:185:ARG:HH12	1:F:774:MET:HE2	1.85	0.42
1:F:509:LYS:O	1:F:518:ARG:NH1	2.52	0.42
1:F:617:PHE:CD1	1:F:626:ILE:HD11	2.55	0.42
1:A:30:LEU:HD23	1:A:390:ILE:HG13	2.01	0.42
1:A:578:LEU:HB2	1:A:623:ASN:O	2.19	0.42
1:A:787:GLY:O	1:A:789:TRP:N	2.52	0.42
1:A:857:TYR:N	1:A:857:TYR:CD2	2.88	0.42
1:B:201:VAL:HG23	1:B:749:THR:HG23	2.02	0.42
1:C:411:VAL:O	1:C:415:ASN:HB2	2.19	0.42
1:C:445:ILE:HG12	1:C:940:LYS:HG3	2.02	0.42
1:D:418:ARG:HH22	1:D:948:PHE:HE2	1.65	0.42
1:E:318:PRO:HG2	1:E:321:LEU:HB2	2.00	0.42
1:E:572:PHE:HA	1:E:668:LEU:CD2	2.47	0.42
1:E:678:THR:O	1:E:678:THR:OG1	2.27	0.42
1:E:925:VAL:O	1:E:928:GLN:N	2.53	0.42
1:F:15:ILE:O	1:F:19:ILE:HG13	2.20	0.42
1:F:540:ARG:O	1:F:543:VAL:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:575:MET:HG2	1:F:666:PHE:HE1	1.85	0.42
1:F:443:VAL:HG12	1:F:891:LEU:HD21	2.01	0.42
1:A:102:ILE:HA	1:A:102:ILE:HD13	1.91	0.42
1:C:706:ALA:HB2	1:C:847:LEU:HD23	2.00	0.42
1:C:800:PRO:HB2	1:C:802:SER:OG	2.19	0.42
1:C:835:LYS:HG2	1:C:836:SER:N	2.35	0.42
1:C:75:LEU:CD1	1:C:92:LEU:HB3	2.49	0.42
1:D:546:LEU:HA	1:D:546:LEU:HD23	1.82	0.42
1:E:1026:PHE:O	1:E:1030:ARG:HB2	2.20	0.42
1:E:154:ILE:HG22	1:E:287:SER:HB3	2.02	0.42
1:E:789:TRP:HB2	1:E:801:PHE:HE2	1.83	0.42
1:E:818:ARG:NH1	1:E:823:PRO:HG3	2.34	0.42
1:F:584:GLN:N	1:F:622:GLN:HB3	2.35	0.42
1:F:742:SER:O	1:F:745:ASP:HB2	2.20	0.42
1:A:3:ASN:O	1:A:4:PHE:C	2.58	0.42
1:A:618:ALA:C	1:A:815:ARG:HH22	2.22	0.42
1:A:634:TRP:N	1:A:634:TRP:CD1	2.85	0.42
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.55	0.42
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.01	0.42
1:B:572:PHE:HD1	1:B:666:PHE:O	2.02	0.42
1:B:712:MET:CE	1:B:839:GLU:HB3	2.50	0.42
1:B:841:MET:HG2	1:B:859:TRP:CH2	2.55	0.42
1:B:57:VAL:HB	1:B:88:VAL:HG23	2.02	0.42
1:B:913:LEU:HD23	1:B:927:PHE:HZ	1.85	0.42
1:C:270:LEU:HD12	1:C:270:LEU:HA	1.56	0.42
1:C:337:ILE:HG13	1:C:392:THR:HG23	2.02	0.42
1:C:456:MET:HB3	1:C:876:LEU:HD21	2.02	0.42
1:C:886:LEU:HA	1:C:886:LEU:HD13	1.71	0.42
1:D:343:THR:O	1:D:346:GLU:HB2	2.20	0.42
1:D:544:LEU:O	1:D:548:ILE:HG13	2.19	0.42
1:E:589:LYS:O	1:E:592:ASN:HB2	2.20	0.42
1:F:892:TYR:C	1:F:894:SER:H	2.22	0.42
1:F:973:ARG:HG2	1:F:977:MET:HE2	2.01	0.42
1:C:692:HIS:CD2	1:C:692:HIS:C	2.93	0.42
1:E:185:ARG:HD3	1:E:185:ARG:HA	1.90	0.42
1:E:310:LEU:HA	1:E:310:LEU:HD12	1.84	0.42
1:E:685:ILE:HG22	1:E:687:GLN:OE1	2.20	0.42
1:F:931:LEU:O	1:F:935:ILE:HG13	2.19	0.42
1:A:472:ILE:HG22	1:A:473:THR:N	2.34	0.41
1:A:545:TYR:HB2	1:A:1021:PHE:HE2	1.85	0.41
1:A:644:VAL:O	1:A:648:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:HG12	1:A:1030:ARG:HD2	2.01	0.41
1:B:990:VAL:HG22	1:B:1004:GLY:C	2.40	0.41
1:B:514:GLY:C	1:B:516:PHE:H	2.23	0.41
1:C:580:ALA:HB1	1:C:724:THR:CG2	2.48	0.41
1:C:587:THR:OG1	1:C:613:ASN:ND2	2.51	0.41
1:C:671:ILE:CG2	1:C:674:LEU:HB2	2.49	0.41
1:D:542:LEU:HA	1:D:542:LEU:HD12	1.82	0.41
1:D:675:GLY:H	1:D:862:MET:HB3	1.84	0.41
1:D:961:ILE:H	1:D:961:ILE:HD12	1.85	0.41
1:E:249:ILE:HD11	1:E:262:LEU:HD22	2.02	0.41
1:E:520:PHE:O	1:E:523:SER:OG	2.38	0.41
1:E:752:ALA:O	1:E:774:MET:HA	2.19	0.41
1:E:776:GLU:CG	1:E:777:ALA:H	2.32	0.41
1:D:583:THR:CG2	1:F:229:GLN:HA	2.45	0.41
1:A:58:GLN:HG3	1:A:818:ARG:HD2	2.03	0.41
1:A:900:SER:HB3	1:A:1029:VAL:HG21	2.01	0.41
1:A:985:GLY:O	1:A:988:PRO:HD2	2.20	0.41
1:B:1015:THR:C	1:B:1017:LEU:H	2.24	0.41
1:B:969:ARG:NH1	1:B:970:MET:HB3	2.34	0.41
1:C:356:TYR:CA	1:C:365:THR:HG21	2.41	0.41
1:C:564:LEU:HD23	1:C:670:ALA:HB3	2.01	0.41
1:C:39:ALA:HB3	1:C:673:GLU:HG2	2.01	0.41
1:D:190:PRO:HB3	1:D:789:TRP:CE3	2.54	0.41
1:D:262:LEU:HD12	1:D:265:VAL:CG2	2.50	0.41
1:D:699:ARG:HD2	1:D:718:PRO:HB3	2.02	0.41
1:D:708:LYS:HB3	1:D:708:LYS:HE3	1.84	0.41
1:D:946:VAL:HG13	1:D:1026:PHE:CD1	2.55	0.41
1:E:754:TRP:CH2	1:E:780:ARG:HA	2.56	0.41
1:F:894:SER:CB	1:F:897:ILE:HG12	2.48	0.41
1:F:944:LEU:HB3	1:F:971:ARG:HE	1.83	0.41
1:A:228:GLN:NE2	1:A:230:LEU:H	2.17	0.41
1:B:5:PHE:HE2	1:B:11:PHE:HD2	1.68	0.41
1:B:425:LEU:HB2	1:B:430:ALA:HB2	2.02	0.41
1:B:459:PHE:CB	1:B:464:GLY:HA2	2.51	0.41
1:C:564:LEU:HG	1:C:565:PRO:HD2	2.01	0.41
1:D:375:VAL:HG21	1:D:481:SER:HA	2.02	0.41
1:D:401:ALA:O	1:D:405:LEU:HG	2.20	0.41
1:D:448:VAL:HG22	1:D:887:CYS:CB	2.44	0.41
1:D:764:ASP:OD1	1:D:765:ARG:HG3	2.20	0.41
1:D:6:ILE:HG13	1:D:7:ASP:N	2.34	0.41
1:D:961:ILE:CD1	1:D:961:ILE:H	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:ARG:NE	3:E:1101:LMT:O3B	2.53	0.41
1:E:119:PRO:HG2	1:E:122:VAL:HB	2.02	0.41
1:E:459:PHE:CE2	1:E:876:LEU:HD12	2.55	0.41
1:E:445:ILE:HG12	1:E:940:LYS:HE3	2.01	0.41
1:E:94:PHE:CZ	1:E:103:ALA:HB1	2.55	0.41
1:F:352:PHE:HD1	1:F:369:THR:OG1	2.04	0.41
1:F:369:THR:O	1:F:373:PRO:HD2	2.20	0.41
1:F:187:TRP:HE3	1:F:775:SER:O	2.03	0.41
1:A:1040:ILE:HD11	1:A:1042:HIS:HB2	2.01	0.41
1:A:183:ALA:HB2	1:A:273:GLU:HG3	2.01	0.41
1:A:832:ALA:HB3	1:A:835:LYS:CD	2.41	0.41
1:A:78:MET:HG3	1:A:92:LEU:HG	2.01	0.41
1:B:255:GLN:HG3	1:B:255:GLN:H	1.59	0.41
1:C:591:LEU:HD11	1:C:625:GLY:HA3	2.01	0.41
1:D:1018:ALA:O	1:D:1022:VAL:HG23	2.20	0.41
1:D:160:ALA:HA	1:D:767:ARG:NE	2.35	0.41
1:D:452:VAL:HG12	1:D:880:SER:OG	2.20	0.41
1:D:841:MET:O	1:D:845:GLU:HG3	2.20	0.41
1:E:273:GLU:OE1	1:E:770:LYS:HD2	2.21	0.41
1:E:534:ILE:HG22	3:E:1101:LMT:C5'	2.49	0.41
1:E:891:LEU:HA	1:E:891:LEU:HD12	1.68	0.41
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.76	0.41
1:B:14:VAL:HG22	1:C:886:LEU:CD1	2.42	0.41
1:B:185:ARG:HD3	1:B:185:ARG:HA	1.84	0.41
1:B:359:LEU:HD13	1:B:417:GLU:HG3	2.01	0.41
1:B:684:LEU:HA	1:B:684:LEU:HD12	1.64	0.41
1:C:443:VAL:HG12	1:C:891:LEU:CD2	2.50	0.41
1:C:525:HIS:C	1:C:525:HIS:CD2	2.92	0.41
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.91	0.41
1:B:237:GLN:CG	1:C:731:ILE:HD11	2.50	0.41
1:C:713:LEU:HD21	1:C:844:MET:SD	2.60	0.41
1:D:57:VAL:HG21	1:D:86:GLY:HA2	2.02	0.41
1:E:362:PHE:O	1:E:366:LEU:HG	2.21	0.41
1:E:588:GLN:NE2	1:E:592:ASN:HD21	2.14	0.41
1:E:617:PHE:HA	1:E:617:PHE:HD1	1.75	0.41
1:F:149:MET:HG3	1:F:154:ILE:HG13	2.03	0.41
1:F:34:GLN:HB2	1:F:333:VAL:CG2	2.35	0.41
1:F:795:ASP:OD2	1:F:797:GLN:HG2	2.21	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.84	0.41
1:A:847:LEU:HD23	1:A:847:LEU:HA	1.86	0.41
1:B:5:PHE:CE2	1:B:11:PHE:HD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:TYR:C	1:B:358:PHE:H	2.24	0.41
1:B:937:LEU:HD23	1:B:937:LEU:HA	1.73	0.41
1:B:987:MET:HA	1:B:1008:MET:HE3	2.03	0.41
1:C:61:VAL:HG21	1:C:122:VAL:HG21	2.03	0.41
1:C:574:THR:HG23	1:C:627:ALA:HB3	2.03	0.41
1:C:644:VAL:CG1	1:C:667:ASN:HB2	2.50	0.41
1:C:858:ASP:OD2	1:C:859:TRP:N	2.50	0.41
1:D:136:PHE:CD2	1:D:292:LYS:HG3	2.56	0.41
1:D:356:TYR:C	1:D:358:PHE:H	2.23	0.41
1:D:420:MET:HE3	1:D:420:MET:HB2	1.93	0.41
1:D:801:PHE:CD1	1:D:804:PHE:HE2	2.39	0.41
1:D:682:PHE:CE2	1:D:857:TYR:HB2	2.56	0.41
1:D:527:TYR:CE2	1:D:968:VAL:HG13	2.56	0.41
1:E:189:ASN:HB3	1:E:192:GLU:HB2	2.02	0.41
1:E:32:VAL:HG12	1:E:390:ILE:HB	2.01	0.41
1:E:537:SER:OG	1:E:540:ARG:NE	2.50	0.41
1:E:597:TYR:CD1	1:E:601:LYS:HD2	2.56	0.41
1:E:997:SER:HA	1:E:1000:GLN:HB2	2.03	0.41
1:F:1043:SER:HB2	1:F:1044:HIS:ND1	2.36	0.41
1:F:897:ILE:HD11	1:F:950:LYS:HE2	2.02	0.41
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.89	0.41
1:A:735:LYS:O	1:A:738:ALA:HB3	2.20	0.41
1:A:127:VAL:O	1:B:113:LEU:HD13	2.21	0.41
1:B:352:PHE:CZ	1:B:362:PHE:HE1	2.39	0.41
1:B:459:PHE:HB3	1:B:464:GLY:HA2	2.02	0.41
1:B:594:VAL:HG22	1:B:655:PHE:CZ	2.56	0.41
1:B:950:LYS:HB2	1:B:950:LYS:HE2	1.73	0.41
1:D:314:GLU:OE1	1:D:323:ILE:HD12	2.20	0.41
1:D:605:ASN:O	1:D:632:LYS:N	2.45	0.41
1:D:684:LEU:HA	1:D:684:LEU:HD12	1.93	0.41
1:A:10:ILE:HG13	1:B:895:TRP:CE2	2.56	0.41
1:A:211:ASN:CG	1:A:240:LEU:HG	2.40	0.41
1:A:706:ALA:HB1	1:A:713:LEU:HD23	2.03	0.41
1:A:944:LEU:HA	1:A:944:LEU:HD23	1.89	0.41
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.88	0.41
1:B:77:TYR:OH	1:B:861:GLY:HA2	2.20	0.41
1:C:594:VAL:HG22	1:C:655:PHE:CE2	2.56	0.41
1:C:751:GLY:O	1:C:753:ALA:N	2.54	0.41
1:D:360:GLN:H	1:D:360:GLN:HG2	1.69	0.41
1:D:388:PHE:CZ	1:D:472:ILE:HD12	2.56	0.41
1:D:727:PHE:CD1	1:D:809:TRP:CE2	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:GLN:NE2	1:E:109:ASN:HB2	2.35	0.41
1:E:544:LEU:O	1:E:547:ILE:HB	2.21	0.41
1:F:578:LEU:HA	1:F:661:ALA:HB1	2.03	0.41
1:A:163:LYS:HD2	1:A:177:LEU:HG	2.03	0.41
1:A:648:THR:HB	1:A:665:ALA:C	2.41	0.41
1:B:291:ILE:HG21	1:B:306:ILE:HD11	2.02	0.41
1:C:937:LEU:HD13	1:C:1011:MET:HE2	2.01	0.41
1:C:952:LEU:HD11	1:C:970:MET:HE2	2.03	0.41
1:C:971:ARG:HH21	1:C:975:ILE:HD11	1.86	0.41
1:D:424:GLY:HA3	1:D:502:LYS:HB3	2.03	0.41
1:D:584:GLN:HB2	1:D:622:GLN:HG2	2.03	0.41
1:E:354:VAL:O	1:E:358:PHE:HB2	2.20	0.41
1:E:699:ARG:HE	1:E:718:PRO:HG3	1.85	0.41
1:E:839:GLU:O	1:E:842:GLU:HB3	2.21	0.41
1:E:841:MET:O	1:E:845:GLU:HG3	2.21	0.41
1:E:887:CYS:O	1:E:890:ALA:HB3	2.21	0.41
1:E:922:THR:O	1:E:924:ASP:N	2.53	0.41
1:F:172:VAL:HG13	1:F:291:ILE:HG23	2.02	0.41
1:F:72:ILE:HG21	1:F:72:ILE:HD13	1.87	0.41
1:F:888:LEU:CD1	1:F:901:VAL:HG11	2.50	0.41
1:A:1041:GLU:H	1:A:1042:HIS:HA	1.86	0.41
1:A:530:SER:CB	3:A:1102:LMT:O2'	2.66	0.41
1:A:245:GLU:O	1:A:249:ILE:HG13	2.20	0.41
1:A:310:LEU:O	1:A:314:GLU:HG3	2.21	0.41
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.85	0.41
1:B:876:LEU:HD23	1:B:879:ILE:HD12	2.03	0.41
1:B:164:ASP:OD2	1:C:67:GLN:HG2	2.21	0.41
1:D:545:TYR:HB2	1:D:1021:PHE:CE2	2.56	0.41
1:D:597:TYR:CD2	1:D:598:TYR:CD1	3.09	0.41
1:D:641:GLU:HG2	1:D:642:ASN:N	2.36	0.41
1:D:682:PHE:O	1:D:826:GLU:HA	2.21	0.41
1:D:451:ALA:HB1	1:D:883:VAL:HG12	2.03	0.41
1:E:514:GLY:C	1:E:516:PHE:H	2.22	0.41
1:E:675:GLY:HA2	1:E:862:MET:SD	2.61	0.41
1:E:750:LEU:HD12	1:E:754:TRP:CD1	2.56	0.41
1:F:36:PRO:HD3	1:F:391:ASN:CG	2.42	0.41
1:A:246:PHE:HA	1:A:249:ILE:HG13	2.02	0.41
1:A:682:PHE:CE2	1:A:857:TYR:HB2	2.56	0.41
1:A:902:MET:C	1:A:904:VAL:H	2.25	0.41
1:B:993:THR:O	1:B:997:SER:HB3	2.21	0.41
1:C:671:ILE:HG21	1:C:674:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1007:VAL:HG12	1:D:1008:MET:N	2.36	0.41
1:D:375:VAL:HG11	1:D:405:LEU:HD22	2.03	0.41
1:D:538:THR:HG21	1:D:1028:VAL:CG2	2.51	0.41
1:D:636:ASP:O	1:D:638:PRO:HD3	2.21	0.41
1:D:201:VAL:HG23	1:D:749:THR:HG23	2.02	0.41
1:E:166:ILE:O	1:E:169:THR:HB	2.20	0.41
1:E:200:PRO:HA	1:E:203:VAL:HG23	2.03	0.41
1:E:680:PHE:CE1	1:E:682:PHE:HB2	2.56	0.41
1:F:151:GLN:NE2	1:F:279:ALA:O	2.54	0.41
1:F:382:VAL:O	1:F:386:PHE:HD2	2.04	0.41
1:F:49:TYR:HB3	1:F:57:VAL:HG12	2.02	0.41
1:A:1030:ARG:HA	1:A:1030:ARG:HH11	1.86	0.40
1:A:525:HIS:O	1:A:528:THR:HG22	2.21	0.40
1:B:242:SER:HB2	1:B:245:GLU:H	1.87	0.40
1:B:448:VAL:HG13	1:B:884:VAL:CG2	2.49	0.40
1:B:459:PHE:HD1	1:B:467:TYR:CD1	2.39	0.40
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.78	0.40
1:B:982:PHE:CD2	1:B:1011:MET:HG3	2.56	0.40
1:C:13:TRP:HH2	1:C:370:ILE:HD13	1.86	0.40
1:C:307:ARG:NE	1:C:325:TYR:OH	2.54	0.40
1:C:365:THR:O	1:C:368:PRO:HD2	2.21	0.40
1:C:396:PHE:O	1:C:400:LEU:HB2	2.21	0.40
1:C:687:GLN:HG3	1:C:688:ALA:N	2.36	0.40
1:A:67:GLN:HG2	1:C:767:ARG:HH12	1.85	0.40
1:D:1034:SER:HG	1:D:1035:ARG:H	1.60	0.40
1:D:467:TYR:HE2	1:D:925:VAL:HG22	1.85	0.40
1:D:485:ALA:O	1:D:490:PRO:HD3	2.21	0.40
1:D:671:ILE:H	1:D:671:ILE:HG13	1.59	0.40
1:D:678:THR:HG22	1:D:837:THR:N	2.36	0.40
1:D:894:SER:HB3	1:D:897:ILE:HB	2.03	0.40
1:D:890:ALA:HB1	1:F:11:PHE:CE1	2.56	0.40
1:F:459:PHE:CE2	1:F:872:GLN:HB3	2.56	0.40
1:F:560:PRO:HB2	1:F:836:SER:OG	2.21	0.40
1:F:979:SER:OG	1:F:1015:THR:HG21	2.20	0.40
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.57	0.40
1:A:801:PHE:HA	1:A:804:PHE:HE2	1.84	0.40
1:C:950:LYS:HG3	1:C:951:ASP:N	2.36	0.40
1:D:144:ASN:HA	1:D:320:GLY:O	2.21	0.40
1:D:332:PHE:O	1:D:336:SER:HB2	2.21	0.40
1:D:574:THR:HG23	1:D:627:ALA:HB3	2.03	0.40
1:D:602:GLU:OE1	1:D:650:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:LYS:HG2	1:E:196:PHE:CE1	2.56	0.40
1:E:555:LEU:HD23	1:E:555:LEU:HA	1.82	0.40
1:F:1032:ARG:O	1:F:1033:PHE:HB2	2.21	0.40
1:F:329:THR:O	1:F:333:VAL:HG23	2.21	0.40
1:F:414:GLU:HG2	1:F:973:ARG:NH1	2.36	0.40
1:F:931:LEU:HD23	1:F:931:LEU:HA	1.72	0.40
1:A:144:ASN:HA	1:A:320:GLY:O	2.21	0.40
1:A:344:LEU:HD22	1:A:402:ILE:CD1	2.52	0.40
1:B:915:ALA:CB	1:B:1009:GLY:HA3	2.41	0.40
1:B:172:VAL:HG13	1:B:291:ILE:HG23	2.02	0.40
1:B:729:ILE:HG22	1:B:731:ILE:HD13	2.03	0.40
1:C:263:ARG:HG2	1:C:263:ARG:O	2.22	0.40
1:C:445:ILE:HG23	1:C:940:LYS:HG3	2.03	0.40
1:C:594:VAL:O	1:C:597:TYR:N	2.55	0.40
1:D:377:LEU:O	1:D:380:PHE:HB2	2.21	0.40
1:D:710:PRO:HA	1:D:713:LEU:O	2.21	0.40
1:D:948:PHE:CD1	1:D:948:PHE:N	2.89	0.40
1:E:294:ALA:HB3	1:E:297:ALA:HB2	2.02	0.40
1:E:30:LEU:CD1	1:E:31:PRO:HD2	2.50	0.40
1:E:416:VAL:HG11	1:E:497:LEU:HD23	2.04	0.40
1:E:639:GLY:O	1:E:643:LYS:HG3	2.21	0.40
1:E:6:ILE:HD11	1:E:435:MET:HG3	2.02	0.40
1:E:267:LYS:HD3	1:E:776:GLU:OE2	2.21	0.40
1:F:102:ILE:HD13	1:F:102:ILE:HA	1.84	0.40
1:F:321:LEU:HD23	1:F:321:LEU:HA	1.75	0.40
1:F:510:LYS:H	1:F:510:LYS:HD3	1.85	0.40
1:F:703:LEU:HD21	1:F:716:VAL:HG12	2.04	0.40
1:F:701:GLN:HE22	1:F:852:PRO:HD3	1.86	0.40
1:A:505:HIS:O	1:A:507:GLU:N	2.55	0.40
1:A:682:PHE:HD2	1:A:683:GLU:N	2.19	0.40
1:A:686:ASP:O	1:A:822:LEU:HD13	2.22	0.40
1:A:400:LEU:CD2	1:A:929:VAL:HG12	2.50	0.40
1:B:195:LYS:HB3	1:B:196:PHE:HD1	1.86	0.40
1:B:137:LEU:HD12	1:B:329:THR:HG22	2.03	0.40
1:B:655:PHE:HB3	1:B:663:VAL:HB	2.03	0.40
1:B:871:ASN:N	1:B:871:ASN:OD1	2.54	0.40
1:B:904:VAL:HG21	1:B:942:ALA:HB2	2.03	0.40
1:B:944:LEU:HD23	1:B:944:LEU:HA	1.78	0.40
1:C:459:PHE:CZ	1:C:876:LEU:HA	2.56	0.40
1:C:591:LEU:HA	1:C:591:LEU:HD23	1.92	0.40
1:C:735:LYS:O	1:C:738:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1101:ERY:C20	2:D:1101:ERY:H313	2.52	0.40
1:D:666:PHE:CD1	1:D:666:PHE:N	2.89	0.40
1:D:70:ASN:OD1	1:D:70:ASN:N	2.54	0.40
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.52	0.40
1:E:641:GLU:HB2	1:E:650:ARG:NH2	2.37	0.40
1:E:950:LYS:NZ	1:E:953:MET:SD	2.94	0.40
1:F:118:LEU:HA	1:F:119:PRO:HD3	1.94	0.40
1:F:783:PRO:O	1:F:786:ILE:HG12	2.21	0.40
1:A:926:TYR:HE1	1:A:999:ALA:HB1	1.86	0.40
1:A:453:PHE:HE2	1:A:932:LEU:HB3	1.83	0.40
1:A:953:MET:HG3	1:A:958:LYS:O	2.22	0.40
1:B:1016:VAL:O	1:B:1016:VAL:HG12	2.21	0.40
1:B:143:ILE:O	1:B:321:LEU:HA	2.21	0.40
1:B:591:LEU:HD11	1:B:625:GLY:HA3	2.04	0.40
1:A:895:TRP:CE2	1:C:10:ILE:HG12	2.56	0.40
1:C:15:ILE:O	1:C:19:ILE:HG13	2.22	0.40
1:C:65:ILE:HG23	1:C:111:LEU:HD23	2.03	0.40
3:D:1103:LMT:H21	3:D:1103:LMT:H1'	1.78	0.40
1:D:201:VAL:O	1:D:204:ILE:HB	2.22	0.40
1:D:666:PHE:HD1	1:D:666:PHE:N	2.20	0.40
1:E:31:PRO:HB2	1:E:389:SER:HB2	2.02	0.40
1:F:588:GLN:NE2	1:F:592:ASN:OD1	2.52	0.40
1:F:986:VAL:CG1	1:F:1008:MET:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1042/1049 (99%)	943 (90%)	86 (8%)	13 (1%)	16 61
1	B	1040/1049 (99%)	955 (92%)	68 (6%)	17 (2%)	12 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1040/1049 (99%)	934 (90%)	88 (8%)	18 (2%)	11	53
1	D	1040/1049 (99%)	943 (91%)	83 (8%)	14 (1%)	15	59
1	E	1040/1049 (99%)	947 (91%)	72 (7%)	21 (2%)	9	50
1	F	1041/1049 (99%)	932 (90%)	81 (8%)	28 (3%)	6	44
All	All	6243/6294 (99%)	5654 (91%)	478 (8%)	111 (2%)	11	52

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	508	GLY
1	B	360	GLN
1	B	509	LYS
1	B	673	GLU
1	B	677	ALA
1	B	1038	GLU
1	C	360	GLN
1	C	893	GLU
1	C	1037	ASN
1	C	1041	GLU
1	D	360	GLN
1	D	508	GLY
1	D	675	GLY
1	D	677	ALA
1	E	358	PHE
1	E	360	GLN
1	E	509	LYS
1	E	673	GLU
1	E	893	GLU
1	E	1039	ASP
1	E	1041	GLU
1	F	134	SER
1	F	360	GLN
1	F	509	LYS
1	F	673	GLU
1	F	691	GLY
1	F	836	SER
1	F	893	GLU
1	F	1033	PHE
1	F	1036	LYS
1	F	1038	GLU

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Mol	Chain	Res	Type
1	F	1043	SER
1	A	991	ILE
1	A	1037	ASN
1	B	638	PRO
1	B	672	VAL
1	B	689	GLY
1	B	893	GLU
1	B	1040	ILE
1	C	146	ASP
1	C	147	GLY
1	C	509	LYS
1	C	689	GLY
1	C	836	SER
1	C	871	ASN
1	D	1036	LYS
1	D	1042	HIS
1	E	638	PRO
1	E	672	VAL
1	E	677	ALA
1	E	1040	ILE
1	F	133	SER
1	F	147	GLY
1	F	511	GLY
1	F	638	PRO
1	F	639	GLY
1	F	689	GLY
1	F	1040	ILE
1	A	133	SER
1	A	263	ARG
1	A	923	ASN
1	A	992	SER
1	A	1043	SER
1	B	263	ARG
1	B	833	PRO
1	C	775	SER
1	C	870	GLY
1	C	1035	ARG
1	D	163	LYS
1	D	775	SER
1	E	511	GLY
1	E	775	SER
1	F	146	ASP

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Mol	Chain	Res	Type
1	F	862	MET
1	B	775	SER
1	C	62	THR
1	D	1034	SER
1	E	134	SER
1	E	263	ARG
1	E	1036	LYS
1	F	263	ARG
1	F	775	SER
1	B	892	TYR
1	B	923	ASN
1	C	6	ILE
1	C	357	LEU
1	D	62	THR
1	D	960	LEU
1	D	1033	PHE
1	E	903	LEU
1	F	507	GLU
1	F	536	ARG
1	F	752	ALA
1	B	676	THR
1	D	133	SER
1	E	62	THR
1	A	1040	ILE
1	C	658	ILE
1	D	751	GLY
1	E	508	GLY
1	F	751	GLY
1	E	639	GLY
1	A	1016	VAL
1	B	639	GLY
1	C	751	GLY
1	E	1016	VAL
1	F	658	ILE
1	A	427	PRO
1	A	910	ILE
1	F	6	ILE

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	850/855 (99%)	788 (93%)	62 (7%)	17 57
1	B	848/855 (99%)	781 (92%)	67 (8%)	15 53
1	C	848/855 (99%)	780 (92%)	68 (8%)	15 52
1	D	848/855 (99%)	775 (91%)	73 (9%)	13 49
1	E	848/855 (99%)	771 (91%)	77 (9%)	12 46
1	F	849/855 (99%)	761 (90%)	88 (10%)	9 39
All	All	5091/5130 (99%)	4656 (92%)	435 (8%)	13 49

All (435) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	21	LEU
1	A	45	ILE
1	A	48	SER
1	A	49	TYR
1	A	93	THR
1	A	151	GLN
1	A	205	THR
1	A	222	THR
1	A	225	VAL
1	A	243	THR
1	A	293	LEU
1	A	310	LEU
1	A	321	LEU
1	A	324	VAL
1	A	336	SER
1	A	343	THR
1	A	360	GLN
1	A	362	PHE
1	A	400	LEU
1	A	428	LYS
1	A	462	SER
1	A	463	THR
1	A	483	LEU
1	A	489	THR
1	A	519	MET

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Mol	Chain	Res	Type
1	A	523	SER
1	A	524	THR
1	A	538	THR
1	A	559	LEU
1	A	561	SER
1	A	575	MET
1	A	634	TRP
1	A	662	MET
1	A	664	PHE
1	A	666	PHE
1	A	671	ILE
1	A	674	LEU
1	A	682	PHE
1	A	687	GLN
1	A	697	GLN
1	A	713	LEU
1	A	716	VAL
1	A	717	ARG
1	A	721	LEU
1	A	748	THR
1	A	760	ASN
1	A	768	VAL
1	A	797	GLN
1	A	804	PHE
1	A	815	ARG
1	A	817	GLU
1	A	843	LEU
1	A	857	TYR
1	A	961	ILE
1	A	964	THR
1	A	968	VAL
1	A	980	LEU
1	A	984	LEU
1	A	986	VAL
1	A	1007	VAL
1	A	1041	GLU
1	B	25	LEU
1	B	28	LEU
1	B	29	LYS
1	B	105	VAL
1	B	128	SER
1	B	131	LYS

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Mol	Chain	Res	Type
1	B	145	THR
1	B	146	ASP
1	B	151	GLN
1	B	196	PHE
1	B	225	VAL
1	B	243	THR
1	B	255	GLN
1	B	259	ARG
1	B	277	ILE
1	B	295	THR
1	B	310	LEU
1	B	321	LEU
1	B	324	VAL
1	B	332	PHE
1	B	336	SER
1	B	353	LEU
1	B	355	MET
1	B	360	GLN
1	B	372	VAL
1	B	400	LEU
1	B	459	PHE
1	B	472	ILE
1	B	489	THR
1	B	519	MET
1	B	524	THR
1	B	561	SER
1	B	571	VAL
1	B	578	LEU
1	B	592	ASN
1	B	602	GLU
1	B	617	PHE
1	B	626	ILE
1	B	634	TRP
1	B	652	THR
1	B	653	ARG
1	B	659	LYS
1	B	672	VAL
1	B	673	GLU
1	B	682	PHE
1	B	687	GLN
1	B	694	LYS
1	B	695	LEU

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Mol	Chain	Res	Type
1	B	708	LYS
1	B	717	ARG
1	B	721	LEU
1	B	748	THR
1	B	768	VAL
1	B	775	SER
1	B	804	PHE
1	B	806	SER
1	B	811	TYR
1	B	835	LYS
1	B	914	LEU
1	B	958	LYS
1	B	961	ILE
1	B	968	VAL
1	B	971	ARG
1	B	980	LEU
1	B	1007	VAL
1	B	1041	GLU
1	B	1043	SER
1	C	3	ASN
1	C	6	ILE
1	C	34	GLN
1	C	44	THR
1	C	48	SER
1	C	49	TYR
1	C	59	ASP
1	C	87	THR
1	C	93	THR
1	C	102	ILE
1	C	104	GLN
1	C	112	GLN
1	C	115	MET
1	C	151	GLN
1	C	174	ASP
1	C	177	LEU
1	C	222	THR
1	C	243	THR
1	C	274	ASN
1	C	300	LEU
1	C	336	SER
1	C	358	PHE
1	C	415	ASN

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Mol	Chain	Res	Type
1	C	432	ARG
1	C	447	MET
1	C	462	SER
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	489	THR
1	C	510	LYS
1	C	519	MET
1	C	524	THR
1	C	538	THR
1	C	540	ARG
1	C	542	LEU
1	C	561	SER
1	C	571	VAL
1	C	578	LEU
1	C	596	HIS
1	C	602	GLU
1	C	626	ILE
1	C	634	TRP
1	C	657	GLN
1	C	659	LYS
1	C	668	LEU
1	C	672	VAL
1	C	674	LEU
1	C	681	ASP
1	C	694	LYS
1	C	714	THR
1	C	716	VAL
1	C	721	LEU
1	C	724	THR
1	C	746	ILE
1	C	775	SER
1	C	804	PHE
1	C	807	SER
1	C	847	LEU
1	C	860	THR
1	C	876	LEU
1	C	895	TRP
1	C	947	GLU
1	C	950	LYS
1	C	958	LYS

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Mol	Chain	Res	Type
1	C	980	LEU
1	C	991	ILE
1	C	1032	ARG
1	D	3	ASN
1	D	21	LEU
1	D	45	ILE
1	D	49	TYR
1	D	146	ASP
1	D	151	GLN
1	D	152	GLU
1	D	177	LEU
1	D	182	TYR
1	D	205	THR
1	D	243	THR
1	D	255	GLN
1	D	293	LEU
1	D	324	VAL
1	D	336	SER
1	D	355	MET
1	D	360	GLN
1	D	362	PHE
1	D	439	GLN
1	D	463	THR
1	D	472	ILE
1	D	483	LEU
1	D	519	MET
1	D	523	SER
1	D	524	THR
1	D	538	THR
1	D	564	LEU
1	D	566	ASP
1	D	571	VAL
1	D	575	MET
1	D	602	GLU
1	D	605	ASN
1	D	626	ILE
1	D	634	TRP
1	D	659	LYS
1	D	662	MET
1	D	666	PHE
1	D	668	LEU
1	D	671	ILE

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Mol	Chain	Res	Type
1	D	674	LEU
1	D	682	PHE
1	D	687	GLN
1	D	697	GLN
1	D	713	LEU
1	D	714	THR
1	D	717	ARG
1	D	721	LEU
1	D	726	GLN
1	D	743	ILE
1	D	748	THR
1	D	757	SER
1	D	768	VAL
1	D	775	SER
1	D	797	GLN
1	D	804	PHE
1	D	806	SER
1	D	815	ARG
1	D	857	TYR
1	D	862	MET
1	D	865	GLN
1	D	901	VAL
1	D	918	PHE
1	D	922	THR
1	D	931	LEU
1	D	958	LYS
1	D	961	ILE
1	D	968	VAL
1	D	980	LEU
1	D	986	VAL
1	D	1007	VAL
1	D	1033	PHE
1	D	1041	GLU
1	D	1042	HIS
1	E	3	ASN
1	E	6	ILE
1	E	25	LEU
1	E	28	LEU
1	E	48	SER
1	E	49	TYR
1	E	60	THR
1	E	93	THR

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Mol	Chain	Res	Type
1	E	105	VAL
1	E	109	ASN
1	E	128	SER
1	E	145	THR
1	E	151	GLN
1	E	174	ASP
1	E	175	VAL
1	E	177	LEU
1	E	196	PHE
1	E	225	VAL
1	E	230	LEU
1	E	255	GLN
1	E	259	ARG
1	E	277	ILE
1	E	293	LEU
1	E	295	THR
1	E	324	VAL
1	E	329	THR
1	E	343	THR
1	E	355	MET
1	E	358	PHE
1	E	372	VAL
1	E	439	GLN
1	E	513	PHE
1	E	519	MET
1	E	523	SER
1	E	524	THR
1	E	526	HIS
1	E	540	ARG
1	E	559	LEU
1	E	561	SER
1	E	563	PHE
1	E	569	GLN
1	E	613	ASN
1	E	626	ILE
1	E	630	SER
1	E	634	TRP
1	E	659	LYS
1	E	662	MET
1	E	668	LEU
1	E	672	VAL
1	E	673	GLU

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Mol	Chain	Res	Type
1	E	678	THR
1	E	687	GLN
1	E	694	LYS
1	E	695	LEU
1	E	697	GLN
1	E	699	ARG
1	E	708	LYS
1	E	713	LEU
1	E	714	THR
1	E	717	ARG
1	E	760	ASN
1	E	775	SER
1	E	804	PHE
1	E	806	SER
1	E	843	LEU
1	E	880	SER
1	E	958	LYS
1	E	961	ILE
1	E	968	VAL
1	E	971	ARG
1	E	980	LEU
1	E	986	VAL
1	E	1007	VAL
1	E	1032	ARG
1	E	1033	PHE
1	E	1041	GLU
1	E	1043	SER
1	F	3	ASN
1	F	6	ILE
1	F	28	LEU
1	F	34	GLN
1	F	45	ILE
1	F	48	SER
1	F	49	TYR
1	F	76	MET
1	F	81	ASN
1	F	87	THR
1	F	88	VAL
1	F	90	ILE
1	F	93	THR
1	F	96	SER
1	F	104	GLN

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Mol	Chain	Res	Type
1	F	112	GLN
1	F	129	VAL
1	F	151	GLN
1	F	174	ASP
1	F	177	LEU
1	F	182	TYR
1	F	189	ASN
1	F	222	THR
1	F	243	THR
1	F	274	ASN
1	F	293	LEU
1	F	300	LEU
1	F	307	ARG
1	F	321	LEU
1	F	336	SER
1	F	362	PHE
1	F	418	ARG
1	F	432	ARG
1	F	447	MET
1	F	448	VAL
1	F	462	SER
1	F	472	ILE
1	F	482	VAL
1	F	489	THR
1	F	493	CYS
1	F	510	LYS
1	F	515	TRP
1	F	519	MET
1	F	524	THR
1	F	538	THR
1	F	540	ARG
1	F	559	LEU
1	F	564	LEU
1	F	571	VAL
1	F	578	LEU
1	F	596	HIS
1	F	602	GLU
1	F	615	PHE
1	F	626	ILE
1	F	630	SER
1	F	634	TRP
1	F	649	MET

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Mol	Chain	Res	Type
1	F	659	LYS
1	F	668	LEU
1	F	672	VAL
1	F	674	LEU
1	F	683	GLU
1	F	695	LEU
1	F	697	GLN
1	F	703	LEU
1	F	721	LEU
1	F	730	ASP
1	F	743	ILE
1	F	775	SER
1	F	804	PHE
1	F	806	SER
1	F	811	TYR
1	F	843	LEU
1	F	853	THR
1	F	862	MET
1	F	865	GLN
1	F	895	TRP
1	F	947	GLU
1	F	958	LYS
1	F	971	ARG
1	F	980	LEU
1	F	986	VAL
1	F	991	ILE
1	F	993	THR
1	F	1033	PHE
1	F	1035	ARG
1	F	1038	GLU
1	F	1044	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	229	GLN
1	A	231	ASN
1	A	361	ASN
1	A	605	ASN
1	B	34	GLN
1	B	228	GLN

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Mol	Chain	Res	Type
1	B	744	ASN
1	C	34	GLN
1	C	622	GLN
1	D	58	GLN
1	D	108	GLN
1	D	109	ASN
1	D	210	GLN
1	D	415	ASN
1	D	517	ASN
1	D	865	GLN
1	D	1037	ASN
1	E	67	GLN
1	E	104	GLN
1	E	231	ASN
1	E	588	GLN
1	E	592	ASN
1	E	667	ASN
1	F	81	ASN
1	F	104	GLN
1	F	108	GLN
1	F	210	GLN
1	F	228	GLN
1	F	231	ASN
1	F	439	GLN
1	F	692	HIS
1	F	726	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	ERY	A	1101	-	53,53,53	1.21	3 (5%)	82,82,82	2.04	23 (28%)
3	LMT	A	1102	-	36,36,36	1.73	7 (19%)	47,47,47	1.49	7 (14%)
3	LMT	A	1103	-	36,36,36	1.76	8 (22%)	47,47,47	1.66	10 (21%)
3	LMT	B	1101	-	36,36,36	1.81	10 (27%)	47,47,47	1.65	10 (21%)
3	LMT	C	1101	-	36,36,36	1.73	9 (25%)	47,47,47	1.08	4 (8%)
2	ERY	D	1101	-	53,53,53	1.26	2 (3%)	82,82,82	1.93	19 (23%)
3	LMT	D	1102	-	36,36,36	1.74	9 (25%)	47,47,47	1.10	3 (6%)
3	LMT	D	1103	-	36,36,36	1.83	9 (25%)	47,47,47	1.49	6 (12%)
3	LMT	E	1101	-	36,36,36	1.77	9 (25%)	47,47,47	1.79	11 (23%)
3	LMT	F	1101	-	36,36,36	1.80	9 (25%)	47,47,47	1.14	4 (8%)

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	ERY	A	1101	-	-	0/72/107/107	0/3/3/3
3	LMT	A	1102	-	-	0/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	0/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	0/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	0/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	0/72/107/107	1/3/3/3
3	LMT	D	1102	-	-	0/21/61/61	0/2/2/2
3	LMT	D	1103	-	-	0/21/61/61	0/2/2/2
3	LMT	E	1101	-	-	0/21/61/61	0/2/2/2
3	LMT	F	1101	-	-	0/21/61/61	0/2/2/2

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1102	LMT	C6'-C5'	-3.20	1.40	1.51
3	A	1103	LMT	C6'-C5'	-3.19	1.40	1.51
3	E	1101	LMT	C6'-C5'	-3.09	1.41	1.51
3	B	1101	LMT	C6'-C5'	-2.94	1.41	1.51
3	C	1101	LMT	C6'-C5'	-2.91	1.41	1.51
3	A	1102	LMT	C6'-C5'	-2.89	1.41	1.51
3	F	1101	LMT	C6'-C5'	-2.87	1.41	1.51
3	D	1103	LMT	C6'-C5'	-2.56	1.42	1.51
3	C	1101	LMT	C3B-C2B	-2.22	1.46	1.52
3	E	1101	LMT	C3B-C2B	-2.15	1.46	1.52
3	B	1101	LMT	C3'-C2'	-2.14	1.46	1.52
3	C	1101	LMT	C3'-C2'	-2.14	1.46	1.52
3	F	1101	LMT	C3'-C2'	-2.14	1.46	1.52
2	A	1101	ERY	C23-C24	2.00	1.58	1.53
3	D	1103	LMT	C5-C4	2.01	1.63	1.51
3	D	1102	LMT	C5-C4	2.01	1.63	1.51
3	F	1101	LMT	C5-C4	2.04	1.63	1.51
2	A	1101	ERY	O6-C17	2.04	1.46	1.42
3	B	1101	LMT	C5-C4	2.06	1.63	1.51
3	F	1101	LMT	O3'-C3'	2.09	1.47	1.43
3	D	1103	LMT	O3'-C3'	2.15	1.48	1.43
3	E	1101	LMT	O3'-C3'	2.18	1.48	1.43
3	A	1103	LMT	O3'-C3'	2.22	1.48	1.43
3	D	1102	LMT	O3'-C3'	2.26	1.48	1.43
3	E	1101	LMT	O2'-C2'	2.33	1.48	1.43
3	A	1102	LMT	O2'-C2'	2.38	1.48	1.43
3	D	1102	LMT	O2'-C2'	2.39	1.48	1.43
3	C	1101	LMT	O3B-C3B	2.42	1.48	1.43
3	B	1101	LMT	O3'-C3'	2.43	1.48	1.43
3	B	1101	LMT	O3B-C3B	2.44	1.48	1.43
2	D	1101	ERY	O9-C22	2.48	1.48	1.41
3	C	1101	LMT	O2'-C2'	2.62	1.49	1.43
3	A	1103	LMT	O5'-C1'	2.63	1.48	1.41
3	A	1103	LMT	O2'-C2'	2.64	1.49	1.43
3	F	1101	LMT	O3B-C3B	2.65	1.49	1.43
3	B	1101	LMT	O2'-C2'	2.67	1.49	1.43
3	D	1103	LMT	O2'-C2'	2.85	1.49	1.43
3	A	1102	LMT	O3B-C3B	2.85	1.49	1.43
3	A	1102	LMT	O5'-C1'	2.89	1.49	1.41
3	D	1102	LMT	O3B-C3B	2.89	1.49	1.43
3	E	1101	LMT	O3B-C3B	2.95	1.49	1.43
3	F	1101	LMT	O5'-C1'	3.06	1.49	1.41
3	E	1101	LMT	O5B-C1B	3.08	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1101	LMT	O5'-C1'	3.11	1.49	1.41
3	E	1101	LMT	O5'-C1'	3.11	1.49	1.41
3	D	1102	LMT	O5'-C1'	3.13	1.49	1.41
3	C	1101	LMT	O5B-C1B	3.19	1.50	1.41
3	A	1103	LMT	O5'-C5'	3.24	1.52	1.44
3	E	1101	LMT	O5'-C5'	3.30	1.52	1.44
3	C	1101	LMT	O5'-C1'	3.32	1.50	1.41
3	C	1101	LMT	O1'-C1'	3.33	1.46	1.40
3	A	1102	LMT	O1'-C1'	3.39	1.46	1.40
3	A	1103	LMT	O3B-C3B	3.40	1.51	1.43
3	B	1101	LMT	O5'-C5'	3.41	1.52	1.44
3	D	1102	LMT	O5B-C1B	3.42	1.50	1.41
3	D	1103	LMT	O3B-C3B	3.48	1.51	1.43
3	D	1103	LMT	O5'-C1'	3.51	1.50	1.41
3	A	1103	LMT	O1'-C1'	3.52	1.46	1.40
3	F	1101	LMT	O5B-C1B	3.68	1.51	1.41
3	F	1101	LMT	O5'-C5'	3.69	1.53	1.44
3	A	1102	LMT	O5B-C1B	3.69	1.51	1.41
3	D	1102	LMT	O5'-C5'	3.75	1.53	1.44
3	A	1102	LMT	O5'-C5'	3.80	1.53	1.44
3	B	1101	LMT	O5B-C1B	3.87	1.51	1.41
3	C	1101	LMT	O5'-C5'	3.89	1.54	1.44
3	D	1102	LMT	O1'-C1'	3.89	1.47	1.40
3	D	1103	LMT	O1'-C1'	4.04	1.47	1.40
3	F	1101	LMT	O1'-C1'	4.06	1.47	1.40
3	D	1103	LMT	O5'-C5'	4.10	1.54	1.44
3	D	1103	LMT	O5B-C1B	4.10	1.52	1.41
3	A	1103	LMT	O5B-C1B	4.24	1.52	1.41
3	B	1101	LMT	O1'-C1'	4.28	1.47	1.40
3	E	1101	LMT	O1'-C1'	4.45	1.48	1.40
2	A	1101	ERY	O2-C1	5.09	1.46	1.34
2	D	1101	ERY	O2-C1	5.94	1.48	1.34

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	ERY	O7-C5-C4	-5.34	102.66	111.49
2	A	1101	ERY	O2-C1-O1	-4.66	114.85	123.88
2	A	1101	ERY	C13-O2-C1	-4.63	110.35	118.10
3	A	1103	LMT	C1'-O5'-C5'	-4.58	104.76	113.74
2	A	1101	ERY	C19-C16-C15	-4.18	102.96	110.21
2	D	1101	ERY	C33-C8-C7	-4.18	101.10	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1101	LMT	O2'-C2'-C3'	-3.65	102.12	110.36
2	D	1101	ERY	C25-C24-N1	-3.51	105.11	115.68
3	B	1101	LMT	C1B-O1B-C4'	-3.45	108.83	118.00
3	E	1101	LMT	C1B-C2B-C3B	-3.35	103.33	109.98
3	D	1103	LMT	C1B-O1B-C4'	-2.99	110.06	118.00
3	C	1101	LMT	C6B-C5B-C4B	-2.98	105.51	112.99
3	B	1101	LMT	O3B-C3B-C2B	-2.95	103.71	110.36
3	C	1101	LMT	C1B-O1B-C4'	-2.85	110.42	118.00
3	B	1101	LMT	C6B-C5B-C4B	-2.71	106.19	112.99
3	D	1102	LMT	O2B-C2B-C1B	-2.65	104.12	110.01
2	D	1101	ERY	C31-C4-C3	-2.62	106.57	111.45
3	A	1102	LMT	C1B-O1B-C4'	-2.59	111.10	118.00
2	A	1101	ERY	C31-C4-C3	-2.58	106.66	111.45
2	D	1101	ERY	O7-C5-C4	-2.55	107.27	111.49
3	C	1101	LMT	O3B-C3B-C2B	-2.54	104.64	110.36
2	A	1101	ERY	O10-C6-C32	-2.49	102.89	108.58
2	D	1101	ERY	C36-C13-C12	-2.44	109.99	115.13
3	E	1101	LMT	O5B-C1B-C2B	-2.38	105.34	110.28
3	E	1101	LMT	C1B-O1B-C4'	-2.36	111.73	118.00
3	E	1101	LMT	O5'-C5'-C4'	-2.28	104.91	109.78
3	B	1101	LMT	O3B-C3B-C4B	-2.26	105.26	110.36
3	A	1102	LMT	O2'-C2'-C3'	-2.26	105.26	110.36
3	A	1103	LMT	O5'-C5'-C4'	-2.13	105.23	109.78
2	A	1101	ERY	C7-C8-C9	-2.10	109.47	113.46
2	A	1101	ERY	O1-C1-C2	-2.09	119.12	124.27
3	F	1101	LMT	C6B-C5B-C4B	-2.06	107.83	112.99
2	D	1101	ERY	O13-C12-C13	-2.02	103.92	107.10
2	D	1101	ERY	C16-C17-C18	-2.01	107.96	111.03
3	D	1103	LMT	O1'-C1'-C2'	2.05	110.52	108.00
3	D	1102	LMT	O1'-C1'-C2'	2.05	110.53	108.00
3	B	1101	LMT	C3'-C4'-C5'	2.06	115.55	110.85
2	A	1101	ERY	C35-C12-C13	2.09	114.42	111.23
3	A	1103	LMT	C1B-O5B-C5B	2.09	117.85	113.74
3	A	1103	LMT	C4B-C3B-C2B	2.09	114.64	110.79
3	E	1101	LMT	O5'-C1'-C2'	2.11	114.67	110.28
3	A	1102	LMT	O5'-C5'-C6'	2.12	111.86	106.38
2	A	1101	ERY	C30-C2-C3	2.14	117.75	113.03
3	A	1102	LMT	O5B-C5B-C4B	2.21	113.88	109.67
3	E	1101	LMT	O5'-C5'-C6'	2.30	112.34	106.38
2	A	1101	ERY	O6-C17-C16	2.31	115.08	111.33
3	B	1101	LMT	C1B-O5B-C5B	2.33	118.31	113.74
2	D	1101	ERY	O5-C16-C17	2.34	107.58	103.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1103	LMT	O5B-C5B-C4B	2.40	114.24	109.67
2	D	1101	ERY	C33-C8-C9	2.45	116.08	109.49
3	D	1103	LMT	O1B-C1B-C2B	2.48	114.27	108.12
3	A	1103	LMT	O5B-C5B-C6B	2.54	112.95	106.38
2	D	1101	ERY	C30-C2-C3	2.54	118.65	113.03
2	A	1101	ERY	O4-C18-C21	2.55	111.99	106.57
2	A	1101	ERY	O9-C26-C27	2.59	112.04	106.69
3	F	1101	LMT	C1'-C2'-C3'	2.61	115.16	109.98
3	B	1101	LMT	C4B-C3B-C2B	2.70	115.76	110.79
2	D	1101	ERY	C22-O9-C26	2.74	117.65	112.97
3	C	1101	LMT	O5B-C5B-C4B	2.75	114.92	109.67
2	A	1101	ERY	O12-C11-C10	2.77	114.38	110.79
3	B	1101	LMT	O5B-C5B-C4B	2.82	115.04	109.67
2	A	1101	ERY	O7-C5-C6	2.84	110.11	106.45
2	A	1101	ERY	O2-C1-C2	2.89	117.40	111.44
2	D	1101	ERY	O4-C18-C21	2.90	112.73	106.57
2	D	1101	ERY	O9-C26-C27	3.01	112.91	106.69
3	F	1101	LMT	C1-O1'-C1'	3.09	119.40	114.00
3	D	1103	LMT	C2'-C3'-C4'	3.11	116.50	109.63
3	A	1102	LMT	O1'-C1'-C2'	3.13	111.85	108.00
2	A	1101	ERY	O7-C22-C23	3.16	115.98	108.12
3	E	1101	LMT	C2'-C3'-C4'	3.17	116.63	109.63
2	A	1101	ERY	O2-C13-C12	3.21	112.70	107.17
2	A	1101	ERY	C15-C16-C17	3.24	111.95	107.82
3	D	1102	LMT	C1'-C2'-C3'	3.25	116.44	109.98
2	A	1101	ERY	C29-N1-C24	3.27	122.73	113.14
3	D	1103	LMT	C3B-C4B-C5B	3.37	116.25	110.23
3	B	1101	LMT	C3B-C4B-C5B	3.42	116.32	110.23
3	A	1103	LMT	O1'-C1'-C2'	3.45	112.25	108.00
2	D	1101	ERY	C20-O5-C16	3.55	125.70	117.64
3	A	1103	LMT	C3B-C4B-C5B	3.62	116.68	110.23
3	D	1103	LMT	C1'-C2'-C3'	3.69	117.30	109.98
2	A	1101	ERY	C3-C4-C5	3.77	117.86	110.85
3	E	1101	LMT	O5B-C5B-C4B	3.79	116.89	109.67
2	D	1101	ERY	C3-C4-C5	3.82	117.96	110.85
3	A	1103	LMT	C1'-C2'-C3'	3.85	117.61	109.98
3	F	1101	LMT	O5B-C5B-C4B	3.92	117.15	109.67
3	A	1103	LMT	C2'-C3'-C4'	4.06	118.59	109.63
2	D	1101	ERY	O2-C13-C36	4.24	115.17	107.37
2	A	1101	ERY	C22-O7-C5	4.26	124.09	116.36
3	A	1102	LMT	C2'-C3'-C4'	4.57	119.73	109.63
3	A	1102	LMT	C1'-C2'-C3'	4.81	119.52	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1101	ERY	C22-O7-C5	5.01	125.44	116.36
2	D	1101	ERY	C29-N1-C24	5.07	128.00	113.14
3	E	1101	LMT	C1'-C2'-C3'	5.07	120.04	109.98
3	E	1101	LMT	O1'-C1'-C2'	5.24	114.45	108.00
2	A	1101	ERY	C20-O5-C16	5.49	130.12	117.64
3	B	1101	LMT	O1'-C1'-C2'	5.65	114.95	108.00
2	D	1101	ERY	O12-C11-C10	6.22	118.84	110.79

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1101	ERY	C22-C23-C24-C25-C26-O9

9 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ERY	6	0
3	A	1102	LMT	5	0
3	A	1103	LMT	9	0
3	B	1101	LMT	5	0
3	C	1101	LMT	2	0
2	D	1101	ERY	12	0
3	D	1102	LMT	1	0
3	D	1103	LMT	5	0
3	E	1101	LMT	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1044/1049 (99%)	0.64	140 (13%)	4	4	46, 78, 106, 147	0
1	B	1042/1049 (99%)	0.65	139 (13%)	4	5	50, 76, 102, 148	0
1	C	1042/1049 (99%)	0.88	169 (16%)	3	3	43, 77, 103, 155	0
1	D	1042/1049 (99%)	0.82	162 (15%)	3	3	45, 86, 112, 147	0
1	E	1042/1049 (99%)	0.82	181 (17%)	2	2	55, 86, 108, 147	0
1	F	1043/1049 (99%)	0.96	212 (20%)	1	1	52, 82, 106, 158	0
All	All	6255/6294 (99%)	0.80	1003 (16%)	3	3	43, 81, 107, 158	0

All (1003) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	720	GLY	16.8
1	F	48	SER	14.6
1	C	719	ASN	14.1
1	F	719	ASN	13.5
1	F	720	GLY	12.3
1	D	619	GLY	11.9
1	C	80	SER	11.2
1	F	79	SER	10.6
1	E	291	ILE	9.5
1	D	621	GLY	9.5
1	E	719	ASN	9.4
1	D	463	THR	9.2
1	E	81	ASN	9.2
1	E	618	ALA	8.9
1	E	720	GLY	8.9
1	E	617	PHE	8.9
1	B	620	ARG	8.7
1	A	619	GLY	8.6
1	B	869	SER	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	617	PHE	8.5
1	F	80	SER	8.2
1	F	442	LEU	8.1
1	F	676	THR	8.1
1	D	620	ARG	8.0
1	F	9	PRO	7.9
1	C	815	ARG	7.8
1	E	681	ASP	7.8
1	F	91	THR	7.6
1	C	836	SER	7.6
1	B	895	TRP	7.5
1	D	462	SER	7.5
1	F	712	MET	7.4
1	E	619	GLY	7.3
1	F	618	ALA	7.3
1	A	618	ALA	7.3
1	C	83	ASP	7.2
1	B	615	PHE	7.2
1	A	615	PHE	7.1
1	C	79	SER	7.1
1	E	290	GLY	7.1
1	D	615	PHE	7.1
1	B	870	GLY	7.1
1	D	866	GLU	7.1
1	D	459	PHE	7.0
1	F	503	GLY	7.0
1	D	719	ASN	7.0
1	A	400	LEU	7.0
1	D	460	GLY	6.9
1	C	619	GLY	6.9
1	D	720	GLY	6.9
1	A	13	TRP	6.9
1	F	675	GLY	6.8
1	D	1038	GLU	6.8
1	C	501	ALA	6.8
1	C	618	ALA	6.8
1	E	943	ILE	6.7
1	D	869	SER	6.7
1	C	9	PRO	6.7
1	F	836	SER	6.6
1	E	615	PHE	6.6
1	C	721	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	F	47	ALA	6.6
1	E	488	LEU	6.5
1	C	835	LYS	6.5
1	C	872	GLN	6.5
1	B	617	PHE	6.5
1	F	406	VAL	6.4
1	C	617	PHE	6.4
1	B	488	LEU	6.4
1	F	405	LEU	6.3
1	B	229	GLN	6.3
1	F	865	GLN	6.3
1	F	46	SER	6.3
1	F	619	GLY	6.2
1	F	81	ASN	6.2
1	D	618	ALA	6.2
1	C	826	GLU	6.2
1	F	711	ASP	6.2
1	F	721	LEU	6.1
1	F	617	PHE	6.1
1	F	826	GLU	6.0
1	D	323	ILE	6.0
1	A	620	ARG	6.0
1	C	871	ASN	6.0
1	A	719	ASN	6.0
1	A	403	GLY	5.9
1	B	79	SER	5.9
1	F	10	ILE	5.9
1	B	403	GLY	5.9
1	C	81	ASN	5.9
1	D	663	VAL	5.9
1	F	69	MET	5.9
1	C	1038	GLU	5.8
1	F	835	LYS	5.8
1	D	1037	ASN	5.8
1	B	943	ILE	5.8
1	E	91	THR	5.7
1	D	870	GLY	5.7
1	C	1039	ASP	5.7
1	F	713	LEU	5.7
1	E	620	ARG	5.7
1	F	815	ARG	5.7
1	C	888	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	79	SER	5.6
1	E	80	SER	5.6
1	D	486	LEU	5.6
1	B	618	ALA	5.6
1	F	230	LEU	5.5
1	F	481	SER	5.5
1	F	837	THR	5.5
1	A	621	GLY	5.5
1	F	13	TRP	5.5
1	D	960	LEU	5.5
1	D	895	TRP	5.5
1	F	407	ASP	5.5
1	C	837	THR	5.5
1	E	680	PHE	5.5
1	E	314	GLU	5.4
1	C	445	ILE	5.4
1	F	869	SER	5.4
1	B	619	GLY	5.4
1	A	404	LEU	5.4
1	F	410	ILE	5.4
1	F	107	VAL	5.4
1	A	445	ILE	5.4
1	E	901	VAL	5.4
1	F	620	ARG	5.3
1	C	712	MET	5.3
1	F	473	THR	5.3
1	E	495	THR	5.3
1	F	445	ILE	5.3
1	E	315	PRO	5.2
1	F	403	GLY	5.2
1	E	308	ALA	5.2
1	C	782	LEU	5.2
1	D	617	PHE	5.2
1	B	621	GLY	5.2
1	F	888	LEU	5.1
1	D	681	ASP	5.1
1	F	449	LEU	5.1
1	B	714	THR	5.1
1	C	494	ALA	5.1
1	F	398	MET	5.1
1	B	716	VAL	5.1
1	E	82	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	715	SER	5.1
1	F	501	ALA	5.0
1	A	89	GLN	5.0
1	E	87	THR	5.0
1	C	620	ARG	5.0
1	A	449	LEU	5.0
1	B	230	LEU	5.0
1	E	944	LEU	5.0
1	E	826	GLU	5.0
1	F	516	PHE	4.9
1	F	89	GLN	4.9
1	B	624	THR	4.9
1	D	11	PHE	4.9
1	A	1040	ILE	4.9
1	D	614	GLY	4.9
1	F	448	VAL	4.9
1	C	405	LEU	4.9
1	B	719	ASN	4.9
1	F	840	ALA	4.8
1	A	938	SER	4.8
1	C	57	VAL	4.8
1	E	92	LEU	4.8
1	A	92	LEU	4.8
1	E	406	VAL	4.8
1	A	486	LEU	4.8
1	F	541	TYR	4.8
1	E	496	MET	4.8
1	E	366	LEU	4.8
1	A	605	ASN	4.8
1	B	613	ASN	4.8
1	A	946	VAL	4.8
1	B	91	THR	4.8
1	B	315	PRO	4.8
1	C	681	ASP	4.7
1	C	834	GLY	4.7
1	D	461	GLY	4.7
1	F	615	PHE	4.7
1	E	489	THR	4.7
1	D	9	PRO	4.7
1	E	616	GLY	4.7
1	C	783	PRO	4.7
1	A	410	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	441	ALA	4.7
1	A	494	ALA	4.6
1	D	81	ASN	4.6
1	C	739	LEU	4.6
1	B	678	THR	4.6
1	E	487	ILE	4.6
1	E	888	LEU	4.6
1	B	80	SER	4.6
1	D	508	GLY	4.6
1	E	89	GLN	4.6
1	E	83	ASP	4.6
1	A	942	ALA	4.5
1	F	488	LEU	4.5
1	C	48	SER	4.5
1	C	448	VAL	4.5
1	D	577	GLN	4.5
1	C	868	LEU	4.5
1	F	839	GLU	4.5
1	A	408	ASP	4.5
1	B	404	LEU	4.5
1	C	711	ASP	4.5
1	A	368	PRO	4.5
1	D	782	LEU	4.5
1	F	937	LEU	4.5
1	F	60	THR	4.4
1	A	401	ALA	4.4
1	A	939	ALA	4.4
1	B	487	ILE	4.4
1	D	815	ARG	4.4
1	A	616	GLY	4.4
1	B	894	SER	4.4
1	A	943	ILE	4.4
1	A	407	ASP	4.4
1	A	402	ILE	4.3
1	C	804	PHE	4.3
1	F	231	ASN	4.3
1	D	400	LEU	4.3
1	F	938	SER	4.3
1	E	408	ASP	4.3
1	E	678	THR	4.3
1	E	937	LEU	4.3
1	F	901	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	225	VAL	4.3
1	E	682	PHE	4.3
1	E	892	TYR	4.3
1	C	684	LEU	4.3
1	C	70	ASN	4.2
1	F	941	ASN	4.2
1	E	815	ARG	4.2
1	D	576	VAL	4.2
1	D	834	GLY	4.2
1	C	310	LEU	4.2
1	C	10	ILE	4.2
1	F	897	ILE	4.2
1	F	892	TYR	4.2
1	F	402	ILE	4.2
1	B	400	LEU	4.1
1	F	895	TRP	4.1
1	F	474	ILE	4.1
1	C	504	ASP	4.1
1	F	3	ASN	4.1
1	E	138	MET	4.1
1	F	868	LEU	4.1
1	A	714	THR	4.1
1	F	502	LYS	4.1
1	E	405	LEU	4.1
1	C	615	PHE	4.1
1	F	679	GLY	4.1
1	E	741	VAL	4.1
1	D	493	CYS	4.1
1	F	889	ALA	4.1
1	F	708	LYS	4.1
1	A	397	GLY	4.0
1	C	403	GLY	4.0
1	C	449	LEU	4.0
1	D	626	ILE	4.0
1	C	402	ILE	4.0
1	F	57	VAL	4.0
1	E	310	LEU	4.0
1	C	362	PHE	4.0
1	C	833	PRO	4.0
1	D	504	ASP	4.0
1	B	486	LEU	4.0
1	E	370	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	839	GLU	3.9
1	C	511	GLY	3.9
1	E	679	GLY	3.9
1	B	439	GLN	3.9
1	E	632	LYS	3.9
1	D	894	SER	3.9
1	C	13	TRP	3.9
1	B	616	GLY	3.9
1	D	401	ALA	3.9
1	C	510	LYS	3.9
1	A	87	THR	3.9
1	D	837	THR	3.9
1	C	503	GLY	3.9
1	A	640	GLU	3.9
1	F	404	LEU	3.8
1	E	834	GLY	3.8
1	E	933	THR	3.8
1	E	677	ALA	3.8
1	F	902	MET	3.8
1	A	43	VAL	3.8
1	F	681	ASP	3.8
1	E	939	ALA	3.8
1	E	78	MET	3.8
1	E	307	ARG	3.8
1	A	1039	ASP	3.8
1	E	367	ILE	3.8
1	E	362	PHE	3.8
1	F	709	HIS	3.8
1	F	484	VAL	3.8
1	F	825	MET	3.8
1	C	54	ALA	3.7
1	D	656	SER	3.7
1	B	407	ASP	3.7
1	F	817	GLU	3.7
1	B	720	GLY	3.7
1	F	7	ASP	3.7
1	C	683	GLU	3.7
1	E	400	LEU	3.7
1	E	900	SER	3.7
1	E	492	LEU	3.7
1	D	322	LYS	3.7
1	F	306	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	943	ILE	3.7
1	B	89	GLN	3.7
1	D	79	SER	3.7
1	B	78	MET	3.7
1	E	435	MET	3.7
1	D	12	ALA	3.7
1	A	91	THR	3.7
1	B	623	ASN	3.7
1	C	935	ILE	3.7
1	D	662	MET	3.6
1	C	937	LEU	3.6
1	D	92	LEU	3.6
1	C	500	ILE	3.6
1	C	621	GLY	3.6
1	A	656	SER	3.6
1	F	577	GLN	3.6
1	A	10	ILE	3.6
1	D	661	ALA	3.6
1	E	432	ARG	3.6
1	E	657	GLN	3.6
1	E	175	VAL	3.6
1	A	369	THR	3.6
1	C	314	GLU	3.6
1	A	496	MET	3.6
1	C	663	VAL	3.6
1	E	817	GLU	3.5
1	C	869	SER	3.5
1	A	9	PRO	3.5
1	E	613	ASN	3.5
1	B	408	ASP	3.5
1	F	540	ARG	3.5
1	C	68	ASN	3.5
1	F	83	ASP	3.5
1	B	534	ILE	3.5
1	D	897	ILE	3.5
1	C	444	GLY	3.5
1	D	83	ASP	3.5
1	C	791	VAL	3.5
1	D	613	ASN	3.5
1	F	512	PHE	3.5
1	D	90	ILE	3.5
1	D	893	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	993	THR	3.5
1	E	32	VAL	3.5
1	D	791	VAL	3.4
1	D	10	ILE	3.4
1	B	866	GLU	3.4
1	B	889	ALA	3.4
1	A	713	LEU	3.4
1	C	722	GLU	3.4
1	B	291	ILE	3.4
1	B	492	LEU	3.4
1	B	90	ILE	3.4
1	F	718	PRO	3.4
1	C	401	ALA	3.4
1	B	830	GLN	3.4
1	E	904	VAL	3.4
1	E	683	GLU	3.4
1	C	889	ALA	3.4
1	B	412	VAL	3.4
1	B	577	GLN	3.4
1	E	88	VAL	3.4
1	E	576	VAL	3.4
1	A	81	ASN	3.4
1	B	177	LEU	3.4
1	D	624	THR	3.4
1	E	934	THR	3.4
1	F	624	THR	3.4
1	F	848	ALA	3.4
1	C	865	GLN	3.4
1	B	5	PHE	3.4
1	A	443	VAL	3.4
1	D	731	ILE	3.4
1	D	833	PRO	3.4
1	F	485	ALA	3.4
1	B	92	LEU	3.4
1	F	504	ASP	3.4
1	A	680	PHE	3.4
1	D	622	GLN	3.4
1	C	463	THR	3.4
1	D	678	THR	3.4
1	F	896	SER	3.4
1	F	942	ALA	3.3
1	B	401	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	706	ALA	3.3
1	C	400	LEU	3.3
1	B	837	THR	3.3
1	D	627	ALA	3.3
1	E	441	ALA	3.3
1	F	832	ALA	3.3
1	C	838	GLY	3.3
1	A	489	THR	3.3
1	D	729	ILE	3.3
1	D	809	TRP	3.3
1	A	90	ILE	3.3
1	A	398	MET	3.3
1	F	408	ASP	3.3
1	A	613	ASN	3.3
1	D	804	PHE	3.3
1	E	866	GLU	3.3
1	A	634	TRP	3.3
1	F	463	THR	3.3
1	E	605	ASN	3.3
1	B	81	ASN	3.3
1	E	513	PHE	3.3
1	A	894	SER	3.3
1	E	869	SER	3.3
1	F	828	LEU	3.3
1	F	444	GLY	3.2
1	A	892	TYR	3.2
1	E	633	ASP	3.2
1	C	69	MET	3.2
1	F	462	SER	3.2
1	F	44	THR	3.2
1	D	5	PHE	3.2
1	D	80	SER	3.2
1	A	88	VAL	3.2
1	A	935	ILE	3.2
1	F	443	VAL	3.2
1	C	817	GLU	3.2
1	A	396	PHE	3.2
1	A	961	ILE	3.2
1	D	487	ILE	3.2
1	D	727	PHE	3.2
1	E	721	LEU	3.2
1	E	827	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	390	ILE	3.2
1	D	89	GLN	3.2
1	D	835	LYS	3.2
1	E	357	LEU	3.2
1	F	626	ILE	3.2
1	F	401	ALA	3.2
1	A	866	GLU	3.2
1	E	292	LYS	3.2
1	B	901	VAL	3.2
1	A	575	MET	3.2
1	E	439	GLN	3.2
1	F	849	SER	3.2
1	C	892	TYR	3.2
1	C	577	GLN	3.1
1	A	681	ASP	3.1
1	C	390	ILE	3.1
1	A	635	ALA	3.1
1	A	873	ALA	3.1
1	F	576	VAL	3.1
1	F	834	GLY	3.1
1	C	488	LEU	3.1
1	A	655	PHE	3.1
1	B	11	PHE	3.1
1	A	399	VAL	3.1
1	F	831	ALA	3.1
1	D	888	LEU	3.1
1	A	246	PHE	3.1
1	C	941	ASN	3.1
1	E	938	SER	3.1
1	C	624	THR	3.1
1	C	576	VAL	3.1
1	E	929	VAL	3.1
1	C	388	PHE	3.1
1	F	621	GLY	3.1
1	F	310	LEU	3.1
1	A	164	ASP	3.1
1	B	495	THR	3.1
1	D	616	GLY	3.1
1	E	902	MET	3.1
1	A	134	SER	3.1
1	C	91	THR	3.1
1	D	575	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	331	PRO	3.0
1	E	409	ALA	3.1
1	E	993	THR	3.0
1	A	657	GLN	3.0
1	D	839	GLU	3.0
1	D	178	PHE	3.0
1	A	874	PRO	3.0
1	D	606	VAL	3.0
1	E	62	THR	3.0
1	D	889	ALA	3.0
1	C	718	PRO	3.0
1	E	891	LEU	3.0
1	D	385	ALA	3.0
1	E	71	GLY	3.0
1	D	961	ILE	3.0
1	E	837	THR	3.0
1	B	494	ALA	3.0
1	C	421	ALA	3.0
1	D	167	SER	3.0
1	F	482	VAL	3.0
1	F	872	GLN	3.0
1	A	83	ASP	3.0
1	C	938	SER	3.0
1	F	409	ALA	3.0
1	C	713	LEU	3.0
1	A	899	PHE	3.0
1	D	403	GLY	3.0
1	B	897	ILE	3.0
1	C	778	LYS	3.0
1	E	396	PHE	3.0
1	A	355	MET	3.0
1	F	62	THR	3.0
1	F	496	MET	2.9
1	E	897	ILE	2.9
1	B	405	LEU	2.9
1	F	739	LEU	2.9
1	C	563	PHE	2.9
1	A	945	ILE	2.9
1	D	623	ASN	2.9
1	A	44	THR	2.9
1	A	178	PHE	2.9
1	C	801	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	867	ARG	2.9
1	A	900	SER	2.9
1	C	742	SER	2.9
1	E	624	THR	2.9
1	D	404	LEU	2.9
1	E	828	LEU	2.9
1	E	835	LYS	2.9
1	F	110	LYS	2.9
1	E	936	GLY	2.9
1	A	376	LEU	2.9
1	C	498	LYS	2.9
1	D	892	TYR	2.9
1	E	311	ALA	2.9
1	F	809	TRP	2.9
1	B	88	VAL	2.9
1	E	289	LEU	2.9
1	E	626	ILE	2.9
1	D	982	PHE	2.9
1	B	836	SER	2.9
1	C	676	THR	2.9
1	D	959	GLY	2.9
1	E	940	LYS	2.9
1	F	175	VAL	2.9
1	B	231	ASN	2.9
1	F	838	GLY	2.9
1	E	369	THR	2.9
1	E	1007	VAL	2.9
1	D	610	PHE	2.9
1	E	942	ALA	2.9
1	F	90	ILE	2.9
1	A	762	PHE	2.9
1	F	940	LYS	2.9
1	F	936	GLY	2.9
1	E	438	ILE	2.8
1	E	746	ILE	2.8
1	B	933	THR	2.8
1	D	665	ALA	2.8
1	F	127	VAL	2.8
1	A	12	ALA	2.8
1	D	733	GLN	2.8
1	E	33	ALA	2.8
1	C	166	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	945	ILE	2.8
1	D	467	TYR	2.8
1	E	895	TRP	2.8
1	B	211	ASN	2.8
1	D	449	LEU	2.8
1	E	404	LEU	2.8
1	D	306	ILE	2.8
1	F	855	VAL	2.8
1	A	167	SER	2.8
1	C	496	MET	2.8
1	D	91	THR	2.8
1	B	829	GLY	2.8
1	C	410	ILE	2.8
1	F	65	ILE	2.8
1	C	674	LEU	2.8
1	D	141	GLY	2.8
1	E	890	ALA	2.8
1	D	510	LYS	2.8
1	A	976	LEU	2.8
1	B	711	ASP	2.8
1	D	87	THR	2.8
1	D	664	PHE	2.8
1	E	229	GLN	2.7
1	C	502	LYS	2.7
1	C	207	ILE	2.7
1	F	746	ILE	2.7
1	E	13	TRP	2.7
1	C	816	LEU	2.7
1	C	516	PHE	2.7
1	E	296	GLY	2.7
1	E	831	ALA	2.7
1	A	607	GLU	2.7
1	D	402	ILE	2.7
1	C	67	GLN	2.7
1	A	442	LEU	2.7
1	B	591	LEU	2.7
1	A	444	GLY	2.7
1	B	815	ARG	2.7
1	F	846	GLN	2.7
1	B	83	ASP	2.7
1	F	59	ASP	2.7
1	F	841	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	663	VAL	2.7
1	C	558	ARG	2.7
1	D	578	LEU	2.7
1	D	49	TYR	2.7
1	E	819	TYR	2.7
1	B	938	SER	2.7
1	E	246	PHE	2.7
1	B	576	VAL	2.7
1	F	495	THR	2.7
1	F	782	LEU	2.7
1	A	82	SER	2.7
1	E	824	SER	2.7
1	F	8	ARG	2.7
1	B	298	ASN	2.7
1	F	159	ALA	2.7
1	A	508	GLY	2.7
1	B	246	PHE	2.7
1	C	398	MET	2.7
1	F	246	PHE	2.7
1	B	175	VAL	2.7
1	B	942	ALA	2.7
1	F	515	TRP	2.7
1	F	704	ALA	2.7
1	F	845	GLU	2.7
1	F	843	LEU	2.7
1	B	841	MET	2.7
1	A	371	ALA	2.7
1	C	741	VAL	2.7
1	A	79	SER	2.6
1	A	453	PHE	2.6
1	A	516	PHE	2.6
1	D	1039	ASP	2.6
1	F	613	ASN	2.6
1	E	714	THR	2.6
1	C	814	PRO	2.6
1	B	428	LYS	2.6
1	C	127	VAL	2.6
1	E	402	ILE	2.6
1	C	982	PHE	2.6
1	E	73	ASP	2.6
1	E	407	ASP	2.6
1	E	830	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	891	LEU	2.6
1	F	477	ALA	2.6
1	C	708	LYS	2.6
1	E	641	GLU	2.6
1	C	406	VAL	2.6
1	D	59	ASP	2.6
1	E	636	ASP	2.6
1	E	782	LEU	2.6
1	C	446	ALA	2.6
1	F	707	ALA	2.6
1	A	815	ARG	2.6
1	C	622	GLN	2.6
1	F	45	ILE	2.6
1	B	491	ALA	2.6
1	A	492	LEU	2.6
1	E	712	MET	2.6
1	D	164	ASP	2.6
1	E	889	ALA	2.6
1	B	835	LYS	2.6
1	D	142	VAL	2.6
1	E	86	GLY	2.6
1	C	932	LEU	2.6
1	A	467	TYR	2.6
1	B	758	TYR	2.6
1	F	82	SER	2.6
1	F	877	TYR	2.6
1	B	406	VAL	2.6
1	F	851	LEU	2.6
1	C	12	ALA	2.6
1	A	80	SER	2.6
1	D	590	VAL	2.6
1	F	715	SER	2.6
1	A	591	LEU	2.6
1	B	937	LEU	2.6
1	E	860	THR	2.6
1	D	246	PHE	2.5
1	C	507	GLU	2.5
1	F	88	VAL	2.5
1	F	856	GLY	2.5
1	D	386	PHE	2.5
1	E	727	PHE	2.5
1	C	389	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	406	VAL	2.5
1	A	632	LYS	2.5
1	E	769	LYS	2.5
1	F	891	LEU	2.5
1	F	867	ARG	2.5
1	C	404	LEU	2.5
1	C	575	MET	2.5
1	A	871	ASN	2.5
1	E	75	LEU	2.5
1	E	778	LYS	2.5
1	E	833	PRO	2.5
1	F	446	ALA	2.5
1	F	612	VAL	2.5
1	F	70	ASN	2.5
1	F	106	GLN	2.5
1	B	899	PHE	2.5
1	F	680	PHE	2.5
1	F	489	THR	2.5
1	E	328	ASP	2.5
1	B	48	SER	2.5
1	E	642	ASN	2.5
1	D	886	LEU	2.5
1	E	541	TYR	2.5
1	B	844	MET	2.5
1	B	888	LEU	2.5
1	D	828	LEU	2.5
1	A	801	PHE	2.5
1	D	943	ILE	2.5
1	F	164	ASP	2.5
1	C	497	LEU	2.4
1	C	578	LEU	2.4
1	C	993	THR	2.4
1	F	294	ALA	2.4
1	F	487	ILE	2.4
1	F	111	LEU	2.4
1	F	884	VAL	2.4
1	A	885	PHE	2.4
1	E	762	PHE	2.4
1	B	939	ALA	2.4
1	B	431	THR	2.4
1	D	640	GLU	2.4
1	B	240	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	895	TRP	2.4
1	E	46	SER	2.4
1	B	409	ALA	2.4
1	A	835	LYS	2.4
1	C	90	ILE	2.4
1	A	367	ILE	2.4
1	C	746	ILE	2.4
1	D	935	ILE	2.4
1	B	762	PHE	2.4
1	F	682	PHE	2.4
1	A	357	LEU	2.4
1	D	591	LEU	2.4
1	E	655	PHE	2.4
1	B	32	VAL	2.4
1	D	431	THR	2.4
1	B	900	SER	2.4
1	E	486	LEU	2.4
1	F	357	LEU	2.4
1	C	616	GLY	2.4
1	C	655	PHE	2.4
1	C	518	ARG	2.4
1	E	47	ALA	2.4
1	C	587	THR	2.4
1	B	176	GLN	2.4
1	B	461	GLY	2.4
1	C	462	SER	2.4
1	D	507	GLU	2.4
1	D	494	ALA	2.4
1	F	12	ALA	2.4
1	C	62	THR	2.4
1	F	211	ASN	2.4
1	E	177	LEU	2.4
1	D	573	MET	2.3
1	D	801	PHE	2.3
1	F	400	LEU	2.3
1	C	745	ASP	2.3
1	C	809	TRP	2.3
1	E	398	MET	2.3
1	D	713	LEU	2.3
1	C	870	GLY	2.3
1	B	59	ASP	2.3
1	B	828	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	500	ILE	2.3
1	A	411	VAL	2.3
1	E	5	PHE	2.3
1	F	1021	PHE	2.3
1	A	893	GLU	2.3
1	D	933	THR	2.3
1	A	47	ALA	2.3
1	A	488	LEU	2.3
1	A	661	ALA	2.3
1	E	658	ILE	2.3
1	B	292	LYS	2.3
1	B	531	VAL	2.3
1	B	741	VAL	2.3
1	C	848	ALA	2.3
1	E	10	ILE	2.3
1	F	92	LEU	2.3
1	F	578	LEU	2.3
1	C	512	PHE	2.3
1	F	14	VAL	2.3
1	D	355	MET	2.3
1	F	121	GLU	2.3
1	A	568	ASP	2.3
1	C	897	ILE	2.3
1	D	407	ASP	2.3
1	F	399	VAL	2.3
1	D	900	SER	2.3
1	F	710	PRO	2.3
1	B	44	THR	2.3
1	F	1037	ASN	2.3
1	E	607	GLU	2.3
1	A	310	LEU	2.3
1	C	33	ALA	2.3
1	E	706	ALA	2.3
1	A	463	THR	2.3
1	B	310	LEU	2.3
1	D	743	ILE	2.3
1	D	926	TYR	2.3
1	F	372	VAL	2.3
1	F	1026	PHE	2.3
1	F	163	LYS	2.3
1	F	494	ALA	2.3
1	E	614	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	519	MET	2.3
1	F	240	LEU	2.3
1	A	606	VAL	2.3
1	A	624	THR	2.2
1	A	1037	ASN	2.2
1	C	828	LEU	2.2
1	F	1023	PRO	2.2
1	D	946	VAL	2.2
1	E	925	VAL	2.2
1	C	942	ALA	2.2
1	D	389	SER	2.2
1	E	429	GLU	2.2
1	A	405	LEU	2.2
1	C	230	LEU	2.2
1	D	778	LYS	2.2
1	D	814	PRO	2.2
1	E	90	ILE	2.2
1	B	484	VAL	2.2
1	D	324	VAL	2.2
1	B	995	ALA	2.2
1	B	536	ARG	2.2
1	B	442	LEU	2.2
1	B	944	LEU	2.2
1	B	680	PHE	2.2
1	C	846	GLN	2.2
1	D	854	GLY	2.2
1	D	310	LEU	2.2
1	D	977	MET	2.2
1	C	278	ILE	2.2
1	F	396	PHE	2.2
1	F	762	PHE	2.2
1	A	330	THR	2.2
1	A	614	GLY	2.2
1	B	290	GLY	2.2
1	C	198	LEU	2.2
1	B	1022	VAL	2.2
1	C	1019	ILE	2.2
1	F	808	ARG	2.2
1	B	174	ASP	2.2
1	C	623	ASN	2.2
1	D	464	GLY	2.2
1	E	440	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	657	GLN	2.2
1	C	989	LEU	2.2
1	B	612	VAL	2.2
1	C	32	VAL	2.2
1	D	307	ARG	2.2
1	D	563	PHE	2.2
1	B	892	TYR	2.2
1	F	939	ALA	2.2
1	C	980	LEU	2.2
1	E	198	LEU	2.2
1	E	442	LEU	2.2
1	F	68	ASN	2.2
1	F	684	LEU	2.2
1	F	1020	PHE	2.2
1	A	626	ILE	2.2
1	B	443	VAL	2.2
1	B	947	GLU	2.2
1	D	140	VAL	2.2
1	D	836	SER	2.2
1	E	718	PRO	2.2
1	F	483	LEU	2.2
1	A	587	THR	2.2
1	F	169	THR	2.2
1	F	558	ARG	2.2
1	F	699	ARG	2.2
1	B	411	VAL	2.2
1	E	930	GLY	2.2
1	E	994	GLY	2.2
1	E	325	TYR	2.2
1	C	976	LEU	2.2
1	D	868	LEU	2.2
1	E	12	ALA	2.2
1	A	470	PHE	2.2
1	C	1037	ASN	2.2
1	F	683	GLU	2.2
1	F	827	ILE	2.2
1	D	690	LEU	2.2
1	B	237	GLN	2.2
1	B	982	PHE	2.2
1	B	3	ASN	2.2
1	D	746	ILE	2.2
1	E	330	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	441	ALA	2.2
1	A	727	PHE	2.2
1	C	1023	PRO	2.2
1	B	402	ILE	2.2
1	F	662	MET	2.2
1	E	211	ASN	2.2
1	B	896	SER	2.1
1	B	718	PRO	2.1
1	D	612	VAL	2.1
1	C	356	TYR	2.1
1	E	634	TRP	2.1
1	A	982	PHE	2.1
1	A	830	GLN	2.1
1	A	490	PRO	2.1
1	C	426	PRO	2.1
1	D	367	ILE	2.1
1	D	940	LYS	2.1
1	F	128	SER	2.1
1	F	731	ILE	2.1
1	D	230	LEU	2.1
1	D	853	THR	2.1
1	C	940	LYS	2.1
1	B	626	ILE	2.1
1	C	291	ILE	2.1
1	C	626	ILE	2.1
1	E	577	GLN	2.1
1	B	219	LEU	2.1
1	B	289	LEU	2.1
1	D	497	LEU	2.1
1	A	958	LYS	2.1
1	D	628	PHE	2.1
1	E	760	ASN	2.1
1	F	933	THR	2.1
1	F	278	ILE	2.1
1	D	976	LEU	2.1
1	C	1026	PHE	2.1
1	E	711	ASP	2.1
1	C	936	GLY	2.1
1	F	86	GLY	2.1
1	B	926	TYR	2.1
1	A	372	VAL	2.1
1	A	48	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	178	PHE	2.1
1	A	817	GLU	2.1
1	A	962	GLU	2.1
1	B	839	GLU	2.1
1	E	661	ALA	2.1
1	D	789	TRP	2.1
1	F	225	VAL	2.1
1	D	433	LYS	2.1
1	D	278	ILE	2.1
1	D	929	VAL	2.1
1	F	929	VAL	2.1
1	B	112	GLN	2.1
1	B	440	GLY	2.1
1	E	210	GLN	2.1
1	F	162	MET	2.1
1	F	816	LEU	2.1
1	D	585	GLU	2.1
1	A	741	VAL	2.1
1	B	43	VAL	2.1
1	D	509	LYS	2.1
1	B	73	ASP	2.1
1	D	390	ILE	2.1
1	A	136	PHE	2.1
1	B	964	THR	2.1
1	F	43	VAL	2.1
1	C	323	ILE	2.1
1	B	886	LEU	2.1
1	A	181	GLN	2.1
1	E	1011	MET	2.1
1	E	1026	PHE	2.1
1	A	193	LEU	2.1
1	B	278	ILE	2.1
1	B	935	ILE	2.1
1	E	625	GLY	2.1
1	A	493	CYS	2.0
1	A	612	VAL	2.0
1	F	890	ALA	2.0
1	C	306	ILE	2.0
1	C	112	GLN	2.0
1	C	818	ARG	2.0
1	F	453	PHE	2.0
1	E	174	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	14	VAL	2.0
1	D	736	ALA	2.0
1	E	297	ALA	2.0
1	A	323	ILE	2.0
1	C	522	LYS	2.0
1	D	518	ARG	2.0
1	D	784	ASP	2.0
1	E	494	ALA	2.0
1	F	932	LEU	2.0
1	D	396	PHE	2.0
1	E	85	THR	2.0
1	E	312	LYS	2.0
1	E	905	VAL	2.0
1	C	736	ALA	2.0
1	D	321	LEU	2.0
1	F	945	ILE	2.0
1	E	31	PRO	2.0
1	C	960	LEU	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
3	LMT	A	1103	35/35	0.68	1.09	6.18	82,95,107,111	0
3	LMT	B	1101	35/35	0.82	0.78	3.06	53,82,105,107	0
3	LMT	F	1101	35/35	0.85	0.98	2.91	48,88,105,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ERY	A	1101	51/51	0.84	1.20	2.63	70,79,90,95	51
3	LMT	A	1102	35/35	0.89	0.54	2.41	28,83,89,94	0
2	ERY	D	1101	51/51	0.75	1.07	2.20	71,84,96,107	51
3	LMT	D	1102	35/35	0.86	0.56	2.05	64,82,96,102	0
3	LMT	C	1101	35/35	0.86	0.52	1.89	64,84,95,96	0
3	LMT	E	1101	35/35	0.85	0.47	1.41	45,79,97,125	0
3	LMT	D	1103	35/35	0.65	0.79	1.04	79,95,103,110	0
4	NI	C	1102	1/1	0.99	0.12	-	72,72,72,72	0
4	NI	E	1102	1/1	0.99	0.13	-	79,79,79,79	0
4	NI	A	1104	1/1	0.98	0.09	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.