



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:05 AM UTC

PDB ID : 6ZTS / pdb_00006zts
EMDB ID : EMD-22165
Title : Assembly intermediates of orthoreovirus captured in the cell
Authors : Sutton, G.C.; Stuart, D.I.
Deposited on : 2020-07-20
Resolution : 6.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

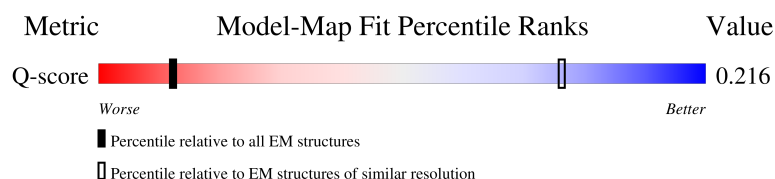
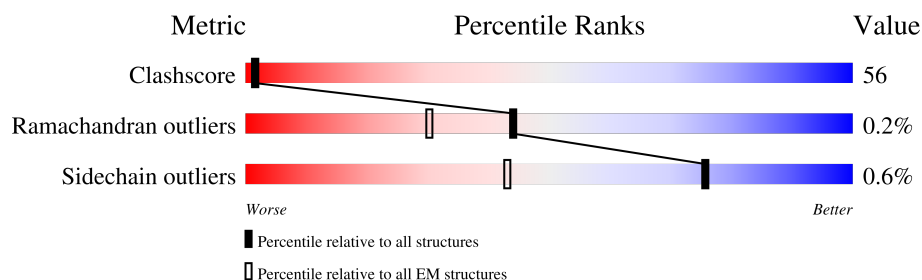
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	531 (6.10 - 7.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	975	21% 27% 71% .
1	B	975	15% 25% 74% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15341 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 Lambda-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	974	Total	C	N	O	S	0	0
			7696	4911	1304	1432	49		
1	B	967	Total	C	N	O	S	0	0
			7645	4883	1296	1417	49		

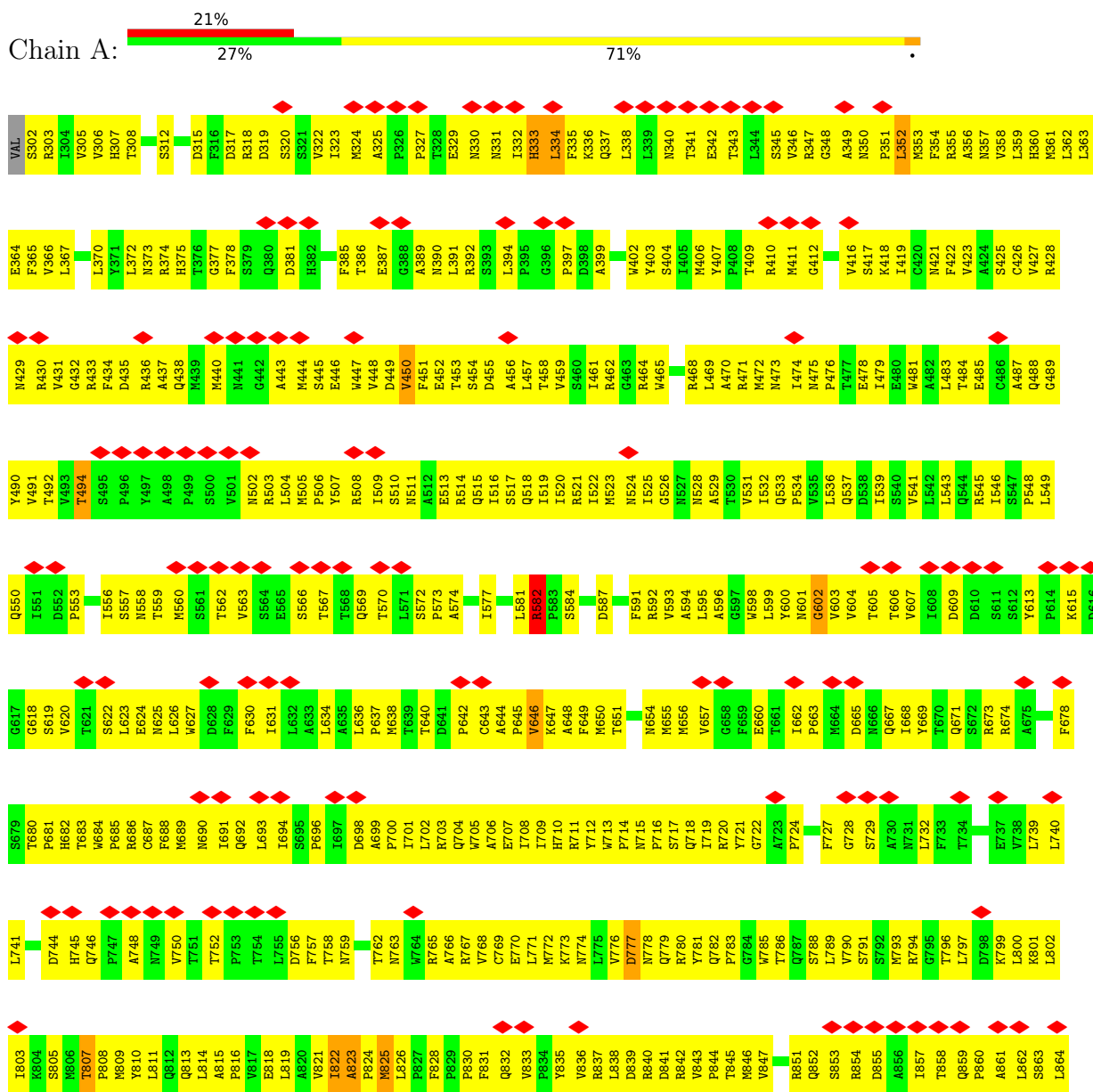
There are 10 discrepancies between the modelled and reference sequences:

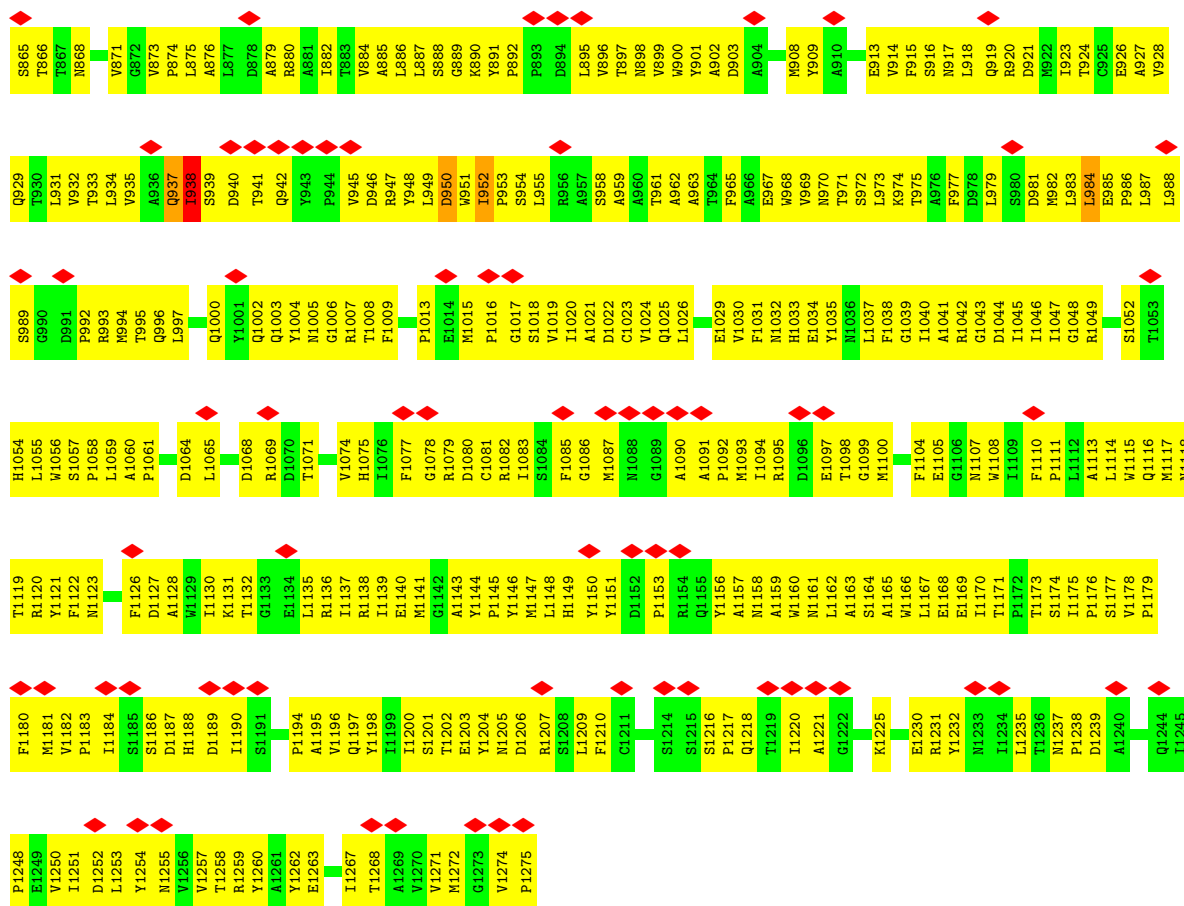
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	LYS	ARG	conflict	UNP A0A023VYS9
A	507	TYR	ARG	conflict	UNP A0A023VYS9
A	973	LEU	MET	conflict	UNP A0A023VYS9
A	1010	ASP	ASN	conflict	UNP A0A023VYS9
A	1163	ALA	THR	conflict	UNP A0A023VYS9
B	336	LYS	ARG	conflict	UNP A0A023VYS9
B	507	TYR	ARG	conflict	UNP A0A023VYS9
B	973	LEU	MET	conflict	UNP A0A023VYS9
B	1010	ASP	ASN	conflict	UNP A0A023VYS9
B	1163	ALA	THR	conflict	UNP A0A023VYS9

3 Residue-property plots

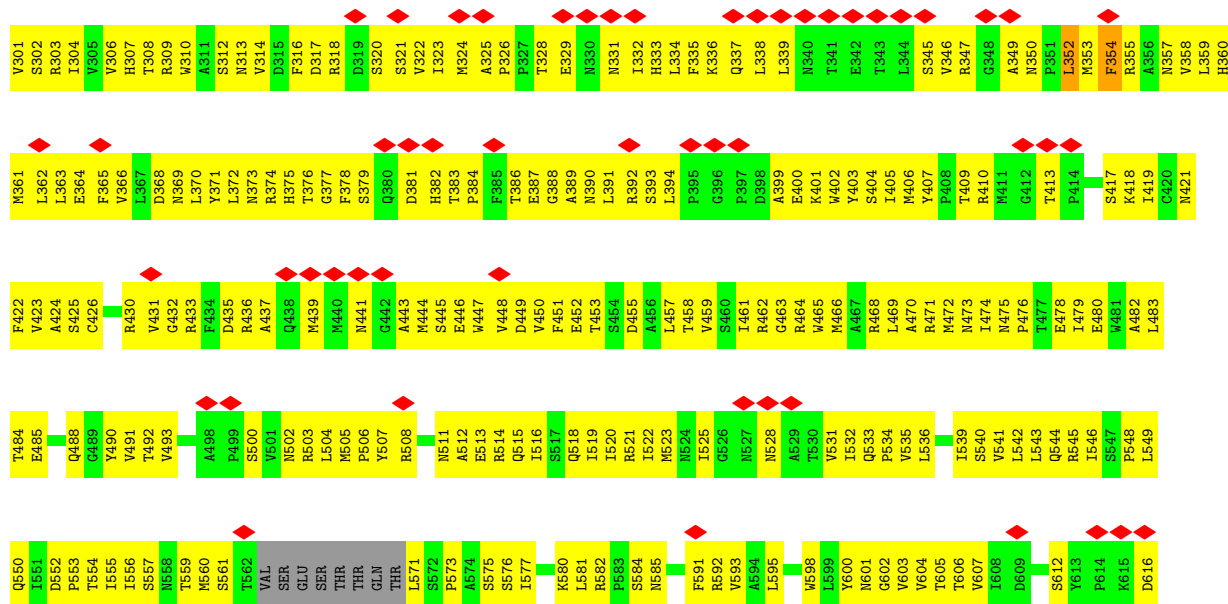
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Lambda-1





• Molecule 1: Lambda-1



Y1254	H1188	D1127	L1065	Y1001	D940	G872	Q812	T751	P885	G817
N1255	D1189	A1128	V1066	Q1002	T941	V873	Q813	T752	R886	G818
V1256	F1067	W1129	F1068	Q1003	Q942	P874	L814	P753	C887	S819
T1258	R1069	K1131	R1069	N1005	Y943	A876	A815	T754	F688	V620
R1269	D1070	T1132	D1070	G1006	P944	L877	V817	T757	M889	T621
A1195	T1071	G1133	T1071	R1007	V945	D878	E818	F758	N690	S622
V1196	P1072	E1134	P1072	T1008	D946	A879	L819	T759	I691	L623
Q1197	H1075	R1135	H1075	F1009	R947	R880	A820	E760	Q692	E824
Y1198	I1076	R1136	I1076	D1010	Y948	A881	V821	E760	N693	N625
I1199	I1077	I1137	I1077	V1011	D949	T882	I822	L761	I694	L626
I1200	G1078	R1138	G1078	E1014	D950	T883	A823	T762	A699	D628
S1201	R1079	E1140	R1079	M1015	W951	V884	P824	N763	P700	F629
T1202	D1080	M1141	D1080	P1016	P952	A885	M825	W764	F700	F630
E1203	C1081	G1142	C1081	G1017	P953	L886	L825	R765	I701	I631
R1204	R1082	A1143	R1082	S1018	S854	L887	P827	A766	L702	L632
N1205	I1083	Y1144	I1083	V1019	L955	S888	P829	R767	Q704	A833
D1206	S1084	Y1145	S1084	I1020	R956	G889	P830	V768	W705	L634
R1207	F1085	Y1146	F1085	A1021	R957	K890	F831	C769	A706	A635
S1208	G1086	M1147	G1086	D1022	A957	Y891	Q832	E770	E707	L636
L1209	M1087	L1148	M1087	C1023	S958	P892	V833	L771	I708	P637
F1210	N1088	H1149	N1088	Y1024	A959	P893	P834	M772	I709	M638
C1211	G1089	Y1150	G1089	Q1025	A960	D894	Y835	K773	H710	T639
T1212	A1090	Y1151	A1090	L1026	T961	L895	V836	N774	R711	T640
N1213	A1091	D1152	A1091	T1027	A962	V896	R837	L775	Y712	M650
S1214	P1092	R1153	P1092	E1029	R963	T897	L838	W776	Y713	T951
S1215	M1093	R1154	M1093	F1030	F965	N898	D839	D777	W714	L652
T1216	I1094	Q1155	I1094	F1031	A966	V899	R840	W778	A653	A654
P1217	R1095	Y1156	R1095	M1032	E967	W900	D841	Q779	N654	N655
Q1218	D1096	A1157	D1096	H1033	W968	A902	R842	R780	M656	M657
T1219	G1099	M1158	G1099	E1034	P969	I905	V843	Y781	G658	G659
I1220	M1100	A1159	M1100	Y1035	N970	Y906	P844	Q782	E660	E661
A1221	W1160	W1160	W1160	M1036	T971	E913	T845	G784	T661	I662
G1222	L1162	L1162	L1162	L1037	L973	V914	N846	A723	I663	P663
P1223	A1163	S1164	A1163	F1038	K974	F915	V847	T786	M664	M664
D1224	S1164	S1164	S1164	F1039	F977	S916	G848	Q787	D665	D665
K1225	A1165	W1166	A1165	I1040	D978	N917	T850	N726	Q667	Q667
H1226	E1105	L1167	E1105	R1041	L979	L918	R851	N725	I668	I668
P1228	G1106	E1168	G1106	G1043	S880	Q919	Q852	A730	Y669	Y669
H1229	M1107	F1169	M1107	D1044	D981	D921	R854	N731	T670	T670
E1230	W1108	F1170	W1108	I1045	M982	N922	D855	L732	Q671	Q671
R1231	F1110	T1171	F1110	I1046	L983	T923	A856	L733	I669	I669
Y1232	P1111	P1172	P1111	I1047	L984	T924	I857	F734	P735	P735
N1233	L1112	T1176	L1112	G1048	E965	T924	T858	L797	P736	P736
I1234	A1113	P1177	A1113	R1049	P986	V928	Q859	D798	E737	E737
L1235	W1114	W1178	W1114	V1050	L987	Q929	P860	L800	R738	R738
T1236	W1115	W1179	W1115	Q1051	L988	T930	A861	L802	L739	L739
N1237	M1117	F1180	M1117	W1056	S989	L931	L862	L740	L740	A675
P1238	M1118	F1181	P1238	S1057	G990	V932	S863	L741	L741	A677
D1239	T1119	W1182	D1239	P1058	P992	T933	L864	I742	I742	F678
A1240	R1120	P1183	A1240	A1059	R993	L934	S805	I743	I743	S679
L1241	Y1121	Y1184	L1241	A1060	M994	V935	S865	D744	D744	T680
P1246	Y1122	T1185	P1246	P1061	T995	A936	T866	Q745	Q745	H682
E1249	P1062	S1186	E1249	P1063	Q996	Q937	T867	H746	H746	T683
V1250	M1123	Q1124	V1250	D1064	L997	S939	T869	V750	V750	W684
I1251	Q1125	F1126	I1251							
D1252			D1252							
L1253			L1253							

4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	
Number of tilted images used	41	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum voxel value	10.927	Depositor
Minimum voxel value	-5.906	Depositor
Average voxel value	0.059	Depositor
Voxel value standard deviation	0.498	Depositor
Recommended contour level	3	Depositor
Tomogram size ($\text{\AA}$)	696.6, 696.6, 696.6	wwPDB
Tomogram dimensions	387, 387, 387	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing ($\text{\AA}$)	1.8, 1.8, 1.8	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/7902	0.71	8/10819 (0.1%)
1	B	0.37	0/7850	0.64	0/10746
All	All	0.37	0/15752	0.68	8/21565 (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
1	A	0	7
1	B	0	1
All	All	0	8

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	825	MET	CA-C-N	10.45	147.29	121.80
1	A	825	MET	C-N-CA	10.45	147.29	121.80
1	A	306	VAL	N-CA-C	-8.11	105.58	113.53
1	A	602	GLY	N-CA-C	-6.63	105.32	115.66
1	A	950	ASP	N-CA-C	-6.15	105.48	114.39
1	A	938	ILE	N-CA-C	-5.76	101.75	109.30
1	A	984	LEU	CA-C-N	5.03	127.22	120.58
1	A	984	LEU	C-N-CA	5.03	127.22	120.58

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	352	LEU	Peptide
1	A	582	ARG	Peptide
1	A	822	ILE	Peptide
1	A	823	ALA	Peptide
1	A	937	GLN	Peptide
1	A	938	ILE	Peptide
1	B	1111	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7696	0	7605	857	0
1	B	7645	0	7559	860	0
All	All	15341	0	15164	1711	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 56.

All (1711) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:GLU:HA	1:B:1261:ALA:H	1.24	1.02
1:B:511:ASN:HA	1:B:514:ARG:HH21	1.25	1.00
1:A:847:VAL:H	1:A:871:VAL:HG11	1.23	0.98
1:A:929:GLN:HB2	1:A:1015:MET:HG2	1.43	0.97
1:A:449:ASP:HA	1:A:1257:VAL:O	1.67	0.95
1:B:1042:ARG:HA	1:B:1142:GLY:O	1.67	0.95
1:A:942:GLN:HE22	1:A:994:MET:HA	1.33	0.94
1:B:333:HIS:HA	1:B:336:LYS:HG2	1.49	0.93
1:A:341:THR:HG23	1:A:350:ASN:HD22	1.33	0.93
1:A:600:TYR:HB3	1:A:603:VAL:HB	1.49	0.93
1:A:1108:TRP:HB2	1:A:1137:ILE:HG12	1.49	0.92
1:B:1108:TRP:HB2	1:B:1137:ILE:HG12	1.53	0.91
1:B:403:TYR:O	1:B:407:TYR:N	2.04	0.90
1:B:1079:ARG:HD2	1:B:1114:LEU:HB3	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:ASP:HB3	1:B:842:ARG:HE	1.38	0.88
1:A:1000:GLN:HE22	1:A:1002:GLN:HB2	1.38	0.87
1:B:1233:ASN:O	1:B:1237:ASN:N	2.06	0.87
1:A:854:ARG:NH2	1:A:862:LEU:O	2.08	0.87
1:A:974:LYS:HA	1:A:979:LEU:HB2	1.57	0.87
1:A:485:GLU:HB3	1:A:720:ARG:HH12	1.39	0.87
1:A:699:ALA:HB1	1:A:702:LEU:HB2	1.54	0.87
1:A:536:LEU:HA	1:A:539:ILE:HD12	1.55	0.86
1:A:354:PHE:HA	1:A:357:ASN:HD21	1.39	0.86
1:A:1079:ARG:NH1	1:A:1114:LEU:H	1.73	0.86
1:B:511:ASN:OD1	1:B:514:ARG:NH2	2.09	0.86
1:A:448:VAL:O	1:A:1258:THR:HA	1.76	0.86
1:B:439:MET:SD	1:B:447:TRP:NE1	2.48	0.85
1:B:301:VAL:HA	1:B:1214:SER:HB2	1.58	0.85
1:B:1003:GLN:OE1	1:B:1005:ASN:ND2	2.11	0.84
1:A:366:VAL:HG21	1:A:1024:VAL:HG12	1.60	0.82
1:A:1187:ASP:OD1	1:A:1188:HIS:ND1	2.12	0.82
1:A:355:ARG:NH2	1:A:952:ILE:O	2.12	0.81
1:B:339:LEU:HD21	1:B:965:PHE:HB2	1.62	0.81
1:B:516:ILE:HA	1:B:519:ILE:HD12	1.62	0.81
1:A:1079:ARG:NH1	1:A:1111:PRO:O	2.13	0.81
1:B:439:MET:SD	1:B:1262:TYR:OH	2.39	0.81
1:B:770:GLU:OE2	1:B:801:LYS:NZ	2.13	0.81
1:B:493:VAL:HB	1:B:1271:VAL:HG12	1.61	0.80
1:A:1147:MET:N	1:A:1178:VAL:O	2.13	0.80
1:A:433:ARG:HD2	1:A:436:ARG:HH21	1.45	0.80
1:A:1032:ASN:O	1:A:1042:ARG:NH1	2.15	0.80
1:A:1095:ARG:HE	1:A:1099:GLY:HA2	1.45	0.80
1:A:879:ALA:HA	1:A:882:ILE:HD12	1.63	0.80
1:A:598:TRP:O	1:A:832:GLN:NE2	2.15	0.80
1:A:1081:CYS:HB3	1:A:1094:ILE:HD11	1.64	0.79
1:B:550:GLN:HE22	1:B:892:PRO:HG3	1.47	0.79
1:B:638:MET:N	1:B:638:MET:SD	2.56	0.79
1:B:965:PHE:HA	1:B:968:TRP:HD1	1.45	0.79
1:A:844:PRO:HA	1:A:1003:GLN:HA	1.65	0.79
1:A:404:SER:HB3	1:A:410:ARG:HB2	1.64	0.79
1:B:392:ARG:O	1:B:403:TYR:OH	1.99	0.79
1:B:654:ASN:ND2	1:B:671:GLN:O	2.14	0.79
1:B:605:THR:N	1:B:873:VAL:O	2.14	0.79
1:B:1154:ARG:HG3	1:B:1155:GLN:HG3	1.65	0.79
1:B:557:SER:O	1:B:561:SER:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1187:ASP:HA	1:B:1220:ILE:H	1.47	0.78
1:A:896:VAL:O	1:A:900:TRP:N	2.12	0.78
1:B:554:THR:O	1:B:557:SER:OG	1.99	0.78
1:B:1061:PRO:HB2	1:B:1065:LEU:HD11	1.64	0.78
1:A:987:LEU:HG	1:A:992:PRO:HB3	1.66	0.78
1:A:1049:ARG:NH2	1:A:1132:THR:O	2.16	0.78
1:A:1128:ALA:O	1:A:1132:THR:N	2.17	0.77
1:A:373:ASN:HB3	1:A:1260:TYR:H	1.48	0.77
1:A:686:ARG:NH2	1:A:689:MET:SD	2.57	0.77
1:B:731:ASN:HB2	1:B:736:PRO:HA	1.66	0.77
1:B:430:ARG:NH2	1:B:1238:PRO:O	2.17	0.77
1:B:1213:ASN:ND2	1:B:1218:GLN:O	2.18	0.77
1:B:543:LEU:HD23	1:B:592:ARG:HB3	1.67	0.77
1:B:1209:LEU:HG	1:B:1225:LYS:HG2	1.65	0.77
1:B:915:PHE:HA	1:B:918:LEU:HG	1.66	0.76
1:A:548:PRO:HB2	1:A:892:PRO:HD2	1.67	0.76
1:B:686:ARG:NH1	1:B:687:CYS:SG	2.57	0.76
1:B:765:ARG:NH1	1:B:803:ILE:O	2.16	0.76
1:B:741:LEU:HG	1:B:743:ILE:H	1.48	0.76
1:A:1048:GLY:HA3	1:A:1136:ARG:HE	1.50	0.76
1:A:351:PRO:HA	1:A:354:PHE:HB2	1.68	0.76
1:B:485:GLU:O	1:B:488:GLN:NE2	2.19	0.76
1:A:1149:HIS:N	1:A:1180:PHE:O	2.19	0.75
1:B:1213:ASN:HB3	1:B:1216:SER:HB3	1.67	0.75
1:A:841:ASP:O	1:A:1005:ASN:N	2.19	0.75
1:A:1045:ILE:HG13	1:A:1047:ILE:HD11	1.68	0.75
1:A:965:PHE:HA	1:A:968:TRP:HD1	1.52	0.75
1:A:1246:GLN:O	1:A:1250:VAL:N	2.19	0.75
1:A:464:ARG:NH1	1:A:1023:CYS:SG	2.60	0.75
1:B:961:THR:O	1:B:964:THR:OG1	2.05	0.74
1:B:445:SER:HB2	1:B:448:VAL:HB	1.69	0.74
1:B:624:GLU:HA	1:B:627:TRP:CD1	2.22	0.74
1:B:741:LEU:HD12	1:B:742:PRO:HD2	1.69	0.74
1:B:745:HIS:O	1:B:746:GLN:NE2	2.20	0.74
1:B:929:GLN:NE2	1:B:1016:PRO:O	2.21	0.74
1:B:1069:ARG:NH1	1:B:1138:ARG:O	2.21	0.74
1:B:452:GLU:O	1:B:1255:ASN:N	2.20	0.74
1:B:1197:GLN:HB3	1:B:1200:ILE:HD11	1.68	0.74
1:A:447:TRP:HB2	1:A:1258:THR:HG22	1.69	0.74
1:B:349:ALA:O	1:B:1175:ILE:N	2.19	0.73
1:B:448:VAL:H	1:B:1259:ARG:H	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:GLN:HA	1:B:521:ARG:HE	1.52	0.73
1:A:929:GLN:NE2	1:A:933:THR:OG1	2.21	0.73
1:B:514:ARG:HH22	1:B:729:SER:N	1.85	0.73
1:A:600:TYR:HB2	1:A:604:VAL:HG22	1.69	0.73
1:A:1030:VAL:HG13	1:A:1248:PRO:HB3	1.71	0.73
1:A:935:VAL:HG22	1:A:941:THR:HB	1.71	0.73
1:B:1028:ALA:O	1:B:1032:ASN:N	2.20	0.73
1:A:563:VAL:HA	1:A:796:THR:HG23	1.69	0.73
1:B:1158:ASN:HD21	1:B:1160:TRP:HB3	1.53	0.73
1:B:1148:LEU:HD13	1:B:1182:VAL:HG11	1.70	0.72
1:B:430:ARG:NH2	1:B:1240:ALA:O	2.21	0.72
1:B:598:TRP:O	1:B:832:GLN:NE2	2.22	0.72
1:A:474:ILE:HD12	1:A:478:GLU:HB3	1.72	0.72
1:A:1080:ASP:HB3	1:A:1097:GLU:HA	1.71	0.72
1:A:1082:ARG:O	1:A:1095:ARG:N	2.21	0.72
1:B:309:ARG:HH22	1:B:318:ARG:H	1.36	0.72
1:B:974:LYS:HD3	1:B:982:MET:HA	1.71	0.72
1:B:446:GLU:HA	1:B:1261:ALA:N	2.04	0.72
1:B:577:ILE:HD12	1:B:580:LYS:HB3	1.72	0.72
1:B:1037:LEU:HA	1:B:1207:ARG:HG3	1.71	0.72
1:A:1146:TYR:HA	1:A:1178:VAL:H	1.55	0.72
1:B:536:LEU:HA	1:B:539:ILE:HD12	1.72	0.72
1:A:1150:TYR:HA	1:A:1182:VAL:HG13	1.70	0.72
1:A:529:ALA:O	1:A:532:ILE:HG12	1.90	0.72
1:B:1231:ARG:NH1	1:B:1251:ILE:O	2.23	0.72
1:B:320:SER:OG	1:B:364:GLU:O	2.08	0.71
1:B:407:TYR:HB2	1:B:410:ARG:HB2	1.72	0.71
1:B:458:THR:HA	1:B:461:ILE:HD12	1.70	0.71
1:B:624:GLU:HA	1:B:627:TRP:HD1	1.54	0.71
1:A:375:HIS:ND1	1:A:1259:ARG:O	2.24	0.71
1:A:937:GLN:NE2	1:A:946:ASP:O	2.22	0.71
1:B:630:PHE:HE1	1:B:772:MET:HG3	1.54	0.71
1:B:621:THR:HA	1:B:785:TRP:HZ2	1.55	0.71
1:A:352:LEU:HD13	1:A:955:LEU:HD22	1.71	0.71
1:B:705:TRP:HA	1:B:708:ILE:HD12	1.72	0.71
1:A:694:ILE:O	1:A:703:ARG:NH1	2.23	0.71
1:A:399:ALA:HA	1:A:402:TRP:CD1	2.25	0.71
1:A:350:ASN:HD21	1:A:352:LEU:HB2	1.55	0.71
1:A:452:GLU:HG2	1:A:1257:VAL:HG21	1.73	0.71
1:A:669:TYR:OH	1:A:682:HIS:O	2.09	0.71
1:A:1159:ALA:HB3	1:A:1197:GLN:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:CYS:HA	1:A:772:MET:HE3	1.72	0.70
1:B:1186:SER:O	1:B:1221:ALA:N	2.24	0.70
1:A:691:ILE:O	1:A:703:ARG:NH1	2.24	0.70
1:B:359:LEU:HD23	1:B:934:LEU:HD12	1.71	0.70
1:A:680:THR:N	1:A:683:THR:OG1	2.24	0.70
1:B:1047:ILE:O	1:B:1136:ARG:HA	1.91	0.70
1:A:1115:TRP:HD1	1:A:1119:THR:HG22	1.57	0.69
1:A:1083:ILE:O	1:A:1121:TYR:OH	2.10	0.69
1:B:846:MET:O	1:B:1001:TYR:HA	1.92	0.69
1:A:407:TYR:HB2	1:A:409:THR:HG22	1.74	0.69
1:A:503:ARG:HG2	1:A:1263:GLU:HB2	1.74	0.69
1:A:582:ARG:NH1	1:A:584:SER:OG	2.26	0.69
1:B:694:ILE:O	1:B:703:ARG:NH1	2.26	0.69
1:A:927:ALA:O	1:A:931:LEU:HG	1.92	0.69
1:A:1107:ASN:C	1:A:1108:TRP:HD1	2.00	0.69
1:B:1120:ARG:NH1	1:B:1170:ILE:O	2.25	0.69
1:B:500:SER:OG	1:B:502:ASN:OD1	2.11	0.69
1:B:706:ALA:HA	1:B:709:ILE:HD12	1.72	0.69
1:B:1094:ILE:O	1:B:1101:MET:HA	1.92	0.69
1:A:462:ARG:HA	1:A:465:TRP:HB3	1.75	0.69
1:A:507:TYR:CZ	1:A:1267:ILE:HD13	2.27	0.69
1:A:656:MET:HG3	1:A:702:LEU:HD21	1.73	0.69
1:A:360:HIS:CD2	1:A:968:TRP:HB3	2.28	0.69
1:A:450:VAL:HG13	1:A:1257:VAL:HB	1.75	0.69
1:A:805:SER:HA	1:A:889:GLY:H	1.55	0.69
1:A:934:LEU:O	1:A:939:SER:OG	2.11	0.69
1:B:729:SER:HB2	1:B:736:PRO:HB3	1.75	0.69
1:B:1084:SER:OG	1:B:1093:MET:O	2.11	0.69
1:A:352:LEU:HD22	1:A:955:LEU:HB2	1.75	0.69
1:A:763:ASN:O	1:A:767:ARG:NH1	2.26	0.69
1:A:1160:TRP:CD1	1:A:1162:LEU:H	2.10	0.69
1:B:541:VAL:O	1:B:544:GLN:NE2	2.26	0.69
1:A:430:ARG:NH1	1:A:1239:ASP:O	2.21	0.69
1:A:941:THR:OG1	1:A:993:ARG:O	2.11	0.69
1:A:1044:ASP:OD1	1:A:1141:MET:N	2.26	0.69
1:A:331:ASN:HB3	1:A:333:HIS:CE1	2.29	0.68
1:B:382:HIS:CE1	1:B:389:ALA:H	2.10	0.68
1:A:748:ALA:HB2	1:A:813:GLN:HB3	1.76	0.68
1:A:1158:ASN:HD21	1:A:1160:TRP:HB3	1.59	0.68
1:A:884:VAL:O	1:A:888:SER:OG	2.12	0.68
1:B:924:THR:HG23	1:B:983:LEU:HD21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:SER:OG	1:A:857:ILE:O	2.10	0.68
1:A:838:LEU:O	1:A:842:ARG:NH2	2.23	0.68
1:A:974:LYS:O	1:A:979:LEU:N	2.27	0.68
1:B:1085:PHE:HA	1:B:1092:PRO:HB3	1.74	0.68
1:B:1186:SER:HB3	1:B:1221:ALA:HB3	1.74	0.68
1:A:681:PRO:HA	1:A:684:TRP:CD2	2.29	0.68
1:A:713:TRP:CD2	1:A:714:PRO:HD2	2.29	0.68
1:B:687:CYS:HA	1:B:693:LEU:HD12	1.76	0.68
1:A:613:TYR:O	1:A:615:LYS:NZ	2.26	0.67
1:B:318:ARG:HG2	1:B:371:TYR:CZ	2.29	0.67
1:B:1158:ASN:OD1	1:B:1161:ASN:N	2.27	0.67
1:B:465:TRP:O	1:B:469:LEU:HG	1.95	0.67
1:A:854:ARG:HD2	1:A:857:ILE:HD12	1.75	0.67
1:B:733:PHE:CD1	1:B:834:PRO:HD3	2.29	0.67
1:A:465:TRP:O	1:A:469:LEU:HG	1.94	0.67
1:A:776:VAL:HG12	1:A:790:VAL:HG13	1.77	0.67
1:B:680:THR:O	1:B:683:THR:OG1	2.09	0.67
1:B:382:HIS:HB3	1:B:387:GLU:HA	1.76	0.67
1:B:630:PHE:CE1	1:B:772:MET:HG3	2.30	0.67
1:B:670:THR:HG22	1:B:672:SER:H	1.57	0.67
1:A:1032:ASN:OD1	1:A:1042:ARG:NH2	2.27	0.67
1:B:713:TRP:HD1	1:B:837:ARG:HE	1.41	0.67
1:B:732:LEU:HD12	1:B:1011:VAL:HG11	1.76	0.67
1:B:844:PRO:HG2	1:B:870:THR:HG21	1.77	0.67
1:A:750:VAL:HG22	1:A:752:THR:H	1.60	0.67
1:B:819:LEU:HA	1:B:822:ILE:HD12	1.76	0.67
1:B:1134:GLU:OE2	1:B:1136:ARG:N	2.27	0.67
1:B:987:LEU:HD13	1:B:992:PRO:HA	1.76	0.67
1:A:681:PRO:HA	1:A:684:TRP:CE3	2.30	0.67
1:B:504:LEU:HD11	1:B:1262:TYR:HB3	1.76	0.67
1:B:1147:MET:N	1:B:1178:VAL:O	2.28	0.67
1:A:601:ASN:OD1	1:A:602:GLY:N	2.28	0.66
1:A:1060:ALA:HB2	1:A:1204:TYR:HD1	1.58	0.66
1:A:1203:GLU:HB2	1:A:1205:ASN:HD21	1.60	0.66
1:B:952:ILE:HG23	1:B:1143:ALA:HB3	1.75	0.66
1:A:1059:LEU:O	1:A:1204:TYR:HA	1.95	0.66
1:B:383:THR:N	1:B:386:THR:OG1	2.21	0.66
1:B:573:PRO:O	1:B:576:SER:OG	2.14	0.66
1:B:1252:ASP:OD1	1:B:1255:ASN:ND2	2.25	0.66
1:A:665:ASP:HB2	1:A:669:TYR:HD1	1.60	0.66
1:A:843:VAL:O	1:A:1004:TYR:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:GLU:HA	1:A:627:TRP:CD1	2.30	0.66
1:B:720:ARG:NH1	1:B:721:TYR:O	2.28	0.66
1:A:419:ILE:H	1:A:419:ILE:HD12	1.60	0.66
1:A:426:CYS:O	1:A:428:ARG:NH1	2.27	0.66
1:A:511:ASN:HA	1:A:514:ARG:HB2	1.78	0.66
1:A:681:PRO:O	1:A:840:ARG:NH2	2.28	0.66
1:A:896:VAL:HB	1:A:899:VAL:HB	1.78	0.66
1:B:686:ARG:HA	1:B:689:MET:HB2	1.78	0.66
1:A:353:MET:HE2	1:A:356:ALA:H	1.60	0.66
1:A:895:LEU:HG	1:A:900:TRP:CD1	2.31	0.66
1:B:1041:ALA:O	1:B:1143:ALA:HA	1.94	0.66
1:A:776:VAL:HG11	1:A:793:MET:HG3	1.76	0.66
1:A:847:VAL:HA	1:A:1000:GLN:O	1.95	0.66
1:B:712:TYR:HB3	1:B:763:ASN:HD21	1.60	0.66
1:B:720:ARG:HH22	1:B:724:PRO:HD2	1.60	0.66
1:B:1129:TRP:CD1	1:B:1129:TRP:H	2.13	0.66
1:A:329:GLU:O	1:A:331:ASN:ND2	2.29	0.65
1:B:306:VAL:HB	1:B:324:MET:SD	2.37	0.65
1:B:1059:LEU:HD11	1:B:1205:ASN:HB2	1.78	0.65
1:B:437:ALA:HB3	1:B:445:SER:HB3	1.77	0.65
1:B:994:MET:SD	1:B:996:GLN:N	2.69	0.65
1:A:472:MET:HB3	1:A:508:ARG:H	1.60	0.65
1:B:962:ALA:O	1:B:966:ALA:N	2.22	0.65
1:A:983:LEU:C	1:A:985:GLU:H	2.03	0.65
1:A:446:GLU:HB3	1:A:1262:TYR:CZ	2.31	0.65
1:B:520:ILE:HG23	1:B:523:MET:HE2	1.78	0.65
1:A:809:MET:SD	1:A:810:TYR:N	2.69	0.65
1:B:810:TYR:HA	1:B:814:LEU:HD13	1.78	0.65
1:B:1065:LEU:O	1:B:1136:ARG:NH2	2.29	0.65
1:A:331:ASN:HB3	1:A:333:HIS:HE1	1.60	0.65
1:A:468:ARG:HA	1:A:471:ARG:CZ	2.27	0.65
1:A:627:TRP:O	1:A:631:ILE:HG12	1.97	0.65
1:B:600:TYR:OH	1:B:828:PHE:O	2.14	0.64
1:A:607:VAL:O	1:A:876:ALA:HA	1.96	0.64
1:A:303:ARG:HB2	1:A:1210:PHE:CG	2.33	0.64
1:A:332:ILE:HG12	1:A:335:PHE:H	1.62	0.64
1:A:624:GLU:HA	1:A:627:TRP:HD1	1.62	0.64
1:A:982:MET:HG2	1:A:986:PRO:HD3	1.79	0.64
1:B:1069:ARG:NH1	1:B:1109:ILE:HA	2.12	0.64
1:A:324:MET:HA	1:A:333:HIS:HB3	1.79	0.64
1:B:601:ASN:ND2	1:B:833:VAL:HB	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:MET:HG3	1:B:890:LYS:HA	1.78	0.64
1:B:841:ASP:HA	1:B:1004:TYR:HD2	1.62	0.64
1:A:713:TRP:O	1:A:837:ARG:NH2	2.30	0.64
1:B:418:LYS:NZ	1:B:1225:LYS:O	2.30	0.64
1:B:449:ASP:OD1	1:B:1258:THR:N	2.30	0.64
1:B:473:ASN:HA	1:B:506:PRO:HA	1.80	0.64
1:A:601:ASN:ND2	1:A:833:VAL:O	2.28	0.64
1:A:708:ILE:HG23	1:A:712:TYR:HD2	1.61	0.64
1:A:381:ASP:HB2	1:A:386:THR:HG21	1.78	0.64
1:A:1115:TRP:HA	1:A:1122:PHE:CE2	2.33	0.64
1:B:794:ARG:HA	1:B:797:LEU:HD12	1.80	0.64
1:A:416:VAL:HG13	1:A:421:ASN:HD21	1.62	0.64
1:B:773:LYS:NZ	1:B:794:ARG:O	2.30	0.64
1:A:355:ARG:O	1:A:359:LEU:HG	1.98	0.64
1:A:1058:PRO:HD3	1:A:1197:GLN:HE22	1.63	0.64
1:B:309:ARG:NH2	1:B:371:TYR:OH	2.31	0.64
1:B:1042:ARG:O	1:B:1144:TYR:OH	2.15	0.64
1:B:1115:TRP:CH2	1:B:1119:THR:HG23	2.33	0.64
1:A:662:ILE:HB	1:A:663:PRO:HD2	1.80	0.64
1:A:841:ASP:HA	1:A:1004:TYR:CD2	2.33	0.64
1:A:845:THR:N	1:A:1002:GLN:O	2.29	0.63
1:A:1247:LEU:HG	1:A:1251:ILE:HG12	1.80	0.63
1:B:773:LYS:HG2	1:B:797:LEU:HD13	1.79	0.63
1:B:951:TRP:HZ3	1:B:1042:ARG:HB3	1.62	0.63
1:B:958:SER:HA	1:B:993:ARG:HH22	1.62	0.63
1:B:1059:LEU:O	1:B:1204:TYR:HA	1.98	0.63
1:B:1187:ASP:HA	1:B:1220:ILE:N	2.11	0.63
1:A:768:VAL:HG22	1:A:772:MET:HE2	1.80	0.63
1:A:468:ARG:HH11	1:A:471:ARG:HH11	1.45	0.63
1:A:1052:SER:O	1:A:1195:ALA:HB3	1.99	0.63
1:B:691:ILE:O	1:B:703:ARG:NH1	2.32	0.63
1:A:494:THR:HG23	1:A:1274:VAL:HG22	1.80	0.63
1:A:343:THR:HG23	1:A:1170:ILE:HD11	1.79	0.63
1:A:484:THR:HA	1:A:487:ALA:HB3	1.79	0.63
1:A:521:ARG:HA	1:A:524:ASN:HB2	1.80	0.63
1:A:974:LYS:NZ	1:A:981:ASP:O	2.31	0.63
1:B:402:TRP:HA	1:B:405:ILE:HD12	1.81	0.63
1:B:516:ILE:O	1:B:520:ILE:HG12	1.98	0.63
1:A:516:ILE:HA	1:A:519:ILE:HD12	1.81	0.63
1:B:333:HIS:HA	1:B:336:LYS:CG	2.27	0.63
1:B:792:SER:O	1:B:796:THR:OG1	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:849:VAL:O	1:B:861:ALA:N	2.31	0.63
1:A:566:SER:HB2	1:A:573:PRO:HD3	1.81	0.62
1:A:473:ASN:O	1:A:508:ARG:NH2	2.31	0.62
1:B:1147:MET:HB2	1:B:1177:SER:OG	2.00	0.62
1:A:1068:ASP:OD1	1:A:1071:THR:N	2.31	0.62
1:B:326:PRO:O	1:B:331:ASN:ND2	2.32	0.62
1:B:869:THR:HG23	1:B:870:THR:H	1.65	0.62
1:B:951:TRP:CZ3	1:B:1042:ARG:HB3	2.34	0.62
1:B:965:PHE:HA	1:B:968:TRP:CD1	2.32	0.62
1:B:1047:ILE:HG23	1:B:1199:ILE:HG13	1.81	0.62
1:B:377:GLY:HA2	1:B:443:ALA:HB3	1.81	0.62
1:B:1189:ASP:HA	1:B:1221:ALA:HB2	1.81	0.62
1:A:673:ARG:HH22	1:B:784:GLY:H	1.47	0.62
1:B:359:LEU:H	1:B:359:LEU:HD12	1.65	0.62
1:B:603:VAL:O	1:B:873:VAL:N	2.22	0.62
1:B:913:GLU:O	1:B:916:SER:OG	2.09	0.62
1:A:419:ILE:O	1:A:423:VAL:HG23	2.00	0.62
1:A:531:VAL:O	1:A:534:PRO:HD2	2.00	0.62
1:B:708:ILE:N	1:B:711:ARG:HH21	1.97	0.62
1:B:882:ILE:O	1:B:886:LEU:HG	2.00	0.62
1:B:1029:GLU:HA	1:B:1032:ASN:HB2	1.82	0.62
1:B:1252:ASP:CG	1:B:1255:ASN:HD21	2.07	0.62
1:A:307:HIS:H	1:A:324:MET:HE1	1.65	0.62
1:A:516:ILE:O	1:A:520:ILE:HG12	2.00	0.62
1:A:705:TRP:HA	1:A:708:ILE:HD12	1.81	0.62
1:B:448:VAL:C	1:B:1258:THR:HA	2.25	0.62
1:B:670:THR:HB	1:B:673:ARG:HB2	1.80	0.62
1:A:553:PRO:HA	1:A:556:ILE:HB	1.81	0.62
1:B:713:TRP:CD1	1:B:837:ARG:HE	2.17	0.62
1:B:897:THR:OG1	1:B:898:ASN:N	2.33	0.62
1:A:506:PRO:HD2	1:A:507:TYR:CZ	2.33	0.62
1:A:913:GLU:O	1:A:917:ASN:N	2.32	0.61
1:B:522:ILE:HA	1:B:525:ILE:HD12	1.81	0.61
1:B:750:VAL:HG21	1:B:814:LEU:HD11	1.80	0.61
1:B:929:GLN:HE22	1:B:1015:MET:HB2	1.65	0.61
1:B:1149:HIS:O	1:B:1182:VAL:N	2.28	0.61
1:B:713:TRP:CD2	1:B:714:PRO:HD2	2.36	0.61
1:A:432:GLY:C	1:A:450:VAL:HG23	2.26	0.61
1:B:931:LEU:O	1:B:935:VAL:HG23	2.01	0.61
1:A:518:GLN:O	1:A:522:ILE:HG12	2.00	0.61
1:B:1047:ILE:HG13	1:B:1199:ILE:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1164:SER:HA	1:B:1167:LEU:HD12	1.81	0.61
1:A:457:LEU:O	1:A:461:ILE:N	2.19	0.61
1:A:636:LEU:HD13	1:A:648:ALA:HB2	1.83	0.61
1:A:941:THR:HG23	1:A:942:GLN:H	1.64	0.61
1:B:476:PRO:HA	1:B:479:ILE:HD12	1.82	0.61
1:B:825:MET:SD	1:B:825:MET:N	2.73	0.61
1:B:1233:ASN:OD1	1:B:1236:THR:OG1	2.19	0.61
1:A:385:PHE:HZ	1:A:412:GLY:HA2	1.64	0.61
1:A:445:SER:OG	1:A:447:TRP:O	2.15	0.61
1:A:483:LEU:O	1:A:487:ALA:N	2.26	0.61
1:A:567:THR:HA	1:A:572:SER:HB2	1.82	0.61
1:A:1156:TYR:HD1	1:A:1194:PRO:HB2	1.65	0.61
1:A:330:ASN:OD1	1:A:1148:LEU:N	2.33	0.61
1:A:418:LYS:HG3	1:A:1217:PRO:HA	1.82	0.61
1:A:858:THR:O	1:A:996:GLN:NE2	2.33	0.61
1:B:1224:ASP:OD1	1:B:1225:LYS:N	2.34	0.61
1:A:662:ILE:HG22	1:A:698:ASP:HB3	1.82	0.61
1:B:355:ARG:NH1	1:B:954:SER:O	2.34	0.61
1:A:649:PHE:CE2	1:A:688:PHE:HB2	2.35	0.61
1:A:705:TRP:NE1	1:A:709:ILE:HD11	2.15	0.60
1:A:1260:TYR:HD2	1:A:1262:TYR:HE2	1.49	0.60
1:B:854:ARG:HH22	1:B:857:ILE:HA	1.65	0.60
1:A:916:SER:HA	1:A:919:GLN:HE21	1.67	0.60
1:A:1046:ILE:HG13	1:A:1202:THR:HG22	1.83	0.60
1:A:362:LEU:O	1:A:366:VAL:HG23	2.02	0.60
1:A:920:ARG:O	1:A:924:THR:OG1	2.15	0.60
1:A:1122:PHE:HB3	1:A:1126:PHE:CE2	2.36	0.60
1:B:423:VAL:HA	1:B:426:CYS:SG	2.41	0.60
1:A:686:ARG:HG3	1:A:690:ASN:CG	2.26	0.60
1:B:450:VAL:O	1:B:1256:VAL:HA	2.01	0.60
1:B:694:ILE:HB	1:B:703:ARG:HH11	1.66	0.60
1:B:776:VAL:O	1:B:782:GLN:NE2	2.34	0.60
1:B:892:PRO:HD2	1:B:895:LEU:HD22	1.82	0.60
1:B:1058:PRO:HB3	1:B:1200:ILE:HG23	1.83	0.60
1:B:1258:THR:HG1	1:B:1260:TYR:HH	1.48	0.60
1:B:312:SER:OG	1:B:314:VAL:O	2.19	0.60
1:B:407:TYR:HD2	1:B:410:ARG:HD3	1.66	0.60
1:B:669:TYR:OH	1:B:682:HIS:O	2.18	0.60
1:B:850:THR:HG23	1:B:860:PRO:HA	1.83	0.60
1:A:600:TYR:HE2	1:A:828:PHE:HE2	1.50	0.60
1:A:865:SER:O	1:A:868:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:ALA:HB1	1:A:1093:MET:HE3	1.82	0.60
1:B:373:ASN:O	1:B:374:ARG:NH1	2.30	0.60
1:B:449:ASP:HB3	1:B:1256:VAL:HB	1.83	0.60
1:A:521:ARG:HD2	1:A:828:PHE:CD1	2.36	0.60
1:A:646:VAL:HG11	1:A:684:TRP:HB3	1.84	0.60
1:A:779:GLN:HA	1:A:782:GLN:CD	2.26	0.60
1:A:974:LYS:HZ2	1:A:983:LEU:HD12	1.66	0.60
1:A:1055:LEU:HD11	1:A:1190:ILE:HD11	1.84	0.60
1:A:1186:SER:HB2	1:A:1221:ALA:HA	1.83	0.60
1:A:409:THR:HG23	1:A:410:ARG:HG3	1.84	0.60
1:A:591:PHE:CE2	1:A:882:ILE:HA	2.37	0.60
1:A:604:VAL:HB	1:A:875:LEU:HD11	1.84	0.60
1:A:863:SER:OG	1:A:866:THR:OG1	2.19	0.60
1:B:634:LEU:HD21	1:B:768:VAL:HG21	1.83	0.60
1:B:1020:ILE:O	1:B:1024:VAL:HG23	2.02	0.60
1:B:1095:ARG:NH1	1:B:1096:ASP:O	2.33	0.60
1:A:900:TRP:HD1	1:A:901:TYR:CD2	2.19	0.60
1:A:920:ARG:NE	1:A:981:ASP:OD2	2.27	0.60
1:A:397:PRO:O	1:A:402:TRP:NE1	2.34	0.59
1:B:417:SER:O	1:B:421:ASN:N	2.24	0.59
1:B:612:SER:HB2	1:B:632:LEU:HD21	1.83	0.59
1:B:853:SER:HB2	1:B:995:THR:H	1.67	0.59
1:B:1069:ARG:HH22	1:B:1110:PHE:N	2.00	0.59
1:B:1075:HIS:CE1	1:B:1106:GLY:HA3	2.37	0.59
1:B:1119:THR:HG22	1:B:1120:ARG:HD3	1.82	0.59
1:A:1231:ARG:HB2	1:A:1232:TYR:CZ	2.37	0.59
1:B:476:PRO:HA	1:B:479:ILE:HB	1.84	0.59
1:B:479:ILE:O	1:B:483:LEU:HG	2.02	0.59
1:B:548:PRO:O	1:B:550:GLN:NE2	2.34	0.59
1:B:782:GLN:OE1	1:B:782:GLN:N	2.36	0.59
1:B:839:ASP:HB3	1:B:842:ARG:NE	2.12	0.59
1:B:1170:ILE:HG12	1:B:1176:PRO:HD2	1.84	0.59
1:B:1175:ILE:HD12	1:B:1176:PRO:HD2	1.84	0.59
1:A:822:ILE:HB	1:A:823:ALA:HA	1.83	0.59
1:B:370:LEU:HD22	1:B:465:TRP:CG	2.37	0.59
1:B:665:ASP:HB3	1:B:686:ARG:CZ	2.31	0.59
1:B:668:ILE:HG22	1:B:673:ARG:NH1	2.17	0.59
1:B:1003:GLN:HB2	1:B:1005:ASN:OD1	2.02	0.59
1:A:359:LEU:O	1:A:363:LEU:HG	2.02	0.59
1:A:514:ARG:NE	1:A:729:SER:O	2.35	0.59
1:A:941:THR:HA	1:A:993:ARG:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:ALA:O	1:B:770:GLU:HG2	2.02	0.59
1:B:773:LYS:NZ	1:B:798:ASP:OD1	2.35	0.59
1:A:357:ASN:N	1:A:357:ASN:OD1	2.36	0.59
1:A:721:TYR:CE2	1:A:824:PRO:HB3	2.37	0.59
1:B:743:ILE:HG22	1:B:744:ASP:H	1.68	0.59
1:B:523:MET:HE3	1:B:989:SER:HB2	1.84	0.59
1:A:740:LEU:HB3	1:A:835:TYR:CE1	2.38	0.59
1:B:332:ILE:HD11	1:B:349:ALA:HB2	1.84	0.59
1:B:525:ILE:HG12	1:B:531:VAL:HG11	1.83	0.59
1:A:974:LYS:NZ	1:A:983:LEU:HD12	2.17	0.59
1:B:1051:GLN:HG2	1:B:1196:VAL:HA	1.85	0.59
1:B:1131:LYS:HZ3	1:B:1160:TRP:CD1	2.20	0.59
1:A:473:ASN:OD1	1:A:505:MET:N	2.32	0.59
1:A:1087:MET:HE1	1:A:1093:MET:HB2	1.84	0.59
1:B:390:ASN:O	1:B:433:ARG:HB2	2.03	0.59
1:B:930:THR:HG23	1:B:1021:ALA:HB2	1.84	0.59
1:A:773:LYS:HE2	1:A:797:LEU:HB3	1.85	0.59
1:A:931:LEU:HD11	1:A:984:LEU:HD13	1.84	0.59
1:A:1064:ASP:N	1:A:1064:ASP:OD1	2.32	0.59
1:B:939:SER:HB3	1:B:956:ARG:HG2	1.85	0.59
1:A:577:ILE:HD13	1:A:627:TRP:CD2	2.38	0.58
1:B:333:HIS:CG	1:B:336:LYS:HE3	2.38	0.58
1:B:559:THR:O	1:B:799:LYS:NZ	2.29	0.58
1:B:985:GLU:O	1:B:989:SER:N	2.36	0.58
1:A:438:GLN:OE1	1:A:440:MET:N	2.34	0.58
1:B:854:ARG:NE	1:B:854:ARG:O	2.36	0.58
1:B:1211:CYS:HA	1:B:1225:LYS:HG3	1.84	0.58
1:A:766:ALA:O	1:A:770:GLU:HG2	2.03	0.58
1:A:801:LYS:HG3	1:A:802:LEU:HG	1.84	0.58
1:A:1201:SER:OG	1:A:1203:GLU:O	2.20	0.58
1:B:374:ARG:H	1:B:1259:ARG:HH21	1.51	0.58
1:A:763:ASN:HB3	1:A:767:ARG:NH2	2.18	0.58
1:A:1079:ARG:HH12	1:A:1111:PRO:C	2.12	0.58
1:A:807:THR:O	1:A:811:LEU:HG	2.02	0.58
1:B:339:LEU:HD11	1:B:965:PHE:HD1	1.69	0.58
1:B:621:THR:HA	1:B:785:TRP:CZ2	2.37	0.58
1:A:471:ARG:HG3	1:A:472:MET:HG3	1.85	0.58
1:A:504:LEU:HG	1:A:506:PRO:HD3	1.84	0.58
1:A:801:LYS:HZ2	1:A:802:LEU:HD11	1.68	0.58
1:B:345:SER:OG	1:B:346:VAL:N	2.36	0.58
1:B:350:ASN:OD1	1:B:352:LEU:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069:ARG:HH11	1:B:1138:ARG:HB3	1.67	0.58
1:A:857:ILE:HD13	1:A:862:LEU:HD13	1.85	0.58
1:A:924:THR:O	1:A:928:VAL:HG23	2.03	0.58
1:A:1216:SER:OG	1:A:1218:GLN:O	2.16	0.58
1:B:941:THR:HG22	1:B:942:GLN:H	1.68	0.58
1:A:1082:ARG:HH21	1:A:1095:ARG:HD2	1.69	0.58
1:B:582:ARG:O	1:B:584:SER:N	2.32	0.58
1:A:1149:HIS:HB2	1:A:1181:MET:SD	2.44	0.58
1:B:371:TYR:C	1:B:462:ARG:HH21	2.12	0.58
1:B:1046:ILE:HG13	1:B:1202:THR:HG22	1.86	0.58
1:B:1078:GLY:N	1:B:1081:CYS:SG	2.76	0.58
1:B:690:ASN:HD21	1:B:692:GLN:HG2	1.68	0.58
1:A:453:THR:HA	1:A:1254:TYR:HA	1.86	0.57
1:A:981:ASP:OD1	1:A:981:ASP:N	2.36	0.57
1:B:453:THR:HA	1:B:1254:TYR:HA	1.85	0.57
1:A:317:ASP:OD1	1:A:318:ARG:N	2.37	0.57
1:A:422:PHE:O	1:A:425:SER:OG	2.21	0.57
1:B:304:ILE:HG13	1:B:1210:PHE:HB2	1.86	0.57
1:B:772:MET:O	1:B:776:VAL:HG13	2.04	0.57
1:B:1030:VAL:O	1:B:1034:GLU:N	2.35	0.57
1:A:983:LEU:H	1:A:985:GLU:CD	2.11	0.57
1:B:376:THR:HG21	1:B:392:ARG:HH11	1.68	0.57
1:B:542:LEU:HB3	1:B:545:ARG:HH21	1.68	0.57
1:B:782:GLN:HB2	1:B:785:TRP:CE2	2.39	0.57
1:B:814:LEU:N	1:B:816:PRO:HD2	2.20	0.57
1:A:1060:ALA:HB2	1:A:1204:TYR:CD1	2.38	0.57
1:B:691:ILE:HG21	1:B:710:HIS:HE1	1.69	0.57
1:A:454:SER:O	1:A:1255:ASN:ND2	2.37	0.57
1:A:810:TYR:HA	1:A:814:LEU:HB2	1.87	0.57
1:A:1079:ARG:HH11	1:A:1114:LEU:H	1.52	0.57
1:B:759:ASN:HD21	1:B:761:LEU:HD12	1.69	0.57
1:B:787:GLN:HG3	1:B:789:LEU:HD22	1.87	0.57
1:B:815:ALA:HA	1:B:818:GLU:HG2	1.86	0.57
1:B:1198:TYR:HB2	1:B:1199:ILE:HD12	1.85	0.57
1:A:429:ASN:O	1:A:431:VAL:N	2.37	0.57
1:A:1230:GLU:HG3	1:A:1231:ARG:HG2	1.87	0.57
1:B:1127:ASP:N	1:B:1127:ASP:OD1	2.36	0.57
1:A:854:ARG:HB3	1:A:857:ILE:HB	1.86	0.57
1:A:1041:ALA:O	1:A:1143:ALA:HA	2.05	0.57
1:A:307:HIS:N	1:A:324:MET:HE1	2.19	0.57
1:A:521:ARG:HD2	1:A:828:PHE:HD1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ILE:HG22	1:A:678:PHE:CE2	2.39	0.57
1:A:807:THR:HG22	1:A:811:LEU:HD11	1.87	0.57
1:A:945:VAL:HG12	1:A:946:ASP:H	1.69	0.57
1:B:681:PRO:HB2	1:B:840:ARG:HE	1.70	0.57
1:A:354:PHE:HD2	1:A:952:ILE:HD11	1.70	0.57
1:A:472:MET:HB2	1:A:506:PRO:HA	1.86	0.57
1:A:1166:TRP:NE1	1:A:1176:PRO:HB2	2.20	0.57
1:A:1120:ARG:HD2	1:A:1121:TYR:N	2.20	0.57
1:B:511:ASN:OD1	1:B:729:SER:N	2.35	0.57
1:B:1087:MET:HG3	1:B:1088:ASN:ND2	2.20	0.57
1:A:303:ARG:HB2	1:A:1210:PHE:CD1	2.40	0.56
1:A:340:ASN:HD21	1:A:348:GLY:C	2.13	0.56
1:A:680:THR:HB	1:A:683:THR:HG23	1.87	0.56
1:A:1123:ASN:ND2	1:A:1168:GLU:OE1	2.36	0.56
1:B:318:ARG:N	1:B:371:TYR:OH	2.37	0.56
1:B:894:ASP:N	1:B:894:ASP:OD1	2.38	0.56
1:A:938:ILE:HA	1:A:947:ARG:CZ	2.35	0.56
1:B:376:THR:OG1	1:B:444:MET:SD	2.59	0.56
1:B:403:TYR:O	1:B:406:MET:N	2.38	0.56
1:B:810:TYR:OH	1:B:901:TYR:OH	2.12	0.56
1:B:1046:ILE:HG21	1:B:1136:ARG:HH21	1.70	0.56
1:A:332:ILE:HD11	1:A:335:PHE:HB2	1.86	0.56
1:A:375:HIS:N	1:A:1260:TYR:O	2.29	0.56
1:A:515:GLN:O	1:A:519:ILE:HG13	2.05	0.56
1:A:777:ASP:HA	1:A:790:VAL:HG11	1.86	0.56
1:B:555:ILE:HD11	1:B:890:LYS:HD3	1.88	0.56
1:B:556:ILE:HD12	1:B:556:ILE:H	1.69	0.56
1:B:902:ALA:HB2	1:B:1274:VAL:O	2.05	0.56
1:B:961:THR:OG1	1:B:962:ALA:N	2.38	0.56
1:B:1057:SER:O	1:B:1060:ALA:N	2.36	0.56
1:A:694:ILE:HB	1:A:703:ARG:HH11	1.69	0.56
1:A:899:VAL:O	1:A:903:ASP:HB2	2.06	0.56
1:A:1131:LYS:HA	1:A:1198:TYR:HE2	1.69	0.56
1:B:676:SER:O	1:B:679:SER:OG	2.22	0.56
1:A:465:TRP:CE2	1:A:469:LEU:HD11	2.40	0.56
1:A:548:PRO:HD2	1:A:891:TYR:CE1	2.40	0.56
1:A:656:MET:HE3	1:A:702:LEU:HG	1.87	0.56
1:A:841:ASP:HB3	1:A:1005:ASN:HB3	1.87	0.56
1:A:958:SER:O	1:A:961:THR:OG1	2.23	0.56
1:B:810:TYR:N	1:B:891:TYR:OH	2.39	0.56
1:A:370:LEU:HB3	1:A:465:TRP:CZ2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:HD11	1:A:506:PRO:HB3	1.88	0.56
1:A:601:ASN:OD1	1:A:833:VAL:N	2.39	0.56
1:B:1007:ARG:NH1	1:B:1008:THR:O	2.38	0.56
1:A:464:ARG:NE	1:A:1022:ASP:OD2	2.38	0.56
1:A:846:MET:HA	1:A:871:VAL:HG21	1.86	0.56
1:A:965:PHE:O	1:A:969:VAL:HG23	2.05	0.56
1:B:473:ASN:OD1	1:B:474:ILE:N	2.38	0.56
1:B:500:SER:H	1:B:503:ARG:NH2	2.04	0.56
1:B:731:ASN:HB3	1:B:734:THR:HG23	1.86	0.56
1:A:484:THR:O	1:A:489:GLY:N	2.38	0.56
1:A:532:ILE:O	1:A:536:LEU:HD23	2.06	0.56
1:A:970:ASN:ND2	1:A:983:LEU:O	2.38	0.56
1:A:1061:PRO:HB2	1:A:1065:LEU:HD12	1.88	0.56
1:A:1260:TYR:CD2	1:A:1262:TYR:HE2	2.24	0.56
1:A:418:LYS:HE2	1:A:1217:PRO:O	2.06	0.56
1:A:864:LEU:HD23	1:A:865:SER:H	1.71	0.56
1:B:519:ILE:O	1:B:523:MET:HG3	2.05	0.56
1:B:632:LEU:O	1:B:636:LEU:HG	2.06	0.56
1:B:666:ASN:HB3	1:B:669:TYR:CD1	2.41	0.56
1:B:1064:ASP:OD1	1:B:1065:LEU:N	2.37	0.56
1:A:320:SER:OG	1:A:364:GLU:O	2.23	0.55
1:A:797:LEU:HD23	1:A:800:LEU:HD12	1.88	0.55
1:B:452:GLU:N	1:B:1255:ASN:O	2.37	0.55
1:B:548:PRO:HB2	1:B:892:PRO:HG2	1.87	0.55
1:A:375:HIS:CD2	1:A:444:MET:HE3	2.42	0.55
1:A:582:ARG:HB2	1:A:880:ARG:NH2	2.21	0.55
1:A:1148:LEU:HA	1:A:1180:PHE:H	1.69	0.55
1:B:475:ASN:O	1:B:478:GLU:HG2	2.06	0.55
1:B:849:VAL:HB	1:B:999:ILE:HD12	1.88	0.55
1:B:1112:LEU:HB3	1:B:1116:GLN:HE21	1.71	0.55
1:A:807:THR:OG1	1:A:885:ALA:O	2.24	0.55
1:A:855:ASP:OD2	1:B:711:ARG:HB3	2.06	0.55
1:A:1058:PRO:HB3	1:A:1200:ILE:HG22	1.88	0.55
1:B:556:ILE:O	1:B:560:MET:N	2.32	0.55
1:B:817:VAL:O	1:B:821:VAL:HG23	2.06	0.55
1:A:967:GLU:O	1:A:971:THR:OG1	2.24	0.55
1:A:1113:ALA:O	1:A:1117:MET:HG3	2.06	0.55
1:A:1115:TRP:HA	1:A:1122:PHE:HE2	1.71	0.55
1:A:646:VAL:HG22	1:A:688:PHE:CE2	2.41	0.55
1:A:1146:TYR:HA	1:A:1178:VAL:N	2.20	0.55
1:B:591:PHE:CE1	1:B:595:LEU:HD21	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1126:PHE:HA	1:B:1129:TRP:CD1	2.42	0.55
1:A:514:ARG:HH22	1:A:518:GLN:HE21	1.54	0.55
1:A:593:VAL:HG23	1:A:594:ALA:H	1.72	0.55
1:A:897:THR:OG1	1:A:898:ASN:N	2.39	0.55
1:A:983:LEU:O	1:A:985:GLU:HG3	2.07	0.55
1:A:1079:ARG:HA	1:A:1114:LEU:HD12	1.88	0.55
1:B:325:ALA:O	1:B:331:ASN:ND2	2.39	0.55
1:B:349:ALA:N	1:B:1175:ILE:O	2.39	0.55
1:B:604:VAL:HA	1:B:873:VAL:N	2.21	0.55
1:B:699:ALA:HB1	1:B:702:LEU:HG	1.89	0.55
1:A:952:ILE:HD12	1:A:953:PRO:HD2	1.89	0.55
1:B:338:LEU:HD11	1:B:361:MET:N	2.22	0.55
1:B:439:MET:HG3	1:B:446:GLU:HB2	1.89	0.55
1:B:468:ARG:N	1:B:471:ARG:HH21	2.05	0.55
1:B:965:PHE:O	1:B:968:TRP:HB2	2.07	0.55
1:B:983:LEU:HD23	1:B:984:LEU:HB2	1.87	0.55
1:B:1104:PHE:HD2	1:B:1129:TRP:CD2	2.24	0.55
1:A:370:LEU:HB3	1:A:465:TRP:CE2	2.40	0.55
1:A:549:LEU:HB2	1:A:891:TYR:HE1	1.72	0.55
1:B:378:PHE:C	1:B:393:SER:HB3	2.32	0.55
1:A:1098:THR:HG23	1:A:1100:MET:HG2	1.89	0.55
1:B:360:HIS:HA	1:B:363:LEU:HD12	1.89	0.55
1:B:546:ILE:HG12	1:B:901:TYR:HE2	1.71	0.55
1:B:684:TRP:CD2	1:B:840:ARG:HB2	2.42	0.55
1:B:850:THR:HA	1:B:861:ALA:H	1.72	0.55
1:A:928:VAL:HG22	1:A:984:LEU:HD21	1.87	0.55
1:A:1026:LEU:O	1:A:1030:VAL:HG23	2.07	0.55
1:B:437:ALA:HB2	1:B:447:TRP:CE3	2.42	0.55
1:B:518:GLN:HG3	1:B:828:PHE:HE1	1.72	0.55
1:B:914:VAL:HA	1:B:917:ASN:ND2	2.22	0.55
1:B:1093:MET:HB3	1:B:1101:MET:C	2.32	0.55
1:B:1151:TYR:CD2	1:B:1181:MET:HG2	2.42	0.55
1:A:713:TRP:HB3	1:A:837:ARG:NH2	2.22	0.54
1:A:1156:TYR:HE1	1:A:1196:VAL:HG23	1.72	0.54
1:B:322:VAL:HA	1:B:365:PHE:CD2	2.42	0.54
1:B:422:PHE:O	1:B:425:SER:OG	2.15	0.54
1:B:502:ASN:O	1:B:504:LEU:HG	2.07	0.54
1:B:807:THR:HG22	1:B:811:LEU:HD21	1.89	0.54
1:A:518:GLN:HG3	1:A:732:LEU:HD11	1.88	0.54
1:A:707:GLU:HA	1:A:710:HIS:CD2	2.42	0.54
1:A:1126:PHE:O	1:A:1130:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:LEU:O	1:B:635:ALA:N	2.40	0.54
1:B:721:TYR:CD2	1:B:739:LEU:HB2	2.42	0.54
1:B:1032:ASN:HA	1:B:1035:TYR:CE2	2.41	0.54
1:A:488:GLN:HB3	1:A:490:TYR:CD2	2.42	0.54
1:A:657:VAL:HG22	1:A:671:GLN:HG3	1.90	0.54
1:A:1057:SER:OG	1:A:1060:ALA:N	2.40	0.54
1:A:1141:MET:HG2	1:A:1144:TYR:HB3	1.88	0.54
1:B:667:GLN:HE21	1:B:668:ILE:HG13	1.72	0.54
1:B:1079:ARG:HH12	1:B:1118:ASN:HD21	1.53	0.54
1:A:353:MET:O	1:A:357:ASN:ND2	2.40	0.54
1:A:763:ASN:O	1:A:767:ARG:HG2	2.07	0.54
1:B:376:THR:H	1:B:444:MET:HB2	1.72	0.54
1:A:557:SER:HA	1:A:560:MET:HG3	1.90	0.54
1:A:788:SER:O	1:A:791:SER:OG	2.15	0.54
1:A:818:GLU:HA	1:A:821:VAL:HG23	1.89	0.54
1:A:969:VAL:O	1:A:973:LEU:HG	2.07	0.54
1:B:374:ARG:H	1:B:1259:ARG:HE	1.56	0.54
1:B:540:SER:O	1:B:544:GLN:HG3	2.08	0.54
1:B:600:TYR:CZ	1:B:830:PRO:HA	2.42	0.54
1:B:666:ASN:OD1	1:B:669:TYR:N	2.36	0.54
1:B:1019:VAL:HA	1:B:1022:ASP:OD2	2.08	0.54
1:A:574:ALA:HA	1:A:577:ILE:HG22	1.89	0.54
1:A:939:SER:OG	1:A:939:SER:O	2.22	0.54
1:B:600:TYR:CE2	1:B:830:PRO:HA	2.42	0.54
1:B:601:ASN:HB3	1:B:832:GLN:HA	1.90	0.54
1:A:302:SER:N	1:A:307:HIS:HB3	2.22	0.54
1:A:796:THR:O	1:A:800:LEU:HG	2.08	0.54
1:A:977:PHE:H	1:A:979:LEU:HD12	1.73	0.54
1:A:1118:ASN:OD1	1:A:1120:ARG:NE	2.41	0.54
1:A:1160:TRP:O	1:A:1163:ALA:N	2.29	0.54
1:A:1260:TYR:HD2	1:A:1262:TYR:CE2	2.26	0.54
1:B:573:PRO:HG3	1:B:793:MET:SD	2.47	0.54
1:B:1158:ASN:ND2	1:B:1160:TRP:HB3	2.23	0.54
1:A:375:HIS:HD2	1:A:444:MET:HE3	1.73	0.54
1:A:971:THR:O	1:A:975:THR:HG23	2.08	0.54
1:B:518:GLN:O	1:B:522:ILE:HG13	2.07	0.54
1:B:601:ASN:H	1:B:832:GLN:HA	1.72	0.54
1:B:837:ARG:HG3	1:B:838:LEU:HG	1.89	0.54
1:A:549:LEU:HA	1:A:890:LYS:O	2.08	0.54
1:A:1147:MET:HE2	1:A:1177:SER:O	2.07	0.54
1:B:474:ILE:HG23	1:B:508:ARG:HH21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:ASP:C	1:B:1082:ARG:HH11	2.15	0.54
1:A:385:PHE:CZ	1:A:412:GLY:HA2	2.43	0.54
1:A:937:GLN:OE1	1:A:947:ARG:HA	2.08	0.54
1:A:1151:TYR:N	1:A:1182:VAL:O	2.40	0.54
1:A:1166:TRP:CE3	1:A:1167:LEU:HG	2.43	0.54
1:A:434:PHE:CD2	1:A:435:ASP:HB2	2.43	0.53
1:A:740:LEU:HB3	1:A:835:TYR:HE1	1.74	0.53
1:A:895:LEU:HG	1:A:900:TRP:NE1	2.23	0.53
1:B:508:ARG:HE	1:B:726:VAL:HG13	1.73	0.53
1:B:851:ARG:H	1:B:861:ALA:HB2	1.73	0.53
1:B:898:ASN:HB2	1:B:1275:PRO:C	2.33	0.53
1:B:1149:HIS:N	1:B:1180:PHE:O	2.34	0.53
1:A:591:PHE:HE2	1:A:882:ILE:HA	1.73	0.53
1:B:376:THR:N	1:B:444:MET:SD	2.81	0.53
1:B:1032:ASN:HA	1:B:1035:TYR:CZ	2.43	0.53
1:B:1069:ARG:HH22	1:B:1110:PHE:H	1.54	0.53
1:A:582:ARG:HB2	1:A:880:ARG:HH21	1.73	0.53
1:B:686:ARG:O	1:B:690:ASN:N	2.41	0.53
1:B:1156:TYR:CE2	1:B:1158:ASN:HA	2.43	0.53
1:A:375:HIS:HA	1:A:392:ARG:HH22	1.74	0.53
1:A:1186:SER:CB	1:A:1221:ALA:HA	2.38	0.53
1:B:482:ALA:O	1:B:485:GLU:N	2.41	0.53
1:B:629:PHE:CZ	1:B:652:LEU:HB2	2.43	0.53
1:B:636:LEU:O	1:B:638:MET:N	2.41	0.53
1:B:639:THR:OG1	1:B:640:THR:N	2.42	0.53
1:B:1232:TYR:O	1:B:1236:THR:HG23	2.08	0.53
1:A:1107:ASN:C	1:A:1108:TRP:CD1	2.85	0.53
1:B:325:ALA:CB	1:B:331:ASN:HA	2.38	0.53
1:B:700:PRO:C	1:B:704:GLN:HE21	2.15	0.53
1:A:378:PHE:CZ	1:A:392:ARG:HD3	2.43	0.53
1:A:851:ARG:HA	1:A:997:LEU:HD22	1.89	0.53
1:A:949:LEU:HG	1:A:951:TRP:CE2	2.44	0.53
1:A:1147:MET:HG3	1:A:1179:PRO:HA	1.90	0.53
1:B:301:VAL:CA	1:B:1214:SER:HB2	2.37	0.53
1:B:379:SER:N	1:B:393:SER:HB3	2.22	0.53
1:B:540:SER:OG	1:B:592:ARG:HB2	2.09	0.53
1:B:721:TYR:CG	1:B:739:LEU:HD22	2.44	0.53
1:B:996:GLN:OE1	1:B:997:LEU:N	2.34	0.53
1:A:810:TYR:HA	1:A:814:LEU:HD23	1.90	0.53
1:A:938:ILE:HG23	1:A:948:TYR:H	1.73	0.53
1:B:480:GLU:O	1:B:484:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:LEU:O	1:B:630:PHE:HB2	2.09	0.53
1:B:1147:MET:HE3	1:B:1179:PRO:HB3	1.90	0.53
1:A:514:ARG:O	1:A:518:GLN:HG2	2.08	0.53
1:A:720:ARG:NH1	1:A:722:GLY:O	2.42	0.53
1:B:433:ARG:HG2	1:B:436:ARG:HH11	1.72	0.53
1:B:548:PRO:HD2	1:B:810:TYR:HE1	1.74	0.53
1:B:1165:ALA:HA	1:B:1168:GLU:CD	2.33	0.53
1:A:529:ALA:HA	1:A:532:ILE:HG23	1.91	0.53
1:A:1002:GLN:HA	1:A:1007:ARG:O	2.09	0.53
1:B:316:PHE:HB2	1:B:371:TYR:CD2	2.43	0.53
1:B:616:ASP:HB3	1:B:674:ARG:HD2	1.91	0.53
1:B:656:MET:SD	1:B:660:GLU:HB2	2.49	0.53
1:B:1000:GLN:HB2	1:B:1010:ASP:OD1	2.09	0.53
1:B:920:ARG:O	1:B:924:THR:OG1	2.18	0.53
1:B:1037:LEU:CA	1:B:1207:ARG:HG3	2.39	0.53
1:B:1166:TRP:CZ3	1:B:1170:ILE:HD11	2.44	0.53
1:B:1232:TYR:HB3	1:B:1235:LEU:HD12	1.90	0.53
1:A:312:SER:HB3	1:A:1259:ARG:HH12	1.74	0.52
1:A:592:ARG:HA	1:A:595:LEU:HD12	1.92	0.52
1:A:759:ASN:HD22	1:A:808:PRO:HB3	1.73	0.52
1:B:355:ARG:HB3	1:B:954:SER:HB2	1.91	0.52
1:B:810:TYR:HA	1:B:814:LEU:HB2	1.91	0.52
1:B:1115:TRP:HH2	1:B:1123:ASN:HD21	1.56	0.52
1:A:644:ALA:HA	1:A:647:LYS:HB2	1.91	0.52
1:B:358:VAL:HG12	1:B:362:LEU:HD23	1.91	0.52
1:B:733:PHE:HD1	1:B:834:PRO:HD3	1.73	0.52
1:B:759:ASN:ND2	1:B:808:PRO:HB2	2.24	0.52
1:A:406:MET:HG3	1:A:452:GLU:HB2	1.91	0.52
1:A:479:ILE:HG13	1:A:483:LEU:HD23	1.90	0.52
1:B:432:GLY:O	1:B:451:PHE:N	2.42	0.52
1:B:792:SER:OG	1:B:793:MET:N	2.43	0.52
1:B:1151:TYR:CZ	1:B:1183:PRO:HB3	2.45	0.52
1:B:1247:LEU:HA	1:B:1249:GLU:N	2.25	0.52
1:A:330:ASN:HA	1:A:1148:LEU:H	1.75	0.52
1:A:851:ARG:O	1:A:995:THR:HA	2.09	0.52
1:A:1044:ASP:CG	1:A:1140:GLU:HA	2.34	0.52
1:B:324:MET:HE3	1:B:1207:ARG:HH21	1.74	0.52
1:B:432:GLY:N	1:B:451:PHE:HB2	2.25	0.52
1:B:846:MET:HB3	1:B:1002:GLN:HG2	1.90	0.52
1:B:1095:ARG:HG2	1:B:1099:GLY:HA2	1.91	0.52
1:A:643:CYS:HG	1:A:684:TRP:CD1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:LEU:HG	1:A:951:TRP:NE1	2.25	0.52
1:B:400:GLU:O	1:B:403:TYR:HB2	2.08	0.52
1:B:406:MET:SD	1:B:453:THR:OG1	2.68	0.52
1:B:777:ASP:OD1	1:B:794:ARG:NE	2.42	0.52
1:B:1234:ILE:HA	1:B:1238:PRO:HA	1.91	0.52
1:A:706:ALA:HA	1:A:709:ILE:HD12	1.92	0.52
1:A:713:TRP:O	1:A:715:ASN:ND2	2.43	0.52
1:A:713:TRP:CE3	1:A:714:PRO:HD2	2.45	0.52
1:A:1158:ASN:ND2	1:A:1160:TRP:HB3	2.24	0.52
1:B:448:VAL:HG12	1:B:1259:ARG:O	2.08	0.52
1:A:533:GLN:HG2	1:A:537:GLN:NE2	2.24	0.52
1:A:651:THR:HA	1:A:654:ASN:ND2	2.25	0.52
1:A:1079:ARG:CZ	1:A:1113:ALA:HB3	2.39	0.52
1:B:448:VAL:H	1:B:1259:ARG:N	2.04	0.52
1:B:686:ARG:HD3	1:B:686:ARG:H	1.75	0.52
1:B:844:PRO:HA	1:B:1003:GLN:HA	1.92	0.52
1:B:1005:ASN:OD1	1:B:1006:GLY:N	2.42	0.52
1:B:1071:THR:HG23	1:B:1072:PRO:O	2.09	0.52
1:A:942:GLN:NE2	1:A:994:MET:HA	2.14	0.52
1:A:1034:GLU:OE1	1:A:1207:ARG:NH1	2.34	0.52
1:A:399:ALA:HB1	1:A:403:TYR:CZ	2.45	0.52
1:B:553:PRO:HG3	1:B:884:VAL:HG11	1.92	0.52
1:B:807:THR:O	1:B:811:LEU:HG	2.10	0.52
1:A:381:ASP:OD1	1:A:391:LEU:HB3	2.10	0.51
1:A:550:GLN:OE1	1:A:890:LYS:HG3	2.10	0.51
1:A:674:ARG:NH2	1:B:786:THR:OG1	2.42	0.51
1:B:307:HIS:C	1:B:310:TRP:HZ3	2.19	0.51
1:B:451:PHE:N	1:B:1256:VAL:HG12	2.25	0.51
1:B:717:SER:OG	1:B:744:ASP:HA	2.10	0.51
1:B:880:ARG:O	1:B:884:VAL:HG23	2.10	0.51
1:B:1049:ARG:HE	1:B:1132:THR:C	2.17	0.51
1:A:523:MET:C	1:A:526:GLY:H	2.19	0.51
1:A:778:ASN:OD1	1:A:779:GLN:N	2.43	0.51
1:A:928:VAL:HA	1:A:931:LEU:HD12	1.92	0.51
1:B:464:ARG:HH22	1:B:1026:LEU:HD21	1.74	0.51
1:B:701:ILE:HG23	1:B:775:LEU:HD11	1.92	0.51
1:B:854:ARG:NH2	1:B:856:ALA:O	2.43	0.51
1:B:1146:TYR:HE2	1:B:1207:ARG:HH11	1.58	0.51
1:A:342:GLU:HB2	1:A:350:ASN:CG	2.35	0.51
1:A:559:THR:HA	1:A:562:THR:HG22	1.91	0.51
1:B:999:ILE:HG13	1:B:1000:GLN:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:ASN:O	1:B:1146:TYR:OH	2.28	0.51
1:A:1054:HIS:HB2	1:A:1056:TRP:CD1	2.46	0.51
1:A:1166:TRP:HE1	1:A:1176:PRO:HB2	1.75	0.51
1:B:313:ASN:HD22	1:B:1259:ARG:HH12	1.57	0.51
1:B:838:LEU:C	1:B:842:ARG:HH21	2.19	0.51
1:A:1232:TYR:HB3	1:A:1235:LEU:HD12	1.91	0.51
1:B:375:HIS:CD2	1:B:444:MET:HB2	2.46	0.51
1:B:809:MET:HB3	1:B:891:TYR:OH	2.10	0.51
1:B:1166:TRP:CH2	1:B:1175:ILE:HD11	2.44	0.51
1:A:358:VAL:O	1:A:362:LEU:HG	2.10	0.51
1:A:407:TYR:C	1:A:409:THR:H	2.19	0.51
1:B:514:ARG:HH22	1:B:728:GLY:C	2.19	0.51
1:B:1158:ASN:HB3	1:B:1161:ASN:ND2	2.26	0.51
1:B:1161:ASN:O	1:B:1164:SER:OG	2.24	0.51
1:A:390:ASN:HB2	1:A:433:ARG:HB3	1.93	0.51
1:A:457:LEU:H	1:A:457:LEU:HD12	1.76	0.51
1:A:714:PRO:O	1:A:837:ARG:NE	2.41	0.51
1:A:1058:PRO:O	1:A:1061:PRO:HD3	2.11	0.51
1:B:307:HIS:O	1:B:310:TRP:HZ3	1.94	0.51
1:B:338:LEU:HD21	1:B:361:MET:HB2	1.92	0.51
1:B:607:VAL:N	1:B:875:LEU:O	2.25	0.51
1:B:840:ARG:O	1:B:843:VAL:HB	2.11	0.51
1:B:1247:LEU:HA	1:B:1249:GLU:H	1.76	0.51
1:A:543:LEU:HD23	1:A:592:ARG:HG3	1.92	0.51
1:A:855:ASP:HB2	1:B:711:ARG:HG2	1.93	0.51
1:A:1002:GLN:HG3	1:A:1008:THR:HG22	1.93	0.51
1:B:307:HIS:CE1	1:B:310:TRP:HB3	2.46	0.51
1:A:985:GLU:N	1:A:986:PRO:HD2	2.26	0.51
1:B:628:ASP:HA	1:B:631:ILE:HD12	1.93	0.51
1:B:853:SER:N	1:B:994:MET:HG2	2.25	0.51
1:B:1121:TYR:O	1:B:1125:GLN:HG2	2.11	0.51
1:B:1149:HIS:O	1:B:1181:MET:HA	2.11	0.51
1:A:340:ASN:HB3	1:A:343:THR:O	2.11	0.50
1:A:406:MET:HE3	1:A:407:TYR:CE1	2.45	0.50
1:A:581:LEU:HG	1:A:880:ARG:NH2	2.27	0.50
1:A:773:LYS:HZ1	1:A:801:LYS:HD3	1.76	0.50
1:A:805:SER:OG	1:A:886:LEU:O	2.15	0.50
1:A:915:PHE:O	1:A:919:GLN:HG2	2.11	0.50
1:A:1043:GLY:O	1:A:1144:TYR:HE2	1.94	0.50
1:B:518:GLN:HG3	1:B:828:PHE:CE1	2.46	0.50
1:B:603:VAL:HG13	1:B:831:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:MET:O	1:B:686:ARG:NH2	2.43	0.50
1:B:1031:PHE:HE1	1:B:1037:LEU:H	1.59	0.50
1:B:1162:LEU:H	1:B:1162:LEU:HD12	1.76	0.50
1:B:1163:ALA:O	1:B:1167:LEU:HG	2.10	0.50
1:A:335:PHE:HE2	1:A:338:LEU:HD23	1.76	0.50
1:A:353:MET:HE3	1:A:355:ARG:H	1.76	0.50
1:A:721:TYR:HD1	1:A:739:LEU:HD11	1.77	0.50
1:B:472:MET:C	1:B:506:PRO:HA	2.36	0.50
1:B:685:PRO:HG2	1:B:688:PHE:HB2	1.93	0.50
1:B:713:TRP:HB3	1:B:837:ARG:HH21	1.76	0.50
1:B:845:THR:O	1:B:865:SER:OG	2.22	0.50
1:B:850:THR:HG22	1:B:852:GLN:H	1.75	0.50
1:B:1166:TRP:CD1	1:B:1179:PRO:HD3	2.47	0.50
1:A:987:LEU:CG	1:A:992:PRO:HB3	2.39	0.50
1:B:338:LEU:HB3	1:B:357:ASN:HB3	1.92	0.50
1:B:898:ASN:O	1:B:901:TYR:N	2.43	0.50
1:B:1150:TYR:HA	1:B:1182:VAL:HG23	1.93	0.50
1:A:609:ASP:HA	1:A:876:ALA:HB1	1.93	0.50
1:A:785:TRP:HB3	1:A:789:LEU:HD23	1.94	0.50
1:A:807:THR:HG21	1:A:886:LEU:HA	1.92	0.50
1:A:895:LEU:HD23	1:A:901:TYR:CE2	2.46	0.50
1:B:374:ARG:H	1:B:1259:ARG:NH2	2.09	0.50
1:B:513:GLU:H	1:B:513:GLU:CD	2.19	0.50
1:B:545:ARG:CZ	1:B:546:ILE:HB	2.41	0.50
1:B:808:PRO:HA	1:B:811:LEU:HD12	1.93	0.50
1:B:934:LEU:O	1:B:938:ILE:HG23	2.11	0.50
1:A:330:ASN:CB	1:A:1147:MET:HB2	2.42	0.50
1:A:468:ARG:HA	1:A:471:ARG:NE	2.27	0.50
1:A:713:TRP:C	1:A:837:ARG:HH21	2.20	0.50
1:A:718:GLN:HA	1:A:739:LEU:O	2.11	0.50
1:B:680:THR:OG1	1:B:683:THR:HG23	2.12	0.50
1:B:956:ARG:HG2	1:B:957:ALA:H	1.76	0.50
1:B:1059:LEU:HD21	1:B:1205:ASN:HB2	1.92	0.50
1:B:1185:SER:HA	1:B:1222:GLY:HA3	1.92	0.50
1:B:1232:TYR:OH	1:B:1253:LEU:HB2	2.12	0.50
1:B:394:LEU:HD12	1:B:399:ALA:HB1	1.92	0.50
1:B:668:ILE:HG22	1:B:673:ARG:HH12	1.77	0.50
1:B:949:LEU:HD13	1:B:952:ILE:HD12	1.94	0.50
1:B:1007:ARG:HG3	1:B:1009:PHE:CZ	2.47	0.50
1:A:543:LEU:HD12	1:A:546:ILE:HB	1.94	0.50
1:A:332:ILE:C	1:A:333:HIS:CG	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:HIS:O	1:A:364:GLU:HG2	2.12	0.50
1:A:510:SER:N	1:A:513:GLU:OE2	2.42	0.50
1:A:537:GLN:O	1:A:541:VAL:HG23	2.11	0.50
1:A:967:GLU:OE2	1:A:971:THR:OG1	2.30	0.50
1:A:1079:ARG:NH2	1:A:1111:PRO:HB2	2.27	0.50
1:A:1159:ALA:CB	1:A:1197:GLN:HA	2.39	0.50
1:B:1062:PRO:HD2	1:B:1065:LEU:HD21	1.94	0.50
1:A:668:ILE:HG23	1:A:673:ARG:HG2	1.94	0.50
1:B:375:HIS:HA	1:B:444:MET:HE2	1.93	0.50
1:B:1062:PRO:HB2	1:B:1064:ASP:OD1	2.11	0.50
1:A:315:ASP:OD2	1:A:372:LEU:HG	2.12	0.49
1:B:473:ASN:CG	1:B:505:MET:H	2.20	0.49
1:B:552:ASP:HB2	1:B:890:LYS:NZ	2.27	0.49
1:B:665:ASP:HB3	1:B:686:ARG:NE	2.27	0.49
1:B:773:LYS:O	1:B:776:VAL:HG22	2.11	0.49
1:B:918:LEU:O	1:B:922:MET:HG2	2.12	0.49
1:B:1105:GLU:O	1:B:1108:TRP:NE1	2.44	0.49
1:A:364:GLU:HA	1:A:367:LEU:HG	1.93	0.49
1:A:600:TYR:HA	1:A:831:PHE:O	2.12	0.49
1:A:1153:PRO:HG3	1:A:1183:PRO:HB2	1.93	0.49
1:B:316:PHE:HE1	1:B:372:LEU:HB2	1.77	0.49
1:A:392:ARG:HG3	1:A:394:LEU:HD11	1.93	0.49
1:A:1022:ASP:O	1:A:1026:LEU:HG	2.12	0.49
1:B:339:LEU:HA	1:B:968:TRP:NE1	2.27	0.49
1:B:406:MET:HE3	1:B:452:GLU:HB2	1.94	0.49
1:B:732:LEU:C	1:B:734:THR:H	2.21	0.49
1:A:438:GLN:HB2	1:A:445:SER:HB2	1.94	0.49
1:A:701:ILE:O	1:A:704:GLN:HB3	2.12	0.49
1:A:810:TYR:OH	1:A:818:GLU:OE2	2.26	0.49
1:A:824:PRO:C	1:A:826:LEU:H	2.19	0.49
1:A:841:ASP:HA	1:A:1004:TYR:HD2	1.77	0.49
1:A:985:GLU:O	1:A:989:SER:OG	2.16	0.49
1:B:504:LEU:O	1:B:1265:PRO:HD2	2.13	0.49
1:B:846:MET:SD	1:B:1000:GLN:HG2	2.52	0.49
1:B:1037:LEU:HB2	1:B:1038:PHE:CE1	2.46	0.49
1:B:1125:GLN:O	1:B:1129:TRP:NE1	2.46	0.49
1:A:342:GLU:O	1:A:1174:SER:OG	2.30	0.49
1:A:406:MET:HG2	1:A:407:TYR:CE2	2.47	0.49
1:A:514:ARG:NH2	1:A:729:SER:OG	2.45	0.49
1:A:545:ARG:HE	1:A:908:MET:HE2	1.78	0.49
1:A:959:ALA:HA	1:A:962:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:MET:HE1	1:B:671:GLN:HA	1.95	0.49
1:B:999:ILE:HG22	1:B:1011:VAL:HB	1.94	0.49
1:B:1026:LEU:O	1:B:1030:VAL:HG23	2.12	0.49
1:A:437:ALA:HB2	1:A:447:TRP:CZ2	2.48	0.49
1:A:708:ILE:HG12	1:A:711:ARG:NH2	2.27	0.49
1:A:765:ARG:HA	1:A:768:VAL:HG12	1.95	0.49
1:A:836:VAL:HG13	1:A:842:ARG:HH21	1.78	0.49
1:A:1170:ILE:HG13	1:A:1171:THR:H	1.78	0.49
1:B:500:SER:H	1:B:503:ARG:HH21	1.61	0.49
1:B:1044:ASP:HA	1:B:1141:MET:HE2	1.94	0.49
1:B:1120:ARG:NH2	1:B:1168:GLU:O	2.46	0.49
1:A:345:SER:OG	1:A:346:VAL:N	2.45	0.49
1:A:634:LEU:HD21	1:A:887:LEU:HD21	1.95	0.49
1:A:680:THR:O	1:A:683:THR:N	2.46	0.49
1:A:773:LYS:NZ	1:A:801:LYS:HD3	2.28	0.49
1:A:972:SER:O	1:A:975:THR:OG1	2.18	0.49
1:A:1058:PRO:O	1:A:1201:SER:OG	2.30	0.49
1:A:1186:SER:OG	1:A:1220:ILE:O	2.22	0.49
1:B:965:PHE:O	1:B:969:VAL:HG23	2.11	0.49
1:A:362:LEU:O	1:A:365:PHE:HB3	2.13	0.49
1:A:456:ALA:HA	1:A:459:VAL:HG23	1.95	0.49
1:A:601:ASN:CG	1:A:833:VAL:H	2.21	0.49
1:A:630:PHE:CD2	1:A:631:ILE:HD13	2.48	0.49
1:A:1002:GLN:HG2	1:A:1003:GLN:N	2.26	0.49
1:A:1054:HIS:HB2	1:A:1056:TRP:HD1	1.78	0.49
1:B:302:SER:OG	1:B:303:ARG:N	2.45	0.49
1:B:607:VAL:O	1:B:876:ALA:HA	2.12	0.49
1:B:985:GLU:O	1:B:989:SER:OG	2.09	0.49
1:B:1114:LEU:HD23	1:B:1114:LEU:H	1.76	0.49
1:A:352:LEU:HD22	1:A:955:LEU:HD13	1.95	0.49
1:A:353:MET:CE	1:A:356:ALA:H	2.26	0.49
1:A:708:ILE:HG23	1:A:712:TYR:CD2	2.45	0.49
1:A:762:THR:HG23	1:A:765:ARG:NH2	2.27	0.49
1:A:1000:GLN:HE21	1:A:1008:THR:HA	1.77	0.49
1:A:1002:GLN:HG2	1:A:1003:GLN:H	1.78	0.49
1:A:1149:HIS:O	1:A:1181:MET:HA	2.11	0.49
1:A:1255:ASN:O	1:A:1257:VAL:HG23	2.13	0.49
1:A:455:ASP:O	1:A:458:THR:OG1	2.18	0.49
1:A:470:ALA:HA	1:A:504:LEU:HD13	1.94	0.49
1:A:839:ASP:HB3	1:A:842:ARG:NE	2.28	0.49
1:A:1118:ASN:HB3	1:A:1122:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:HIS:HB3	1:A:1259:ARG:HB3	1.95	0.48
1:A:680:THR:O	1:A:683:THR:OG1	2.27	0.48
1:A:851:ARG:HG2	1:A:852:GLN:OE1	2.11	0.48
1:B:437:ALA:HB2	1:B:447:TRP:CD2	2.47	0.48
1:B:444:MET:SD	1:B:1259:ARG:HG3	2.52	0.48
1:A:464:ARG:HD2	1:A:1023:CYS:SG	2.52	0.48
1:A:494:THR:O	1:A:1272:MET:HB2	2.13	0.48
1:A:913:GLU:HG3	1:A:914:VAL:N	2.27	0.48
1:A:1247:LEU:HD21	1:A:1251:ILE:HG23	1.95	0.48
1:B:667:GLN:CD	1:B:667:GLN:H	2.21	0.48
1:B:967:GLU:OE2	1:B:971:THR:HG23	2.13	0.48
1:A:302:SER:C	1:A:305:VAL:HA	2.38	0.48
1:A:507:TYR:CE1	1:A:1267:ILE:HG21	2.48	0.48
1:A:1047:ILE:HD13	1:A:1139:ILE:HD13	1.94	0.48
1:B:455:ASP:O	1:B:459:VAL:HG23	2.13	0.48
1:B:848:GLY:HA2	1:B:863:SER:OG	2.12	0.48
1:B:1170:ILE:HG12	1:B:1175:ILE:HD12	1.94	0.48
1:A:354:PHE:HA	1:A:357:ASN:ND2	2.17	0.48
1:A:514:ARG:HH12	1:A:518:GLN:CG	2.27	0.48
1:A:526:GLY:O	1:A:528:ASN:ND2	2.46	0.48
1:A:593:VAL:HG23	1:A:594:ALA:N	2.27	0.48
1:B:492:THR:O	1:B:1271:VAL:HA	2.13	0.48
1:A:336:LYS:HD2	1:A:337:GLN:HG3	1.96	0.48
1:A:370:LEU:HD13	1:A:465:TRP:CZ3	2.48	0.48
1:A:1151:TYR:CD2	1:A:1181:MET:HB3	2.49	0.48
1:B:376:THR:H	1:B:444:MET:CB	2.27	0.48
1:B:987:LEU:HD22	1:B:991:ASP:O	2.13	0.48
1:B:1044:ASP:C	1:B:1141:MET:HE2	2.38	0.48
1:A:719:ILE:HG23	1:A:739:LEU:HD12	1.95	0.48
1:B:435:ASP:C	1:B:436:ARG:HD3	2.37	0.48
1:B:928:VAL:HA	1:B:931:LEU:HB3	1.96	0.48
1:B:940:ASP:HB2	1:B:956:ARG:HD2	1.96	0.48
1:A:343:THR:OG1	1:A:1174:SER:OG	2.13	0.48
1:A:759:ASN:HD22	1:A:808:PRO:CB	2.25	0.48
1:A:982:MET:CG	1:A:986:PRO:HD3	2.44	0.48
1:B:806:MET:HB3	1:B:891:TYR:CE1	2.49	0.48
1:B:864:LEU:HD23	1:B:867:THR:HB	1.96	0.48
1:A:355:ARG:NH2	1:A:950:ASP:HA	2.28	0.48
1:A:514:ARG:HH22	1:A:518:GLN:NE2	2.11	0.48
1:A:600:TYR:CE2	1:A:830:PRO:HA	2.49	0.48
1:A:756:ASP:OD1	1:A:758:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:LEU:HA	1:A:774:ASN:HD22	1.78	0.48
1:A:1157:ALA:O	1:A:1196:VAL:N	2.29	0.48
1:B:760:GLU:HA	1:B:763:ASN:HB3	1.94	0.48
1:A:458:THR:HB	1:A:462:ARG:CZ	2.44	0.48
1:A:502:ASN:HB3	1:A:1262:TYR:CD1	2.49	0.48
1:A:514:ARG:HB3	1:A:514:ARG:CZ	2.43	0.48
1:A:745:HIS:CD2	1:A:816:PRO:HG2	2.49	0.48
1:A:914:VAL:HA	1:A:917:ASN:HB2	1.94	0.48
1:A:953:PRO:HG2	1:A:1141:MET:HE3	1.96	0.48
1:B:707:GLU:C	1:B:711:ARG:HE	2.22	0.48
1:B:1106:GLY:O	1:B:1136:ARG:HB2	2.14	0.48
1:A:335:PHE:CE2	1:A:338:LEU:HD23	2.48	0.48
1:A:375:HIS:HE1	1:A:447:TRP:HA	1.79	0.48
1:A:417:SER:HA	1:A:1217:PRO:HD3	1.94	0.48
1:A:720:ARG:HD2	1:A:721:TYR:O	2.14	0.48
1:A:841:ASP:C	1:A:1004:TYR:HB3	2.39	0.48
1:A:660:GLU:OE2	1:A:700:PRO:HD2	2.14	0.47
1:A:1081:CYS:HA	1:A:1095:ARG:O	2.13	0.47
1:B:323:ILE:HG13	1:B:334:LEU:HD21	1.96	0.47
1:B:437:ALA:HB1	1:B:439:MET:HG2	1.96	0.47
1:B:511:ASN:HB3	1:B:515:GLN:NE2	2.29	0.47
1:B:779:GLN:H	1:B:782:GLN:NE2	2.12	0.47
1:B:937:GLN:HA	1:B:946:ASP:O	2.14	0.47
1:B:977:PHE:C	1:B:979:LEU:H	2.21	0.47
1:B:1158:ASN:HD21	1:B:1160:TRP:CB	2.24	0.47
1:A:375:HIS:CD2	1:A:444:MET:HB3	2.49	0.47
1:A:718:GLN:HA	1:A:741:LEU:HG	1.95	0.47
1:A:766:ALA:HB3	1:A:767:ARG:NH1	2.28	0.47
1:A:836:VAL:HG13	1:A:842:ARG:NH2	2.28	0.47
1:A:1020:ILE:H	1:A:1020:ILE:HD12	1.78	0.47
1:A:1086:GLY:HA2	1:A:1091:ALA:C	2.39	0.47
1:B:375:HIS:CG	1:B:376:THR:N	2.82	0.47
1:B:981:ASP:N	1:B:981:ASP:OD1	2.47	0.47
1:B:1068:ASP:O	1:B:1071:THR:HB	2.14	0.47
1:B:1227:ILE:HG23	1:B:1229:VAL:HG13	1.95	0.47
1:B:401:LYS:O	1:B:405:ILE:HG13	2.15	0.47
1:B:560:MET:HE3	1:B:803:ILE:HD11	1.96	0.47
1:B:721:TYR:CZ	1:B:739:LEU:HD13	2.49	0.47
1:B:735:PRO:HB2	1:B:738:VAL:HG23	1.96	0.47
1:B:839:ASP:CG	1:B:842:ARG:HG3	2.38	0.47
1:B:1040:ILE:HG23	1:B:1144:TYR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1232:TYR:HE1	1:B:1253:LEU:H	1.61	0.47
1:A:504:LEU:HD12	1:A:505:MET:N	2.30	0.47
1:A:686:ARG:HH21	1:A:689:MET:HB2	1.79	0.47
1:A:1209:LEU:HD23	1:A:1225:LYS:HD3	1.96	0.47
1:B:1047:ILE:HD13	1:B:1139:ILE:HG12	1.96	0.47
1:B:1126:PHE:C	1:B:1129:TRP:HD1	2.22	0.47
1:B:1160:TRP:HA	1:B:1163:ALA:HB3	1.96	0.47
1:A:378:PHE:CD2	1:A:392:ARG:HA	2.50	0.47
1:A:1021:ALA:HA	1:A:1024:VAL:HG22	1.96	0.47
1:B:321:SER:OG	1:B:323:ILE:HG12	2.14	0.47
1:B:322:VAL:HA	1:B:365:PHE:HD2	1.78	0.47
1:B:662:ILE:HD12	1:B:663:PRO:HD2	1.95	0.47
1:A:359:LEU:O	1:A:362:LEU:N	2.48	0.47
1:A:446:GLU:HG3	1:A:502:ASN:ND2	2.30	0.47
1:A:549:LEU:HD12	1:A:890:LYS:HB3	1.95	0.47
1:A:619:SER:OG	1:A:620:VAL:N	2.45	0.47
1:A:619:SER:N	1:A:655:MET:HA	2.30	0.47
1:A:657:VAL:HA	1:A:671:GLN:NE2	2.29	0.47
1:A:916:SER:HA	1:A:919:GLN:NE2	2.28	0.47
1:A:1083:ILE:HA	1:A:1094:ILE:HA	1.97	0.47
1:A:1231:ARG:HB3	1:A:1253:LEU:H	1.79	0.47
1:B:1031:PHE:HA	1:B:1034:GLU:O	2.14	0.47
1:B:1079:ARG:HH21	1:B:1117:MET:HE2	1.78	0.47
1:A:317:ASP:CG	1:A:319:ASP:H	2.23	0.47
1:A:387:GLU:HG2	1:A:428:ARG:HD3	1.97	0.47
1:A:458:THR:HA	1:A:461:ILE:HB	1.97	0.47
1:A:716:PRO:HA	1:A:741:LEU:O	2.13	0.47
1:A:744:ASP:O	1:A:746:GLN:NE2	2.45	0.47
1:A:965:PHE:HA	1:A:968:TRP:CD1	2.41	0.47
1:A:1068:ASP:HA	1:A:1138:ARG:NH1	2.29	0.47
1:A:1082:ARG:HB2	1:A:1095:ARG:HB3	1.97	0.47
1:A:1165:ALA:O	1:A:1169:GLU:HG3	2.15	0.47
1:B:325:ALA:HB1	1:B:331:ASN:HA	1.97	0.47
1:B:528:ASN:OD1	1:B:531:VAL:HG23	2.15	0.47
1:B:1069:ARG:NH2	1:B:1140:GLU:OE2	2.47	0.47
1:B:1208:SER:O	1:B:1208:SER:OG	2.22	0.47
1:A:345:SER:CB	1:A:347:ARG:H	2.27	0.47
1:A:900:TRP:CD1	1:A:901:TYR:CD2	3.02	0.47
1:A:1044:ASP:H	1:A:1202:THR:HG1	1.63	0.47
1:A:1246:GLN:HB3	1:A:1250:VAL:HB	1.97	0.47
1:B:920:ARG:HG3	1:B:983:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:935:VAL:O	1:B:938:ILE:HG12	2.15	0.47
1:A:649:PHE:CZ	1:A:688:PHE:HB2	2.49	0.47
1:A:681:PRO:HG3	1:A:843:VAL:HG21	1.97	0.47
1:A:696:PRO:HB3	1:A:703:ARG:HD3	1.97	0.47
1:A:1188:HIS:HE1	1:A:1220:ILE:HA	1.80	0.47
1:B:332:ILE:HG13	1:B:335:PHE:HB2	1.97	0.47
1:B:382:HIS:CG	1:B:388:GLY:H	2.33	0.47
1:B:446:GLU:HG2	1:B:1261:ALA:HB3	1.95	0.47
1:B:795:GLY:HA2	1:B:798:ASP:OD2	2.15	0.47
1:B:1187:ASP:HB3	1:B:1218:GLN:O	2.14	0.47
1:A:377:GLY:O	1:A:392:ARG:HD2	2.15	0.47
1:A:458:THR:HB	1:A:462:ARG:NH2	2.29	0.47
1:A:472:MET:HB2	1:A:506:PRO:CA	2.45	0.47
1:A:524:ASN:OD1	1:A:986:PRO:HG3	2.15	0.47
1:A:656:MET:HG3	1:A:702:LEU:HD11	1.96	0.47
1:A:1046:ILE:HG22	1:A:1136:ARG:NH2	2.30	0.47
1:A:1115:TRP:CD1	1:A:1119:THR:HG22	2.46	0.47
1:B:949:LEU:O	1:B:952:ILE:N	2.42	0.47
1:B:967:GLU:OE2	1:B:970:ASN:HB3	2.15	0.47
1:B:1064:ASP:C	1:B:1066:VAL:H	2.22	0.47
1:B:1069:ARG:NH1	1:B:1138:ARG:HB3	2.30	0.47
1:B:1107:ASN:C	1:B:1108:TRP:HD1	2.23	0.47
1:A:345:SER:OG	1:A:347:ARG:N	2.46	0.46
1:A:372:LEU:HD13	1:A:374:ARG:HH21	1.80	0.46
1:A:447:TRP:HB2	1:A:1258:THR:CG2	2.42	0.46
1:A:570:THR:OG1	1:A:789:LEU:HD22	2.15	0.46
1:A:1020:ILE:O	1:A:1024:VAL:HG13	2.14	0.46
1:A:1041:ALA:HB3	1:A:1144:TYR:CE1	2.51	0.46
1:A:1104:PHE:HB3	1:A:1135:LEU:HD22	1.97	0.46
1:B:334:LEU:HA	1:B:337:GLN:OE1	2.15	0.46
1:B:360:HIS:CE1	1:B:968:TRP:HB3	2.50	0.46
1:B:724:PRO:HA	1:B:728:GLY:CA	2.44	0.46
1:A:913:GLU:CD	1:A:917:ASN:HD21	2.24	0.46
1:A:920:ARG:NH1	1:A:924:THR:OG1	2.48	0.46
1:A:969:VAL:HG12	1:A:973:LEU:HD11	1.97	0.46
1:A:1039:GLY:O	1:A:1145:PRO:HA	2.16	0.46
1:A:708:ILE:O	1:A:712:TYR:N	2.41	0.46
1:A:847:VAL:N	1:A:871:VAL:HG11	2.08	0.46
1:A:1114:LEU:HA	1:A:1117:MET:SD	2.56	0.46
1:B:375:HIS:HA	1:B:444:MET:CE	2.45	0.46
1:B:376:THR:O	1:B:444:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:GLU:O	1:B:1260:TYR:HD2	1.98	0.46
1:B:549:LEU:HD13	1:B:891:TYR:CE2	2.50	0.46
1:B:959:ALA:CB	1:B:992:PRO:HB3	2.44	0.46
1:A:492:THR:OG1	1:A:1274:VAL:HB	2.15	0.46
1:A:509:ILE:HG13	1:A:727:PHE:HA	1.98	0.46
1:A:514:ARG:HH12	1:A:518:GLN:CD	2.24	0.46
1:A:630:PHE:HD2	1:A:631:ILE:HD13	1.80	0.46
1:A:650:MET:SD	1:A:685:PRO:HG2	2.55	0.46
1:A:1150:TYR:HA	1:A:1182:VAL:CG1	2.42	0.46
1:B:713:TRP:CB	1:B:837:ARG:HH21	2.28	0.46
1:B:720:ARG:NH1	1:B:722:GLY:O	2.49	0.46
1:B:969:VAL:O	1:B:973:LEU:HG	2.16	0.46
1:B:974:LYS:HZ3	1:B:982:MET:HG2	1.79	0.46
1:B:1041:ALA:HB3	1:B:1144:TYR:CE1	2.50	0.46
1:A:458:THR:HA	1:A:461:ILE:HD12	1.98	0.46
1:A:533:GLN:HB3	1:A:534:PRO:HD3	1.98	0.46
1:A:606:THR:OG1	1:A:640:THR:N	2.47	0.46
1:A:623:LEU:HA	1:A:626:LEU:HG	1.97	0.46
1:A:687:CYS:HA	1:A:690:ASN:HB2	1.98	0.46
1:A:780:ARG:C	1:A:783:PRO:HD2	2.39	0.46
1:A:807:THR:N	1:A:889:GLY:HA3	2.31	0.46
1:A:854:ARG:HH11	1:A:857:ILE:HD12	1.80	0.46
1:A:1131:LYS:HB2	1:A:1160:TRP:CZ3	2.50	0.46
1:A:1231:ARG:HA	1:A:1252:ASP:OD1	2.16	0.46
1:B:355:ARG:NH2	1:B:954:SER:H	2.13	0.46
1:B:750:VAL:HG11	1:B:814:LEU:HD11	1.97	0.46
1:A:323:ILE:O	1:A:333:HIS:HB3	2.15	0.46
1:A:370:LEU:HD22	1:A:465:TRP:CD2	2.51	0.46
1:A:446:GLU:HB3	1:A:1262:TYR:CE1	2.50	0.46
1:A:810:TYR:O	1:A:815:ALA:N	2.37	0.46
1:A:811:LEU:O	1:A:816:PRO:HD3	2.15	0.46
1:B:464:ARG:NH1	1:B:1023:CYS:SG	2.81	0.46
1:B:476:PRO:O	1:B:480:GLU:HG3	2.15	0.46
1:B:602:GLY:HA2	1:B:833:VAL:HG23	1.98	0.46
1:B:685:PRO:O	1:B:689:MET:HG3	2.16	0.46
1:B:771:LEU:O	1:B:775:LEU:HD13	2.15	0.46
1:B:841:ASP:HA	1:B:1004:TYR:CD2	2.46	0.46
1:B:1079:ARG:NH2	1:B:1117:MET:HE2	2.31	0.46
1:A:484:THR:HG22	1:A:489:GLY:HA2	1.98	0.46
1:A:949:LEU:HB3	1:A:952:ILE:CG2	2.45	0.46
1:B:350:ASN:HD21	1:B:353:MET:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:GLU:HA	1:B:710:HIS:ND1	2.30	0.46
1:B:812:GLN:HG2	1:B:813:GLN:HG3	1.98	0.46
1:B:883:THR:HA	1:B:886:LEU:HD12	1.97	0.46
1:A:558:ASN:HB3	1:A:803:ILE:HD11	1.98	0.46
1:A:681:PRO:HB3	1:A:840:ARG:HB2	1.98	0.46
1:A:928:VAL:O	1:A:932:VAL:HG13	2.16	0.46
1:B:600:TYR:HE2	1:B:828:PHE:CE2	2.33	0.46
1:B:607:VAL:HG22	1:B:875:LEU:C	2.40	0.46
1:B:844:PRO:O	1:B:870:THR:HG23	2.15	0.46
1:B:1023:CYS:O	1:B:1026:LEU:HB2	2.16	0.46
1:B:1067:PHE:HE2	1:B:1136:ARG:HB3	1.81	0.46
1:B:1069:ARG:HD2	1:B:1109:ILE:HD12	1.97	0.46
1:B:1100:MET:HE3	1:B:1101:MET:O	2.16	0.46
1:A:427:VAL:HB	1:A:429:ASN:OD1	2.16	0.46
1:A:434:PHE:HB2	1:A:451:PHE:CE1	2.51	0.46
1:A:772:MET:O	1:A:776:VAL:HG23	2.16	0.46
1:A:988:LEU:HA	1:A:988:LEU:HD23	1.70	0.46
1:B:339:LEU:HA	1:B:968:TRP:HE1	1.80	0.46
1:B:476:PRO:O	1:B:479:ILE:HB	2.16	0.46
1:B:1166:TRP:CE2	1:B:1176:PRO:HG2	2.51	0.46
1:A:327:PRO:O	1:A:1148:LEU:HD11	2.16	0.46
1:A:354:PHE:CZ	1:A:1145:PRO:HD3	2.50	0.46
1:A:433:ARG:CD	1:A:436:ARG:HH21	2.24	0.46
1:A:790:VAL:C	1:A:794:ARG:HH21	2.23	0.46
1:B:473:ASN:HD21	1:B:504:LEU:HA	1.81	0.46
1:B:532:ILE:HA	1:B:535:VAL:HG23	1.97	0.46
1:A:523:MET:SD	1:A:526:GLY:HA3	2.56	0.45
1:A:919:GLN:O	1:A:923:ILE:HG12	2.17	0.45
1:A:959:ALA:O	1:A:963:ALA:N	2.32	0.45
1:A:1000:GLN:HA	1:A:1009:PHE:O	2.16	0.45
1:B:606:THR:OG1	1:B:639:THR:OG1	2.24	0.45
1:B:705:TRP:O	1:B:709:ILE:HG13	2.16	0.45
1:B:708:ILE:HG13	1:B:711:ARG:NH2	2.31	0.45
1:B:898:ASN:HA	1:B:1274:VAL:HG12	1.98	0.45
1:A:318:ARG:HE	1:A:977:PHE:HA	1.81	0.45
1:A:361:MET:HA	1:A:364:GLU:OE2	2.15	0.45
1:A:1000:GLN:NE2	1:A:1002:GLN:HB2	2.20	0.45
1:B:402:TRP:O	1:B:405:ILE:HB	2.14	0.45
1:B:493:VAL:HB	1:B:1271:VAL:CG1	2.40	0.45
1:B:657:VAL:HG22	1:B:671:GLN:NE2	2.31	0.45
1:B:1075:HIS:HB3	1:B:1077:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1134:GLU:HG2	1:B:1136:ARG:HG3	1.99	0.45
1:A:320:SER:O	1:A:322:VAL:HG23	2.16	0.45
1:A:605:THR:OG1	1:A:873:VAL:O	2.25	0.45
1:A:845:THR:OG1	1:A:1002:GLN:HB3	2.17	0.45
1:A:973:LEU:O	1:A:979:LEU:HD13	2.17	0.45
1:B:543:LEU:HD21	1:B:595:LEU:HD12	1.98	0.45
1:B:582:ARG:HB2	1:B:585:ASN:HD21	1.80	0.45
1:B:600:TYR:HA	1:B:832:GLN:HG2	1.99	0.45
1:B:666:ASN:HB3	1:B:669:TYR:CG	2.52	0.45
1:B:1069:ARG:HD3	1:B:1138:ARG:HB3	1.97	0.45
1:B:577:ILE:HG13	1:B:581:LEU:HD23	1.97	0.45
1:B:960:ALA:HA	1:B:963:ALA:HB3	1.97	0.45
1:A:687:CYS:HB3	1:A:693:LEU:HD12	1.99	0.45
1:B:560:MET:HA	1:B:799:LYS:NZ	2.32	0.45
1:B:1050:VAL:O	1:B:1197:GLN:NE2	2.48	0.45
1:B:1051:GLN:NE2	1:B:1196:VAL:HG13	2.32	0.45
1:A:355:ARG:NH1	1:A:950:ASP:OD1	2.50	0.45
1:A:604:VAL:HB	1:A:875:LEU:CD1	2.47	0.45
1:A:929:GLN:O	1:A:932:VAL:HG22	2.17	0.45
1:B:355:ARG:NE	1:B:950:ASP:HA	2.31	0.45
1:B:374:ARG:H	1:B:1259:ARG:NE	2.14	0.45
1:B:511:ASN:HA	1:B:514:ARG:NH2	2.10	0.45
1:B:618:GLY:HA3	1:B:655:MET:HG2	1.98	0.45
1:B:959:ALA:HB2	1:B:992:PRO:HB3	1.99	0.45
1:B:1049:ARG:HD2	1:B:1051:GLN:HE21	1.81	0.45
1:B:1147:MET:C	1:B:1179:PRO:HA	2.42	0.45
1:A:343:THR:HG23	1:A:1170:ILE:CD1	2.46	0.45
1:A:762:THR:HG23	1:A:765:ARG:HH22	1.82	0.45
1:A:873:VAL:HG23	1:A:875:LEU:HD11	1.97	0.45
1:A:937:GLN:CD	1:A:938:ILE:H	2.25	0.45
1:A:1033:HIS:HB2	1:A:1034:GLU:OE2	2.16	0.45
1:A:1075:HIS:N	1:A:1107:ASN:O	2.33	0.45
1:A:1110:PHE:CD1	1:A:1114:LEU:HD22	2.52	0.45
1:A:1188:HIS:CE1	1:A:1220:ILE:HA	2.52	0.45
1:B:601:ASN:N	1:B:831:PHE:O	2.47	0.45
1:A:389:ALA:HB2	1:A:431:VAL:HG13	1.99	0.45
1:A:745:HIS:CD2	1:A:813:GLN:HA	2.51	0.45
1:A:1038:PHE:O	1:A:1040:ILE:HG12	2.17	0.45
1:A:1087:MET:N	1:A:1090:ALA:O	2.32	0.45
1:B:400:GLU:HA	1:B:403:TYR:CD2	2.51	0.45
1:B:520:ILE:HA	1:B:523:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:MET:HG3	1:A:909:TYR:OH	2.16	0.45
1:A:926:GLU:OE1	1:A:1018:SER:HA	2.17	0.45
1:A:937:GLN:HG3	1:A:938:ILE:HG12	1.99	0.45
1:B:450:VAL:C	1:B:1256:VAL:HA	2.42	0.45
1:B:769:CYS:SG	1:B:797:LEU:HB3	2.57	0.45
1:B:933:THR:O	1:B:937:GLN:HG3	2.16	0.45
1:B:1043:GLY:O	1:B:1144:TYR:HE2	2.00	0.45
1:B:1131:LYS:HZ3	1:B:1160:TRP:CG	2.34	0.45
1:B:1203:GLU:OE2	1:B:1205:ASN:ND2	2.34	0.45
1:A:657:VAL:HA	1:A:671:GLN:HE21	1.82	0.45
1:B:548:PRO:HB3	1:B:900:TRP:CE2	2.52	0.45
1:B:606:THR:HA	1:B:875:LEU:HB3	1.99	0.45
1:B:685:PRO:HB2	1:B:687:CYS:SG	2.57	0.45
1:B:1236:THR:OG1	1:B:1237:ASN:N	2.50	0.45
1:A:345:SER:C	1:A:347:ARG:H	2.24	0.44
1:A:746:GLN:HB3	1:A:813:GLN:HE21	1.82	0.44
1:A:818:GLU:HA	1:A:821:VAL:CG2	2.47	0.44
1:A:890:LYS:HA	1:A:890:LYS:HD2	1.85	0.44
1:A:1019:VAL:HG23	1:A:1020:ILE:HD12	1.98	0.44
1:B:591:PHE:CZ	1:B:595:LEU:HD11	2.51	0.44
1:B:653:ALA:O	1:B:657:VAL:HG23	2.17	0.44
1:A:363:LEU:O	1:A:367:LEU:HG	2.18	0.44
1:A:375:HIS:NE2	1:A:445:SER:O	2.50	0.44
1:A:470:ALA:HA	1:A:504:LEU:CD1	2.46	0.44
1:A:692:GLN:CD	1:A:703:ARG:HH22	2.25	0.44
1:A:1015:MET:SD	1:A:1016:PRO:HD2	2.57	0.44
1:A:1077:PHE:CE1	1:A:1108:TRP:HB3	2.52	0.44
1:B:765:ARG:HD2	1:B:801:LYS:HA	1.99	0.44
1:B:943:TYR:CG	1:B:944:PRO:HD2	2.52	0.44
1:A:502:ASN:ND2	1:A:1262:TYR:HE1	2.15	0.44
1:A:756:ASP:OD1	1:A:757:PHE:N	2.51	0.44
1:A:818:GLU:O	1:A:821:VAL:HB	2.17	0.44
1:A:853:SER:OG	1:A:854:ARG:N	2.50	0.44
1:A:916:SER:O	1:A:920:ARG:HB2	2.16	0.44
1:A:1267:ILE:O	1:A:1271:VAL:HG23	2.17	0.44
1:B:484:THR:HA	1:B:491:VAL:HG12	1.99	0.44
1:B:552:ASP:HB3	1:B:555:ILE:CD1	2.46	0.44
1:B:684:TRP:CE3	1:B:840:ARG:HB2	2.52	0.44
1:B:713:TRP:HB3	1:B:837:ARG:NH2	2.32	0.44
1:B:898:ASN:N	1:B:898:ASN:OD1	2.50	0.44
1:A:434:PHE:HB2	1:A:451:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:TRP:HE3	1:A:708:ILE:HD12	1.82	0.44
1:A:1171:THR:C	1:A:1173:THR:H	2.25	0.44
1:A:1237:ASN:HA	1:A:1238:PRO:HD3	1.83	0.44
1:B:503:ARG:HA	1:B:1263:GLU:O	2.18	0.44
1:B:582:ARG:HH12	1:B:880:ARG:HD2	1.81	0.44
1:B:810:TYR:H	1:B:891:TYR:HH	1.64	0.44
1:B:1007:ARG:NH1	1:B:1008:THR:H	2.16	0.44
1:B:1039:GLY:O	1:B:1145:PRO:HA	2.17	0.44
1:B:1049:ARG:HA	1:B:1197:GLN:O	2.17	0.44
1:B:1069:ARG:CZ	1:B:1109:ILE:HA	2.48	0.44
1:A:350:ASN:CG	1:A:352:LEU:H	2.24	0.44
1:A:519:ILE:HD11	1:A:1013:PRO:HB3	1.98	0.44
1:A:600:TYR:CZ	1:A:830:PRO:HB3	2.53	0.44
1:B:947:ARG:HH22	1:B:956:ARG:HA	1.82	0.44
1:B:1036:ASN:O	1:B:1038:PHE:N	2.50	0.44
1:B:1203:GLU:CD	1:B:1205:ASN:HD21	2.23	0.44
1:A:409:THR:OG1	1:A:410:ARG:N	2.50	0.44
1:A:476:PRO:O	1:A:479:ILE:HG22	2.18	0.44
1:B:433:ARG:HA	1:B:450:VAL:HG12	1.99	0.44
1:B:433:ARG:CD	1:B:436:ARG:HD2	2.47	0.44
1:B:468:ARG:HA	1:B:471:ARG:HE	1.83	0.44
1:B:479:ILE:HD11	1:B:505:MET:HG2	1.99	0.44
1:B:715:ASN:HA	1:B:716:PRO:HD3	1.87	0.44
1:B:806:MET:H	1:B:889:GLY:C	2.25	0.44
1:B:929:GLN:O	1:B:933:THR:OG1	2.28	0.44
1:B:1107:ASN:N	1:B:1108:TRP:HD1	2.16	0.44
1:B:1111:PRO:O	1:B:1112:LEU:HG	2.17	0.44
1:A:509:ILE:CG1	1:A:727:PHE:HA	2.48	0.44
1:A:1164:SER:HA	1:A:1167:LEU:HD12	2.00	0.44
1:B:905:ILE:O	1:B:906:TYR:C	2.61	0.44
1:B:1056:TRP:CZ3	1:B:1061:PRO:HB3	2.52	0.44
1:B:1058:PRO:HG2	1:B:1180:PHE:CD2	2.53	0.44
1:B:1187:ASP:HA	1:B:1219:THR:HA	2.00	0.44
1:A:355:ARG:CZ	1:A:950:ASP:HA	2.47	0.44
1:A:1114:LEU:O	1:A:1117:MET:HB2	2.18	0.44
1:A:1162:LEU:HD13	1:A:1162:LEU:HA	1.89	0.44
1:B:470:ALA:C	1:B:472:MET:H	2.26	0.44
1:B:896:VAL:HG12	1:B:898:ASN:OD1	2.18	0.44
1:B:1065:LEU:H	1:B:1065:LEU:HG	1.62	0.44
1:B:1141:MET:HE3	1:B:1144:TYR:CZ	2.53	0.44
1:B:1156:TYR:CZ	1:B:1158:ASN:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:HIS:NE2	1:A:746:GLN:O	2.51	0.44
1:A:860:PRO:HG3	1:A:996:GLN:CD	2.43	0.44
1:B:413:THR:HG21	1:B:424:ALA:N	2.33	0.44
1:B:482:ALA:O	1:B:483:LEU:C	2.61	0.44
1:B:591:PHE:CE2	1:B:595:LEU:HD11	2.53	0.44
1:B:869:THR:HG23	1:B:870:THR:N	2.31	0.44
1:B:1138:ARG:HG2	1:B:1140:GLU:OE1	2.18	0.44
1:A:915:PHE:HE2	1:A:1268:THR:HA	1.83	0.43
1:A:982:MET:HA	1:A:985:GLU:CD	2.43	0.43
1:A:1015:MET:HG3	1:A:1017:GLY:H	1.83	0.43
1:B:392:ARG:HG2	1:B:394:LEU:HD21	1.99	0.43
1:B:550:GLN:HE22	1:B:892:PRO:CG	2.25	0.43
1:B:712:TYR:HB3	1:B:763:ASN:ND2	2.30	0.43
1:B:724:PRO:HA	1:B:728:GLY:C	2.43	0.43
1:B:804:LYS:HD2	1:B:804:LYS:H	1.82	0.43
1:B:1106:GLY:H	1:B:1134:GLU:CD	2.25	0.43
1:B:1141:MET:HE3	1:B:1144:TYR:CE2	2.53	0.43
1:A:502:ASN:HB3	1:A:1262:TYR:HD1	1.83	0.43
1:A:982:MET:HA	1:A:985:GLU:OE1	2.18	0.43
1:B:352:LEU:HB2	1:B:353:MET:HE2	1.99	0.43
1:B:536:LEU:HB3	1:B:593:VAL:HG13	1.99	0.43
1:B:721:TYR:CE2	1:B:739:LEU:HD13	2.53	0.43
1:B:1040:ILE:HA	1:B:1144:TYR:O	2.18	0.43
1:A:325:ALA:HB3	1:A:331:ASN:HA	2.00	0.43
1:A:452:GLU:CD	1:A:1257:VAL:HG11	2.43	0.43
1:A:705:TRP:O	1:A:709:ILE:HG13	2.18	0.43
1:A:840:ARG:HD3	1:A:1004:TYR:CZ	2.53	0.43
1:A:1071:THR:O	1:A:1074:VAL:HG13	2.19	0.43
1:B:332:ILE:O	1:B:336:LYS:N	2.51	0.43
1:B:432:GLY:H	1:B:451:PHE:HB2	1.83	0.43
1:B:605:THR:O	1:B:875:LEU:N	2.51	0.43
1:B:635:ALA:HB2	1:B:883:THR:OG1	2.18	0.43
1:A:681:PRO:HB2	1:A:1004:TYR:CE1	2.54	0.43
1:A:897:THR:HA	1:A:901:TYR:CD1	2.53	0.43
1:B:383:THR:O	1:B:386:THR:N	2.43	0.43
1:B:824:PRO:HG2	1:B:825:MET:SD	2.58	0.43
1:B:1096:ASP:HB3	1:B:1099:GLY:H	1.83	0.43
1:A:390:ASN:CG	1:A:433:ARG:HH21	2.26	0.43
1:A:472:MET:HB3	1:A:508:ARG:N	2.32	0.43
1:A:515:GLN:O	1:A:518:GLN:HB2	2.19	0.43
1:A:773:LYS:HG3	1:A:797:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ILE:O	1:B:423:VAL:HG23	2.19	0.43
1:B:750:VAL:HB	1:B:809:MET:SD	2.59	0.43
1:B:790:VAL:O	1:B:794:ARG:HB2	2.19	0.43
1:B:905:ILE:HD12	1:B:1274:VAL:H	1.84	0.43
1:B:1146:TYR:OH	1:B:1207:ARG:HD2	2.18	0.43
1:B:1147:MET:HE2	1:B:1177:SER:O	2.19	0.43
1:A:717:SER:O	1:A:740:LEU:HA	2.18	0.43
1:B:401:LYS:O	1:B:404:SER:OG	2.28	0.43
1:B:418:LYS:NZ	1:B:1224:ASP:OD1	2.49	0.43
1:B:905:ILE:CD1	1:B:1274:VAL:HG23	2.49	0.43
1:B:1045:ILE:HG23	1:B:1141:MET:CE	2.48	0.43
1:A:484:THR:CG2	1:A:489:GLY:HA2	2.48	0.43
1:A:587:ASP:N	1:A:587:ASP:OD1	2.51	0.43
1:A:680:THR:O	1:A:684:TRP:CD1	2.72	0.43
1:A:717:SER:O	1:A:740:LEU:HD23	2.19	0.43
1:A:1159:ALA:N	1:A:1196:VAL:O	2.28	0.43
1:B:366:VAL:C	1:B:368:ASP:H	2.26	0.43
1:B:533:GLN:N	1:B:534:PRO:HD2	2.34	0.43
1:B:591:PHE:O	1:B:595:LEU:HG	2.18	0.43
1:A:353:MET:HE2	1:A:356:ALA:N	2.29	0.43
1:A:465:TRP:CZ3	1:A:469:LEU:HD21	2.54	0.43
1:A:491:VAL:HA	1:A:902:ALA:HB2	2.01	0.43
1:A:853:SER:HB2	1:A:996:GLN:OE1	2.19	0.43
1:A:1025:GLN:O	1:A:1029:GLU:OE1	2.35	0.43
1:A:1108:TRP:O	1:A:1137:ILE:HA	2.18	0.43
1:B:592:ARG:HA	1:B:595:LEU:HD12	2.01	0.43
1:B:1213:ASN:CB	1:B:1216:SER:HB3	2.43	0.43
1:A:375:HIS:ND1	1:A:448:VAL:HG22	2.34	0.43
1:A:513:GLU:HA	1:A:516:ILE:HD12	2.00	0.43
1:A:515:GLN:HG2	1:A:732:LEU:HD22	2.00	0.43
1:A:591:PHE:C	1:A:593:VAL:H	2.26	0.43
1:A:623:LEU:HD12	1:A:626:LEU:HD12	2.01	0.43
1:A:667:GLN:H	1:A:667:GLN:HG3	1.53	0.43
1:A:701:ILE:H	1:A:701:ILE:HG13	1.59	0.43
1:A:1082:ARG:O	1:A:1094:ILE:HG13	2.19	0.43
1:A:1083:ILE:HB	1:A:1121:TYR:CE2	2.53	0.43
1:A:1272:MET:HB2	1:A:1272:MET:HE2	1.92	0.43
1:B:309:ARG:NH2	1:B:318:ARG:H	2.09	0.43
1:B:328:THR:HA	1:B:1150:TYR:CE1	2.54	0.43
1:B:359:LEU:O	1:B:362:LEU:HG	2.19	0.43
1:B:379:SER:OG	1:B:391:LEU:O	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:GLU:C	1:B:1260:TYR:HA	2.43	0.43
1:B:601:ASN:HB3	1:B:832:GLN:CA	2.49	0.43
1:B:623:LEU:O	1:B:626:LEU:HB3	2.19	0.43
1:A:507:TYR:CE1	1:A:1267:ILE:HD13	2.54	0.43
1:A:582:ARG:HD2	1:A:584:SER:HB3	2.00	0.43
1:A:769:CYS:SG	1:A:801:LYS:HB3	2.58	0.43
1:A:1151:TYR:HB3	1:A:1181:MET:CE	2.49	0.43
1:B:376:THR:HG21	1:B:392:ARG:HD2	2.00	0.43
1:B:406:MET:HE3	1:B:406:MET:HB3	1.79	0.43
1:B:667:GLN:NE2	1:B:668:ILE:HG13	2.34	0.43
1:A:669:TYR:CD1	1:A:685:PRO:HA	2.54	0.42
1:B:462:ARG:HA	1:B:465:TRP:HB3	2.01	0.42
1:B:622:SER:HB3	1:B:625:ASN:CG	2.43	0.42
1:B:847:VAL:O	1:B:847:VAL:HG13	2.19	0.42
1:B:853:SER:HB2	1:B:995:THR:N	2.31	0.42
1:B:1147:MET:HB3	1:B:1179:PRO:HA	2.01	0.42
1:B:1219:THR:O	1:B:1220:ILE:HD13	2.18	0.42
1:A:665:ASP:HB2	1:A:669:TYR:CD1	2.46	0.42
1:A:724:PRO:HA	1:A:728:GLY:N	2.34	0.42
1:A:786:THR:O	1:A:789:LEU:HB3	2.19	0.42
1:A:914:VAL:O	1:A:918:LEU:N	2.34	0.42
1:A:967:GLU:CD	1:A:967:GLU:C	2.87	0.42
1:A:1108:TRP:CD1	1:A:1108:TRP:N	2.87	0.42
1:A:1127:ASP:OD1	1:A:1128:ALA:N	2.45	0.42
1:B:355:ARG:CZ	1:B:950:ASP:HA	2.48	0.42
1:B:370:LEU:HB3	1:B:465:TRP:CE2	2.54	0.42
1:B:630:PHE:CD1	1:B:772:MET:HE2	2.54	0.42
1:B:739:LEU:HD12	1:B:739:LEU:HA	1.89	0.42
1:B:1036:ASN:ND2	1:B:1205:ASN:HB3	2.34	0.42
1:B:1056:TRP:HE3	1:B:1057:SER:C	2.26	0.42
1:A:534:PRO:HA	1:A:537:GLN:CD	2.44	0.42
1:A:700:PRO:HG2	1:A:701:ILE:HG13	2.01	0.42
1:A:1087:MET:HE2	1:A:1090:ALA:HB3	2.00	0.42
1:A:1131:LYS:HZ1	1:A:1160:TRP:CD1	2.36	0.42
1:A:1153:PRO:HD3	1:A:1184:ILE:H	1.84	0.42
1:B:307:HIS:ND1	1:B:310:TRP:HB3	2.35	0.42
1:B:601:ASN:ND2	1:B:835:TYR:HE2	2.17	0.42
1:B:763:ASN:O	1:B:767:ARG:HG2	2.19	0.42
1:B:827:PRO:HA	1:B:917:ASN:HD21	1.85	0.42
1:B:1042:ARG:CA	1:B:1142:GLY:O	2.54	0.42
1:B:1138:ARG:NE	1:B:1202:THR:HG21	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HA	1:A:305:VAL:N	2.34	0.42
1:A:330:ASN:HB3	1:A:1147:MET:HB2	2.01	0.42
1:A:334:LEU:O	1:A:337:GLN:N	2.48	0.42
1:A:558:ASN:HD22	1:A:888:SER:HB3	1.83	0.42
1:A:874:PRO:HG3	1:B:790:VAL:HG21	2.01	0.42
1:A:1034:GLU:O	1:A:1037:LEU:HG	2.19	0.42
1:B:439:MET:HB2	1:B:446:GLU:OE1	2.19	0.42
1:B:1049:ARG:HD3	1:B:1131:LYS:O	2.19	0.42
1:A:330:ASN:N	1:A:1148:LEU:O	2.52	0.42
1:A:953:PRO:HG3	1:A:1141:MET:O	2.18	0.42
1:A:1116:GLN:OE1	1:A:1174:SER:N	2.53	0.42
1:A:1119:THR:O	1:A:1123:ASN:ND2	2.52	0.42
1:A:1160:TRP:HB2	1:A:1198:TYR:CZ	2.54	0.42
1:B:465:TRP:CE2	1:B:469:LEU:HD11	2.54	0.42
1:B:691:ILE:O	1:B:694:ILE:N	2.45	0.42
1:B:1115:TRP:HE3	1:B:1122:PHE:CD2	2.37	0.42
1:B:1180:PHE:O	1:B:1182:VAL:HG13	2.19	0.42
1:A:711:ARG:HG3	1:A:712:TYR:CD1	2.55	0.42
1:A:898:ASN:OD1	1:A:899:VAL:N	2.51	0.42
1:B:381:ASP:O	1:B:382:HIS:ND1	2.53	0.42
1:B:430:ARG:HE	1:B:1238:PRO:HB2	1.84	0.42
1:B:637:PRO:HG2	1:B:764:TRP:CE2	2.54	0.42
1:B:773:LYS:HB3	1:B:794:ARG:NH2	2.34	0.42
1:B:1111:PRO:O	1:B:1140:GLU:HB2	2.19	0.42
1:A:517:SER:HB3	1:A:921:ASP:HB3	2.01	0.42
1:A:521:ARG:O	1:A:525:ILE:HG12	2.20	0.42
1:A:562:THR:O	1:A:799:LYS:HB2	2.20	0.42
1:A:680:THR:H	1:A:683:THR:CG2	2.33	0.42
1:A:839:ASP:HB3	1:A:842:ARG:CZ	2.50	0.42
1:A:900:TRP:O	1:A:903:ASP:HB3	2.19	0.42
1:A:902:ALA:O	1:A:1275:PRO:HA	2.20	0.42
1:A:1105:GLU:O	1:A:1108:TRP:NE1	2.53	0.42
1:A:1110:PHE:HD1	1:A:1114:LEU:HD22	1.84	0.42
1:A:1231:ARG:HB2	1:A:1232:TYR:CE2	2.54	0.42
1:B:403:TYR:HD2	1:B:410:ARG:HH21	1.68	0.42
1:B:864:LEU:HD22	1:B:868:ASN:HB3	2.01	0.42
1:B:930:THR:HG1	1:B:1018:SER:HG	1.57	0.42
1:B:1107:ASN:HA	1:B:1136:ARG:O	2.19	0.42
1:B:1112:LEU:HD23	1:B:1112:LEU:HA	1.87	0.42
1:B:1115:TRP:CZ3	1:B:1119:THR:HA	2.55	0.42
1:A:431:VAL:HG23	1:A:1254:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:ILE:CB	1:A:823:ALA:HA	2.48	0.42
1:A:854:ARG:N	1:A:863:SER:HB2	2.34	0.42
1:B:372:LEU:HB3	1:B:374:ARG:HH12	1.84	0.42
1:B:623:LEU:HG	1:B:627:TRP:NE1	2.34	0.42
1:B:685:PRO:HG2	1:B:688:PHE:CB	2.50	0.42
1:B:1165:ALA:HA	1:B:1168:GLU:OE1	2.20	0.42
1:A:375:HIS:CE1	1:A:448:VAL:HG13	2.54	0.42
1:A:392:ARG:HG3	1:A:394:LEU:CD1	2.50	0.42
1:A:546:ILE:O	1:A:895:LEU:HD21	2.20	0.42
1:A:622:SER:OG	1:A:625:ASN:OD1	2.22	0.42
1:A:713:TRP:HB3	1:A:837:ARG:HH21	1.82	0.42
1:A:781:TYR:CE2	1:A:790:VAL:HG22	2.55	0.42
1:B:325:ALA:HB3	1:B:331:ASN:HA	2.01	0.42
1:B:354:PHE:O	1:B:358:VAL:HG23	2.20	0.42
1:B:441:ASN:HB2	1:B:1261:ALA:HB1	2.00	0.42
1:B:450:VAL:H	1:B:1257:VAL:H	1.68	0.42
1:B:859:GLN:HG3	1:B:860:PRO:HD2	2.02	0.42
1:B:1166:TRP:HE1	1:B:1177:SER:C	2.27	0.42
1:A:478:GLU:HA	1:A:481:TRP:CE3	2.55	0.42
1:A:643:CYS:O	1:A:647:LYS:N	2.47	0.42
1:A:979:LEU:HD12	1:A:979:LEU:H	1.85	0.42
1:A:1069:ARG:HA	1:A:1074:VAL:HG11	2.02	0.42
1:A:1075:HIS:ND1	1:A:1108:TRP:NE1	2.68	0.42
1:B:307:HIS:CE1	1:B:308:THR:O	2.73	0.42
1:B:307:HIS:NE2	1:B:308:THR:O	2.53	0.42
1:B:455:ASP:OD1	1:B:457:LEU:HB3	2.20	0.42
1:B:507:TYR:HB3	1:B:727:PHE:CZ	2.55	0.42
1:B:619:SER:H	1:B:625:ASN:HD22	1.68	0.42
1:B:1141:MET:HE3	1:B:1141:MET:HB2	1.90	0.42
1:B:1153:PRO:HG3	1:B:1184:ILE:H	1.84	0.42
1:B:1237:ASN:ND2	1:B:1239:ASP:OD2	2.53	0.42
1:A:592:ARG:H	1:A:592:ARG:HD2	1.85	0.41
1:A:646:VAL:HG22	1:A:688:PHE:CD2	2.55	0.41
1:A:857:ILE:HG22	1:A:859:GLN:H	1.85	0.41
1:A:1031:PHE:CE1	1:A:1035:TYR:HA	2.55	0.41
1:A:1189:ASP:O	1:A:1190:ILE:HG23	2.20	0.41
1:B:307:HIS:CG	1:B:308:THR:N	2.88	0.41
1:B:409:THR:OG1	1:B:431:VAL:HG11	2.20	0.41
1:B:504:LEU:H	1:B:1265:PRO:HD3	1.84	0.41
1:B:559:THR:HG21	1:B:803:ILE:HG12	2.01	0.41
1:B:987:LEU:HD22	1:B:991:ASP:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:THR:HG1	1:A:640:THR:H	1.68	0.41
1:A:790:VAL:O	1:A:793:MET:HB3	2.20	0.41
1:A:816:PRO:HA	1:A:819:LEU:HG	2.02	0.41
1:A:938:ILE:CG2	1:A:947:ARG:HB3	2.50	0.41
1:A:1087:MET:HB2	1:A:1090:ALA:HB3	2.02	0.41
1:A:1231:ARG:HB3	1:A:1253:LEU:N	2.35	0.41
1:B:326:PRO:HB2	1:B:329:GLU:HB2	2.02	0.41
1:B:352:LEU:HB2	1:B:353:MET:CE	2.50	0.41
1:B:449:ASP:HA	1:B:1257:VAL:C	2.46	0.41
1:B:490:TYR:HB3	1:B:1274:VAL:HG22	2.01	0.41
1:B:773:LYS:HA	1:B:776:VAL:HG22	2.02	0.41
1:B:840:ARG:O	1:B:1004:TYR:HB3	2.21	0.41
1:B:999:ILE:HG13	1:B:1000:GLN:N	2.34	0.41
1:B:1067:PHE:HB2	1:B:1071:THR:HG21	2.02	0.41
1:B:1069:ARG:NH2	1:B:1110:PHE:N	2.68	0.41
1:B:1147:MET:O	1:B:1148:LEU:HD23	2.20	0.41
1:A:660:GLU:OE1	1:A:699:ALA:HA	2.19	0.41
1:A:732:LEU:H	1:A:831:PHE:HE1	1.62	0.41
1:A:853:SER:HB2	1:A:996:GLN:NE2	2.35	0.41
1:A:861:ALA:O	1:A:864:LEU:HD22	2.21	0.41
1:A:863:SER:O	1:A:866:THR:N	2.51	0.41
1:A:949:LEU:HB3	1:A:952:ILE:HG22	2.02	0.41
1:B:313:ASN:ND2	1:B:1259:ARG:HH22	2.19	0.41
1:B:669:TYR:HA	1:B:678:PHE:CZ	2.55	0.41
1:B:773:LYS:HZ2	1:B:797:LEU:HB2	1.85	0.41
1:B:884:VAL:HA	1:B:887:LEU:HB3	2.02	0.41
1:B:934:LEU:HD22	1:B:937:GLN:NE2	2.34	0.41
1:B:1166:TRP:CE3	1:B:1167:LEU:HD23	2.55	0.41
1:A:673:ARG:NH2	1:B:784:GLY:H	2.17	0.41
1:A:1019:VAL:O	1:A:1022:ASP:HB3	2.20	0.41
1:A:1085:PHE:C	1:A:1092:PRO:HA	2.46	0.41
1:A:1151:TYR:O	1:A:1184:ILE:HG13	2.19	0.41
1:B:468:ARG:HA	1:B:468:ARG:HD2	1.68	0.41
1:B:475:ASN:HB3	1:B:478:GLU:CD	2.46	0.41
1:B:602:GLY:H	1:B:832:GLN:HA	1.84	0.41
1:B:652:LEU:HD23	1:B:705:TRP:CD1	2.55	0.41
1:B:720:ARG:HH22	1:B:724:PRO:CD	2.28	0.41
1:B:1151:TYR:O	1:B:1183:PRO:HA	2.20	0.41
1:B:1213:ASN:O	1:B:1214:SER:C	2.63	0.41
1:A:327:PRO:HA	1:A:331:ASN:HD21	1.86	0.41
1:A:330:ASN:CG	1:A:1147:MET:HB2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:HG3	1:A:365:PHE:N	2.36	0.41
1:A:533:GLN:HG2	1:A:537:GLN:HE21	1.86	0.41
1:A:596:ALA:O	1:A:599:LEU:HD23	2.20	0.41
1:A:969:VAL:C	1:A:973:LEU:HG	2.45	0.41
1:A:1058:PRO:HB2	1:A:1200:ILE:HA	2.03	0.41
1:B:368:ASP:HB3	1:B:369:ASN:ND2	2.35	0.41
1:B:375:HIS:HD2	1:B:444:MET:N	2.18	0.41
1:B:659:PHE:CD1	1:B:781:TYR:HD1	2.39	0.41
1:B:684:TRP:CE2	1:B:840:ARG:HB2	2.55	0.41
1:B:778:ASN:HB2	1:B:780:ARG:HG3	2.02	0.41
1:B:1121:TYR:O	1:B:1122:PHE:C	2.63	0.41
1:B:1259:ARG:HD2	1:B:1260:TYR:H	1.86	0.41
1:A:355:ARG:NH2	1:A:954:SER:H	2.19	0.41
1:A:995:THR:C	1:A:996:GLN:HG3	2.45	0.41
1:A:1147:MET:HG3	1:A:1179:PRO:CA	2.50	0.41
1:B:383:THR:HB	1:B:384:PRO:HD2	2.02	0.41
1:B:407:TYR:CD2	1:B:410:ARG:HD3	2.50	0.41
1:B:545:ARG:HH12	1:B:546:ILE:HD12	1.85	0.41
1:B:556:ILE:HD11	1:B:888:SER:HB3	2.02	0.41
1:B:682:HIS:CD2	1:B:682:HIS:H	2.38	0.41
1:B:691:ILE:HB	1:B:703:ARG:NE	2.36	0.41
1:B:1007:ARG:NH1	1:B:1008:THR:N	2.69	0.41
1:B:1059:LEU:C	1:B:1061:PRO:HD3	2.45	0.41
1:A:342:GLU:HB3	1:A:1173:THR:OG1	2.21	0.41
1:A:359:LEU:O	1:A:360:HIS:C	2.64	0.41
1:A:404:SER:O	1:A:411:MET:HE3	2.21	0.41
1:A:1120:ARG:HD2	1:A:1121:TYR:H	1.84	0.41
1:A:1156:TYR:CG	1:A:1157:ALA:N	2.88	0.41
1:A:1203:GLU:HB2	1:A:1205:ASN:ND2	2.32	0.41
1:B:355:ARG:NE	1:B:952:ILE:O	2.51	0.41
1:B:476:PRO:HD3	1:B:505:MET:HE3	2.01	0.41
1:B:994:MET:HE3	1:B:994:MET:HB3	1.95	0.41
1:B:1051:GLN:HB3	1:B:1194:PRO:O	2.20	0.41
1:B:1076:ILE:HA	1:B:1109:ILE:HB	2.02	0.41
1:A:385:PHE:N	1:A:385:PHE:CD1	2.88	0.41
1:A:475:ASN:OD1	1:A:475:ASN:N	2.53	0.41
1:A:852:GLN:HB3	1:A:853:SER:H	1.74	0.41
1:A:1000:GLN:HE21	1:A:1008:THR:CA	2.34	0.41
1:B:512:ALA:HA	1:B:515:GLN:OE1	2.20	0.41
1:B:603:VAL:C	1:B:872:GLY:HA2	2.45	0.41
1:B:634:LEU:O	1:B:638:MET:HE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:GLU:OE1	1:B:701:ILE:HB	2.19	0.41
1:B:754:THR:OG1	1:B:806:MET:HA	2.21	0.41
1:B:915:PHE:HA	1:B:918:LEU:CG	2.43	0.41
1:B:1095:ARG:CG	1:B:1099:GLY:HA2	2.50	0.41
1:A:473:ASN:HB2	1:A:504:LEU:CD1	2.51	0.41
1:A:475:ASN:HA	1:A:476:PRO:HD3	1.95	0.41
1:A:478:GLU:O	1:A:481:TRP:HE3	2.03	0.41
1:A:548:PRO:HG3	1:A:895:LEU:HD13	2.03	0.41
1:A:607:VAL:HG22	1:A:875:LEU:C	2.45	0.41
1:A:637:PRO:C	1:A:638:MET:HE2	2.46	0.41
1:A:708:ILE:HG12	1:A:711:ARG:HH22	1.86	0.41
1:A:720:ARG:HE	1:A:720:ARG:HB3	1.64	0.41
1:A:763:ASN:HB3	1:A:767:ARG:HH22	1.86	0.41
1:A:917:ASN:O	1:A:920:ARG:HB3	2.19	0.41
1:A:1170:ILE:HG13	1:A:1171:THR:N	2.36	0.41
1:B:317:ASP:OD1	1:B:318:ARG:N	2.53	0.41
1:B:531:VAL:HG12	1:B:532:ILE:HG13	2.03	0.41
1:B:654:ASN:HD22	1:B:672:SER:HA	1.85	0.41
1:B:681:PRO:HA	1:B:684:TRP:CD1	2.56	0.41
1:B:928:VAL:O	1:B:931:LEU:HB3	2.21	0.41
1:B:1007:ARG:HH11	1:B:1008:THR:H	1.69	0.41
1:B:1022:ASP:O	1:B:1026:LEU:HD23	2.21	0.41
1:B:1045:ILE:HG23	1:B:1141:MET:HE1	2.03	0.41
1:B:1160:TRP:HB2	1:B:1198:TYR:CZ	2.56	0.41
1:A:343:THR:HG21	1:A:349:ALA:H	1.85	0.41
1:A:618:GLY:C	1:A:655:MET:HA	2.46	0.41
1:A:1003:GLN:O	1:A:1006:GLY:N	2.52	0.41
1:A:1075:HIS:N	1:A:1075:HIS:CD2	2.88	0.41
1:A:1151:TYR:CD2	1:A:1181:MET:HE3	2.56	0.41
1:A:1151:TYR:HB3	1:A:1181:MET:HE3	2.02	0.41
1:A:1170:ILE:HD12	1:A:1170:ILE:HA	1.91	0.41
1:B:338:LEU:HD13	1:B:338:LEU:HA	1.81	0.41
1:B:678:PHE:HA	1:B:683:THR:HG21	2.02	0.41
1:B:805:SER:HB2	1:B:887:LEU:O	2.21	0.41
1:B:1093:MET:HG2	1:B:1103:PRO:N	2.36	0.41
1:B:1138:ARG:O	1:B:1139:ILE:HD13	2.21	0.41
1:B:1258:THR:OG1	1:B:1260:TYR:OH	2.21	0.41
1:A:427:VAL:HG13	1:A:1235:LEU:O	2.21	0.40
1:A:595:LEU:O	1:A:598:TRP:HB2	2.20	0.40
1:A:600:TYR:HE2	1:A:828:PHE:CE2	2.34	0.40
1:A:813:GLN:O	1:A:816:PRO:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:ARG:CZ	1:A:1111:PRO:HG2	2.51	0.40
1:A:1160:TRP:HB2	1:A:1198:TYR:CE1	2.56	0.40
1:A:1170:ILE:HG12	1:A:1175:ILE:CA	2.51	0.40
1:B:542:LEU:HA	1:B:545:ARG:HE	1.86	0.40
1:B:603:VAL:HG13	1:B:831:PHE:CE2	2.55	0.40
1:B:759:ASN:HD21	1:B:808:PRO:HB2	1.84	0.40
1:B:764:TRP:O	1:B:768:VAL:HG13	2.21	0.40
1:B:810:TYR:HA	1:B:814:LEU:HD22	2.02	0.40
1:B:827:PRO:HA	1:B:917:ASN:ND2	2.36	0.40
1:B:930:THR:HG21	1:B:1020:ILE:HB	2.04	0.40
1:A:351:PRO:HA	1:A:354:PHE:CG	2.56	0.40
1:A:569:GLN:O	1:A:789:LEU:HD13	2.21	0.40
1:A:929:GLN:NE2	1:A:929:GLN:O	2.54	0.40
1:A:1164:SER:O	1:A:1167:LEU:N	2.54	0.40
1:B:401:LYS:HE3	1:B:401:LYS:HB3	1.96	0.40
1:B:654:ASN:HA	1:B:657:VAL:HG23	2.03	0.40
1:B:841:ASP:HB3	1:B:1005:ASN:HB3	2.03	0.40
1:B:878:ASP:OD1	1:B:880:ARG:N	2.51	0.40
1:B:986:PRO:O	1:B:990:GLY:N	2.54	0.40
1:B:1116:GLN:HB2	1:B:1117:MET:SD	2.61	0.40
1:A:307:HIS:CG	1:A:308:THR:N	2.89	0.40
1:A:307:HIS:CG	1:A:323:ILE:HG22	2.56	0.40
1:A:403:TYR:O	1:A:407:TYR:N	2.37	0.40
1:A:642:PRO:O	1:A:645:PRO:HD2	2.21	0.40
1:A:797:LEU:HA	1:A:800:LEU:HD12	2.03	0.40
1:A:949:LEU:HG	1:A:951:TRP:CZ2	2.56	0.40
1:A:1040:ILE:C	1:A:1146:TYR:HE2	2.28	0.40
1:A:1059:LEU:HD12	1:A:1206:ASP:OD1	2.21	0.40
1:A:1078:GLY:O	1:A:1079:ARG:HD3	2.21	0.40
1:A:1164:SER:O	1:A:1167:LEU:HB2	2.21	0.40
1:B:346:VAL:HB	1:B:347:ARG:HG3	2.02	0.40
1:B:463:GLY:HA2	1:B:466:MET:HE3	2.02	0.40
1:B:637:PRO:HA	1:B:713:TRP:CH2	2.57	0.40
1:B:949:LEU:HB3	1:B:952:ILE:HD12	2.03	0.40
1:B:977:PHE:C	1:B:979:LEU:N	2.78	0.40
1:A:364:GLU:HG3	1:A:365:PHE:H	1.86	0.40
1:A:1003:GLN:HB2	1:A:1005:ASN:OD1	2.21	0.40
1:A:1095:ARG:HA	1:A:1100:MET:O	2.21	0.40
1:B:318:ARG:HH21	1:B:370:LEU:C	2.29	0.40
1:B:338:LEU:HD12	1:B:360:HIS:HB3	2.02	0.40
1:B:375:HIS:CD2	1:B:443:ALA:H	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:TYR:HD2	1:B:410:ARG:NH2	2.18	0.40
1:B:430:ARG:HG3	1:B:1238:PRO:HB3	2.03	0.40
1:B:518:GLN:NE2	1:B:830:PRO:O	2.51	0.40
1:B:571:LEU:HB3	1:B:575:SER:OG	2.21	0.40
1:A:334:LEU:HD23	1:A:334:LEU:N	2.36	0.40
1:A:438:GLN:NE2	1:A:443:ALA:O	2.47	0.40
1:A:511:ASN:CA	1:A:514:ARG:HB2	2.50	0.40
1:A:853:SER:HB2	1:A:996:GLN:CD	2.46	0.40
1:A:929:GLN:HG2	1:A:1017:GLY:HA2	2.03	0.40
1:A:940:ASP:OD2	1:A:947:ARG:HD2	2.21	0.40
1:A:952:ILE:CD1	1:A:1143:ALA:HB3	2.52	0.40
1:A:1002:GLN:NE2	1:A:1006:GLY:O	2.54	0.40
1:B:333:HIS:CD2	1:B:336:LYS:HE3	2.56	0.40
1:B:545:ARG:NH2	1:B:546:ILE:HB	2.36	0.40
1:B:763:ASN:OD1	1:B:767:ARG:NH1	2.55	0.40
1:B:1178:VAL:O	1:B:1178:VAL:HG13	2.22	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	972/975 (100%)	783 (81%)	187 (19%)	2 (0%)	43	78
1	B	963/975 (99%)	806 (84%)	156 (16%)	1 (0%)	48	83
All	All	1935/1950 (99%)	1589 (82%)	343 (18%)	3 (0%)	44	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1111	PRO
1	A	1161	ASN

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Mol	Chain	Res	Type
1	A	582	ARG

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	861/862 (100%)	854 (99%)	7 (1%)	73	80
1	B	854/862 (99%)	850 (100%)	4 (0%)	81	83
All	All	1715/1724 (100%)	1704 (99%)	11 (1%)	76	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	HIS
1	A	450	VAL
1	A	494	THR
1	A	646	VAL
1	A	777	ASP
1	A	807	THR
1	A	952	ILE
1	B	352	LEU
1	B	354	PHE
1	B	1212	THR
1	B	1227	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	A	350	ASN
1	A	515	GLN
1	A	528	ASN
1	A	654	ASN
1	A	671	GLN

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Mol	Chain	Res	Type
1	A	715	ASN
1	A	774	ASN
1	A	813	GLN
1	A	832	GLN
1	A	917	ASN
1	A	919	GLN
1	A	929	GLN
1	A	1000	GLN
1	A	1149	HIS
1	A	1205	ASN
1	A	1246	GLN
1	B	313	ASN
1	B	331	ASN
1	B	360	HIS
1	B	382	HIS
1	B	524	ASN
1	B	558	ASN
1	B	585	ASN
1	B	601	ASN
1	B	671	GLN
1	B	690	ASN
1	B	704	GLN
1	B	710	HIS
1	B	715	ASN
1	B	759	ASN
1	B	787	GLN
1	B	852	GLN
1	B	917	ASN
1	B	929	GLN
1	B	942	GLN
1	B	1036	ASN
1	B	1051	GLN
1	B	1088	ASN
1	B	1107	ASN
1	B	1116	GLN
1	B	1118	ASN
1	B	1197	GLN
1	B	1255	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

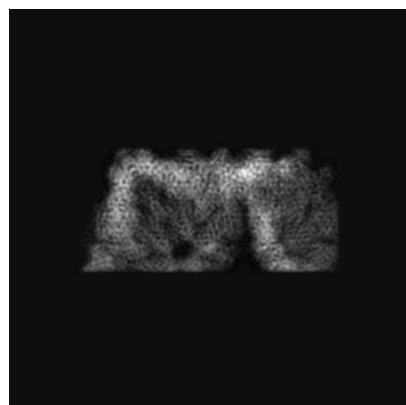
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

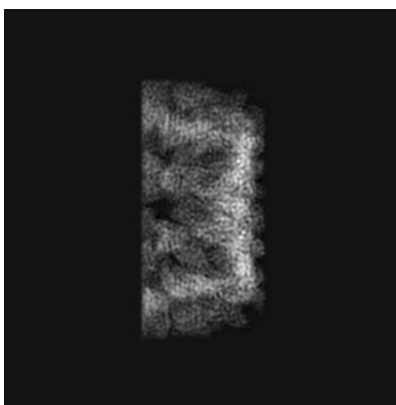
6 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22165. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

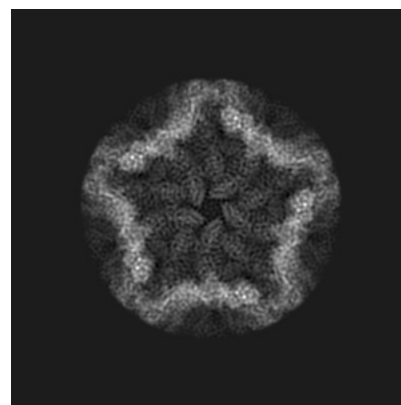
6.1 Orthogonal projections [i](#)



X



Y



Z

The images above show the tomogram projected in three orthogonal directions.

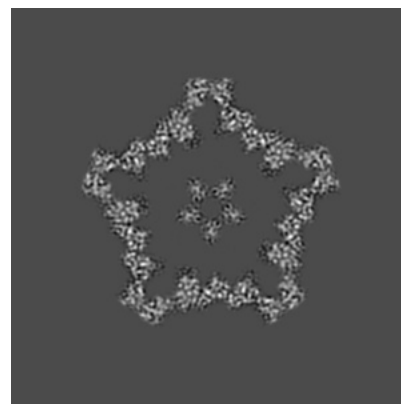
6.2 Central slices [i](#)



X Index: 193



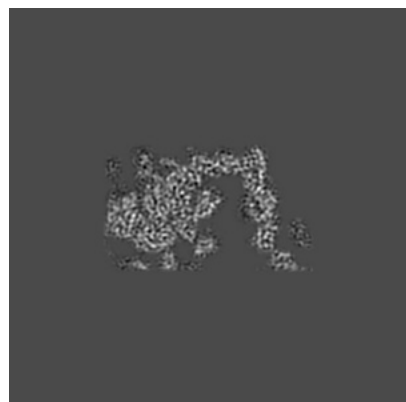
Y Index: 193



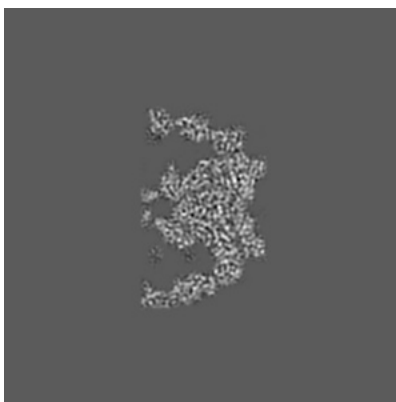
Z Index: 193

The images above show central slices of the tomogram in three orthogonal directions.

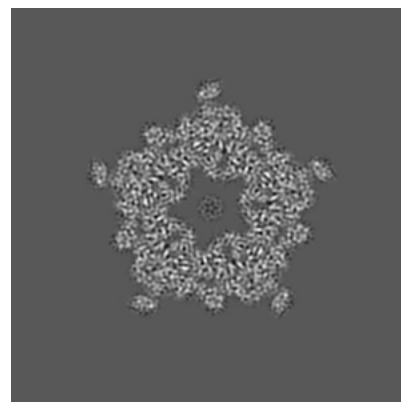
6.3 Largest variance slices [i](#)



X Index: 117



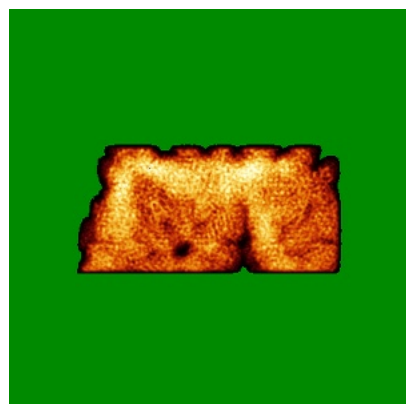
Y Index: 112



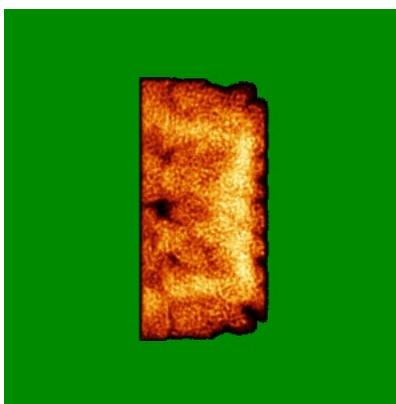
Z Index: 230

The images above show the largest variance slices of the tomogram in three orthogonal directions.

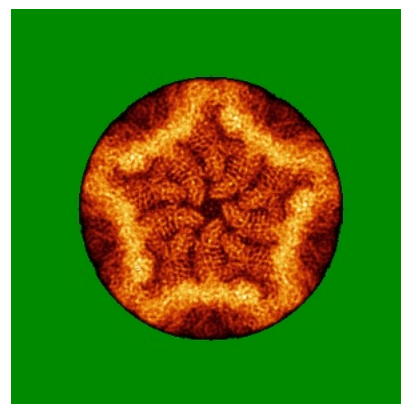
6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

The images above show the tomogram projected in three orthogonal directions.

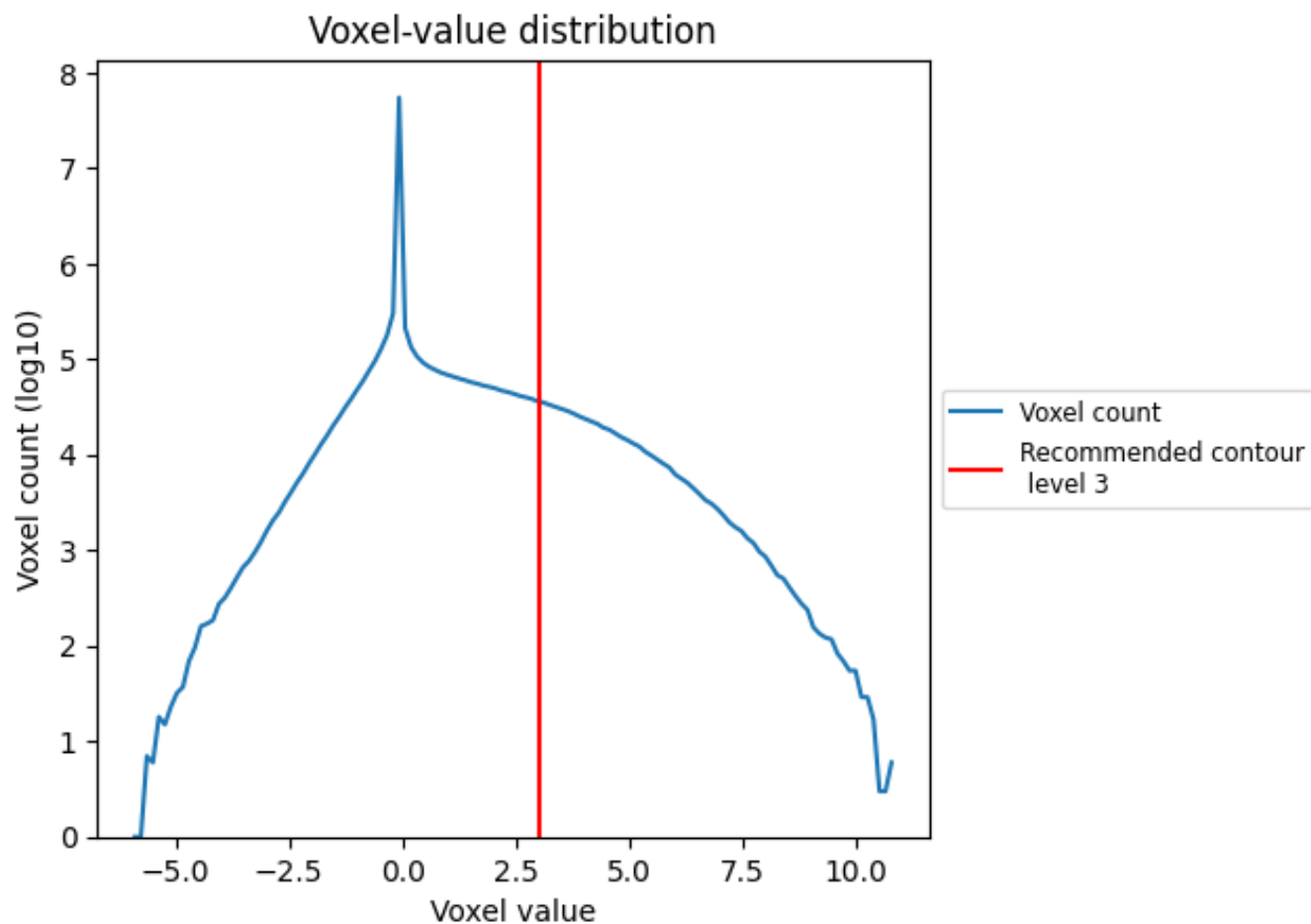
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis [i](#)

This section contains the results of statistical analysis of the tomogram.

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22165 and PDB model 6ZTS. Per-residue inclusion information can be found in section 3 on page 4.

8.1 Map-model overlay [i](#)

This section was not generated.

8.2 Q-score mapped to coordinate model [i](#)

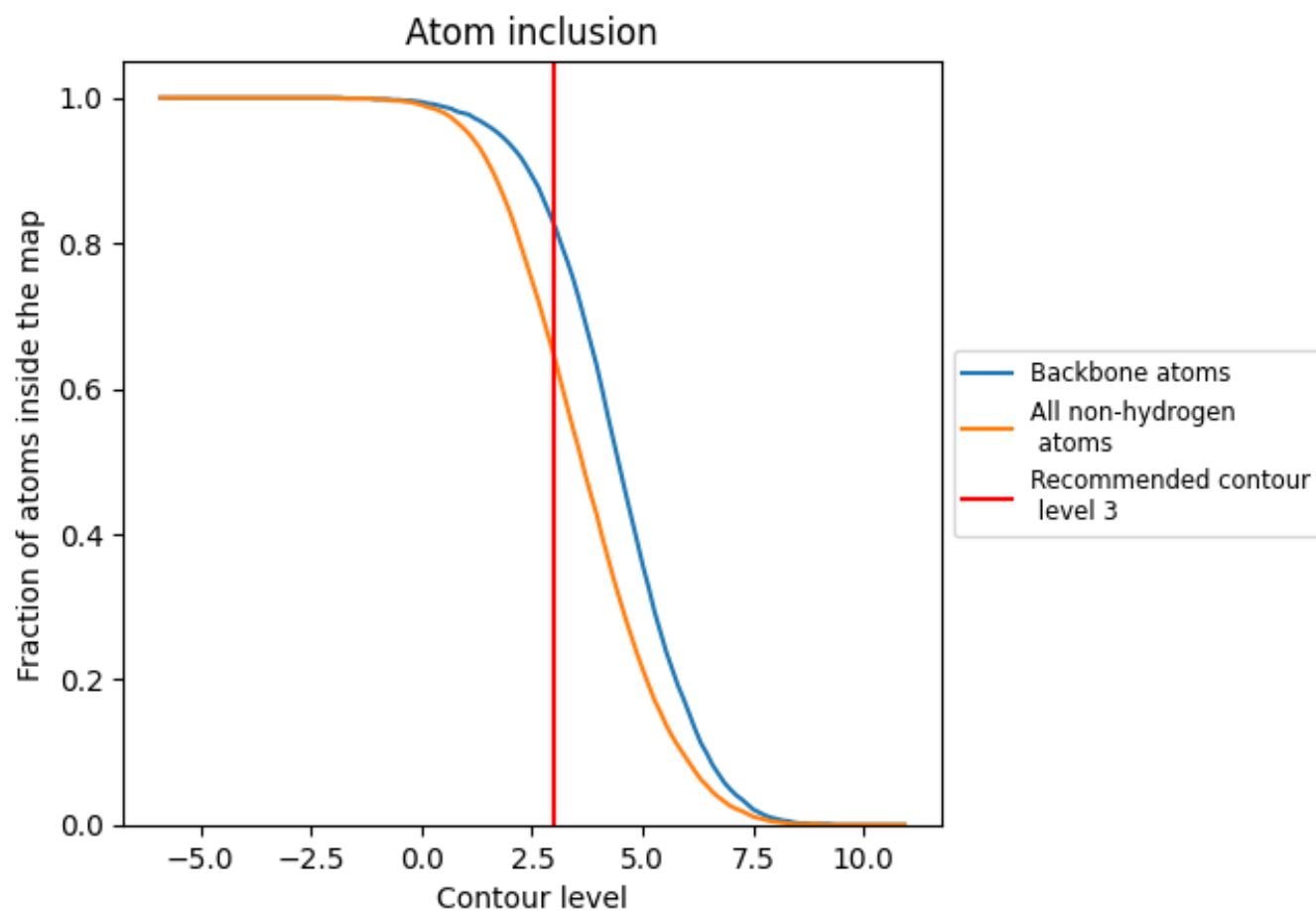


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.2160
A	0.6350	0.2110
B	0.6550	0.2220

