



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:19 pm BST

PDB ID : 3SHF  
Title : Crystal structure of the R265S mutant of full-length murine Apaf-1  
Authors : Eschenburg, S.; Reubold, T.F.  
Deposited on : 2011-06-16  
Resolution : 3.55 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

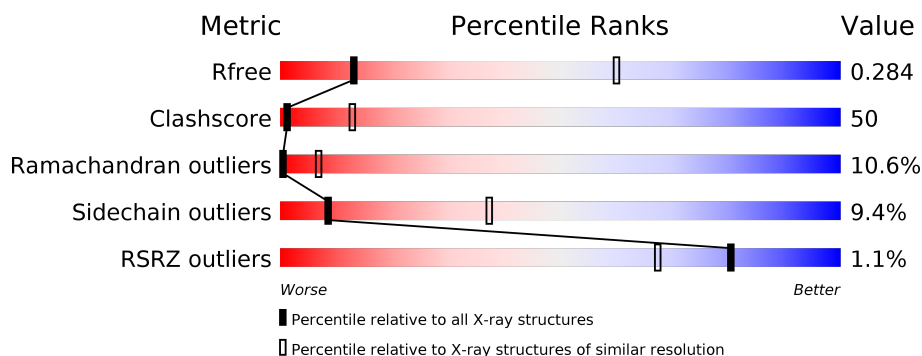
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1256	<div> <div></div> <div>29%</div> <div>48%</div> <div>12%</div> <div>10%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

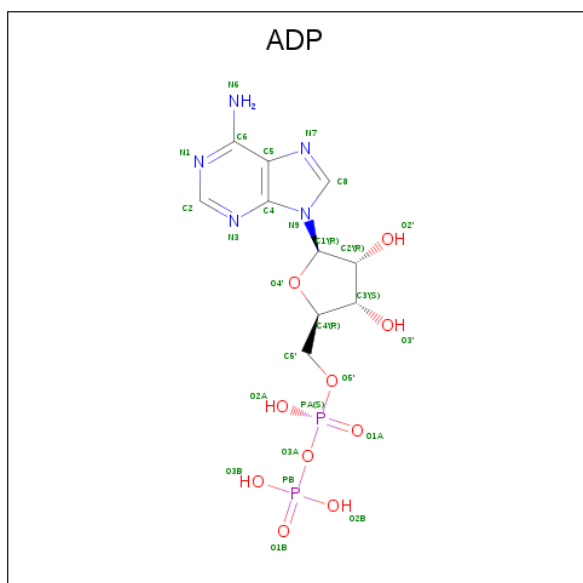
- Molecule 1 is a protein called Apoptotic peptidase activating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1133	9010	5712	1551	1692	55	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

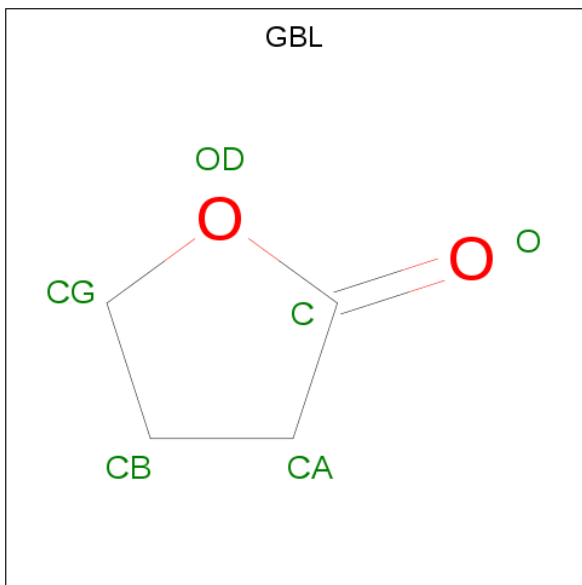
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP A2RRK8
A	-5	ALA	-	EXPRESSION TAG	UNP A2RRK8
A	-4	MET	-	EXPRESSION TAG	UNP A2RRK8
A	-3	ASP	-	EXPRESSION TAG	UNP A2RRK8
A	-2	PRO	-	EXPRESSION TAG	UNP A2RRK8
A	-1	GLU	-	EXPRESSION TAG	UNP A2RRK8
A	0	PHE	-	EXPRESSION TAG	UNP A2RRK8
A	265	SER	ARG	ENGINEERED MUTATION	UNP A2RRK8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is GAMMA-BUTYROLACTONE (three-letter code: GBL) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		

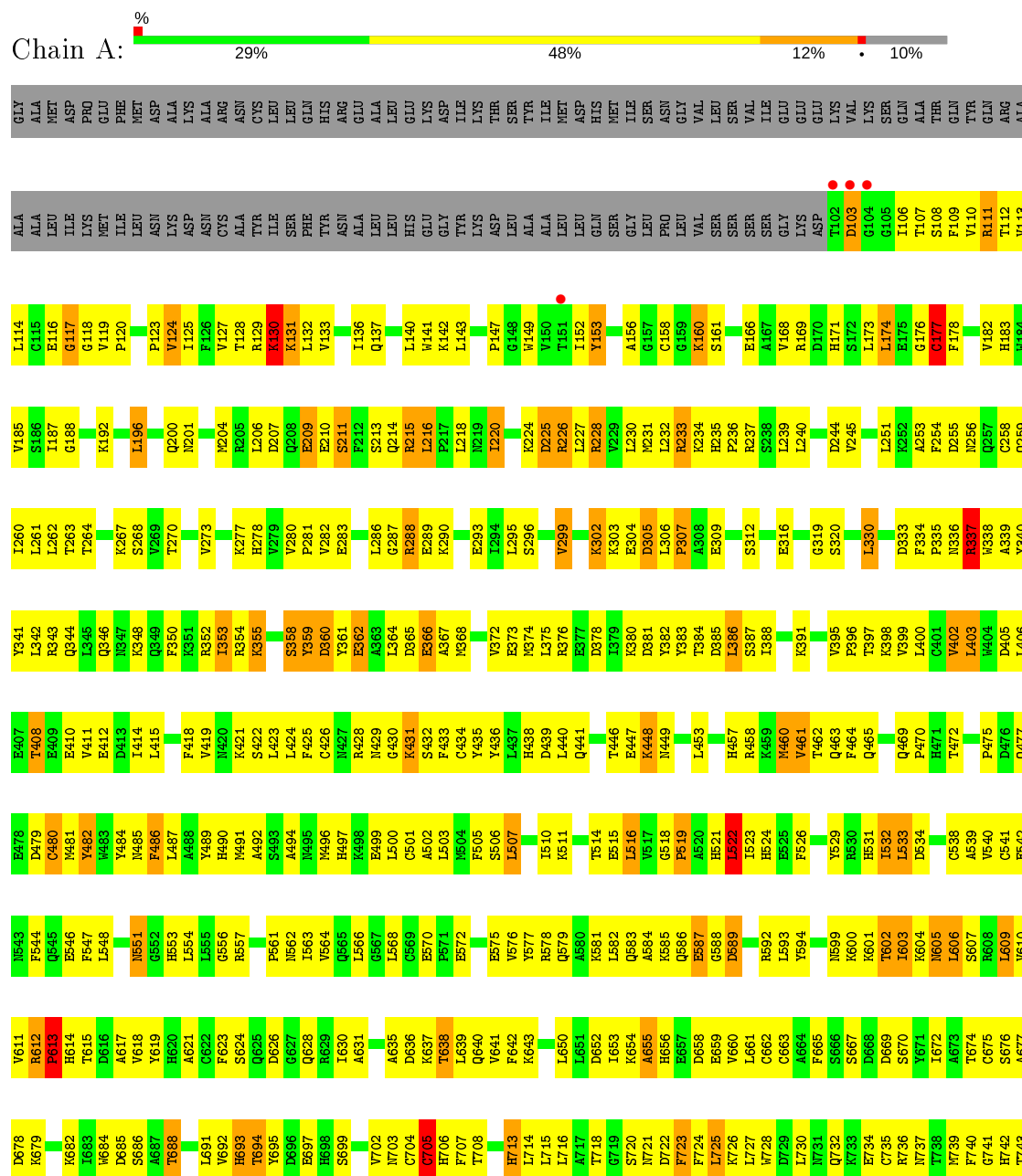
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		

### 3 Residue-property plots

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

- Molecule 1: Apoptotic peptidase activating factor 1



T1207	L1142	D1080	F1011	Q947	B879	G810	N744
S1210	A1143	F1081	T1012	C968	G880	D811	S745
S1211	T1144	T1082	A1013	L948	H881	R812	V746
Q1212	G1145	C1083	D1014	I949	L882	R813	N747
T1213	D1146	H1084	G1015	A950	G951	R814	H748
F1214	D1147	T1087	K1016	K952	H884	V815	C749
	N1148	V1088	T1017	T953	V888	R750	R750
	G1149	V1086	L1018	G954	F894	F751	F751
	I1150	S1089	I1019	Q955	M889	S752	S752
	I1151	S1090	E1023	I956	F890	P753	P753
	R1152	C1091	E1024	D957	S891	D754	D754
	I1153	A1092	S1025	Y958	P892	D755	D755
	H1154	I1083	S1026	L959	D893	E756	E756
	N1155	S1094	V1027	P960	G894	L757	L757
	V1156	S1095	I1028	E961	S895	L758	L758
	H1225	D1096	Q1029	A962	S896	A759	A759
	V1226	A1097	V1029	Q963	F897	S760	S760
	D1158	T1098	V1030	V964	L898	C761	C761
	G1159	T1098	M1031	C967	T899	S762	S762
	Q1160	S1101	M1032	C968	D902	A763	A763
	L1161	S1102	Q1033	L969	D903	D764	D764
	L1162	T1103	Q1041	S970	Q904	L767	L767
	H1163	S1104	A1042	P971	T905	R768	R768
	S1164	A1105	H1043	H972	I906	L769	L769
	C1165	D1106	Q1044	L973	R907	W770	W770
	A1166	K1107	E1045	E974	V908	D771	D771
	P1167	T1108	T1046	Y975	W909	V772	V772
	I1168	A1109	V1047	V976	E910	R773	R773
	S1169	K1110	K1048	A977	K913	S774	S774
	VAL	I1111	D1049	F978	Q844	A775	A775
	GLU	W1112	F1050	G979	Y845	R778	R778
	GLY	S1113	R1051	D980	C846	V783	V783
	THR	F1114	L1058	E981	D847	K784	K784
	ALA	D1115	L1059	D982	F849	R785	R785
	THR	L1116	S1060	G983	S849	F786	F786
	H1177	L1117	Q1054	A984	P850	F787	F787
	G1178	S1118	R1057	L985	W856	LEU	LEU
	G1179	P1119	L1058	K986	SER	SER	SER
	W1180	L1120	L1059	I987	GLU	GLU	GLU
	V1181	H1121	S1060	I988	ASP	ASP	ASP
	T1182	E1122	W1061	E989	PRO	PRO	PRO
	D1183	L1123	S1062	E990	D796	D796	D796
	V1184	K1124	F1063	P991	V797	V797	V797
	C1185	G1125	D1064	R992	E798	E798	E798
	F1186	H1126	G1065	R993	V799	V799	V799
	S1187	G1128	T1066	R994	M868	M868	M868
	D1189	C1129	V1067	V995	V801	V801	V801
	S1190	V1130	K1068	S998	K802	K802	K802
	K1191	R1131	V1069	G1001	C803	C803	C803
	T1192	C1132	W1070	H1002	S804	S804	S804
	L1193	S1133	M1071	I1003	S805	S805	S805
	V1194	F1135	V1072	K1003	W806	W806	W806
		S1136	T1074	V1006	D809	D809	D809
	K1201	L1137	G1075	R1007			
	W1202	D1138	A1076	H1008			
	W1203	G1139	I1077	I1009			
	N1204	I1140	E1078	G945			
	V1205	L1141	R1079	Q1010			
	A1206						

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.88Å 111.82Å 244.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.55 48.85 – 3.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.55) 99.6 (48.85-3.55)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.230 , 0.305 0.229 , 0.284	Depositor DCC
$R_{free}$ test set	8050 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	98.8	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 78.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.45	0/9206	0.72	5/12465 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	761	CYS	CA-CB-SG	-6.36	102.55	114.00
1	A	922	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	460	MET	N-CA-C	-5.66	95.71	111.00
1	A	796	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	705	CYS	CA-CB-SG	5.06	123.12	114.00

There are no chirality outliers.

There are no planarity outliers.

### 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	9010	0	8875	902	0
2	A	27	0	12	3	0
3	A	12	0	12	1	0
4	A	73	0	0	3	0
All	All	9122	0	8899	902	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 50.

All (902) 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:A:216:LEU:HD12	1:A:216:LEU:H	1.13	1.08
1:A:182:VAL:HG12	1:A:239:LEU:HB3	1.36	1.06
1:A:1108:THR:HG21	1:A:1124:LYS:HA	1.35	1.05
1:A:288:ARG:N	1:A:288:ARG:HE	1.58	1.00
1:A:785:ARG:HH11	1:A:785:ARG:HG3	1.28	0.97
1:A:992:ASN:HD21	1:A:995:VAL:N	1.63	0.96
1:A:342:LEU:O	1:A:346:GLN:HG2	1.64	0.96
1:A:288:ARG:H	1:A:288:ARG:NE	1.62	0.96
1:A:1150:GLU:HA	1:A:1166:ALA:HB1	1.45	0.96
1:A:575:GLU:HG2	1:A:578:ARG:HH11	1.29	0.94
1:A:785:ARG:HD2	1:A:785:ARG:H	1.29	0.94
1:A:612:ARG:HG3	1:A:905:THR:HG22	1.49	0.94
1:A:856:VAL:HG12	1:A:866:LEU:HB3	1.49	0.92
1:A:1002:HIS:HA	1:A:1003:LYS:HZ3	1.31	0.92
1:A:1029:VAL:HG11	1:A:1072:VAL:HG13	1.52	0.91
1:A:1084:HIS:ND1	1:A:1107:LYS:HE2	1.85	0.91
1:A:896:SER:HB2	1:A:909:TRP:O	1.69	0.91
1:A:1107:LYS:HD2	1:A:1108:THR:H	1.34	0.90
1:A:603:ILE:HG22	1:A:604:LYS:H	1.34	0.90
1:A:675:CYS:HB2	1:A:702:VAL:HG11	1.54	0.89
1:A:767:LEU:HD11	1:A:813:ILE:HD13	1.53	0.89
1:A:659:GLU:O	1:A:676:SER:HB2	1.71	0.89
1:A:1167:PRO:HD2	1:A:1203:TRP:HH2	1.39	0.88
1:A:682:LYS:HG2	1:A:694:THR:HG22	1.54	0.87
1:A:618:VAL:HG11	1:A:906:ILE:HD11	1.54	0.87
1:A:760:SER:HB3	1:A:770:TRP:HZ3	1.38	0.87
1:A:658:ASP:OD2	1:A:677:ALA:HB3	1.73	0.86
1:A:1016:LYS:HG2	1:A:1033:GLN:OE1	1.76	0.86
1:A:1112:TRP:HA	1:A:1120:LEU:HG	1.55	0.86
1:A:1139:GLY:O	1:A:1140:ILE:HG22	1.75	0.86
1:A:732:GLN:HG2	1:A:734:GLU:H	1.36	0.86
1:A:785:ARG:HD2	1:A:785:ARG:N	1.92	0.84
1:A:1012:THR:HA	1:A:1052:LEU:HD21	1.59	0.84
1:A:1053:LEU:HB3	1:A:1057:ARG:HG3	1.58	0.84
1:A:1140:ILE:HG13	1:A:1156:VAL:HB	1.58	0.84
1:A:1151:ILE:H	1:A:1166:ALA:HB2	1.43	0.84
1:A:529:TYR:O	1:A:533:LEU:HB2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:GLY:HA3	1:A:1152:ARG:HH12	1.44	0.82
1:A:1167:PRO:HD2	1:A:1203:TRP:CH2	2.14	0.82
1:A:1112:TRP:HB3	1:A:1119:PRO:HA	1.61	0.82
1:A:714:LEU:HD23	1:A:714:LEU:O	1.80	0.81
1:A:920:ILE:HG23	1:A:921:VAL:HG23	1.61	0.81
1:A:448:LYS:NZ	1:A:449:ASN:HD21	1.78	0.81
1:A:971:PRO:O	1:A:972:HIS:HB2	1.78	0.81
1:A:1151:ILE:HD11	1:A:1193:LEU:HD21	1.61	0.80
1:A:153:TYR:HE2	1:A:281:PRO:HG3	1.46	0.80
1:A:826:ILE:O	1:A:826:ILE:HG12	1.80	0.80
1:A:1071:ASN:HD21	1:A:1074:THR:HB	1.48	0.79
1:A:1138:ASP:O	1:A:1140:ILE:N	2.13	0.79
1:A:1074:THR:O	1:A:1076:ARG:N	2.16	0.79
1:A:1091:CYS:HB2	1:A:1102:SER:O	1.83	0.79
1:A:1106:ASP:O	1:A:1107:LYS:HB3	1.83	0.79
1:A:132:LEU:HD13	1:A:282:VAL:HG22	1.64	0.79
1:A:1136:SER:O	1:A:1138:ASP:N	2.14	0.78
1:A:538:CYS:HB2	1:A:540:VAL:HG23	1.65	0.78
1:A:910:GLU:HG3	1:A:913:LYS:HB3	1.65	0.78
1:A:546:GLU:HG2	1:A:612:ARG:HH22	1.46	0.78
1:A:1146:ASP:HB3	1:A:1150:GLU:O	1.83	0.78
1:A:1003:LYS:CE	1:A:1003:LYS:H	1.97	0.78
1:A:1053:LEU:HD23	1:A:1059:LEU:HB2	1.66	0.77
1:A:893:ASP:OD2	1:A:895:SER:HB3	1.85	0.77
1:A:309:GLU:HG2	1:A:339:ALA:HA	1.66	0.77
1:A:1091:CYS:HB3	1:A:1103:THR:HA	1.66	0.77
1:A:220:ILE:HD12	1:A:220:ILE:H	1.49	0.77
1:A:946:LEU:HD23	1:A:964:VAL:HG11	1.65	0.77
1:A:1112:TRP:HD1	1:A:1119:PRO:HB3	1.49	0.76
1:A:692:VAL:O	1:A:693:HIS:HB2	1.85	0.76
1:A:663:CYS:HB3	1:A:674:THR:HG22	1.66	0.76
1:A:228:ARG:HG3	1:A:256:ASN:HB3	1.67	0.76
1:A:619:TYR:HE2	1:A:635:ALA:HB2	1.51	0.76
1:A:364:LEU:CD2	1:A:440:LEU:HB3	2.16	0.75
1:A:1003:LYS:H	1:A:1003:LYS:HE2	1.48	0.75
1:A:364:LEU:HD22	1:A:440:LEU:HB3	1.68	0.75
1:A:531:HIS:CD2	1:A:532:ILE:HG22	2.22	0.75
1:A:930:PHE:CD2	1:A:1227:SER:HA	2.22	0.75
1:A:288:ARG:H	1:A:288:ARG:HE	0.82	0.75
1:A:940:VAL:HG13	1:A:964:VAL:CG2	2.16	0.75
1:A:228:ARG:HB3	1:A:228:ARG:NH1	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:ARG:H	1:A:785:ARG:CD	2.00	0.74
1:A:382:TYR:CE2	1:A:414:ILE:HD13	2.23	0.74
1:A:337:ARG:HH21	1:A:374:MET:HE3	1.52	0.73
1:A:760:SER:CB	1:A:770:TRP:HZ3	2.01	0.73
1:A:992:ASN:HD21	1:A:995:VAL:H	1.35	0.73
1:A:785:ARG:NH1	1:A:785:ARG:HG3	1.98	0.73
1:A:305:ASP:O	1:A:307:PRO:HD3	1.88	0.73
1:A:864:VAL:O	1:A:878:CYS:HB3	1.88	0.73
1:A:214:GLN:HG2	1:A:215:ARG:H	1.51	0.73
1:A:1141:LEU:HD11	1:A:1162:LEU:HD22	1.71	0.73
1:A:804:CYS:HB2	1:A:815:VAL:HG12	1.70	0.72
1:A:153:TYR:CE2	1:A:281:PRO:HG3	2.25	0.72
1:A:408:THR:HG22	1:A:412:GLU:OE1	1.89	0.72
1:A:130:LYS:HD2	1:A:131:LYS:H	1.53	0.72
1:A:107:THR:C	1:A:109:PHE:H	1.93	0.71
1:A:129:ARG:HB3	1:A:131:LYS:HZ3	1.54	0.71
1:A:1029:VAL:HG11	1:A:1072:VAL:CG1	2.19	0.71
1:A:382:TYR:HD2	1:A:414:ILE:HG21	1.54	0.71
1:A:426:CYS:HB3	1:A:435:TYR:CD1	2.26	0.71
1:A:460:MET:O	1:A:461:VAL:HG22	1.90	0.71
1:A:382:TYR:HE2	1:A:414:ILE:HD13	1.55	0.71
1:A:491:MET:HE2	1:A:503:LEU:HD22	1.73	0.71
1:A:396:PRO:HG2	1:A:399:VAL:HG23	1.72	0.71
1:A:762:SER:O	1:A:801:VAL:HG22	1.90	0.71
1:A:714:LEU:HD21	1:A:730:LEU:HB2	1.71	0.71
1:A:1042:ALA:HB1	1:A:1044:GLN:HG3	1.72	0.71
1:A:178:PHE:CD1	1:A:239:LEU:HB2	2.26	0.71
1:A:446:THR:HG23	1:A:453:LEU:HD11	1.70	0.71
1:A:623:PHE:CD2	1:A:891:SER:HA	2.26	0.71
1:A:718:THR:O	1:A:725:LEU:HD23	1.90	0.71
1:A:841:SER:HB2	1:A:860:SER:OG	1.90	0.71
1:A:938:LEU:HD23	1:A:947:GLN:O	1.91	0.71
1:A:974:GLU:HG2	1:A:975:TYR:N	2.04	0.70
1:A:233:ARG:O	1:A:234:LYS:HB3	1.92	0.70
1:A:656:HIS:HE1	1:A:674:THR:OG1	1.74	0.70
1:A:656:HIS:HB3	1:A:678:ASP:OD2	1.90	0.70
1:A:675:CYS:HB2	1:A:702:VAL:CG1	2.21	0.70
1:A:618:VAL:HG23	1:A:904:GLN:HA	1.73	0.70
1:A:196:LEU:O	1:A:200:GLN:HG3	1.90	0.69
1:A:561:PRO:HB2	1:A:566:LEU:HD11	1.75	0.69
1:A:1212:GLN:C	1:A:1212:GLN:HE21	1.96	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:ILE:HG23	1:A:956:ILE:HD11	1.75	0.69
1:A:960:PRO:O	1:A:961:GLU:HB2	1.91	0.69
1:A:568:LEU:HD23	1:A:577:TYR:HE2	1.56	0.69
1:A:1107:LYS:CD	1:A:1108:THR:H	2.06	0.69
1:A:107:THR:OG1	1:A:110:VAL:HG23	1.93	0.69
1:A:532:ILE:HD12	1:A:532:ILE:O	1.92	0.69
1:A:1107:LYS:HB3	1:A:1107:LYS:HZ2	1.57	0.69
1:A:395:VAL:O	1:A:434:CYS:HA	1.93	0.69
1:A:713:HIS:H	1:A:713:HIS:CD2	2.08	0.69
1:A:742:HIS:CE1	1:A:768:ARG:HG3	2.28	0.69
1:A:614:HIS:CE1	1:A:640:GLN:HG3	2.28	0.68
1:A:986:LYS:HG2	1:A:998:SER:HB3	1.74	0.68
1:A:879:ARG:HH12	1:A:882:LEU:HG	1.57	0.68
1:A:1151:ILE:H	1:A:1166:ALA:CB	2.05	0.68
1:A:216:LEU:HD12	1:A:216:LEU:N	1.98	0.68
1:A:400:LEU:HD13	1:A:415:LEU:HD11	1.75	0.68
1:A:334:PHE:HB3	1:A:337:ARG:HD3	1.74	0.68
1:A:131:LYS:H	1:A:131:LYS:HD3	1.58	0.68
1:A:661:LEU:HD12	1:A:702:VAL:O	1.94	0.68
1:A:1008:HIS:HB2	1:A:1049:ASP:OD1	1.94	0.67
1:A:448:LYS:HZ2	1:A:449:ASN:HD21	1.40	0.67
1:A:507:LEU:HD12	1:A:579:GLN:HB3	1.75	0.67
1:A:448:LYS:HG2	1:A:449:ASN:ND2	2.09	0.67
1:A:464:PHE:CE1	1:A:487:LEU:HD22	2.29	0.67
1:A:396:PRO:HD2	1:A:399:VAL:HG21	1.74	0.67
1:A:1091:CYS:CB	1:A:1103:THR:HA	2.24	0.67
1:A:938:LEU:HD12	1:A:969:LEU:HG	1.76	0.67
1:A:920:ILE:HG23	1:A:921:VAL:N	2.09	0.67
1:A:1116:LEU:HD12	1:A:1116:LEU:H	1.59	0.66
1:A:723:PHE:HD1	1:A:723:PHE:N	1.93	0.66
1:A:176:GLY:O	1:A:177:CYS:HB2	1.94	0.66
1:A:149:TRP:CZ2	1:A:273:VAL:HG21	2.31	0.66
1:A:849:SER:OG	1:A:850:PRO:HD2	1.95	0.66
1:A:270:THR:O	1:A:277:LYS:HE2	1.94	0.66
1:A:245:VAL:HG11	1:A:251:LEU:HD13	1.77	0.66
1:A:522:LEU:HD22	1:A:526:PHE:HE2	1.61	0.66
1:A:638:THR:HB	1:A:653:ILE:O	1.95	0.66
1:A:255:ASP:OD2	1:A:273:VAL:HG23	1.94	0.66
1:A:744:ASN:CG	1:A:745:SER:H	1.99	0.66
1:A:539:ALA:C	1:A:541:CYS:H	1.98	0.66
1:A:942:ASN:H	1:A:942:ASN:ND2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:HB3	1:A:131:LYS:NZ	2.11	0.66
1:A:1248:LEU:HD22	1:A:1249:GLU:HG2	1.78	0.66
1:A:723:PHE:CD1	1:A:723:PHE:N	2.62	0.66
1:A:1211:SER:C	1:A:1213:THR:H	1.97	0.66
1:A:1019:ILE:N	1:A:1019:ILE:HD12	2.11	0.65
1:A:1160:GLN:C	1:A:1161:LEU:HD12	2.16	0.65
1:A:1211:SER:O	1:A:1213:THR:N	2.29	0.65
1:A:201:ASN:HA	1:A:204:MET:HE3	1.77	0.65
1:A:665:PHE:CE1	1:A:672:ILE:HD11	2.32	0.65
1:A:1064:ASP:HB2	1:A:1066:THR:OG1	1.97	0.65
1:A:1141:LEU:HD11	1:A:1162:LEU:CD2	2.26	0.65
1:A:458:ARG:HG3	1:A:496:MET:CE	2.27	0.65
1:A:107:THR:OG1	1:A:109:PHE:HB3	1.97	0.65
1:A:902:ASP:C	1:A:904:GLN:H	1.99	0.65
1:A:685:ASP:OD2	1:A:688:THR:HG23	1.97	0.65
1:A:1059:LEU:HD11	1:A:1067:VAL:CG1	2.27	0.64
1:A:802:LYS:O	1:A:803:CYS:O	2.16	0.64
1:A:218:LEU:HD22	1:A:518:GLY:CA	2.27	0.64
1:A:1053:LEU:HD12	1:A:1054:GLN:H	1.61	0.64
1:A:1248:LEU:CD2	1:A:1249:GLU:HG2	2.27	0.64
1:A:1042:ALA:C	1:A:1044:GLN:H	1.98	0.64
1:A:1054:GLN:HB2	1:A:1057:ARG:HD3	1.78	0.64
1:A:514:THR:HA	1:A:518:GLY:O	1.98	0.64
1:A:898:LEU:HD12	1:A:898:LEU:C	2.18	0.64
1:A:924:GLN:HG2	1:A:1236:VAL:HG12	1.79	0.64
1:A:1074:THR:HG22	1:A:1076:ARG:HB2	1.80	0.64
1:A:942:ASN:H	1:A:942:ASN:HD22	1.45	0.64
1:A:713:HIS:H	1:A:713:HIS:HD2	1.46	0.63
1:A:742:HIS:HE1	1:A:768:ARG:HG3	1.61	0.63
1:A:1107:LYS:CG	1:A:1108:THR:N	2.61	0.63
1:A:1001:GLY:O	1:A:1002:HIS:HB2	1.99	0.63
1:A:1071:ASN:ND2	1:A:1074:THR:HB	2.13	0.63
1:A:676:SER:O	1:A:702:VAL:HG12	1.98	0.63
1:A:376:ARG:HB2	1:A:376:ARG:HH11	1.63	0.63
1:A:1110:LYS:HE2	1:A:1122:GLU:OE2	1.97	0.63
1:A:946:LEU:CD2	1:A:964:VAL:HG11	2.28	0.63
1:A:599:ASN:HB2	1:A:602:THR:OG1	1.99	0.63
1:A:1125:GLY:HA3	1:A:1152:ARG:NH1	2.14	0.63
1:A:1237:ASP:O	1:A:1239:LEU:N	2.32	0.63
1:A:697:GLU:HB3	1:A:726:LYS:HE3	1.81	0.63
1:A:114:LEU:HD11	1:A:169:ARG:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:PRO:O	1:A:972:HIS:CB	2.47	0.62
1:A:399:VAL:O	1:A:402:VAL:HG23	1.97	0.62
1:A:942:ASN:N	1:A:942:ASN:HD22	1.96	0.62
1:A:337:ARG:HG3	1:A:341:TYR:CE2	2.35	0.62
1:A:1140:ILE:HG23	1:A:1140:ILE:O	1.99	0.62
1:A:237:ARG:HH11	1:A:237:ARG:HG2	1.65	0.62
1:A:919:ALA:HB2	1:A:947:GLN:OE1	2.00	0.62
1:A:337:ARG:HH21	1:A:374:MET:CE	2.13	0.62
1:A:402:VAL:O	1:A:463:GLN:HB3	2.00	0.62
1:A:722:ASP:C	1:A:723:PHE:HD1	2.03	0.62
1:A:1227:SER:HB3	1:A:1232:THR:HB	1.81	0.61
1:A:1135:PHE:CE1	1:A:1142:LEU:HG	2.35	0.61
1:A:1236:VAL:HG23	1:A:1242:LEU:HD23	1.81	0.61
1:A:1236:VAL:CG2	1:A:1242:LEU:HD23	2.29	0.61
1:A:1248:LEU:HD23	1:A:1249:GLU:H	1.64	0.61
1:A:1108:THR:CG2	1:A:1124:LYS:HA	2.21	0.61
1:A:303:LYS:H	1:A:306:LEU:HG	1.66	0.61
1:A:881:HIS:HE1	1:A:907:ARG:HG3	1.65	0.61
1:A:1065:GLY:HA3	1:A:1084:HIS:O	2.01	0.61
1:A:1097:ALA:O	1:A:1098:THR:HB	2.01	0.61
1:A:1135:PHE:CD1	1:A:1142:LEU:HB2	2.36	0.61
1:A:210:GLU:HG2	1:A:214:GLN:HG3	1.82	0.61
1:A:804:CYS:CB	1:A:815:VAL:HG12	2.29	0.61
1:A:251:LEU:HD11	1:A:262:LEU:HD13	1.81	0.61
1:A:1153:ILE:O	1:A:1162:LEU:HB3	2.01	0.60
1:A:215:ARG:HH12	1:A:557:ARG:HD3	1.65	0.60
1:A:974:GLU:HA	1:A:991:PRO:HD3	1.82	0.60
1:A:1135:PHE:HD1	1:A:1142:LEU:HB2	1.64	0.60
1:A:879:ARG:NH1	1:A:882:LEU:HG	2.16	0.60
1:A:239:LEU:HD12	1:A:240:LEU:H	1.66	0.60
1:A:499:GLU:O	1:A:502:ALA:HB3	2.02	0.60
1:A:1107:LYS:HG2	1:A:1108:THR:N	2.17	0.60
1:A:341:TYR:HA	1:A:344:GLN:HG2	1.81	0.60
1:A:484:TYR:CE2	1:A:516:LEU:HD12	2.36	0.60
1:A:532:ILE:C	1:A:532:ILE:HD12	2.22	0.60
1:A:551:ASN:HD22	1:A:566:LEU:HD22	1.66	0.60
1:A:470:PRO:HB3	1:A:503:LEU:CD1	2.31	0.60
1:A:821:VAL:O	1:A:822:LEU:HD13	2.02	0.60
1:A:563:ILE:O	1:A:563:ILE:HG13	2.02	0.59
1:A:970:SER:HB3	1:A:1011:PHE:CE2	2.38	0.59
1:A:547:PHE:CD1	1:A:576:VAL:HG11	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ASP:O	1:A:638:THR:HG23	2.03	0.59
1:A:918:SER:OG	1:A:920:ILE:HG22	2.02	0.59
1:A:1003:LYS:HE3	1:A:1024:ASP:OD1	2.02	0.59
1:A:302:LYS:HE2	1:A:304:GLU:HG3	1.83	0.59
1:A:376:ARG:HB2	1:A:376:ARG:NH1	2.17	0.59
1:A:1058:LEU:HD23	1:A:1058:LEU:O	2.03	0.59
1:A:1084:HIS:CE1	1:A:1107:LYS:HE2	2.37	0.59
1:A:1059:LEU:HD12	1:A:1068:LYS:O	2.02	0.59
1:A:1126:HIS:ND1	1:A:1146:ASP:HB2	2.17	0.59
1:A:1131:ARG:O	1:A:1132:CYS:HB3	2.03	0.59
1:A:117:GLY:HA3	1:A:182:VAL:O	2.02	0.59
1:A:1121:HIS:HB3	1:A:1158:ASP:O	2.03	0.59
1:A:1191:LYS:HA	1:A:1205:VAL:HG21	1.85	0.59
1:A:215:ARG:HD2	1:A:556:GLY:O	2.02	0.59
1:A:603:ILE:HG22	1:A:604:LYS:N	2.14	0.59
1:A:161:SER:HB2	2:A:1250:ADP:O2A	2.03	0.59
1:A:977:ALA:HB2	1:A:987:ILE:HG12	1.84	0.59
1:A:1093:ILE:HG13	1:A:1095:SER:H	1.68	0.59
1:A:534:ASP:HB2	1:A:541:CYS:HB2	1.84	0.58
1:A:926:ILE:HG22	1:A:939:ALA:CB	2.32	0.58
1:A:1194:VAL:HG23	1:A:1202:TRP:CD1	2.37	0.58
1:A:360:ASP:OD1	1:A:440:LEU:HD21	2.03	0.58
1:A:448:LYS:HG2	1:A:449:ASN:HD22	1.67	0.58
1:A:491:MET:HE3	1:A:500:LEU:HD12	1.84	0.58
1:A:1131:ARG:O	1:A:1131:ARG:HG2	2.02	0.58
1:A:262:LEU:HD23	1:A:262:LEU:H	1.68	0.58
1:A:568:LEU:HD23	1:A:577:TYR:CE2	2.37	0.58
1:A:1107:LYS:HB3	1:A:1107:LYS:NZ	2.17	0.58
1:A:113:VAL:HG11	1:A:174:LEU:HD21	1.84	0.58
1:A:353:ILE:HG12	1:A:354:ARG:H	1.68	0.58
1:A:522:LEU:HD22	1:A:526:PHE:CE2	2.37	0.58
1:A:1116:LEU:HD12	1:A:1116:LEU:N	2.19	0.58
1:A:1146:ASP:CB	1:A:1150:GLU:HB3	2.34	0.58
1:A:639:LEU:O	1:A:640:GLN:HG2	2.03	0.58
1:A:921:VAL:HB	1:A:942:ASN:OD1	2.03	0.58
1:A:1059:LEU:HD11	1:A:1067:VAL:HG12	1.84	0.58
1:A:714:LEU:CD2	1:A:730:LEU:HB2	2.34	0.58
1:A:846:CYS:HB2	1:A:857:ILE:HG22	1.84	0.58
1:A:938:LEU:HD11	1:A:976:VAL:CG2	2.34	0.58
1:A:1003:LYS:N	1:A:1003:LYS:HE2	2.17	0.58
1:A:1042:ALA:HB1	1:A:1044:GLN:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLU:O	1:A:600:LYS:HE2	2.04	0.58
1:A:760:SER:CB	1:A:770:TRP:CZ3	2.85	0.58
1:A:1177:HIS:CD2	1:A:1178:GLY:H	2.20	0.58
1:A:604:LYS:HD3	1:A:606:LEU:HD21	1.85	0.58
1:A:938:LEU:HD13	1:A:967:CYS:SG	2.44	0.58
1:A:481:MET:O	1:A:482:TYR:C	2.42	0.58
1:A:953:THR:HG22	1:A:953:THR:O	2.02	0.58
1:A:1111:ILE:HD13	1:A:1111:ILE:C	2.25	0.58
1:A:382:TYR:CD2	1:A:414:ILE:HG21	2.38	0.58
1:A:130:LYS:HD2	1:A:131:LYS:HD3	1.85	0.57
1:A:1116:LEU:CD1	1:A:1116:LEU:H	2.18	0.57
1:A:1129:CYS:SG	1:A:1147:ASP:HB2	2.44	0.57
1:A:619:TYR:CE2	1:A:635:ALA:HB2	2.36	0.57
1:A:811:ASP:HA	1:A:826:ILE:HG21	1.84	0.57
1:A:938:LEU:HG	1:A:948:LEU:HD22	1.85	0.57
1:A:1116:LEU:C	1:A:1118:SER:H	2.08	0.57
1:A:630:ILE:HD12	1:A:642:PHE:HE2	1.69	0.57
1:A:705:CYS:HB3	1:A:718:THR:HG22	1.87	0.57
1:A:225:ASP:O	1:A:227:LEU:N	2.38	0.57
1:A:1027:ILE:HG13	1:A:1047:VAL:HG21	1.86	0.57
1:A:1222:LYS:O	1:A:1223:LYS:O	2.23	0.57
1:A:330:LEU:HD22	1:A:341:TYR:CE2	2.40	0.57
1:A:511:LYS:HE3	1:A:515:GLU:OE2	2.05	0.57
1:A:767:LEU:HD23	1:A:768:ARG:N	2.20	0.57
1:A:783:VAL:HG12	1:A:786:PHE:HE2	1.69	0.57
1:A:224:LYS:O	1:A:227:LEU:HB3	2.05	0.57
1:A:762:SER:OG	1:A:763:ALA:N	2.38	0.57
1:A:130:LYS:HA	1:A:133:VAL:HG23	1.86	0.57
1:A:192:LYS:HE3	4:A:1266:HOH:O	2.04	0.57
1:A:430:GLY:C	1:A:432:SER:H	2.07	0.57
1:A:1183:ASP:OD1	1:A:1223:LYS:HE3	2.04	0.56
1:A:697:GLU:CB	1:A:726:LYS:HE3	2.35	0.56
1:A:938:LEU:HD11	1:A:976:VAL:HG23	1.87	0.56
1:A:1210:SER:OG	1:A:1211:SER:N	2.37	0.56
1:A:682:LYS:HG2	1:A:694:THR:CG2	2.30	0.56
1:A:768:ARG:HB2	1:A:770:TRP:CZ3	2.40	0.56
1:A:842:THR:O	1:A:842:THR:HG22	2.05	0.56
1:A:987:ILE:HD11	1:A:1018:LEU:HD11	1.87	0.56
1:A:410:GLU:O	1:A:414:ILE:HG13	2.05	0.56
1:A:358:SER:HB3	1:A:361:TYR:HB2	1.87	0.56
1:A:532:ILE:HG13	1:A:533:LEU:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LEU:HD23	1:A:640:GLN:H	1.70	0.56
1:A:856:VAL:HG13	1:A:890:PHE:CZ	2.41	0.56
1:A:968:CYS:HB2	1:A:1009:ILE:HG23	1.86	0.56
1:A:1151:ILE:HD11	1:A:1193:LEU:CD2	2.34	0.56
1:A:1167:PRO:O	1:A:1168:ILE:HB	2.05	0.56
1:A:626:ASP:OD1	1:A:628:GLN:HB2	2.06	0.56
1:A:1237:ASP:C	1:A:1239:LEU:H	2.08	0.56
1:A:228:ARG:HH11	1:A:228:ARG:HB3	1.71	0.56
1:A:384:THR:HG23	1:A:449:ASN:OD1	2.05	0.56
1:A:1187:SER:OG	1:A:1188:PRO:HD2	2.06	0.56
1:A:1113:SER:O	1:A:1115:ASP:N	2.38	0.56
1:A:128:THR:O	1:A:130:LYS:HE3	2.06	0.56
1:A:519:PRO:O	1:A:523:ILE:HG13	2.05	0.56
1:A:588:GLY:O	1:A:589:ASP:HB2	2.06	0.56
1:A:1066:THR:HA	1:A:1081:PHE:O	2.06	0.55
1:A:803:CYS:SG	1:A:846:CYS:C	2.84	0.55
1:A:448:LYS:NZ	1:A:449:ASN:ND2	2.52	0.55
1:A:1177:HIS:CG	1:A:1178:GLY:H	2.25	0.55
1:A:1113:SER:C	1:A:1115:ASP:H	2.09	0.55
1:A:237:ARG:O	1:A:237:ARG:HG3	2.06	0.55
1:A:1102:SER:HB2	1:A:1111:ILE:CG1	2.37	0.55
1:A:1121:HIS:CB	1:A:1158:ASP:O	2.55	0.55
1:A:449:ASN:HD22	1:A:449:ASN:N	2.05	0.55
1:A:951:GLY:O	1:A:952:LYS:HB3	2.06	0.55
1:A:1155:ASN:OD1	1:A:1160:GLN:HB2	2.06	0.55
1:A:1152:ARG:HG2	1:A:1164:SER:OG	2.06	0.55
1:A:1165:CYS:C	1:A:1167:PRO:HD3	2.27	0.55
1:A:926:ILE:HG22	1:A:939:ALA:HB2	1.88	0.55
1:A:946:LEU:HD12	1:A:959:LEU:HD12	1.88	0.55
1:A:1029:VAL:HG12	1:A:1029:VAL:O	2.07	0.55
1:A:395:VAL:O	1:A:434:CYS:CA	2.55	0.55
1:A:539:ALA:C	1:A:541:CYS:N	2.59	0.55
1:A:814:ILE:HG22	1:A:823:LEU:HD13	1.89	0.55
1:A:286:LEU:HG	1:A:287:GLY:H	1.71	0.55
1:A:302:LYS:O	1:A:303:LYS:HB2	2.05	0.55
1:A:491:MET:HE1	1:A:503:LEU:HB3	1.89	0.55
1:A:662:CYS:SG	1:A:663:CYS:N	2.80	0.55
1:A:921:VAL:HG13	1:A:1240:GLY:HA3	1.88	0.55
1:A:917:ASN:HD21	1:A:947:GLN:HE22	1.55	0.55
1:A:940:VAL:HG13	1:A:964:VAL:HG23	1.89	0.55
1:A:107:THR:C	1:A:109:PHE:N	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:O	1:A:234:LYS:CB	2.55	0.54
1:A:366:GLU:O	1:A:367:ALA:C	2.46	0.54
1:A:1217:ASN:N	1:A:1217:ASN:HD22	2.04	0.54
1:A:1102:SER:HB2	1:A:1111:ILE:HG12	1.89	0.54
1:A:722:ASP:C	1:A:723:PHE:CD1	2.81	0.54
1:A:406:LEU:HB2	1:A:411:VAL:CG2	2.37	0.54
1:A:361:TYR:O	1:A:362:GLU:C	2.46	0.54
1:A:400:LEU:CD1	1:A:415:LEU:HD11	2.38	0.54
1:A:426:CYS:HB3	1:A:435:TYR:HD1	1.70	0.54
1:A:225:ASP:O	1:A:226:ARG:C	2.46	0.54
1:A:415:LEU:HA	1:A:418:PHE:HD2	1.71	0.54
1:A:802:LYS:O	1:A:803:CYS:C	2.45	0.54
1:A:1237:ASP:OD1	1:A:1241:ILE:HB	2.08	0.54
1:A:774:SER:O	1:A:775:ALA:HB3	2.08	0.54
1:A:1053:LEU:CD2	1:A:1059:LEU:HB2	2.36	0.53
1:A:1063:PHE:HA	1:A:1087:THR:HA	1.90	0.53
1:A:470:PRO:HB3	1:A:503:LEU:HD12	1.90	0.53
1:A:1072:VAL:HG12	1:A:1073:ILE:N	2.22	0.53
1:A:1231:ARG:CZ	1:A:1231:ARG:HB2	2.37	0.53
1:A:835:ILE:HD12	1:A:867:TRP:CE3	2.43	0.53
1:A:951:GLY:O	1:A:952:LYS:CB	2.56	0.53
1:A:511:LYS:O	1:A:515:GLU:HG3	2.07	0.53
1:A:302:LYS:HE2	1:A:304:GLU:CG	2.38	0.53
1:A:953:THR:O	1:A:954:GLY:C	2.46	0.53
1:A:1152:ARG:HG2	1:A:1164:SER:CB	2.39	0.53
1:A:497:HIS:HA	1:A:532:ILE:HD11	1.90	0.53
1:A:1128:GLY:O	1:A:1129:CYS:HB3	2.09	0.53
1:A:1155:ASN:HD21	1:A:1160:GLN:CG	2.21	0.53
1:A:226:ARG:O	1:A:230:LEU:HG	2.09	0.53
1:A:1042:ALA:C	1:A:1044:GLN:N	2.62	0.53
1:A:592:ARG:O	1:A:593:LEU:HB2	2.09	0.53
1:A:720:SER:OG	1:A:721:ASN:N	2.41	0.53
1:A:653:ILE:HG21	1:A:684:TRP:CZ3	2.44	0.53
1:A:196:LEU:HD12	1:A:196:LEU:O	2.09	0.53
1:A:1204:ASN:ND2	1:A:1207:THR:O	2.42	0.52
1:A:1211:SER:C	1:A:1213:THR:N	2.62	0.52
1:A:1012:THR:HG22	1:A:1013:ALA:N	2.24	0.52
1:A:1140:ILE:CG1	1:A:1156:VAL:HB	2.34	0.52
1:A:388:ILE:HB	1:A:457:HIS:CE1	2.44	0.52
1:A:739:MET:HG2	1:A:770:TRP:CD1	2.44	0.52
1:A:920:ILE:HG23	1:A:921:VAL:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD13	1:A:259:GLN:HB3	1.92	0.52
1:A:438:HIS:HB3	1:A:441:GLN:HE21	1.74	0.52
1:A:960:PRO:O	1:A:961:GLU:CB	2.58	0.52
1:A:760:SER:HB3	1:A:770:TRP:CZ3	2.31	0.52
1:A:1048:LYS:HB3	1:A:1061:TRP:CZ3	2.45	0.52
1:A:605:ASN:O	1:A:606:LEU:C	2.48	0.52
1:A:752:SER:O	1:A:753:PRO:C	2.47	0.52
1:A:209:GLU:HB3	1:A:211:SER:OG	2.10	0.52
1:A:1062:SER:OG	1:A:1063:PHE:N	2.43	0.52
1:A:1163:HIS:CD2	1:A:1207:THR:HA	2.44	0.52
1:A:660:VAL:HA	1:A:676:SER:HB2	1.92	0.52
1:A:1019:ILE:HG21	1:A:1058:LEU:HD11	1.91	0.52
1:A:123:PRO:O	1:A:124:VAL:C	2.49	0.52
1:A:352:ARG:HB2	1:A:447:GLU:HG2	1.91	0.52
1:A:381:ASP:O	1:A:384:THR:HB	2.10	0.52
1:A:704:CYS:HB2	1:A:747:ASN:O	2.10	0.52
1:A:207:ASP:OD2	1:A:230:LEU:HD11	2.10	0.51
1:A:846:CYS:HA	1:A:856:VAL:O	2.10	0.51
1:A:992:ASN:ND2	1:A:995:VAL:HB	2.26	0.51
1:A:119:VAL:HG13	1:A:120:PRO:HD2	1.93	0.51
1:A:196:LEU:HD12	1:A:200:GLN:HG3	1.91	0.51
1:A:182:VAL:HA	1:A:239:LEU:O	2.10	0.51
1:A:309:GLU:HG3	1:A:342:LEU:HD22	1.91	0.51
1:A:980:ASP:OD1	1:A:982:ASP:N	2.41	0.51
1:A:469:GLN:HB3	1:A:472:THR:OG1	2.10	0.51
1:A:708:THR:CG2	1:A:715:LEU:HB2	2.39	0.51
1:A:859:LEU:HG	1:A:860:SER:H	1.76	0.51
1:A:903:ASP:O	1:A:905:THR:HG23	2.10	0.51
1:A:970:SER:O	1:A:971:PRO:C	2.49	0.51
1:A:183:HIS:HB2	1:A:240:LEU:HD12	1.93	0.51
1:A:771:ASP:HB2	1:A:778:ARG:HH11	1.75	0.51
1:A:1191:LYS:HA	1:A:1205:VAL:CG2	2.41	0.51
1:A:1087:THR:O	1:A:1105:ALA:HB1	2.10	0.51
1:A:477:GLN:HB3	1:A:479:ASP:OD1	2.10	0.51
1:A:215:ARG:NH1	1:A:557:ARG:HA	2.24	0.51
1:A:704:CYS:SG	1:A:749:CYS:N	2.84	0.51
1:A:879:ARG:HD3	1:A:1239:LEU:HD13	1.93	0.51
1:A:1194:VAL:HG13	1:A:1194:VAL:O	2.11	0.51
1:A:245:VAL:HG21	1:A:262:LEU:HD12	1.92	0.51
1:A:340:TYR:O	1:A:343:ARG:HB3	2.11	0.51
1:A:919:ALA:HB3	1:A:956:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD23	1:A:256:ASN:HD22	1.75	0.51
1:A:336:ASN:O	1:A:338:TRP:N	2.42	0.51
1:A:529:TYR:O	1:A:533:LEU:CB	2.54	0.51
1:A:924:GLN:OE1	1:A:1222:LYS:HD2	2.10	0.51
1:A:1072:VAL:C	1:A:1073:ILE:HG13	2.31	0.51
1:A:160:LYS:HB2	2:A:1250:ADP:O1B	2.11	0.51
1:A:980:ASP:HB3	1:A:984:ALA:O	2.11	0.51
1:A:1083:CYS:O	1:A:1084:HIS:CG	2.64	0.51
1:A:736:ARG:O	1:A:737:ASN:ND2	2.44	0.51
1:A:980:ASP:CG	1:A:981:GLU:N	2.63	0.51
1:A:841:SER:HB2	1:A:860:SER:CB	2.40	0.50
1:A:1097:ALA:O	1:A:1098:THR:CB	2.59	0.50
1:A:1157:SER:HB2	1:A:1160:GLN:NE2	2.26	0.50
1:A:130:LYS:HD2	1:A:131:LYS:N	2.21	0.50
1:A:1136:SER:O	1:A:1137:LEU:C	2.49	0.50
1:A:1146:ASP:CB	1:A:1150:GLU:O	2.58	0.50
1:A:1202:TRP:C	1:A:1203:TRP:CD1	2.83	0.50
1:A:239:LEU:HD12	1:A:240:LEU:N	2.25	0.50
1:A:343:ARG:HH21	1:A:343:ARG:HG3	1.76	0.50
1:A:485:ASN:O	1:A:486:PHE:CG	2.65	0.50
1:A:902:ASP:C	1:A:904:GLN:N	2.63	0.50
1:A:704:CYS:O	1:A:718:THR:HA	2.12	0.50
1:A:920:ILE:CG2	1:A:921:VAL:N	2.74	0.50
1:A:534:ASP:CB	1:A:541:CYS:HB2	2.42	0.50
1:A:722:ASP:OD2	1:A:724:PHE:HD2	1.95	0.50
1:A:107:THR:HG21	1:A:171:HIS:HB2	1.94	0.50
1:A:396:PRO:HD2	1:A:399:VAL:CG2	2.40	0.50
1:A:461:VAL:CG2	1:A:462:THR:N	2.75	0.50
1:A:479:ASP:O	1:A:480:CYS:C	2.49	0.50
1:A:814:ILE:CD1	1:A:848:PHE:HB2	2.41	0.50
1:A:861:GLN:O	1:A:863:CYS:N	2.35	0.50
1:A:130:LYS:HA	1:A:133:VAL:CG2	2.42	0.50
1:A:141:TRP:C	1:A:143:LEU:H	2.14	0.50
1:A:185:VAL:HG12	1:A:187:ILE:HG13	1.92	0.50
1:A:604:LYS:C	1:A:606:LEU:H	2.15	0.50
1:A:108:SER:HA	1:A:111:ARG:CD	2.42	0.49
1:A:133:VAL:HG21	4:A:1259:HOH:O	2.12	0.49
1:A:1017:THR:HA	1:A:1031:ASN:HA	1.94	0.49
1:A:1227:SER:HB2	1:A:1228:PRO:CD	2.41	0.49
1:A:133:VAL:HG13	1:A:166:GLU:HB3	1.94	0.49
1:A:723:PHE:CE2	1:A:744:ASN:HA	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:LEU:H	1:A:866:LEU:HD23	1.77	0.49
1:A:1017:THR:HA	1:A:1030:TRP:O	2.12	0.49
1:A:1179:GLY:O	1:A:1180:TRP:HB2	2.12	0.49
1:A:835:ILE:HG22	1:A:872:ARG:HG2	1.95	0.49
1:A:756:GLU:O	1:A:772:VAL:HG23	2.13	0.49
1:A:612:ARG:CG	1:A:905:THR:HG22	2.34	0.49
1:A:942:ASN:N	1:A:942:ASN:ND2	2.55	0.49
1:A:1107:LYS:CD	1:A:1108:THR:N	2.74	0.49
1:A:1191:LYS:O	1:A:1205:VAL:HG13	2.12	0.49
1:A:1120:LEU:HD13	1:A:1158:ASP:OD1	2.13	0.49
1:A:1141:LEU:HD13	1:A:1155:ASN:HA	1.94	0.49
1:A:743:THR:HB	1:A:764:ASP:CB	2.43	0.49
1:A:869:ILE:HG22	1:A:870:ASP:N	2.28	0.49
1:A:130:LYS:NZ	1:A:131:LYS:HD2	2.28	0.49
1:A:295:LEU:O	1:A:299:VAL:HG22	2.13	0.49
1:A:735:CYS:SG	1:A:737:ASN:O	2.71	0.49
1:A:1094:SER:O	1:A:1096:ASP:N	2.45	0.49
1:A:1107:LYS:HD2	1:A:1108:THR:N	2.15	0.49
1:A:531:HIS:NE2	1:A:532:ILE:HG22	2.28	0.49
1:A:784:LYS:C	1:A:786:PHE:H	2.15	0.49
1:A:831:LEU:C	1:A:831:LEU:HD23	2.32	0.49
1:A:1047:VAL:HA	1:A:1062:SER:HB2	1.94	0.48
1:A:785:ARG:NH2	1:A:831:LEU:HD12	2.28	0.48
1:A:1046:THR:O	1:A:1047:VAL:C	2.49	0.48
1:A:398:LYS:O	1:A:402:VAL:HG22	2.14	0.48
1:A:609:LEU:HD12	1:A:610:VAL:N	2.28	0.48
1:A:796:ASP:O	1:A:797:VAL:O	2.31	0.48
1:A:1161:LEU:O	1:A:1162:LEU:O	2.31	0.48
1:A:931:GLN:HG3	1:A:934:GLU:O	2.13	0.48
1:A:1024:ASP:OD1	1:A:1026:VAL:HG12	2.13	0.48
1:A:1231:ARG:O	1:A:1231:ARG:HG2	2.13	0.48
1:A:245:VAL:HG11	1:A:251:LEU:CD1	2.44	0.48
1:A:251:LEU:HD11	1:A:262:LEU:CD1	2.43	0.48
1:A:361:TYR:O	1:A:364:LEU:N	2.47	0.48
1:A:449:ASN:N	1:A:449:ASN:ND2	2.60	0.48
1:A:482:TYR:O	1:A:486:PHE:HB2	2.13	0.48
1:A:811:ASP:C	1:A:826:ILE:HG22	2.34	0.48
1:A:228:ARG:HG2	1:A:232:LEU:HD12	1.95	0.48
1:A:348:LYS:N	1:A:348:LYS:HD2	2.29	0.48
1:A:987:ILE:HD11	1:A:1018:LEU:CD1	2.43	0.48
1:A:119:VAL:HG12	1:A:120:PRO:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:HIS:HE1	1:A:640:GLN:HG3	1.76	0.48
1:A:214:GLN:HG2	1:A:215:ARG:N	2.24	0.48
1:A:216:LEU:CD1	1:A:216:LEU:H	1.90	0.48
1:A:364:LEU:O	1:A:365:ASP:C	2.51	0.48
1:A:758:LEU:HD23	1:A:759:ALA:N	2.28	0.48
1:A:944:ARG:HG2	1:A:961:GLU:O	2.14	0.48
1:A:978:PHE:C	1:A:978:PHE:CD2	2.87	0.48
1:A:1019:ILE:N	1:A:1019:ILE:CD1	2.77	0.48
1:A:1146:ASP:HB3	1:A:1150:GLU:HB3	1.95	0.48
1:A:385:ASP:C	1:A:387:SER:H	2.17	0.48
1:A:752:SER:HB2	1:A:806:TRP:CZ2	2.49	0.48
1:A:908:VAL:HG12	1:A:909:TRP:N	2.29	0.48
1:A:994:ARG:O	1:A:995:VAL:C	2.52	0.48
1:A:1224:ILE:HD13	1:A:1235:THR:HB	1.96	0.48
1:A:835:ILE:HG13	1:A:835:ILE:O	2.14	0.48
1:A:239:LEU:HD12	1:A:259:GLN:O	2.14	0.47
1:A:809:ASP:N	1:A:809:ASP:OD2	2.47	0.47
1:A:106:ILE:HG22	1:A:107:THR:N	2.30	0.47
1:A:1131:ARG:HG3	1:A:1131:ARG:HH11	1.78	0.47
1:A:152:ILE:HB	1:A:263:THR:HG22	1.96	0.47
1:A:415:LEU:HA	1:A:418:PHE:CD2	2.48	0.47
1:A:487:LEU:O	1:A:491:MET:HG3	2.13	0.47
1:A:624:SER:HB2	1:A:669:ASP:OD1	2.14	0.47
1:A:707:PHE:CZ	1:A:716:LEU:HD12	2.48	0.47
1:A:814:ILE:HA	1:A:822:LEU:O	2.13	0.47
1:A:1053:LEU:CD1	1:A:1054:GLN:H	2.27	0.47
1:A:1189:ASP:OD1	1:A:1191:LYS:HB2	2.14	0.47
1:A:137:GLN:HG2	1:A:173:LEU:HD22	1.96	0.47
1:A:237:ARG:HG2	1:A:237:ARG:NH1	2.29	0.47
1:A:534:ASP:CG	1:A:541:CYS:HB2	2.35	0.47
1:A:630:ILE:HB	1:A:642:PHE:CE2	2.49	0.47
1:A:682:LYS:HE2	1:A:694:THR:CG2	2.45	0.47
1:A:1027:ILE:CG1	1:A:1047:VAL:HG21	2.44	0.47
1:A:406:LEU:HB2	1:A:411:VAL:HG22	1.94	0.47
1:A:635:ALA:C	1:A:637:LYS:H	2.16	0.47
1:A:899:THR:O	1:A:906:ILE:HA	2.15	0.47
1:A:980:ASP:O	1:A:1006:VAL:HG23	2.13	0.47
1:A:225:ASP:C	1:A:227:LEU:N	2.64	0.47
1:A:692:VAL:O	1:A:693:HIS:CB	2.59	0.47
1:A:340:TYR:CZ	1:A:344:GLN:NE2	2.83	0.47
1:A:801:VAL:HG23	1:A:801:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HG22	2:A:1250:ADP:N1	2.30	0.47
1:A:375:LEU:HD21	1:A:423:LEU:CD1	2.44	0.47
1:A:541:CYS:O	1:A:542:GLU:C	2.52	0.47
1:A:870:ASP:OD1	1:A:871:SER:N	2.48	0.47
1:A:1062:SER:C	1:A:1064:ASP:H	2.18	0.47
1:A:1101:SER:O	1:A:1112:TRP:CZ3	2.68	0.47
1:A:1212:GLN:O	1:A:1213:THR:O	2.33	0.47
1:A:231:MET:O	1:A:236:PRO:HA	2.15	0.47
1:A:431:LYS:HA	1:A:431:LYS:NZ	2.30	0.47
1:A:587:GLU:OE1	1:A:592:ARG:HD2	2.15	0.47
1:A:604:LYS:O	1:A:606:LEU:HD22	2.14	0.47
1:A:744:ASN:ND2	1:A:763:ALA:HB3	2.30	0.47
1:A:832:LEU:CD1	1:A:832:LEU:N	2.78	0.47
1:A:1002:HIS:HA	1:A:1003:LYS:NZ	2.16	0.47
1:A:1012:THR:O	1:A:1013:ALA:C	2.53	0.47
1:A:109:PHE:O	1:A:110:VAL:C	2.53	0.47
1:A:1106:ASP:O	1:A:1107:LYS:CB	2.60	0.47
1:A:1184:VAL:HB	1:A:1193:LEU:HD11	1.97	0.47
1:A:1229:ASP:OD2	1:A:1229:ASP:N	2.45	0.47
1:A:207:ASP:C	1:A:209:GLU:H	2.17	0.47
1:A:293:GLU:O	1:A:296:SER:HB3	2.15	0.47
1:A:218:LEU:HD12	1:A:557:ARG:CZ	2.45	0.47
1:A:230:LEU:O	1:A:235:HIS:HB2	2.15	0.47
1:A:453:LEU:HD13	3:A:1251:GBL:HBC1	1.96	0.47
1:A:507:LEU:O	1:A:510:ILE:HB	2.14	0.47
1:A:603:ILE:CG2	1:A:604:LYS:H	2.17	0.47
1:A:838:GLY:O	1:A:839:HIS:C	2.52	0.47
1:A:1182:THR:O	1:A:1183:ASP:HB2	2.15	0.47
1:A:383:TYR:CE1	1:A:423:LEU:HB3	2.50	0.47
1:A:799:VAL:HG22	1:A:818:LYS:HD3	1.96	0.47
1:A:112:THR:O	1:A:116:GLU:HG2	2.15	0.46
1:A:309:GLU:HG3	1:A:342:LEU:CD2	2.44	0.46
1:A:954:GLY:O	1:A:956:ILE:HD13	2.14	0.46
1:A:312:SER:O	1:A:316:GLU:HG2	2.15	0.46
1:A:337:ARG:CB	1:A:340:TYR:HB3	2.45	0.46
1:A:1042:ALA:HB1	1:A:1044:GLN:OE1	2.14	0.46
1:A:1113:SER:C	1:A:1115:ASP:N	2.69	0.46
1:A:1148:ASN:O	1:A:1168:ILE:HD12	2.15	0.46
1:A:336:ASN:C	1:A:338:TRP:H	2.18	0.46
1:A:754:ASP:O	1:A:756:GLU:N	2.45	0.46
1:A:496:MET:HB3	1:A:499:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:THR:O	1:A:955:GLN:N	2.48	0.46
1:A:309:GLU:O	1:A:312:SER:N	2.47	0.46
1:A:706:HIS:CD2	1:A:707:PHE:N	2.83	0.46
1:A:1140:ILE:HA	1:A:1156:VAL:HB	1.98	0.46
1:A:492:ALA:C	1:A:494:ALA:H	2.18	0.46
1:A:846:CYS:O	1:A:847:ASP:HB2	2.16	0.46
1:A:1191:LYS:O	1:A:1205:VAL:HG22	2.16	0.46
1:A:130:LYS:HD2	1:A:131:LYS:CD	2.45	0.46
1:A:227:LEU:HD23	1:A:256:ASN:ND2	2.30	0.46
1:A:562:ASN:OD1	1:A:564:VAL:HG23	2.16	0.46
1:A:938:LEU:CD1	1:A:976:VAL:HG23	2.46	0.46
1:A:866:LEU:N	1:A:866:LEU:HD23	2.31	0.46
1:A:923:LYS:HD2	1:A:940:VAL:HG11	1.98	0.46
1:A:1072:VAL:CG1	1:A:1073:ILE:N	2.79	0.46
1:A:1126:HIS:CE1	1:A:1146:ASP:HB2	2.51	0.46
1:A:542:GLU:O	1:A:546:GLU:N	2.26	0.46
1:A:941:ASP:OD2	1:A:943:ILE:N	2.45	0.46
1:A:946:LEU:CD1	1:A:959:LEU:HD12	2.46	0.46
1:A:113:VAL:HG11	1:A:174:LEU:CD2	2.45	0.45
1:A:1140:ILE:HD11	1:A:1156:VAL:O	2.16	0.45
1:A:563:ILE:HA	1:A:566:LEU:HD12	1.98	0.45
1:A:708:THR:HG23	1:A:715:LEU:HB2	1.97	0.45
1:A:862:TYR:HB2	1:A:881:HIS:O	2.15	0.45
1:A:1201:LYS:HG3	1:A:1212:GLN:HA	1.98	0.45
1:A:149:TRP:O	1:A:278:HIS:N	2.50	0.45
1:A:353:ILE:HG23	1:A:354:ARG:HG3	1.98	0.45
1:A:679:LYS:CD	1:A:699:SER:O	2.65	0.45
1:A:847:ASP:OD2	1:A:889:MET:HB2	2.16	0.45
1:A:1103:THR:HG23	1:A:1112:TRP:CZ2	2.51	0.45
1:A:187:ILE:HG22	1:A:188:GLY:N	2.31	0.45
1:A:1014:ASP:OD2	1:A:1016:LYS:HE3	2.17	0.45
1:A:1123:LEU:HB3	1:A:1154:TRP:CE3	2.52	0.45
1:A:130:LYS:HZ3	1:A:131:LYS:HD2	1.81	0.45
1:A:604:LYS:CG	1:A:606:LEU:HD22	2.47	0.45
1:A:679:LYS:HD2	1:A:699:SER:O	2.15	0.45
1:A:1229:ASP:OD1	1:A:1231:ARG:HB3	2.17	0.45
1:A:123:PRO:O	1:A:125:ILE:N	2.50	0.45
1:A:218:LEU:HD22	1:A:518:GLY:HA3	1.97	0.45
1:A:917:ASN:ND2	1:A:947:GLN:HE22	2.14	0.45
1:A:1101:SER:OG	1:A:1114:PHE:CE1	2.70	0.45
1:A:1237:ASP:OD2	1:A:1243:TYR:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:N	1:A:288:ARG:NE	2.36	0.45
1:A:411:VAL:O	1:A:415:LEU:HG	2.15	0.45
1:A:584:ALA:C	1:A:586:GLN:H	2.19	0.45
1:A:624:SER:HA	1:A:665:PHE:CD2	2.52	0.45
1:A:693:HIS:CD2	1:A:694:THR:H	2.35	0.45
1:A:756:GLU:O	1:A:757:LEU:HD23	2.16	0.45
1:A:1122:GLU:OE1	1:A:1124:LYS:HD2	2.16	0.45
1:A:1137:LEU:O	1:A:1138:ASP:CB	2.65	0.45
1:A:147:PRO:HA	1:A:259:GLN:HG2	1.98	0.45
1:A:376:ARG:CB	1:A:376:ARG:NH1	2.80	0.45
1:A:695:TYR:HD1	1:A:728:TRP:CE3	2.34	0.45
1:A:1218:GLY:HA3	1:A:1239:LEU:HG	1.98	0.45
1:A:405:ASP:O	1:A:406:LEU:HD23	2.16	0.45
1:A:491:MET:CE	1:A:500:LEU:HD12	2.46	0.45
1:A:136:ILE:HD13	1:A:152:ILE:CD1	2.47	0.45
1:A:928:VAL:HG12	1:A:929:VAL:N	2.31	0.45
1:A:604:LYS:HD3	1:A:606:LEU:CD2	2.46	0.45
1:A:667:SER:HB3	1:A:708:THR:O	2.17	0.45
1:A:695:TYR:CD1	1:A:728:TRP:CE3	3.05	0.45
1:A:251:LEU:HD21	1:A:262:LEU:CD1	2.48	0.44
1:A:974:GLU:O	1:A:990:LEU:N	2.49	0.44
1:A:1064:ASP:HB2	1:A:1066:THR:HG1	1.82	0.44
1:A:254:PHE:HB3	1:A:260:ILE:CD1	2.47	0.44
1:A:391:LYS:HD3	1:A:439:ASP:CB	2.47	0.44
1:A:586:GLN:O	1:A:587:GLU:HB3	2.17	0.44
1:A:724:PHE:HE1	1:A:740:PHE:HD2	1.65	0.44
1:A:744:ASN:CG	1:A:745:SER:N	2.67	0.44
1:A:920:ILE:CG2	1:A:921:VAL:H	2.29	0.44
1:A:1102:SER:HB2	1:A:1111:ILE:CB	2.47	0.44
1:A:1153:ILE:HD13	1:A:1153:ILE:N	2.32	0.44
1:A:421:LYS:O	1:A:422:SER:HB2	2.18	0.44
1:A:639:LEU:HD23	1:A:640:GLN:N	2.32	0.44
1:A:618:VAL:CG1	1:A:906:ILE:HD11	2.36	0.44
1:A:961:GLU:HG2	1:A:978:PHE:CZ	2.53	0.44
1:A:1012:THR:OG1	1:A:1017:THR:HB	2.18	0.44
1:A:1143:ALA:HB2	1:A:1186:PHE:CZ	2.52	0.44
1:A:708:THR:HA	1:A:751:PHE:CD2	2.52	0.44
1:A:804:CYS:SG	1:A:804:CYS:O	2.76	0.44
1:A:383:TYR:HB2	1:A:418:PHE:CE1	2.52	0.44
1:A:540:VAL:O	1:A:540:VAL:HG12	2.17	0.44
1:A:785:ARG:CG	1:A:785:ARG:NH1	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:LYS:HG3	1:A:941:ASP:O	2.18	0.44
1:A:1156:VAL:O	1:A:1156:VAL:HG12	2.16	0.44
1:A:232:LEU:O	1:A:233:ARG:HB2	2.17	0.44
1:A:302:LYS:C	1:A:304:GLU:H	2.21	0.44
1:A:358:SER:O	1:A:359:TYR:O	2.36	0.44
1:A:553:HIS:ND1	1:A:554:LEU:HG	2.32	0.44
1:A:604:LYS:HG2	1:A:606:LEU:HD22	1.99	0.44
1:A:756:GLU:C	1:A:772:VAL:HG23	2.37	0.44
1:A:615:THR:O	1:A:904:GLN:NE2	2.50	0.44
1:A:952:LYS:O	1:A:953:THR:OG1	2.23	0.44
1:A:480:CYS:O	1:A:481:MET:C	2.56	0.44
1:A:1027:ILE:HG22	1:A:1028:GLN:N	2.33	0.44
1:A:116:GLU:O	1:A:118:GLY:N	2.50	0.44
1:A:137:GLN:O	1:A:140:LEU:HB2	2.18	0.44
1:A:448:LYS:CG	1:A:449:ASN:ND2	2.79	0.44
1:A:501:CYS:O	1:A:505:PHE:HB2	2.18	0.44
1:A:1132:CYS:O	1:A:1133:SER:HB3	2.18	0.44
1:A:1133:SER:HB3	1:A:1144:THR:HA	2.00	0.44
1:A:228:ARG:HB3	1:A:228:ARG:CZ	2.46	0.44
1:A:643:LYS:HG3	1:A:650:LEU:HD11	2.00	0.44
1:A:721:ASN:HA	1:A:745:SER:OG	2.17	0.44
1:A:803:CYS:SG	1:A:846:CYS:O	2.76	0.44
1:A:1151:ILE:O	1:A:1151:ILE:HG12	2.17	0.43
1:A:127:VAL:HG23	1:A:127:VAL:O	2.18	0.43
1:A:136:ILE:HD13	1:A:152:ILE:HD13	2.00	0.43
1:A:373:GLU:OE1	1:A:380:LYS:NZ	2.50	0.43
1:A:672:ILE:O	1:A:684:TRP:HD1	2.00	0.43
1:A:692:VAL:O	1:A:692:VAL:HG12	2.17	0.43
1:A:888:VAL:O	1:A:888:VAL:HG13	2.17	0.43
1:A:1191:LYS:C	1:A:1205:VAL:HG13	2.39	0.43
1:A:1242:LEU:HD13	1:A:1244:ILE:HG13	2.00	0.43
1:A:415:LEU:O	1:A:419:VAL:HG23	2.18	0.43
1:A:727:LEU:HD21	1:A:758:LEU:HD12	2.00	0.43
1:A:706:HIS:ND1	1:A:750:ARG:HD3	2.33	0.43
1:A:869:ILE:O	1:A:870:ASP:OD1	2.35	0.43
1:A:562:ASN:HD21	1:A:564:VAL:HB	1.82	0.43
1:A:653:ILE:HG22	1:A:654:LYS:N	2.33	0.43
1:A:428:ARG:HG2	1:A:433:PHE:HE2	1.83	0.43
1:A:1023:GLU:C	1:A:1046:THR:HG23	2.39	0.43
1:A:1226:VAL:HG23	1:A:1226:VAL:O	2.17	0.43
1:A:158:CYS:SG	1:A:160:LYS:HD3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:VAL:O	1:A:1073:ILE:CB	2.67	0.43
1:A:1221:LEU:C	1:A:1222:LYS:HG3	2.39	0.43
1:A:604:LYS:HE2	1:A:606:LEU:HD13	2.00	0.43
1:A:986:LYS:HG2	1:A:998:SER:CB	2.46	0.43
1:A:1007:ARG:N	1:A:1007:ARG:NE	2.66	0.43
1:A:1110:LYS:HG2	1:A:1122:GLU:HG3	2.01	0.43
1:A:1183:ASP:O	1:A:1184:VAL:HG13	2.18	0.43
1:A:214:GLN:O	1:A:215:ARG:HB3	2.19	0.43
1:A:280:VAL:O	1:A:280:VAL:HG12	2.19	0.43
1:A:350:PHE:O	4:A:1255:HOH:O	2.21	0.43
1:A:652:ASP:O	1:A:652:ASP:OD1	2.36	0.43
1:A:641:VAL:HG21	1:A:672:ILE:CD1	2.48	0.43
1:A:736:ARG:O	1:A:737:ASN:CG	2.57	0.43
1:A:903:ASP:O	1:A:904:GLN:HG3	2.18	0.43
1:A:989:GLU:HG3	1:A:992:ASN:HB3	2.00	0.43
1:A:114:LEU:HD21	1:A:168:VAL:O	2.18	0.43
1:A:1227:SER:CB	1:A:1232:THR:HB	2.47	0.43
1:A:522:LEU:O	1:A:526:PHE:HD2	2.02	0.43
1:A:621:ALA:HA	1:A:631:ALA:O	2.18	0.43
1:A:714:LEU:C	1:A:714:LEU:HD23	2.37	0.43
1:A:695:TYR:HB3	1:A:728:TRP:CZ3	2.54	0.43
1:A:835:ILE:HD12	1:A:867:TRP:CD2	2.54	0.43
1:A:932:GLU:C	1:A:934:GLU:H	2.22	0.43
1:A:1061:TRP:N	1:A:1061:TRP:CD1	2.87	0.43
1:A:1083:CYS:O	1:A:1084:HIS:CD2	2.72	0.43
1:A:147:PRO:HB3	1:A:258:CYS:O	2.18	0.43
1:A:706:HIS:ND1	1:A:750:ARG:HA	2.33	0.43
1:A:743:THR:HB	1:A:764:ASP:HB2	2.00	0.43
1:A:1006:VAL:C	1:A:1007:ARG:HE	2.21	0.42
1:A:1202:TRP:N	1:A:1202:TRP:CD1	2.87	0.42
1:A:309:GLU:H	1:A:309:GLU:CD	2.21	0.42
1:A:553:HIS:CE1	1:A:554:LEU:HG	2.54	0.42
1:A:739:MET:HG2	1:A:770:TRP:NE1	2.34	0.42
1:A:1113:SER:OG	1:A:1116:LEU:HD13	2.19	0.42
1:A:131:LYS:HB2	1:A:131:LYS:HE2	1.83	0.42
1:A:137:GLN:HG2	1:A:173:LEU:CD2	2.49	0.42
1:A:187:ILE:HG22	1:A:188:GLY:O	2.19	0.42
1:A:541:CYS:O	1:A:544:PHE:N	2.52	0.42
1:A:581:LYS:HE2	1:A:1248:LEU:HD21	2.01	0.42
1:A:378:ASP:N	1:A:378:ASP:OD2	2.50	0.42
1:A:896:SER:CB	1:A:909:TRP:O	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:GLY:HA2	1:A:1006:VAL:CG2	2.50	0.42
1:A:107:THR:O	1:A:109:PHE:N	2.51	0.42
1:A:153:TYR:CD1	1:A:267:LYS:HB3	2.54	0.42
1:A:228:ARG:CG	1:A:256:ASN:HB3	2.44	0.42
1:A:149:TRP:CE2	1:A:273:VAL:HG21	2.54	0.42
1:A:333:ASP:O	1:A:334:PHE:CD1	2.72	0.42
1:A:630:ILE:HD12	1:A:642:PHE:CE2	2.53	0.42
1:A:865:GLU:OE1	1:A:874:LYS:HE2	2.20	0.42
1:A:924:GLN:NE2	1:A:1236:VAL:O	2.51	0.42
1:A:953:THR:O	1:A:955:GLN:HB2	2.20	0.42
1:A:1093:ILE:C	1:A:1095:SER:H	2.21	0.42
1:A:290:LYS:O	1:A:293:GLU:HB3	2.20	0.42
1:A:465:GLN:HE21	1:A:465:GLN:HB2	1.71	0.42
1:A:713:HIS:N	1:A:713:HIS:CD2	2.80	0.42
1:A:1029:VAL:HG21	1:A:1072:VAL:HG22	2.01	0.42
1:A:290:LYS:O	1:A:293:GLU:N	2.52	0.42
1:A:628:GLN:OE1	1:A:628:GLN:HA	2.19	0.42
1:A:978:PHE:CD2	1:A:978:PHE:O	2.72	0.42
1:A:1009:ILE:HG23	1:A:1009:ILE:O	2.19	0.42
1:A:1032:TRP:O	1:A:1033:GLN:CB	2.68	0.42
1:A:1123:LEU:HB3	1:A:1154:TRP:CZ3	2.55	0.42
1:A:1146:ASP:CG	1:A:1147:ASP:N	2.73	0.42
1:A:1233:TYR:HB2	1:A:1245:LEU:HB2	2.01	0.42
1:A:594:TYR:O	1:A:1248:LEU:HB2	2.20	0.42
1:A:670:SER:O	1:A:686:SER:HB3	2.20	0.42
1:A:682:LYS:HE2	1:A:694:THR:HG21	2.01	0.42
1:A:785:ARG:CZ	1:A:831:LEU:HD12	2.50	0.42
1:A:603:ILE:HA	1:A:920:ILE:HG13	2.01	0.42
1:A:1007:ARG:CD	1:A:1007:ARG:N	2.83	0.42
1:A:183:HIS:NE2	1:A:206:LEU:HD21	2.35	0.42
1:A:352:ARG:C	1:A:353:ILE:O	2.58	0.42
1:A:438:HIS:O	1:A:439:ASP:C	2.57	0.42
1:A:572:GLU:HA	1:A:577:TYR:CD1	2.54	0.42
1:A:888:VAL:HA	1:A:898:LEU:O	2.19	0.42
1:A:1044:GLN:HG2	1:A:1068:LYS:HZ3	1.83	0.42
1:A:1090:SER:HB2	1:A:1132:CYS:HA	2.02	0.42
1:A:1140:ILE:CA	1:A:1156:VAL:HB	2.50	0.42
1:A:386:LEU:HD23	1:A:386:LEU:N	2.35	0.42
1:A:215:ARG:NH1	1:A:557:ARG:HD3	2.34	0.42
1:A:586:GLN:O	1:A:587:GLU:CB	2.68	0.42
1:A:835:ILE:HG22	1:A:872:ARG:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:O	1:A:388:ILE:HG13	2.18	0.42
1:A:482:TYR:OH	1:A:490:HIS:NE2	2.34	0.42
1:A:1129:CYS:SG	1:A:1129:CYS:O	2.78	0.41
1:A:1131:ARG:NH1	1:A:1131:ARG:HG3	2.35	0.41
1:A:458:ARG:HG3	1:A:496:MET:HE1	2.01	0.41
1:A:492:ALA:C	1:A:494:ALA:N	2.73	0.41
1:A:506:SER:O	1:A:510:ILE:HG12	2.20	0.41
1:A:607:SER:HB3	1:A:909:TRP:CZ3	2.55	0.41
1:A:827:HIS:C	1:A:829:SER:N	2.73	0.41
1:A:941:ASP:CG	1:A:942:ASN:N	2.74	0.41
1:A:990:LEU:O	1:A:991:PRO:C	2.58	0.41
1:A:1071:ASN:OD1	1:A:1072:VAL:O	2.38	0.41
1:A:1089:LEU:O	1:A:1104:SER:O	2.38	0.41
1:A:228:ARG:HG2	1:A:232:LEU:CD1	2.49	0.41
1:A:289:GLU:OE1	1:A:303:LYS:HE2	2.20	0.41
1:A:464:PHE:CD1	1:A:487:LEU:HD13	2.54	0.41
1:A:972:HIS:O	1:A:973:LEU:HB2	2.20	0.41
1:A:1191:LYS:HA	1:A:1205:VAL:HG11	2.00	0.41
1:A:1237:ASP:C	1:A:1239:LEU:N	2.73	0.41
1:A:158:CYS:SG	1:A:160:LYS:CD	3.08	0.41
1:A:655:ALA:HA	1:A:684:TRP:CH2	2.55	0.41
1:A:945:GLY:N	1:A:958:TYR:OH	2.47	0.41
1:A:1003:LYS:H	1:A:1003:LYS:NZ	2.16	0.41
1:A:1042:ALA:HA	1:A:1070:TRP:HH2	1.85	0.41
1:A:424:LEU:O	1:A:425:PHE:CD2	2.73	0.41
1:A:786:PHE:N	1:A:786:PHE:CD2	2.87	0.41
1:A:130:LYS:HD3	1:A:131:LYS:HG3	2.02	0.41
1:A:207:ASP:C	1:A:209:GLU:N	2.73	0.41
1:A:1116:LEU:C	1:A:1118:SER:N	2.74	0.41
1:A:1132:CYS:O	1:A:1133:SER:CB	2.69	0.41
1:A:352:ARG:CZ	1:A:361:TYR:CE2	3.04	0.41
1:A:510:ILE:O	1:A:514:THR:HG23	2.20	0.41
1:A:582:LEU:O	1:A:584:ALA:N	2.54	0.41
1:A:918:SER:OG	1:A:920:ILE:CG2	2.66	0.41
1:A:1016:LYS:O	1:A:1017:THR:CB	2.68	0.41
1:A:1116:LEU:O	1:A:1118:SER:N	2.47	0.41
1:A:152:ILE:HD11	1:A:261:LEU:HD11	2.01	0.41
1:A:546:GLU:HA	1:A:612:ARG:HH12	1.85	0.41
1:A:849:SER:HB2	1:A:890:PHE:CE2	2.56	0.41
1:A:857:ILE:HG13	1:A:857:ILE:O	2.21	0.41
1:A:868:ASN:C	1:A:868:ASN:ND2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:LEU:O	1:A:1090:SER:O	2.39	0.41
1:A:430:GLY:C	1:A:432:SER:N	2.73	0.41
1:A:706:HIS:HD2	1:A:707:PHE:H	1.68	0.41
1:A:368:MET:O	1:A:372:VAL:HG23	2.21	0.41
1:A:396:PRO:O	1:A:398:LYS:N	2.54	0.41
1:A:677:ALA:C	1:A:679:LYS:H	2.23	0.41
1:A:945:GLY:HA3	1:A:959:LEU:O	2.20	0.41
1:A:1131:ARG:CG	1:A:1131:ARG:O	2.69	0.41
1:A:319:GLY:O	1:A:320:SER:C	2.60	0.41
1:A:353:ILE:O	1:A:354:ARG:C	2.59	0.41
1:A:521:HIS:O	1:A:524:HIS:N	2.53	0.41
1:A:825:ASP:OD1	1:A:828:THR:HG23	2.21	0.41
1:A:844:GLN:HG2	1:A:844:GLN:H	1.58	0.41
1:A:970:SER:O	1:A:973:LEU:N	2.53	0.41
1:A:1231:ARG:HG3	1:A:1247:VAL:HB	2.03	0.41
1:A:403:LEU:HG	1:A:460:MET:SD	2.61	0.41
1:A:601:LYS:HE3	1:A:601:LYS:HB2	1.81	0.41
1:A:611:VAL:HG12	1:A:613:PRO:HD3	2.03	0.41
1:A:1223:LYS:HD3	1:A:1225:HIS:CE1	2.56	0.40
1:A:337:ARG:O	1:A:338:TRP:C	2.59	0.40
1:A:482:TYR:C	1:A:482:TYR:CD1	2.94	0.40
1:A:458:ARG:NH1	1:A:496:MET:HE2	2.37	0.40
1:A:582:LEU:O	1:A:583:GLN:C	2.59	0.40
1:A:846:CYS:HA	1:A:857:ILE:HA	2.03	0.40
1:A:881:HIS:CE1	1:A:907:ARG:HG3	2.52	0.40
1:A:1044:GLN:CG	1:A:1068:LYS:HZ3	2.34	0.40
1:A:1146:ASP:CG	1:A:1147:ASP:H	2.25	0.40
1:A:302:LYS:O	1:A:303:LYS:CB	2.69	0.40
1:A:1061:TRP:HA	1:A:1066:THR:O	2.22	0.40
1:A:354:ARG:O	1:A:355:LYS:C	2.59	0.40
1:A:448:LYS:HZ3	1:A:449:ASN:ND2	2.18	0.40
1:A:726:LYS:HD3	1:A:728:TRP:CH2	2.56	0.40
1:A:869:ILE:CG2	1:A:870:ASP:N	2.85	0.40
1:A:1090:SER:CB	1:A:1132:CYS:HA	2.51	0.40
1:A:930:PHE:CE2	1:A:1227:SER:HA	2.56	0.40
1:A:218:LEU:HD22	1:A:518:GLY:HA2	2.04	0.40
1:A:286:LEU:HG	1:A:287:GLY:N	2.36	0.40
1:A:431:LYS:HZ3	1:A:431:LYS:HA	1.85	0.40
1:A:601:LYS:O	1:A:603:ILE:O	2.40	0.40
1:A:1069:VAL:CG2	1:A:1079:ARG:HB2	2.52	0.40
1:A:1076:ARG:NH1	1:A:1078:GLU:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HB	1:A:290:LYS:HD2	2.02	0.40
1:A:153:TYR:HA	1:A:264:THR:O	2.21	0.40
1:A:585:LYS:HD2	1:A:1249:GLU:OE1	2.22	0.40
1:A:584:ALA:C	1:A:586:GLN:N	2.75	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1127/1256 (90%)	765 (68%)	242 (22%)	120 (11%)	<b>0</b> <b>7</b>

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	VAL
1	A	174	LEU
1	A	177	CYS
1	A	253	ALA
1	A	337	ARG
1	A	359	TYR
1	A	362	GLU
1	A	397	THR
1	A	408	THR
1	A	533	LEU
1	A	587	GLU
1	A	655	ALA
1	A	693	HIS
1	A	755	ASP
1	A	797	VAL
1	A	803	CYS
1	A	839	HIS

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Mol	Chain	Res	Type
1	A	862	TYR
1	A	953	THR
1	A	954	GLY
1	A	972	HIS
1	A	1032	TRP
1	A	1044	GLN
1	A	1054	GLN
1	A	1073	ILE
1	A	1087	THR
1	A	1095	SER
1	A	1098	THR
1	A	1107	LYS
1	A	1129	CYS
1	A	1137	LEU
1	A	1139	GLY
1	A	1162	LEU
1	A	1168	ILE
1	A	1212	GLN
1	A	1213	THR
1	A	1214	PHE
1	A	1223	LYS
1	A	1238	ASN
1	A	117	GLY
1	A	130	LYS
1	A	142	LYS
1	A	244	ASP
1	A	302	LYS
1	A	355	LYS
1	A	386	LEU
1	A	480	CYS
1	A	603	ILE
1	A	606	LEU
1	A	880	GLY
1	A	884	TRP
1	A	933	ASN
1	A	952	LYS
1	A	1075	GLY
1	A	1090	SER
1	A	1114	PHE
1	A	1120	LEU
1	A	1133	SER
1	A	1247	VAL

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Mol	Chain	Res	Type
1	A	156	ALA
1	A	160	LYS
1	A	211	SER
1	A	226	ARG
1	A	228	ARG
1	A	233	ARG
1	A	283	GLU
1	A	307	PRO
1	A	448	LYS
1	A	605	ASN
1	A	617	ALA
1	A	785	ARG
1	A	842	THR
1	A	861	GLN
1	A	962	ALA
1	A	995	VAL
1	A	1015	GLY
1	A	1025	SER
1	A	1053	LEU
1	A	1063	PHE
1	A	1101	SER
1	A	1132	CYS
1	A	1182	THR
1	A	103	ASP
1	A	111	ARG
1	A	220	ILE
1	A	335	PRO
1	A	475	PRO
1	A	486	PHE
1	A	589	ASP
1	A	749	CYS
1	A	818	LYS
1	A	841	SER
1	A	847	ASP
1	A	955	GLN
1	A	961	GLU
1	A	1117	LEU
1	A	1180	TRP
1	A	1207	THR
1	A	213	SER
1	A	215	ARG
1	A	268	SER

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Mol	Chain	Res	Type
1	A	353	ILE
1	A	360	ASP
1	A	482	TYR
1	A	522	LEU
1	A	609	LEU
1	A	613	PRO
1	A	741	GLY
1	A	838	GLY
1	A	1007	ARG
1	A	1017	THR
1	A	1167	PRO
1	A	753	PRO
1	A	963	GLN
1	A	1047	VAL
1	A	1140	ILE
1	A	1185	CYS
1	A	519	PRO
1	A	964	VAL
1	A	945	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1005/1109 (91%)	911 (91%)	94 (9%)	8 37

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASP
1	A	130	LYS
1	A	131	LYS
1	A	153	TYR
1	A	177	CYS
1	A	196	LEU
1	A	209	GLU

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Mol	Chain	Res	Type
1	A	216	LEU
1	A	225	ASP
1	A	288	ARG
1	A	299	VAL
1	A	305	ASP
1	A	330	LEU
1	A	337	ARG
1	A	358	SER
1	A	366	GLU
1	A	402	VAL
1	A	403	LEU
1	A	429	ASN
1	A	431	LYS
1	A	436	TYR
1	A	461	VAL
1	A	489	TYR
1	A	507	LEU
1	A	516	LEU
1	A	522	LEU
1	A	532	ILE
1	A	548	LEU
1	A	551	ASN
1	A	602	THR
1	A	612	ARG
1	A	613	PRO
1	A	638	THR
1	A	688	THR
1	A	691	LEU
1	A	694	THR
1	A	703	ASN
1	A	705	CYS
1	A	713	HIS
1	A	723	PHE
1	A	725	LEU
1	A	751	PHE
1	A	752	SER
1	A	784	LYS
1	A	785	ARG
1	A	812	LYS
1	A	822	LEU
1	A	826	ILE
1	A	832	LEU

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Mol	Chain	Res	Type
1	A	842	THR
1	A	844	GLN
1	A	863	CYS
1	A	866	LEU
1	A	868	ASN
1	A	870	ASP
1	A	871	SER
1	A	879	ARG
1	A	902	ASP
1	A	904	GLN
1	A	922	LEU
1	A	938	LEU
1	A	942	ASN
1	A	946	LEU
1	A	948	LEU
1	A	956	ILE
1	A	963	GLN
1	A	967	CYS
1	A	974	GLU
1	A	980	ASP
1	A	992	ASN
1	A	1003	LYS
1	A	1007	ARG
1	A	1016	LYS
1	A	1024	ASP
1	A	1031	ASN
1	A	1041	GLN
1	A	1045	GLU
1	A	1051	ARG
1	A	1053	LEU
1	A	1061	TRP
1	A	1064	ASP
1	A	1071	ASN
1	A	1096	ASP
1	A	1107	LYS
1	A	1111	ILE
1	A	1112	TRP
1	A	1137	LEU
1	A	1151	ILE
1	A	1160	GLN
1	A	1185	CYS
1	A	1212	GLN

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Mol	Chain	Res	Type
1	A	1223	LYS
1	A	1242	LEU
1	A	1248	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	137	GLN
1	A	138	GLN
1	A	208	GLN
1	A	214	GLN
1	A	390	GLN
1	A	429	ASN
1	A	449	ASN
1	A	465	GLN
1	A	477	GLN
1	A	543	ASN
1	A	586	GLN
1	A	605	ASN
1	A	656	HIS
1	A	709	ASN
1	A	712	ASN
1	A	713	HIS
1	A	737	ASN
1	A	782	ASN
1	A	836	HIS
1	A	844	GLN
1	A	868	ASN
1	A	917	ASN
1	A	924	GLN
1	A	933	ASN
1	A	942	ASN
1	A	963	GLN
1	A	992	ASN
1	A	1002	HIS
1	A	1008	HIS
1	A	1031	ASN
1	A	1041	GLN
1	A	1071	ASN
1	A	1160	GLN
1	A	1163	HIS

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Mol	Chain	Res	Type
1	A	1177	HIS
1	A	1212	GLN
1	A	1217	ASN
1	A	1225	HIS

### 5.3.3 RNA [i](#)

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GBL	A	1252	-	6,6,6	0.69	0	7,7,7	0.77	0
3	GBL	A	1251	-	6,6,6	0.98	0	7,7,7	0.78	0
2	ADP	A	1250	-	24,29,29	1.44	3 (12%)	29,45,45	1.80	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GBL	A	1252	-	-	-	0/1/1/1
3	GBL	A	1251	-	-	-	0/1/1/1
2	ADP	A	1250	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1250	ADP	O4'-C1'	4.19	1.46	1.41
2	A	1250	ADP	PB-O3B	2.37	1.64	1.54
2	A	1250	ADP	C6-N6	2.04	1.41	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1250	ADP	PA-O3A-PB	-5.73	113.15	132.83
2	A	1250	ADP	N3-C2-N1	-4.48	121.67	128.68
2	A	1250	ADP	C3'-C2'-C1'	3.31	105.95	100.98
2	A	1250	ADP	C4-C5-N7	-2.35	106.95	109.40

There are no chirality outliers.

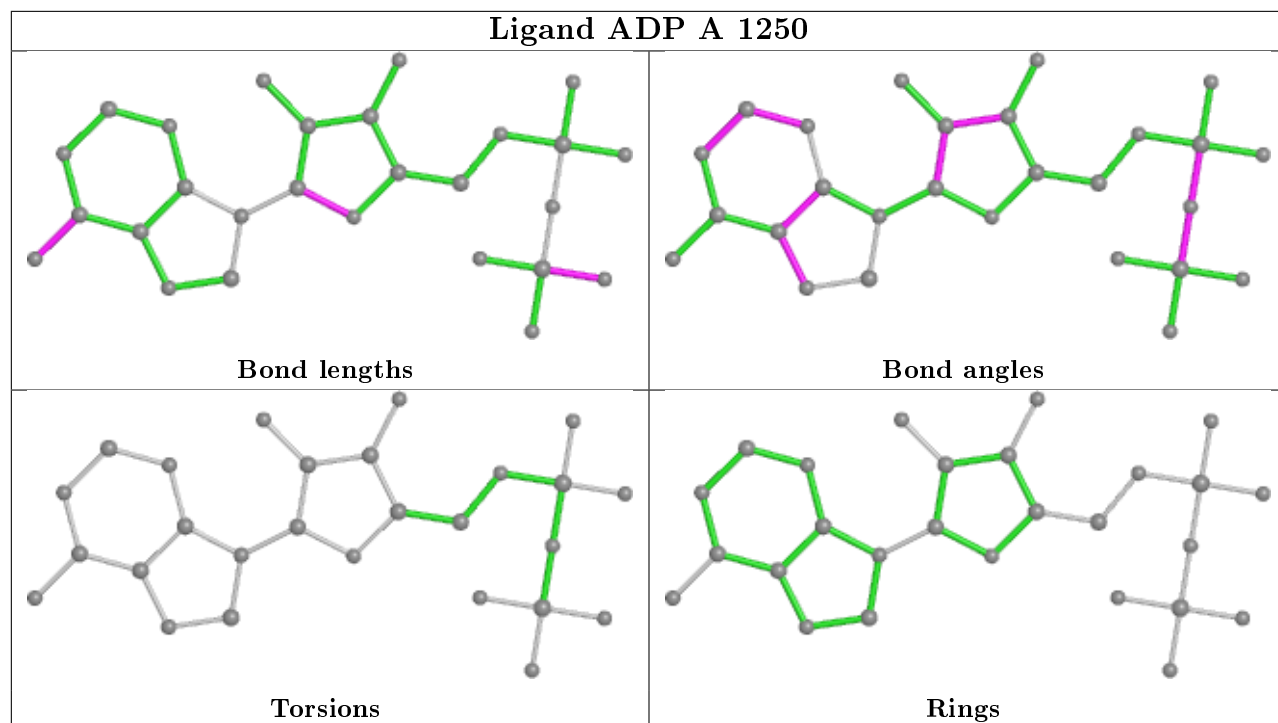
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1251	GBL	1	0
2	A	1250	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1133/1256 (90%)	-0.14	13 (1%) 80 67	74, 106, 140, 175	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ASP	5.2
1	A	102	THR	4.7
1	A	1124	LYS	4.3
1	A	1177	HIS	3.9
1	A	104	GLY	3.4
1	A	1122	GLU	2.7
1	A	1121	HIS	2.6
1	A	1178	GLY	2.5
1	A	151	THR	2.4
1	A	1153	ILE	2.4
1	A	1154	TRP	2.2
1	A	1144	THR	2.2
1	A	834	GLU	2.1

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

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

### 6.3 Carbohydrates [i](#)

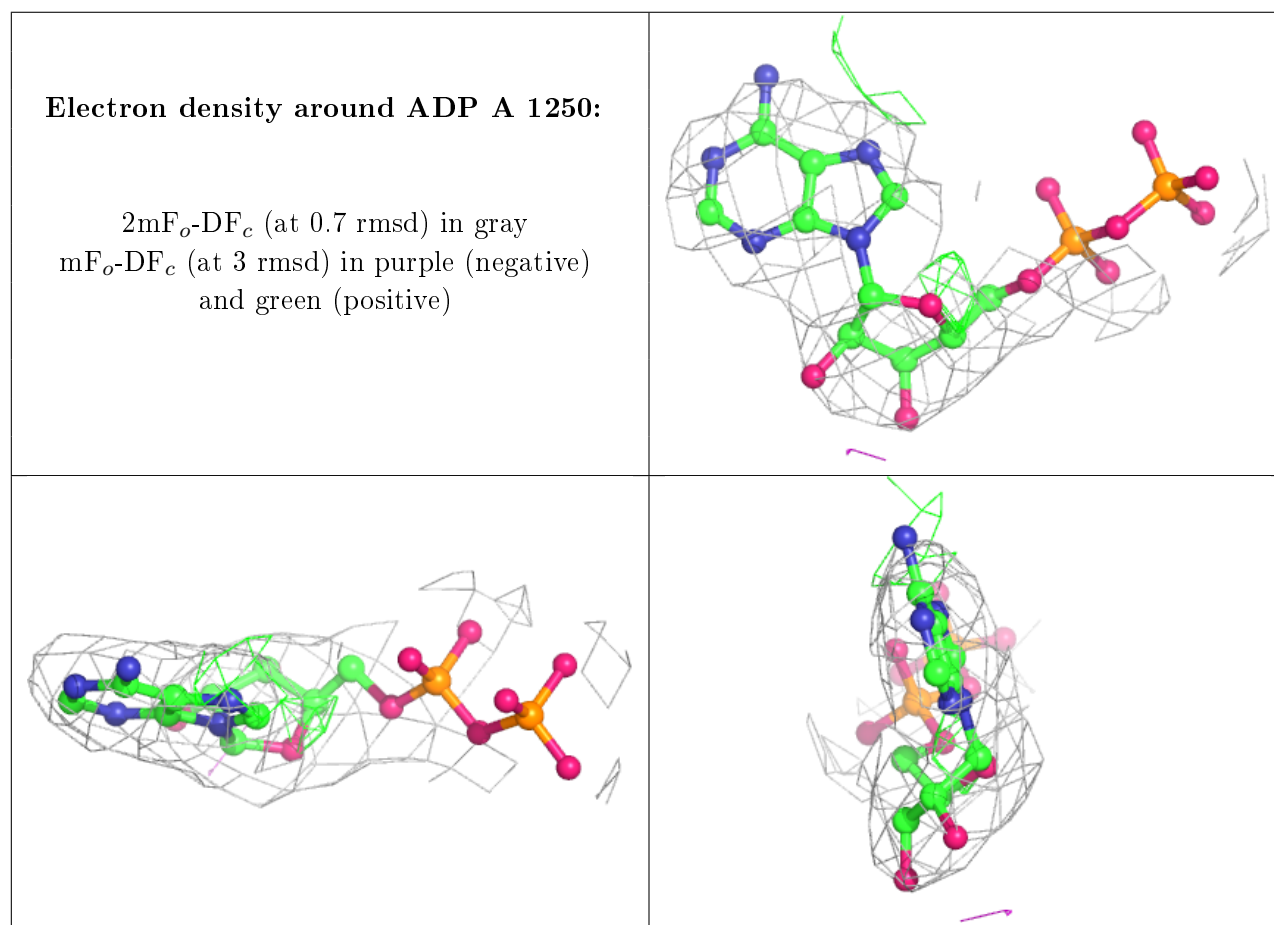
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GBL	A	1251	6/6	0.92	0.26	91,92,92,93	0
2	ADP	A	1250	27/27	0.94	0.21	81,86,90,90	0
3	GBL	A	1252	6/6	0.96	0.24	100,101,102,103	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.