



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 08:13 PM GMT

PDB ID : 1K32  
Title : Crystal structure of the tricorn protease  
Authors : Brandstetter, H.; Kim, J.-S.; Groll, M.; Huber, R.  
Deposited on : 2001-10-01  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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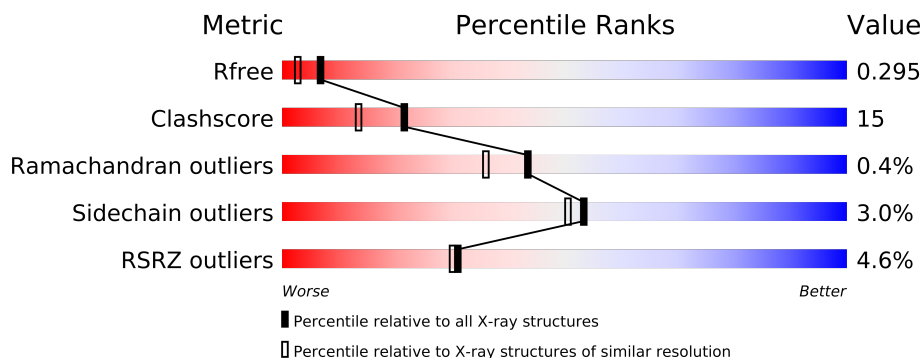
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1045	
1	B	1045	
1	C	1045	
1	D	1045	
1	E	1045	
1	F	1045	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 51456 atoms, of which 0 are hydrogen and 0 are deuterium.

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 tricorn protease.

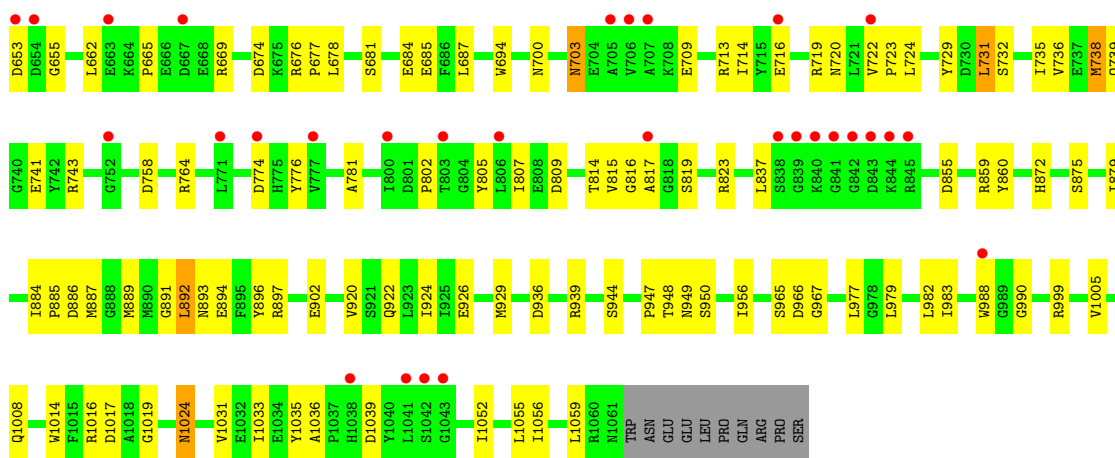
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	B	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	C	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	D	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	E	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	F	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	401	Total	O	0	0
			401	401		
2	B	395	Total	O	0	0
			395	395		
2	C	398	Total	O	0	0
			398	398		
2	D	401	Total	O	0	0
			401	401		
2	E	405	Total	O	0	0
			405	405		
2	F	394	Total	O	0	0
			394	394		

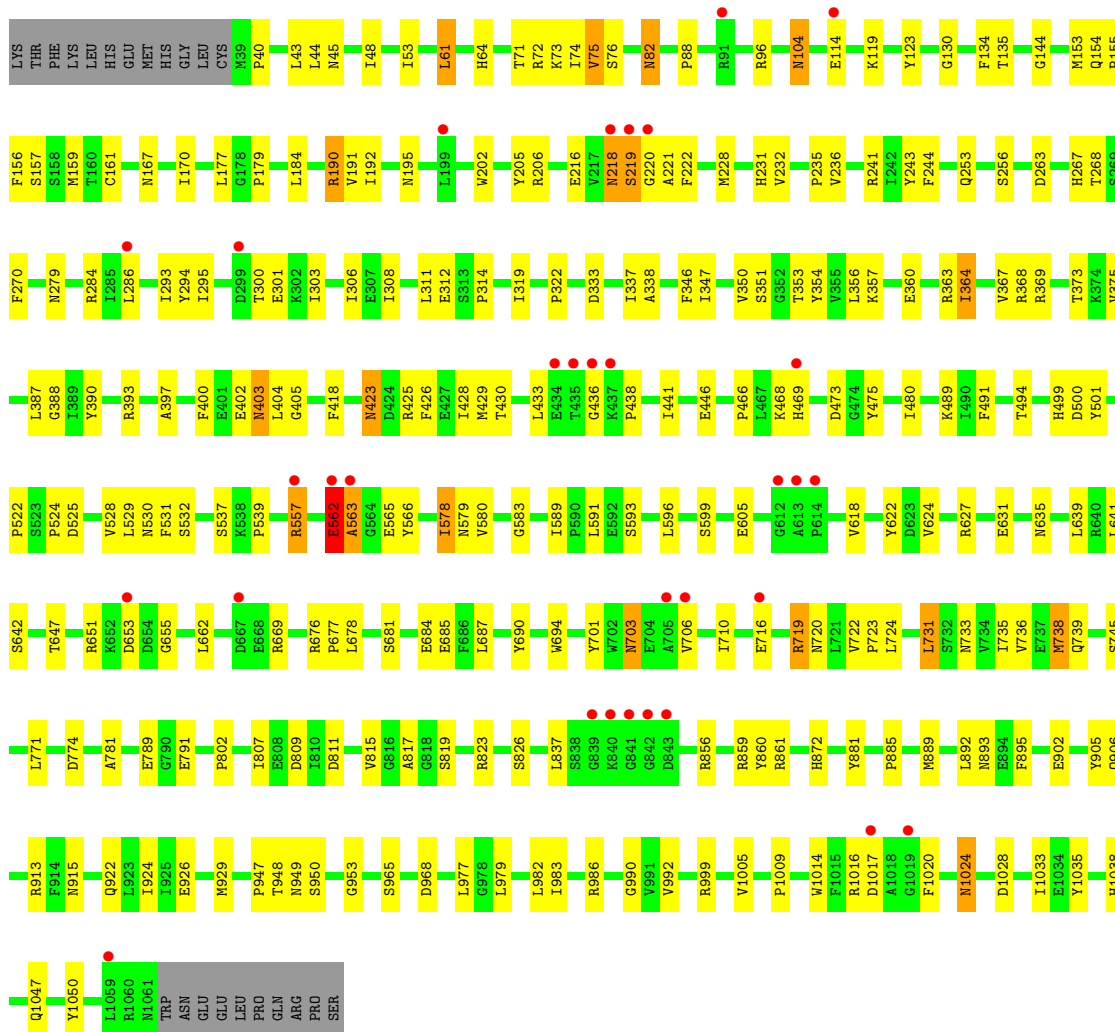






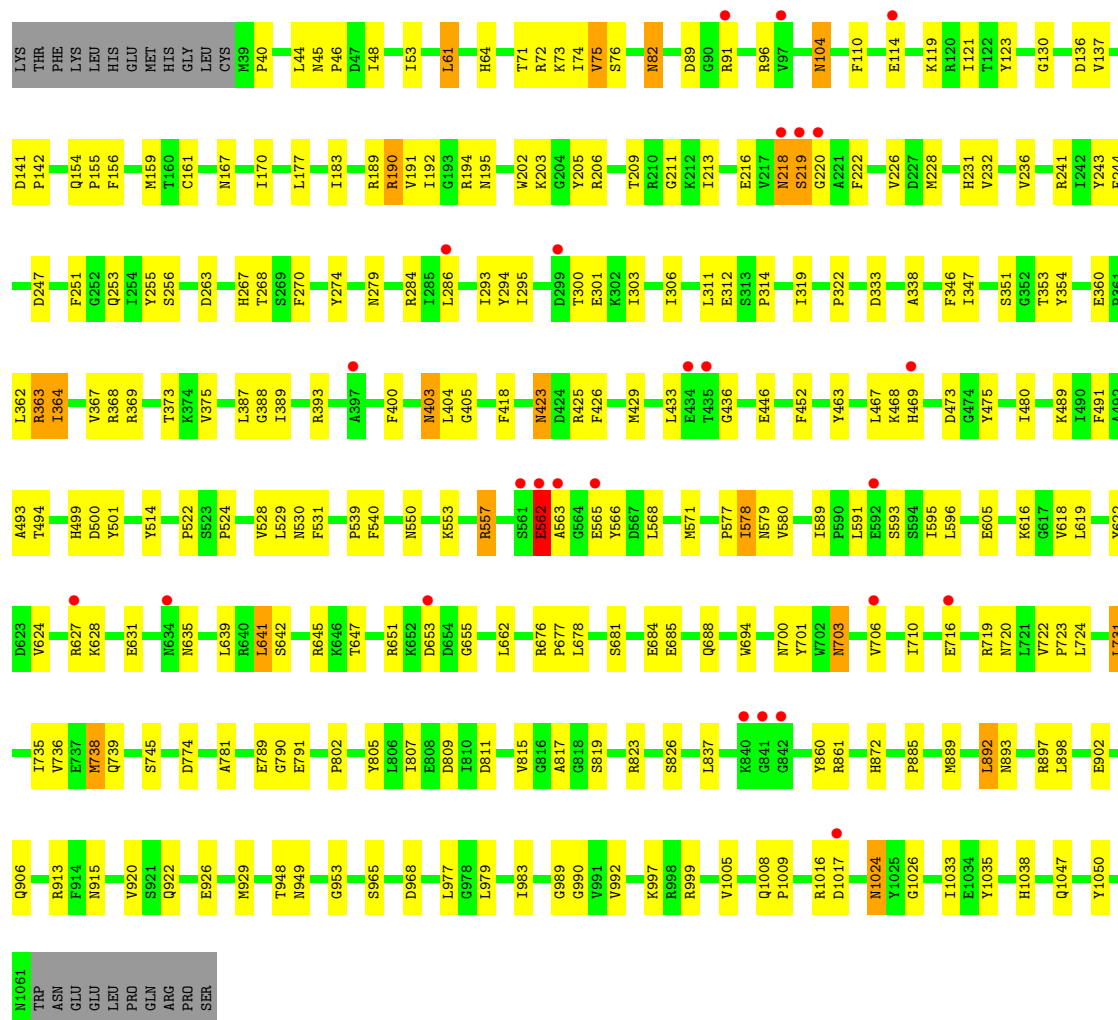
• Molecule 1: tricorn protease

Chain D:



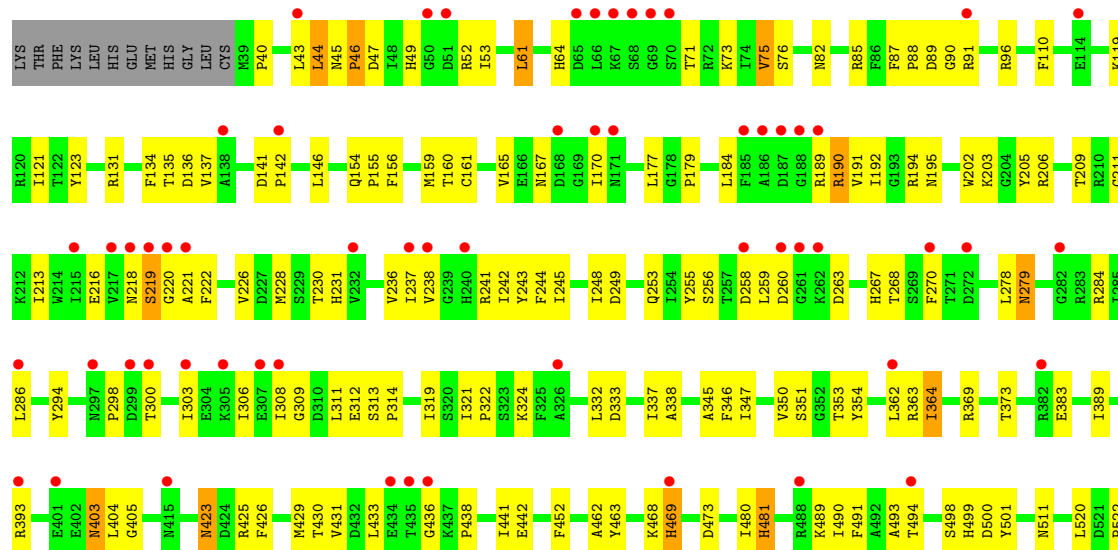
• Molecule 1: tricorn protease

Chain E:



• Molecule 1: tricorn protease

Chain F:



R1060	S523	K633	D730	G839	I966
N1061	P524	R634	L731	K840	A967
TRP		N635	S732	G841	I968
ASN	S537			G842	T959
GLU	K538	L639	I735	D843	
LEU	P539	R640	V736	K844	S965
PRO	P543	L641	E737		
GLN	P546	S642	M738	Y860	L977
ARG		T647	Q739	R861	G978
PRO	T552		G740	V864	L979
SER	R557	R651	S745	H872	L982
		K652	D756		I983
	S561	D653	R761	I882	G984
E562	R562	G655		I883	
A563		L662	C767	I884	W988
G564				P885	G989
E565		D667	L771	M889	G990
Y566		E668	D772	M890	V991
D567		R669	G773	L892	V992
			D774		G993
M571		D674	H775	N893	I994
		Y776		E894	
P577		P677	K780	R897	R999
I578		L678	A781	L898	V1005
V580		S681	Y782	F899	Q1008
		I682			P1009
G583		H683	E789	E902	R1016
I889		E684	G790	Y905	D1017
P590		L687	E791		
L591			I800	V912	F1020
E592		W694	D801	R913	
S593		N700	P802	F914	N1024
S594				N915	
I595			Y805	V920	V1031
E605		N703	L806	S921	E1032
		E704	I807	Q922	I1033
Y609		Y706	D811	L923	E1034
		A707		I924	Y1035
G612		K708	V815	E925	A1036
A613		E709	G816	E926	P1037
		S711	A817		H1038
K616		E712	S818	M929	D1039
G617		E716	N820		
V618				D936	G1043
					K1044
Y622		R719	R823	R939	D1045
D623		N720	V824		F1046
V624		L721	L825	S944	Q1047
		V722	S826		I1048
K628		P723	F827	P947	
		L724	K828	T948	L1052
E631		Y729	L837	N949	L1055
V632			S838	S960	I1056
					L1059



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.86Å 246.00Å 159.04Å 90.00° 105.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 37.48 – 1.98	Depositor EDS
% Data completeness (in resolution range)	78.6 (20.00-2.00) 81.6 (37.48-1.98)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.245 , 0.264 0.258 , 0.295	Depositor DCC
$R_{free}$ test set	20086 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 42.0	EDS
Estimated twinning fraction	0.054 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	9 of 400057 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	51456	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.40	0/8367	0.66	1/11311 (0.0%)
1	B	0.40	0/8367	0.66	2/11311 (0.0%)
1	C	0.36	0/8367	0.62	1/11311 (0.0%)
1	D	0.39	0/8367	0.65	1/11311 (0.0%)
1	E	0.38	0/8367	0.65	1/11311 (0.0%)
1	F	0.36	0/8367	0.62	1/11311 (0.0%)
All	All	0.38	0/50202	0.64	7/67866 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	364	ILE	N-CA-C	-6.20	94.25	111.00
1	A	364	ILE	N-CA-C	-5.63	95.81	111.00
1	E	364	ILE	N-CA-C	-5.41	96.39	111.00
1	B	79	GLY	N-CA-C	-5.28	99.89	113.10
1	D	364	ILE	N-CA-C	-5.23	96.87	111.00
1	B	364	ILE	N-CA-C	-5.15	97.10	111.00
1	F	364	ILE	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8177	0	8003	256	0
1	B	8177	0	8003	265	0
1	C	8177	0	8003	272	0
1	D	8177	0	8003	226	0
1	E	8177	0	8003	249	0
1	F	8177	0	8003	275	0
2	A	401	0	0	12	0
2	B	395	0	0	8	0
2	C	398	0	0	18	0
2	D	401	0	0	9	0
2	E	405	0	0	10	0
2	F	394	0	0	10	0
All	All	51456	0	48018	1453	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (1453) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:155:PRO:HG2	1:F:159:MET:HE1	1.33	1.09
1:B:155:PRO:HG2	1:B:159:MET:HE1	1.36	1.07
1:C:155:PRO:HG2	1:C:159:MET:HE1	1.37	1.06
1:D:155:PRO:HG2	1:D:159:MET:HE1	1.35	1.03
1:B:983:ILE:HG23	1:B:1033:ILE:HD13	1.41	1.02
1:A:983:ILE:HG23	1:A:1033:ILE:HD13	1.41	0.99
1:D:983:ILE:HG23	1:D:1033:ILE:HD12	1.43	0.97
1:A:155:PRO:HG2	1:A:159:MET:HE1	1.46	0.95
1:F:154:GLN:HB3	1:F:159:MET:HE3	1.47	0.95
1:C:983:ILE:HG23	1:C:1033:ILE:HD13	1.49	0.94
1:D:53:ILE:HG23	1:D:286:LEU:HD21	1.48	0.93
1:B:104:ASN:HD22	1:B:104:ASN:H	1.12	0.93
1:A:948:THR:H	1:B:922:GLN:HE22	1.16	0.92
1:E:155:PRO:HG2	1:E:159:MET:HE1	1.49	0.91
1:F:983:ILE:HG23	1:F:1033:ILE:HD13	1.50	0.90
1:E:53:ILE:HG23	1:E:286:LEU:HD21	1.53	0.89
1:B:253:GLN:HE22	1:B:270:PHE:H	1.20	0.89
1:C:154:GLN:HB3	1:C:159:MET:HE3	1.54	0.88
1:A:922:GLN:HE22	1:B:948:THR:H	1.21	0.88
1:A:789:GLU:HG3	1:B:577:PRO:HG3	1.55	0.87
1:D:253:GLN:HE22	1:D:270:PHE:H	1.23	0.87
1:C:922:GLN:HE22	1:D:948:THR:H	1.15	0.87
1:B:480:ILE:H	1:B:494:THR:HG22	1.38	0.87
1:B:468:LYS:HD2	1:B:473:ASP:HB2	1.58	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:480:ILE:H	1:F:494:THR:HG22	1.39	0.86
1:F:468:LYS:HD2	1:F:473:ASP:HB2	1.57	0.85
1:C:268:THR:HG22	1:C:303:ILE:HD11	1.56	0.85
1:E:104:ASN:H	1:E:104:ASN:HD22	1.23	0.85
1:B:539:PRO:HG2	1:B:578:ILE:HG23	1.58	0.85
1:C:104:ASN:H	1:C:104:ASN:HD22	1.22	0.85
1:E:922:GLN:HE22	1:F:948:THR:H	1.22	0.85
1:A:161:CYS:SG	2:A:2394:HOH:O	2.35	0.84
1:A:104:ASN:HD22	1:A:104:ASN:H	1.21	0.84
1:F:539:PRO:HG2	1:F:578:ILE:HG23	1.56	0.84
1:C:73:LYS:HD3	1:C:76:SER:HB3	1.60	0.84
1:A:480:ILE:H	1:A:494:THR:HG22	1.41	0.84
1:F:73:LYS:HD3	1:F:76:SER:HB3	1.59	0.83
1:F:322:PRO:HB3	1:F:678:LEU:HD13	1.59	0.83
1:E:40:PRO:HG2	1:E:724:LEU:HD22	1.59	0.83
1:E:403:ASN:ND2	1:E:405:GLY:H	1.76	0.83
1:D:104:ASN:H	1:D:104:ASN:HD22	1.26	0.82
1:A:253:GLN:HE22	1:A:270:PHE:H	1.22	0.81
1:E:983:ILE:HG23	1:E:1033:ILE:HD12	1.63	0.81
1:B:489:LYS:HG3	1:B:491:PHE:CE1	2.15	0.81
1:E:789:GLU:HG3	1:F:577:PRO:HG3	1.61	0.81
1:E:948:THR:H	1:F:922:GLN:HE22	1.29	0.81
1:C:40:PRO:HG2	1:C:724:LEU:HD22	1.61	0.80
1:F:268:THR:HG22	1:F:303:ILE:HD11	1.62	0.80
1:D:468:LYS:HD2	1:D:473:ASP:HB2	1.63	0.80
1:A:322:PRO:HG3	1:A:678:LEU:HD13	1.63	0.80
1:D:48:ILE:HB	1:D:286:LEU:HD22	1.64	0.79
1:F:404:LEU:HD22	1:F:429:MET:HE2	1.65	0.79
1:C:577:PRO:HG3	1:D:789:GLU:HG3	1.63	0.78
1:B:284:ARG:HD3	2:B:3393:HOH:O	1.81	0.78
1:E:539:PRO:HG2	1:E:578:ILE:HG23	1.65	0.78
1:A:557:ARG:NH2	1:E:393:ARG:HH12	1.80	0.78
1:B:161:CYS:SG	2:B:3394:HOH:O	2.40	0.78
1:E:154:GLN:HB3	1:E:159:MET:HE3	1.65	0.78
1:A:948:THR:H	1:B:922:GLN:NE2	1.82	0.78
1:A:404:LEU:HD22	1:A:429:MET:HE2	1.66	0.77
1:B:154:GLN:HB3	1:B:159:MET:HE3	1.67	0.77
1:F:403:ASN:ND2	1:F:405:GLY:H	1.82	0.77
1:D:662:LEU:HD23	1:D:662:LEU:O	1.84	0.77
1:E:161:CYS:SG	2:E:6394:HOH:O	2.42	0.77
1:F:694:TRP:HA	1:F:738:MET:CE	2.15	0.77
1:F:253:GLN:HE22	1:F:270:PHE:H	1.33	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:403:ASN:HD22	1:C:405:GLY:H	1.33	0.77
1:C:403:ASN:ND2	1:C:405:GLY:H	1.81	0.77
1:C:539:PRO:HG2	1:C:578:ILE:HG23	1.66	0.76
1:A:268:THR:HG22	1:A:303:ILE:HD11	1.67	0.76
1:C:480:ILE:H	1:C:494:THR:HG22	1.50	0.76
1:A:73:LYS:HD3	1:A:76:SER:HB3	1.67	0.76
1:C:578:ILE:HG12	1:C:580:VAL:HG23	1.67	0.76
1:A:293:ILE:HG22	1:A:306:ILE:HD12	1.68	0.76
1:A:284:ARG:HD3	2:A:2393:HOH:O	1.84	0.76
1:E:662:LEU:O	1:E:662:LEU:HD23	1.86	0.76
1:B:73:LYS:HD3	1:B:76:SER:HB3	1.68	0.76
1:B:206:ARG:H	1:B:1024:ASN:HD21	1.32	0.75
1:D:40:PRO:HG2	1:D:724:LEU:HD22	1.67	0.75
1:F:403:ASN:HD22	1:F:405:GLY:H	1.35	0.75
1:A:539:PRO:HG2	1:A:578:ILE:HG23	1.68	0.75
1:F:350:VAL:HG21	1:F:669:ARG:HH11	1.51	0.75
1:F:82:ASN:HD21	1:F:96:ARG:HH21	1.33	0.75
1:C:948:THR:H	1:D:922:GLN:HE22	1.33	0.75
1:A:154:GLN:HB3	1:A:159:MET:HE3	1.69	0.74
1:D:53:ILE:CG2	1:D:286:LEU:HD21	2.16	0.74
1:E:403:ASN:HD22	1:E:405:GLY:H	1.35	0.74
1:C:167:ASN:HB2	1:C:170:ILE:HB	1.68	0.74
1:C:286:LEU:HD12	1:C:294:TYR:O	1.87	0.74
1:A:353:THR:HG23	1:A:354:TYR:CD1	2.23	0.74
1:A:489:LYS:HG3	1:A:491:PHE:CE1	2.22	0.74
1:E:253:GLN:HE22	1:E:270:PHE:H	1.34	0.74
1:B:206:ARG:H	1:B:1024:ASN:ND2	1.85	0.74
1:D:268:THR:HG22	1:D:303:ILE:HD11	1.69	0.74
1:B:295:ILE:HG13	1:B:306:ILE:HD11	1.68	0.74
1:B:480:ILE:H	1:B:494:THR:CG2	2.00	0.73
1:D:578:ILE:HG12	1:D:580:VAL:HG23	1.70	0.73
1:A:40:PRO:HG2	1:A:724:LEU:HD22	1.69	0.73
1:F:206:ARG:H	1:F:1024:ASN:ND2	1.86	0.73
1:E:268:THR:HG22	1:E:303:ILE:HD11	1.69	0.73
1:E:480:ILE:H	1:E:494:THR:HG22	1.54	0.73
1:A:468:LYS:HD2	1:A:473:ASP:HB2	1.70	0.73
1:B:286:LEU:HD12	1:B:294:TYR:O	1.88	0.73
1:F:206:ARG:H	1:F:1024:ASN:HD21	1.37	0.72
1:C:468:LYS:HD2	1:C:473:ASP:HB2	1.70	0.72
1:B:202:TRP:CH2	1:B:745:SER:HB3	2.24	0.72
1:F:578:ILE:HG12	1:F:580:VAL:HG23	1.70	0.72
1:B:350:VAL:HG21	1:B:669:ARG:HH11	1.53	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:351:SER:OG	1:B:353:THR:HG22	1.88	0.72
1:C:161:CYS:SG	2:C:4394:HOH:O	2.47	0.72
1:E:922:GLN:NE2	1:F:948:THR:H	1.86	0.72
1:B:681:SER:HB3	1:B:684:GLU:HG2	1.70	0.72
1:A:350:VAL:HG21	1:A:669:ARG:HH11	1.54	0.72
1:B:40:PRO:HG2	1:B:724:LEU:HD22	1.72	0.71
1:D:161:CYS:SG	2:D:5394:HOH:O	2.48	0.71
1:F:155:PRO:CG	1:F:159:MET:HE1	2.17	0.71
1:F:286:LEU:HD12	1:F:294:TYR:O	1.90	0.71
1:C:253:GLN:HE22	1:C:270:PHE:H	1.37	0.71
1:A:351:SER:OG	1:A:353:THR:HG22	1.91	0.71
1:C:694:TRP:HA	1:C:738:MET:CE	2.21	0.71
1:D:73:LYS:HD3	1:D:76:SER:HB3	1.73	0.71
1:D:403:ASN:ND2	1:D:405:GLY:H	1.87	0.71
1:A:480:ILE:H	1:A:494:THR:CG2	2.04	0.71
1:A:922:GLN:NE2	1:B:948:THR:H	1.86	0.71
1:A:206:ARG:H	1:A:1024:ASN:ND2	1.88	0.71
1:D:404:LEU:HD22	1:D:429:MET:HE2	1.72	0.70
1:D:403:ASN:HD22	1:D:405:GLY:H	1.38	0.70
1:A:205:TYR:HA	1:A:1024:ASN:HD21	1.57	0.70
1:C:322:PRO:HB3	1:C:678:LEU:HD13	1.72	0.69
1:E:468:LYS:HD2	1:E:473:ASP:HB2	1.74	0.69
1:F:82:ASN:ND2	1:F:96:ARG:HH21	1.90	0.69
1:B:268:THR:HG22	1:B:303:ILE:HD11	1.71	0.69
1:B:82:ASN:ND2	1:B:96:ARG:HH21	1.90	0.69
1:F:40:PRO:HG2	1:F:724:LEU:CD2	2.21	0.69
1:D:206:ARG:H	1:D:1024:ASN:ND2	1.90	0.69
1:F:662:LEU:HD23	1:F:662:LEU:O	1.92	0.69
1:B:557:ARG:NE	1:D:393:ARG:HH22	1.91	0.69
1:F:61:LEU:HB3	1:F:75:VAL:HG13	1.73	0.69
1:D:351:SER:OG	1:D:353:THR:HG22	1.93	0.69
1:F:774:ASP:HA	1:F:817:ALA:HB2	1.74	0.68
1:A:577:PRO:HG3	1:B:789:GLU:HG3	1.75	0.68
1:D:404:LEU:HD22	1:D:429:MET:CE	2.22	0.68
1:A:393:ARG:HH22	1:C:557:ARG:NE	1.91	0.68
1:B:430:THR:HG23	1:B:441:ILE:HD11	1.75	0.68
1:E:530:ASN:ND2	1:E:531:PHE:H	1.90	0.68
1:B:404:LEU:HD22	1:B:429:MET:HE2	1.74	0.68
1:C:350:VAL:HG21	1:C:669:ARG:HH11	1.58	0.68
1:F:480:ILE:H	1:F:494:THR:CG2	2.07	0.68
1:F:892:LEU:HD13	1:F:920:VAL:HG21	1.73	0.68
1:B:363:ARG:HG3	1:B:688:GLN:NE2	2.09	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:681:SER:HB3	1:C:684:GLU:HG2	1.74	0.68
1:A:53:ILE:HG23	1:A:286:LEU:HD21	1.75	0.68
1:E:73:LYS:HD3	1:E:76:SER:HB3	1.74	0.68
1:D:977:LEU:HB2	1:D:979:LEU:CD1	2.24	0.68
1:D:190:ARG:NH2	1:D:222:PHE:HZ	1.93	0.67
1:E:322:PRO:HG3	1:E:678:LEU:HD13	1.75	0.67
1:E:53:ILE:CG2	1:E:286:LEU:HD21	2.23	0.67
1:F:351:SER:OG	1:F:353:THR:HG22	1.93	0.67
1:E:205:TYR:HA	1:E:1024:ASN:HD21	1.58	0.67
1:C:922:GLN:NE2	1:D:948:THR:H	1.89	0.67
1:B:40:PRO:HG2	1:B:724:LEU:CD2	2.24	0.67
1:F:236:VAL:HG23	1:F:243:TYR:HB2	1.76	0.67
1:C:635:ASN:HB3	1:C:653:ASP:OD1	1.95	0.67
1:A:222:PHE:H	1:A:1038:HIS:HD2	1.42	0.67
1:C:190:ARG:NH2	1:C:222:PHE:HZ	1.91	0.67
1:B:404:LEU:HD22	1:B:429:MET:CE	2.24	0.67
1:D:703:ASN:HD22	1:D:703:ASN:C	1.98	0.67
1:A:350:VAL:HG21	1:A:669:ARG:NH1	2.10	0.67
1:E:190:ARG:NH2	1:E:222:PHE:HZ	1.93	0.67
1:F:53:ILE:HG23	1:F:286:LEU:HD21	1.77	0.67
1:B:72:ARG:HG3	1:E:72:ARG:HG3	1.75	0.67
1:F:982:LEU:O	1:F:983:ILE:HD12	1.95	0.66
1:A:393:ARG:HH12	1:C:557:ARG:HD2	1.59	0.66
1:D:913:ARG:HH21	1:D:1047:GLN:HE21	1.42	0.66
1:D:480:ILE:H	1:D:494:THR:HG22	1.60	0.66
1:D:681:SER:O	1:D:684:GLU:HG2	1.95	0.66
1:D:154:GLN:HB3	1:D:159:MET:HE3	1.78	0.66
1:B:489:LYS:HG3	1:B:491:PHE:HE1	1.57	0.66
1:D:286:LEU:HD12	1:D:294:TYR:O	1.96	0.66
1:A:681:SER:HB3	1:A:684:GLU:HG2	1.77	0.66
1:D:539:PRO:HG2	1:D:578:ILE:HG23	1.76	0.66
1:D:40:PRO:HG2	1:D:724:LEU:CD2	2.26	0.66
1:D:206:ARG:H	1:D:1024:ASN:HD21	1.43	0.66
1:E:284:ARG:HD3	2:E:6393:HOH:O	1.95	0.66
1:F:977:LEU:HB2	1:F:979:LEU:HD13	1.78	0.66
1:E:403:ASN:HD22	1:E:403:ASN:C	1.99	0.66
1:A:893:ASN:OD1	1:B:522:PRO:HD3	1.96	0.66
1:E:404:LEU:HD22	1:E:429:MET:HE2	1.77	0.65
1:A:522:PRO:HD3	1:B:893:ASN:OD1	1.95	0.65
1:E:48:ILE:HB	1:E:286:LEU:HD22	1.77	0.65
1:C:61:LEU:CB	1:C:75:VAL:HG13	2.26	0.65
1:D:61:LEU:CB	1:D:75:VAL:HG13	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:628:LYS:HE3	2:F:7366:HOH:O	1.95	0.65
1:D:446:GLU:OE1	1:D:468:LYS:HE2	1.97	0.65
1:C:46:PRO:HB2	1:C:286:LEU:CD2	2.26	0.65
1:E:206:ARG:H	1:E:1024:ASN:ND2	1.94	0.65
1:B:774:ASP:HA	1:B:817:ALA:HB2	1.78	0.65
1:B:593:SER:O	1:B:624:VAL:HG22	1.96	0.65
1:B:256:SER:OG	1:B:267:HIS:HE1	1.80	0.65
1:F:982:LEU:C	1:F:983:ILE:HD12	2.17	0.65
1:E:591:LEU:HD11	1:E:662:LEU:HD21	1.79	0.64
1:B:53:ILE:HG23	1:B:286:LEU:HD21	1.79	0.64
1:F:179:PRO:HG2	2:F:7045:HOH:O	1.96	0.64
1:A:552:THR:HG21	1:A:578:ILE:HD12	1.78	0.64
1:C:480:ILE:H	1:C:494:THR:CG2	2.10	0.64
1:C:74:ILE:HG13	1:C:75:VAL:HG12	1.78	0.64
1:B:61:LEU:CB	1:B:75:VAL:HG13	2.27	0.64
1:C:662:LEU:HD23	1:C:662:LEU:O	1.96	0.64
1:E:293:ILE:HG22	1:E:306:ILE:HD12	1.78	0.64
1:B:82:ASN:HD21	1:B:96:ARG:HH21	1.45	0.64
1:E:353:THR:HG23	1:E:354:TYR:CD1	2.32	0.64
1:F:694:TRP:HA	1:F:738:MET:HE1	1.78	0.64
1:F:161:CYS:SG	2:F:7394:HOH:O	2.55	0.64
1:C:322:PRO:HA	1:C:678:LEU:HD22	1.80	0.64
1:D:530:ASN:ND2	1:D:531:PHE:H	1.96	0.64
1:A:286:LEU:HD12	1:A:294:TYR:O	1.97	0.64
1:A:46:PRO:HB2	1:A:286:LEU:HD21	1.80	0.64
1:B:46:PRO:HB2	1:B:286:LEU:CD2	2.27	0.64
1:B:222:PHE:H	1:B:1038:HIS:HD2	1.46	0.64
1:A:628:LYS:HE3	2:A:2366:HOH:O	1.98	0.64
1:A:46:PRO:HB2	1:A:286:LEU:CD2	2.28	0.64
1:B:350:VAL:HG21	1:B:669:ARG:NH1	2.12	0.64
1:B:403:ASN:HD22	1:B:405:GLY:H	1.46	0.64
1:A:774:ASP:HA	1:A:817:ALA:HB2	1.78	0.64
1:F:872:HIS:HE1	1:F:902:GLU:OE1	1.81	0.64
1:C:948:THR:H	1:D:922:GLN:NE2	1.95	0.63
1:B:403:ASN:ND2	1:B:405:GLY:H	1.96	0.63
1:C:104:ASN:H	1:C:104:ASN:ND2	1.94	0.63
1:C:694:TRP:HA	1:C:738:MET:HE1	1.79	0.63
1:A:206:ARG:H	1:A:1024:ASN:HD21	1.44	0.63
1:C:155:PRO:CG	1:C:159:MET:HE1	2.21	0.63
1:C:40:PRO:HG2	1:C:724:LEU:CD2	2.28	0.63
1:A:815:VAL:HA	1:A:819:SER:HB3	1.81	0.63
1:A:493:ALA:HA	1:A:571:MET:HG3	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:789:GLU:OE2	2:A:2230:HOH:O	2.15	0.63
1:D:53:ILE:HG23	1:D:286:LEU:CD2	2.27	0.63
1:F:350:VAL:HG21	1:F:669:ARG:NH1	2.12	0.63
1:D:977:LEU:HB2	1:D:979:LEU:HD13	1.80	0.63
1:A:684:GLU:HG3	1:A:685:GLU:N	2.14	0.63
1:B:618:VAL:HG23	1:B:633:LYS:O	1.99	0.63
1:F:681:SER:O	1:F:684:GLU:HG2	1.99	0.63
1:B:353:THR:HG23	1:B:354:TYR:CD1	2.34	0.63
1:D:403:ASN:HD22	1:D:403:ASN:C	2.01	0.63
1:A:889:MET:SD	1:B:522:PRO:HG2	2.38	0.63
1:E:312:GLU:HG2	1:E:314:PRO:HD3	1.80	0.63
1:A:522:PRO:HG2	1:B:889:MET:SD	2.39	0.62
1:A:61:LEU:HB2	1:A:75:VAL:HG13	1.81	0.62
1:B:578:ILE:HG12	1:B:580:VAL:HG23	1.81	0.62
1:F:195:ASN:O	1:F:231:HIS:HE1	1.83	0.62
1:D:155:PRO:HG2	1:D:159:MET:CE	2.22	0.62
1:F:40:PRO:HG2	1:F:724:LEU:HD22	1.82	0.62
1:D:494:THR:HG21	1:D:500:ASP:OD1	1.99	0.62
1:A:40:PRO:HG2	1:A:724:LEU:CD2	2.29	0.62
1:B:241:ARG:NH1	1:B:263:ASP:OD1	2.33	0.62
1:B:319:ILE:HG23	1:B:677:PRO:HB3	1.80	0.62
1:C:403:ASN:HD22	1:C:403:ASN:C	2.03	0.62
1:F:61:LEU:CB	1:F:75:VAL:HG13	2.30	0.62
1:C:628:LYS:HE3	2:C:4366:HOH:O	1.99	0.62
1:B:64:HIS:HD2	1:B:71:THR:OG1	1.82	0.62
1:F:404:LEU:HD22	1:F:429:MET:CE	2.28	0.62
1:E:446:GLU:OE1	1:E:468:LYS:HE2	2.00	0.62
1:B:363:ARG:HD2	1:B:365:ARG:NH2	2.15	0.62
1:E:489:LYS:HG3	1:E:491:PHE:CE1	2.35	0.62
1:D:815:VAL:HA	1:D:819:SER:HB3	1.82	0.62
1:D:716:GLU:HG2	1:D:720:ASN:HD21	1.64	0.62
1:F:716:GLU:HG2	1:F:720:ASN:HD21	1.64	0.62
1:E:53:ILE:HD11	1:E:295:ILE:HD11	1.82	0.62
1:F:999:ARG:HG2	1:F:1005:VAL:HG22	1.81	0.62
1:D:82:ASN:HD21	1:D:96:ARG:HH21	1.48	0.62
1:A:489:LYS:HG3	1:A:491:PHE:HE1	1.65	0.61
1:F:736:VAL:HA	1:F:739:GLN:HE21	1.64	0.61
1:A:189:ARG:HD2	1:A:216:GLU:O	1.99	0.61
1:B:913:ARG:HH21	1:B:1047:GLN:HE21	1.47	0.61
1:A:387:LEU:HD13	1:A:388:GLY:N	2.15	0.61
1:F:489:LYS:HG3	1:F:491:PHE:CE1	2.36	0.61
1:E:130:GLY:HA3	2:E:6163:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:480:ILE:N	1:B:494:THR:HG22	2.12	0.61
1:E:716:GLU:HG2	1:E:720:ASN:ND2	2.16	0.61
1:C:256:SER:OG	1:C:267:HIS:HE1	1.84	0.61
1:A:403:ASN:ND2	1:A:405:GLY:H	1.97	0.61
1:F:46:PRO:HB2	1:F:286:LEU:CD2	2.30	0.61
1:D:716:GLU:HG2	1:D:720:ASN:ND2	2.14	0.61
1:D:694:TRP:HA	1:D:738:MET:CE	2.31	0.61
1:D:489:LYS:HG3	1:D:491:PHE:CE1	2.35	0.61
1:F:423:ASN:C	1:F:423:ASN:HD22	2.04	0.61
1:B:190:ARG:NH2	1:B:222:PHE:HZ	1.98	0.61
1:B:393:ARG:HH12	1:F:557:ARG:HD2	1.66	0.61
1:A:1031:VAL:HG12	1:A:1033:ILE:HD11	1.83	0.61
1:F:167:ASN:HB2	1:F:170:ILE:HB	1.83	0.61
1:F:253:GLN:HB2	1:F:255:TYR:CE1	2.36	0.61
1:A:241:ARG:NH1	1:A:263:ASP:OD1	2.33	0.61
1:E:53:ILE:HG23	1:E:286:LEU:CD2	2.29	0.60
1:E:635:ASN:HB3	1:E:653:ASP:OD1	2.01	0.60
1:C:236:VAL:HG23	1:C:243:TYR:HB2	1.82	0.60
1:E:404:LEU:HD22	1:E:429:MET:CE	2.31	0.60
1:B:393:ARG:HH12	1:F:557:ARG:CZ	2.13	0.60
1:A:662:LEU:HD23	1:A:662:LEU:O	2.02	0.60
1:D:190:ARG:HH21	1:D:190:ARG:HB2	1.66	0.60
1:C:279:ASN:ND2	2:C:4071:HOH:O	2.32	0.60
1:F:694:TRP:HA	1:F:738:MET:HE2	1.84	0.60
1:D:61:LEU:HB2	1:D:75:VAL:HG13	1.82	0.60
1:C:593:SER:O	1:C:624:VAL:HG22	2.00	0.60
1:E:40:PRO:HG2	1:E:724:LEU:CD2	2.32	0.60
1:B:155:PRO:CG	1:B:159:MET:HE1	2.22	0.60
1:A:498:SER:HB2	2:A:3192:HOH:O	2.01	0.60
1:E:977:LEU:HB2	1:E:979:LEU:HD13	1.84	0.60
1:B:684:GLU:HG3	1:B:685:GLU:N	2.16	0.60
1:C:681:SER:O	1:C:684:GLU:HG2	2.01	0.60
1:C:195:ASN:O	1:C:231:HIS:HE1	1.85	0.60
1:A:256:SER:OG	1:A:267:HIS:HE1	1.84	0.60
1:C:423:ASN:HD22	1:C:423:ASN:C	2.04	0.60
1:E:622:TYR:OH	1:E:627:ARG:HG2	2.01	0.59
1:E:206:ARG:H	1:E:1024:ASN:HD21	1.50	0.59
1:B:322:PRO:HB3	1:B:678:LEU:HD13	1.83	0.59
1:A:480:ILE:N	1:A:494:THR:HG22	2.14	0.59
1:B:206:ARG:N	1:B:1024:ASN:HD21	2.00	0.59
1:E:716:GLU:HG2	1:E:720:ASN:HD21	1.66	0.59
1:A:230:THR:HG21	1:A:248:ILE:HA	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:872:HIS:HE1	1:C:902:GLU:OE1	1.85	0.59
1:E:367:VAL:CG1	1:E:375:VAL:HG21	2.32	0.59
1:C:309:GLY:O	1:C:311:LEU:HD13	2.03	0.59
1:A:489:LYS:HE2	1:A:491:PHE:HZ	1.67	0.59
1:A:222:PHE:H	1:A:1038:HIS:CD2	2.19	0.59
1:B:61:LEU:HB2	1:B:75:VAL:HG13	1.83	0.59
1:E:489:LYS:HE2	1:E:491:PHE:HZ	1.66	0.59
1:D:82:ASN:ND2	1:D:96:ARG:HH21	2.00	0.59
1:A:393:ARG:HH12	1:C:557:ARG:NH2	2.01	0.59
1:C:61:LEU:HB3	1:C:75:VAL:HG13	1.83	0.59
1:D:642:SER:HB2	1:D:647:THR:HB	1.83	0.59
1:B:872:HIS:HE1	1:B:902:GLU:OE1	1.85	0.59
1:E:155:PRO:HD2	1:E:159:MET:HE3	1.85	0.59
1:B:662:LEU:O	1:B:662:LEU:HD23	2.02	0.59
1:F:988:TRP:CZ3	1:F:990:GLY:HA3	2.38	0.59
1:C:322:PRO:HG2	1:C:674:ASP:OD1	2.02	0.59
1:A:202:TRP:CH2	1:A:745:SER:HB3	2.38	0.59
1:E:676:ARG:HD2	2:E:6370:HOH:O	2.02	0.59
1:C:404:LEU:HD22	1:C:429:MET:HE2	1.85	0.59
1:B:46:PRO:HB2	1:B:286:LEU:HD21	1.85	0.59
1:F:256:SER:OG	1:F:267:HIS:HE1	1.86	0.59
1:E:913:ARG:HH21	1:E:1047:GLN:HE21	1.49	0.59
1:F:1045:ASP:HB3	1:F:1048:ILE:HG22	1.85	0.59
1:A:64:HIS:HD2	1:A:71:THR:OG1	1.85	0.59
1:F:52:ARG:HG3	1:F:52:ARG:HH21	1.68	0.59
1:C:999:ARG:HG2	1:C:1005:VAL:HG22	1.84	0.59
1:E:61:LEU:CB	1:E:75:VAL:HG13	2.33	0.58
1:E:82:ASN:HD21	1:E:96:ARG:HH21	1.51	0.58
1:E:681:SER:O	1:E:684:GLU:HG2	2.03	0.58
1:B:589:ILE:HD13	1:B:641:LEU:HD12	1.85	0.58
1:D:190:ARG:NH2	1:D:222:PHE:CZ	2.71	0.58
1:D:190:ARG:NH2	1:D:216:GLU:OE2	2.35	0.58
1:E:681:SER:HB3	1:E:684:GLU:HG2	1.85	0.58
1:D:256:SER:OG	1:D:267:HIS:HE1	1.86	0.58
1:E:82:ASN:ND2	1:E:96:ARG:HH21	2.01	0.58
1:D:622:TYR:OH	1:D:627:ARG:HG2	2.03	0.58
1:A:82:ASN:ND2	1:A:96:ARG:HH21	2.01	0.58
1:B:119:LYS:NZ	1:B:823:ARG:HH22	2.01	0.58
1:E:333:ASP:CG	1:E:369:ARG:HE	2.06	0.58
1:B:628:LYS:HE3	2:B:3366:HOH:O	2.03	0.58
1:B:293:ILE:HG22	1:B:306:ILE:HD12	1.86	0.58
1:E:61:LEU:HB3	1:E:75:VAL:HG13	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:947:PRO:HD2	1:C:950:SER:HB3	1.86	0.58
1:C:889:MET:SD	1:D:522:PRO:HG2	2.44	0.58
1:F:403:ASN:C	1:F:403:ASN:HD22	2.07	0.58
1:C:43:LEU:O	1:C:44:LEU:HG	2.04	0.58
1:D:872:HIS:HE1	1:D:902:GLU:OE1	1.86	0.58
1:E:190:ARG:NH2	1:E:222:PHE:CZ	2.72	0.58
1:B:781:ALA:HB2	1:B:802:PRO:HG2	1.86	0.58
1:B:104:ASN:ND2	1:B:104:ASN:H	1.89	0.57
1:F:319:ILE:HG23	1:F:677:PRO:HB3	1.85	0.57
1:F:815:VAL:HA	1:F:819:SER:HB3	1.85	0.57
1:E:64:HIS:HD2	1:E:71:THR:OG1	1.87	0.57
1:E:104:ASN:ND2	1:E:104:ASN:H	1.99	0.57
1:E:104:ASN:N	1:E:104:ASN:HD22	1.91	0.57
1:A:872:HIS:HE1	1:A:902:GLU:OE1	1.87	0.57
1:D:322:PRO:HB3	1:D:678:LEU:HD13	1.85	0.57
1:E:694:TRP:HA	1:E:738:MET:CE	2.34	0.57
1:C:530:ASN:ND2	1:C:531:PHE:H	2.02	0.57
1:F:884:ILE:HD13	1:F:924:ILE:HD13	1.86	0.57
1:F:735:ILE:O	1:F:739:GLN:HG3	2.04	0.57
1:F:618:VAL:HG23	1:F:633:LYS:O	2.03	0.57
1:D:635:ASN:HB3	1:D:653:ASP:OD1	2.04	0.57
1:E:202:TRP:CH2	1:E:745:SER:HB3	2.39	0.57
1:F:947:PRO:HD2	1:F:950:SER:HB3	1.85	0.57
1:F:218:ASN:O	1:F:219:SER:C	2.43	0.57
1:F:350:VAL:CG2	1:F:669:ARG:HH11	2.15	0.57
1:B:557:ARG:CZ	1:D:393:ARG:HH12	2.18	0.57
1:C:524:PRO:HD3	1:D:605:GLU:HG2	1.87	0.57
1:B:390:TYR:HD1	1:B:397:ALA:HB2	1.69	0.57
1:D:965:SER:HA	1:D:990:GLY:O	2.03	0.57
1:A:319:ILE:HG23	1:A:677:PRO:HB3	1.87	0.57
1:E:815:VAL:HA	1:E:819:SER:HB3	1.86	0.57
1:D:684:GLU:HG3	1:D:685:GLU:N	2.19	0.57
1:C:230:THR:HG21	1:C:248:ILE:HA	1.87	0.57
1:C:319:ILE:HG23	1:C:677:PRO:HB3	1.86	0.56
1:D:489:LYS:HG3	1:D:491:PHE:HE1	1.70	0.56
1:A:346:PHE:C	1:A:347:ILE:HD12	2.25	0.56
1:F:642:SER:HB2	1:F:647:THR:HB	1.87	0.56
1:D:241:ARG:NH1	1:D:263:ASP:OD1	2.37	0.56
1:C:350:VAL:HG21	1:C:669:ARG:NH1	2.19	0.56
1:E:351:SER:OG	1:E:353:THR:HG22	2.05	0.56
1:D:694:TRP:HA	1:D:738:MET:HE1	1.87	0.56
1:F:216:GLU:OE1	1:F:219:SER:HA	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:807:ILE:HG12	1:E:837:LEU:CD2	2.35	0.56
1:E:232:VAL:HG13	1:E:244:PHE:CD1	2.41	0.56
1:D:360:GLU:HB2	1:D:364:ILE:HD11	1.86	0.56
1:F:202:TRP:CH2	1:F:745:SER:HB3	2.40	0.56
1:F:308:ILE:HG22	1:F:311:LEU:HD11	1.87	0.56
1:A:104:ASN:ND2	1:A:104:ASN:H	1.98	0.56
1:B:489:LYS:HE2	1:B:491:PHE:HZ	1.71	0.56
1:D:205:TYR:HA	1:D:1024:ASN:HD21	1.70	0.56
1:B:811:ASP:OD1	1:E:676:ARG:NH1	2.39	0.56
1:F:562:GLU:O	1:F:563:ALA:HB3	2.06	0.56
1:A:605:GLU:CG	1:B:524:PRO:HD3	2.36	0.56
1:B:153:MET:HG3	1:B:859:ARG:CZ	2.35	0.56
1:F:312:GLU:HG2	1:F:314:PRO:HD3	1.87	0.56
1:F:965:SER:HA	1:F:990:GLY:O	2.06	0.56
1:D:999:ARG:HG2	1:D:1005:VAL:HG22	1.86	0.56
1:F:353:THR:HG23	1:F:354:TYR:CD1	2.40	0.56
1:D:284:ARG:HD3	2:D:5393:HOH:O	2.05	0.56
1:A:423:ASN:HD22	1:A:423:ASN:C	2.09	0.56
1:A:429:MET:HE3	1:A:438:PRO:HB2	1.87	0.56
1:A:965:SER:HA	1:A:990:GLY:O	2.06	0.56
1:B:499:HIS:HD2	2:B:3176:HOH:O	1.89	0.56
1:E:872:HIS:HE1	1:E:902:GLU:OE1	1.89	0.56
1:E:568:LEU:HB3	1:E:571:MET:HE2	1.87	0.56
1:D:312:GLU:HG2	1:D:314:PRO:HD3	1.86	0.56
1:E:1016:ARG:O	1:E:1017:ASP:HB2	2.06	0.56
1:A:403:ASN:HD22	1:A:405:GLY:H	1.54	0.55
1:E:499:HIS:HE1	2:E:6239:HOH:O	1.89	0.55
1:C:53:ILE:HG23	1:C:286:LEU:HD21	1.87	0.55
1:D:353:THR:HG23	1:D:354:TYR:CD1	2.41	0.55
1:B:493:ALA:HA	1:B:571:MET:HG3	1.88	0.55
1:B:977:LEU:HB2	1:B:979:LEU:HD13	1.88	0.55
1:E:605:GLU:HG2	1:F:524:PRO:HD3	1.88	0.55
1:C:929:MET:HA	1:C:929:MET:CE	2.36	0.55
1:A:293:ILE:CG2	1:A:306:ILE:HD12	2.36	0.55
1:E:190:ARG:NH2	1:E:216:GLU:OE2	2.40	0.55
1:E:593:SER:O	1:E:624:VAL:HG22	2.05	0.55
1:B:167:ASN:HB2	1:B:170:ILE:HB	1.87	0.55
1:C:565:GLU:HG2	1:C:566:TYR:N	2.21	0.55
1:B:494:THR:HG21	1:B:500:ASP:OD1	2.06	0.55
1:A:681:SER:O	1:A:684:GLU:HG2	2.06	0.55
1:F:635:ASN:HB3	1:F:653:ASP:OD1	2.07	0.55
1:D:929:MET:HA	1:D:929:MET:CE	2.36	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:236:VAL:CG2	1:F:243:TYR:HB2	2.36	0.55
1:D:184:LEU:HB2	1:D:191:VAL:HB	1.88	0.55
1:F:431:VAL:HG22	1:F:438:PRO:HB3	1.88	0.55
1:E:731:LEU:HD22	1:E:735:ILE:HG13	1.88	0.55
1:E:480:ILE:H	1:E:494:THR:CG2	2.18	0.55
1:B:228:MET:HE3	1:B:232:VAL:CG2	2.36	0.55
1:B:423:ASN:HD22	1:B:423:ASN:C	2.09	0.55
1:F:565:GLU:HG2	1:F:566:TYR:N	2.21	0.55
1:C:522:PRO:HD3	1:D:893:ASN:OD1	2.05	0.55
1:E:494:THR:HG21	1:E:500:ASP:OD1	2.07	0.55
1:F:258:ASP:C	1:F:260:ASP:H	2.10	0.55
1:D:346:PHE:C	1:D:347:ILE:HD12	2.27	0.55
1:A:155:PRO:HD2	1:A:159:MET:HE3	1.88	0.55
1:E:286:LEU:CD1	1:E:295:ILE:HG12	2.36	0.55
1:B:189:ARG:HD2	1:B:216:GLU:O	2.07	0.55
1:F:913:ARG:HH21	1:F:1047:GLN:HE21	1.55	0.55
1:B:155:PRO:HG2	1:B:159:MET:CE	2.25	0.55
1:B:88:PRO:HG3	1:B:144:GLY:HA2	1.89	0.55
1:D:295:ILE:HG13	1:D:306:ILE:HD11	1.87	0.54
1:C:694:TRP:HA	1:C:738:MET:HE2	1.87	0.54
1:B:892:LEU:HD13	1:B:920:VAL:HG21	1.89	0.54
1:A:119:LYS:NZ	1:A:823:ARG:HH22	2.05	0.54
1:D:565:GLU:HG2	1:D:566:TYR:N	2.22	0.54
1:C:965:SER:HA	1:C:990:GLY:O	2.08	0.54
1:D:681:SER:HB3	1:D:684:GLU:HG2	1.88	0.54
1:F:618:VAL:HG21	1:F:631:GLU:HG3	1.89	0.54
1:F:43:LEU:O	1:F:44:LEU:HG	2.08	0.54
1:C:321:ILE:HB	1:C:324:LYS:HG3	1.89	0.54
1:C:61:LEU:HB2	1:C:75:VAL:HG13	1.88	0.54
1:F:872:HIS:CE1	1:F:902:GLU:OE1	2.61	0.54
1:F:489:LYS:HG3	1:F:491:PHE:HE1	1.71	0.54
1:C:241:ARG:HB2	1:C:243:TYR:CE1	2.42	0.54
1:C:774:ASP:HA	1:C:817:ALA:HB2	1.88	0.54
1:E:155:PRO:CD	1:E:159:MET:HE3	2.38	0.54
1:E:530:ASN:ND2	1:E:531:PHE:N	2.55	0.54
1:A:220:GLY:O	1:A:1038:HIS:HB3	2.08	0.54
1:D:591:LEU:HD11	1:D:662:LEU:HD21	1.89	0.54
1:E:167:ASN:HB2	1:E:170:ILE:HB	1.90	0.54
1:D:104:ASN:H	1:D:104:ASN:ND2	2.00	0.54
1:E:948:THR:H	1:F:922:GLN:NE2	2.03	0.54
1:D:480:ILE:H	1:D:494:THR:CG2	2.19	0.54
1:F:332:LEU:HD11	1:F:338:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:524:PRO:HD3	1:B:605:GLU:CG	2.36	0.54
1:A:736:VAL:HA	1:A:739:GLN:HE21	1.72	0.54
1:D:983:ILE:CG2	1:D:1033:ILE:HD12	2.28	0.54
1:E:156:PHE:CD1	1:E:159:MET:HE1	2.43	0.54
1:C:351:SER:OG	1:C:353:THR:HG22	2.07	0.54
1:B:676:ARG:NH1	1:E:811:ASP:OD1	2.41	0.54
1:C:589:ILE:HG21	1:C:641:LEU:HD11	1.89	0.54
1:A:706:VAL:HG12	1:A:710:ILE:HD12	1.89	0.54
1:F:184:LEU:HD13	1:F:237:ILE:HG13	1.90	0.54
1:F:49:HIS:CD2	1:F:90:GLY:HA3	2.43	0.54
1:F:498:SER:OG	1:F:499:HIS:N	2.40	0.54
1:C:700:ASN:HD22	1:C:1008:GLN:NE2	2.06	0.54
1:B:546:PRO:CG	1:B:567:ASP:HB3	2.38	0.54
1:C:562:GLU:O	1:C:563:ALA:HB3	2.08	0.54
1:D:807:ILE:HG12	1:D:837:LEU:CD2	2.38	0.54
1:C:206:ARG:H	1:C:1024:ASN:ND2	2.06	0.54
1:D:64:HIS:HD2	1:D:71:THR:OG1	1.91	0.54
1:F:1036:ALA:O	1:F:1039:ASP:HB2	2.08	0.54
1:B:703:ASN:C	1:B:703:ASN:HD22	2.12	0.54
1:E:286:LEU:HD12	1:E:294:TYR:O	2.07	0.53
1:F:87:PHE:HB3	1:F:88:PRO:HD2	1.90	0.53
1:A:494:THR:HG21	1:A:500:ASP:OD1	2.08	0.53
1:B:393:ARG:HH22	1:F:557:ARG:NE	2.06	0.53
1:F:222:PHE:H	1:F:1038:HIS:HD2	1.53	0.53
1:B:355:VAL:HG12	1:B:676:ARG:HH21	1.74	0.53
1:B:218:ASN:HB3	1:B:221:ALA:HB3	1.90	0.53
1:A:363:ARG:HG3	1:A:688:GLN:NE2	2.23	0.53
1:F:253:GLN:NE2	1:F:268:THR:OG1	2.39	0.53
1:B:681:SER:CB	1:B:684:GLU:HG2	2.37	0.53
1:C:522:PRO:HG2	1:D:889:MET:SD	2.47	0.53
1:A:913:ARG:HH21	1:A:1047:GLN:HE21	1.55	0.53
1:B:789:GLU:OE2	2:B:3230:HOH:O	2.19	0.53
1:E:241:ARG:NH1	1:E:263:ASP:OD1	2.41	0.53
1:E:475:TYR:OH	1:F:949:ASN:ND2	2.37	0.53
1:A:703:ASN:C	1:A:703:ASN:HD22	2.11	0.53
1:E:220:GLY:O	1:E:1038:HIS:HB3	2.09	0.53
1:B:61:LEU:HB3	1:B:75:VAL:HG13	1.91	0.53
1:A:319:ILE:CG2	1:A:677:PRO:HB3	2.39	0.53
1:C:1036:ALA:O	1:C:1039:ASP:HB2	2.09	0.53
1:F:206:ARG:N	1:F:1024:ASN:HD21	2.04	0.53
1:C:190:ARG:NH2	1:C:222:PHE:CZ	2.75	0.53
1:A:676:ARG:NH1	1:D:811:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:568:LEU:HB3	1:E:571:MET:CE	2.39	0.53
1:F:190:ARG:NH2	1:F:222:PHE:HZ	2.07	0.53
1:A:156:PHE:HB2	1:A:159:MET:HE2	1.91	0.53
1:C:524:PRO:HD3	1:D:605:GLU:CG	2.39	0.53
1:B:546:PRO:HG2	1:B:567:ASP:HB3	1.91	0.53
1:C:82:ASN:HD21	1:C:96:ARG:HD3	1.71	0.53
1:F:64:HIS:HD2	1:F:71:THR:OG1	1.91	0.53
1:A:562:GLU:O	1:A:563:ALA:HB3	2.09	0.53
1:F:253:GLN:HB2	1:F:255:TYR:HE1	1.74	0.53
1:C:46:PRO:HB2	1:C:286:LEU:HD21	1.90	0.53
1:F:618:VAL:CG2	1:F:631:GLU:HG3	2.39	0.53
1:A:167:ASN:HB2	1:A:170:ILE:HB	1.90	0.53
1:D:418:PHE:HA	1:D:433:LEU:HG	1.89	0.53
1:C:722:VAL:N	1:C:723:PRO:HD2	2.24	0.53
1:F:977:LEU:HB2	1:F:979:LEU:CD1	2.39	0.53
1:D:61:LEU:HB3	1:D:75:VAL:HG13	1.90	0.53
1:C:241:ARG:NH1	1:C:263:ASP:HB3	2.24	0.53
1:A:82:ASN:HD21	1:A:96:ARG:HH21	1.56	0.53
1:D:319:ILE:HG23	1:D:677:PRO:HB3	1.91	0.53
1:C:393:ARG:HH22	1:E:557:ARG:NE	2.07	0.53
1:F:700:ASN:HD22	1:F:1008:GLN:NE2	2.07	0.53
1:F:134:PHE:O	1:F:135:THR:HB	2.09	0.53
1:A:88:PRO:HG3	1:A:144:GLY:HA2	1.91	0.53
1:B:982:LEU:C	1:B:983:ILE:HD12	2.29	0.52
1:E:295:ILE:HG13	1:E:306:ILE:HD11	1.90	0.52
1:F:735:ILE:O	1:F:738:MET:HG3	2.09	0.52
1:C:404:LEU:HD22	1:C:429:MET:CE	2.39	0.52
1:A:61:LEU:CB	1:A:75:VAL:HG13	2.39	0.52
1:A:423:ASN:ND2	1:A:425:ARG:HB2	2.24	0.52
1:F:249:ASP:HB2	2:F:7014:HOH:O	2.09	0.52
1:B:337:ILE:HG22	1:B:338:ALA:N	2.24	0.52
1:B:706:VAL:HG12	1:B:710:ILE:HD12	1.91	0.52
1:C:53:ILE:HD11	1:C:295:ILE:HD11	1.92	0.52
1:A:393:ARG:NH1	1:C:557:ARG:HD2	2.24	0.52
1:F:1052:ILE:O	1:F:1056:ILE:HG13	2.10	0.52
1:D:333:ASP:CG	1:D:369:ARG:HE	2.12	0.52
1:D:913:ARG:HH21	1:D:1047:GLN:NE2	2.07	0.52
1:D:179:PRO:HG2	2:D:5045:HOH:O	2.09	0.52
1:E:524:PRO:HD3	1:F:605:GLU:CG	2.39	0.52
1:C:716:GLU:HG2	1:C:720:ASN:ND2	2.24	0.52
1:E:403:ASN:HD22	1:E:404:LEU:N	2.06	0.52
1:B:319:ILE:CG2	1:B:677:PRO:HB3	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:642:SER:HB2	1:E:647:THR:HB	1.91	0.52
1:F:729:TYR:O	1:F:732:SER:HB3	2.09	0.52
1:B:155:PRO:HD2	1:B:159:MET:HE3	1.90	0.52
1:D:155:PRO:CG	1:D:159:MET:HE1	2.23	0.52
1:C:249:ASP:HB2	2:C:4014:HOH:O	2.08	0.52
1:C:308:ILE:HG22	1:C:311:LEU:HD11	1.91	0.52
1:C:676:ARG:HD2	2:C:4370:HOH:O	2.08	0.52
1:F:123:TYR:OH	1:F:823:ARG:HD3	2.10	0.52
1:F:123:TYR:HB3	1:F:826:SER:OG	2.09	0.52
1:C:333:ASP:CG	1:C:369:ARG:HE	2.13	0.52
1:B:815:VAL:HA	1:B:819:SER:HB3	1.91	0.52
1:F:593:SER:O	1:F:624:VAL:HG22	2.10	0.52
1:E:781:ALA:HB2	1:E:802:PRO:HG2	1.91	0.52
1:A:982:LEU:C	1:A:983:ILE:HD12	2.30	0.52
1:A:190:ARG:NH2	1:A:222:PHE:HZ	2.07	0.52
1:D:557:ARG:HD2	1:F:393:ARG:HH12	1.75	0.52
1:B:467:LEU:C	1:B:467:LEU:HD12	2.29	0.52
1:B:156:PHE:HB2	1:B:159:MET:HE2	1.92	0.52
1:A:580:VAL:HG22	1:A:622:TYR:CD2	2.44	0.52
1:E:216:GLU:OE1	1:E:219:SER:HA	2.10	0.52
1:B:913:ARG:HH21	1:B:1047:GLN:NE2	2.08	0.52
1:C:807:ILE:HG12	1:C:837:LEU:CD2	2.40	0.52
1:C:184:LEU:HD13	1:C:237:ILE:HG13	1.90	0.52
1:C:52:ARG:HH21	1:C:52:ARG:HG3	1.75	0.52
1:C:350:VAL:CG2	1:C:669:ARG:HH11	2.23	0.52
1:A:781:ALA:HB2	1:A:802:PRO:HG2	1.90	0.52
1:A:206:ARG:N	1:A:1024:ASN:HD21	2.07	0.52
1:B:190:ARG:NH2	1:B:222:PHE:CZ	2.77	0.52
1:A:363:ARG:HD2	1:A:365:ARG:NH2	2.25	0.52
1:D:885:PRO:O	1:D:915:ASN:HA	2.09	0.52
1:B:387:LEU:HD13	1:B:388:GLY:N	2.24	0.52
1:D:156:PHE:HD1	1:D:159:MET:CE	2.23	0.51
1:C:684:GLU:HG3	1:C:685:GLU:N	2.24	0.51
1:E:684:GLU:HG3	1:E:685:GLU:N	2.24	0.51
1:F:222:PHE:H	1:F:1038:HIS:CD2	2.28	0.51
1:B:314:PRO:HD2	1:B:726:LYS:HG2	1.92	0.51
1:F:651:ARG:NH2	1:F:655:GLY:O	2.42	0.51
1:A:475:TYR:OH	1:B:949:ASN:ND2	2.43	0.51
1:E:156:PHE:HD1	1:E:159:MET:HE1	1.76	0.51
1:E:578:ILE:CD1	1:E:595:ILE:HD12	2.41	0.51
1:A:681:SER:CB	1:A:684:GLU:HG2	2.39	0.51
1:D:202:TRP:CH2	1:D:745:SER:HB3	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:562:GLU:O	1:D:563:ALA:HB3	2.10	0.51
1:D:1016:ARG:O	1:D:1017:ASP:HB2	2.10	0.51
1:B:965:SER:HA	1:B:990:GLY:O	2.10	0.51
1:F:1055:LEU:O	1:F:1059:LEU:HD13	2.10	0.51
1:C:776:TYR:CD1	1:C:816:GLY:HA2	2.45	0.51
1:F:241:ARG:NH1	1:F:263:ASP:OD1	2.44	0.51
1:F:430:THR:HG23	1:F:441:ILE:HD11	1.92	0.51
1:E:889:MET:SD	1:F:522:PRO:HG2	2.50	0.51
1:E:155:PRO:HG2	1:E:159:MET:CE	2.32	0.51
1:E:222:PHE:H	1:E:1038:HIS:CD2	2.28	0.51
1:B:222:PHE:H	1:B:1038:HIS:CD2	2.28	0.51
1:C:489:LYS:HG3	1:C:491:PHE:CE1	2.45	0.51
1:C:703:ASN:HD22	1:C:703:ASN:C	2.13	0.51
1:C:893:ASN:OD1	1:D:522:PRO:HD3	2.11	0.51
1:D:130:GLY:HA3	2:D:5163:HOH:O	2.10	0.51
1:E:522:PRO:HG2	1:F:889:MET:SD	2.50	0.51
1:C:242:ILE:O	1:C:256:SER:HA	2.10	0.51
1:B:393:ARG:HH12	1:F:557:ARG:CD	2.23	0.51
1:B:589:ILE:HD13	1:B:641:LEU:CD1	2.41	0.51
1:F:589:ILE:HG21	1:F:641:LEU:HD11	1.91	0.51
1:C:802:PRO:O	1:C:805:TYR:HB2	2.11	0.51
1:C:494:THR:HG21	1:C:500:ASP:OD1	2.11	0.51
1:F:238:VAL:HG11	1:F:298:PRO:HG2	1.93	0.51
1:B:205:TYR:HA	1:B:1024:ASN:HD21	1.76	0.51
1:C:736:VAL:HA	1:C:739:GLN:HE21	1.76	0.51
1:D:123:TYR:HB3	1:D:826:SER:OG	2.11	0.51
1:B:315:GLU:OE2	1:E:119:LYS:HD2	2.11	0.51
1:C:278:LEU:HD23	1:C:287:PHE:HB3	1.92	0.51
1:A:1031:VAL:HG12	1:A:1033:ILE:CD1	2.40	0.51
1:F:205:TYR:HA	1:F:1024:ASN:HD21	1.76	0.51
1:E:530:ASN:HD22	1:E:531:PHE:H	1.55	0.51
1:D:593:SER:O	1:D:624:VAL:HG22	2.11	0.51
1:E:156:PHE:HD1	1:E:159:MET:CE	2.24	0.50
1:B:446:GLU:OE1	1:B:468:LYS:HE2	2.11	0.50
1:C:350:VAL:HG23	1:C:351:SER:N	2.26	0.50
1:E:700:ASN:HD22	1:E:1008:GLN:NE2	2.09	0.50
1:F:245:ILE:HD11	1:F:278:LEU:HG	1.92	0.50
1:F:156:PHE:H	1:F:159:MET:CE	2.24	0.50
1:B:373:THR:HG21	1:B:393:ARG:HD2	1.92	0.50
1:A:134:PHE:O	1:A:135:THR:HB	2.12	0.50
1:A:43:LEU:HD13	1:A:308:ILE:HD12	1.92	0.50
1:C:153:MET:HG3	1:C:859:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:703:ASN:HD22	1:E:703:ASN:C	2.13	0.50
1:F:53:ILE:HG23	1:F:286:LEU:CD2	2.39	0.50
1:D:676:ARG:HD2	2:D:5370:HOH:O	2.11	0.50
1:F:493:ALA:HA	1:F:571:MET:HG3	1.92	0.50
1:E:46:PRO:HB2	1:E:286:LEU:CD2	2.41	0.50
1:E:578:ILE:HG12	1:E:580:VAL:HG23	1.94	0.50
1:C:709:GLU:OE2	1:C:713:ARG:HD3	2.11	0.50
1:D:236:VAL:HG23	1:D:243:TYR:HB2	1.93	0.50
1:A:156:PHE:CD1	1:A:159:MET:HE1	2.47	0.50
1:F:552:THR:HG21	1:F:578:ILE:HD12	1.94	0.50
1:B:363:ARG:HG3	1:B:688:GLN:HE22	1.76	0.50
1:D:190:ARG:HH21	1:D:190:ARG:CG	2.24	0.50
1:B:393:ARG:HH12	1:F:557:ARG:NH2	2.10	0.50
1:A:48:ILE:HB	1:A:286:LEU:HD22	1.94	0.50
1:B:286:LEU:HD11	1:B:293:ILE:CG2	2.42	0.50
1:C:256:SER:OG	1:C:267:HIS:CE1	2.65	0.50
1:C:317:ARG:HD3	1:F:823:ARG:HD2	1.93	0.50
1:E:913:ARG:HH21	1:E:1047:GLN:NE2	2.09	0.50
1:C:206:ARG:H	1:C:1024:ASN:HD21	1.59	0.50
1:C:716:GLU:HG2	1:C:720:ASN:HD21	1.77	0.50
1:C:332:LEU:HD11	1:C:338:ALA:HB2	1.94	0.50
1:F:46:PRO:HB2	1:F:286:LEU:HD21	1.92	0.50
1:E:977:LEU:HB2	1:E:979:LEU:CD1	2.40	0.50
1:B:872:HIS:CE1	1:B:902:GLU:OE1	2.65	0.50
1:E:694:TRP:HA	1:E:738:MET:HE2	1.93	0.50
1:E:618:VAL:HG21	1:E:631:GLU:HG3	1.94	0.50
1:D:557:ARG:NE	1:F:393:ARG:HH22	2.10	0.50
1:A:317:ARG:HD3	1:D:823:ARG:HD2	1.92	0.50
1:F:452:PHE:HB3	1:F:463:TYR:HB3	1.94	0.50
1:C:815:VAL:HA	1:C:819:SER:HB3	1.92	0.50
1:E:286:LEU:HD13	1:E:295:ILE:HG12	1.94	0.49
1:B:681:SER:O	1:B:684:GLU:HG2	2.12	0.49
1:B:403:ASN:HD22	1:B:403:ASN:C	2.16	0.49
1:F:616:LYS:HE2	1:F:653:ASP:CB	2.42	0.49
1:E:618:VAL:CG2	1:E:631:GLU:HG3	2.41	0.49
1:F:333:ASP:CG	1:F:369:ARG:HE	2.14	0.49
1:A:992:VAL:HG11	1:A:1009:PRO:HB2	1.93	0.49
1:E:965:SER:HA	1:E:990:GLY:O	2.12	0.49
1:C:731:LEU:HD22	1:C:735:ILE:HG13	1.95	0.49
1:C:732:SER:O	1:C:736:VAL:HG23	2.12	0.49
1:E:123:TYR:HB3	1:E:826:SER:OG	2.10	0.49
1:D:350:VAL:HG21	1:D:669:ARG:HH11	1.76	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:228:MET:HE1	1:C:244:PHE:CE1	2.47	0.49
1:F:177:LEU:HD13	1:F:192:ILE:HD11	1.94	0.49
1:F:639:LEU:HD23	1:F:639:LEU:C	2.33	0.49
1:A:498:SER:OG	1:A:499:HIS:N	2.44	0.49
1:C:988:TRP:CZ3	1:C:990:GLY:HA3	2.47	0.49
1:F:346:PHE:C	1:F:347:ILE:HD12	2.32	0.49
1:A:236:VAL:HG23	1:A:243:TYR:HB2	1.93	0.49
1:C:218:ASN:O	1:C:221:ALA:N	2.45	0.49
1:E:300:THR:O	1:E:301:GLU:HB3	2.12	0.49
1:E:46:PRO:HB2	1:E:286:LEU:HD23	1.94	0.49
1:A:605:GLU:HG2	1:B:524:PRO:HD3	1.93	0.49
1:E:256:SER:OG	1:E:267:HIS:HE1	1.95	0.49
1:C:363:ARG:NH2	1:C:365:ARG:HH22	2.11	0.49
1:C:155:PRO:HB3	1:C:860:TYR:HA	1.94	0.49
1:A:626:THR:O	1:A:627:ARG:HB2	2.12	0.49
1:A:205:TYR:CE1	1:A:207:GLY:HA3	2.48	0.49
1:E:736:VAL:HA	1:E:739:GLN:HE21	1.77	0.49
1:B:134:PHE:O	1:B:135:THR:HB	2.12	0.49
1:C:156:PHE:HD1	1:C:159:MET:CE	2.26	0.49
1:A:155:PRO:CD	1:A:159:MET:HE3	2.43	0.49
1:B:104:ASN:N	1:B:104:ASN:HD22	1.93	0.49
1:D:706:VAL:HG12	1:D:710:ILE:CD1	2.43	0.49
1:D:774:ASP:HA	1:D:817:ALA:HB2	1.94	0.49
1:B:286:LEU:HD11	1:B:293:ILE:HG22	1.94	0.49
1:F:716:GLU:HG2	1:F:720:ASN:ND2	2.27	0.49
1:C:641:LEU:HD22	1:C:645:ARG:HA	1.94	0.49
1:E:524:PRO:HD3	1:F:605:GLU:HG2	1.94	0.49
1:C:218:ASN:O	1:C:219:SER:C	2.50	0.49
1:E:346:PHE:C	1:E:347:ILE:HD12	2.33	0.49
1:D:206:ARG:N	1:D:1024:ASN:HD21	2.09	0.49
1:C:884:ILE:HD13	1:C:924:ILE:HD13	1.94	0.49
1:D:618:VAL:CG2	1:D:631:GLU:HG3	2.42	0.49
1:D:268:THR:CG2	1:D:303:ILE:HD11	2.40	0.49
1:B:350:VAL:CG2	1:B:669:ARG:HH11	2.23	0.49
1:F:189:ARG:HD2	1:F:216:GLU:O	2.13	0.49
1:F:994:ILE:HG22	1:F:1008:GLN:O	2.13	0.49
1:C:141:ASP:HB2	1:C:142:PRO:HD2	1.93	0.49
1:E:589:ILE:HG21	1:E:641:LEU:HD11	1.95	0.49
1:D:167:ASN:HB2	1:D:170:ILE:HB	1.94	0.49
1:B:156:PHE:HD1	1:B:159:MET:CE	2.26	0.49
1:D:1033:ILE:HD11	1:D:1050:TYR:CD2	2.48	0.49
1:A:589:ILE:HD13	1:A:641:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:256:SER:OG	1:F:267:HIS:CE1	2.65	0.48
1:E:400:PHE:CD2	1:E:436:GLY:HA3	2.48	0.48
1:B:580:VAL:HG22	1:B:622:TYR:CD2	2.48	0.48
1:A:286:LEU:HD11	1:A:293:ILE:CG2	2.42	0.48
1:E:965:SER:N	1:E:968:ASP:OD2	2.43	0.48
1:D:367:VAL:CG1	1:D:375:VAL:HG21	2.43	0.48
1:E:499:HIS:HD2	2:E:6176:HOH:O	1.95	0.48
1:C:337:ILE:HG22	1:C:338:ALA:N	2.28	0.48
1:F:890:MET:O	1:F:894:GLU:HG2	2.12	0.48
1:A:882:ILE:HD11	1:A:899:PHE:HA	1.94	0.48
1:F:722:VAL:N	1:F:723:PRO:HD2	2.29	0.48
1:E:577:PRO:HG3	1:F:789:GLU:HG3	1.95	0.48
1:C:639:LEU:HD23	1:C:639:LEU:C	2.33	0.48
1:D:468:LYS:CD	1:D:473:ASP:HB2	2.38	0.48
1:A:578:ILE:HG12	1:A:580:VAL:HG23	1.94	0.48
1:A:676:ARG:HD2	2:A:2370:HOH:O	2.13	0.48
1:F:706:VAL:HG12	1:F:710:ILE:CD1	2.42	0.48
1:B:709:GLU:OE2	1:B:713:ARG:HD3	2.14	0.48
1:F:213:ILE:HB	1:F:226:VAL:HB	1.95	0.48
1:A:155:PRO:CG	1:A:159:MET:HE1	2.31	0.48
1:B:53:ILE:CD1	1:B:306:ILE:HD13	2.42	0.48
1:F:897:ARG:HG2	1:F:898:LEU:HD12	1.96	0.48
1:A:977:LEU:HB2	1:A:979:LEU:HD13	1.96	0.48
1:C:977:LEU:HB2	1:C:979:LEU:HD13	1.95	0.48
1:A:1016:ARG:O	1:A:1017:ASP:HB2	2.13	0.48
1:B:524:PRO:HB3	1:B:531:PHE:CE2	2.49	0.48
1:C:929:MET:HA	1:C:929:MET:HE3	1.95	0.48
1:C:205:TYR:HA	1:C:1024:ASN:HD21	1.77	0.48
1:C:119:LYS:NZ	1:C:823:ARG:HH22	2.12	0.48
1:A:499:HIS:HD2	2:A:2176:HOH:O	1.95	0.48
1:F:309:GLY:O	1:F:311:LEU:HD13	2.14	0.48
1:E:167:ASN:O	1:E:170:ILE:HG12	2.13	0.48
1:E:802:PRO:O	1:E:805:TYR:HB2	2.13	0.48
1:F:284:ARG:HD3	2:F:7393:HOH:O	2.13	0.48
1:B:639:LEU:HD23	1:B:639:LEU:C	2.34	0.48
1:C:735:ILE:O	1:C:739:GLN:HG3	2.13	0.48
1:C:241:ARG:HB2	1:C:243:TYR:HE1	1.79	0.48
1:A:791:GLU:CD	1:A:861:ARG:HE	2.16	0.48
1:D:430:THR:HG23	1:D:441:ILE:HD11	1.96	0.48
1:C:78:LEU:HB2	2:C:4254:HOH:O	2.13	0.48
1:B:505:PHE:CE2	1:B:512:LEU:HD13	2.48	0.48
1:C:238:VAL:HG11	1:C:298:PRO:HG2	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:999:ARG:HG2	1:E:1005:VAL:HG22	1.95	0.48
1:A:218:ASN:HB3	1:A:221:ALA:HB3	1.95	0.48
1:E:53:ILE:CD1	1:E:306:ILE:HD13	2.44	0.48
1:E:983:ILE:HG23	1:E:1033:ILE:CD1	2.38	0.48
1:A:556:PRO:HD3	1:E:354:TYR:CD1	2.49	0.48
1:B:425:ARG:O	1:B:426:PHE:HB2	2.14	0.48
1:B:230:THR:HG21	1:B:248:ILE:HA	1.95	0.48
1:C:605:GLU:HG2	1:D:524:PRO:HD3	1.95	0.48
1:B:562:GLU:O	1:B:563:ALA:HB3	2.14	0.48
1:F:403:ASN:HD22	1:F:404:LEU:N	2.12	0.47
1:C:681:SER:CB	1:C:684:GLU:HG2	2.42	0.47
1:D:913:ARG:NH2	1:D:1047:GLN:HE21	2.10	0.47
1:B:498:SER:HB2	2:B:2192:HOH:O	2.13	0.47
1:C:48:ILE:HG12	1:C:49:HIS:N	2.28	0.47
1:D:425:ARG:O	1:D:426:PHE:HB2	2.13	0.47
1:C:297:ASN:O	1:C:301:GLU:N	2.44	0.47
1:E:155:PRO:CG	1:E:159:MET:HE1	2.35	0.47
1:E:578:ILE:HD12	1:E:595:ILE:HD12	1.96	0.47
1:A:53:ILE:CD1	1:A:306:ILE:HD13	2.45	0.47
1:E:194:ARG:O	1:E:211:GLY:HA2	2.14	0.47
1:D:228:MET:HE1	1:D:232:VAL:HG22	1.96	0.47
1:B:360:GLU:HB2	1:B:364:ILE:HD11	1.97	0.47
1:F:681:SER:HB3	1:F:684:GLU:HG2	1.97	0.47
1:A:314:PRO:HD2	1:A:726:LYS:HG2	1.94	0.47
1:A:270:PHE:CD2	1:A:289:LYS:HE2	2.50	0.47
1:A:337:ILE:HD11	1:A:350:VAL:HG12	1.95	0.47
1:B:355:VAL:CG1	1:B:676:ARG:HH21	2.26	0.47
1:F:218:ASN:O	1:F:221:ALA:N	2.48	0.47
1:C:64:HIS:HD2	1:C:71:THR:OG1	1.97	0.47
1:C:956:ILE:HG22	1:C:1055:LEU:HD11	1.96	0.47
1:E:565:GLU:HG2	1:E:566:TYR:N	2.28	0.47
1:A:63:GLU:OE1	1:A:72:ARG:NH1	2.48	0.47
1:C:253:GLN:HB2	1:C:255:TYR:CE1	2.49	0.47
1:F:319:ILE:CG2	1:F:677:PRO:HB3	2.44	0.47
1:A:393:ARG:HH12	1:C:557:ARG:CD	2.25	0.47
1:C:236:VAL:CG2	1:C:243:TYR:HB2	2.44	0.47
1:C:231:HIS:HD2	2:C:4052:HOH:O	1.97	0.47
1:D:872:HIS:CE1	1:D:902:GLU:OE1	2.66	0.47
1:C:110:PHE:CD2	1:C:121:ILE:HG13	2.50	0.47
1:A:349:ASP:OD2	1:A:353:THR:HG22	2.15	0.47
1:C:425:ARG:O	1:C:426:PHE:HB2	2.15	0.47
1:E:493:ALA:HA	1:E:571:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:350:VAL:CG2	1:D:669:ARG:HH11	2.27	0.47
1:B:43:LEU:HD13	1:B:308:ILE:HD12	1.96	0.47
1:B:1016:ARG:O	1:B:1017:ASP:HB2	2.13	0.47
1:C:949:ASN:ND2	1:D:475:TYR:OH	2.40	0.47
1:E:701:TYR:O	1:F:939:ARG:HD3	2.14	0.47
1:C:537:SER:HB3	1:C:583:GLY:O	2.15	0.47
1:A:155:PRO:HG2	1:A:159:MET:CE	2.30	0.47
1:C:982:LEU:C	1:C:983:ILE:HD12	2.35	0.47
1:E:293:ILE:CG2	1:E:306:ILE:HD12	2.45	0.47
1:B:53:ILE:HD11	1:B:295:ILE:HD11	1.95	0.47
1:E:228:MET:HE1	1:E:244:PHE:CE1	2.49	0.47
1:A:309:GLY:O	1:A:311:LEU:HD13	2.14	0.47
1:F:442:GLU:OE2	1:F:481:HIS:HD2	1.98	0.47
1:C:218:ASN:HB3	1:C:221:ALA:HB3	1.97	0.47
1:B:736:VAL:HA	1:B:739:GLN:HE21	1.79	0.47
1:A:327:GLU:O	1:A:328:ASP:C	2.53	0.47
1:E:110:PHE:CD2	1:E:121:ILE:HG13	2.50	0.47
1:F:791:GLU:CD	1:F:861:ARG:HE	2.18	0.47
1:A:401:GLU:N	1:A:401:GLU:OE2	2.43	0.47
1:C:286:LEU:HD11	1:C:293:ILE:HG22	1.96	0.47
1:B:557:ARG:NH2	1:D:393:ARG:HH12	2.12	0.47
1:E:319:ILE:HG23	1:E:677:PRO:HB3	1.96	0.47
1:F:537:SER:HB3	1:F:583:GLY:O	2.15	0.47
1:E:425:ARG:O	1:E:426:PHE:HB2	2.15	0.47
1:D:293:ILE:HG22	1:D:306:ILE:HD12	1.97	0.47
1:B:61:LEU:HB3	1:B:75:VAL:CG1	2.45	0.47
1:A:43:LEU:CD1	1:A:308:ILE:HD12	2.45	0.47
1:D:651:ARG:NH2	1:D:655:GLY:O	2.41	0.47
1:B:367:VAL:CG1	1:B:375:VAL:HG21	2.44	0.47
1:A:156:PHE:HD1	1:A:159:MET:CE	2.27	0.47
1:C:578:ILE:CG1	1:C:580:VAL:HG23	2.43	0.47
1:D:74:ILE:HG13	1:D:75:VAL:HG12	1.96	0.47
1:E:562:GLU:O	1:E:563:ALA:HB3	2.15	0.47
1:C:939:ARG:HD3	1:D:701:TYR:O	2.14	0.47
1:A:623:ASP:O	1:A:627:ARG:N	2.47	0.46
1:A:205:TYR:CZ	1:A:207:GLY:HA3	2.50	0.46
1:A:190:ARG:HH21	1:A:190:ARG:CG	2.28	0.46
1:C:676:ARG:NH1	1:F:811:ASP:OD1	2.48	0.46
1:C:758:ASP:HB3	2:C:4314:HOH:O	2.15	0.46
1:C:328:ASP:O	1:C:339:PHE:HA	2.14	0.46
1:C:1016:ARG:O	1:C:1017:ASP:HB2	2.15	0.46
1:C:493:ALA:HA	1:C:571:MET:HG3	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:203:LYS:HG2	1:E:274:TYR:CZ	2.50	0.46
1:E:501:TYR:CD2	1:E:501:TYR:N	2.82	0.46
1:E:373:THR:HG21	1:E:393:ARG:HD2	1.96	0.46
1:E:591:LEU:CD1	1:E:662:LEU:HD21	2.43	0.46
1:C:46:PRO:CG	1:C:286:LEU:HG	2.45	0.46
1:A:337:ILE:HG22	1:A:338:ALA:N	2.31	0.46
1:F:820:ASN:O	1:F:824:VAL:HG23	2.14	0.46
1:C:430:THR:HG23	1:C:441:ILE:HD11	1.97	0.46
1:A:949:ASN:ND2	1:B:475:TYR:OH	2.47	0.46
1:E:268:THR:CG2	1:E:303:ILE:HD11	2.41	0.46
1:A:393:ARG:NH1	1:C:557:ARG:NH2	2.62	0.46
1:D:222:PHE:H	1:D:1038:HIS:CD2	2.34	0.46
1:F:642:SER:HB3	1:F:647:THR:H	1.80	0.46
1:F:781:ALA:HB2	1:F:802:PRO:HG2	1.97	0.46
1:E:195:ASN:O	1:E:231:HIS:HE1	1.98	0.46
1:C:860:TYR:OH	1:C:885:PRO:HD3	2.14	0.46
1:D:222:PHE:H	1:D:1038:HIS:HD2	1.64	0.46
1:B:220:GLY:O	1:B:1038:HIS:HB3	2.15	0.46
1:C:92:LYS:HD3	1:C:110:PHE:CD1	2.50	0.46
1:D:731:LEU:HD22	1:D:735:ILE:HG13	1.97	0.46
1:E:550:ASN:HB3	1:E:553:LYS:HG3	1.96	0.46
1:D:986:ARG:HD3	1:D:1028:ASP:OD2	2.16	0.46
1:B:393:ARG:HH12	1:F:557:ARG:NE	2.14	0.46
1:A:872:HIS:CE1	1:A:902:GLU:OE1	2.67	0.46
1:F:589:ILE:HB	1:F:596:LEU:HB2	1.96	0.46
1:F:463:TYR:CE1	1:F:481:HIS:HB2	2.51	0.46
1:E:423:ASN:HD22	1:E:423:ASN:C	2.18	0.46
1:A:511:ASN:ND2	1:A:543:PRO:HA	2.30	0.46
1:C:580:VAL:HG22	1:C:622:TYR:CD2	2.51	0.46
1:A:167:ASN:O	1:A:170:ILE:HG12	2.15	0.46
1:D:1014:TRP:HB2	1:D:1020:PHE:CE2	2.50	0.46
1:A:110:PHE:HE2	1:A:146:LEU:HD22	1.81	0.46
1:D:300:THR:O	1:D:301:GLU:HB3	2.16	0.46
1:F:511:ASN:HD22	1:F:543:PRO:HA	1.81	0.46
1:E:53:ILE:HD12	1:E:306:ILE:HD13	1.97	0.46
1:B:228:MET:HE1	1:B:244:PHE:CE1	2.51	0.46
1:C:641:LEU:HD23	1:C:642:SER:H	1.81	0.46
1:A:992:VAL:CG1	1:A:1009:PRO:HB2	2.46	0.46
1:A:228:MET:HE1	1:A:244:PHE:CE1	2.51	0.46
1:A:618:VAL:CG2	1:A:631:GLU:HG3	2.46	0.46
1:B:700:ASN:HD22	1:B:1008:GLN:NE2	2.12	0.46
1:C:596:LEU:N	1:C:596:LEU:CD2	2.78	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:929:MET:CE	1:E:929:MET:HA	2.46	0.46
1:B:591:LEU:CD1	1:B:662:LEU:HD21	2.46	0.46
1:B:641:LEU:HD23	1:B:642:SER:H	1.80	0.46
1:A:355:VAL:HG12	1:A:676:ARG:HH21	1.81	0.46
1:A:425:ARG:O	1:A:426:PHE:HB2	2.16	0.46
1:E:735:ILE:O	1:E:739:GLN:HG3	2.16	0.46
1:C:855:ASP:HA	2:C:4221:HOH:O	2.16	0.46
1:B:565:GLU:HG2	1:B:566:TYR:N	2.30	0.46
1:A:639:LEU:HD23	1:A:639:LEU:C	2.36	0.46
1:C:892:LEU:HD13	1:C:920:VAL:HG21	1.96	0.46
1:F:423:ASN:ND2	1:F:425:ARG:HB2	2.32	0.46
1:F:190:ARG:NH2	1:F:222:PHE:CZ	2.84	0.46
1:E:123:TYR:OH	1:E:823:ARG:HD3	2.15	0.46
1:F:511:ASN:ND2	1:F:543:PRO:HA	2.30	0.46
1:E:992:VAL:HG11	1:E:1009:PRO:HB2	1.98	0.46
1:E:997:LYS:NZ	2:E:7168:HOH:O	2.47	0.46
1:B:156:PHE:CD1	1:B:159:MET:HE1	2.52	0.45
1:A:403:ASN:C	1:A:403:ASN:HD22	2.18	0.45
1:D:190:ARG:CB	1:D:190:ARG:HH21	2.28	0.45
1:E:218:ASN:O	1:E:220:GLY:N	2.49	0.45
1:E:368:ARG:O	1:E:375:VAL:HG23	2.16	0.45
1:F:369:ARG:HH21	1:F:369:ARG:HG3	1.79	0.45
1:E:562:GLU:HB3	1:E:563:ALA:H	1.60	0.45
1:D:387:LEU:HD13	1:D:388:GLY:N	2.31	0.45
1:A:807:ILE:HG12	1:A:837:LEU:CD2	2.46	0.45
1:B:442:GLU:OE2	1:B:481:HIS:HD2	1.97	0.45
1:E:706:VAL:HG12	1:E:710:ILE:CD1	2.46	0.45
1:A:1032:GLU:OE1	1:A:1034:GLU:OE2	2.34	0.45
1:F:959:THR:O	1:F:984:GLY:HA3	2.15	0.45
1:E:897:ARG:HG2	1:E:898:LEU:HD12	1.98	0.45
1:E:61:LEU:HD13	1:E:74:ILE:HD11	1.97	0.45
1:E:228:MET:HE1	1:E:232:VAL:HG22	1.98	0.45
1:A:418:PHE:HA	1:A:433:LEU:HG	1.98	0.45
1:B:369:ARG:HD2	1:B:371:GLY:H	1.80	0.45
1:B:579:ASN:ND2	1:B:627:ARG:NH1	2.64	0.45
1:E:418:PHE:HA	1:E:433:LEU:HG	1.98	0.45
1:B:195:ASN:O	1:B:231:HIS:HE1	1.99	0.45
1:D:528:VAL:HG12	1:D:529:LEU:N	2.31	0.45
1:B:578:ILE:CD1	1:B:595:ILE:HD12	2.46	0.45
1:C:681:SER:HB3	1:C:684:GLU:CG	2.45	0.45
1:E:589:ILE:HB	1:E:596:LEU:HB2	1.97	0.45
1:A:1055:LEU:O	1:A:1059:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:906:GLN:O	1:D:953:GLY:HA3	2.16	0.45
1:A:156:PHE:HD1	1:A:159:MET:HE1	1.81	0.45
1:F:580:VAL:HG22	1:F:622:TYR:CD2	2.52	0.45
1:D:373:THR:HG21	1:D:393:ARG:HD2	1.98	0.45
1:A:347:ILE:N	1:A:347:ILE:HD12	2.32	0.45
1:E:596:LEU:N	1:E:596:LEU:HD22	2.31	0.45
1:A:249:ASP:HB2	2:A:2014:HOH:O	2.16	0.45
1:D:402:GLU:HG3	1:D:438:PRO:HD3	1.98	0.45
1:A:369:ARG:HD2	1:A:371:GLY:H	1.81	0.45
1:A:57:CYS:HB3	1:A:62:TRP:CD1	2.51	0.45
1:E:790:GLY:HA2	2:E:6244:HOH:O	2.17	0.45
1:E:528:VAL:HG12	1:E:529:LEU:N	2.31	0.45
1:F:136:ASP:OD2	1:F:137:VAL:N	2.42	0.45
1:B:393:ARG:NH1	1:F:557:ARG:HD2	2.32	0.45
1:C:589:ILE:HD13	1:C:641:LEU:HD12	1.99	0.45
1:E:641:LEU:HD22	1:E:645:ARG:HA	1.98	0.45
1:D:232:VAL:HG13	1:D:244:PHE:CD1	2.52	0.45
1:C:886:ASP:O	1:C:891:GLY:HA3	2.17	0.45
1:D:44:LEU:HD22	1:D:733:ASN:ND2	2.32	0.45
1:D:690:TYR:CE2	1:D:719:ARG:HB2	2.52	0.45
1:F:1016:ARG:O	1:F:1017:ASP:HB2	2.16	0.45
1:B:53:ILE:HD13	1:B:306:ILE:HD13	1.98	0.45
1:C:781:ALA:HB2	1:C:802:PRO:HG2	1.98	0.45
1:E:619:LEU:HD13	1:E:639:LEU:CD1	2.47	0.45
1:E:1033:ILE:HD11	1:E:1050:TYR:CD2	2.51	0.45
1:B:63:GLU:OE1	1:B:72:ARG:NH1	2.50	0.45
1:B:977:LEU:HB2	1:B:979:LEU:CD1	2.47	0.45
1:E:893:ASN:OD1	1:F:522:PRO:HD3	2.16	0.45
1:D:537:SER:HB3	1:D:583:GLY:O	2.17	0.45
1:C:642:SER:HB2	1:C:647:THR:HB	1.99	0.45
1:E:467:LEU:C	1:E:467:LEU:HD12	2.37	0.45
1:F:860:TYR:CZ	1:F:864:VAL:HG21	2.52	0.45
1:A:393:ARG:HH12	1:C:557:ARG:CZ	2.30	0.45
1:D:235:PRO:HA	1:D:243:TYR:O	2.17	0.45
1:A:591:LEU:CD1	1:A:596:LEU:HD23	2.47	0.45
1:C:463:TYR:CE1	1:C:481:HIS:HB2	2.52	0.45
1:E:360:GLU:HB2	1:E:364:ILE:HD11	1.99	0.45
1:A:430:THR:HG23	1:A:441:ILE:HD11	1.99	0.45
1:F:141:ASP:HB2	1:F:142:PRO:HD2	1.98	0.45
1:E:885:PRO:O	1:E:915:ASN:HA	2.17	0.45
1:A:565:GLU:HG2	1:A:566:TYR:N	2.32	0.45
1:F:300:THR:HG22	1:F:300:THR:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:295:ILE:CG1	1:B:306:ILE:HD11	2.41	0.44
1:C:642:SER:HB3	1:C:647:THR:H	1.82	0.44
1:D:736:VAL:HA	1:D:739:GLN:HE21	1.82	0.44
1:B:309:GLY:O	1:B:311:LEU:HD13	2.18	0.44
1:A:195:ASN:O	1:A:231:HIS:HE1	2.00	0.44
1:F:912:VAL:O	1:F:915:ASN:HB2	2.17	0.44
1:A:929:MET:HA	1:A:929:MET:CE	2.47	0.44
1:A:403:ASN:HD22	1:A:404:LEU:N	2.16	0.44
1:F:731:LEU:HD22	1:F:735:ILE:CD1	2.47	0.44
1:B:441:ILE:HG23	1:B:483:TYR:CD1	2.52	0.44
1:C:279:ASN:HD22	1:C:279:ASN:HA	1.63	0.44
1:C:308:ILE:CG2	1:C:311:LEU:HD11	2.47	0.44
1:C:82:ASN:ND2	1:C:96:ARG:HH21	2.14	0.44
1:F:321:ILE:HB	1:F:324:LYS:HG3	1.99	0.44
1:F:47:ASP:OD1	1:F:85:ARG:HA	2.17	0.44
1:D:681:SER:HB3	1:D:684:GLU:CG	2.47	0.44
1:E:367:VAL:HG13	1:E:375:VAL:HG21	1.97	0.44
1:B:641:LEU:CD2	1:B:645:ARG:HA	2.48	0.44
1:A:228:MET:HE1	1:A:232:VAL:HG22	1.99	0.44
1:E:213:ILE:HB	1:E:226:VAL:HB	1.99	0.44
1:D:722:VAL:N	1:D:723:PRO:HD2	2.33	0.44
1:D:319:ILE:HA	1:D:678:LEU:O	2.18	0.44
1:B:988:TRP:CZ3	1:B:990:GLY:HA3	2.52	0.44
1:E:387:LEU:HD13	1:E:388:GLY:N	2.32	0.44
1:E:989:GLY:HA2	1:E:1026:GLY:HA2	2.00	0.44
1:B:1031:VAL:O	1:B:1033:ILE:HD12	2.17	0.44
1:A:404:LEU:HD22	1:A:429:MET:CE	2.42	0.44
1:F:738:MET:C	1:F:738:MET:SD	2.96	0.44
1:C:403:ASN:HD22	1:C:404:LEU:N	2.15	0.44
1:B:681:SER:HB3	1:B:684:GLU:CG	2.44	0.44
1:D:530:ASN:HD22	1:D:531:PHE:H	1.66	0.44
1:E:347:ILE:HD12	1:E:347:ILE:N	2.31	0.44
1:F:228:MET:HE1	1:F:244:PHE:CE1	2.53	0.44
1:C:203:LYS:O	1:C:743:ARG:HG2	2.17	0.44
1:C:130:GLY:HA3	2:C:4163:HOH:O	2.17	0.44
1:A:624:VAL:HG23	1:A:625:LYS:N	2.33	0.44
1:D:781:ALA:HB2	1:D:802:PRO:HG2	1.98	0.44
1:F:45:ASN:N	1:F:45:ASN:ND2	2.64	0.44
1:B:91:ARG:NH2	1:B:114:GLU:OE1	2.50	0.44
1:A:557:ARG:CZ	1:E:393:ARG:HH22	2.31	0.44
1:C:515:LEU:HD23	1:C:539:PRO:HA	1.99	0.44
1:F:350:VAL:CG2	1:F:669:ARG:NH1	2.80	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:253:GLN:NE2	1:E:268:THR:OG1	2.48	0.44
1:A:913:ARG:HH21	1:A:1047:GLN:NE2	2.16	0.44
1:E:452:PHE:HB3	1:E:463:TYR:HB3	2.00	0.44
1:B:327:GLU:O	1:B:328:ASP:O	2.35	0.44
1:C:289:LYS:HA	2:C:4095:HOH:O	2.17	0.44
1:B:890:MET:O	1:B:894:GLU:HG2	2.16	0.44
1:A:986:ARG:HD3	1:A:1028:ASP:OD2	2.16	0.44
1:B:501:TYR:CD2	1:B:501:TYR:N	2.85	0.44
1:C:651:ARG:NH2	1:C:655:GLY:O	2.46	0.44
1:F:578:ILE:CD1	1:F:595:ILE:HD12	2.47	0.44
1:F:253:GLN:HE21	1:F:253:GLN:HA	1.83	0.44
1:D:190:ARG:HH22	1:D:216:GLU:CD	2.21	0.44
1:D:218:ASN:O	1:D:220:GLY:N	2.50	0.44
1:A:82:ASN:HD21	1:A:96:ARG:HD3	1.82	0.44
1:E:694:TRP:HA	1:E:738:MET:HE1	2.00	0.44
1:D:618:VAL:HG21	1:D:631:GLU:HG3	1.98	0.44
1:F:131:ARG:NH2	2:F:7157:HOH:O	2.50	0.44
1:E:45:ASN:N	1:E:45:ASN:ND2	2.65	0.44
1:F:480:ILE:N	1:F:494:THR:HG22	2.20	0.44
1:E:104:ASN:N	1:E:104:ASN:ND2	2.62	0.44
1:C:579:ASN:ND2	1:C:627:ARG:NH1	2.66	0.44
1:A:622:TYR:OH	1:A:627:ARG:HG2	2.18	0.44
1:D:642:SER:HB3	1:D:647:THR:H	1.83	0.44
1:F:308:ILE:HG22	1:F:311:LEU:CD1	2.48	0.44
1:F:913:ARG:HH21	1:F:1047:GLN:NE2	2.15	0.44
1:C:363:ARG:HH21	1:C:365:ARG:HH22	1.64	0.44
1:B:735:ILE:O	1:B:739:GLN:HG3	2.18	0.44
1:A:618:VAL:HG21	1:A:631:GLU:HG3	1.99	0.44
1:C:247:ASP:HA	1:C:251:PHE:O	2.18	0.44
1:A:834:ARG:HG3	1:A:846:ASP:OD2	2.18	0.44
1:C:179:PRO:HG2	2:C:4045:HOH:O	2.16	0.44
1:F:501:TYR:CD2	1:F:501:TYR:N	2.86	0.44
1:A:253:GLN:HE22	1:A:270:PHE:N	2.03	0.44
1:A:429:MET:HE3	1:A:438:PRO:CB	2.48	0.44
1:A:53:ILE:HD13	1:A:306:ILE:CD1	2.48	0.44
1:A:350:VAL:CG2	1:A:669:ARG:HH11	2.27	0.44
1:E:218:ASN:O	1:E:219:SER:C	2.56	0.44
1:B:393:ARG:NH1	1:F:557:ARG:CZ	2.80	0.44
1:B:499:HIS:HE1	2:B:3239:HOH:O	2.00	0.44
1:C:142:PRO:HD3	1:C:185:PHE:CD2	2.53	0.44
1:A:218:ASN:O	1:A:219:SER:C	2.55	0.44
1:B:623:ASP:O	1:B:627:ARG:N	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:57:CYS:HB3	1:C:62:TRP:NE1	2.33	0.44
1:C:284:ARG:HD3	2:C:4393:HOH:O	2.16	0.44
1:E:514:TYR:CZ	1:E:540:PHE:HB2	2.53	0.44
1:E:61:LEU:HB2	1:E:75:VAL:HG13	2.00	0.43
1:B:390:TYR:CD1	1:B:397:ALA:HB2	2.53	0.43
1:C:218:ASN:O	1:C:220:GLY:N	2.51	0.43
1:B:994:ILE:HG22	1:B:1008:GLN:O	2.18	0.43
1:F:776:TYR:CD1	1:F:816:GLY:HA2	2.53	0.43
1:A:1031:VAL:CG1	1:A:1033:ILE:HD11	2.48	0.43
1:C:729:TYR:O	1:C:732:SER:HB3	2.19	0.43
1:B:556:PRO:HD3	1:D:354:TYR:CD1	2.53	0.43
1:B:170:ILE:HD13	1:B:820:ASN:HB2	2.00	0.43
1:D:347:ILE:N	1:D:347:ILE:HD12	2.33	0.43
1:D:525:ASP:HB3	1:D:528:VAL:O	2.18	0.43
1:E:639:LEU:HD23	1:E:639:LEU:C	2.39	0.43
1:C:1014:TRP:CD1	1:C:1019:GLY:HA2	2.53	0.43
1:E:363:ARG:HG3	1:E:688:GLN:NE2	2.33	0.43
1:A:123:TYR:HB3	1:A:826:SER:OG	2.17	0.43
1:E:89:ASP:CG	1:E:91:ARG:HG3	2.38	0.43
1:F:53:ILE:HD13	1:F:306:ILE:CD1	2.49	0.43
1:B:82:ASN:HD21	1:B:96:ARG:HD3	1.84	0.43
1:D:218:ASN:O	1:D:219:SER:C	2.57	0.43
1:E:189:ARG:HD2	1:E:216:GLU:O	2.18	0.43
1:C:965:SER:C	1:C:967:GLY:N	2.71	0.43
1:F:220:GLY:O	1:F:1038:HIS:HB3	2.19	0.43
1:F:141:ASP:HB2	1:F:142:PRO:CD	2.48	0.43
1:F:882:ILE:HD11	1:F:899:PHE:HA	2.00	0.43
1:D:791:GLU:CD	1:D:861:ARG:HE	2.21	0.43
1:D:639:LEU:HD23	1:D:639:LEU:C	2.38	0.43
1:A:53:ILE:HD13	1:A:306:ILE:HD13	2.01	0.43
1:C:286:LEU:HD11	1:C:293:ILE:CG2	2.49	0.43
1:A:190:ARG:NH2	1:A:222:PHE:CZ	2.87	0.43
1:E:190:ARG:CG	1:E:190:ARG:HH21	2.30	0.43
1:C:308:ILE:HG22	1:C:311:LEU:CD1	2.48	0.43
1:C:373:THR:HG21	1:C:393:ARG:HD2	2.00	0.43
1:A:401:GLU:H	1:A:401:GLU:CD	2.20	0.43
1:D:466:PRO:HB3	2:D:5183:HOH:O	2.17	0.43
1:D:195:ASN:O	1:D:231:HIS:HE1	2.01	0.43
1:D:43:LEU:HD13	1:D:308:ILE:HD12	2.01	0.43
1:A:638:ASP:HB3	1:A:651:ARG:HB3	2.00	0.43
1:F:337:ILE:HG22	1:F:338:ALA:N	2.33	0.43
1:F:184:LEU:HB2	1:F:191:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:314:PRO:HD2	1:B:726:LYS:CG	2.48	0.43
1:F:706:VAL:O	1:F:710:ILE:HG13	2.19	0.43
1:E:177:LEU:HD13	1:E:192:ILE:HD11	2.00	0.43
1:E:949:ASN:HB2	2:F:7075:HOH:O	2.18	0.43
1:A:142:PRO:HD3	1:A:185:PHE:CD2	2.53	0.43
1:A:557:ARG:CZ	1:E:393:ARG:HH12	2.29	0.43
1:D:530:ASN:ND2	1:D:531:PHE:N	2.64	0.43
1:A:628:LYS:HB3	1:A:628:LYS:HE2	1.88	0.43
1:E:489:LYS:HG3	1:E:491:PHE:HE1	1.78	0.43
1:C:872:HIS:CE1	1:C:902:GLU:OE1	2.67	0.43
1:F:218:ASN:HB3	1:F:221:ALA:HB3	1.99	0.43
1:F:442:GLU:OE2	1:F:490:ILE:HD13	2.18	0.43
1:F:802:PRO:O	1:F:805:TYR:HB2	2.18	0.43
1:B:436:GLY:O	1:B:438:PRO:HD3	2.18	0.43
1:C:528:VAL:HG21	1:C:896:TYR:CD2	2.53	0.43
1:D:905:TYR:HB2	2:D:5042:HOH:O	2.18	0.43
1:B:552:THR:HG21	1:B:578:ILE:HD12	2.00	0.43
1:F:319:ILE:HA	1:F:678:LEU:O	2.19	0.43
1:E:319:ILE:HA	1:E:678:LEU:O	2.19	0.43
1:E:616:LYS:HE2	1:E:653:ASP:CB	2.49	0.43
1:E:61:LEU:HB3	1:E:75:VAL:CG1	2.49	0.43
1:A:706:VAL:HG12	1:A:710:ILE:CD1	2.49	0.43
1:F:389:ILE:HD11	1:F:433:LEU:HB3	2.00	0.43
1:E:906:GLN:O	1:E:953:GLY:HA3	2.19	0.43
1:B:637:THR:OG1	1:B:651:ARG:HG3	2.19	0.43
1:D:501:TYR:CD2	1:D:501:TYR:N	2.86	0.43
1:D:982:LEU:C	1:D:983:ILE:HD12	2.39	0.43
1:C:53:ILE:HD13	1:C:306:ILE:CD1	2.48	0.43
1:A:333:ASP:CG	1:A:369:ARG:HE	2.22	0.43
1:B:400:PHE:CD2	1:B:436:GLY:HA3	2.54	0.43
1:E:774:ASP:HA	1:E:817:ALA:HB2	2.00	0.43
1:F:546:PRO:HG2	1:F:567:ASP:HB3	1.99	0.43
1:D:157:SER:HB3	1:D:856:ARG:NH1	2.34	0.43
1:C:312:GLU:HG2	1:C:314:PRO:HD3	2.00	0.43
1:F:780:LYS:HD3	1:F:782:TYR:CZ	2.54	0.43
1:D:771:LEU:C	1:D:771:LEU:HD13	2.39	0.43
1:C:622:TYR:OH	1:C:627:ARG:HG2	2.19	0.43
1:A:190:ARG:NH2	1:A:190:ARG:HG3	2.34	0.43
1:A:61:LEU:CB	1:A:75:VAL:CG1	2.96	0.43
1:A:61:LEU:HB3	1:A:75:VAL:CG1	2.49	0.43
1:D:965:SER:N	1:D:968:ASP:OD2	2.50	0.43
1:C:119:LYS:NZ	1:C:823:ARG:NH2	2.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:327:GLU:O	1:B:328:ASP:C	2.57	0.43
1:C:498:SER:HB2	2:C:5192:HOH:O	2.18	0.43
1:E:651:ARG:NH2	1:E:655:GLY:O	2.46	0.43
1:F:194:ARG:O	1:F:211:GLY:HA2	2.18	0.43
1:D:337:ILE:HG22	1:D:338:ALA:N	2.34	0.43
1:D:400:PHE:CD2	1:D:436:GLY:HA3	2.53	0.43
1:B:155:PRO:CD	1:B:159:MET:HE3	2.48	0.43
1:D:694:TRP:HA	1:D:738:MET:HE2	2.01	0.43
1:F:633:LYS:HE2	1:F:633:LYS:HB2	1.87	0.43
1:B:218:ASN:O	1:B:219:SER:C	2.57	0.43
1:A:43:LEU:C	1:A:44:LEU:HG	2.38	0.43
1:D:428:ILE:HG23	1:D:441:ILE:HB	2.01	0.43
1:C:605:GLU:CG	1:D:524:PRO:HD3	2.49	0.43
1:E:860:TYR:OH	1:E:885:PRO:HD3	2.19	0.43
1:B:637:THR:OG1	1:B:651:ARG:CG	2.67	0.43
1:A:373:THR:HA	1:A:392:TYR:CZ	2.54	0.43
1:F:53:ILE:CG2	1:F:286:LEU:HD21	2.46	0.42
1:D:480:ILE:N	1:D:494:THR:HG22	2.30	0.42
1:D:241:ARG:HH12	1:D:263:ASP:HB3	1.84	0.42
1:C:1055:LEU:O	1:C:1059:LEU:HD13	2.19	0.42
1:B:626:THR:O	1:B:627:ARG:HB2	2.18	0.42
1:B:235:PRO:HA	1:B:243:TYR:O	2.19	0.42
1:C:1031:VAL:O	1:C:1033:ILE:HD12	2.19	0.42
1:F:731:LEU:HD22	1:F:735:ILE:HG13	2.01	0.42
1:B:404:LEU:HD22	1:B:429:MET:HE1	2.01	0.42
1:D:929:MET:HA	1:D:929:MET:HE3	2.01	0.42
1:E:731:LEU:CD2	1:E:735:ILE:HG13	2.49	0.42
1:E:241:ARG:NH1	1:E:263:ASP:HB3	2.34	0.42
1:F:241:ARG:HH12	1:F:263:ASP:CG	2.22	0.42
1:B:739:GLN:NE2	2:B:3141:HOH:O	2.52	0.42
1:C:936:ASP:HB2	1:C:944:SER:HB2	2.01	0.42
1:A:994:ILE:HG22	1:A:1008:GLN:O	2.18	0.42
1:B:184:LEU:HB2	1:B:191:VAL:HB	1.99	0.42
1:D:992:VAL:HG11	1:D:1009:PRO:HB2	2.00	0.42
1:C:156:PHE:HD1	1:C:159:MET:HE1	1.84	0.42
1:F:1031:VAL:HG12	1:F:1033:ILE:HD11	2.01	0.42
1:C:922:GLN:HE22	1:D:948:THR:N	1.98	0.42
1:B:319:ILE:HA	1:B:678:LEU:O	2.19	0.42
1:B:676:ARG:HA	1:B:677:PRO:HD3	1.91	0.42
1:F:425:ARG:O	1:F:426:PHE:HB2	2.19	0.42
1:C:562:GLU:HB3	1:C:563:ALA:H	1.65	0.42
1:D:177:LEU:HD13	1:D:192:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:390:TYR:HD1	1:D:397:ALA:HB2	1.84	0.42
2:C:4075:HOH:O	1:D:949:ASN:HB2	2.18	0.42
1:F:146:LEU:HD23	1:F:165:VAL:HG21	2.01	0.42
1:F:110:PHE:CD2	1:F:121:ILE:HG13	2.54	0.42
1:D:45:ASN:N	1:D:45:ASN:ND2	2.64	0.42
1:F:1031:VAL:O	1:F:1033:ILE:HD12	2.19	0.42
1:A:46:PRO:CG	1:A:286:LEU:HG	2.49	0.42
1:A:578:ILE:CD1	1:A:595:ILE:HD12	2.49	0.42
1:B:562:GLU:HB3	1:B:563:ALA:H	1.59	0.42
1:C:764:ARG:HB3	1:C:855:ASP:OD1	2.19	0.42
1:B:321:ILE:HB	1:B:324:LYS:HG3	2.01	0.42
1:C:809:ASP:HB3	1:C:814:THR:HA	2.01	0.42
1:E:216:GLU:OE1	1:E:220:GLY:N	2.52	0.42
1:C:61:LEU:HB3	1:C:75:VAL:CG1	2.48	0.42
1:E:913:ARG:NH2	1:E:1047:GLN:HE21	2.15	0.42
1:B:228:MET:CE	1:B:232:VAL:HG22	2.49	0.42
1:D:368:ARG:O	1:D:375:VAL:CG2	2.67	0.42
1:B:367:VAL:HG12	1:B:375:VAL:HG21	2.01	0.42
1:E:389:ILE:HD11	1:E:433:LEU:HB3	2.01	0.42
1:E:279:ASN:ND2	2:E:6071:HOH:O	2.52	0.42
1:A:892:LEU:HD13	1:A:920:VAL:HG21	2.01	0.42
1:C:894:GLU:OE2	1:C:897:ARG:HD2	2.19	0.42
1:A:390:TYR:HD1	1:A:397:ALA:HB2	1.85	0.42
1:A:579:ASN:ND2	1:A:627:ARG:NH1	2.68	0.42
1:B:167:ASN:O	1:B:170:ILE:HG12	2.20	0.42
1:A:312:GLU:HG2	1:A:314:PRO:HD3	2.01	0.42
1:E:897:ARG:HB2	1:F:520:LEU:HD12	2.01	0.42
1:B:1045:ASP:HB3	1:B:1048:ILE:HG22	2.01	0.42
1:A:890:MET:O	1:A:894:GLU:HG2	2.19	0.42
1:A:157:SER:HB2	2:A:2397:HOH:O	2.19	0.42
1:F:936:ASP:HB2	1:F:944:SER:HB2	2.02	0.42
1:A:53:ILE:HG23	1:A:286:LEU:CD2	2.48	0.42
1:A:676:ARG:HA	1:A:677:PRO:HD3	1.89	0.42
1:C:596:LEU:N	1:C:596:LEU:HD22	2.35	0.42
1:E:926:GLU:CG	1:F:926:GLU:HG2	2.50	0.42
1:A:811:ASP:HB2	1:A:828:LYS:HE2	2.01	0.42
1:C:258:ASP:C	1:C:260:ASP:H	2.21	0.42
1:A:469:HIS:CG	1:A:470:GLY:N	2.86	0.42
1:C:926:GLU:CG	1:D:926:GLU:HG2	2.50	0.42
1:A:315:GLU:OE2	1:D:119:LYS:HD2	2.20	0.42
1:C:295:ILE:HG13	1:C:306:ILE:HD11	2.02	0.42
1:B:53:ILE:HG12	1:B:286:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:530:ASN:ND2	1:C:531:PHE:N	2.66	0.42
1:D:357:LYS:HB2	1:D:676:ARG:HH12	1.84	0.42
1:F:462:ALA:HA	1:F:481:HIS:O	2.20	0.42
1:C:887:MET:HB3	1:C:966:ASP:OD2	2.20	0.42
1:F:110:PHE:CE2	1:F:121:ILE:HG13	2.55	0.42
1:E:926:GLU:HG2	1:F:926:GLU:CG	2.49	0.42
1:F:230:THR:HG21	1:F:248:ILE:HA	2.02	0.42
1:C:1052:ILE:O	1:C:1056:ILE:HG13	2.19	0.42
1:D:153:MET:HG3	1:D:859:ARG:NH1	2.35	0.42
1:E:362:LEU:HA	1:E:362:LEU:HD23	1.84	0.42
1:F:362:LEU:HA	1:F:362:LEU:HD23	1.91	0.42
1:D:286:LEU:HD13	1:D:295:ILE:HG12	2.00	0.42
1:F:494:THR:HG21	1:F:500:ASP:OD1	2.20	0.42
1:D:494:THR:CG2	1:D:500:ASP:OD1	2.65	0.42
1:B:373:THR:HA	1:B:392:TYR:CZ	2.54	0.42
1:B:153:MET:HG3	1:B:859:ARG:NH1	2.34	0.42
1:B:217:VAL:HG23	1:B:218:ASN:N	2.35	0.42
1:C:153:MET:HG3	1:C:859:ARG:CZ	2.50	0.42
1:C:499:HIS:HD2	2:C:4176:HOH:O	2.02	0.42
1:A:635:ASN:HB3	1:A:653:ASP:OD1	2.19	0.42
1:C:367:VAL:CG1	1:C:375:VAL:HG21	2.50	0.42
1:A:501:TYR:CD2	1:A:501:TYR:N	2.87	0.42
1:F:929:MET:HA	1:F:929:MET:CE	2.49	0.42
1:C:362:LEU:HA	1:C:362:LEU:HD23	1.85	0.42
1:F:469:HIS:HD1	1:F:473:ASP:CG	2.23	0.42
1:C:350:VAL:HG11	1:C:669:ARG:NH1	2.35	0.42
1:E:206:ARG:N	1:E:1024:ASN:HD21	2.16	0.42
1:A:189:ARG:HB2	1:A:216:GLU:HB3	2.01	0.42
1:F:436:GLY:O	1:F:438:PRO:HD3	2.20	0.42
1:F:345:ALA:HB2	1:F:364:ILE:HG21	2.01	0.42
1:B:807:ILE:HG12	1:B:837:LEU:CD2	2.50	0.42
1:B:1031:VAL:HG12	1:B:1033:ILE:HD11	2.01	0.41
1:F:322:PRO:HG2	1:F:674:ASP:OD1	2.19	0.41
1:D:216:GLU:OE1	1:D:219:SER:HA	2.20	0.41
1:C:423:ASN:ND2	1:C:427:GLU:H	2.18	0.41
1:B:641:LEU:HD22	1:B:645:ARG:HA	2.02	0.41
1:C:977:LEU:HB2	1:C:979:LEU:CD1	2.49	0.41
1:E:423:ASN:ND2	1:E:425:ARG:HB2	2.35	0.41
1:D:390:TYR:CD1	1:D:397:ALA:HB2	2.55	0.41
1:D:589:ILE:HB	1:D:596:LEU:HB2	2.02	0.41
1:B:989:GLY:HA2	1:B:1026:GLY:HA2	2.03	0.41
1:C:117:GLU:HA	1:F:313:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.78	0.41
1:C:446:GLU:OE1	1:C:468:LYS:HE2	2.19	0.41
1:C:616:LYS:HE2	1:C:653:ASP:CB	2.49	0.41
1:B:119:LYS:HZ1	1:B:823:ARG:HH22	1.66	0.41
1:F:811:ASP:HB2	1:F:828:LYS:HE2	2.02	0.41
1:A:428:ILE:HG23	1:A:441:ILE:HB	2.02	0.41
1:F:203:LYS:HD3	1:F:740:GLY:C	2.41	0.41
1:C:402:GLU:HG3	1:C:438:PRO:HD3	2.02	0.41
1:B:278:LEU:HD23	1:B:287:PHE:HB3	2.02	0.41
1:B:469:HIS:CG	1:B:470:GLY:N	2.88	0.41
1:F:253:GLN:NE2	1:F:253:GLN:HA	2.35	0.41
1:C:241:ARG:HH12	1:C:263:ASP:HB3	1.84	0.41
1:B:425:ARG:HB3	1:B:427:GLU:HG3	2.02	0.41
1:B:731:LEU:HD22	1:B:735:ILE:HG13	2.02	0.41
1:A:228:MET:HE3	1:A:232:VAL:HG21	2.02	0.41
1:B:871:VAL:HG22	1:B:1052:ILE:HD11	2.01	0.41
1:C:875:SER:HB2	1:C:879:ILE:HG13	2.02	0.41
1:B:156:PHE:H	1:B:159:MET:CE	2.34	0.41
1:D:155:PRO:HB3	1:D:860:TYR:HA	2.02	0.41
1:E:253:GLN:HB2	1:E:255:TYR:CE1	2.55	0.41
1:D:218:ASN:O	1:D:221:ALA:N	2.53	0.41
1:D:241:ARG:NH1	1:D:263:ASP:HB3	2.35	0.41
1:C:82:ASN:HD21	1:C:96:ARG:HH21	1.67	0.41
1:D:676:ARG:NH2	2:D:5370:HOH:O	2.53	0.41
1:D:368:ARG:O	1:D:375:VAL:HG23	2.21	0.41
1:A:110:PHE:CD2	1:A:121:ILE:HG13	2.54	0.41
1:F:905:TYR:HB2	2:F:7042:HOH:O	2.18	0.41
1:F:807:ILE:HG12	1:F:837:LEU:CD2	2.50	0.41
1:E:247:ASP:HA	1:E:251:PHE:O	2.20	0.41
1:B:401:GLU:N	1:B:401:GLU:OE2	2.47	0.41
1:D:881:TYR:O	1:D:902:GLU:HG3	2.20	0.41
1:E:642:SER:HB3	1:E:647:THR:H	1.84	0.41
1:C:184:LEU:HB2	1:C:191:VAL:HB	2.01	0.41
1:D:735:ILE:O	1:D:739:GLN:HG3	2.20	0.41
1:B:78:LEU:HD11	1:B:118:ILE:HD11	2.02	0.41
1:F:992:VAL:HG11	1:F:1009:PRO:HB2	2.02	0.41
1:D:947:PRO:HD2	1:D:950:SER:HB3	2.02	0.41
1:F:89:ASP:OD1	1:F:91:ARG:HG3	2.21	0.41
1:B:46:PRO:CG	1:B:286:LEU:HG	2.50	0.41
1:C:319:ILE:HA	1:C:678:LEU:O	2.20	0.41
1:B:618:VAL:CG2	1:B:631:GLU:HG3	2.51	0.41
1:C:43:LEU:HD13	1:C:308:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:524:PRO:HD3	1:B:605:GLU:HG3	2.01	0.41
1:D:228:MET:HE1	1:D:244:PHE:CE1	2.55	0.41
1:F:767:CYS:HA	1:F:780:LYS:O	2.20	0.41
1:A:194:ARG:O	1:A:211:GLY:HA2	2.21	0.41
1:F:155:PRO:HB3	1:F:860:TYR:HA	2.03	0.41
1:A:1031:VAL:O	1:A:1033:ILE:HD12	2.21	0.41
1:A:295:ILE:HG13	1:A:306:ILE:HD11	2.02	0.41
1:D:703:ASN:C	1:D:703:ASN:ND2	2.71	0.41
1:B:74:ILE:HG13	1:B:75:VAL:HG12	2.02	0.41
1:E:74:ILE:HG13	1:E:75:VAL:HG12	2.03	0.41
1:E:228:MET:HE2	1:E:244:PHE:CZ	2.56	0.41
1:B:228:MET:CE	1:B:244:PHE:CE1	3.04	0.41
1:B:423:ASN:ND2	1:B:425:ARG:HB2	2.36	0.41
1:B:333:ASP:CG	1:B:369:ARG:HE	2.24	0.41
1:F:912:VAL:HG22	1:F:958:ILE:O	2.21	0.41
1:B:1055:LEU:O	1:B:1059:LEU:HD13	2.21	0.41
1:D:423:ASN:HD22	1:D:423:ASN:C	2.24	0.41
1:C:350:VAL:CG2	1:C:669:ARG:NH1	2.83	0.41
1:F:170:ILE:HD13	1:F:820:ASN:HB2	2.02	0.41
1:C:118:ILE:HG22	1:F:314:PRO:HA	2.02	0.41
1:F:119:LYS:NZ	1:F:823:ARG:HH22	2.19	0.41
1:E:722:VAL:N	1:E:723:PRO:HD2	2.36	0.41
1:E:791:GLU:CD	1:E:861:ARG:HE	2.24	0.41
1:D:155:PRO:HD2	1:D:159:MET:HE3	2.02	0.41
1:A:156:PHE:CD1	1:A:159:MET:CE	3.04	0.41
1:C:253:GLN:HB2	1:C:255:TYR:HE1	1.86	0.41
1:E:580:VAL:HG22	1:E:622:TYR:CD2	2.56	0.41
1:C:480:ILE:N	1:C:494:THR:HG22	2.28	0.41
1:D:268:THR:HG22	1:D:303:ILE:CD1	2.45	0.41
1:F:46:PRO:HB2	1:F:286:LEU:HD23	2.02	0.41
1:D:190:ARG:NH2	1:D:190:ARG:CG	2.83	0.41
1:F:628:LYS:HE2	1:F:628:LYS:HB3	1.88	0.41
1:B:624:VAL:HG23	1:B:625:LYS:N	2.36	0.41
1:F:160:THR:O	1:F:179:PRO:HA	2.21	0.41
1:B:591:LEU:HD11	1:B:662:LEU:HD21	2.02	0.41
1:F:242:ILE:O	1:F:256:SER:HA	2.21	0.41
1:B:119:LYS:NZ	1:B:823:ARG:NH2	2.69	0.41
1:E:1016:ARG:O	1:E:1017:ASP:CB	2.69	0.41
1:C:96:ARG:NH2	1:C:133:MET:HB3	2.35	0.41
1:A:802:PRO:O	1:A:805:TYR:HB2	2.21	0.41
1:B:965:SER:N	1:B:968:ASP:OD2	2.51	0.41
1:D:599:SER:HB3	1:D:618:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:591:LEU:HD12	1:A:596:LEU:HD23	2.02	0.41
1:F:706:VAL:HG12	1:F:710:ILE:HD11	2.02	0.41
1:E:565:GLU:CG	1:E:566:TYR:N	2.83	0.41
1:F:546:PRO:CG	1:F:567:ASP:HB3	2.51	0.41
1:A:886:ASP:O	1:A:891:GLY:HA3	2.21	0.41
1:F:708:LYS:O	1:F:712:GLU:HG3	2.21	0.41
1:C:714:ILE:HG21	1:C:741:GLU:HG3	2.03	0.41
1:E:136:ASP:OD2	1:E:137:VAL:N	2.44	0.41
1:D:895:PHE:CE2	1:D:924:ILE:HG23	2.56	0.41
1:B:694:TRP:HA	1:B:738:MET:CE	2.51	0.41
1:E:236:VAL:HG23	1:E:243:TYR:HB2	2.03	0.41
1:F:383:GLU:HA	1:F:383:GLU:OE2	2.20	0.41
1:A:85:ARG:HD3	2:A:2104:HOH:O	2.21	0.41
1:C:253:GLN:NE2	1:C:268:THR:OG1	2.49	0.41
1:F:739:GLN:NE2	2:F:7141:HOH:O	2.53	0.41
1:F:591:LEU:HD11	1:F:662:LEU:HD21	2.03	0.41
1:B:123:TYR:OH	1:B:823:ARG:HD3	2.21	0.41
1:B:628:LYS:HB3	1:B:628:LYS:HE2	1.94	0.41
1:B:892:LEU:HA	1:B:892:LEU:HD12	1.96	0.41
1:C:393:ARG:HH12	1:E:557:ARG:HD2	1.86	0.41
1:C:216:GLU:OE1	1:C:219:SER:HA	2.21	0.41
1:A:72:ARG:HG3	1:D:72:ARG:HG3	2.03	0.41
1:C:887:MET:O	1:C:920:VAL:HG22	2.21	0.41
1:A:130:GLY:HA3	2:A:2163:HOH:O	2.20	0.41
1:B:346:PHE:C	1:B:347:ILE:HD12	2.42	0.41
1:A:286:LEU:HD11	1:A:293:ILE:HG22	2.03	0.40
1:C:735:ILE:O	1:C:738:MET:HG3	2.21	0.40
1:D:403:ASN:HD22	1:D:404:LEU:N	2.19	0.40
1:C:947:PRO:HG3	2:C:4038:HOH:O	2.20	0.40
1:B:498:SER:OG	1:B:499:HIS:N	2.54	0.40
1:E:731:LEU:HD22	1:E:735:ILE:CD1	2.52	0.40
1:B:337:ILE:CG2	1:B:338:ALA:N	2.84	0.40
1:F:373:THR:HG21	1:F:393:ARG:HD2	2.03	0.40
1:F:956:ILE:HG22	1:F:1055:LEU:HD11	2.01	0.40
1:A:308:ILE:HG22	1:A:311:LEU:HD11	2.02	0.40
1:A:110:PHE:CE2	1:A:146:LEU:HD22	2.55	0.40
1:A:618:VAL:HG23	1:A:633:LYS:O	2.20	0.40
1:C:499:HIS:HE1	2:C:4239:HOH:O	2.04	0.40
1:C:194:ARG:O	1:C:211:GLY:HA2	2.22	0.40
1:D:499:HIS:HD2	2:D:5176:HOH:O	2.04	0.40
1:D:134:PHE:O	1:D:135:THR:HB	2.21	0.40
1:A:466:PRO:HB3	2:A:2183:HOH:O	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:297:ASN:O	1:B:301:GLU:N	2.46	0.40
1:C:210:ARG:HH21	1:C:210:ARG:HG2	1.87	0.40
1:C:183:ILE:HG23	1:C:183:ILE:O	2.21	0.40
1:F:155:PRO:HD2	1:F:159:MET:HE3	2.04	0.40
1:B:156:PHE:HD1	1:B:159:MET:HE1	1.84	0.40
1:E:872:HIS:CE1	1:E:902:GLU:OE1	2.72	0.40
1:B:332:LEU:HD11	1:B:338:ALA:HB2	2.03	0.40
1:E:338:ALA:HA	1:E:346:PHE:O	2.21	0.40
1:C:300:THR:O	1:C:301:GLU:HB3	2.21	0.40
1:F:929:MET:HE3	1:F:929:MET:HA	2.02	0.40
1:D:88:PRO:HG3	1:D:144:GLY:HA2	2.01	0.40
1:B:690:TYR:OH	1:B:718:TYR:HB2	2.21	0.40
1:C:175:LEU:O	1:C:176:ASN:HB2	2.21	0.40
1:A:350:VAL:CG2	1:A:669:ARG:NH1	2.83	0.40
1:C:423:ASN:ND2	1:C:425:ARG:HB2	2.36	0.40
1:B:811:ASP:HB2	1:B:828:LYS:HE2	2.03	0.40
1:C:141:ASP:HB2	1:C:142:PRO:CD	2.51	0.40
1:A:589:ILE:HB	1:A:596:LEU:HB2	2.04	0.40
1:B:860:TYR:OH	1:B:885:PRO:HD3	2.21	0.40
1:F:279:ASN:ND2	2:F:7071:HOH:O	2.54	0.40
1:B:559:MET:HG2	1:D:356:LEU:HD11	2.02	0.40
1:E:892:LEU:HD13	1:E:920:VAL:HG21	2.03	0.40
1:C:633:LYS:HE2	1:C:633:LYS:HB2	1.88	0.40
1:E:446:GLU:CD	1:E:468:LYS:HG3	2.42	0.40
1:A:387:LEU:HD12	1:A:400:PHE:CE1	2.56	0.40
1:B:123:TYR:HB3	1:B:826:SER:OG	2.22	0.40
1:F:884:ILE:HA	1:F:885:PRO:HD2	1.83	0.40
1:A:319:ILE:HG23	1:A:677:PRO:CB	2.51	0.40
1:A:235:PRO:HA	1:A:243:TYR:O	2.20	0.40
1:E:628:LYS:HE3	2:E:6366:HOH:O	2.22	0.40
1:E:183:ILE:HA	1:E:191:VAL:O	2.21	0.40
1:A:731:LEU:HD22	1:A:735:ILE:HG13	2.04	0.40
1:F:640:ARG:HG2	1:F:640:ARG:HH21	1.86	0.40
1:C:156:PHE:H	1:C:159:MET:CE	2.35	0.40
1:A:270:PHE:CE2	1:A:289:LYS:HE2	2.56	0.40
1:C:578:ILE:O	1:C:580:VAL:N	2.50	0.40
1:A:489:LYS:HE2	1:A:491:PHE:CZ	2.53	0.40
1:B:342:ARG:NE	1:B:685:GLU:OE1	2.51	0.40
1:B:530:ASN:ND2	1:B:531:PHE:H	2.20	0.40
1:C:589:ILE:HG21	1:C:641:LEU:CD1	2.52	0.40
1:E:619:LEU:HD13	1:E:639:LEU:HD13	2.04	0.40
1:E:141:ASP:HB2	1:E:142:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:703:ASN:C	1:F:703:ASN:HD22	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1045 (98%)	979 (96%)	38 (4%)	4 (0%)	43	36
1	B	1021/1045 (98%)	977 (96%)	41 (4%)	3 (0%)	50	44
1	C	1021/1045 (98%)	961 (94%)	53 (5%)	7 (1%)	30	20
1	D	1021/1045 (98%)	979 (96%)	38 (4%)	4 (0%)	43	36
1	E	1021/1045 (98%)	975 (96%)	43 (4%)	3 (0%)	50	44
1	F	1021/1045 (98%)	971 (95%)	44 (4%)	6 (1%)	33	24
All	All	6126/6270 (98%)	5842 (95%)	257 (4%)	27 (0%)	43	36

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ASP
1	B	328	ASP
1	C	219	SER
1	C	579	ASN
1	D	219	SER
1	E	219	SER
1	F	219	SER
1	F	579	ASN
1	A	562	GLU
1	B	562	GLU
1	B	579	ASN
1	C	562	GLU
1	E	562	GLU
1	E	579	ASN

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Mol	Chain	Res	Type
1	F	562	GLU
1	F	563	ALA
1	D	562	GLU
1	A	219	SER
1	C	328	ASP
1	D	563	ALA
1	D	579	ASN
1	F	259	LEU
1	A	579	ASN
1	C	563	ALA
1	C	665	PRO
1	C	45	ASN
1	F	682	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	883/904 (98%)	857 (97%)	26 (3%)	55	52
1	B	883/904 (98%)	853 (97%)	30 (3%)	49	45
1	C	883/904 (98%)	860 (97%)	23 (3%)	59	58
1	D	883/904 (98%)	856 (97%)	27 (3%)	52	49
1	E	883/904 (98%)	857 (97%)	26 (3%)	55	52
1	F	883/904 (98%)	857 (97%)	26 (3%)	55	52
All	All	5298/5424 (98%)	5140 (97%)	158 (3%)	53	50

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	46	PRO
1	A	61	LEU
1	A	104	ASN
1	A	190	ARG
1	A	279	ASN

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Mol	Chain	Res	Type
1	A	311	LEU
1	A	313	SER
1	A	363	ARG
1	A	375	VAL
1	A	403	ASN
1	A	423	ASN
1	A	469	HIS
1	A	562	GLU
1	A	578	ILE
1	A	641	LEU
1	A	678	LEU
1	A	687	LEU
1	A	703	ASN
1	A	719	ARG
1	A	731	LEU
1	A	738	MET
1	A	929	MET
1	A	965	SER
1	A	1024	ASN
1	A	1035	TYR
1	B	44	LEU
1	B	61	LEU
1	B	75	VAL
1	B	104	ASN
1	B	114	GLU
1	B	153	MET
1	B	190	ARG
1	B	279	ASN
1	B	311	LEU
1	B	313	SER
1	B	330	SER
1	B	363	ARG
1	B	403	ASN
1	B	423	ASN
1	B	469	HIS
1	B	481	HIS
1	B	557	ARG
1	B	562	GLU
1	B	578	ILE
1	B	641	LEU
1	B	678	LEU
1	B	687	LEU

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Mol	Chain	Res	Type
1	B	703	ASN
1	B	717	LYS
1	B	719	ARG
1	B	731	LEU
1	B	738	MET
1	B	892	LEU
1	B	1024	ASN
1	B	1035	TYR
1	C	61	LEU
1	C	75	VAL
1	C	82	ASN
1	C	104	ASN
1	C	279	ASN
1	C	353	THR
1	C	363	ARG
1	C	403	ASN
1	C	423	ASN
1	C	469	HIS
1	C	481	HIS
1	C	557	ARG
1	C	562	GLU
1	C	578	ILE
1	C	641	LEU
1	C	687	LEU
1	C	703	ASN
1	C	719	ARG
1	C	731	LEU
1	C	738	MET
1	C	892	LEU
1	C	1024	ASN
1	C	1035	TYR
1	D	61	LEU
1	D	75	VAL
1	D	82	ASN
1	D	104	ASN
1	D	114	GLU
1	D	190	ARG
1	D	218	ASN
1	D	279	ASN
1	D	311	LEU
1	D	363	ARG
1	D	403	ASN

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Mol	Chain	Res	Type
1	D	423	ASN
1	D	469	HIS
1	D	532	SER
1	D	557	ARG
1	D	562	GLU
1	D	578	ILE
1	D	641	LEU
1	D	687	LEU
1	D	703	ASN
1	D	719	ARG
1	D	731	LEU
1	D	738	MET
1	D	809	ASP
1	D	892	LEU
1	D	1024	ASN
1	D	1035	TYR
1	E	44	LEU
1	E	61	LEU
1	E	75	VAL
1	E	82	ASN
1	E	104	ASN
1	E	114	GLU
1	E	190	ARG
1	E	209	THR
1	E	218	ASN
1	E	311	LEU
1	E	363	ARG
1	E	403	ASN
1	E	423	ASN
1	E	469	HIS
1	E	557	ARG
1	E	562	GLU
1	E	578	ILE
1	E	641	LEU
1	E	703	ASN
1	E	719	ARG
1	E	731	LEU
1	E	738	MET
1	E	809	ASP
1	E	892	LEU
1	E	1024	ASN
1	E	1035	TYR

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Mol	Chain	Res	Type
1	F	44	LEU
1	F	46	PRO
1	F	61	LEU
1	F	75	VAL
1	F	190	ARG
1	F	209	THR
1	F	279	ASN
1	F	363	ARG
1	F	403	ASN
1	F	423	ASN
1	F	469	HIS
1	F	481	HIS
1	F	557	ARG
1	F	562	GLU
1	F	578	ILE
1	F	641	LEU
1	F	687	LEU
1	F	703	ASN
1	F	719	ARG
1	F	731	LEU
1	F	738	MET
1	F	892	LEU
1	F	929	MET
1	F	1008	GLN
1	F	1024	ASN
1	F	1035	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (193) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	64	HIS
1	A	82	ASN
1	A	104	ASN
1	A	176	ASN
1	A	253	GLN
1	A	267	HIS
1	A	279	ASN
1	A	403	ASN
1	A	415	ASN
1	A	423	ASN
1	A	481	HIS

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Mol	Chain	Res	Type
1	A	497	ASN
1	A	499	HIS
1	A	511	ASN
1	A	530	ASN
1	A	579	ASN
1	A	611	GLN
1	A	635	ASN
1	A	703	ASN
1	A	733	ASN
1	A	739	GLN
1	A	867	ASN
1	A	872	HIS
1	A	922	GLN
1	A	930	ASN
1	A	949	ASN
1	A	1008	GLN
1	A	1024	ASN
1	A	1038	HIS
1	A	1047	GLN
1	B	45	ASN
1	B	64	HIS
1	B	82	ASN
1	B	104	ASN
1	B	253	GLN
1	B	267	HIS
1	B	279	ASN
1	B	403	ASN
1	B	415	ASN
1	B	423	ASN
1	B	481	HIS
1	B	497	ASN
1	B	499	HIS
1	B	511	ASN
1	B	530	ASN
1	B	579	ASN
1	B	611	GLN
1	B	635	ASN
1	B	703	ASN
1	B	733	ASN
1	B	739	GLN
1	B	867	ASN
1	B	872	HIS

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Mol	Chain	Res	Type
1	B	922	GLN
1	B	930	ASN
1	B	949	ASN
1	B	1008	GLN
1	B	1024	ASN
1	B	1038	HIS
1	B	1047	GLN
1	C	45	ASN
1	C	49	HIS
1	C	64	HIS
1	C	82	ASN
1	C	104	ASN
1	C	195	ASN
1	C	253	GLN
1	C	267	HIS
1	C	279	ASN
1	C	403	ASN
1	C	423	ASN
1	C	497	ASN
1	C	499	HIS
1	C	511	ASN
1	C	530	ASN
1	C	579	ASN
1	C	611	GLN
1	C	635	ASN
1	C	703	ASN
1	C	720	ASN
1	C	733	ASN
1	C	739	GLN
1	C	867	ASN
1	C	872	HIS
1	C	922	GLN
1	C	930	ASN
1	C	949	ASN
1	C	1008	GLN
1	C	1024	ASN
1	C	1038	HIS
1	C	1047	GLN
1	D	45	ASN
1	D	49	HIS
1	D	64	HIS
1	D	82	ASN

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Mol	Chain	Res	Type
1	D	104	ASN
1	D	253	GLN
1	D	267	HIS
1	D	279	ASN
1	D	403	ASN
1	D	415	ASN
1	D	423	ASN
1	D	481	HIS
1	D	497	ASN
1	D	499	HIS
1	D	511	ASN
1	D	530	ASN
1	D	569	ASN
1	D	611	GLN
1	D	635	ASN
1	D	703	ASN
1	D	720	ASN
1	D	733	ASN
1	D	739	GLN
1	D	867	ASN
1	D	872	HIS
1	D	922	GLN
1	D	930	ASN
1	D	937	ASN
1	D	949	ASN
1	D	1008	GLN
1	D	1024	ASN
1	D	1038	HIS
1	D	1047	GLN
1	E	45	ASN
1	E	49	HIS
1	E	64	HIS
1	E	82	ASN
1	E	104	ASN
1	E	253	GLN
1	E	267	HIS
1	E	279	ASN
1	E	403	ASN
1	E	415	ASN
1	E	423	ASN
1	E	481	HIS
1	E	497	ASN

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Mol	Chain	Res	Type
1	E	499	HIS
1	E	511	ASN
1	E	530	ASN
1	E	569	ASN
1	E	611	GLN
1	E	635	ASN
1	E	703	ASN
1	E	720	ASN
1	E	733	ASN
1	E	739	GLN
1	E	867	ASN
1	E	872	HIS
1	E	901	ASN
1	E	922	GLN
1	E	930	ASN
1	E	949	ASN
1	E	1008	GLN
1	E	1024	ASN
1	E	1038	HIS
1	E	1047	GLN
1	F	45	ASN
1	F	64	HIS
1	F	82	ASN
1	F	104	ASN
1	F	145	ASN
1	F	176	ASN
1	F	253	GLN
1	F	267	HIS
1	F	279	ASN
1	F	403	ASN
1	F	415	ASN
1	F	423	ASN
1	F	481	HIS
1	F	497	ASN
1	F	499	HIS
1	F	511	ASN
1	F	530	ASN
1	F	569	ASN
1	F	579	ASN
1	F	611	GLN
1	F	635	ASN
1	F	703	ASN

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Mol	Chain	Res	Type
1	F	720	ASN
1	F	733	ASN
1	F	739	GLN
1	F	867	ASN
1	F	872	HIS
1	F	901	ASN
1	F	922	GLN
1	F	930	ASN
1	F	949	ASN
1	F	1008	GLN
1	F	1024	ASN
1	F	1038	HIS
1	F	1047	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1022/1045 (97%)	0.18	23 (2%)	57 57	14, 26, 43, 56	19 (1%)
1	B	1022/1045 (97%)	0.18	21 (2%)	60 61	16, 26, 43, 55	19 (1%)
1	C	1022/1045 (97%)	0.62	87 (8%)	11 10	20, 33, 46, 56	19 (1%)
1	D	1022/1045 (97%)	0.22	32 (3%)	47 46	18, 28, 45, 54	19 (1%)
1	E	1022/1045 (97%)	0.20	26 (2%)	54 54	17, 28, 45, 55	19 (1%)
1	F	1022/1045 (97%)	0.58	91 (8%)	10 9	21, 32, 46, 55	19 (1%)
All	All	6132/6270 (97%)	0.33	280 (4%)	31 30	14, 30, 45, 56	114 (1%)

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	841	GLY	9.3
1	C	219	SER	8.6
1	F	219	SER	8.2
1	F	220	GLY	7.9
1	E	219	SER	7.1
1	F	563	ALA	7.0
1	C	841	GLY	6.8
1	D	219	SER	6.8
1	E	220	GLY	6.7
1	C	220	GLY	6.4
1	C	218	ASN	6.0
1	E	218	ASN	5.7
1	D	220	GLY	5.4
1	C	217	VAL	5.3
1	C	188	GLY	5.3
1	D	841	GLY	5.0
1	C	563	ALA	4.9
1	F	840	LYS	4.9
1	B	563	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	238	VAL	4.8
1	C	842	GLY	4.8
1	D	563	ALA	4.7
1	F	839	GLY	4.7
1	C	840	LYS	4.5
1	D	842	GLY	4.4
1	B	841	GLY	4.4
1	F	67	LYS	4.4
1	C	221	ALA	4.4
1	B	218	ASN	4.3
1	F	188	GLY	4.3
1	F	706	VAL	4.2
1	C	300	THR	4.2
1	C	843	ASP	4.1
1	F	843	ASP	4.1
1	C	817	ALA	4.1
1	F	69	GLY	4.1
1	C	706	VAL	4.0
1	C	66	LEU	4.0
1	C	116	GLY	4.0
1	C	237	ILE	3.9
1	C	114	GLU	3.9
1	F	774	ASP	3.9
1	D	435	THR	3.9
1	C	562	GLU	3.8
1	F	299	ASP	3.8
1	C	774	ASP	3.8
1	F	705	ALA	3.8
1	D	469	HIS	3.7
1	C	299	ASP	3.7
1	F	393	ARG	3.7
1	C	839	GLY	3.6
1	C	67	LYS	3.6
1	D	218	ASN	3.6
1	D	840	LYS	3.6
1	D	706	VAL	3.6
1	F	401	GLU	3.5
1	F	262	LYS	3.5
1	C	142	PRO	3.5
1	F	771	LEU	3.5
1	C	707	ALA	3.5
1	F	842	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	561	SER	3.5
1	F	806	LEU	3.4
1	E	469	HIS	3.4
1	F	434	GLU	3.4
1	F	187	ASP	3.4
1	A	563	ALA	3.4
1	D	436	GLY	3.4
1	C	187	ASP	3.4
1	F	217	VAL	3.4
1	F	704	GLU	3.4
1	F	218	ASN	3.3
1	C	806	LEU	3.3
1	D	434	GLU	3.3
1	C	397	ALA	3.3
1	C	69	GLY	3.3
1	D	286	LEU	3.3
1	D	1019	GLY	3.3
1	C	777	VAL	3.2
1	F	238	VAL	3.2
1	C	239	GLY	3.2
1	F	817	ALA	3.2
1	C	303	ILE	3.2
1	F	722	VAL	3.2
1	C	318	ILE	3.1
1	F	66	LEU	3.1
1	F	488	ARG	3.1
1	F	435	THR	3.1
1	C	654	ASP	3.1
1	F	260	ASP	3.1
1	F	305	LYS	3.1
1	D	653	ASP	3.1
1	A	839	GLY	3.0
1	F	221	ALA	3.0
1	F	612	GLY	3.0
1	C	752	GLY	3.0
1	C	50	GLY	2.9
1	F	272	ASP	2.9
1	F	91	ARG	2.9
1	F	50	GLY	2.9
1	F	362	LEU	2.9
1	F	114	GLU	2.9
1	D	716	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	299	ASP	2.9
1	C	845	ARG	2.9
1	E	842	GLY	2.9
1	D	843	ASP	2.9
1	C	68	SER	2.9
1	F	300	THR	2.9
1	B	434	GLU	2.9
1	B	435	THR	2.9
1	C	286	LEU	2.8
1	F	1059	LEU	2.8
1	F	307	GLU	2.8
1	F	716	GLU	2.8
1	C	667	ASP	2.8
1	E	434	GLU	2.8
1	E	299	ASP	2.8
1	B	488	ARG	2.8
1	C	393	ARG	2.7
1	F	841	GLY	2.7
1	F	70	SER	2.7
1	F	562	GLU	2.7
1	C	51	ASP	2.7
1	F	51	ASP	2.7
1	C	434	GLU	2.7
1	F	297	ASN	2.7
1	C	844	LYS	2.7
1	C	1043	GLY	2.7
1	E	841	GLY	2.7
1	B	628	LYS	2.6
1	C	613	ALA	2.6
1	E	91	ARG	2.6
1	F	215	ILE	2.6
1	A	842	GLY	2.6
1	B	39	MET	2.6
1	F	773	GLY	2.6
1	A	437	LYS	2.6
1	E	706	VAL	2.6
1	A	434	GLU	2.6
1	C	612	GLY	2.6
1	D	613	ALA	2.6
1	E	563	ALA	2.6
1	C	803	THR	2.6
1	D	667	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	243	TYR	2.6
1	C	561	SER	2.6
1	A	494	THR	2.6
1	C	168	ASP	2.6
1	C	469	HIS	2.6
1	C	653	ASP	2.5
1	E	1017	ASP	2.5
1	C	91	ARG	2.5
1	A	840	LYS	2.5
1	E	840	LYS	2.5
1	F	844	LYS	2.5
1	C	487	GLY	2.5
1	C	1041	LEU	2.5
1	B	842	GLY	2.5
1	C	1042	SER	2.5
1	A	199	LEU	2.5
1	E	653	ASP	2.5
1	F	186	ALA	2.5
1	B	469	HIS	2.5
1	F	469	HIS	2.5
1	D	705	ALA	2.5
1	D	839	GLY	2.5
1	C	722	VAL	2.5
1	C	435	THR	2.4
1	C	1038	HIS	2.4
1	E	435	THR	2.4
1	D	557	ARG	2.4
1	F	65	ASP	2.4
1	C	401	GLU	2.4
1	C	488	ARG	2.4
1	D	562	GLU	2.4
1	B	612	GLY	2.4
1	F	68	SER	2.4
1	B	924	ILE	2.4
1	A	67	LYS	2.4
1	A	1059	LEU	2.4
1	E	562	GLU	2.4
1	F	436	GLY	2.4
1	A	562	GLU	2.4
1	A	39	MET	2.4
1	F	185	PHE	2.4
1	B	286	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	1043	GLY	2.4
1	C	144	GLY	2.4
1	C	705	ALA	2.4
1	A	218	ASN	2.4
1	D	114	GLU	2.4
1	B	923	LEU	2.3
1	C	271	THR	2.3
1	D	1059	LEU	2.3
1	F	761	ARG	2.3
1	C	236	VAL	2.3
1	F	171	ASN	2.3
1	F	189	ARG	2.3
1	C	494	THR	2.3
1	D	437	LYS	2.3
1	B	562	GLU	2.3
1	F	258	ASP	2.3
1	B	1017	ASP	2.3
1	C	838	SER	2.3
1	F	237	ILE	2.3
1	E	397	ALA	2.2
1	A	488	ARG	2.2
1	D	91	ARG	2.2
1	C	297	ASN	2.2
1	F	415	ASN	2.2
1	A	469	HIS	2.2
1	C	258	ASP	2.2
1	F	756	ASP	2.2
1	F	494	THR	2.2
1	C	382	ARG	2.2
1	A	928	LEU	2.2
1	F	138	ALA	2.2
1	F	775	HIS	2.2
1	E	592	GLU	2.2
1	F	613	ALA	2.2
1	F	653	ASP	2.2
1	A	286	LEU	2.2
1	F	170	ILE	2.2
1	C	65	ASP	2.2
1	D	612	GLY	2.2
1	B	928	LEU	2.2
1	C	800	ILE	2.2
1	F	308	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	262	LYS	2.2
1	F	326	ALA	2.2
1	C	202	TRP	2.2
1	F	286	LEU	2.1
1	A	653	ASP	2.1
1	D	1017	ASP	2.1
1	A	330	SER	2.1
1	C	988	TRP	2.1
1	F	261	GLY	2.1
1	A	1017	ASP	2.1
1	C	771	LEU	2.1
1	E	286	LEU	2.1
1	E	627	ARG	2.1
1	F	142	PRO	2.1
1	F	628	LYS	2.1
1	E	114	GLU	2.1
1	F	667	ASP	2.1
1	B	705	ALA	2.1
1	D	614	PRO	2.1
1	F	303	ILE	2.1
1	B	494	THR	2.1
1	A	217	VAL	2.1
1	C	165	VAL	2.1
1	B	167	ASN	2.1
1	C	185	PHE	2.1
1	F	270	PHE	2.1
1	B	437	LYS	2.1
1	E	565	GLU	2.1
1	F	282	GLY	2.1
1	C	308	ILE	2.1
1	F	800	ILE	2.1
1	C	415	ASN	2.1
1	F	609	TYR	2.1
1	C	445	ARG	2.1
1	F	43	LEU	2.1
1	F	168	ASP	2.1
1	C	663	GLU	2.1
1	F	232	VAL	2.1
1	F	1020	PHE	2.1
1	F	382	ARG	2.1
1	C	716	GLU	2.0
1	D	199	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	716	GLU	2.0
1	E	97	VAL	2.0
1	A	705	ALA	2.0
1	C	439	THR	2.0
1	F	557	ARG	2.0
1	E	634	ASN	2.0
1	F	240	HIS	2.0
1	C	70	SER	2.0
1	E	561	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.