



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 08:30 PM EDT

PDB ID : 5TAX
EMDB ID: : EMD-8388
Title : Structure of rabbit RyR1 (ryanodine dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-10
Resolution : 6.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

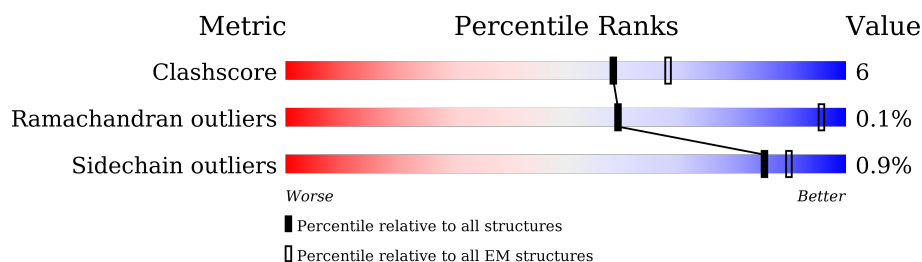
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	80% 19% .
1	F	108	78% 21% .
1	H	108	79% 20% .
1	J	108	76% 23% .
2	B	4416	83% 12% 5%
2	E	4416	83% 12% 5%
2	G	4416	83% 12% 5%
2	I	4416	83% 12% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	


- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

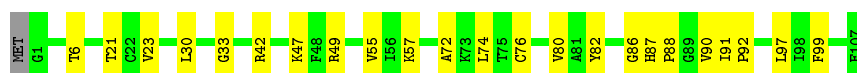
Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0

3 Residue-property plots

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

- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




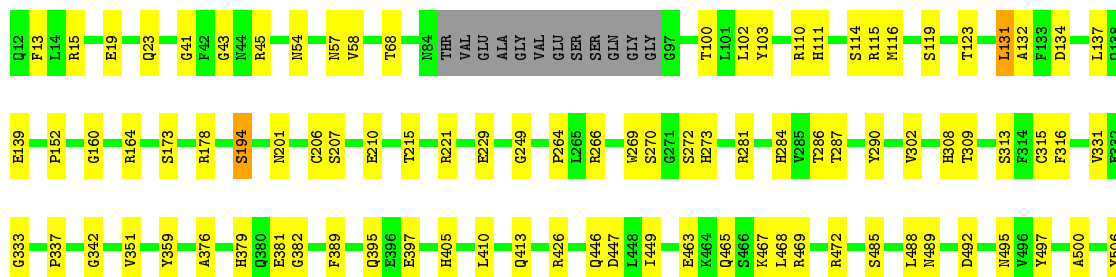
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 

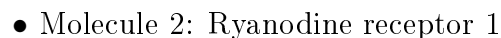


- Molecule 2: Ryanodine receptor 1

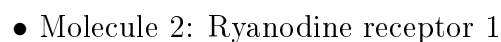
Chain B: 



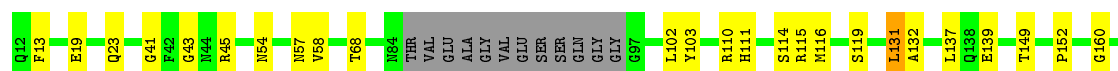
M4231	L3985	Q3830	X3365	K2810	F2340	LEU	R1976	GLU	R1725	L1600	V1149	Y1024	E876	L719	R534
E4232	H9994	S3831	X3369	I2823	V2363	PRO	R1976	GLU	S1726	W1605	M1152	N1035	E880	H720	R534
L4233		Q3833	GLU			ALA	P2002	GLU	R1727	I1153	D1154	N1035	E880	Q735	K550
S4236	H9998	M3836	X3552	E2830	L2357	GLU	Q2003	GLU	R1728	V1615	D1154	N1035	R886	H736	L551
F4237	K4002	M3836	X3556	GLU	G2375	GLU	Q2005	GLU	L1731	GLU	N1158	R1044	I887	L737	D552
T4241	I4019	D3843	R2104	ARG	G2378	GLU	Q2006	GLU	I1735	THR			W891	P740	R553
M4558	N4034	Q3850	Q2107	THR	A2378	GLU	N2007	GLU	R1743	ARG	I1161	E1064	T892		L575
T4561	L4059	A3853	G2132	LVS	P2395	GLU	P2022	GLU	G1764	ALA	L1164	PRO	G894	S745	L575
R4563	D4063	V3874	R2136	THR	G2132	GLU	P2023	GLU	L1771	E1622	L1166	ASP	R897	C746	E580
L4577	K4067	F3880	K2189	ARG	R2028	GLU	L2024	GLU	R1772	GLY		GLN			L583
Y4580	V4081	L3884	Y2192	ARG	F2034	GLU	L2023	GLU	H1775	GLU	L1189	VAL	P905	L776	L589
K4581			GLU	ARG		GLU	L2038	GLU	A1784	VAL	P1190	ASN		P779	V599
V4582	R4085	Q3889	N2196	GLU	L2038	GLU	L2038	GLU	A1788	M1637	V1199	GLN	H911		L600
P4586	I4088	N3896	R2199	ALA	C2042	GLU	C2042	GLU	GLY	A1638	G1200	SER		S782	
GLY		N3897	G2226	GLN	G2043	GLU	G2043	GLU	ALA	L1639	H1201	TRP	P914	F783	L606
ASP	T4104	D3898	V2229	THR	G2048	GLU	G2048	GLU	VAL	Q1631	I1216	D1070	R918	S784	C609
GLY	G4105	F3899	F2235	GLU		GLU		GLU	E1793	E1637	P1243	R1073	L929	G786	H610
ASP	P4106	Q3900	F2235	GLU		GLU		GLU	A1794	L1653	P1247	R1076	L932	K788	R615
MET		N3901	F2235	GLU		GLU		GLU	P1795	Q1660	E1256	A1077	K952	R790	S616
GLU	F4110	T3910	Y2238	GLU		GLU		GLU	A1796	Q1664	E1256	E1078		G794	L626
GLY		T3911	Y2238	GLU		GLU		GLU	R1797	S1664	R1259	K1079	Y859		P627
SER	M4120	T3911	Y2238	GLU		GLU		GLU	I1802	L1667	M1260	S1080		G798	E630
ALA	R4137	D3932	L2257	GLU		GLU		GLU	L1807	R1668	C1269	Y1081	L972	Y808	T635
ALA	P4158	W3935	L2265	THR		THR		THR	L1808	L1667		F1092			
GLY		Y3936	G2266	SER		SER		SER	D1828	R1671	A1273	V1095		R820	T635
LEU	R4161	Y3937	T2271	LEU		LEU		LEU	P1840	L1676	X1286	G1103	L977	L823	L637
ALA	N4163	D3941	P2272	SER		SER		SER	V1841	G1677	X1457	W1104	T978	H338	P646
GLY	F4163	Q3946	L2273	LEU		LEU		LEU	L1844	L1685	X1461	A1105	A980		H647
SER	L4166	N3950	D2274	SER		SER		SER	L1844	L1685	X1461	R1106	T983	P842	L648
GLY	Y4173	M3955	A2277	LEU		LEU		LEU	L1848	H1688	X1461	P1107			F649
GLY	R4180	M3955	E2285	GLU		GLU		GLU	L1848	Q1691	X1473	E1108	R987	H848	R652
SER	I4181	K3959	L2286	THR		THR		THR	I1853	A1697	X1497	L1109	A989	P853	F664
TRP	E4182	Q3960	L2286	VAL		VAL		VAL	F1854	L1698	X1516	P1111			
GLY	I4183	N3963	Q2291	ARG		ARG		ARG	V1859	L1708	X1516	L1120	A1009	D857	V671
SER	M4184	M3963	Q2291	LEU		LEU		LEU	V1859	R1708	X1516	L1120	VAL	THR	
GLY			D2294	VAL		VAL		VAL	M1865	A1709	X1519	V1123	GLN	VAL	H681
ALA	R4188	E3967	L2295	LVS		LVS		LVS	M1865	E1874	X1526	Q1130	ASP	GLN	L682
GLY	S4198	F2929	L2295	LVS		LVS		LVS	E1874	Y1710	X1526	Q1130	ILE	GLN	R683
GLU		G3971	V2298	LVS		LVS		LVS	GLU	Y1712	X1529	P1138	PRO		
ALA	M4201	P2972	R2330	GLU		GLU		GLU	GLU	Y1718	X1529	P1138	ALA	L867	V695
ALA		C3973	R2330	LVS		LVS		LVS	GLU	H1719	P1593	G1140	ARG	I870	V707
GLY	E4227	N3976	L2335	PRO		PRO		PRO	GLU	H1719	P1593	G1140	ARG	I870	
ASP	A4228	E4229	R2336	GLU		GLU		GLU	GLU	L1720	Q1598	R1141	ASN		
GLU		L3980	F2337	GLU		GLU		GLU	GLU	E1721	Q1598	R1141	PRO	K873	D717
ASP	K4230		Q1973	GLU		GLU		GLU	GLU		M1599	V1148	R1020		G718



K873	Y1024	Q735	R534	G333	G160	Q12
E880	M1035	H736	K550	P337	R164	F13
R886	R1044	L737	L551	G342	S173	E19
I887		P740	R553	G342	S173	Q23
W891	M1052	E741	L575	V351	R178	G41
T892	I1053	D742	L575	Y359	T184	P42
F893	E1054	S745	E580	A376	L189	G43
G894	PRO	C746				M44
PRO	R1055		I583	H379	S194	R45
ASP		L750	I586			N54
GLN	R902	R758	L589	G382	M201	N54
GLU	R903	I759	L589			N57
PRO	H004	N760		F389	C206	V58
SER	R905		V599	Q395	S207	
GLN	P914	L776	L600	Q395	E210	T68
VAL		P779	L606	E396		
GLU	R918			E397		N84
ASN					T215	
GLN	R929	S782	C609	H405		THR
SER	L929	F783	R610	H405	R221	VAL
ARG		S784		L410		GLU
TRP	L932	A785	R615			ALA
		G786	S616	Q413	E229	GLY
D1070	G940	F787	R617	Q413	G249	VAL
R1073		K788		R426		GLU
R1076	K952	F789	L626		P264	SER
A1077	Y959	R790		Q446	R265	SER
E1078		G794	E630	D447	R266	GLN
K1079				L448		GLY
S1080	A968		T635	I449	W269	GLY
Y1081		G798	N636		S270	G97
	L972		L637	E463	G271	
F1092		Y808		K464	S272	L102
	L977		P646	Q465	H273	Y103
V1095	T978	R820	N647	S466		R110
G1103	P979		L648	K467	R281	H111
V1104	A980	L823	F649	L468		
A1105	T983	H838	R652	R469	H284	S114
L1106					V285	R115
P1107	R987	P842	F664	R472	T286	M116
E1108	R988			S435	T287	
L1109	A989	H848	V671		Y290	S119
R1110				L488		
P1111	A1009	P853	H681	N489	V302	T123
	VAL		L682			L131
L1120	GLN	D857	R683	D492	R308	A132
ASP	ASP	THR		T309		F133
V1123	PRO	VAL	V695	N495	S313	D134
	PRO	GLN		Y497	F314	
Q1130	ALA	S611	V707			L137
	ARG			A500	F316	Q138
P1138	ASN	L867	D717			E139
F1139	ASN		G718	Y506	V321	
G1140	PRO	I870	L719			P152
L1141			W720			
	P1620					



83% 12% 5%



F3880	W3661	LYS	P2395	Q2005	GLU	R1725	Y1599	M1152	Y1024	K873	D717	Y506	V331	R164
L3884	D6696	LYS	GLY	L2006	GLU	R1728	L1600	I1153	Y1024	E876	G718	Y506	E332	Y172
Q3889	Q3700	THR	ARG	N2007	GLU	R1728	W1605	D1154	N1035	G333	L719	R534	G333	S173
N3896	L3703	ARG	ASP	P2022	GLU	L1731	V1615	N1158	R1044	E880	Q735	K550	P337	R178
N3897	S3706	ILE	ARG	L2023	GLU	I1735	GLU	I1161	E1054	R886	H736	L551	G342	T184
D3898	L3710	GLN	ARG	P2024	ASP	R1743	THR	L1164	PRO	I887	L737	B552	Y351	L189
F3899	T3711	ALA	ARG	L2027	GLU	R1743	ARG	L1165	PRO	W891	P740	L551	Y359	L189
Q3900	E3712	HIS	ALA	R2028	GLU	G1764	ALA	G1166	ASP	T892	S745	L575	Y359	L189
N3901	E3712	GLN	PHE	F2034	LYS	G1764	GLY	G1166	GLN	Y893	C746	E580	A376	S194
T3910	C3733	THR	GLY	L2038	GLU	L1771	E1622	L1169	PRO	G894	L776	E580	A376	N201
T3911	H3734	ASP	GLU	C2042	ASP	R1772	W1626	L1189	SER	R897	L750	E583	H379	C206
D3932	G3738	GLU	PRO	G2043	GLU	A1784	A1627	P1190	GLN	Q380	R758	E583	Y359	S207
W3935	N3741	GLY	GLU	G2049	GLU	A1788	Q1631	V1199	ASN	H904	L776	E583	A376	E210
Y3936	GLY	LYS	GLU	GLU	LYS	ALA	Q1631	G1200	GLN	P905	L776	E583	A376	E210
Y3937	ALA	GLU	GLU	GLU	GLU	GLY	M1637	H1201	SER	P914	P779	E583	A376	T215
D3941	GLU	ASP	ASP	GLU	ASP	ALA	A1638	L1202	ARG	S782	S782	E583	A376	R221
Q3946	E3747	ALA	ALA	PRO	GLU	E1793	Q1631	I1216	TRP	R918	S784	E583	A376	E229
N3950	V3751	GLU	GLU	GLU	GLU	A1794	Q1631	Q1220	D1070	L929	A785	E583	A376	G249
N3955	K3756	LEU	GLU	GLU	GLU	P1795	Q1631	P1243	R1073	L932	G786	E583	A376	P264
K3959	R3762	SER	SER	SER	ALA	R1796	Q1631	P1247	E1078	K952	V788	E583	A376	R266
Q3960	Q3766	ARG	ARG	ARG	PRO	A1797	Q1631	E1256	S1080	Y859	R790	E583	A376	W269
N3963	Q3781	LEU	LEU	LEU	GLY	D1828	L1667	R1259	Y1081	A968	G794	E583	A376	S270
E3967	S3784	SER	SER	SER	LYS	P1840	R1668	M1260	E1091	L972	G798	E583	A376	G271
G3971	K3787	THR	ASP	THR	ASP	V1841	L1671	G1269	F1092	L977	Y808	E583	A376	H273
C3973	S3803	VAL	L1922	THR	L1922	L1844	L1676	X1286	V1095	T978	R820	E583	A376	R281
N3976	I3804	ARG	L1931	VAL	L1931	L1848	G1677	G1677	G1103	P979	L823	E583	A376	H284
L3980	L3805	LEU	P1932	ARG	P1932	L1848	L1685	X1457	A1105	A980	H838	E583	A376	T286
L3985	N3809	VAL	V1935	VAL	V1935	L1853	H1688	X1461	R1106	T863	P842	E583	A376	T287
H3994	L3817	LYS	A1960	LYS	A1960	F1864	H1688	X1473	P1107	R837	R842	E583	A376	Y290
H3998	F3829	LYS	R1964	LYS	R1964	V1859	A1697	X1497	E1108	L988	R848	E583	A376	Y302
K4002	I3832	GLU	Y1965	GLU	Y1965	M1865	L1698	X1516	R1110	A989	R852	E583	A376	V302
L4019	Q3833	LYS	V1966	LYS	V1966	E1874	L1698	X1516	P1111	A1009	P853	E583	A376	H308
M4034	M3836	PRO	L1969	PRO	L1969	GLU	R1708	X1519	L1120	VAL	T857	E583	A376	T309
L4059	Q3850	GLU	L1969	GLU	L1969	GLU	A1709	X1519	L1120	GLN	THR	E583	A376	S313
	A3853	GLU	L1969	GLU	L1969	GLU	Y1710	X1526	V1123	ILE	VAL	E583	A376	F314
		THR	L1969	GLU	L1969	GLU	Y1712	X1526	G1140	ALA	GLN	E583	A376	C315
		GLU	L1969	GLU	L1969	GLU	Y1718	X1529	R1141	ARG	I861	E583	A376	F316
		THR	L1969	GLU	L1969	GLU	H1719	X1529	V1148	ASN	L867	E583	A376	E321
		GLU	L1969	GLU	L1969	GLU	L1720	X1529	V1149	PRO	I870	E583	A376	K322
		GLU	L1969	GLU	L1969	GLU	E1721	X1598	Q1598	R1020		E583	A376	A500

L4928	Q4700	Y4580	D4063
L4935	W4701	K4581	K4067
	W4702	K4582	
K4957	P4712	P4586	V4081
C4958		P4587	
P4959	Y4715	GLY	R4085
L4960		GLY	
C4961	K4718	ASP	L4088
G4962		ASP	
L4963	W4743	NET	T4104
G4964		GLU	G4105
	A4746	GLY	P4106
P4968		SER	
	W4778	ALA	F4110
H4978		ALA	
	V4782	GLY	N4120
E4981		ASP	
E4982	T4785	LEU	R4137
H4983	D4786	ALA	
N4984		GLY	P4158
L4985	F4789	ALA	
A4986		GLY	R4161
	W4796	SER	L4162
L4995	W4797	GLY	P4163
	W4798	GLY	
		GLY	L4166
R5017	A4811	SER	
		GLY	Y4173
G5025	D4815	TRP	
S5026		GLY	R4180
G5027	K4821	SER	L4181
	T4822	GLY	A4182
		ALA	L4183
S5037	T4825	GLY	M4184
		GLU	
	M4833	GLU	R4188
		ALA	
	M4839	GLU	S4198
	V4843	GLY	
		ASP	M4201
	T4852	GLU	
	R4860	ASP	E4227
	C4876	GLU	A4228
		GLY	L4229
	M4880	M4626	K4230
	T4881	M4627	M4231
	C4882	V4628	E4232
			L4233
	H4886	P4641	S4236
	P4904	R4673	
	R4913	E4674	M4558
		L4681	T4561
		Y4687	L4562
			R4563
	V4924	V4697	L4577
		K4698	
		C4699	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.29	0/834	0.53	0/1123
1	F	0.29	0/834	0.53	0/1123
1	H	0.29	0/834	0.53	0/1123
1	J	0.29	0/834	0.53	0/1123
2	B	0.29	0/25428	0.54	7/34534 (0.0%)
2	E	0.29	0/25428	0.54	7/34534 (0.0%)
2	G	0.29	0/25428	0.54	7/34534 (0.0%)
2	I	0.29	0/25428	0.54	7/34534 (0.0%)
All	All	0.29	0/105048	0.54	28/142628 (0.0%)

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
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	8.10	133.93	115.30
2	I	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	B	131	LEU	CA-CB-CG	8.08	133.88	115.30
2	G	131	LEU	CA-CB-CG	8.07	133.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4985	LEU	CA-CB-CG	7.05	131.51	115.30
2	B	4985	LEU	CA-CB-CG	7.04	131.49	115.30
2	I	4985	LEU	CA-CB-CG	7.04	131.48	115.30
2	G	4985	LEU	CA-CB-CG	7.03	131.47	115.30
2	I	1140	GLY	C-N-CA	6.89	138.93	121.70
2	B	1140	GLY	C-N-CA	6.89	138.93	121.70
2	E	1140	GLY	C-N-CA	6.89	138.93	121.70
2	G	1140	GLY	C-N-CA	6.88	138.90	121.70
2	E	1676	LEU	CA-CB-CG	6.50	130.25	115.30
2	G	1676	LEU	CA-CB-CG	6.50	130.24	115.30
2	B	1676	LEU	CA-CB-CG	6.49	130.23	115.30
2	I	1676	LEU	CA-CB-CG	6.48	130.21	115.30
2	E	1600	LEU	CA-CB-CG	6.40	130.02	115.30
2	B	1600	LEU	CA-CB-CG	6.39	130.00	115.30
2	G	1600	LEU	CA-CB-CG	6.38	129.99	115.30
2	I	1600	LEU	CA-CB-CG	6.38	129.98	115.30
2	I	977	LEU	CA-CB-CG	5.36	127.63	115.30
2	G	977	LEU	CA-CB-CG	5.36	127.62	115.30
2	E	977	LEU	CA-CB-CG	5.35	127.60	115.30
2	B	977	LEU	CA-CB-CG	5.35	127.60	115.30
2	B	1667	LEU	CA-CB-CG	5.07	126.96	115.30
2	I	1667	LEU	CA-CB-CG	5.07	126.95	115.30
2	E	1667	LEU	CA-CB-CG	5.06	126.93	115.30
2	G	1667	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	194	SER	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	194	SER	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	194	SER	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-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 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	818	0	824	13	0
1	F	818	0	824	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	818	0	824	12	0
1	J	818	0	824	15	0
2	B	29499	0	24741	329	0
2	E	29499	0	24742	325	0
2	G	29499	0	24741	322	0
2	I	29499	0	24742	324	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102262	1338	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 6.

All (1338) 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)
2:I:4182:GLU:OE2	2:I:4983:HIS:NE2	1.64	1.31
2:E:4182:GLU:OE2	2:E:4983:HIS:NE2	1.64	1.29
2:G:4182:GLU:OE2	2:G:4983:HIS:NE2	1.64	1.29
2:B:4182:GLU:OE2	2:B:4983:HIS:NE2	1.64	1.27
2:G:4982:GLU:OE1	2:G:5027:CYS:SG	1.98	1.22
2:I:4982:GLU:OE1	2:I:5027:CYS:SG	1.98	1.21
2:B:4982:GLU:OE1	2:B:5027:CYS:SG	1.98	1.21
2:E:4982:GLU:OE1	2:E:5027:CYS:SG	1.98	1.20
2:E:4230:LYS:HG3	2:E:4959:PHE:CZ	1.89	1.07
2:G:4230:LYS:HG3	2:G:4959:PHE:CZ	1.89	1.06
2:B:4230:LYS:HG3	2:B:4959:PHE:CZ	1.89	1.06
2:I:4230:LYS:HG3	2:I:4959:PHE:CZ	1.89	1.06
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.50	1.00
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.50	1.00
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.50	0.99
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.50	0.99
2:I:4230:LYS:HG3	2:I:4959:PHE:HZ	1.30	0.96
2:B:4230:LYS:HG3	2:B:4959:PHE:HZ	1.30	0.94
2:G:4230:LYS:HG3	2:G:4959:PHE:HZ	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4230:LYS:HG3	2:E:4959:PHE:HZ	1.30	0.92
2:G:4230:LYS:HD2	2:G:4959:PHE:CZ	2.06	0.91
2:I:4230:LYS:HD2	2:I:4959:PHE:CZ	2.06	0.90
2:E:4230:LYS:HD2	2:E:4959:PHE:CZ	2.06	0.90
2:B:4230:LYS:HD2	2:B:4959:PHE:CZ	2.06	0.89
2:B:4230:LYS:CG	2:B:4959:PHE:CZ	2.59	0.85
2:I:4230:LYS:CG	2:I:4959:PHE:CZ	2.59	0.85
2:G:4230:LYS:CG	2:G:4959:PHE:CZ	2.59	0.84
2:E:4230:LYS:CG	2:E:4959:PHE:CZ	2.59	0.84
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.61	0.83
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.61	0.82
2:G:4968:PHE:CZ	2:G:4978:HIS:ND1	2.48	0.82
2:B:4968:PHE:CZ	2:B:4978:HIS:ND1	2.48	0.82
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.61	0.82
2:I:4968:PHE:CZ	2:I:4978:HIS:ND1	2.48	0.82
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.61	0.81
2:E:4230:LYS:CD	2:E:4959:PHE:CZ	2.63	0.81
2:G:4230:LYS:CD	2:G:4959:PHE:CZ	2.63	0.81
2:E:4968:PHE:CZ	2:E:4978:HIS:ND1	2.48	0.81
2:I:4230:LYS:CD	2:I:4959:PHE:CZ	2.63	0.81
2:B:4230:LYS:CD	2:B:4959:PHE:CZ	2.63	0.81
2:G:4957:LYS:HZ3	2:G:4957:LYS:HB2	1.55	0.72
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.56	0.71
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.56	0.71
2:G:4957:LYS:HG3	2:G:4964:GLY:CA	2.22	0.70
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.56	0.70
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.56	0.70
2:B:4957:LYS:HG3	2:B:4964:GLY:CA	2.22	0.70
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.56	0.70
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.56	0.69
2:E:4957:LYS:HG3	2:E:4964:GLY:CA	2.22	0.69
2:I:4957:LYS:HG3	2:I:4964:GLY:CA	2.22	0.69
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.56	0.69
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.58	0.69
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.58	0.69
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.56	0.69
2:B:4957:LYS:HG3	2:B:4964:GLY:HA2	1.75	0.69
2:G:4957:LYS:HG3	2:G:4964:GLY:HA2	1.76	0.68
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.58	0.68
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.58	0.67
2:I:4957:LYS:HG3	2:I:4964:GLY:HA2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4968:PHE:CZ	2:I:4978:HIS:HE1	2.09	0.67
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.76	0.67
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.76	0.67
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.76	0.66
2:G:4968:PHE:CZ	2:G:4978:HIS:HE1	2.09	0.66
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.76	0.66
2:E:4968:PHE:CZ	2:E:4978:HIS:HE1	2.09	0.66
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.60	0.66
2:E:4957:LYS:HG3	2:E:4964:GLY:HA2	1.76	0.66
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.77	0.66
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.60	0.66
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.31	0.65
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.60	0.65
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.77	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.44	0.65
2:E:379:HIS:HD2	2:E:382:GLY:H	1.44	0.65
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.31	0.65
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.60	0.65
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.31	0.65
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.77	0.65
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.31	0.65
2:B:626:LEU:HD23	2:B:630:GLU:H	1.62	0.64
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.09	0.64
2:G:626:LEU:HD23	2:G:630:GLU:H	1.62	0.64
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.78	0.64
2:E:626:LEU:HD23	2:E:630:GLU:H	1.62	0.64
2:I:379:HIS:HD2	2:I:382:GLY:H	1.44	0.64
2:B:379:HIS:HD2	2:B:382:GLY:H	1.44	0.64
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.63	0.64
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.63	0.64
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.80	0.63
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.80	0.63
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.80	0.63
2:I:626:LEU:HD23	2:I:630:GLU:H	1.62	0.63
2:E:4957:LYS:CG	2:E:4964:GLY:HA2	2.29	0.63
2:B:4957:LYS:CG	2:B:4964:GLY:HA2	2.29	0.62
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.81	0.62
2:E:111:HIS:HD2	2:E:114:SER:H	1.47	0.62
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.80	0.62
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.82	0.62
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:331:VAL:HG12	2:I:333:GLY:H	1.64	0.62
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.82	0.62
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.82	0.62
2:I:4063:ASP:OD2	2:I:4067:LYS:NZ	2.33	0.62
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.82	0.62
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.82	0.62
2:I:4957:LYS:CG	2:I:4964:GLY:HA2	2.29	0.62
2:E:4063:ASP:OD2	2:E:4067:LYS:NZ	2.33	0.62
2:G:4957:LYS:CG	2:G:4964:GLY:HA2	2.29	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.64	0.62
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.81	0.62
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.62
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.63	0.61
2:B:4063:ASP:OD2	2:B:4067:LYS:NZ	2.33	0.61
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.82	0.61
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.81	0.61
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.61
2:G:331:VAL:HG12	2:G:333:GLY:H	1.64	0.61
1:F:87:HIS:H	1:F:91:ILE:HB	1.65	0.61
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.61
2:B:111:HIS:HD2	2:B:114:SER:H	1.47	0.61
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.82	0.61
2:G:4063:ASP:OD2	2:G:4067:LYS:NZ	2.33	0.61
2:B:132:ALA:HA	2:B:194:SER:HB2	1.83	0.61
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.61
2:B:4198:SER:HB3	2:B:4201:ASN:HB2	1.83	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.64	0.61
1:A:87:HIS:H	1:A:91:ILE:HB	1.66	0.61
2:E:132:ALA:HA	2:E:194:SER:HB2	1.83	0.61
1:H:87:HIS:H	1:H:91:ILE:HB	1.66	0.61
2:B:4957:LYS:HZ3	2:B:4957:LYS:HB2	1.65	0.61
2:E:4198:SER:HB3	2:E:4201:ASN:HB2	1.83	0.61
2:G:111:HIS:HD2	2:G:114:SER:H	1.47	0.61
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	1.83	0.60
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	1.83	0.60
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.83	0.60
2:G:4198:SER:HB3	2:G:4201:ASN:HB2	1.83	0.60
2:I:111:HIS:HD2	2:I:114:SER:H	1.47	0.60
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.81	0.60
1:J:87:HIS:H	1:J:91:ILE:HB	1.66	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:ALA:HA	2:I:194:SER:HB2	1.83	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.60
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.83	0.60
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.81	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.60
2:E:4957:LYS:HB2	2:E:4957:LYS:HZ3	1.66	0.60
2:G:132:ALA:HA	2:G:194:SER:HB2	1.83	0.60
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.83	0.60
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.67	0.60
2:I:4198:SER:HB3	2:I:4201:ASN:HB2	1.83	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.60
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.84	0.60
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.67	0.60
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.84	0.60
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.84	0.60
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.35	0.60
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.35	0.60
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.83	0.60
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.84	0.60
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.83	0.59
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.83	0.59
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.35	0.59
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.84	0.59
2:I:683:ARG:NH1	2:I:707:VAL:O	2.36	0.59
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.84	0.59
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	1.83	0.59
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.36	0.59
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	1.83	0.59
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.59
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.67	0.59
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.84	0.59
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.36	0.59
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.59
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.59
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.68	0.59
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.68	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.83	0.59
2:E:315:CYS:SG	2:E:316:PHE:N	2.77	0.58
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.67	0.58
2:E:683:ARG:NH1	2:E:707:VAL:O	2.36	0.58
2:B:315:CYS:SG	2:B:316:PHE:N	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.35	0.58
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.83	0.58
2:B:683:ARG:NH1	2:B:707:VAL:O	2.36	0.58
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.85	0.58
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.84	0.58
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.84	0.58
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.58
2:G:315:CYS:SG	2:G:316:PHE:N	2.77	0.58
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.58
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.85	0.58
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.85	0.58
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.37	0.58
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.85	0.58
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.86	0.58
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.22	0.58
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.86	0.58
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.85	0.58
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.37	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.86	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.37	0.58
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.37	0.58
2:G:683:ARG:NH1	2:G:707:VAL:O	2.36	0.58
2:I:119:SER:H	2:I:137:LEU:HA	1.69	0.58
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.85	0.58
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.58
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.86	0.57
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.85	0.57
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.37	0.57
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.86	0.57
2:G:1865:MET:SD	2:G:1865:MET:N	2.77	0.57
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.37	0.57
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.86	0.57
2:B:119:SER:H	2:B:137:LEU:HA	1.69	0.57
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.86	0.57
2:E:1865:MET:SD	2:E:1865:MET:N	2.77	0.57
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.37	0.57
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.36	0.57
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.68	0.57
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.37	0.57
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.73	0.57
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.86	0.57
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.86	0.57
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.86	0.57
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.37	0.57
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.85	0.57
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.68	0.57
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.86	0.57
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.86	0.57
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.87	0.57
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.36	0.57
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.85	0.57
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.85	0.57
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
2:I:4978:HIS:CE1	2:I:5027:CYS:SG	2.98	0.57
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.86	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:B:1865:MET:SD	2:B:1865:MET:N	2.77	0.57
2:E:4978:HIS:CE1	2:E:5027:CYS:SG	2.98	0.57
2:G:4957:LYS:NZ	2:G:4957:LYS:HB2	2.20	0.57
2:I:1865:MET:SD	2:I:1865:MET:N	2.77	0.57
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.78	0.57
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.85	0.57
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.86	0.57
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.37	0.57
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.86	0.56
2:E:4957:LYS:HB2	2:E:4957:LYS:NZ	2.20	0.56
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.87	0.56
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.73	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.70	0.56
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.86	0.56
2:E:4180:ARG:HH22	2:E:4981:GLU:HA	1.71	0.56
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.86	0.56
2:G:4180:ARG:HH22	2:G:4981:GLU:HA	1.71	0.56
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.37	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.56
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.78	0.56
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.87	0.56
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.88	0.56
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.85	0.56
2:G:4978:HIS:CE1	2:G:5027:CYS:SG	2.98	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.70	0.56
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.86	0.56
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.37	0.56
2:G:119:SER:H	2:G:137:LEU:HA	1.69	0.56
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.86	0.56
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.78	0.56
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.87	0.56
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.86	0.56
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.78	0.56
2:E:119:SER:H	2:E:137:LEU:HA	1.69	0.56
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.22	0.56
2:I:4957:LYS:HB2	2:I:4957:LYS:NZ	2.20	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.39	0.56
2:B:4180:ARG:HH22	2:B:4981:GLU:HA	1.70	0.56
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.88	0.56
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.70	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.39	0.56
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.88	0.56
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.39	0.56
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.39	0.56
2:B:4978:HIS:CE1	2:B:5027:CYS:SG	2.98	0.56
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.87	0.56
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.86	0.56
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.87	0.56
2:G:4968:PHE:HZ	2:G:4978:HIS:HE1	1.54	0.56
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.22	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.71	0.56
2:I:4180:ARG:HH22	2:I:4981:GLU:HA	1.70	0.56
2:B:3932:ASP:HA	2:B:3935:TRP:HD1	1.71	0.56
2:E:2479:LEU:O	2:E:2487:UNK:N	2.39	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.88	0.56
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.88	0.55
2:E:3932:ASP:HA	2:E:3935:TRP:HD1	1.71	0.55
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.38	0.55
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.89	0.55
2:I:4968:PHE:HZ	2:I:4978:HIS:HE1	1.54	0.55
2:B:4983:HIS:H	2:B:4983:HIS:CD2	2.22	0.55
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.88	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:G:3932:ASP:HA	2:G:3935:TRP:HD1	1.71	0.55
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.88	0.55
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.55
2:I:4983:HIS:N	2:I:4983:HIS:CD2	2.73	0.55
2:B:4957:LYS:NZ	2:B:4957:LYS:HB2	2.20	0.55
2:B:606:LEU:O	2:B:617:ASN:ND2	2.40	0.55
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.89	0.55
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.89	0.55
2:B:2479:LEU:O	2:B:2487:UNK:N	2.39	0.55
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.89	0.55
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.38	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.89	0.55
2:G:4184:MET:HE1	2:G:4188:ARG:HE	1.72	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.88	0.55
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.89	0.54
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.73	0.54
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.88	0.54
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.89	0.54
2:I:1667:LEU:O	2:I:1671:ARG:NH1	2.41	0.54
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.88	0.54
2:I:3932:ASP:HA	2:I:3935:TRP:HD1	1.71	0.54
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.89	0.54
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.90	0.54
2:I:2479:LEU:O	2:I:2487:UNK:N	2.39	0.54
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.89	0.54
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.89	0.54
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.89	0.54
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.89	0.54
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.89	0.54
2:G:2479:LEU:O	2:G:2487:UNK:N	2.39	0.54
2:B:1667:LEU:O	2:B:1671:ARG:NH1	2.41	0.54
2:E:2298:VAL:HG21	2:E:2335:LEU:HD21	1.90	0.54
2:E:606:LEU:O	2:E:617:ASN:ND2	2.40	0.54
2:G:606:LEU:O	2:G:617:ASN:ND2	2.40	0.54
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.89	0.54
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.96	0.54
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.88	0.54
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.89	0.54
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.41	0.54
2:G:1667:LEU:O	2:G:1671:ARG:NH1	2.41	0.54
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.89	0.54
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.89	0.54
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.41	0.54
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.41	0.54
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.73	0.54
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.41	0.54
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.90	0.54
2:I:606:LEU:O	2:I:617:ASN:ND2	2.40	0.54
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.38	0.54
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.89	0.54
2:I:4059:LEU:O	2:I:4063:ASP:N	2.36	0.54
2:I:4957:LYS:HZ3	2:I:4957:LYS:HB2	1.72	0.54
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.54
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.90	0.54
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.38	0.54
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.96	0.54
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.41	0.54
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.89	0.53
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.91	0.53
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.89	0.53
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.41	0.53
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.90	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.91	0.53
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.89	0.53
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.89	0.53
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.41	0.53
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.90	0.53
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.90	0.53
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.90	0.53
2:B:4137:ARG:NH1	2:B:4173:TYR:OH	2.42	0.53
2:E:4184:MET:HE1	2:E:4188:ARG:HE	1.74	0.53
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.90	0.53
2:I:2298:VAL:HG21	2:I:2335:LEU:HD21	1.90	0.53
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.73	0.53
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.73	0.53
2:G:2298:VAL:HG21	2:G:2335:LEU:HD21	1.90	0.53
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.42	0.53
1:J:6:THR:HA	1:J:72:ALA:HA	1.91	0.53
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.41	0.53
2:B:2298:VAL:HG21	2:B:2335:LEU:HD21	1.90	0.53
2:E:1667:LEU:O	2:E:1671:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.41	0.53
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.42	0.53
1:F:6:THR:HA	1:F:72:ALA:HA	1.91	0.53
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.91	0.53
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.90	0.53
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.89	0.53
2:B:4968:PHE:HZ	2:B:4978:HIS:HE1	1.54	0.53
2:G:41:GLY:O	2:G:45:ARG:NH1	2.42	0.53
1:H:6:THR:HA	1:H:72:ALA:HA	1.91	0.53
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.91	0.53
2:I:4184:MET:HE1	2:I:4188:ARG:HE	1.73	0.53
1:A:6:THR:HA	1:A:72:ALA:HA	1.91	0.53
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.91	0.53
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.96	0.53
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.42	0.53
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.73	0.53
2:I:266:ARG:NH2	2:I:272:SER:OG	2.42	0.53
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.82	0.53
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.42	0.53
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.90	0.53
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.90	0.53
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.74	0.53
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.91	0.53
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.90	0.53
2:G:173:SER:HB3	2:G:178:ARG:H	1.74	0.53
2:I:173:SER:HB3	2:I:178:ARG:H	1.74	0.53
2:I:647:ASN:ND2	2:I:820:ARG:O	2.42	0.53
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.41	0.53
2:B:4184:MET:HE1	2:B:4188:ARG:HE	1.73	0.52
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.41	0.52
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.41	0.52
2:E:4137:ARG:NH1	2:E:4173:TYR:OH	2.42	0.52
2:E:41:GLY:O	2:E:45:ARG:NH1	2.42	0.52
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.96	0.52
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.91	0.52
2:I:3734:HIS:O	2:I:3738:GLY:N	2.43	0.52
2:I:4137:ARG:NH1	2:I:4173:TYR:OH	2.42	0.52
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.89	0.52
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3734:HIS:O	2:E:3738:GLY:N	2.43	0.52
2:E:4231:MET:HE3	2:E:4960:ILE:HG23	1.91	0.52
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.91	0.52
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	1.92	0.52
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.91	0.52
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.91	0.52
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.52
2:B:173:SER:HB3	2:B:178:ARG:H	1.74	0.52
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.91	0.52
2:G:13:PHE:HA	2:G:164:ARG:HA	1.92	0.52
2:B:313:SER:HB3	2:B:351:VAL:HB	1.92	0.52
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	1.92	0.52
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.42	0.52
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.92	0.52
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.39	0.52
2:G:4137:ARG:NH1	2:G:4173:TYR:OH	2.42	0.52
2:B:266:ARG:NH2	2:B:272:SER:OG	2.42	0.52
2:E:13:PHE:HA	2:E:164:ARG:HA	1.92	0.52
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.82	0.52
2:G:266:ARG:NH2	2:G:272:SER:OG	2.42	0.52
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.90	0.52
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.74	0.52
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.91	0.52
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	1.92	0.52
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.90	0.52
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.91	0.52
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.74	0.52
2:G:3734:HIS:O	2:G:3738:GLY:N	2.43	0.52
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.39	0.52
2:E:173:SER:HB3	2:E:178:ARG:H	1.74	0.52
2:B:41:GLY:O	2:B:45:ARG:NH1	2.42	0.51
2:E:266:ARG:NH2	2:E:272:SER:OG	2.42	0.51
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.51
2:I:13:PHE:HA	2:I:164:ARG:HA	1.92	0.51
2:I:4833:ASN:ND2	2:I:4935:LEU:O	2.44	0.51
2:I:4958:CYS:SG	2:I:4961:CYS:N	2.84	0.51
1:A:82:TYR:O	1:A:86:GLY:N	2.44	0.51
2:E:4833:ASN:ND2	2:E:4935:LEU:O	2.44	0.51
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.92	0.51
2:G:264:PRO:HG2	2:G:270:SER:HB2	1.92	0.51
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:PHE:HA	2:B:164:ARG:HA	1.92	0.51
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.92	0.51
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.91	0.51
2:E:264:PRO:HG2	2:E:270:SER:HB2	1.92	0.51
2:E:4968:PHE:HZ	2:E:4978:HIS:HE1	1.54	0.51
2:G:313:SER:HB3	2:G:351:VAL:HB	1.92	0.51
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.39	0.51
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.92	0.51
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	1.92	0.51
2:I:41:GLY:O	2:I:45:ARG:NH1	2.42	0.51
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.51
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.92	0.51
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.74	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.82	0.51
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.42	0.51
2:G:647:ASN:ND2	2:G:820:ARG:O	2.42	0.51
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.93	0.51
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.38	0.51
2:B:264:PRO:HG2	2:B:270:SER:HB2	1.92	0.51
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.93	0.51
2:B:4833:ASN:ND2	2:B:4935:LEU:O	2.44	0.51
1:F:82:TYR:O	1:F:86:GLY:N	2.44	0.51
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.92	0.51
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.93	0.51
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.93	0.51
2:G:4958:CYS:SG	2:G:4961:CYS:N	2.84	0.51
2:I:264:PRO:HG2	2:I:270:SER:HB2	1.92	0.51
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.76	0.51
2:B:4958:CYS:SG	2:B:4961:CYS:N	2.84	0.51
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.92	0.51
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.93	0.51
2:E:313:SER:HB3	2:E:351:VAL:HB	1.92	0.51
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.93	0.51
1:H:82:TYR:O	1:H:86:GLY:N	2.44	0.51
2:I:313:SER:HB3	2:I:351:VAL:HB	1.92	0.51
1:J:82:TYR:O	1:J:86:GLY:N	2.44	0.51
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.50
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.76	0.50
2:G:4833:ASN:ND2	2:G:4935:LEU:O	2.44	0.50
2:B:3734:HIS:O	2:B:3738:GLY:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.92	0.50
2:E:4958:CYS:SG	2:E:4961:CYS:N	2.84	0.50
2:I:68:THR:N	2:I:110:ARG:O	2.44	0.50
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.94	0.50
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.92	0.50
2:E:68:THR:N	2:E:110:ARG:O	2.44	0.50
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.92	0.50
2:G:4230:LYS:HG3	2:G:4959:PHE:CE2	2.44	0.50
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.76	0.50
2:B:68:THR:N	2:B:110:ARG:O	2.44	0.50
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.93	0.50
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.39	0.50
2:E:647:ASN:ND2	2:E:820:ARG:O	2.42	0.50
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.94	0.50
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.82	0.50
2:I:4182:GLU:OE2	2:I:4983:HIS:CD2	2.57	0.50
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.93	0.50
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.42	0.50
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.94	0.50
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.94	0.50
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.93	0.50
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.93	0.50
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.94	0.50
2:B:3751:VAL:O	2:B:3756:LYS:NZ	2.45	0.50
2:B:978:THR:HB	2:B:980:ALA:H	1.77	0.50
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.94	0.50
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.77	0.50
2:I:978:THR:HB	2:I:980:ALA:H	1.77	0.50
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.93	0.50
2:E:3751:VAL:O	2:E:3756:LYS:NZ	2.45	0.50
2:I:3751:VAL:O	2:I:3756:LYS:NZ	2.45	0.50
2:I:4978:HIS:HE1	2:I:5027:CYS:SG	2.35	0.50
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.45	0.49
2:B:647:ASN:ND2	2:B:820:ARG:O	2.42	0.49
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.94	0.49
2:E:359:TYR:HA	2:E:376:ALA:HA	1.94	0.49
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.94	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.92	0.49
2:G:221:ARG:NH2	2:G:397:GLU:OE2	2.45	0.49
2:G:3941:ASP:HA	2:G:4002:LYS:HE3	1.94	0.49
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.92	0.49
2:B:3941:ASP:HA	2:B:4002:LYS:HE3	1.94	0.49
2:B:4978:HIS:HE1	2:B:5027:CYS:SG	2.35	0.49
2:E:3941:ASP:HA	2:E:4002:LYS:HE3	1.94	0.49
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.45	0.49
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.94	0.49
2:B:4962:GLY:HA3	2:B:5025:GLY:HA2	1.95	0.49
2:E:4978:HIS:HE1	2:E:5027:CYS:SG	2.35	0.49
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.93	0.49
2:G:68:THR:N	2:G:110:ARG:O	2.44	0.49
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.77	0.49
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.38	0.49
2:E:221:ARG:NH2	2:E:397:GLU:OE2	2.45	0.49
2:E:4230:LYS:HG3	2:E:4959:PHE:CE2	2.44	0.49
2:E:4962:GLY:HA3	2:E:5025:GLY:HA2	1.95	0.49
2:G:359:TYR:HA	2:G:376:ALA:HA	1.94	0.49
2:B:284:HIS:HB3	2:B:287:THR:HB	1.94	0.49
2:B:4059:LEU:O	2:B:4063:ASP:N	2.36	0.49
2:E:395:GLN:HG3	2:E:397:GLU:H	1.78	0.49
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.93	0.49
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.45	0.49
2:B:485:SER:O	2:B:489:ASN:N	2.40	0.49
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.95	0.49
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.94	0.49
2:G:3751:VAL:O	2:G:3756:LYS:NZ	2.45	0.49
2:G:395:GLN:HG3	2:G:397:GLU:H	1.78	0.49
2:I:4231:MET:CE	2:I:4960:ILE:HG23	2.43	0.49
2:B:4231:MET:CE	2:B:4960:ILE:HG23	2.43	0.49
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.95	0.49
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.95	0.49
2:E:776:LEU:HG	2:E:848:HIS:HA	1.95	0.49
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.94	0.49
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.94	0.49
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.94	0.49
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.95	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.94	0.49
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.46	0.49
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.76	0.49
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.77	0.49
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.95	0.49
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:615:ARG:NH2	2:B:1677:GLY:O	2.43	0.49
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.95	0.49
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.95	0.49
2:B:4230:LYS:HG3	2:B:4959:PHE:CE2	2.44	0.48
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.45	0.48
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.95	0.48
2:G:284:HIS:HB3	2:G:287:THR:HB	1.94	0.48
2:G:4978:HIS:HE1	2:G:5027:CYS:SG	2.35	0.48
2:I:4833:ASN:HD21	2:I:4935:LEU:HG	1.78	0.48
2:B:359:TYR:HA	2:B:376:ALA:HA	1.94	0.48
2:B:43:GLY:N	2:B:447:ASP:OD2	2.43	0.48
2:B:776:LEU:HG	2:B:848:HIS:HA	1.95	0.48
2:E:867:LEU:HB3	2:E:929:LEU:HD13	1.95	0.48
2:G:978:THR:HB	2:G:980:ALA:H	1.77	0.48
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	2.48	0.48
2:B:4833:ASN:HD21	2:B:4935:LEU:HG	1.78	0.48
2:E:4962:GLY:H	2:E:5025:GLY:N	2.12	0.48
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.95	0.48
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.79	0.48
2:I:3941:ASP:HA	2:I:4002:LYS:HE3	1.94	0.48
2:I:4962:GLY:H	2:I:5025:GLY:N	2.12	0.48
2:B:1516:UNK:N	2:B:1529:UNK:O	2.47	0.48
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.43	0.48
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.95	0.48
2:E:4833:ASN:HD21	2:E:4935:LEU:HG	1.78	0.48
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.43	0.48
2:I:4962:GLY:HA3	2:I:5025:GLY:HA2	1.95	0.48
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.96	0.48
2:E:43:GLY:N	2:E:447:ASP:OD2	2.43	0.48
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.46	0.48
2:E:978:THR:HB	2:E:980:ALA:H	1.77	0.48
2:G:1516:UNK:N	2:G:1529:UNK:O	2.47	0.48
2:G:4962:GLY:HA3	2:G:5025:GLY:HA2	1.95	0.48
2:G:867:LEU:HB3	2:G:929:LEU:HD13	1.95	0.48
2:I:1660:GLN:O	2:I:1664:SER:N	2.47	0.48
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.94	0.48
2:I:359:TYR:HA	2:I:376:ALA:HA	1.94	0.48
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.79	0.48
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.38	0.48
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.77	0.48
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4233:LEU:HA	2:E:4236:SER:HB3	1.95	0.48
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.46	0.48
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.94	0.48
2:G:4231:MET:CE	2:G:4960:ILE:HG23	2.43	0.48
2:G:4962:GLY:H	2:G:5025:GLY:N	2.12	0.48
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.94	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.94	0.48
2:E:1516:UNK:N	2:E:1529:UNK:O	2.47	0.48
2:E:2285:GLU:HG3	2:E:2286:LEU:HG	1.96	0.48
2:E:284:HIS:HB3	2:E:287:THR:HB	1.94	0.48
2:E:4059:LEU:O	2:E:4063:ASP:N	2.36	0.48
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.95	0.48
2:G:4059:LEU:O	2:G:4063:ASP:N	2.36	0.48
2:G:4833:ASN:HD21	2:G:4935:LEU:HG	1.78	0.48
2:I:615:ARG:NH2	2:I:1677:GLY:O	2.43	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.95	0.48
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.95	0.48
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.95	0.48
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.79	0.48
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.96	0.48
2:I:1516:UNK:N	2:I:1529:UNK:O	2.47	0.48
2:I:284:HIS:HB3	2:I:287:THR:HB	1.94	0.48
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.95	0.48
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.94	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.78	0.48
2:B:867:LEU:HB3	2:B:929:LEU:HD13	1.95	0.48
2:E:3900:GLN:NE2	2:E:3967:GLU:O	2.47	0.48
2:E:4231:MET:CE	2:E:4960:ILE:HG23	2.43	0.48
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.47	0.48
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.95	0.48
2:I:395:GLN:HG3	2:I:397:GLU:H	1.78	0.48
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.95	0.48
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.79	0.48
2:G:2285:GLU:HG3	2:G:2286:LEU:HG	1.96	0.48
1:J:57:LYS:HB2	1:J:80:VAL:HB	1.96	0.48
2:B:2285:GLU:HG3	2:B:2286:LEU:HG	1.96	0.47
2:E:4230:LYS:HD2	2:E:4959:PHE:CE2	2.49	0.47
1:F:57:LYS:HB2	1:F:80:VAL:HB	1.96	0.47
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.95	0.47
2:G:776:LEU:HG	2:G:848:HIS:HA	1.95	0.47
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.96	0.47
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.95	0.47
2:B:1685:LEU:HD22	2:B:1718:ILE:HG21	1.96	0.47
2:B:4233:LEU:HA	2:B:4236:SER:HB3	1.95	0.47
2:E:983:THR:O	2:E:987:ARG:N	2.47	0.47
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.47	0.47
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.47	0.47
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.95	0.47
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.47	0.47
2:G:3900:GLN:NE2	2:G:3967:GLU:O	2.47	0.47
2:G:4230:LYS:HD2	2:G:4959:PHE:CE2	2.48	0.47
2:I:116:MET:HB2	2:I:137:LEU:HD12	1.96	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.47	0.47
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.47	0.47
1:A:57:LYS:HB2	1:A:80:VAL:HB	1.96	0.47
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.95	0.47
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.97	0.47
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.47	0.47
2:G:116:MET:HB2	2:G:137:LEU:HD12	1.96	0.47
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.43	0.47
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.48	0.47
2:G:1685:LEU:HD22	2:G:1718:ILE:HG21	1.96	0.47
2:I:2285:GLU:HG3	2:I:2286:LEU:HG	1.96	0.47
2:I:4231:MET:HE3	2:I:4960:ILE:HG23	1.95	0.47
2:I:4586:PRO:HB3	2:I:4628:VAL:HG21	1.97	0.47
2:I:983:THR:O	2:I:987:ARG:N	2.47	0.47
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.94	0.47
2:B:221:ARG:NH2	2:B:397:GLU:OE2	2.45	0.47
2:E:1685:LEU:HD22	2:E:1718:ILE:HG21	1.96	0.47
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.30	0.47
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.96	0.47
2:G:983:THR:O	2:G:987:ARG:N	2.47	0.47
2:B:3900:GLN:NE2	2:B:3967:GLU:O	2.47	0.47
2:B:4182:GLU:OE2	2:B:4983:HIS:CD2	2.57	0.47
2:B:4822:THR:O	2:B:4825:THR:OG1	2.32	0.47
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.97	0.47
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.97	0.47
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.38	0.47
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.97	0.47
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.97	0.47
2:G:4233:LEU:HA	2:G:4236:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3900:GLN:NE2	2:I:3967:GLU:O	2.47	0.47
2:E:4558:ASN:HB2	2:E:4561:THR:HB	1.97	0.47
2:G:1660:GLN:O	2:G:1664:SER:N	2.47	0.47
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.97	0.47
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.97	0.47
2:I:894:GLY:HA3	2:I:903:LEU:HD22	1.97	0.47
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.97	0.47
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.97	0.47
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.47	0.47
2:B:4586:PRO:HB3	2:B:4628:VAL:HG21	1.97	0.47
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.95	0.47
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.96	0.47
2:G:4586:PRO:HB3	2:G:4628:VAL:HG21	1.97	0.47
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.80	0.47
1:H:57:LYS:HB2	1:H:80:VAL:HB	1.96	0.47
2:I:468:LEU:HB3	2:I:472:ARG:HH12	1.80	0.47
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.47	0.47
2:B:4962:GLY:H	2:B:5025:GLY:N	2.12	0.47
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.80	0.47
2:E:4158:PRO:HA	2:E:4161:ARG:HB2	1.97	0.47
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.97	0.47
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.80	0.46
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.97	0.46
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.97	0.46
2:G:4158:PRO:HA	2:G:4161:ARG:HB2	1.97	0.46
2:I:4233:LEU:HA	2:I:4236:SER:HB3	1.95	0.46
2:I:488:LEU:O	2:I:492:ASP:N	2.45	0.46
2:I:867:LEU:HB3	2:I:929:LEU:HD13	1.95	0.46
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.96	0.46
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.43	0.46
2:E:468:LEU:HB3	2:E:472:ARG:HH12	1.80	0.46
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.80	0.46
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.97	0.46
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.96	0.46
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.98	0.46
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.97	0.46
2:E:1660:GLN:O	2:E:1664:SER:N	2.47	0.46
2:E:615:ARG:NH2	2:E:1677:GLY:O	2.43	0.46
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.97	0.46
2:G:3528:UNK:HA	2:E:1220:GLN:NE2	2.30	0.46
2:G:4697:VAL:O	2:G:4701:TRP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:894:GLY:HA3	2:G:903:LEU:HD22	1.97	0.46
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.43	0.46
2:B:116:MET:HB2	2:B:137:LEU:HD12	1.96	0.46
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.96	0.46
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.81	0.46
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.47	0.46
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.98	0.46
1:J:21:THR:HA	1:J:49:ARG:HA	1.98	0.46
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.80	0.46
2:B:4558:ASN:HB2	2:B:4561:THR:HB	1.97	0.46
2:E:116:MET:HB2	2:E:137:LEU:HD12	1.96	0.46
2:E:286:THR:HA	2:E:405:HIS:HB2	1.98	0.46
2:E:4882:CYS:SG	2:E:4886:HIS:NE2	2.89	0.46
2:G:4182:GLU:OE2	2:G:4983:HIS:CD2	2.57	0.46
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.98	0.46
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.80	0.46
2:I:4558:ASN:HB2	2:I:4561:THR:HB	1.97	0.46
2:B:4231:MET:HE3	2:B:4960:ILE:HG23	1.97	0.46
2:B:468:LEU:HB3	2:B:472:ARG:HH12	1.80	0.46
2:B:870:ILE:HD12	2:B:873:LYS:HB2	1.98	0.46
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.97	0.46
2:E:4957:LYS:HG3	2:E:4964:GLY:HA3	1.96	0.46
2:E:870:ILE:HD12	2:E:873:LYS:HB2	1.98	0.46
2:G:4957:LYS:HG3	2:G:4964:GLY:HA3	1.97	0.46
1:H:21:THR:HA	1:H:49:ARG:HA	1.98	0.46
2:I:3696:ASP:O	2:I:3700:GLN:N	2.46	0.46
2:I:786:GLY:HA2	2:I:1631:GLN:HA	1.98	0.46
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.80	0.46
2:I:870:ILE:HD12	2:I:873:LYS:HB2	1.98	0.46
2:B:786:GLY:HA2	2:B:1631:GLN:HA	1.98	0.46
2:B:983:THR:O	2:B:987:ARG:N	2.47	0.46
2:E:4924:VAL:HG12	2:E:4928:LEU:HD12	1.98	0.46
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.80	0.46
2:G:286:THR:HA	2:G:405:HIS:HB2	1.98	0.46
2:G:4960:ILE:O	2:G:4960:ILE:HG22	2.16	0.46
2:G:870:ILE:HD12	2:G:873:LYS:HB2	1.98	0.46
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.81	0.46
2:E:786:GLY:HA2	2:E:1631:GLN:HA	1.98	0.46
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.97	0.46
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.98	0.46
2:G:786:GLY:HA2	2:G:1631:GLN:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.47	0.46
2:I:4230:LYS:HG3	2:I:4959:PHE:CE2	2.44	0.46
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.97	0.46
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.81	0.46
2:B:894:GLY:HA3	2:B:903:LEU:HD22	1.97	0.46
2:E:2375:GLY:HA3	2:E:2378:ALA:HB3	1.98	0.46
2:E:4586:PRO:HB3	2:E:4628:VAL:HG21	1.97	0.46
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.98	0.46
2:I:4697:VAL:O	2:I:4701:TRP:N	2.47	0.46
2:I:4882:CYS:SG	2:I:4886:HIS:NE2	2.89	0.46
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.98	0.46
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.98	0.46
2:B:4924:VAL:HG12	2:B:4928:LEU:HD12	1.98	0.46
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.46
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.81	0.46
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.48	0.46
1:F:21:THR:HA	1:F:49:ARG:HA	1.98	0.46
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.81	0.46
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.81	0.46
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.96	0.46
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.98	0.46
2:I:2517:UNK:O	2:I:2521:UNK:N	2.49	0.46
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.45
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	1.98	0.45
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.98	0.45
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.45
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.99	0.45
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.98	0.45
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.98	0.45
2:I:4960:ILE:O	2:I:4960:ILE:HG22	2.16	0.45
2:I:880:GLU:OE1	2:I:968:ALA:N	2.47	0.45
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.97	0.45
2:B:4158:PRO:HA	2:B:4161:ARG:HB2	1.97	0.45
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.45
2:G:468:LEU:HB3	2:G:472:ARG:HH12	1.80	0.45
2:I:790:ARG:HG2	2:I:1627:ALA:HA	1.98	0.45
2:I:794:GLY:H	2:I:798:GLY:HA3	1.82	0.45
2:B:2517:UNK:O	2:B:2521:UNK:N	2.49	0.45
2:B:4882:CYS:SG	2:B:4886:HIS:NE2	2.89	0.45
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.45
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.98	0.45
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.97	0.45
1:A:21:THR:HA	1:A:49:ARG:HA	1.98	0.45
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.98	0.45
2:B:2375:GLY:HA3	2:B:2378:ALA:HB3	1.98	0.45
2:E:1148:VAL:HB	2:E:1165:ASN:HA	1.98	0.45
2:E:2517:UNK:O	2:E:2521:UNK:N	2.49	0.45
2:E:894:GLY:HA3	2:E:903:LEU:HD22	1.97	0.45
2:G:2517:UNK:O	2:G:2521:UNK:N	2.49	0.45
2:G:485:SER:HA	2:G:488:LEU:HB2	1.99	0.45
2:G:794:GLY:H	2:G:798:GLY:HA3	1.82	0.45
2:I:1148:VAL:HB	2:I:1165:ASN:HA	1.98	0.45
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.52	0.45
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.81	0.45
2:I:3943:ILE:HD11	2:I:4002:LYS:HZ3	1.81	0.45
2:I:4059:LEU:HD13	2:I:4166:LEU:HB3	1.99	0.45
2:B:1660:GLN:O	2:B:1664:SER:N	2.47	0.45
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.81	0.45
2:B:266:ARG:NH2	2:B:269:TRP:O	2.50	0.45
2:B:2874:MET:O	2:B:2878:LEU:N	2.42	0.45
2:E:4782:VAL:O	2:E:4785:THR:OG1	2.30	0.45
2:G:266:ARG:NH2	2:G:269:TRP:O	2.50	0.45
2:G:4059:LEU:HD13	2:G:4166:LEU:HB3	1.99	0.45
2:I:2375:GLY:HA3	2:I:2378:ALA:HB3	1.98	0.45
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.46	0.45
2:B:4957:LYS:HG3	2:B:4964:GLY:HA3	1.96	0.45
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.97	0.45
2:E:4059:LEU:HD13	2:E:4166:LEU:HB3	1.99	0.45
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.99	0.45
2:I:4158:PRO:HA	2:I:4161:ARG:HB2	1.97	0.45
2:I:4957:LYS:HG3	2:I:4964:GLY:HA3	1.96	0.45
2:B:2587:UNK:O	2:B:2591:UNK:N	2.50	0.45
2:B:286:THR:HA	2:B:405:HIS:HB2	1.98	0.45
2:B:4059:LEU:HD13	2:B:4166:LEU:HB3	1.99	0.45
2:B:794:GLY:H	2:B:798:GLY:HA3	1.82	0.45
2:E:485:SER:HA	2:E:488:LEU:HB2	1.99	0.45
2:E:892:THR:N	2:E:902:ARG:O	2.48	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.52	0.45
2:I:221:ARG:NH2	2:I:397:GLU:OE2	2.45	0.45
2:I:495:ASN:HD21	2:I:550:LYS:HE3	1.82	0.45
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3658:LYS:HA	2:B:3661:TRP:CE2	2.52	0.45
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	1.99	0.45
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.98	0.45
2:B:4697:VAL:O	2:B:4701:TRP:N	2.47	0.45
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.99	0.45
2:E:4960:ILE:HG22	2:E:4960:ILE:O	2.16	0.45
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	1.99	0.45
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.98	0.45
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.34	0.45
2:G:4924:VAL:HG12	2:G:4928:LEU:HD12	1.98	0.45
2:G:495:ASN:HD21	2:G:550:LYS:HE3	1.82	0.45
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	1.99	0.45
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.82	0.45
2:E:2235:PHE:HA	2:E:2238:TYR:HD2	1.82	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.82	0.45
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.98	0.45
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.99	0.45
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.99	0.45
2:I:286:THR:HA	2:I:405:HIS:HB2	1.98	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.52	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.82	0.45
2:E:2874:MET:O	2:E:2878:LEU:N	2.42	0.45
2:E:794:GLY:H	2:E:798:GLY:HA3	1.82	0.45
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.45
2:G:790:ARG:HG2	2:G:1627:ALA:HA	1.98	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.52	0.45
2:G:2235:PHE:HA	2:G:2238:TYR:HD2	1.82	0.45
2:G:2375:GLY:HA3	2:G:2378:ALA:HB3	1.98	0.45
2:G:4558:ASN:HB2	2:G:4561:THR:HB	1.97	0.45
2:G:652:ARG:HB2	2:G:750:LEU:HD13	1.99	0.45
2:I:43:GLY:N	2:I:447:ASP:OD2	2.43	0.45
2:I:4924:VAL:HG12	2:I:4928:LEU:HD12	1.98	0.45
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.98	0.44
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.99	0.44
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.98	0.44
2:G:1148:VAL:HB	2:G:1165:ASN:HA	1.98	0.44
2:G:2034:PHE:O	2:G:2038:LEU:N	2.50	0.44
2:G:4798:MET:HG3	2:G:4811:ALA:HB3	1.99	0.44
2:G:4848:VAL:O	2:G:4852:THR:N	2.50	0.44
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.82	0.44
2:I:1457:UNK:N	2:I:1497:UNK:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1105:ALA:O	2:B:1189:LEU:N	2.51	0.44
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.99	0.44
2:B:4848:VAL:O	2:B:4852:THR:N	2.50	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.70	0.44
2:B:4960:ILE:HG22	2:B:4960:ILE:O	2.16	0.44
2:B:495:ASN:HD21	2:B:550:LYS:HE3	1.82	0.44
2:E:2034:PHE:O	2:E:2038:LEU:N	2.50	0.44
2:G:3943:ILE:HD11	2:G:4002:LYS:HZ3	1.83	0.44
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.99	0.44
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.51	0.44
2:I:2587:UNK:O	2:I:2591:UNK:N	2.50	0.44
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.48	0.44
2:B:2235:PHE:HA	2:B:2238:TYR:HD2	1.82	0.44
2:E:206:CYS:SG	2:E:207:SER:N	2.90	0.44
2:E:2587:UNK:O	2:E:2591:UNK:N	2.50	0.44
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.99	0.44
2:E:54:ASN:O	2:E:58:VAL:N	2.47	0.44
2:G:1105:ALA:N	2:G:1189:LEU:O	2.50	0.44
2:G:4959:PHE:CD2	2:G:4959:PHE:O	2.70	0.44
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.81	0.44
2:I:4798:MET:HG3	2:I:4811:ALA:HB3	2.00	0.44
2:I:485:SER:HA	2:I:488:LEU:HB2	1.99	0.44
2:B:1457:UNK:N	2:B:1497:UNK:O	2.50	0.44
2:B:2034:PHE:O	2:B:2038:LEU:N	2.50	0.44
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.51	0.44
2:B:290:TYR:O	2:B:302:VAL:N	2.51	0.44
2:E:790:ARG:HG2	2:E:1627:ALA:HA	1.98	0.44
2:E:266:ARG:NH2	2:E:269:TRP:O	2.49	0.44
2:E:4848:VAL:O	2:E:4852:THR:N	2.50	0.44
2:E:495:ASN:HD21	2:E:550:LYS:HE3	1.82	0.44
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.99	0.44
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.51	0.44
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.99	0.44
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.98	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CD2	2.70	0.44
2:B:215:THR:HG22	2:B:273:HIS:HA	2.00	0.44
2:B:4782:VAL:O	2:B:4785:THR:OG1	2.30	0.44
2:E:290:TYR:O	2:E:302:VAL:N	2.51	0.44
2:E:551:LEU:HD11	2:E:589:LEU:HD13	2.00	0.44
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.82	0.44
2:I:206:CYS:SG	2:I:207:SER:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2235:PHE:HA	2:I:2238:TYR:HD2	1.82	0.44
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.99	0.44
2:B:1148:VAL:HB	2:B:1165:ASN:HA	1.98	0.44
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.99	0.44
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.00	0.44
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.99	0.44
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.51	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.52	0.44
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.98	0.44
2:E:4798:MET:HG3	2:E:4811:ALA:HB3	1.99	0.44
2:E:488:LEU:O	2:E:492:ASP:N	2.45	0.44
2:E:4959:PHE:CD2	2:E:4959:PHE:O	2.70	0.44
2:E:4959:PHE:CG	2:E:4959:PHE:O	2.70	0.44
2:G:206:CYS:SG	2:G:207:SER:N	2.90	0.44
2:G:914:PRO:O	2:G:918:ARG:N	2.48	0.44
2:I:266:ARG:NH2	2:I:269:TRP:O	2.50	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.82	0.44
2:B:790:ARG:HG2	2:B:1627:ALA:HA	1.98	0.44
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.00	0.44
2:G:4959:PHE:CG	2:G:4959:PHE:O	2.70	0.44
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.81	0.44
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.82	0.44
2:I:4848:VAL:O	2:I:4852:THR:N	2.51	0.44
2:I:681:HIS:O	2:I:784:SER:N	2.45	0.44
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	2.00	0.44
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.44
2:B:485:SER:HA	2:B:488:LEU:HB2	1.99	0.44
2:B:4959:PHE:CD2	2:B:4959:PHE:O	2.70	0.44
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.99	0.44
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.00	0.44
2:G:43:GLY:N	2:G:447:ASP:OD2	2.43	0.44
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.48	0.44
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	2.00	0.44
2:I:2034:PHE:O	2:I:2038:LEU:N	2.50	0.44
2:I:485:SER:O	2:I:489:ASN:N	2.40	0.44
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	1.99	0.44
2:E:1841:VAL:HG13	2:E:1844:LEU:HD23	2.00	0.44
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	1.99	0.44
2:G:2353:VAL:O	2:G:2357:LEU:N	2.51	0.44
2:G:2587:UNK:O	2:G:2591:UNK:N	2.50	0.44
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1841:VAL:HG13	2:I:1844:LEU:HD23	2.00	0.44
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.00	0.44
2:I:4959:PHE:CG	2:I:4959:PHE:O	2.70	0.44
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.00	0.44
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.83	0.43
2:E:1105:ALA:O	2:E:1189:LEU:N	2.51	0.43
2:E:1105:ALA:N	2:E:1189:LEU:O	2.50	0.43
2:E:1457:UNK:N	2:E:1497:UNK:O	2.50	0.43
2:G:215:THR:HG22	2:G:273:HIS:HA	2.00	0.43
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.00	0.43
2:G:892:THR:N	2:G:902:ARG:O	2.48	0.43
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	2.00	0.43
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	1.99	0.43
2:I:914:PRO:O	2:I:918:ARG:N	2.48	0.43
2:B:1841:VAL:HG13	2:B:1844:LEU:HD23	2.00	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.90	0.43
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	1.99	0.43
2:E:4697:VAL:O	2:E:4701:TRP:N	2.47	0.43
2:E:575:LEU:HD22	2:E:609:CYS:HB3	2.00	0.43
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.00	0.43
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.43
2:G:488:LEU:O	2:G:492:ASP:N	2.45	0.43
2:G:551:LEU:HD11	2:G:589:LEU:HD13	2.00	0.43
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.99	0.43
2:I:551:LEU:HD11	2:I:589:LEU:HD13	2.00	0.43
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.82	0.43
2:B:4798:MET:HG3	2:B:4811:ALA:HB3	1.99	0.43
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.00	0.43
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.00	0.43
2:E:880:GLU:OE1	2:E:968:ALA:N	2.48	0.43
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.00	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.52	0.43
2:G:3805:LEU:HG	2:G:3805:LEU:H	1.74	0.43
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.00	0.43
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.00	0.43
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.99	0.43
2:E:4182:GLU:OE2	2:E:4983:HIS:CD2	2.57	0.43
2:G:1457:UNK:N	2:G:1497:UNK:O	2.50	0.43
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.88	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:B:551:LEU:HD11	2:B:589:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:215:THR:HG22	2:E:273:HIS:HA	2.00	0.43
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.99	0.43
2:G:485:SER:O	2:G:489:ASN:N	2.40	0.43
2:G:575:LEU:HD22	2:G:609:CYS:HB3	2.00	0.43
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.99	0.43
2:I:290:TYR:O	2:I:302:VAL:N	2.51	0.43
2:I:4230:LYS:HD2	2:I:4959:PHE:CE2	2.48	0.43
2:B:2353:VAL:O	2:B:2357:LEU:N	2.51	0.43
2:B:3552:UNK:O	2:B:3556:UNK:N	2.52	0.43
2:E:1154:ASP:O	2:E:1158:ASN:N	2.52	0.43
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.52	0.43
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.51	0.43
2:E:4984:ASN:ND2	2:E:4986:ALA:HB3	2.33	0.43
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.52	0.43
2:G:4984:ASN:ND2	2:G:4986:ALA:HB3	2.33	0.43
2:G:683:ARG:HG2	2:G:717:ASP:HB3	2.01	0.43
2:G:880:GLU:OE1	2:G:968:ALA:N	2.48	0.43
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.01	0.43
2:B:3994:HIS:O	2:B:3998:HIS:ND1	2.46	0.43
2:B:575:LEU:HD22	2:B:609:CYS:HB3	2.00	0.43
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.83	0.43
2:E:2353:VAL:O	2:E:2357:LEU:N	2.51	0.43
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.00	0.43
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.89	0.43
2:G:1105:ALA:O	2:G:1189:LEU:N	2.51	0.43
2:I:1269:CYS:HA	2:I:1473:UNK:HA	2.01	0.43
2:I:215:THR:HG22	2:I:273:HIS:HA	2.00	0.43
2:I:4982:GLU:HB3	2:I:4983:HIS:H	1.71	0.43
2:I:4984:ASN:ND2	2:I:4986:ALA:HB3	2.33	0.43
2:I:929:LEU:HD23	2:I:932:LEU:HD12	2.01	0.43
2:B:683:ARG:HG2	2:B:717:ASP:HB3	2.01	0.43
2:B:892:THR:N	2:B:902:ARG:O	2.48	0.43
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.01	0.43
2:E:929:LEU:HD23	2:E:932:LEU:HD12	2.01	0.43
2:G:1841:VAL:HG13	2:G:1844:LEU:HD23	2.00	0.43
2:G:290:TYR:O	2:G:302:VAL:N	2.51	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.84	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.52	0.43
2:I:3552:UNK:O	2:I:3556:UNK:N	2.52	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.99	0.43
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4984:ASN:ND2	2:B:4986:ALA:HB3	2.33	0.43
2:G:929:LEU:HD23	2:G:932:LEU:HD12	2.01	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.83	0.43
2:B:1154:ASP:O	2:B:1158:ASN:N	2.52	0.43
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.43
2:B:4962:GLY:H	2:B:5025:GLY:HA2	1.84	0.43
2:B:929:LEU:HD23	2:B:932:LEU:HD12	2.01	0.43
2:E:1269:CYS:HA	2:E:1473:UNK:HA	2.01	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.83	0.43
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.52	0.43
2:I:683:ARG:HG2	2:I:717:ASP:HB3	2.01	0.43
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.84	0.42
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.48	0.42
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.01	0.42
2:E:3552:UNK:O	2:E:3556:UNK:N	2.52	0.42
2:I:2874:MET:O	2:I:2878:LEU:N	2.42	0.42
2:B:1105:ALA:N	2:B:1189:LEU:O	2.50	0.42
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.01	0.42
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	2.00	0.42
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.85	0.42
2:E:379:HIS:CD2	2:E:382:GLY:H	2.32	0.42
2:E:4962:GLY:H	2:E:5025:GLY:HA2	1.84	0.42
2:I:4962:GLY:H	2:I:5025:GLY:HA2	1.84	0.42
2:B:3703:LEU:HA	2:B:3706:SER:HB3	2.01	0.42
2:B:54:ASN:O	2:B:58:VAL:N	2.47	0.42
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.84	0.42
2:E:3832:ILE:O	2:E:3836:MET:N	2.50	0.42
2:E:4968:PHE:CE1	2:E:4978:HIS:ND1	2.76	0.42
2:E:683:ARG:HG2	2:E:717:ASP:HB3	2.01	0.42
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.00	0.42
2:B:842:PRO:HD3	2:B:1073:ARG:HG3	2.02	0.42
2:B:1286:UNK:HA	2:B:1461:UNK:HA	2.02	0.42
2:G:3552:UNK:O	2:G:3556:UNK:N	2.52	0.42
2:I:2132:GLY:O	2:I:2136:ARG:N	2.51	0.42
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.84	0.42
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.52	0.42
2:E:3696:ASP:O	2:E:3700:GLN:N	2.46	0.42
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.02	0.42
2:E:914:PRO:O	2:E:918:ARG:N	2.48	0.42
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.84	0.42
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.01	0.42
2:I:3703:LEU:HA	2:I:3706:SER:HB3	2.01	0.42
2:I:575:LEU:HD22	2:I:609:CYS:HB3	2.00	0.42
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	2.02	0.42
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.85	0.42
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	2.02	0.42
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	2.02	0.42
2:E:4712:PRO:HB2	2:E:4718:LYS:HA	2.01	0.42
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	2.02	0.42
2:I:842:PRO:HD3	2:I:1073:ARG:HG3	2.02	0.42
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	2.02	0.42
2:I:2810:LYS:O	2:I:2814:LYS:N	2.43	0.42
2:I:4712:PRO:HB2	2:I:4718:LYS:HA	2.01	0.42
2:I:4822:THR:O	2:I:4825:THR:OG1	2.32	0.42
1:J:7:ILE:N	1:J:71:ARG:O	2.48	0.42
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.02	0.42
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.01	0.42
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.34	0.42
2:E:1668:ARG:HA	2:E:1671:ARG:HH11	1.85	0.42
2:E:3361:UNK:O	2:E:3365:UNK:N	2.53	0.42
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	2.02	0.42
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.01	0.42
2:G:3832:ILE:O	2:G:3836:MET:N	2.50	0.42
2:G:4982:GLU:HB3	2:G:4983:HIS:H	1.71	0.42
2:G:4962:GLY:H	2:G:5025:GLY:HA2	1.84	0.42
2:I:1668:ARG:HA	2:I:1671:ARG:HH11	1.85	0.42
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.02	0.42
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.88	0.42
2:B:1668:ARG:HA	2:B:1671:ARG:HH11	1.85	0.42
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.84	0.42
2:B:488:LEU:O	2:B:492:ASP:N	2.45	0.42
2:B:4892:ARG:HD3	2:I:4918:ILE:HD13	2.02	0.42
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.01	0.42
2:G:1286:UNK:HA	2:G:1461:UNK:HA	2.02	0.42
2:G:1668:ARG:HA	2:G:1671:ARG:HH11	1.85	0.42
2:G:3840:SER:OG	2:G:3875:MET:O	2.34	0.42
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.02	0.42
2:B:2132:GLY:O	2:B:2136:ARG:N	2.51	0.42
2:B:3696:ASP:O	2:B:3700:GLN:N	2.46	0.42
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.01	0.42
2:E:3994:HIS:O	2:E:3998:HIS:ND1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.34	0.42
2:G:3361:UNK:O	2:G:3365:UNK:N	2.53	0.42
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.01	0.42
2:G:4231:MET:HE3	2:G:4960:ILE:HG23	2.02	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.02	0.42
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.84	0.42
2:I:892:THR:N	2:I:902:ARG:O	2.48	0.42
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.01	0.42
2:B:876:GLU:O	2:B:880:GLU:N	2.51	0.42
2:E:1966:VAL:HA	2:E:1969:LEU:HB3	2.02	0.42
2:E:3703:LEU:HA	2:E:3706:SER:HB3	2.01	0.42
2:G:1697:ALA:HB1	2:G:1708:ARG:HB3	2.02	0.42
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.84	0.42
2:G:1966:VAL:HA	2:G:1969:LEU:HB3	2.02	0.42
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.33	0.42
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.84	0.42
2:B:1697:ALA:HB1	2:B:1708:ARG:HB3	2.02	0.41
2:B:1966:VAL:HA	2:B:1969:LEU:HB3	2.02	0.41
2:B:3832:ILE:O	2:B:3836:MET:N	2.50	0.41
2:E:842:PRO:HD3	2:E:1073:ARG:HG3	2.02	0.41
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.84	0.41
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.83	0.41
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	2.01	0.41
2:G:3663:LEU:H	2:G:3663:LEU:HG	1.76	0.41
1:H:7:ILE:N	1:H:71:ARG:O	2.48	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.02	0.41
2:B:3361:UNK:O	2:B:3365:UNK:N	2.53	0.41
2:B:4982:GLU:HB3	2:B:4983:HIS:H	1.71	0.41
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.01	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.01	0.41
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.01	0.41
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.85	0.41
2:E:1697:ALA:HB1	2:E:1708:ARG:HB3	2.02	0.41
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.38	0.41
2:E:4821:LYS:HB3	2:E:4821:LYS:HE2	1.96	0.41
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.01	0.41
2:G:3703:LEU:HA	2:G:3706:SER:HB3	2.01	0.41
2:G:842:PRO:HD3	2:G:1073:ARG:HG3	2.02	0.41
2:I:1697:ALA:HB1	2:I:1708:ARG:HB3	2.02	0.41
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.01	0.41
2:I:1966:VAL:HA	2:I:1969:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:342:GLY:HA2	2:I:389:PHE:HB2	2.03	0.41
2:I:940:GLY:O	2:I:1052:ASN:N	2.52	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.01	0.41
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.85	0.41
2:B:3880:PHE:O	2:B:3884:LEU:N	2.54	0.41
2:B:3937:TYR:HB3	2:B:4002:LYS:HZ3	1.85	0.41
2:B:4712:PRO:HB2	2:B:4718:LYS:HA	2.01	0.41
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.02	0.41
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.03	0.41
2:G:2132:GLY:O	2:G:2136:ARG:N	2.51	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:I:1286:UNK:HA	2:I:1461:UNK:HA	2.02	0.41
2:I:15:ARG:HG2	2:I:100:THR:HA	2.03	0.41
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	2.02	0.41
2:I:3361:UNK:O	2:I:3365:UNK:N	2.53	0.41
2:I:4702:ASP:OD1	2:I:4778:TRP:NE1	2.48	0.41
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	2.02	0.41
2:B:914:PRO:O	2:B:918:ARG:N	2.48	0.41
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.03	0.41
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.85	0.41
2:I:2950:UNK:O	2:I:2954:UNK:N	2.54	0.41
2:I:4163:PHE:HA	2:I:4166:LEU:HB2	2.02	0.41
2:B:1269:CYS:HA	2:B:1473:UNK:HA	2.01	0.41
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.02	0.41
2:E:4106:PRO:O	2:E:4110:PHE:N	2.53	0.41
2:G:1256:GLU:HG2	2:G:1273:ALA:HB3	2.03	0.41
2:G:2810:LYS:O	2:G:2814:LYS:N	2.42	0.41
2:G:3365:UNK:O	2:G:3369:UNK:N	2.54	0.41
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.46	0.41
2:I:1256:GLU:HG2	2:I:1273:ALA:HB3	2.03	0.41
2:I:379:HIS:CD2	2:I:382:GLY:H	2.32	0.41
2:B:342:GLY:HA2	2:B:389:PHE:HB2	2.03	0.41
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.41
2:E:2950:UNK:O	2:E:2954:UNK:N	2.54	0.41
2:E:3365:UNK:O	2:E:3369:UNK:N	2.54	0.41
2:G:123:THR:OG1	2:G:134:ASP:OD1	2.39	0.41
2:I:2353:VAL:O	2:I:2357:LEU:N	2.51	0.41
2:I:3365:UNK:O	2:I:3369:UNK:N	2.54	0.41
2:B:1130:GLN:HG2	2:B:1138:PRO:HA	2.03	0.41
2:B:379:HIS:CD2	2:B:382:GLY:H	2.32	0.41
2:E:876:GLU:O	2:E:880:GLU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.84	0.41
2:G:3880:PHE:O	2:G:3884:LEU:N	2.54	0.41
2:B:15:ARG:HG2	2:B:100:THR:HA	2.03	0.41
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.86	0.41
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.52	0.41
2:E:102:LEU:HB3	2:E:160:GLY:HA2	2.03	0.41
2:E:4163:PHE:HA	2:E:4166:LEU:HB2	2.02	0.41
2:G:1938:GLN:HA	2:G:1941:ASN:HD22	1.86	0.41
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.86	0.41
2:G:54:ASN:O	2:G:58:VAL:N	2.47	0.41
2:I:4782:VAL:O	2:I:4785:THR:OG1	2.30	0.41
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.89	0.41
2:I:734:GLY:O	2:I:736:HIS:ND1	2.54	0.41
2:I:911:HIS:O	2:I:918:ARG:NH2	2.52	0.41
2:B:102:LEU:HB3	2:B:160:GLY:HA2	2.03	0.41
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.39	0.41
2:B:1256:GLU:HG2	2:B:1273:ALA:HB3	2.03	0.41
2:B:1938:GLN:HA	2:B:1941:ASN:HD22	1.86	0.41
2:B:4780:PHE:HA	2:B:4783:ILE:HD12	2.03	0.41
2:B:911:HIS:O	2:B:918:ARG:NH2	2.52	0.41
2:E:379:HIS:CD2	2:E:381:GLU:H	2.39	0.41
2:E:446:GLN:HA	2:E:449:ILE:HD12	2.03	0.41
2:G:102:LEU:HB3	2:G:160:GLY:HA2	2.03	0.41
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.02	0.41
2:G:2874:MET:O	2:G:2878:LEU:N	2.42	0.41
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.03	0.41
2:B:2950:UNK:O	2:B:2954:UNK:N	2.54	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.54	0.41
2:B:379:HIS:CD2	2:B:381:GLU:H	2.39	0.41
2:B:4237:PHE:O	2:B:4241:THR:OG1	2.33	0.41
2:E:342:GLY:HA2	2:E:389:PHE:HB2	2.03	0.41
2:E:3880:PHE:O	2:E:3884:LEU:N	2.53	0.41
2:E:4822:THR:O	2:E:4825:THR:OG1	2.32	0.41
2:E:485:SER:O	2:E:489:ASN:N	2.40	0.41
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.86	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.88	0.40
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.39	0.40
2:B:309:THR:O	2:B:313:SER:OG	2.39	0.40
2:B:4163:PHE:HA	2:B:4166:LEU:HB2	2.02	0.40
2:B:446:GLN:HA	2:B:449:ILE:HD12	2.03	0.40
2:E:1256:GLU:HG2	2:E:1273:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1286:UNK:HA	2:E:1461:UNK:HA	2.02	0.40
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.86	0.40
2:G:1130:GLN:HG2	2:G:1138:PRO:HA	2.03	0.40
2:G:342:GLY:HA2	2:G:389:PHE:HB2	2.02	0.40
2:G:4962:GLY:H	2:G:5025:GLY:CA	2.34	0.40
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.86	0.40
2:G:897:ARG:HD2	2:G:905:PRO:HG3	2.04	0.40
2:I:4106:PRO:O	2:I:4110:PHE:N	2.53	0.40
2:I:4780:PHE:HA	2:I:4783:ILE:HD12	2.03	0.40
2:I:4962:GLY:H	2:I:5025:GLY:CA	2.34	0.40
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	2.03	0.40
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.87	0.40
2:G:4712:PRO:HB2	2:G:4718:LYS:HA	2.01	0.40
2:G:940:GLY:O	2:G:1052:ASN:N	2.52	0.40
2:I:1105:ALA:O	2:I:1189:LEU:N	2.51	0.40
2:I:102:LEU:HB3	2:I:160:GLY:HA2	2.03	0.40
2:I:309:THR:O	2:I:313:SER:OG	2.39	0.40
2:I:3880:PHE:O	2:I:3884:LEU:N	2.54	0.40
2:B:4984:ASN:HD21	2:B:4986:ALA:HB3	1.86	0.40
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	2.03	0.40
2:E:184:THR:HA	2:E:189:LEU:HA	2.03	0.40
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.40
2:G:184:THR:HA	2:G:189:LEU:HA	2.03	0.40
2:G:3662:ILE:H	2:G:3662:ILE:HG13	1.79	0.40
2:G:4176:PRO:O	2:G:4202:ARG:NH2	2.55	0.40
2:G:4984:ASN:HD21	2:G:4986:ALA:HB3	1.87	0.40
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.39	0.40
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.40
2:I:4957:LYS:NZ	2:I:4957:LYS:CB	2.83	0.40
2:I:876:GLU:O	2:I:880:GLU:N	2.51	0.40
2:B:3843:ASP:H	2:B:3874:VAL:HG13	1.87	0.40
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	2.03	0.40
2:B:897:ARG:HD2	2:B:905:PRO:HG3	2.04	0.40
2:E:321:GLU:HB3	2:E:322:LYS:H	1.73	0.40
2:G:4578:LEU:O	2:E:4880:MET:HG3	2.21	0.40
2:E:4982:GLU:HB3	2:E:4983:HIS:H	1.71	0.40
2:E:897:ARG:HD2	2:E:905:PRO:HG3	2.04	0.40
2:G:2950:UNK:O	2:G:2954:UNK:N	2.54	0.40
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.57	0.40
2:B:4106:PRO:O	2:B:4110:PHE:N	2.53	0.40
2:E:1090:PHE:HD2	2:E:1202:LEU:HD11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:149:THR:N	2:E:172:VAL:O	2.54	0.40
2:E:4702:ASP:OD1	2:E:4778:TRP:NE1	2.48	0.40
2:E:4962:GLY:H	2:E:5025:GLY:CA	2.34	0.40
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.38	0.40
2:G:446:GLN:HA	2:G:449:ILE:HD12	2.03	0.40
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.89	0.40
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	F	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	H	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	J	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4416 (73%)	2899 (90%)	332 (10%)	4 (0%)	56	90
2	E	3235/4416 (73%)	2900 (90%)	331 (10%)	4 (0%)	56	90
2	G	3235/4416 (73%)	2900 (90%)	331 (10%)	4 (0%)	56	90
2	I	3235/4416 (73%)	2900 (90%)	331 (10%)	4 (0%)	56	90
All	All	13360/18096 (74%)	11967 (90%)	1377 (10%)	16 (0%)	59	90

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	I	1708	ARG
2	G	1708	ARG

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Mol	Chain	Res	Type
2	E	1708	ARG
2	B	4641	PRO
2	I	4641	PRO
2	G	4641	PRO
2	E	4641	PRO
2	B	1932	PRO
2	I	1932	PRO
2	G	1932	PRO
2	E	1932	PRO
2	B	1840	PRO
2	I	1840	PRO
2	G	1840	PRO
2	E	1840	PRO

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2471 (99%)	22 (1%)	84	93
2	E	2493/3022 (82%)	2471 (99%)	22 (1%)	84	93
2	G	2493/3022 (82%)	2471 (99%)	22 (1%)	84	93
2	I	2493/3022 (82%)	2471 (99%)	22 (1%)	84	93
All	All	10324/12444 (83%)	10236 (99%)	88 (1%)	85	93

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG

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Mol	Chain	Res	Type
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4166	LEU
2	B	4201	ASN
2	B	4796	MET
2	B	4839	MET
2	B	4957	LYS
2	B	4958	CYS
2	B	4983	HIS
2	B	4995	LEU
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4166	LEU
2	I	4201	ASN
2	I	4796	MET
2	I	4839	MET
2	I	4957	LYS
2	I	4958	CYS
2	I	4983	HIS
2	I	4995	LEU

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Mol	Chain	Res	Type
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4166	LEU
2	G	4201	ASN
2	G	4796	MET
2	G	4839	MET
2	G	4957	LYS
2	G	4958	CYS
2	G	4983	HIS
2	G	4995	LEU
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4166	LEU
2	E	4201	ASN
2	E	4796	MET
2	E	4839	MET
2	E	4957	LYS
2	E	4958	CYS

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Mol	Chain	Res	Type
2	E	4983	HIS
2	E	4995	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	71	GLN
2	B	105	HIS
2	B	111	HIS
2	B	273	HIS
2	B	379	HIS
2	B	413	GLN
2	B	479	GLN
2	B	1598	GLN
2	B	1660	GLN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1941	ASN
2	B	2007	ASN
2	B	2127	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	3976	ASN
2	B	3994	HIS
2	B	4034	ASN
2	B	4054	ASN

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Mol	Chain	Res	Type
2	B	4120	ASN
2	B	4209	GLN
2	B	4833	ASN
2	B	4978	HIS
2	I	57	ASN
2	I	71	GLN
2	I	105	HIS
2	I	111	HIS
2	I	273	HIS
2	I	379	HIS
2	I	413	GLN
2	I	479	GLN
2	I	1598	GLN
2	I	1660	GLN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1941	ASN
2	I	2007	ASN
2	I	2127	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	3976	ASN
2	I	3994	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4833	ASN
2	I	4978	HIS
2	G	57	ASN
2	G	71	GLN
2	G	105	HIS
2	G	111	HIS
2	G	273	HIS
2	G	379	HIS
2	G	413	GLN

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Mol	Chain	Res	Type
2	G	479	GLN
2	G	1598	GLN
2	G	1660	GLN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1941	ASN
2	G	2007	ASN
2	G	2127	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3976	ASN
2	G	3994	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4833	ASN
2	G	4973	HIS
2	G	4978	HIS
2	E	57	ASN
2	E	71	GLN
2	E	105	HIS
2	E	111	HIS
2	E	273	HIS
2	E	379	HIS
2	E	413	GLN
2	E	479	GLN
2	E	1598	GLN
2	E	1660	GLN
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1941	ASN
2	E	2007	ASN
2	E	2127	GLN

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Mol	Chain	Res	Type
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	3976	ASN
2	E	3994	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4833	ASN
2	E	4978	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.58
1	I	4345:UNK	C	4540:PHE	N	74.58
1	G	4345:UNK	C	4540:PHE	N	74.58
1	E	4345:UNK	C	4540:PHE	N	74.58
1	B	3613:UNK	C	3639:THR	N	46.52
1	I	3613:UNK	C	3639:THR	N	46.52
1	G	3613:UNK	C	3639:THR	N	46.52
1	E	3613:UNK	C	3639:THR	N	46.52
1	B	4253:GLU	C	4320:UNK	N	29.50
1	I	4253:GLU	C	4320:UNK	N	29.50
1	G	4253:GLU	C	4320:UNK	N	29.50
1	E	4253:GLU	C	4320:UNK	N	29.50
1	B	3163:UNK	C	3170:UNK	N	16.19
1	I	3163:UNK	C	3170:UNK	N	16.19
1	G	3163:UNK	C	3170:UNK	N	16.18
1	E	3163:UNK	C	3170:UNK	N	16.18
1	B	3063:UNK	C	3134:UNK	N	14.97
1	I	3063:UNK	C	3134:UNK	N	14.97
1	G	3063:UNK	C	3134:UNK	N	14.97
1	E	3063:UNK	C	3134:UNK	N	14.97
1	B	3468:UNK	C	3511:UNK	N	14.26
1	I	3468:UNK	C	3511:UNK	N	14.26
1	G	3468:UNK	C	3511:UNK	N	14.26
1	E	3468:UNK	C	3511:UNK	N	14.26
1	B	2703:UNK	C	2734:ASN	N	13.16
1	I	2703:UNK	C	2734:ASN	N	13.16
1	G	2703:UNK	C	2734:ASN	N	13.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	2703:UNK	C	2734:ASN	N	13.16
1	B	3236:UNK	C	3241:UNK	N	12.69
1	I	3236:UNK	C	3241:UNK	N	12.69
1	G	3236:UNK	C	3241:UNK	N	12.69
1	E	3236:UNK	C	3241:UNK	N	12.69
1	B	2976:UNK	C	2995:UNK	N	12.19
1	I	2976:UNK	C	2995:UNK	N	12.19
1	G	2976:UNK	C	2995:UNK	N	12.19
1	E	2976:UNK	C	2995:UNK	N	12.19
1	B	1564:UNK	C	1573:MET	N	12.11
1	I	1564:UNK	C	1573:MET	N	12.11
1	G	1564:UNK	C	1573:MET	N	12.11
1	E	1564:UNK	C	1573:MET	N	12.11
1	B	3254:UNK	C	3261:UNK	N	8.68
1	I	3254:UNK	C	3261:UNK	N	8.68
1	G	3254:UNK	C	3261:UNK	N	8.68
1	E	3254:UNK	C	3261:UNK	N	8.68
1	B	1297:UNK	C	1430:UNK	N	5.91
1	I	1297:UNK	C	1430:UNK	N	5.91
1	G	1297:UNK	C	1430:UNK	N	5.91
1	E	1297:UNK	C	1430:UNK	N	5.91
1	B	2479:LEU	C	2487:UNK	N	3.40
1	I	2479:LEU	C	2487:UNK	N	3.40
1	G	2479:LEU	C	2487:UNK	N	3.40
1	E	2479:LEU	C	2487:UNK	N	3.40
1	B	2939:ARG	C	2942:UNK	N	3.21
1	I	2939:ARG	C	2942:UNK	N	3.21
1	G	2939:ARG	C	2942:UNK	N	3.21
1	E	2939:ARG	C	2942:UNK	N	3.21