



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:10 pm BST

PDB ID : 1R9S
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COM-
PLEX, MATCHED NUCLEOTIDE
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2003-10-30
Resolution : 4.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

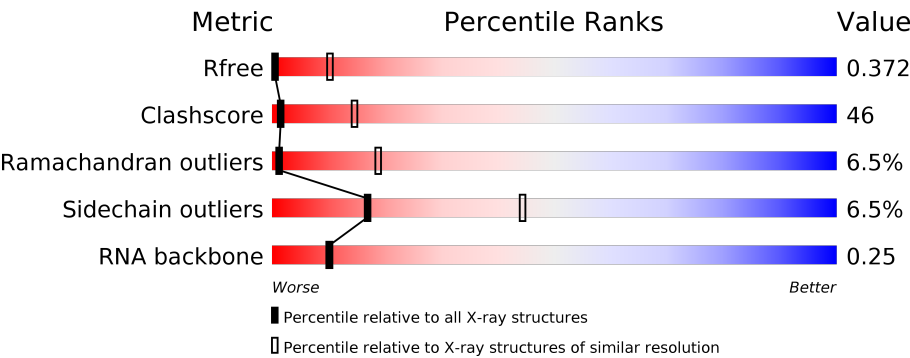
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.25 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	1017 (4.72-3.78)
Clashscore	141614	1059 (4.72-3.80)
Ramachandran outliers	138981	1014 (4.72-3.80)
Sidechain outliers	138945	1018 (4.72-3.78)
RNA backbone	3102	1057 (5.50-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	R	10	<div><div>50%</div><div>50%</div></div>
2	T	14	<div><div>21%</div><div>64%</div><div>14%</div></div>
3	A	1733	<div><div>31%</div><div>41%</div><div>7%</div><div>20%</div></div>
4	B	1224	<div><div>32%</div><div>51%</div><div>7%</div><div>10%</div></div>
5	C	318	<div><div>37%</div><div>40%</div><div>7%</div><div>16%</div></div>
6	E	215	<div><div>40%</div><div>56%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
7	F	155	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	UTP	R	3000	X	-	-	-
15	ZN	I	204	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28491 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 RNA chain called RNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 2 is a DNA chain called DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	14	Total	C	N	O	P	0	0	0
			279	135	48	83	13			

- Molecule 3 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1381	Total	C	N	O	S	0	0	0
			10857	6851	1899	2046	61			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

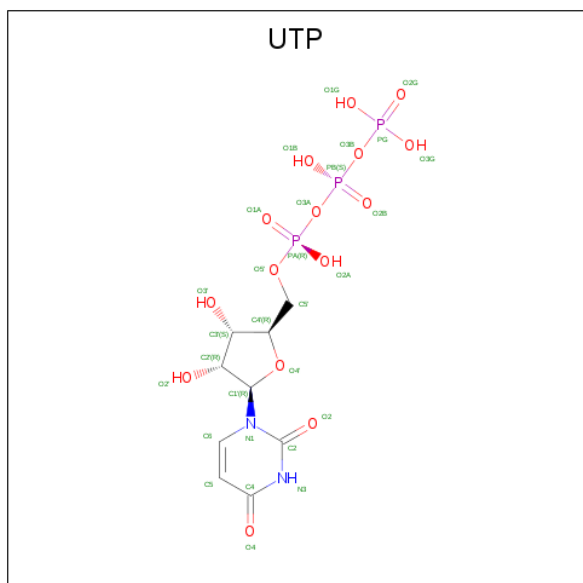
- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	R	1	Total	Mg	0	0
			1	1		
13	A	1	Total	Mg	0	0
			1	1		

- Molecule 14 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	R	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	1	Total	Zn	0	0
			1	1		
15	B	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	C	1	Total	Zn	0	0
			1	1		
15	A	2	Total	Zn	0	0
			2	2		
15	L	1	Total	Zn	0	0
			1	1		

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

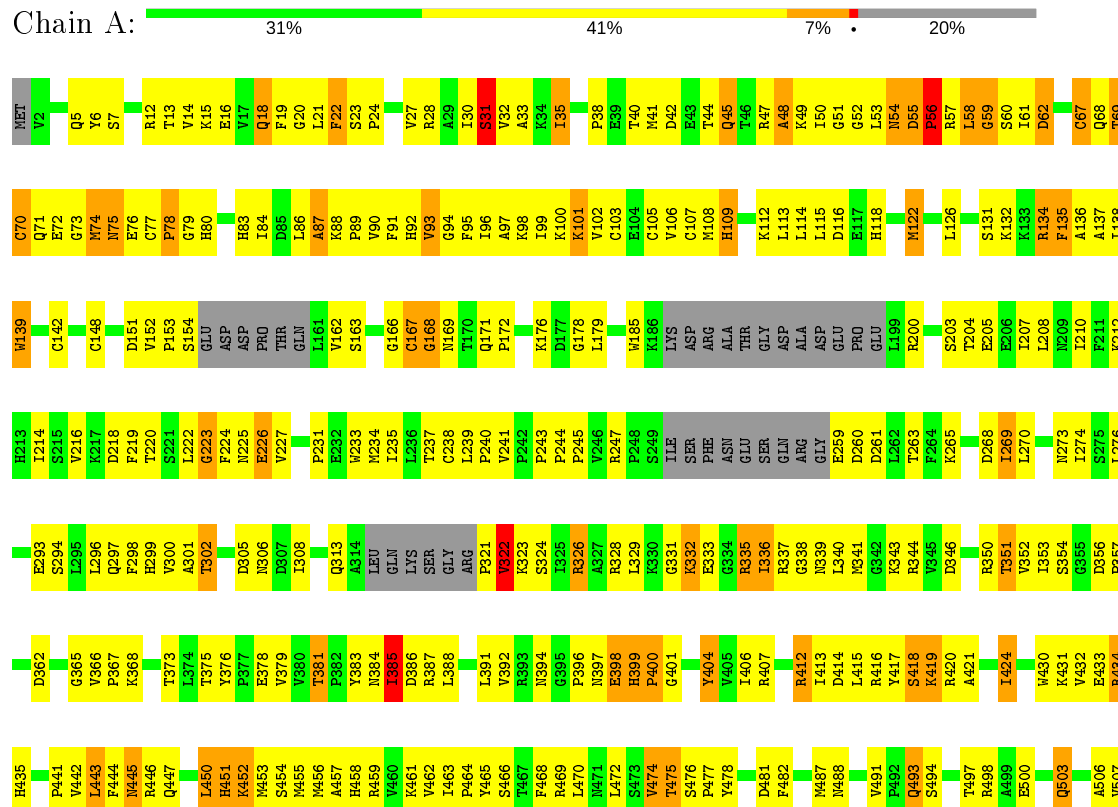
- Molecule 1: RNA strand



- Molecule 2: DNA strand



- Molecule 3: DNA-directed RNA polymerase II largest subunit



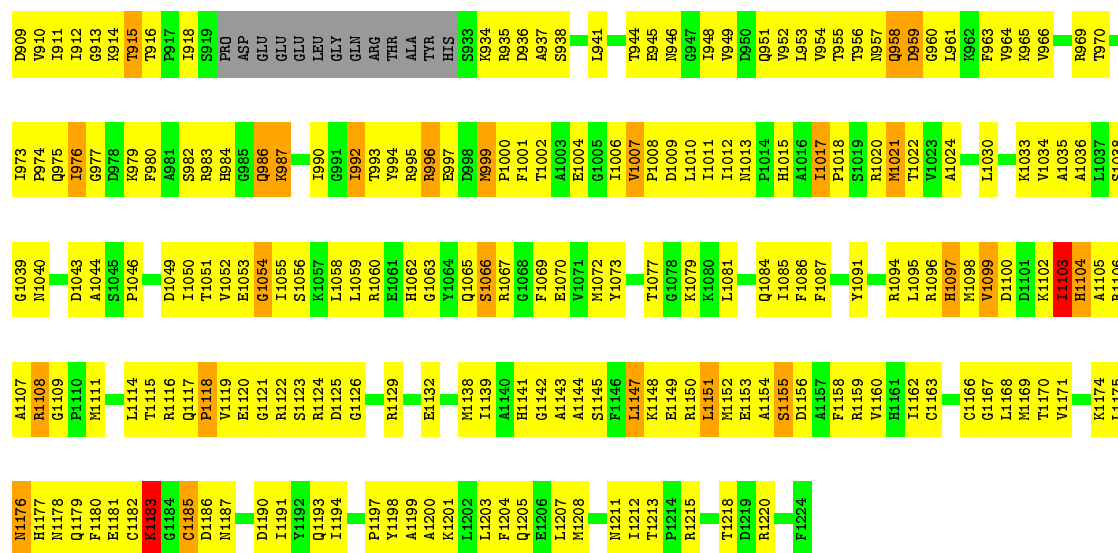
THR	GLY	G1439	T1376	G1310	I1237	E1168	V1098	R1030	N953	E879	F814	K651	S573	P508
SER	SER	A1440	T1377	V1311	I1238	I1169	P1099	Y1035	N954	K880	F815	V652	G574	
PRO	ASN	D1441	Q1378	M1312	I1239	Q1170	R1100	L1036	P955	R881	R816	V653	K575	I511
SER	ASP	F1442	G1379		C1240	Q1171	L1101	R1037	L956	L957	A817	N654	Q576	V512
TYR	ALA	V1443	G1380	E1315	L1241	L1172	K1102	T1038	N958	N736	G819	N737	I577	S513
SER	MET	M1444	L1381	V1316	V1242	H1173	E1103	L1039	N959	N738	G820	N739	L578	P514
PRO	ALA	T1445	T1382	M1317	V1243		I1104	K1039	N960	K738	G821	L657	S579	Q515
THR	GLY	ASP	S1383	T1318	ARG	L1176	L1105	Q1040	R961	D739	R822	L658	V560	S516
SER	GLY	GLU	V1384	T1319	PRO	LEU	L1106	A1041	R962	L740	E823	S663	N684	M517
PRO	PHE	GLU	T1385	P1320	LYS	ASP	N1107	F1042	R962	N741	G824	S664	K518	K518
SER	THR	GLU	R1386	G1321	SER	GLU	V1107	D1043	R963	N742	L824	S665	P519	P519
TYR	ALA	LEU	G1387	T1322	LEU	GLU	M1111	V1044	I964	V743	R825	G665	G520	G520
SER	TYR	VAL	H1388	D1323	ASP	ALA	K1112	V1045	Q965	K744	D826	I666	M521	M521
PRO	GLY	LYS	F1389	F1324	ALA	GLU	T1113	L1046	Q968	Q745	T827	G667	G522	G522
THR	GLY	THR	N1390	T1325	GLU	GLN	P1114	S1047	E894	I670	A828	I671	R590	I523
SER	ALA	MET	R1391	R1326	THR	SER	S1115	M1048	R896	S751	R829	A672	F591	V524
PRO	ASP	PRO	S1392	I1327	GLU	ASP	L1116	I1049	R896	K752	G830	D672	D592	Q525
SER	TYR	GLU	N1393	I1328	ASP	PHE	T1117	E1050	R897	G753	G831	G673	T595	L528
TYR	GLY	LYS	T1394	T1329	Q1187	Q1188	V1118	A1051	D874	S754	G832	G674	T596	G529
SER	GLU	LYS	G1395	M1330	S1189	S1189	E1121	Q1052	R975	F755	T834	T652	T597	C529
PRO	ALA	ILE	A1396	S1331	I1189	P1190	P1122	L1054	S979	I756	G835	I683	L597	I531
THR	THR	GLU	L1397	F1332	F1191	M1191			L981	N757	I837	N603	S599	R532
PRO	PRO	ILE	R1398	D1334	L1192	L1193	A1126	V1057	T982	I758	G838	A686	I608	K533
SER	PHE	GLU	K1399	K1261	L1193	L1193	D1127	V1058	T982	A759	R839	I679	I603	I634
TYR	GLY	ASP	S1401	K1262	R1194	R1194	Q1128	H1059	L983	Q760	R840	G694	T535	T535
SER	ALA	GLY	F1402	E1263	E1264		E1129	P1060	R984	I682	L841	M605	L597	L536
THR	GLY	GLN	E1403	E1267			P1122	F1053	L985	A763	L842	L606	R537	R537
GLY	GLY	ASP	A1404	M1268	M1269	M1202	A1126	V1066	Q994	C764	K843	I607	D638	D638
THR	GLY	GLY	T1405	L1268	E1270		D1127	G1065	L988	Q768	L845	V693	T539	T539
PRO	ALA	GLY	V1406	K1269	L1271		Q1128	V1066	L988	E771	E846	V690	I612	I641
SER	PRO	VAL	E1407	E1271	L1271		Q1128	G1065	L988	E771	E846	V690	I612	I641
TYR	THR	THR	I1408	E1272	L1272		I1138	G1066	L988	E771	E846	V690	I612	I641
SER	GLY	PRO	L1409	E1273	L1273		I1139	A1068	L988	E771	E846	V690	I612	I641
THR	GLY	TYR	F1410	E1274	L1274		H1140	A1069	L988	E771	E846	V690	I612	I641
SER	GLY	SER	A1411	E1275	L1275		T1141	A1070	L988	E771	E846	V690	I612	I641
PRO	GLY	GLU	A1412	E1276	L1276		H1141	A1071	L988	E771	E846	V690	I612	I641
GLY	VAL	SER	G1413	E1277	L1277		T1142	A1072	L988	E771	E846	V690	I612	I641
VAL	SER	SER	A1414	E1278	L1278		L1143	A1073	L988	E771	E846	V690	I612	I641
TYR	SER	LEU	S1415	E1279	L1279		T1144	A1074	L988	E771	E846	V690	I612	I641
SER	SER	LEU	A1416	E1280	L1280		T1145	A1075	L988	E771	E846	V690	I612	I641
PRO	PRO	VAL	A1417	E1281	L1281		T1146	A1076	L988	E771	E846	V690	I612	I641
GLY	GLY	ASN	L1418	E1282	L1282		T1147	A1077	L988	E771	E846	V690	I612	I641
SER	PHE	ALA	D1419	E1283	L1283		T1148	A1078	L988	E771	E846	V690	I612	I641
PRO	SER	ASP	D1420	E1284	L1284		T1149	A1079	L988	E771	E846	V690	I612	I641
SER	PRO	LEU	V1421	E1285	L1285		T1150	A1080	L988	E771	E846	V690	I612	I641
TYR	THR	ASP	G1422	E1286	L1286		T1151	A1081	L988	E771	E846	V690	I612	I641
SER	VAL	VAL	V1423	E1287	L1287		T1152	A1082	L988	E771	E846	V690	I612	I641
PRO	PRO	LYS	S1425	E1288	L1288		T1153	A1083	L988	E771	E846	V690	I612	I641
THR	THR	ASP	V1428	E1289	L1289		T1154	A1084	L988	E771	E846	V690	I612	I641
PRO	LEU	LEU	I1429	E1290	L1290		T1155	A1085	L988	E771	E846	V690	I612	I641
SER	PRO	MET	L1430	E1291	L1291		T1156	A1086	L988	E771	E846	V690	I612	I641
TYR	THR	PHE	G1431	E1292	L1292		T1157	A1087	L988	E771	E846	V690	I612	I641
SER	SER	SER	Q1432	E1293	L1293		T1158	A1088	L988	E771	E846	V690	I612	I641
PRO	PRO	PRO	P1435	E1294	L1294		T1159	A1089	L988	E771	E846	V690	I612	I641
THR	ALA	LEU	V1436	E1295	L1295		T1160	A1090	L988	E771	E846	V690	I612	I641
THR	TYR	VAL	G1437	E1296	L1296		T1161	A1091	L988	E771	E846	V690	I612	I641
PRO	SER	ASP	T1438	E1297	L1297		T1162	A1092	L988	E771	E846	V690	I612	I641
SER	PRO	SER	P1439	E1298	L1298		T1163	A1093	L988	E771	E846	V690	I612	I641
TYR	PRO	PRO	G1440	E1299	L1299		T1164	A1094	L988	E771	E846	V690	I612	I641
GLY	GLY	GLY	T1441	E1300	L1300		T1165	A1095	L988	E771	E846	V690	I612	I641
SER	GLY	GLY	V1442	E1301	L1301		T1166	A1096	L988	E771	E846	V690	I612	I641
PRO	PRO	PRO	P1443	E1302	L1302		T1167	A1097	L988	E771	E846	V690	I612	I641
THR	GLY	GLY	T1444	E1303	L1303		T1168	A1098	L988	E771	E846	V690	I612	I641
GLY	GLY	GLY	V1445	E1304	L1304		T1169	A1099	L988	E771	E846	V690	I612	I641
SER	GLY	GLY	ASP	E1305	L1305		T1170	A1100	L988	E771	E846	V690	I612	I641
THR	GLY	GLY	GLU	E1306	L1306		T1171	A1101	L988	E771	E846	V690	I612	I641
SER	PHE	GLU	T1385	E1307	L1307		T1172	A1102	L988	E771	E846	V690	I612	I641
PRO	THR	THR	R1386	E1308	L1308		T1173	A1103	L988	E771	E846	V690	I612	I641
SER	THR	THR	M1367	E1309	L1309		T1174	A1104	L988	E771	E846	V690	I612	I641
TYR	THR	THR	M1368	E1310	L1310		T1175	A1105	L988	E771	E846	V690	I612	I641
PRO	PRO	SER	A1369	E1311	L1311		T1176	A1106	L988	E771	E846	V690	I612	I641
PRO	PRO	PRO	V1372	E1312	L1312		T1177	A1107	L988	E771	E846	V690	I612	I641
THR	ALA	LEU	D1373	E1313	L1313		T1178	A1108	L988	E771	E846	V690	I612	I641
TYR	TYR	VAL	G1374	E1314	L1314		T1179	A1109	L988	E771	E846	V690	I612	I641
PRO	SER	ASP	T1308	E1315	L1315		T1180	A1110	L988	E771	E846	V690	I612	I641
SER	PRO	SER	M1375	E1316	L1316		T1181	A1111	L988	E771	E846	V690	I612	I641

[illegible]

- Molecule 4: DNA-directed RNA polymerase II 140 kDa polypeptide

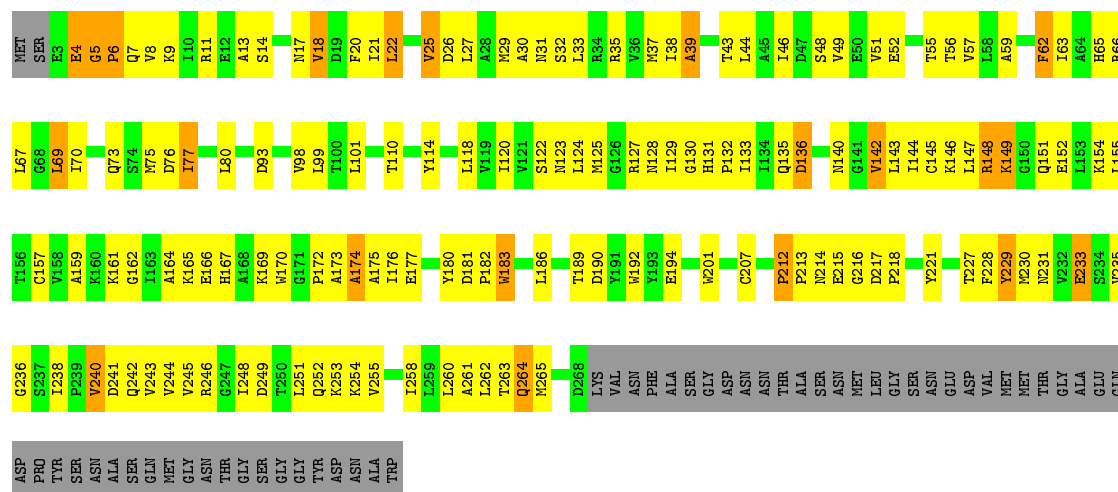
Chain B: 32% 51% 7% 10%

D837	P765	L702	V633	T556	L483	D407	ARG	T268	D198	K134	D66	MET
S838		I703	Y634	F557	M484	A408	ARG	I269	M199	ARG	I70	SER
M839	Q770	A704	R485	L558	R485	GLY	GLY	K270	G200	THR	LEU	ASP
I840		M705	P636	S559	Y487	G410	THR	A271	G201	Y202	GLU	LEU
M841	M773	Q706	L637	T637	Y488		ALA		G202	T487	GLU	ALA
M842		P707	F638	G562	S489	F417	LEU	P274	F203	GLU	GLN	ASN
Q843	Q776	E708	I639	M563		K418	GLY	Y275	I204	ALA	LEU	SER
E844	A777	D709	V640		I1E	T419	I1E	Y276	I204	ALA	ALA	GLU
S845	M778	L710	E641	L566	R496	L420	LVS	K277	G206	ASP	GLN	LVS
I846	G779	E711	D642	E567		F421	LVS	Q278	M207	VAL	HIS	TVR
D847	V760	P712	D643	E644	M499	K422	I345	D279	S208	PRO	THR	TVR
R848	F761	A715	E644	V570	T500	K423	K347	I280	E209	GLY	THR	ASP
G849	L762	ASN	G647	P571	P501		R348	P281	K210	ARG	THR	GLU
L850	M784	GLU	H648	H572	I502	K426	I349	I282	V211	GLU	SER	ASP
F851		GLU	Q573	Q573	GLY	D427	Q350	V283	L212	LEU	ASP	PRO
		ASN	K649	S574	ASP	I428	Y351	I284	L213	LVS	ASN	TVR
F855	V767	GLU	E650	P575	ASP	F429	A352	I285	A214	TVR	I1E	GLY
F856	R768	ASP	L651	D576	GLY	R430	A352	F286	Q215	GLU	SER	PHE
R857	M769	ASP	K652	A577	LVS	Y431	I355	R287	E216	LEU	ARG	GLU
S858	D790	D722	R653	T578	LEU	M432		A288	R217	I1E	LVS	D20
R859	R791	V723	R654	V580	A509		K358		R217	ALA	TVR	E21
M860	M792			R589	E510	T435	E359	I291	M221	GLU	GLY	S22
D861	A793	A726	I658	F581	P511	V436	F360	I292	I90	GLU	GLY	A23
		R727	A589	V582	R512	E437	L361	P293	V225	SER	S91	P24
K864	L795	GLU	N660	N583	Q513	GLU	P362	D294	F226	GLU	F92	I25
K865			G584	G584	L514	ALA	H363	K227	G93	ASP	T26	T26
R866	V797	V731	A663	V585	H515	HIS	I364	E296	K228	ASP	ASP	A27
T871	V798	S732	T664	V586	N516	ASP	T365	I297	A229	SER	Y96	E28
E872	P799	H733	E665	H587	T517	PHE	Q366	L298	A230	GLU	V97	D29
Q800	H734	H734	V666	G588	H518	ASN	L367	E299	P231	SER	T98	S30
R801	A735	A735	Q667	H589	M519	MET	E368	H300	P232	GLY	R99	X31
F874	P802	T736	D668	H590	G520	LVS	G369		P233	K164	P100	
R875	L803	T737	I1E	L521	L521	L446	F370	I234	P234	M101	V102	I34
K876		F738	GLU	R601	V522	A447	E371	D304	S235	S335	S35	S35
R877	T805	T739	GLY	T602	L603		S372	D307	H236	G168	I167	A36
Q878	T806	H740	GLY	L603	A525	A450	R373	X308	V237	R169	F37	F37
R879	R807	E742	PHE	R604	E526			Q309	A238	L170	S405	F38
T880	A808	E742	ASP	R605	T527	L457	F376	M310	E239	P171	D106	R39
N881	M809	I743	GLU				F377	L311	I240	I172	G107	F39
L882		H744	VAL	I609	G530	L461	L378	E312	M173	M173	T109	L43
L883	L812	P745	GLU		Q531	A462	G379	X313	S242	L174		
R884	K813	S746	E678	E612	Q531	T463	X380	L314	A243	R175	L112	Q46
	F814	M747	V679	V613	L535	G464	S381	K315	L244			Q47
	R815	I748	T680	S614	V536	N465	I382	P316		M178	P114	
	L815	L749	M615	W466	K537	W466	N383	C317	G247	C179	Q115	S50
Q821	Q821	G750	S682	I616	N538	G467	R384	V318	S248	Y180	F51	F51
N822	N822	V751	S683	L539	L539	GLU	I385	E319	R249	L181	R118	N52
E823	E823	A752		I619		GLN	L386	D320	F250		L119	Q53
						LVS	L387	G321	R120		L121	Q54
L824	L824	A753	M686	K622	M642	LVS	C388	F322	T253		N121	V55
G825	G825	E754	E687	E623	I545	LVS	A389	V323		D188	L122	D66
A826	A826	I755	R688	R622	I545	ALA		L122	V256	L189	T123	T58
I827	I827	I756	L689	L624	S546	MET		T123	K257	Y190	I124	T58
		P757	V657	K625	V647	SER		I124			S125	L59
		F758	E648	I626	G548	SER	R392			X491		Q60
X830	X830	F758	T549	T627	T549	ARG	K393	T329	G260	L192	S126	D61
S831	S831	F759	I692	F627	M552		D394	A330	R261	K193	G127	I62
G832	G832	D760	I693	T628	M552		D396	L331	E262	E194	L128	I62
N833	N833	H761	D629	A630	G478			F332	G263	C195	F129	I63
S906	S906	T762	R635	A630	V479			F333				I63
G907	G907	Q763	G631	I554	S480		R405	I334		X496	V130	G54
			I554	I554			L406	G325			D431	R55



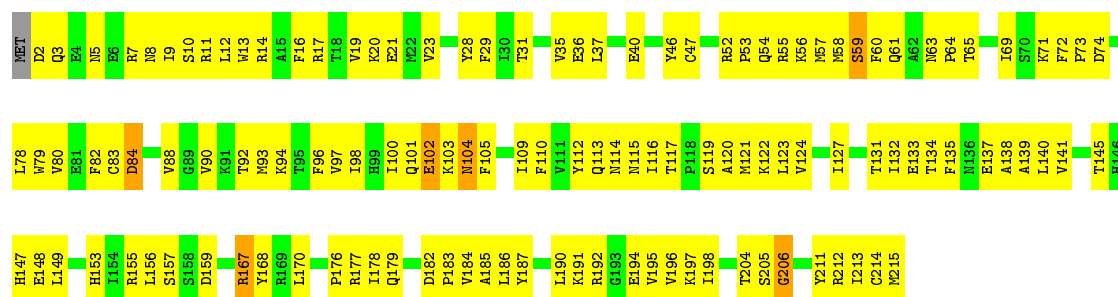
• Molecule 5: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 37% 40% 7% 16%



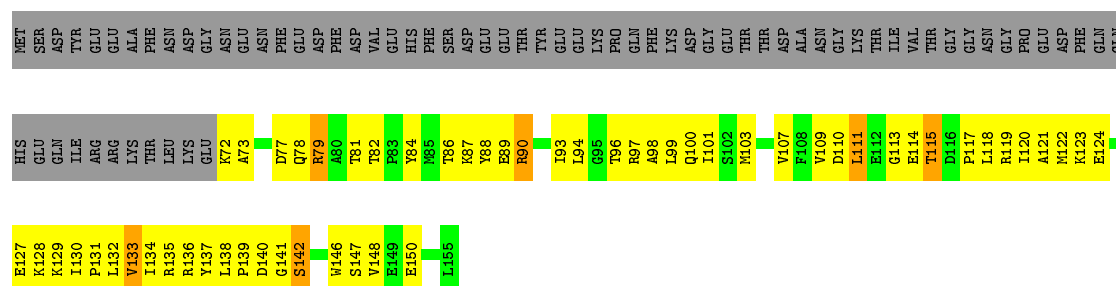
• Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E: 40% 56%



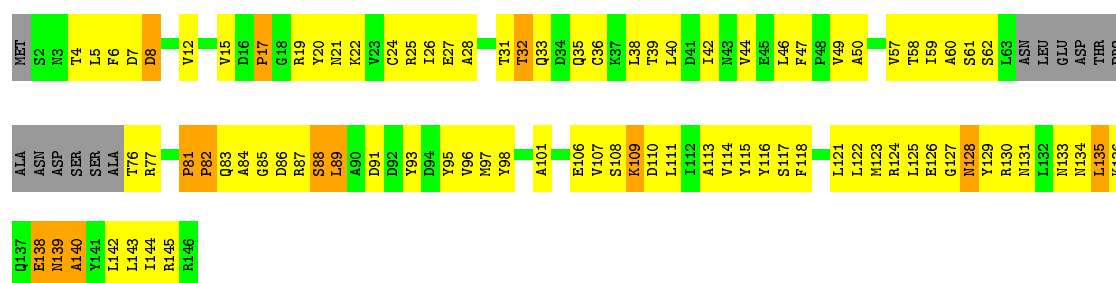
• Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F: 



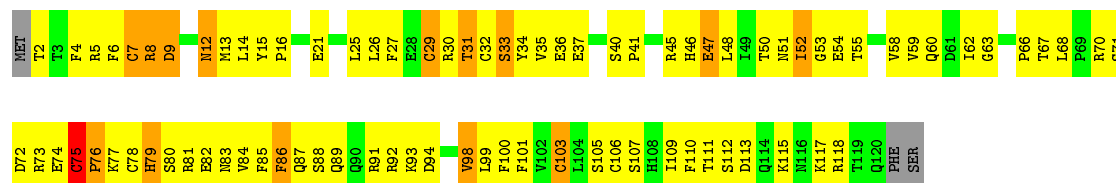
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H: 



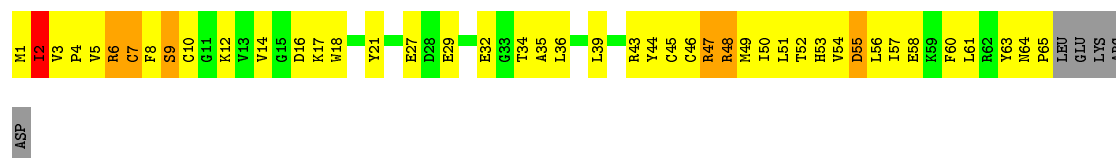
- Molecule 9: DNA-directed RNA polymerase II 14.2 kDa polypeptide

Chain I: 



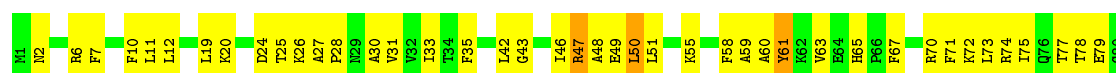
- Molecule 10: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J: 



- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.65Å 222.34Å 194.32Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	40.00 – 4.25 39.94 – 4.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.00-4.25) 84.6 (39.94-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.13Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.349 , 0.398 0.319 , 0.372	Depositor DCC
R_{free} test set	5207 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	96.8	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 104.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	28491	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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

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	R	3.97	33/244 (13.5%)	3.92	44/380 (11.6%)
2	T	4.38	37/311 (11.9%)	3.99	55/477 (11.5%)
3	A	0.41	0/11048	0.71	5/14936 (0.0%)
4	B	0.46	0/8890	0.72	1/11990 (0.0%)
5	C	0.48	0/2133	0.76	2/2891 (0.1%)
6	E	0.36	0/1788	0.65	0/2406
7	F	0.40	0/691	0.64	0/933
8	H	0.40	0/1086	0.73	0/1470
9	I	0.48	0/989	0.76	1/1331 (0.1%)
10	J	0.53	0/541	0.78	0/727
11	K	0.46	0/937	0.68	0/1265
12	L	0.48	0/365	0.78	0/485
All	All	0.72	70/29023 (0.2%)	0.92	108/39291 (0.3%)

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	R	0	1
2	T	1	2
All	All	1	3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	3	DG	O3'-P	-35.59	1.18	1.61
2	T	4	DA	O3'-P	-30.26	1.24	1.61
1	R	10	A	P-OP1	-23.82	1.08	1.49
1	R	5	A	O3'-P	-22.75	1.33	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	3	DG	C3'-O3'	-20.45	1.17	1.44
1	R	10	A	P-O5'	18.42	1.78	1.59
2	T	7	DC	O3'-P	-17.97	1.39	1.61
2	T	7	DC	O5'-C5'	14.34	1.78	1.42
1	R	5	A	P-O5'	13.14	1.72	1.59
2	T	2	DC	C3'-O3'	13.04	1.60	1.44
1	R	7	A	C5'-C4'	-12.56	1.36	1.51
1	R	4	G	P-OP1	12.19	1.69	1.49
1	R	1	A	O3'-P	-11.94	1.46	1.61
2	T	9	DC	C4'-O4'	-11.93	1.33	1.45
2	T	6	DC	C3'-O3'	-11.70	1.28	1.44
2	T	3	DG	P-OP1	11.43	1.68	1.49
1	R	8	G	C3'-O3'	11.15	1.57	1.42
2	T	8	DT	P-OP2	11.14	1.67	1.49
1	R	10	A	C5'-C4'	-11.06	1.38	1.51
1	R	4	G	O3'-P	10.78	1.74	1.61
1	R	9	G	O3'-P	10.10	1.73	1.61
2	T	9	DC	C3'-O3'	-9.95	1.31	1.44
2	T	9	DC	C4'-C3'	-9.74	1.42	1.52
1	R	4	G	C3'-O3'	9.40	1.55	1.42
2	T	9	DC	N1-C2	-9.31	1.30	1.40
1	R	6	G	P-OP2	9.08	1.64	1.49
1	R	2	U	P-OP2	8.68	1.63	1.49
2	T	7	DC	C3'-O3'	-8.68	1.32	1.44
2	T	9	DC	P-O5'	8.46	1.68	1.59
2	T	9	DC	O3'-P	-7.94	1.51	1.61
2	T	7	DC	C3'-C2'	-7.88	1.42	1.52
2	T	5	DT	C3'-O3'	-7.87	1.33	1.44
2	T	7	DC	P-O5'	7.87	1.67	1.59
1	R	10	A	P-OP2	-7.69	1.35	1.49
2	T	4	DA	P-O5'	-7.69	1.52	1.59
1	R	2	U	C3'-O3'	-7.51	1.31	1.42
2	T	1	DA	C3'-O3'	7.48	1.53	1.44
2	T	10	DT	P-OP1	-6.76	1.37	1.49
1	R	9	G	C4'-C3'	-6.73	1.45	1.53
1	R	3	C	C3'-O3'	6.64	1.51	1.42
2	T	3	DG	C4'-C3'	-6.41	1.46	1.52
2	T	7	DC	N1-C2	-6.37	1.33	1.40
1	R	9	G	P-OP1	-6.30	1.38	1.49
1	R	1	A	C3'-O3'	6.26	1.50	1.42
2	T	11	DC	N1-C6	6.25	1.40	1.37
2	T	5	DT	P-OP2	6.13	1.59	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	7	A	P-O5'	-5.96	1.53	1.59
2	T	11	DC	N1-C2	-5.86	1.34	1.40
2	T	5	DT	O3'-P	5.80	1.68	1.61
2	T	6	DC	C4'-C3'	-5.79	1.46	1.52
2	T	5	DT	C4'-C3'	-5.79	1.46	1.52
1	R	6	G	N9-C4	5.78	1.42	1.38
1	R	7	A	O3'-P	-5.69	1.54	1.61
2	T	13	DA	C3'-O3'	-5.66	1.36	1.44
2	T	7	DC	C2'-C1'	-5.58	1.46	1.52
1	R	4	G	C3'-C2'	-5.54	1.46	1.52
1	R	6	G	C5-C4	5.45	1.42	1.38
1	R	8	G	O3'-P	-5.45	1.54	1.61
2	T	9	DC	C2-N3	-5.37	1.31	1.35
2	T	9	DC	N1-C6	5.33	1.40	1.37
2	T	4	DA	C3'-O3'	-5.27	1.37	1.44
1	R	5	A	C3'-O3'	5.25	1.49	1.42
1	R	6	G	O3'-P	-5.25	1.54	1.61
1	R	9	G	C3'-O3'	-5.24	1.34	1.42
2	T	11	DC	C5-C6	5.22	1.38	1.34
1	R	9	G	C5'-C4'	5.20	1.57	1.51
1	R	8	G	P-OP1	-5.19	1.40	1.49
2	T	9	DC	C2'-C1'	-5.13	1.47	1.52
1	R	6	G	O4'-C1'	5.06	1.48	1.41
1	R	6	G	C8-N7	5.05	1.33	1.30

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	3	DG	O3'-P-O5'	-28.04	50.72	104.00
1	R	9	G	P-O3'-C3'	28.01	153.31	119.70
1	R	4	G	OP2-P-O3'	-25.63	48.80	105.20
2	T	3	DG	P-O3'-C3'	-25.44	89.17	119.70
2	T	7	DC	O5'-P-OP1	25.27	141.02	110.70
2	T	6	DC	OP1-P-O3'	-22.05	56.68	105.20
2	T	13	DA	OP1-P-O3'	-21.51	57.88	105.20
1	R	8	G	OP1-P-O3'	-16.21	69.53	105.20
1	R	3	C	O3'-P-O5'	-15.99	73.63	104.00
2	T	7	DC	O4'-C4'-C3'	-14.92	97.05	106.00
1	R	8	G	OP2-P-O3'	14.83	137.82	105.20
1	R	4	G	O3'-P-O5'	13.83	130.28	104.00
1	R	3	C	OP1-P-O3'	13.81	135.59	105.20
2	T	7	DC	C4'-C3'-C2'	13.53	115.28	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	7	DC	C5'-C4'-C3'	13.28	138.00	114.10
2	T	6	DC	OP2-P-O3'	12.92	133.62	105.20
2	T	13	DA	OP2-P-O3'	12.62	132.96	105.20
1	R	4	G	O5'-P-OP1	-12.45	94.49	105.70
1	R	6	G	OP1-P-OP2	-12.30	101.14	119.60
2	T	3	DG	C4'-C3'-C2'	11.85	113.76	103.10
2	T	9	DC	C4'-C3'-O3'	11.67	138.88	109.70
1	R	9	G	O5'-P-OP1	11.23	124.18	110.70
2	T	9	DC	O5'-P-OP2	-10.82	95.96	105.70
1	R	4	G	P-O3'-C3'	10.69	132.53	119.70
1	R	7	A	O5'-P-OP2	-10.66	96.11	105.70
2	T	3	DG	O4'-C4'-C3'	-10.54	99.68	106.00
2	T	7	DC	C4'-C3'-O3'	10.46	135.85	109.70
2	T	3	DG	O5'-P-OP1	-9.93	96.76	105.70
2	T	9	DC	O5'-P-OP1	9.92	122.61	110.70
1	R	1	A	C2'-C3'-O3'	9.87	131.21	109.50
1	R	9	G	OP1-P-O3'	9.77	126.69	105.20
1	R	5	A	O5'-P-OP2	-9.66	97.00	105.70
1	R	7	A	P-O5'-C5'	-9.38	105.88	120.90
1	R	10	A	O5'-P-OP1	-9.38	97.26	105.70
1	R	5	A	C5'-C4'-C3'	9.34	130.95	116.00
1	R	9	G	O3'-P-O5'	-9.22	86.48	104.00
1	R	4	G	OP1-P-O3'	9.12	125.26	105.20
1	R	5	A	C2'-C3'-O3'	9.01	129.31	109.50
1	R	5	A	OP2-P-O3'	8.82	124.61	105.20
2	T	9	DC	O4'-C1'-N1	8.76	114.13	108.00
1	R	9	G	OP1-P-OP2	-8.66	106.61	119.60
1	R	10	A	O5'-P-OP2	8.35	120.72	110.70
1	R	2	U	OP1-P-OP2	-8.30	107.15	119.60
1	R	1	A	OP2-P-O3'	8.22	123.30	105.20
2	T	2	DC	OP1-P-O3'	8.21	123.27	105.20
2	T	3	DG	OP1-P-OP2	-8.19	107.32	119.60
1	R	10	A	C5'-C4'-C3'	8.09	128.95	116.00
2	T	11	DC	O4'-C1'-N1	8.09	113.66	108.00
1	R	10	A	O5'-C5'-C4'	-8.00	96.51	111.70
2	T	5	DT	O5'-P-OP1	7.97	120.27	110.70
1	R	5	A	OP1-P-O3'	7.96	122.72	105.20
2	T	5	DT	OP1-P-OP2	-7.89	107.76	119.60
2	T	9	DC	C4'-C3'-C2'	7.82	110.14	103.10
1	R	6	G	O5'-P-OP2	-7.79	98.69	105.70
1	R	2	U	O5'-P-OP2	-7.61	98.85	105.70
2	T	9	DC	C2-N1-C1'	-7.46	110.60	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4	DA	OP1-P-O3'	-7.42	88.88	105.20
2	T	8	DT	O5'-P-OP2	-7.35	99.09	105.70
2	T	9	DC	C5'-C4'-O4'	7.04	122.67	109.30
2	T	11	DC	O4'-C1'-C2'	6.99	111.50	105.90
2	T	6	DC	C4'-C3'-O3'	6.90	126.96	109.70
1	R	10	A	OP1-P-OP2	-6.90	109.25	119.60
2	T	7	DC	OP2-P-O3'	6.86	120.30	105.20
2	T	6	DC	O4'-C4'-C3'	-6.79	101.78	104.50
2	T	10	DT	C6-N1-C1'	6.79	130.58	120.40
2	T	7	DC	O4'-C1'-C2'	6.73	111.28	105.90
1	R	6	G	C5'-C4'-O4'	6.73	117.17	109.10
2	T	5	DT	OP2-P-O3'	-6.70	90.47	105.20
1	R	1	A	P-O3'-C3'	6.58	127.59	119.70
2	T	3	DG	OP1-P-O3'	6.52	119.54	105.20
1	R	6	G	P-O5'-C5'	-6.47	110.54	120.90
2	T	6	DC	C4'-C3'-C2'	6.37	108.83	103.10
3	A	1392	SER	N-CA-C	6.30	128.02	111.00
1	R	7	A	C4'-C3'-O3'	6.29	125.58	113.00
2	T	8	DT	O5'-P-OP1	6.21	118.16	110.70
2	T	9	DC	N1-C2-O2	-6.21	115.18	118.90
1	R	9	G	O5'-P-OP2	6.19	118.13	110.70
5	C	39	ALA	N-CA-C	6.05	127.34	111.00
2	T	10	DT	C2-N1-C1'	-5.96	108.66	118.20
1	R	10	A	N9-C1'-C2'	5.91	121.68	114.00
1	R	6	G	N3-C4-N9	5.86	129.52	126.00
2	T	8	DT	O3'-P-O5'	-5.85	92.89	104.00
1	R	5	A	P-O3'-C3'	5.83	126.70	119.70
3	A	398	GLU	N-CA-C	-5.78	95.41	111.00
1	R	4	G	OP1-P-OP2	-5.75	110.98	119.60
1	R	6	G	OP1-P-O3'	5.74	117.82	105.20
1	R	10	A	P-O5'-C5'	5.72	130.05	120.90
2	T	5	DT	P-O5'-C5'	-5.72	111.75	120.90
5	C	183	TRP	N-CA-C	-5.62	95.84	111.00
2	T	3	DG	C4'-C3'-O3'	5.61	123.71	109.70
2	T	10	DT	O4'-C1'-N1	5.60	111.92	108.00
1	R	1	A	OP1-P-O3'	5.60	117.52	105.20
2	T	13	DA	O3'-P-O5'	5.53	114.50	104.00
2	T	7	DC	N1-C2-O2	-5.48	115.61	118.90
2	T	9	DC	C6-N1-C1'	5.48	127.37	120.80
2	T	3	DG	OP2-P-O3'	5.37	117.01	105.20
2	T	14	DT	N1-C1'-C2'	5.34	122.75	112.60
4	B	647	GLY	N-CA-C	5.22	126.15	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	2	DC	OP1-P-OP2	-5.21	111.79	119.60
3	A	750	GLY	N-CA-C	-5.21	100.08	113.10
2	T	8	DT	OP1-P-OP2	-5.20	111.80	119.60
3	A	1403	GLU	N-CA-C	5.20	125.05	111.00
2	T	9	DC	C5-C6-N1	-5.16	118.42	121.00
9	I	75	CYS	N-CA-C	-5.16	97.06	111.00
2	T	7	DC	C1'-O4'-C4'	5.08	115.18	110.10
3	A	452	LYS	N-CA-C	-5.07	97.32	111.00
2	T	1	DA	OP1-P-O3'	5.05	116.31	105.20
2	T	4	DA	C4'-C3'-C2'	5.03	107.63	103.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	7	DC	C3'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	10	A	Sidechain
2	T	7	DC	Sidechain
2	T	9	DC	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	217	0	110	48	0
2	T	279	0	160	69	0
3	A	10857	0	10959	1037	18
4	B	8720	0	8746	901	13
5	C	2095	0	2052	164	0
6	E	1752	0	1776	133	0
7	F	679	0	701	67	0
8	H	1068	0	1040	134	0
9	I	971	0	933	105	59
10	J	532	0	544	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	919	0	929	85	0
12	L	363	0	388	55	0
13	A	1	0	0	0	0
13	R	1	0	0	0	0
14	R	29	0	8	8	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	2	0
15	J	1	0	0	1	0
15	L	1	0	0	0	0
All	All	28491	0	28346	2619	59

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 46.

All (2619) 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:R:10:A:OP1	1:R:10:A:P	1.08	1.47
2:T:6:DC:H2''	2:T:7:DC:C5'	1.54	1.36
2:T:7:DC:C5'	2:T:7:DC:O5'	1.78	1.30
3:A:567:LYS:HB2	3:A:568:PRO:HD2	1.18	1.17
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.15
2:T:6:DC:C2'	2:T:7:DC:H5'	1.75	1.15
4:B:345:LYS:HA	4:B:348:ARG:HE	1.11	1.15
3:A:666:ILE:HD11	4:B:1030:LEU:HD13	1.27	1.12
12:L:60:ARG:HG3	12:L:61:THR:H	1.05	1.12
3:A:1329:THR:HG22	3:A:1331:SER:H	1.16	1.11
3:A:855:THR:HG21	3:A:857:ARG:HE	1.12	1.11
6:E:124:VAL:HG13	6:E:132:ILE:HB	1.33	1.10
4:B:1051:THR:HG22	4:B:1053:GLU:H	1.00	1.09
3:A:1364:ASN:ND2	3:A:1366:ARG:HG2	1.65	1.09
4:B:570:VAL:HB	4:B:573:GLN:HB3	1.36	1.08
1:R:8:G:O2'	1:R:9:G:H5'	1.55	1.06
4:B:512:ARG:HH21	4:B:535:LEU:HD11	1.17	1.06
3:A:1161:THR:HG22	3:A:1163:ILE:H	1.18	1.06
3:A:704:ALA:HB2	3:A:710:LEU:HG	1.34	1.06
2:T:1:DA:H2''	2:T:2:DC:O5'	1.46	1.05
2:T:1:DA:C2	2:T:2:DC:H5	1.74	1.05
4:B:708:GLU:HG3	4:B:709:ASP:H	1.17	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:287:ARG:HG2	4:B:292:ILE:HA	1.38	1.04
3:A:93:VAL:HG13	3:A:301:ALA:HB1	1.33	1.03
5:C:80:LEU:HD22	5:C:129:ILE:HD11	1.41	1.03
4:B:1159:ARG:HE	4:B:1193:GLN:NE2	1.56	1.03
7:F:81:THR:HG21	7:F:136:ARG:HD3	1.38	1.03
4:B:977:GLY:HA3	4:B:1099:VAL:HG21	1.41	1.03
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.39	1.02
3:A:567:LYS:CB	3:A:568:PRO:HD2	1.91	1.01
4:B:1159:ARG:NE	4:B:1193:GLN:HE21	1.57	1.00
3:A:902:LEU:HG	3:A:926:GLN:HG3	1.40	1.00
5:C:57:VAL:HG11	10:J:60:PHE:HB3	1.44	1.00
4:B:1002:THR:HG22	4:B:1006:ILE:H	1.22	0.99
11:K:113:THR:O	11:K:114:LEU:HB2	1.60	0.99
3:A:913:LEU:HD12	3:A:914:GLU:H	1.25	0.99
4:B:120:ARG:HG2	4:B:955:THR:HG21	1.40	0.99
5:C:56:THR:HG22	5:C:57:VAL:H	1.28	0.98
6:E:135:PHE:HB3	6:E:140:LEU:HD11	1.45	0.98
4:B:842:ASN:ND2	4:B:845:SER:H	1.62	0.97
3:A:567:LYS:HB3	8:H:96:VAL:H	1.26	0.97
4:B:174:LEU:O	4:B:175:ARG:HB2	1.64	0.97
4:B:1100:ASP:HA	4:B:1103:ILE:HD11	1.46	0.97
2:T:1:DA:C2	2:T:2:DC:C5	2.53	0.97
5:C:167:HIS:CD2	5:C:169:LYS:H	1.83	0.96
1:R:5:A:C2	1:R:6:G:C5	2.52	0.96
4:B:1051:THR:HG22	4:B:1053:GLU:N	1.81	0.96
4:B:200:GLY:HA2	4:B:202:TYR:CE2	2.02	0.95
4:B:392:ARG:HH21	9:I:52:ILE:HD11	1.30	0.95
4:B:639:ILE:HD11	4:B:691:GLU:HG3	1.47	0.94
4:B:737:THR:HG21	9:I:66:PRO:O	1.68	0.94
3:A:244:PRO:HG2	3:A:245:PRO:HD3	1.46	0.94
3:A:1116:LEU:HD12	3:A:1329:THR:OG1	1.67	0.94
3:A:338:GLY:HA2	4:B:1129:ARG:HH22	1.33	0.94
3:A:783:THR:HG22	3:A:784:LEU:HG	1.48	0.93
4:B:824:ILE:HG12	10:J:48:ARG:HH12	1.32	0.93
4:B:1159:ARG:HD3	4:B:1193:GLN:HG3	1.47	0.93
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.47	0.92
4:B:955:THR:HG22	4:B:956:THR:H	1.31	0.92
3:A:1435:PRO:HA	3:A:1439:GLY:O	1.69	0.92
3:A:1281:ARG:HD2	3:A:1309:ASP:OD2	1.68	0.92
12:L:60:ARG:HG3	12:L:61:THR:N	1.85	0.92
10:J:46:CYS:HG	15:J:101:ZN:ZN	0.78	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:9:G:C6	1:R:10:A:N6	2.37	0.91
5:C:73:GLN:HE21	5:C:75:MET:H	1.14	0.91
3:A:15:LYS:HB3	4:B:1220:ARG:HG2	1.51	0.91
3:A:381:THR:HG22	3:A:383:TYR:H	1.35	0.91
3:A:1399:ARG:HB3	3:A:1408:ILE:HD13	1.50	0.91
3:A:1194:ARG:NH2	3:A:1237:ILE:HD13	1.87	0.90
4:B:1002:THR:HG22	4:B:1006:ILE:N	1.84	0.90
4:B:842:ASN:HD22	4:B:845:SER:H	1.17	0.90
4:B:956:THR:HA	4:B:961:LEU:O	1.71	0.90
5:C:22:LEU:HD22	5:C:25:VAL:HG21	1.53	0.90
3:A:1105:LEU:HD22	3:A:1384:VAL:HG21	1.53	0.90
3:A:590:ARG:NH1	3:A:590:ARG:HG3	1.86	0.90
4:B:955:THR:HG22	4:B:956:THR:N	1.85	0.90
9:I:75:CYS:HG	15:I:204:ZN:ZN	0.68	0.90
7:F:93:ILE:HD11	7:F:134:ILE:HD11	1.54	0.90
3:A:351:THR:HG23	4:B:1103:ILE:HA	1.53	0.90
4:B:1159:ARG:HE	4:B:1193:GLN:HE21	0.93	0.89
9:I:111:THR:HG22	9:I:113:ASP:N	1.86	0.89
3:A:868:TYR:HD2	3:A:1058:VAL:HG21	1.38	0.89
3:A:1410:PHE:CD2	4:B:1212:ILE:HD11	2.08	0.89
6:E:5:ASN:HD21	6:E:52:ARG:HG2	1.35	0.89
4:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.89
2:T:2:DC:H2'	2:T:3:DG:C8	2.07	0.89
3:A:567:LYS:HB2	3:A:568:PRO:CD	2.02	0.88
3:A:549:MET:SD	3:A:577:ILE:HD12	2.12	0.88
4:B:1077:THR:HG22	4:B:1079:LYS:H	1.35	0.88
4:B:955:THR:CG2	4:B:956:THR:H	1.87	0.88
1:R:9:G:O6	1:R:10:A:N6	2.07	0.88
3:A:886:ILE:HD11	3:A:943:LEU:HB3	1.56	0.87
3:A:666:ILE:CD1	4:B:1030:LEU:HD13	2.04	0.87
4:B:512:ARG:HH21	4:B:535:LEU:CD1	1.88	0.87
3:A:567:LYS:NZ	8:H:46:LEU:HB2	1.87	0.87
3:A:590:ARG:HH11	3:A:590:ARG:HG3	1.37	0.87
4:B:1065:GLN:HE21	4:B:1067:ARG:N	1.73	0.87
5:C:57:VAL:HG11	10:J:60:PHE:CB	2.03	0.87
3:A:61:ILE:HG22	3:A:62:ASP:H	1.37	0.87
4:B:1072:MET:HE3	4:B:1085:ILE:HB	1.56	0.87
4:B:345:LYS:CA	4:B:348:ARG:HE	1.87	0.87
4:B:744:HIS:HD2	4:B:746:SER:H	1.22	0.87
2:T:8:DT:H2''	2:T:9:DC:O5'	1.74	0.87
3:A:1192:LEU:HD11	3:A:1239:ARG:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:667:GLY:HA2	3:A:670:ILE:HD12	1.56	0.87
3:A:337:ARG:NH1	3:A:839:ARG:HH12	1.72	0.87
5:C:44:LEU:HB2	5:C:77:ILE:HD11	1.55	0.87
3:A:962:ARG:HA	3:A:965:GLN:HE21	1.38	0.86
2:T:3:DG:H5'	3:A:836:TYR:CD1	2.09	0.86
4:B:130:VAL:HG21	4:B:167:ILE:HD12	1.56	0.86
4:B:977:GLY:HA3	4:B:1099:VAL:CG2	2.04	0.86
3:A:605:MET:HE3	3:A:614:PHE:O	1.75	0.86
2:T:11:DC:H2''	2:T:12:DG:H5'	1.56	0.86
3:A:1242:VAL:HG12	3:A:1243:VAL:H	1.40	0.86
4:B:1106:ARG:HH21	4:B:1109:GLY:H	1.24	0.86
4:B:801:LYS:O	10:J:52:THR:HG23	1.75	0.86
4:B:912:ILE:O	4:B:938:SER:HB2	1.76	0.86
5:C:167:HIS:HD2	5:C:169:LYS:H	0.90	0.85
3:A:269:ILE:HD11	3:A:300:VAL:HA	1.57	0.85
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.11	0.85
4:B:345:LYS:HA	4:B:348:ARG:NE	1.91	0.85
3:A:417:TYR:O	3:A:418:SER:HB2	1.75	0.85
3:A:1348:LEU:HD23	3:A:1372:VAL:HG13	1.59	0.85
2:T:6:DC:H4'	3:A:447:GLN:NE2	1.91	0.85
3:A:1039:LYS:O	3:A:1043:ASP:HB2	1.76	0.85
1:R:5:A:N1	1:R:6:G:C6	2.44	0.84
3:A:709:THR:HG21	9:I:93:LYS:O	1.78	0.84
4:B:1106:ARG:NH1	4:B:1118:PRO:HB3	1.91	0.84
8:H:125:LEU:HG	8:H:130:ARG:NH1	1.92	0.84
6:E:177:ARG:HD3	6:E:215:MET:SD	2.18	0.84
3:A:1118:VAL:CG2	3:A:1306:LEU:HB2	2.08	0.84
3:A:1390:ASN:ND2	3:A:1399:ARG:HA	1.93	0.84
11:K:12:LEU:HD12	11:K:12:LEU:H	1.42	0.84
2:T:9:DC:OP1	4:B:1123:SER:HB3	1.77	0.84
4:B:228:LYS:HD3	4:B:234:ILE:HD13	1.57	0.84
2:T:6:DC:H4'	3:A:447:GLN:HE22	1.42	0.83
7:F:147:SER:OG	7:F:150:GLU:HG3	1.78	0.83
4:B:1002:THR:CG2	4:B:1006:ILE:H	1.91	0.83
4:B:200:GLY:HA2	4:B:202:TYR:HE2	1.43	0.83
4:B:637:LEU:HD12	4:B:693:ILE:HD12	1.60	0.83
4:B:519:TRP:HZ2	4:B:705:MET:HE1	1.42	0.83
5:C:11:ARG:NH2	5:C:229:TYR:HD2	1.77	0.82
3:A:535:THR:HG21	3:A:617:VAL:H	1.43	0.82
3:A:565:ILE:HG23	3:A:567:LYS:HG2	1.62	0.82
3:A:885:THR:HG23	3:A:893:PHE:HE1	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:108:VAL:HG12	4:B:109:THR:H	1.42	0.82
4:B:269:ILE:HD11	4:B:386:LEU:HD21	1.62	0.82
3:A:683:ILE:HD11	3:A:764:CYS:HB2	1.61	0.82
6:E:2:ASP:O	6:E:3:GLN:HG2	1.78	0.82
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.61	0.82
4:B:999:MET:HG3	4:B:1000:PRO:HD2	1.61	0.82
3:A:563:PRO:HG3	3:A:572:TRP:CZ2	2.14	0.81
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.62	0.81
8:H:93:TYR:HB3	8:H:144:ILE:O	1.80	0.81
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.61	0.81
3:A:1017:LEU:HB2	6:E:206:GLY:H	1.45	0.81
4:B:1106:ARG:HE	4:B:1109:GLY:N	1.79	0.81
4:B:800:GLN:HB3	10:J:52:THR:CG2	2.11	0.81
3:A:208:LEU:HD22	3:A:212:LYS:HE3	1.62	0.81
3:A:742:ASN:HA	3:A:745:GLN:HB2	1.63	0.81
4:B:1106:ARG:HE	4:B:1109:GLY:H	1.29	0.81
5:C:37:MET:HG2	5:C:243:VAL:HG12	1.62	0.81
4:B:121:ASN:HD22	4:B:121:ASN:N	1.79	0.81
9:I:50:THR:CG2	9:I:52:ILE:HG23	2.11	0.81
3:A:472:LEU:O	3:A:475:THR:HB	1.81	0.81
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.11	0.81
4:B:899:ILE:HD11	4:B:911:ILE:HA	1.62	0.80
3:A:337:ARG:NH1	3:A:839:ARG:NH1	2.29	0.80
4:B:244:LEU:O	4:B:249:ARG:HG2	1.81	0.80
5:C:148:ARG:NH1	10:J:64:ASN:HA	1.96	0.80
3:A:406:ILE:HB	3:A:431:LYS:HB2	1.61	0.80
3:A:868:TYR:CE1	3:A:1064:VAL:HG11	2.17	0.80
4:B:1106:ARG:HH21	4:B:1109:GLY:N	1.78	0.80
4:B:796:LEU:HB3	4:B:799:PRO:HG3	1.63	0.80
9:I:75:CYS:SG	9:I:78:CYS:SG	2.80	0.80
4:B:1100:ASP:HA	4:B:1103:ILE:CD1	2.12	0.80
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.12	0.80
2:T:6:DC:C2'	2:T:7:DC:C5'	2.45	0.80
3:A:523:ILE:HD12	3:A:622:VAL:CG2	2.12	0.80
3:A:1118:VAL:HG22	3:A:1306:LEU:HB2	1.64	0.79
4:B:519:TRP:CZ2	4:B:705:MET:HE1	2.16	0.79
1:R:5:A:H2'	1:R:6:G:C8	2.18	0.79
3:A:93:VAL:CG1	3:A:301:ALA:HB1	2.11	0.79
4:B:313:MET:HE3	4:B:386:LEU:HD22	1.62	0.79
3:A:40:THR:HG22	3:A:41:MET:HG3	1.64	0.79
4:B:293:PRO:HG2	4:B:296:GLU:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:3:DG:H5'	3:A:836:TYR:CE1	2.18	0.79
4:B:487:THR:HG22	4:B:489:SER:H	1.48	0.79
3:A:298:PHE:O	3:A:302:THR:HB	1.83	0.79
3:A:32:VAL:HG21	3:A:68:GLN:NE2	1.97	0.79
4:B:1065:GLN:HE21	4:B:1067:ARG:H	1.29	0.79
4:B:1106:ARG:NH2	4:B:1109:GLY:H	1.79	0.79
5:C:56:THR:HG22	5:C:57:VAL:N	1.97	0.79
3:A:768:GLN:CG	3:A:816:HIS:HA	2.13	0.79
3:A:913:LEU:HD12	3:A:914:GLU:N	1.98	0.79
3:A:1299:VAL:HG12	3:A:1300:LYS:H	1.47	0.78
4:B:834:ASN:HB3	4:B:840:ILE:HG13	1.63	0.78
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.63	0.78
3:A:1281:ARG:O	3:A:1282:VAL:HG23	1.83	0.78
3:A:666:ILE:HD13	4:B:1030:LEU:HD22	1.65	0.78
8:H:5:LEU:HD11	8:H:135:LEU:HG	1.63	0.78
3:A:58:LEU:HD22	3:A:80:HIS:O	1.83	0.78
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.66	0.78
3:A:353:ILE:HD13	3:A:487:MET:CE	2.14	0.78
3:A:313:GLN:HB2	3:A:322:VAL:CG2	2.14	0.78
4:B:102:VAL:HG23	4:B:112:LEU:HB2	1.65	0.78
3:A:783:THR:HG21	3:A:815:PHE:CZ	2.19	0.78
4:B:855:PHE:HZ	4:B:857:ARG:NH1	1.81	0.78
3:A:679:ILE:HG23	3:A:729:ALA:HB1	1.63	0.78
3:A:70:CYS:O	3:A:72:GLU:HG2	1.84	0.78
4:B:392:ARG:NH2	9:I:52:ILE:HD11	1.98	0.78
4:B:583:ASN:HD21	4:B:628:THR:HB	1.49	0.78
4:B:496:ARG:NH1	4:B:539:LEU:HB2	1.99	0.77
5:C:165:LYS:O	11:K:6:ARG:NH1	2.17	0.77
3:A:313:GLN:HB2	3:A:322:VAL:HG23	1.64	0.77
3:A:901:LEU:H	3:A:926:GLN:NE2	1.82	0.77
4:B:1100:ASP:OD1	4:B:1103:ILE:HD11	1.84	0.77
4:B:102:VAL:CG2	4:B:112:LEU:HB2	2.13	0.77
8:H:123:MET:HE3	8:H:142:LEU:HD22	1.66	0.77
4:B:842:ASN:ND2	4:B:845:SER:N	2.31	0.77
4:B:1166:CYS:O	4:B:1168:LEU:N	2.18	0.77
10:J:12:LYS:O	10:J:14:VAL:HG23	1.85	0.77
11:K:47:ARG:HH11	11:K:47:ARG:HB3	1.49	0.77
3:A:855:THR:HG21	3:A:857:ARG:NE	1.95	0.77
4:B:232:SER:OG	4:B:234:ILE:HD12	1.84	0.77
3:A:1438:THR:HB	4:B:1144:ALA:HB3	1.66	0.77
3:A:31:SER:CB	3:A:83:HIS:HB2	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:10:CYS:SG	10:J:46:CYS:SG	2.83	0.77
3:A:1345:ARG:HD2	3:A:1373:ASP:OD1	1.84	0.77
3:A:23:SER:HB3	3:A:233:TRP:CZ2	2.19	0.77
3:A:24:PRO:HB3	3:A:237:THR:HB	1.67	0.76
4:B:708:GLU:HG3	4:B:709:ASP:N	1.98	0.76
3:A:326:ARG:HG2	3:A:1406:VAL:HG21	1.67	0.76
3:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.49	0.76
3:A:896:ARG:HD3	3:A:897:TYR:CE1	2.21	0.76
4:B:1096:ARG:O	4:B:1097:HIS:HB2	1.85	0.76
4:B:707:PRO:HG2	4:B:708:GLU:H	1.49	0.76
3:A:549:MET:HE1	3:A:656:TRP:HD1	1.49	0.76
4:B:899:ILE:CD1	4:B:911:ILE:HA	2.16	0.76
6:E:69:ILE:HG23	6:E:73:PRO:HA	1.68	0.76
3:A:399:HIS:O	3:A:401:GLY:N	2.17	0.76
3:A:353:ILE:HD13	3:A:487:MET:HE3	1.67	0.76
2:T:6:DC:H2"	2:T:7:DC:H5'	0.79	0.76
3:A:223:GLY:O	3:A:1415:SER:HA	1.86	0.76
4:B:842:ASN:HD22	4:B:845:SER:N	1.83	0.76
5:C:166:GLU:HG3	11:K:10:PHE:HZ	1.51	0.76
5:C:57:VAL:CG1	10:J:60:PHE:HB3	2.15	0.76
3:A:1094:VAL:HG13	3:A:1113:THR:HG21	1.66	0.76
4:B:996:ARG:NH2	5:C:174:ALA:O	2.19	0.76
3:A:336:ILE:HD12	3:A:1405:THR:HG21	1.68	0.75
5:C:124:LEU:O	5:C:127:ARG:HG2	1.85	0.75
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.68	0.75
3:A:469:ARG:HH21	4:B:976:ILE:HD13	1.50	0.75
4:B:118:ARG:HG3	4:B:204:ILE:HD13	1.68	0.75
4:B:211:VAL:HG21	4:B:483:LEU:HD13	1.67	0.75
4:B:711:GLU:N	4:B:712:PRO:HD3	2.01	0.75
4:B:882:THR:HG22	4:B:884:ARG:H	1.50	0.75
3:A:1323:ASP:OD1	3:A:1325:THR:HB	1.85	0.75
3:A:41:MET:HA	3:A:49:LYS:HA	1.68	0.75
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.50	0.75
7:F:111:LEU:N	7:F:111:LEU:HD12	2.02	0.75
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.52	0.75
3:A:1436:ILE:HG22	3:A:1437:GLY:H	1.52	0.74
3:A:265:LYS:NZ	3:A:323:LYS:H	1.84	0.74
4:B:62:ILE:HG23	4:B:418:LYS:HG2	1.69	0.74
12:L:38:LEU:O	12:L:39:SER:HB3	1.85	0.74
4:B:118:ARG:HH22	4:B:194:GLU:CD	1.90	0.74
3:A:1146:VAL:HG11	3:A:1202:MET:SD	2.27	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2:DC:OP1	3:A:1403:GLU:O	2.04	0.74
3:A:458:HIS:CE1	3:A:507:VAL:HG21	2.22	0.74
3:A:1436:ILE:HG22	3:A:1437:GLY:N	2.03	0.74
3:A:575:LYS:HB3	3:A:612:ILE:CG2	2.17	0.74
3:A:535:THR:CG2	3:A:616:VAL:HA	2.17	0.74
4:B:708:GLU:CG	4:B:709:ASP:H	1.97	0.74
3:A:693:VAL:HG21	3:A:721:PHE:HE1	1.51	0.74
6:E:61:GLN:HE21	6:E:105:PHE:HE2	1.34	0.74
3:A:853:ASP:OD1	3:A:855:THR:HB	1.88	0.74
3:A:95:PHE:O	3:A:99:ILE:HG13	1.85	0.74
4:B:521:LEU:HD22	4:B:633:VAL:HG12	1.69	0.74
4:B:423:LYS:HA	4:B:426:LYS:HE2	1.68	0.74
4:B:46:GLN:HG3	4:B:47:GLN:N	2.03	0.74
3:A:443:LEU:HD21	3:A:455:MET:HB3	1.70	0.74
4:B:770:GLN:HG2	4:B:983:ARG:O	1.86	0.74
3:A:154:SER:HB3	3:A:162:VAL:CG2	2.17	0.74
3:A:710:LEU:H	3:A:710:LEU:HD12	1.52	0.74
3:A:1436:ILE:CG2	4:B:1142:GLY:HA2	2.17	0.74
3:A:1299:VAL:HG12	3:A:1300:LYS:N	2.02	0.74
5:C:167:HIS:HD2	5:C:169:LYS:N	1.76	0.74
8:H:5:LEU:HB3	8:H:133:ASN:O	1.88	0.74
11:K:65:HIS:CD2	11:K:67:PHE:H	2.06	0.74
3:A:541:ILE:HG21	3:A:549:MET:HE3	1.68	0.73
4:B:172:ILE:HD13	4:B:178:ASN:HB3	1.70	0.73
4:B:363:HIS:O	4:B:364:ILE:HB	1.88	0.73
3:A:500:GLU:OE2	4:B:1145:SER:HB2	1.88	0.73
4:B:542:MET:HE3	4:B:747:MET:HG3	1.67	0.73
11:K:65:HIS:HD2	11:K:67:PHE:H	1.35	0.73
3:A:828:ALA:HB2	4:B:530:GLY:HA2	1.70	0.73
4:B:651:LEU:HD11	4:B:707:PRO:HB3	1.69	0.73
2:T:1:DA:N3	2:T:1:DA:H2'	2.03	0.73
3:A:1441:PHE:CZ	7:F:89:GLU:HA	2.23	0.73
3:A:321:PRO:O	3:A:322:VAL:HB	1.87	0.73
3:A:417:TYR:O	3:A:418:SER:CB	2.36	0.73
3:A:857:ARG:HD3	3:A:861:GLY:O	1.88	0.73
6:E:124:VAL:HA	6:E:132:ILE:HD12	1.70	0.73
3:A:341:MET:HE1	3:A:1401:SER:HB2	1.70	0.73
3:A:268:ASP:HB3	3:A:299:HIS:CE1	2.23	0.73
6:E:61:GLN:NE2	6:E:105:PHE:HE2	1.86	0.73
3:A:32:VAL:HB	3:A:57:ARG:HD2	1.71	0.73
4:B:1106:ARG:NE	4:B:1109:GLY:H	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:534:LEU:O	3:A:574:GLY:HA3	1.88	0.73
8:H:35:GLN:HB3	8:H:111:LEU:HD21	1.70	0.73
1:R:10:A:OP1	1:R:10:A:OP2	1.99	0.73
3:A:567:LYS:HB3	8:H:96:VAL:N	2.02	0.73
3:A:691:LEU:HD11	3:A:695:LYS:HE3	1.71	0.73
3:A:75:ASN:O	3:A:76:GLU:HB3	1.88	0.73
4:B:234:ILE:H	4:B:234:ILE:HD12	1.54	0.73
4:B:313:MET:CE	4:B:386:LEU:HD22	2.19	0.73
1:R:9:G:N1	1:R:10:A:N6	2.36	0.73
3:A:1152:ILE:HG23	3:A:1260:LEU:HD23	1.71	0.73
4:B:708:GLU:O	4:B:710:LEU:N	2.22	0.73
4:B:980:PHE:CE2	4:B:1094:ARG:HG3	2.23	0.73
4:B:570:VAL:HG21	4:B:573:GLN:NE2	2.04	0.72
4:B:542:MET:HG3	4:B:747:MET:HE3	1.69	0.72
3:A:868:TYR:CD2	3:A:1058:VAL:HG21	2.23	0.72
3:A:445:ASN:HB2	3:A:455:MET:HG2	1.70	0.72
3:A:899:VAL:HB	3:A:929:LEU:HD12	1.71	0.72
4:B:193:LYS:HD3	4:B:787:VAL:HG11	1.70	0.72
4:B:542:MET:HE1	4:B:743:ILE:HG21	1.70	0.72
8:H:89:LEU:C	8:H:91:ASP:H	1.90	0.72
3:A:1399:ARG:HB2	3:A:1408:ILE:HG21	1.70	0.72
3:A:337:ARG:NE	3:A:839:ARG:HH22	1.88	0.72
3:A:925:LEU:O	3:A:929:LEU:HD23	1.88	0.72
4:B:570:VAL:HB	4:B:573:GLN:CB	2.18	0.72
3:A:598:LEU:HD22	8:H:25:ARG:NH1	2.05	0.72
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.88	0.72
3:A:1258:HIS:ND1	3:A:1262:LYS:HE3	2.04	0.72
11:K:55:LYS:HD3	11:K:78:THR:CB	2.20	0.72
1:R:4:G:H1	2:T:11:DC:H42	1.37	0.72
3:A:48:ALA:O	3:A:49:LYS:HG3	1.89	0.72
3:A:901:LEU:HG	3:A:926:GLN:HE21	1.55	0.72
4:B:879:ARG:HB3	4:B:883:LEU:HD23	1.70	0.72
3:A:1209:MET:SD	3:A:1236:LEU:HB3	2.30	0.72
4:B:429:PHE:HA	4:B:432:MET:HE2	1.71	0.72
4:B:58:THR:O	4:B:62:ILE:HG13	1.89	0.72
2:T:2:DC:H2'	2:T:3:DG:H8	1.55	0.72
3:A:399:HIS:HB3	3:A:400:PRO:HD3	1.70	0.72
3:A:445:ASN:CB	3:A:455:MET:HG2	2.19	0.72
4:B:745:PRO:O	4:B:748:ILE:HG12	1.88	0.72
3:A:1397:LEU:O	3:A:1400:CYS:HB2	1.89	0.72
3:A:567:LYS:HD3	8:H:95:TYR:CD1	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:340:LEU:HD21	4:B:1200:ALA:HB2	1.72	0.71
4:B:1007:VAL:HG22	4:B:1008:PRO:HD2	1.71	0.71
5:C:18:VAL:HG23	5:C:240:VAL:HG11	1.72	0.71
6:E:168:TYR:HB3	6:E:170:LEU:HD21	1.72	0.71
4:B:309:GLN:HG3	9:I:52:ILE:HD13	1.72	0.71
4:B:637:LEU:CD1	4:B:693:ILE:HD12	2.20	0.71
4:B:737:THR:HG23	9:I:66:PRO:CB	2.20	0.71
9:I:74:GLU:HB3	9:I:79:HIS:HA	1.70	0.71
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.71	0.71
3:A:567:LYS:HE3	8:H:46:LEU:HD12	1.72	0.71
14:R:3000:UTP:O2	2:T:4:DA:C2	2.44	0.71
3:A:575:LYS:HB3	3:A:612:ILE:HG23	1.71	0.71
4:B:1066:SER:O	4:B:1067:ARG:HD3	1.90	0.71
4:B:108:VAL:HG12	4:B:109:THR:N	2.06	0.71
3:A:672:ASP:HB2	3:A:736:ASN:OD1	1.90	0.71
3:A:675:THR:HG21	3:A:736:ASN:ND2	2.06	0.71
4:B:281:PRO:HG2	4:B:284:ILE:HD12	1.73	0.71
4:B:792:MET:HA	4:B:856:PHE:O	1.91	0.71
3:A:1015:VAL:HG12	3:A:1019:CYS:SG	2.31	0.70
3:A:855:THR:HG23	3:A:857:ARG:HG3	1.72	0.70
3:A:900:ASP:OD2	3:A:903:ASN:HB2	1.90	0.70
4:B:555:ILE:HD13	4:B:587:HIS:CE1	2.26	0.70
3:A:225:ASN:O	3:A:227:VAL:N	2.21	0.70
4:B:1056:SER:HB3	4:B:1066:SER:HB2	1.73	0.70
1:R:5:A:C2	1:R:6:G:C6	2.79	0.70
3:A:451:HIS:NE2	3:A:1074:GLU:HG3	2.07	0.70
4:B:839:MET:HE3	4:B:1010:LEU:HD11	1.72	0.70
3:A:367:PRO:HB3	3:A:466:SER:HA	1.73	0.70
3:A:343:LYS:HE3	4:B:1151:LEU:O	1.92	0.70
3:A:675:THR:CB	3:A:736:ASN:HD21	2.04	0.70
3:A:994:GLN:HE22	3:A:1023:ARG:HE	1.38	0.70
4:B:636:PRO:O	4:B:637:LEU:HG	1.90	0.70
4:B:957:ASN:HD22	4:B:961:LEU:HD12	1.57	0.70
6:E:56:LYS:HG3	6:E:84:ASP:HB2	1.73	0.70
8:H:49:VAL:HG12	8:H:50:ALA:N	2.07	0.70
3:A:44:THR:O	3:A:45:GLN:HB2	1.91	0.70
4:B:955:THR:HG23	12:L:54:ARG:O	1.91	0.70
4:B:65:GLU:HG3	4:B:66:ASP:H	1.56	0.70
3:A:351:THR:HG21	4:B:1103:ILE:HG23	1.72	0.70
3:A:463:ILE:HB	3:A:464:PRO:HD2	1.74	0.70
3:A:503:GLN:HE21	7:F:90:ARG:NH2	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:638:PHE:CE1	4:B:743:ILE:HA	2.26	0.70
3:A:1095:THR:HG22	3:A:1100:ARG:HB2	1.74	0.69
11:K:55:LYS:HD3	11:K:78:THR:HB	1.72	0.69
12:L:60:ARG:CG	12:L:61:THR:H	1.94	0.69
3:A:1208:THR:HB	3:A:1211:GLN:HG3	1.74	0.69
2:T:8:DT:C2'	2:T:9:DC:O5'	2.39	0.69
4:B:378:LEU:O	4:B:382:ILE:HG13	1.92	0.69
3:A:472:LEU:HD11	4:B:835:GLN:NE2	2.07	0.69
12:L:47:ARG:HG2	12:L:52:GLY:HA2	1.72	0.69
3:A:335:ARG:HA	3:A:339:ASN:HD22	1.56	0.69
4:B:130:VAL:HG12	4:B:131:ASP:N	2.07	0.69
3:A:383:TYR:HB3	7:F:115:THR:HG22	1.73	0.69
4:B:293:PRO:HG2	4:B:296:GLU:HB3	1.74	0.69
4:B:54:PHE:HA	4:B:58:THR:HB	1.74	0.69
5:C:80:LEU:HD22	5:C:129:ILE:CD1	2.21	0.69
3:A:567:LYS:HE3	8:H:46:LEU:CD1	2.22	0.69
4:B:463:THR:CG2	4:B:465:ASN:HD22	2.05	0.69
8:H:36:CYS:SG	8:H:130:ARG:NH2	2.65	0.69
3:A:1332:PHE:H	3:A:1332:PHE:HD2	1.38	0.69
3:A:414:ASP:OD1	3:A:416:ARG:HG2	1.93	0.69
7:F:81:THR:HG21	7:F:136:ARG:CD	2.20	0.69
2:T:1:DA:N1	2:T:2:DC:C5	2.61	0.69
3:A:392:VAL:HG13	3:A:415:LEU:HD11	1.74	0.69
3:A:763:ALA:O	3:A:803:SER:HB3	1.92	0.69
3:A:340:LEU:HD13	3:A:1429:ILE:HG23	1.74	0.69
3:A:443:LEU:HD22	3:A:455:MET:HE2	1.73	0.69
3:A:768:GLN:HG2	3:A:816:HIS:HA	1.75	0.69
3:A:786:HIS:HE1	4:B:742:GLU:OE1	1.76	0.69
4:B:314:LEU:O	4:B:317:CYS:HB2	1.92	0.69
4:B:884:ARG:O	4:B:936:ASP:HB3	1.93	0.69
5:C:39:ALA:HA	5:C:164:ALA:HB3	1.75	0.68
6:E:83:CYS:SG	6:E:88:VAL:HG22	2.32	0.68
3:A:1111:MET:HE1	3:A:1114:PRO:HA	1.74	0.68
3:A:391:LEU:HD22	3:A:400:PRO:O	1.93	0.68
4:B:288:ALA:HB1	4:B:331:LEU:HD12	1.75	0.68
3:A:1390:ASN:HD22	3:A:1399:ARG:HA	1.57	0.68
3:A:584:ASN:O	3:A:637:LYS:HE3	1.92	0.68
4:B:46:GLN:HG3	4:B:47:GLN:H	1.59	0.68
4:B:22:SER:O	4:B:654:ARG:HD2	1.94	0.68
4:B:542:MET:CE	4:B:747:MET:HG3	2.22	0.68
3:A:693:VAL:CG2	3:A:721:PHE:HE1	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:72:GLU:OE2	4:B:1175:LEU:HD12	1.92	0.68
4:B:954:VAL:O	12:L:55:ILE:O	2.11	0.68
3:A:599:SER:HB2	3:A:603:ASN:H	1.58	0.68
4:B:280:ILE:CD1	4:B:334:ILE:HG12	2.23	0.68
5:C:51:VAL:HG22	5:C:155:LEU:HD22	1.76	0.68
3:A:563:PRO:HB2	3:A:565:ILE:O	1.94	0.68
4:B:562:GLY:HA3	4:B:590:HIS:CE1	2.29	0.68
8:H:7:ASP:O	8:H:8:ASP:HB2	1.92	0.68
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.09	0.68
3:A:858:ASN:HD22	3:A:858:ASN:C	1.95	0.68
3:A:535:THR:HG21	3:A:617:VAL:N	2.08	0.68
4:B:709:ASP:O	4:B:710:LEU:HD23	1.94	0.68
4:B:986:GLN:OE1	4:B:986:GLN:HA	1.92	0.68
3:A:590:ARG:HH11	3:A:590:ARG:CG	2.06	0.68
5:C:254:LYS:HB3	11:K:42:LEU:HD11	1.75	0.68
3:A:994:GLN:HE21	3:A:1019:CYS:HB3	1.59	0.67
4:B:280:ILE:HG22	4:B:285:ILE:HG13	1.76	0.67
4:B:842:ASN:ND2	4:B:844:SER:HB2	2.09	0.67
2:T:1:DA:C6	2:T:2:DC:C5	2.81	0.67
4:B:514:LEU:HD12	4:B:515:HIS:N	2.09	0.67
5:C:166:GLU:HG3	11:K:10:PHE:CZ	2.29	0.67
4:B:121:ASN:HA	4:B:207:GLY:HA3	1.77	0.67
7:F:109:VAL:HG12	7:F:110:ASP:N	2.10	0.67
5:C:5:GLY:O	5:C:7:GLN:HG3	1.95	0.67
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.76	0.67
9:I:53:GLY:O	9:I:89:GLN:HB2	1.94	0.67
9:I:75:CYS:SG	9:I:103:CYS:SG	2.92	0.67
3:A:535:THR:HG21	3:A:616:VAL:HA	1.75	0.67
3:A:351:THR:CG2	4:B:1103:ILE:HG23	2.24	0.67
5:C:8:VAL:HG12	5:C:9:LYS:N	2.09	0.67
3:A:814:PHE:O	3:A:817:ALA:HB3	1.95	0.67
4:B:1147:LEU:HD22	4:B:1151:LEU:HD22	1.77	0.67
4:B:976:ILE:O	4:B:990:ILE:HB	1.94	0.67
4:B:711:GLU:N	4:B:712:PRO:CD	2.57	0.67
4:B:864:LYS:HB3	4:B:872:GLU:H	1.59	0.67
2:T:1:DA:C1'	3:A:1386:ARG:HH12	2.08	0.67
3:A:16:GLU:HB3	3:A:1418:LEU:HD11	1.77	0.67
3:A:450:LEU:HD13	3:A:1074:GLU:HG2	1.77	0.67
3:A:694:THR:O	3:A:698:GLN:HG3	1.94	0.67
5:C:260:LEU:O	5:C:264:GLN:HG3	1.95	0.67
5:C:93:ASP:O	5:C:127:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1:DA:C4	2:T:2:DC:C5	2.83	0.67
4:B:566:LEU:HD13	4:B:588:GLY:HA2	1.77	0.67
3:A:1267:MET:HA	3:A:1271:ILE:HD12	1.77	0.66
3:A:1342:GLU:OE2	6:E:212:ARG:NH1	2.28	0.66
3:A:828:ALA:CB	4:B:530:GLY:HA2	2.25	0.66
4:B:711:GLU:H	4:B:712:PRO:HD3	1.60	0.66
4:B:882:THR:HG21	4:B:935:ARG:HA	1.75	0.66
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.30	0.66
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.77	0.66
4:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.77	0.66
3:A:305:ASP:HB3	3:A:308:ILE:HD11	1.77	0.66
3:A:897:TYR:CD2	3:A:936:LEU:HD13	2.30	0.66
3:A:525:GLN:CB	4:B:835:GLN:HG2	2.25	0.66
4:B:957:ASN:O	4:B:959:ASP:N	2.29	0.66
3:A:1348:LEU:HD21	3:A:1375:MET:SD	2.35	0.66
3:A:446:ARG:HH11	3:A:446:ARG:HG2	1.59	0.66
3:A:453:MET:HB3	3:A:477:PRO:HB3	1.76	0.66
4:B:986:GLN:HE22	4:B:1020:ARG:CZ	2.08	0.66
6:E:127:ILE:O	6:E:127:ILE:HG13	1.93	0.66
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.31	0.66
9:I:55:THR:HG23	9:I:58:VAL:HG21	1.76	0.66
3:A:1333:ILE:O	3:A:1336:MET:HB3	1.96	0.66
3:A:1364:ASN:ND2	3:A:1365:TYR:N	2.43	0.66
3:A:590:ARG:HB3	3:A:605:MET:N	2.10	0.66
4:B:1002:THR:HG23	4:B:1004:GLU:N	2.10	0.66
5:C:98:VAL:C	5:C:99:LEU:HD23	2.16	0.66
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.77	0.66
3:A:1042:PHE:CE2	3:A:1046:LEU:HD11	2.31	0.66
4:B:1051:THR:CG2	4:B:1053:GLU:H	1.93	0.66
3:A:76:GLU:OE2	4:B:1159:ARG:NH1	2.28	0.66
4:B:287:ARG:NH2	4:B:294:ASP:OD2	2.28	0.66
3:A:90:VAL:CG1	3:A:297:GLN:HA	2.26	0.66
5:C:56:THR:HG21	5:C:145:CYS:SG	2.35	0.66
6:E:93:MET:HE2	6:E:120:ALA:HB1	1.77	0.66
8:H:97:MET:HE2	8:H:142:LEU:HD23	1.76	0.66
12:L:45:ALA:O	12:L:46:VAL:HG23	1.95	0.66
3:A:381:THR:HG22	3:A:383:TYR:N	2.09	0.66
4:B:363:HIS:O	4:B:364:ILE:CB	2.44	0.66
3:A:741:ASN:HD22	3:A:741:ASN:C	1.99	0.66
4:B:1106:ARG:CZ	4:B:1109:GLY:H	2.07	0.66
4:B:349:ILE:O	4:B:352:ALA:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:32:CYS:SG	9:I:33:SER:N	2.69	0.66
4:B:311:LEU:HB3	9:I:4:PHE:CZ	2.31	0.66
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.76	0.66
2:T:6:DC:C4	2:T:7:DC:C5	2.84	0.66
4:B:751:VAL:O	4:B:754:SER:HB2	1.95	0.66
3:A:1193:LEU:HB2	3:A:1260:LEU:HD11	1.78	0.66
3:A:306:ASN:HD21	3:A:324:SER:H	1.43	0.66
4:B:1001:PHE:CZ	4:B:1073:TYR:HB2	2.30	0.66
5:C:11:ARG:HH21	5:C:229:TYR:HD2	1.44	0.66
6:E:176:PRO:O	6:E:212:ARG:HA	1.95	0.66
3:A:751:SER:O	3:A:752:LYS:HG2	1.95	0.65
3:A:95:PHE:HE2	3:A:1414:ALA:HB2	1.62	0.65
3:A:914:GLU:HB2	3:A:979:SER:O	1.95	0.65
3:A:715:GLU:O	3:A:719:VAL:HG23	1.96	0.65
4:B:128:LEU:HB3	4:B:167:ILE:O	1.95	0.65
4:B:211:VAL:HG23	4:B:483:LEU:HB2	1.78	0.65
4:B:603:LEU:HB3	4:B:609:ILE:HG13	1.76	0.65
7:F:111:LEU:H	7:F:111:LEU:HD12	1.62	0.65
5:C:8:VAL:HG12	5:C:9:LYS:H	1.60	0.65
12:L:51:CYS:O	12:L:53:HIS:N	2.28	0.65
3:A:994:GLN:HE22	3:A:1023:ARG:NE	1.95	0.65
3:A:329:LEU:HD23	3:A:335:ARG:HG3	1.78	0.65
3:A:816:HIS:CE1	4:B:764:SER:HB2	2.30	0.65
4:B:293:PRO:HG2	4:B:296:GLU:HB2	1.79	0.65
1:R:8:G:N2	2:T:8:DT:N3	2.45	0.65
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.78	0.65
3:A:1242:VAL:HG12	3:A:1243:VAL:N	2.12	0.65
4:B:911:ILE:CG2	4:B:966:VAL:HG11	2.26	0.65
5:C:22:LEU:HD22	5:C:25:VAL:CG2	2.25	0.65
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.27	0.65
3:A:1319:VAL:HG13	3:A:1320:PRO:HD2	1.79	0.65
4:B:1197:PRO:HG2	4:B:1200:ALA:HB2	1.79	0.65
4:B:805:THR:HG21	4:B:815:ARG:HE	1.62	0.65
12:L:48:CYS:SG	12:L:49:LYS:N	2.70	0.65
4:B:512:ARG:NH2	4:B:535:LEU:HD11	2.02	0.65
14:R:3000:UTP:O2	2:T:4:DA:H2	1.80	0.65
3:A:381:THR:HG21	3:A:383:TYR:CD1	2.31	0.65
4:B:1162:ILE:HD11	4:B:1194:ILE:HD13	1.77	0.65
4:B:120:ARG:CG	4:B:955:THR:HG21	2.23	0.65
4:B:824:ILE:CG1	10:J:48:ARG:HH12	2.08	0.64
10:J:9:SER:OG	10:J:48:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:109:VAL:HG21	7:F:124:GLU:HA	1.79	0.64
7:F:96:THR:O	7:F:100:GLN:HG3	1.97	0.64
3:A:1444:MET:HE1	7:F:135:ARG:NE	2.12	0.64
4:B:1170:THR:O	4:B:1170:THR:HG22	1.97	0.64
5:C:241:ASP:HB3	11:K:109:TRP:CE2	2.32	0.64
6:E:96:PHE:CZ	6:E:100:ILE:HD11	2.32	0.64
8:H:12:VAL:HA	8:H:28:ALA:CB	2.28	0.64
2:T:1:DA:N1	2:T:2:DC:H5	1.94	0.64
3:A:87:ALA:HB3	3:A:276:LEU:HD23	1.79	0.64
3:A:475:THR:HG22	3:A:476:SER:N	2.12	0.64
3:A:512:VAL:HA	3:A:519:PRO:HA	1.79	0.64
4:B:788:ARG:NH1	4:B:790:ASP:OD1	2.31	0.64
4:B:879:ARG:HB3	4:B:883:LEU:CD2	2.27	0.64
3:A:1035:TYR:O	3:A:1037:LEU:N	2.30	0.64
3:A:1224:LEU:HD12	3:A:1241:ARG:O	1.97	0.64
4:B:46:GLN:HE22	4:B:496:ARG:HA	1.62	0.64
4:B:649:LYS:HE2	4:B:738:PHE:O	1.96	0.64
8:H:107:VAL:HG21	8:H:126:GLU:HG3	1.79	0.64
3:A:1115:SER:HA	3:A:1308:THR:HG22	1.77	0.64
3:A:1394:THR:CG2	3:A:1395:GLY:N	2.61	0.64
3:A:901:LEU:HA	3:A:907:THR:HG23	1.80	0.64
4:B:1001:PHE:CE1	4:B:1073:TYR:HB2	2.33	0.64
4:B:25:ILE:HG22	4:B:29:ASP:HB2	1.79	0.64
5:C:114:TYR:CD2	5:C:140:ASN:HB3	2.32	0.64
4:B:446:LEU:O	4:B:447:ALA:HB3	1.97	0.64
2:T:4:DA:H2''	2:T:5:DT:H5'	1.80	0.64
6:E:124:VAL:HG22	6:E:132:ILE:HG21	1.78	0.64
3:A:244:PRO:CG	3:A:245:PRO:HD3	2.27	0.64
3:A:381:THR:CG2	3:A:383:TYR:H	2.09	0.64
3:A:84:ILE:HG23	3:A:239:LEU:HB3	1.80	0.64
4:B:842:ASN:HD21	4:B:844:SER:HB2	1.63	0.64
12:L:40:LEU:HD13	12:L:44:ASP:CG	2.19	0.64
3:A:225:ASN:O	3:A:226:GLU:HG2	1.99	0.63
4:B:1034:VAL:HG23	4:B:1059:LEU:HB2	1.80	0.63
1:R:5:A:H2'	1:R:6:G:O4'	1.98	0.63
3:A:778:GLY:HA3	4:B:516:ASN:HB2	1.80	0.63
4:B:515:HIS:HD2	4:B:517:THR:OG1	1.81	0.63
3:A:1402:PHE:CD2	3:A:1403:GLU:HG3	2.33	0.63
3:A:1436:ILE:HB	4:B:1144:ALA:HB2	1.80	0.63
4:B:114:PRO:HG3	4:B:181:LEU:HD11	1.79	0.63
4:B:1201:LYS:O	4:B:1205:GLN:HG3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:577:ALA:HB1	4:B:589:VAL:CG1	2.27	0.63
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.33	0.63
3:A:108:MET:O	3:A:109:HIS:HB2	1.99	0.63
4:B:525:ALA:O	4:B:527:THR:HG22	1.98	0.63
4:B:604:ARG:HG2	4:B:604:ARG:O	1.98	0.63
8:H:31:THR:O	8:H:32:THR:CB	2.47	0.63
3:A:579:SER:OG	3:A:612:ILE:HG22	1.97	0.63
3:A:709:THR:HB	3:A:712:GLU:H	1.64	0.63
4:B:1104:HIS:HB2	4:B:1122:ARG:HD2	1.80	0.63
6:E:100:ILE:HG23	6:E:105:PHE:HB2	1.80	0.63
3:A:523:ILE:HD12	3:A:622:VAL:HG22	1.79	0.63
7:F:86:THR:OG1	7:F:89:GLU:HG3	1.98	0.63
2:T:1:DA:H1'	3:A:1386:ARG:HH12	1.64	0.63
4:B:1187:ASN:OD1	4:B:1190:ASP:HB3	1.99	0.63
4:B:914:LYS:HB3	4:B:937:ALA:O	1.98	0.63
3:A:871:ASP:OD2	6:E:204:THR:HG23	1.99	0.63
4:B:913:GLY:HA2	4:B:938:SER:HB3	1.81	0.63
6:E:96:PHE:O	6:E:100:ILE:HG13	1.99	0.63
6:E:156:LEU:HD12	6:E:195:VAL:HG12	1.81	0.63
1:R:5:A:C4	1:R:6:G:N7	2.67	0.63
14:R:3000:UTP:N3	2:T:4:DA:N1	2.46	0.63
4:B:496:ARG:HH11	4:B:539:LEU:HB2	1.62	0.62
9:I:7:CYS:HB2	9:I:29:CYS:HB2	1.81	0.62
2:T:11:DC:H2'	2:T:12:DG:C8	2.34	0.62
3:A:871:ASP:HB3	6:E:204:THR:HG22	1.82	0.62
12:L:55:ILE:HG13	12:L:56:LEU:H	1.63	0.62
3:A:629:LEU:HD13	3:A:645:LEU:HD21	1.79	0.62
4:B:1106:ARG:HD2	4:B:1126:GLY:O	1.99	0.62
4:B:39:ARG:HE	4:B:665:GLU:HG2	1.64	0.62
4:B:780:VAL:HG21	10:J:56:LEU:CD1	2.29	0.62
5:C:173:ALA:O	5:C:174:ALA:HB3	2.00	0.62
3:A:1074:GLU:HB3	3:A:1075:PRO:CD	2.29	0.62
3:A:418:SER:O	3:A:420:ARG:N	2.32	0.62
3:A:523:ILE:HD12	3:A:622:VAL:HG21	1.80	0.62
3:A:73:GLY:O	3:A:75:ASN:N	2.32	0.62
3:A:982:THR:HG22	3:A:984:LYS:H	1.64	0.62
7:F:97:ARG:O	7:F:101:ILE:HG13	1.99	0.62
5:C:166:GLU:HA	11:K:6:ARG:HB3	1.82	0.62
3:A:1212:VAL:O	3:A:1216:ILE:HG13	1.99	0.62
4:B:1002:THR:HG23	4:B:1004:GLU:H	1.64	0.62
3:A:871:ASP:HB3	6:E:204:THR:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:235:VAL:HG21	10:J:6:ARG:HH21	1.65	0.62
3:A:33:ALA:O	3:A:83:HIS:HB3	1.99	0.62
3:A:268:ASP:HB3	3:A:299:HIS:ND1	2.14	0.62
4:B:208:SER:OG	4:B:210:LYS:HD3	1.99	0.62
4:B:373:ARG:NE	4:B:567:GLU:OE2	2.29	0.62
6:E:78:LEU:C	6:E:78:LEU:HD23	2.20	0.62
3:A:672:ASP:OD1	3:A:674:PRO:HD2	2.00	0.62
4:B:195:CYS:HB3	4:B:782:LEU:HD22	1.81	0.62
4:B:616:ILE:N	4:B:616:ILE:HD12	2.15	0.62
4:B:549:THR:HB	4:B:628:THR:CG2	2.30	0.62
7:F:135:ARG:HG2	7:F:137:TYR:CE1	2.34	0.62
12:L:34:CYS:SG	12:L:51:CYS:SG	2.98	0.62
2:T:11:DC:H2''	2:T:12:DG:C5'	2.29	0.62
4:B:1072:MET:CE	4:B:1085:ILE:HB	2.28	0.62
4:B:25:ILE:HG22	4:B:26:THR:H	1.65	0.62
6:E:93:MET:O	6:E:97:VAL:HG23	2.00	0.62
7:F:111:LEU:H	7:F:111:LEU:CD1	2.13	0.62
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.34	0.62
3:A:328:ARG:O	3:A:335:ARG:HG2	1.99	0.61
3:A:338:GLY:HA2	4:B:1129:ARG:NH2	2.10	0.61
3:A:590:ARG:HB3	3:A:605:MET:H	1.63	0.61
4:B:221:ASN:OD1	4:B:242:SER:HA	1.98	0.61
4:B:446:LEU:O	4:B:447:ALA:CB	2.48	0.61
7:F:109:VAL:HG23	7:F:124:GLU:HG2	1.82	0.61
8:H:49:VAL:HG12	8:H:50:ALA:H	1.62	0.61
11:K:63:VAL:O	11:K:63:VAL:CG2	2.48	0.61
3:A:1054:LEU:O	3:A:1057:VAL:HG23	1.99	0.61
3:A:689:LYS:O	3:A:693:VAL:HG23	1.99	0.61
3:A:855:THR:CG2	3:A:857:ARG:HG3	2.30	0.61
3:A:898:ARG:HB2	3:A:933:TYR:CE1	2.34	0.61
4:B:211:VAL:O	4:B:480:SER:HA	2.01	0.61
4:B:29:ASP:HB3	4:B:658:ILE:CD1	2.30	0.61
3:A:354:SER:HA	3:A:482:PHE:CD2	2.34	0.61
3:A:549:MET:SD	3:A:577:ILE:CD1	2.87	0.61
3:A:88:LYS:HD2	3:A:293:GLU:CD	2.20	0.61
3:A:961:ARG:O	3:A:965:GLN:HG3	2.00	0.61
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.29	0.61
1:R:9:G:OP1	4:B:776:GLN:NE2	2.33	0.61
3:A:709:THR:OG1	3:A:712:GLU:HG3	2.00	0.61
4:B:839:MET:HE3	4:B:1010:LEU:CD1	2.30	0.61
6:E:178:ILE:HG23	6:E:214:CYS:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:5:ASN:ND2	6:E:52:ARG:HG2	2.12	0.61
3:A:1021:LEU:O	3:A:1025:ARG:HG2	2.00	0.61
3:A:1437:GLY:HA3	7:F:88:TYR:CD2	2.36	0.61
3:A:789:LYS:HG3	9:I:67:THR:HB	1.83	0.61
4:B:803:LEU:H	4:B:822:ASN:HD21	1.48	0.61
9:I:8:ARG:HG3	9:I:9:ASP:N	2.16	0.61
3:A:821:ARG:HG3	3:A:825:ILE:HD11	1.82	0.61
5:C:49:VAL:HG21	5:C:67:LEU:HD12	1.82	0.61
3:A:1364:ASN:HD22	3:A:1364:ASN:C	2.04	0.61
3:A:915:SER:O	3:A:919:ILE:HG13	2.00	0.61
4:B:582:VAL:HG22	4:B:626:ILE:HB	1.82	0.61
3:A:1111:MET:HE1	3:A:1330:ASN:OD1	2.00	0.61
3:A:148:CYS:O	3:A:168:GLY:HA2	1.99	0.61
12:L:51:CYS:HB2	12:L:53:HIS:CD2	2.35	0.61
3:A:1192:LEU:HD22	3:A:1239:ARG:NH2	2.16	0.61
3:A:506:ALA:HB1	3:A:508:PRO:HD2	1.83	0.61
4:B:185:THR:HG23	4:B:188:ASP:OD2	2.01	0.61
7:F:138:LEU:HB3	7:F:139:PRO:HD2	1.83	0.61
9:I:103:CYS:SG	9:I:106:CYS:SG	2.99	0.61
10:J:48:ARG:HE	10:J:49:MET:HE2	1.66	0.61
3:A:1317:MET:HA	3:A:1322:ILE:HD11	1.81	0.61
3:A:565:ILE:CG2	3:A:567:LYS:HG2	2.31	0.61
3:A:736:ASN:O	3:A:737:LEU:C	2.38	0.61
4:B:1102:LYS:O	4:B:1104:HIS:N	2.32	0.61
4:B:57:TYR:CD1	4:B:57:TYR:N	2.68	0.61
5:C:123:ASN:HD22	5:C:125:MET:HG2	1.66	0.61
5:C:46:ILE:HA	5:C:159:ALA:HA	1.82	0.61
3:A:337:ARG:CZ	3:A:839:ARG:NH1	2.64	0.60
3:A:824:LEU:O	3:A:827:THR:HB	2.00	0.60
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.83	0.60
4:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.31	0.60
3:A:306:ASN:OD1	3:A:324:SER:HB3	2.01	0.60
4:B:995:ARG:NH1	4:B:995:ARG:HB2	2.16	0.60
3:A:1132:LYS:O	3:A:1135:ARG:HB3	2.01	0.60
3:A:219:PHE:O	3:A:222:LEU:N	2.33	0.60
3:A:445:ASN:HB2	3:A:454:SER:O	2.00	0.60
3:A:511:ILE:HA	3:A:521:MET:HE3	1.83	0.60
8:H:106:GLU:C	8:H:108:SER:H	2.02	0.60
3:A:1293:SER:OG	3:A:1294:PRO:HD2	2.01	0.60
3:A:528:LEU:O	3:A:531:ILE:HG22	2.01	0.60
3:A:1158:PRO:HB3	3:A:1241:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:322:VAL:O	3:A:323:LYS:HG3	2.01	0.60
4:B:913:GLY:HA2	4:B:938:SER:CB	2.31	0.60
6:E:78:LEU:HD23	6:E:79:TRP:N	2.16	0.60
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.01	0.60
3:A:1208:THR:O	3:A:1212:VAL:HG23	2.01	0.60
3:A:567:LYS:O	3:A:569:LYS:N	2.35	0.60
3:A:86:LEU:HA	3:A:273:ASN:OD1	2.02	0.60
4:B:114:PRO:HB3	4:B:174:LEU:HD11	1.82	0.60
11:K:90:ALA:O	11:K:94:ILE:HG13	2.01	0.60
3:A:896:ARG:NH2	3:A:1030:ARG:HH21	2.00	0.60
6:E:47:CYS:HA	6:E:53:PRO:HA	1.83	0.60
7:F:101:ILE:HD12	7:F:121:ALA:HB2	1.82	0.60
2:T:1:DA:C6	2:T:2:DC:C4	2.90	0.60
3:A:1223:ASP:HA	3:A:1243:VAL:CG1	2.32	0.60
10:J:1:MET:N	10:J:56:LEU:HB2	2.17	0.60
3:A:1115:SER:O	3:A:1329:THR:HG23	2.02	0.60
4:B:1169:MET:HE1	4:B:1201:LYS:O	2.01	0.60
4:B:299:GLU:OE1	4:B:571:PRO:HG2	2.01	0.60
4:B:778:MET:CE	4:B:1094:ARG:HD3	2.32	0.60
4:B:787:VAL:O	4:B:787:VAL:HG12	2.00	0.60
3:A:231:PRO:HA	3:A:234:MET:HE2	1.83	0.60
3:A:31:SER:OG	3:A:83:HIS:HB2	2.02	0.60
3:A:567:LYS:CG	3:A:568:PRO:HD2	2.31	0.60
3:A:779:PHE:CZ	4:B:517:THR:HA	2.37	0.60
4:B:686:ASN:C	4:B:688:GLY:H	2.04	0.60
9:I:85:PHE:CD1	9:I:99:LEU:HD22	2.37	0.60
3:A:503:GLN:HE21	7:F:90:ARG:HH21	1.47	0.59
4:B:1174:LYS:HB2	4:B:1179:GLN:O	2.02	0.59
4:B:479:VAL:HG12	4:B:480:SER:N	2.17	0.59
4:B:198:ASP:OD1	4:B:485:ARG:NH2	2.34	0.59
5:C:244:VAL:O	5:C:248:ILE:HG13	2.03	0.59
2:T:1:DA:C6	2:T:2:DC:N4	2.70	0.59
3:A:1402:PHE:CE2	3:A:1403:GLU:HG3	2.37	0.59
3:A:68:GLN:HE22	3:A:80:HIS:HB3	1.67	0.59
8:H:89:LEU:C	8:H:91:ASP:N	2.55	0.59
9:I:15:TYR:O	9:I:27:PHE:HA	2.02	0.59
2:T:11:DC:H2'	2:T:12:DG:H8	1.66	0.59
3:A:239:LEU:HD12	3:A:240:PRO:HD2	1.83	0.59
3:A:76:GLU:O	3:A:76:GLU:HG3	2.02	0.59
4:B:975:GLN:HG2	4:B:976:ILE:H	1.67	0.59
10:J:1:MET:H2	10:J:56:LEU:HB2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:44:THR:O	3:A:44:THR:HG22	2.02	0.59
3:A:567:LYS:CB	3:A:568:PRO:CD	2.67	0.59
4:B:463:THR:HG22	4:B:465:ASN:HD22	1.66	0.59
8:H:84:ALA:HA	8:H:87:ARG:CG	2.32	0.59
3:A:469:ARG:NH2	4:B:976:ILE:HD13	2.17	0.59
9:I:106:CYS:HG	15:I:204:ZN:ZN	1.16	0.59
2:T:1:DA:C2'	2:T:2:DC:O5'	2.38	0.59
3:A:151:ASP:HA	3:A:162:VAL:O	2.02	0.59
3:A:68:GLN:HE22	3:A:80:HIS:CB	2.15	0.59
4:B:217:ARG:NH1	4:B:407:ASP:OD1	2.35	0.59
4:B:512:ARG:NH2	4:B:535:LEU:CD1	2.61	0.59
5:C:166:GLU:CG	11:K:10:PHE:HZ	2.14	0.59
5:C:56:THR:CG2	5:C:57:VAL:H	2.09	0.59
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.84	0.59
12:L:26:THR:O	12:L:27:LEU:HB3	2.01	0.59
3:A:57:ARG:O	3:A:68:GLN:HG3	2.03	0.59
3:A:704:ALA:HB2	3:A:710:LEU:CG	2.23	0.59
4:B:90:ILE:HD12	4:B:432:MET:SD	2.42	0.59
4:B:211:VAL:CG2	4:B:483:LEU:HD13	2.32	0.59
4:B:642:ASP:O	4:B:644:GLU:N	2.36	0.59
4:B:912:ILE:HD11	4:B:966:VAL:HG23	1.84	0.59
8:H:139:ASN:O	8:H:140:ALA:HB2	2.02	0.59
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.66	0.59
3:A:1018:PHE:O	3:A:1021:LEU:HB3	2.03	0.59
3:A:1336:MET:CE	3:A:1381:LEU:HG	2.33	0.59
3:A:1385:THR:HG22	3:A:1386:ARG:H	1.68	0.59
3:A:93:VAL:HG11	3:A:308:ILE:CD1	2.33	0.59
6:E:29:PHE:HB2	6:E:65:THR:HG22	1.83	0.59
8:H:109:LYS:NZ	8:H:109:LYS:HB2	2.18	0.59
3:A:1394:THR:HG22	3:A:1395:GLY:N	2.17	0.59
3:A:596:THR:O	3:A:598:LEU:N	2.36	0.59
4:B:1117:GLN:HG3	4:B:1156:ASP:OD1	2.02	0.59
4:B:46:GLN:O	4:B:408:LEU:HD23	2.03	0.59
4:B:642:ASP:HB3	4:B:649:LYS:HD2	1.85	0.59
3:A:1004:ASN:ND2	6:E:167:ARG:HD2	2.18	0.59
4:B:848:ARG:NH1	10:J:8:PHE:O	2.35	0.59
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.33	0.59
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.35	0.59
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.83	0.59
3:A:896:ARG:HD3	3:A:897:TYR:HE1	1.67	0.59
4:B:1171:VAL:CG1	4:B:1191:ILE:HD13	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1159:ARG:CD	4:B:1193:GLN:HE21	2.15	0.59
4:B:519:TRP:C	4:B:519:TRP:CD1	2.76	0.59
5:C:18:VAL:HG23	5:C:240:VAL:CG1	2.33	0.59
6:E:61:GLN:HB2	6:E:79:TRP:CE3	2.38	0.59
3:A:840:ARG:HB3	3:A:1384:VAL:HG12	1.85	0.58
3:A:90:VAL:HG11	3:A:297:GLN:HA	1.84	0.58
3:A:385:ILE:HG22	3:A:386:ASP:N	2.18	0.58
3:A:482:PHE:CD1	4:B:836:GLU:HB2	2.38	0.58
6:E:156:LEU:HD12	6:E:195:VAL:CG1	2.33	0.58
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.33	0.58
3:A:756:ILE:HG22	3:A:757:ASN:N	2.17	0.58
3:A:901:LEU:H	3:A:926:GLN:HE21	1.50	0.58
4:B:860:MET:HG2	4:B:861:ASP:N	2.18	0.58
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.33	0.58
3:A:107:CYS:HB2	3:A:114:LEU:CD2	2.32	0.58
3:A:444:PHE:HB3	3:A:458:HIS:HD2	1.68	0.58
4:B:1106:ARG:HH12	4:B:1118:PRO:HB3	1.67	0.58
4:B:806:THR:HB	4:B:809:MET:HG3	1.85	0.58
4:B:958:GLN:O	4:B:960:GLY:N	2.33	0.58
3:A:1325:THR:O	6:E:148:GLU:HB2	2.04	0.58
3:A:97:ALA:HA	3:A:100:LYS:HE3	1.84	0.58
3:A:1308:THR:HG21	3:A:1310:GLY:O	2.04	0.58
3:A:663:SER:OG	3:A:664:THR:N	2.34	0.58
4:B:405:ARG:NH1	4:B:632:ARG:HG2	2.17	0.58
4:B:666:TYR:C	4:B:668:ASP:H	2.06	0.58
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.85	0.58
3:A:1161:THR:HG22	3:A:1163:ILE:N	2.03	0.58
4:B:287:ARG:NH1	4:B:324:ILE:O	2.37	0.58
4:B:779:GLY:HA2	4:B:796:LEU:HB2	1.85	0.58
6:E:46:TYR:HA	6:E:57:MET:SD	2.43	0.58
10:J:48:ARG:HE	10:J:49:MET:CE	2.16	0.58
11:K:47:ARG:HD3	11:K:59:ALA:O	2.04	0.58
3:A:1155:ASP:OD2	3:A:1161:THR:HG23	2.04	0.58
3:A:1364:ASN:ND2	3:A:1364:ASN:C	2.56	0.58
3:A:742:ASN:CA	3:A:745:GLN:HB2	2.33	0.58
4:B:205:ILE:N	4:B:205:ILE:HD12	2.19	0.58
4:B:744:HIS:CD2	4:B:746:SER:H	2.13	0.58
7:F:81:THR:HG22	7:F:82:THR:N	2.18	0.58
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.38	0.58
12:L:49:LYS:O	12:L:50:ASP:HB2	2.03	0.58
3:A:225:ASN:ND2	3:A:227:VAL:HB	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:ASP:OD1	3:A:261:ASP:N	2.37	0.58
3:A:849:MET:HE1	3:A:1061:GLY:HA2	1.86	0.58
4:B:1201:LYS:HE2	4:B:1205:GLN:NE2	2.18	0.58
4:B:589:VAL:HG12	4:B:590:HIS:N	2.18	0.58
3:A:1042:PHE:HE2	3:A:1046:LEU:HD11	1.66	0.58
3:A:1074:GLU:O	3:A:1076:ALA:N	2.37	0.58
3:A:28:ARG:HG2	3:A:83:HIS:CE1	2.39	0.58
4:B:101:MET:HB2	4:B:169:ARG:HH12	1.69	0.58
7:F:111:LEU:C	7:F:113:GLY:H	2.07	0.58
7:F:127:GLU:O	7:F:129:LYS:HG3	2.03	0.58
3:A:1149:ALA:HB2	9:I:47:GLU:HA	1.84	0.58
9:I:47:GLU:OE1	9:I:50:THR:HG23	2.04	0.58
4:B:955:THR:OG1	12:L:55:ILE:HA	2.04	0.58
3:A:418:SER:O	3:A:419:LYS:C	2.39	0.58
3:A:524:VAL:HG12	3:A:525:GLN:H	1.69	0.58
4:B:1077:THR:HG22	4:B:1079:LYS:N	2.13	0.58
4:B:93:GLY:N	4:B:131:ASP:O	2.37	0.58
4:B:980:PHE:CE1	4:B:990:ILE:HD11	2.39	0.58
5:C:148:ARG:HG3	10:J:61:LEU:O	2.03	0.58
3:A:1420:ASP:O	3:A:1421:CYS:HB2	2.04	0.57
4:B:973:ILE:HG23	4:B:974:PRO:HD2	1.86	0.57
8:H:81:PRO:CB	8:H:82:PRO:CD	2.81	0.57
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.39	0.57
3:A:1143:LEU:HD23	3:A:1267:MET:HB3	1.86	0.57
3:A:225:ASN:HD22	3:A:227:VAL:HB	1.69	0.57
4:B:803:LEU:N	4:B:822:ASN:HD21	2.02	0.57
4:B:855:PHE:HZ	4:B:857:ARG:HH11	1.52	0.57
5:C:175:ALA:HB3	10:J:43:ARG:NH2	2.20	0.57
6:E:213:ILE:O	6:E:213:ILE:HG23	2.04	0.57
1:R:9:G:N1	1:R:10:A:C6	2.71	0.57
3:A:1400:CYS:SG	3:A:1409:LEU:HG	2.44	0.57
3:A:41:MET:HB3	3:A:48:ALA:O	2.04	0.57
4:B:1147:LEU:HD22	4:B:1151:LEU:CD2	2.34	0.57
4:B:25:ILE:HG22	4:B:29:ASP:CB	2.34	0.57
4:B:653:VAL:HG22	4:B:689:LEU:HB3	1.85	0.57
4:B:701:ILE:HD11	4:B:703:ILE:HD11	1.86	0.57
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.85	0.57
3:A:1399:ARG:CB	3:A:1408:ILE:HD13	2.28	0.57
3:A:353:ILE:HG22	3:A:468:PHE:HB2	1.85	0.57
6:E:61:GLN:HB2	6:E:79:TRP:HE3	1.69	0.57
9:I:78:CYS:SG	9:I:106:CYS:SG	3.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1:DA:C4	2:T:2:DC:C6	2.92	0.57
3:A:399:HIS:O	3:A:435:HIS:HD2	1.87	0.57
3:A:337:ARG:CD	3:A:839:ARG:HH22	2.17	0.57
3:A:92:HIS:HD2	3:A:94:GLY:H	1.53	0.57
4:B:1079:LYS:HA	5:C:27:LEU:HD21	1.87	0.57
4:B:1077:THR:CG2	4:B:1079:LYS:HB2	2.34	0.57
4:B:23:ALA:O	4:B:654:ARG:HB3	2.04	0.57
7:F:111:LEU:N	7:F:111:LEU:CD1	2.67	0.57
11:K:65:HIS:HD2	11:K:67:PHE:N	2.02	0.57
3:A:1111:MET:CE	3:A:1114:PRO:HA	2.35	0.57
3:A:76:GLU:O	3:A:76:GLU:CG	2.53	0.57
3:A:901:LEU:N	3:A:926:GLN:NE2	2.50	0.57
5:C:251:LEU:O	5:C:255:VAL:HG23	2.04	0.57
2:T:1:DA:C5	2:T:2:DC:C5	2.93	0.57
3:A:1332:PHE:N	3:A:1332:PHE:CD2	2.72	0.57
4:B:1116:ARG:HD2	4:B:1198:TYR:CG	2.40	0.57
4:B:801:LYS:O	10:J:52:THR:CG2	2.52	0.57
4:B:979:LYS:HG2	4:B:1095:LEU:HD12	1.87	0.57
5:C:258:ILE:O	5:C:261:ALA:HB3	2.04	0.57
6:E:157:SER:C	6:E:159:ASP:H	2.07	0.57
7:F:97:ARG:NE	7:F:124:GLU:OE1	2.31	0.57
11:K:46:ILE:HG22	11:K:50:LEU:HD12	1.86	0.57
3:A:1295:THR:HG23	3:A:1297:GLU:OE1	2.03	0.57
3:A:1281:ARG:HB2	3:A:1309:ASP:HB2	1.86	0.57
3:A:1315:GLU:O	3:A:1318:THR:HG23	2.04	0.57
3:A:1329:THR:HG22	3:A:1331:SER:N	2.01	0.57
3:A:1342:GLU:HG2	6:E:212:ARG:NH1	2.20	0.57
3:A:537:ARG:HB2	8:H:20:TYR:CE2	2.39	0.57
3:A:879:GLU:OE2	3:A:962:ARG:NH2	2.37	0.57
4:B:756:ILE:O	4:B:759:PRO:HD3	2.04	0.57
4:B:806:THR:OG1	4:B:809:MET:HE3	2.04	0.57
5:C:37:MET:HG2	5:C:243:VAL:CG1	2.34	0.57
9:I:111:THR:HG22	9:I:112:SER:N	2.19	0.57
2:T:1:DA:N3	2:T:2:DC:C5	2.71	0.57
3:A:101:LYS:O	3:A:105:CYS:HB2	2.04	0.57
3:A:414:ASP:O	3:A:417:TYR:O	2.22	0.57
3:A:710:LEU:HD12	3:A:710:LEU:N	2.20	0.57
3:A:882:SER:HA	3:A:952:ALA:O	2.05	0.57
3:A:69:THR:HB	4:B:1174:LYS:HE2	1.87	0.57
11:K:50:LEU:CD1	11:K:73:LEU:HD21	2.35	0.57
1:R:5:A:C4	1:R:6:G:C8	2.93	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:166:GLY:O	3:A:167:CYS:HB3	2.03	0.57
3:A:93:VAL:HG22	3:A:301:ALA:HA	1.85	0.57
4:B:57:TYR:HD1	4:B:57:TYR:N	2.03	0.57
8:H:6:PHE:HE1	8:H:130:ARG:HE	1.53	0.57
8:H:89:LEU:HD22	8:H:91:ASP:OD2	2.05	0.57
2:T:6:DC:C5	2:T:7:DC:C5	2.93	0.57
3:A:1342:GLU:HG3	6:E:198:ILE:HG21	1.86	0.56
3:A:1364:ASN:ND2	3:A:1366:ARG:N	2.53	0.56
3:A:672:ASP:HB3	3:A:675:THR:OG1	2.05	0.56
3:A:886:ILE:CD1	3:A:943:LEU:HB3	2.31	0.56
4:B:130:VAL:HG12	4:B:131:ASP:H	1.67	0.56
7:F:87:LYS:HE2	7:F:88:TYR:CZ	2.39	0.56
1:R:10:A:H61	2:T:6:DC:N4	2.03	0.56
3:A:98:LYS:O	3:A:102:VAL:HG23	2.05	0.56
3:A:40:THR:HG21	3:A:259:GLU:OE2	2.04	0.56
3:A:577:ILE:O	3:A:580:VAL:HG23	2.04	0.56
3:A:974:ASP:HB2	8:H:136:LYS:NZ	2.20	0.56
4:B:1051:THR:HG22	4:B:1052:VAL:N	2.17	0.56
3:A:401:GLY:O	3:A:435:HIS:CD2	2.58	0.56
4:B:23:ALA:HB1	4:B:24:PRO:HD2	1.85	0.56
4:B:429:PHE:HA	4:B:432:MET:CE	2.35	0.56
4:B:522:VAL:HG11	4:B:537:LYS:HB3	1.86	0.56
4:B:955:THR:HG1	12:L:55:ILE:HA	1.71	0.56
5:C:229:TYR:N	5:C:229:TYR:CD1	2.74	0.56
5:C:242:GLN:HE21	5:C:246:ARG:HE	1.54	0.56
8:H:5:LEU:CD1	8:H:135:LEU:HG	2.34	0.56
8:H:97:MET:CE	8:H:142:LEU:HD23	2.35	0.56
8:H:82:PRO:O	8:H:83:GLN:HB2	2.04	0.56
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.69	0.56
3:A:1389:PHE:O	3:A:1392:SER:HB3	2.05	0.56
3:A:452:LYS:HB3	4:B:1141:HIS:CE1	2.40	0.56
4:B:243:ALA:HA	4:B:250:PHE:O	2.05	0.56
4:B:704:ALA:HB1	4:B:710:LEU:HD12	1.87	0.56
6:E:46:TYR:CE2	6:E:58:MET:HA	2.40	0.56
4:B:311:LEU:HB3	9:I:4:PHE:CE2	2.40	0.56
9:I:7:CYS:O	9:I:8:ARG:O	2.24	0.56
1:R:5:A:C2	1:R:6:G:C4	2.93	0.56
3:A:665:GLY:HA3	4:B:1086:PHE:CD1	2.41	0.56
5:C:145:CYS:SG	5:C:146:LYS:N	2.79	0.56
8:H:89:LEU:HD22	8:H:91:ASP:CG	2.25	0.56
3:A:885:THR:O	3:A:885:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:984:HIS:HB3	4:B:1022:THR:OG1	2.05	0.56
5:C:131:HIS:O	5:C:132:PRO:C	2.43	0.56
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.44	0.56
5:C:99:LEU:HD23	5:C:99:LEU:N	2.20	0.56
3:A:1300:LYS:NZ	3:A:1300:LYS:HB3	2.20	0.56
3:A:35:ILE:HG12	3:A:52:GLY:O	2.06	0.56
3:A:547:LEU:HD22	11:K:58:PHE:CD1	2.41	0.56
3:A:875:ALA:HB2	3:A:1366:ARG:HD2	1.88	0.56
4:B:864:LYS:HD3	4:B:871:THR:OG1	2.05	0.56
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.86	0.56
3:A:185:TRP:CZ3	3:A:200:ARG:HG2	2.40	0.56
3:A:401:GLY:C	3:A:435:HIS:CD2	2.79	0.56
4:B:839:MET:CE	4:B:980:PHE:HB2	2.35	0.56
5:C:242:GLN:NE2	5:C:246:ARG:HE	2.02	0.56
3:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.70	0.56
5:C:248:ILE:CD1	11:K:101:LEU:HD22	2.35	0.56
3:A:1328:TYR:CG	3:A:1329:THR:N	2.74	0.56
3:A:1365:TYR:O	3:A:1366:ARG:C	2.43	0.56
4:B:983:ARG:HD2	4:B:1091:TYR:HB3	1.86	0.56
4:B:1180:PHE:O	4:B:1181:GLU:HB2	2.05	0.56
4:B:361:LEU:N	4:B:362:PRO:CD	2.69	0.56
4:B:566:LEU:HD22	4:B:586:TRP:O	2.06	0.56
7:F:99:LEU:HD12	7:F:99:LEU:O	2.06	0.56
8:H:59:ILE:HG22	8:H:60:ALA:N	2.20	0.56
9:I:111:THR:CG2	9:I:112:SER:N	2.69	0.56
3:A:1261:LYS:HA	3:A:1264:GLU:HB3	1.88	0.56
4:B:1022:THR:HG23	4:B:1022:THR:O	2.05	0.56
4:B:1171:VAL:HG11	4:B:1191:ILE:HD13	1.88	0.56
3:A:825:ILE:HD12	4:B:513:GLN:NE2	2.21	0.56
1:R:8:G:N2	2:T:8:DT:C4	2.74	0.56
3:A:1017:LEU:HD23	6:E:204:THR:O	2.06	0.55
4:B:515:HIS:H	4:B:518:HIS:CD2	2.24	0.55
6:E:61:GLN:NE2	6:E:105:PHE:CE2	2.71	0.55
3:A:50:ILE:C	3:A:52:GLY:H	2.09	0.55
3:A:1436:ILE:HG22	4:B:1142:GLY:HA2	1.87	0.55
4:B:120:ARG:NH1	12:L:54:ARG:NH1	2.54	0.55
4:B:34:ILE:O	4:B:37:PHE:HB3	2.06	0.55
4:B:63:ILE:HA	4:B:421:PHE:CE2	2.42	0.55
4:B:556:THR:HG22	4:B:557:PHE:N	2.20	0.55
4:B:566:LEU:HD13	4:B:588:GLY:CA	2.37	0.55
4:B:980:PHE:HE1	4:B:990:ILE:HD11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:106:GLU:C	8:H:108:SER:N	2.57	0.55
3:A:216:VAL:O	3:A:219:PHE:HB2	2.06	0.55
3:A:843:LYS:HG3	3:A:1402:PHE:HD1	1.72	0.55
3:A:849:MET:CE	3:A:1061:GLY:HA2	2.36	0.55
4:B:898:LEU:HD22	4:B:964:VAL:HG11	1.89	0.55
5:C:162:GLY:HA3	5:C:170:TRP:CE2	2.41	0.55
9:I:7:CYS:C	9:I:8:ARG:O	2.43	0.55
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.89	0.55
3:A:1096:SER:O	3:A:1099:PRO:HG2	2.06	0.55
3:A:548:ASN:HA	11:K:60:ALA:HB1	1.87	0.55
4:B:121:ASN:ND2	4:B:121:ASN:N	2.50	0.55
4:B:794:ASN:C	4:B:795:ILE:HD12	2.26	0.55
4:B:864:LYS:N	4:B:872:GLU:OE1	2.39	0.55
4:B:120:ARG:HE	4:B:955:THR:CG2	2.20	0.55
3:A:1339:LEU:HD13	6:E:147:HIS:CD2	2.41	0.55
6:E:195:VAL:HG22	6:E:213:ILE:CB	2.37	0.55
12:L:26:THR:HG22	12:L:27:LEU:N	2.21	0.55
3:A:463:ILE:HD11	3:A:469:ARG:HG3	1.89	0.55
3:A:556:TRP:CE3	3:A:558:GLY:HA2	2.40	0.55
3:A:838:GLN:O	3:A:842:VAL:HG23	2.06	0.55
3:A:963:ILE:HD12	3:A:1049:ILE:HG12	1.88	0.55
5:C:238:ILE:HG23	5:C:242:GLN:HB2	1.89	0.55
3:A:1364:ASN:HD21	3:A:1366:ARG:HG2	1.67	0.55
5:C:55:THR:HB	5:C:152:GLU:H	1.70	0.55
5:C:57:VAL:HG11	10:J:60:PHE:HB2	1.88	0.55
5:C:70:ILE:HD11	5:C:144:ILE:HG12	1.88	0.55
8:H:89:LEU:O	8:H:91:ASP:N	2.37	0.55
3:A:556:TRP:CD2	3:A:558:GLY:HA2	2.42	0.55
4:B:25:ILE:HD11	4:B:653:VAL:HB	1.89	0.55
4:B:864:LYS:HG3	4:B:865:LYS:N	2.21	0.55
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.47	0.55
11:K:61:TYR:HA	11:K:72:LYS:O	2.06	0.55
12:L:63:ARG:O	12:L:64:LEU:O	2.25	0.55
3:A:23:SER:HB3	3:A:233:TRP:CE2	2.41	0.55
10:J:32:GLU:O	10:J:36:LEU:HG	2.07	0.55
3:A:451:HIS:CE1	3:A:1074:GLU:HG3	2.42	0.55
3:A:517:ASN:ND2	3:A:1362:TYR:HE2	2.05	0.55
3:A:710:LEU:H	3:A:710:LEU:CD1	2.19	0.55
3:A:89:PRO:O	3:A:204:THR:HG21	2.07	0.55
6:E:195:VAL:HG22	6:E:213:ILE:HB	1.88	0.55
4:B:308:TRP:CH2	9:I:45:ARG:HG2	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1308:THR:CG2	3:A:1310:GLY:O	2.54	0.54
3:A:399:HIS:O	3:A:435:HIS:CD2	2.60	0.54
3:A:533:LYS:O	3:A:535:THR:N	2.40	0.54
3:A:885:THR:O	3:A:940:ARG:HG3	2.07	0.54
4:B:195:CYS:CB	4:B:782:LEU:HD22	2.37	0.54
3:A:356:ASP:OD2	11:K:65:HIS:HE1	1.90	0.54
3:A:1116:LEU:O	3:A:1308:THR:HB	2.07	0.54
3:A:1193:LEU:HD21	3:A:1267:MET:HE2	1.88	0.54
3:A:233:TRP:C	3:A:235:ILE:N	2.60	0.54
3:A:337:ARG:NE	3:A:839:ARG:NH2	2.55	0.54
3:A:902:LEU:HD21	3:A:923:LEU:HD23	1.90	0.54
4:B:756:ILE:HG21	4:B:759:PRO:HB3	1.90	0.54
4:B:780:VAL:HG21	10:J:56:LEU:HD13	1.88	0.54
4:B:911:ILE:HD11	4:B:941:LEU:CD1	2.37	0.54
6:E:46:TYR:CD2	6:E:58:MET:HG2	2.42	0.54
3:A:974:ASP:HB2	8:H:136:LYS:HZ1	1.73	0.54
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.88	0.54
3:A:350:ARG:HB2	3:A:488:ASN:OD1	2.08	0.54
3:A:443:LEU:HD13	3:A:455:MET:HE1	1.90	0.54
3:A:515:GLN:HG3	3:A:516:SER:N	2.22	0.54
3:A:741:ASN:ND2	3:A:743:VAL:H	2.05	0.54
4:B:1051:THR:CG2	4:B:1052:VAL:N	2.70	0.54
4:B:542:MET:HE2	4:B:747:MET:HE2	1.89	0.54
5:C:101:LEU:HD13	5:C:118:LEU:HD23	1.88	0.54
5:C:183:TRP:CZ2	5:C:207:CYS:HB3	2.42	0.54
6:E:168:TYR:HB3	6:E:170:LEU:CD2	2.36	0.54
7:F:118:LEU:O	7:F:122:MET:HG3	2.08	0.54
2:T:1:DA:HI'	3:A:1386:ARG:NH1	2.22	0.54
3:A:563:PRO:HG3	3:A:572:TRP:CE2	2.42	0.54
4:B:1034:VAL:HG12	4:B:1035:ALA:N	2.23	0.54
4:B:179:CYS:SG	4:B:181:LEU:HB2	2.47	0.54
5:C:13:ALA:O	11:K:114:LEU:HD13	2.08	0.54
6:E:197:LYS:HG3	6:E:211:TYR:CE2	2.42	0.54
12:L:27:LEU:HD13	12:L:37:LYS:HB3	1.90	0.54
1:R:9:G:H1	1:R:10:A:N6	2.04	0.54
3:A:1341:ILE:HD12	3:A:1379:GLY:O	2.07	0.54
3:A:1375:MET:HG2	3:A:1382:THR:O	2.08	0.54
3:A:619:LYS:O	3:A:623:GLY:N	2.38	0.54
3:A:809:THR:O	3:A:810:PRO:C	2.46	0.54
2:T:3:DG:C5'	3:A:836:TYR:CD1	2.87	0.54
3:A:898:ARG:HD2	3:A:899:VAL:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:102:VAL:HG22	4:B:112:LEU:HD22	1.88	0.54
6:E:153:HIS:CE1	6:E:184:VAL:HG11	2.43	0.54
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.22	0.54
3:A:1116:LEU:H	3:A:1308:THR:HG22	1.72	0.54
3:A:154:SER:HB3	3:A:162:VAL:HG23	1.89	0.54
3:A:38:PRO:N	3:A:270:LEU:HD23	2.22	0.54
3:A:821:ARG:O	3:A:822:GLU:C	2.46	0.54
3:A:92:HIS:CD2	3:A:94:GLY:H	2.26	0.54
4:B:172:ILE:HD13	4:B:178:ASN:CB	2.37	0.54
3:A:15:LYS:HD2	4:B:1220:ARG:HE	1.72	0.54
4:B:758:PHE:C	4:B:760:ASP:H	2.11	0.54
4:B:784:ASN:ND2	4:B:788:ARG:HD2	2.23	0.54
4:B:837:ASP:OD1	4:B:1020:ARG:NH2	2.41	0.54
6:E:176:PRO:HD2	6:E:211:TYR:O	2.07	0.54
7:F:109:VAL:HG13	7:F:127:GLU:OE1	2.07	0.54
3:A:852:TYR:CE2	7:F:136:ARG:HG2	2.42	0.54
4:B:783:THR:HA	10:J:60:PHE:HE1	1.72	0.54
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.67	0.54
3:A:367:PRO:HB3	3:A:465:TYR:O	2.08	0.54
7:F:72:LYS:N	7:F:142:SER:HA	2.22	0.54
1:R:9:G:C4	1:R:10:A:N7	2.76	0.54
3:A:226:GLU:HG2	3:A:227:VAL:HG23	1.90	0.54
3:A:590:ARG:O	3:A:591:PHE:HB2	2.08	0.54
3:A:646:PHE:O	3:A:650:GLN:HG3	2.08	0.54
3:A:867:ILE:HG22	3:A:872:GLY:N	2.22	0.54
4:B:406:LEU:HD12	4:B:545:ILE:HD11	1.89	0.54
4:B:680:THR:HG22	4:B:681:TRP:H	1.72	0.54
12:L:51:CYS:C	12:L:53:HIS:H	2.12	0.54
1:R:8:G:C2'	1:R:9:G:H5'	2.36	0.54
3:A:1366:ARG:O	3:A:1369:ALA:HB3	2.08	0.54
4:B:288:ALA:HB1	4:B:331:LEU:CD1	2.38	0.54
4:B:549:THR:HB	4:B:628:THR:HG23	1.89	0.54
4:B:28:GLU:CD	4:B:807:ARG:HH22	2.10	0.54
5:C:248:ILE:HD13	11:K:101:LEU:HD22	1.89	0.54
7:F:107:VAL:HG12	7:F:109:VAL:H	1.72	0.54
8:H:32:THR:HG22	8:H:33:GLN:HG3	1.90	0.54
9:I:2:THR:HG22	9:I:2:THR:O	2.07	0.54
3:A:1073:GLY:O	3:A:1076:ALA:HB3	2.07	0.53
3:A:1222:ASN:O	3:A:1223:ASP:HB3	2.06	0.53
3:A:225:ASN:C	3:A:227:VAL:H	2.10	0.53
3:A:738:LYS:HB2	3:A:740:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:845:LEU:N	3:A:845:LEU:HD23	2.22	0.53
4:B:515:HIS:H	4:B:518:HIS:HD2	1.55	0.53
6:E:23:VAL:HG12	6:E:28:TYR:HB2	1.89	0.53
3:A:567:LYS:NZ	8:H:95:TYR:CE1	2.71	0.53
3:A:122:MET:O	3:A:126:LEU:HG	2.07	0.53
3:A:1341:ILE:HD12	3:A:1379:GLY:C	2.28	0.53
3:A:353:ILE:HD13	3:A:487:MET:HE2	1.88	0.53
3:A:608:ILE:HD12	3:A:613:ILE:CD1	2.39	0.53
6:E:78:LEU:HD21	6:E:109:ILE:HD12	1.90	0.53
7:F:94:LEU:HD21	7:F:122:MET:HA	1.89	0.53
10:J:52:THR:O	10:J:52:THR:HG22	2.08	0.53
3:A:114:LEU:HD22	3:A:171:GLN:NE2	2.23	0.53
3:A:90:VAL:HG13	3:A:297:GLN:HA	1.90	0.53
4:B:235:SER:OG	4:B:236:HIS:HD2	1.91	0.53
4:B:644:GLU:HG3	4:B:654:ARG:HH22	1.74	0.53
4:B:755:ILE:CG2	4:B:755:ILE:O	2.55	0.53
4:B:842:ASN:HD22	4:B:845:SER:CB	2.21	0.53
5:C:46:ILE:HD13	5:C:157:CYS:CB	2.38	0.53
9:I:46:HIS:CD2	9:I:48:LEU:HD21	2.44	0.53
3:A:557:ASP:OD2	3:A:559:VAL:HB	2.08	0.53
3:A:741:ASN:ND2	3:A:741:ASN:C	2.62	0.53
4:B:292:ILE:H	4:B:293:PRO:HD2	1.73	0.53
11:K:63:VAL:HG23	11:K:63:VAL:O	2.08	0.53
3:A:1205:LYS:O	3:A:1207:LEU:N	2.41	0.53
3:A:399:HIS:C	3:A:401:GLY:H	2.10	0.53
3:A:852:TYR:CZ	7:F:136:ARG:HG2	2.44	0.53
3:A:738:LYS:HZ1	5:C:194:GLU:C	2.11	0.53
9:I:29:CYS:O	9:I:29:CYS:SG	2.66	0.53
3:A:768:GLN:HG2	3:A:816:HIS:CA	2.38	0.53
4:B:1069:PHE:HA	4:B:1085:ILE:O	2.08	0.53
4:B:1177:HIS:HB3	4:B:1179:GLN:HE21	1.74	0.53
4:B:479:VAL:HG12	4:B:480:SER:H	1.72	0.53
4:B:405:ARG:HA	4:B:631:GLY:O	2.09	0.53
5:C:189:THR:HG22	5:C:190:ASP:N	2.24	0.53
3:A:1161:THR:HG22	3:A:1162:VAL:N	2.24	0.53
3:A:134:ARG:HH12	3:A:220:THR:HG22	1.74	0.53
3:A:1365:TYR:O	3:A:1367:HIS:N	2.42	0.53
4:B:120:ARG:HB2	4:B:122:LEU:HG	1.91	0.53
4:B:205:ILE:HD11	4:B:461:LEU:HD23	1.90	0.53
5:C:241:ASP:O	5:C:245:VAL:HG23	2.08	0.53
1:R:10:A:O5'	1:R:10:A:OP1	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1094:VAL:HG13	3:A:1113:THR:CG2	2.37	0.53
3:A:1220:PHE:O	3:A:1222:ASN:N	2.42	0.53
3:A:1225:PHE:CE2	3:A:1227:ILE:HD11	2.43	0.53
3:A:339:ASN:O	3:A:343:LYS:HG2	2.07	0.53
3:A:384:ASN:OD1	3:A:385:ILE:N	2.42	0.53
3:A:387:ARG:O	3:A:391:LEU:HG	2.09	0.53
3:A:552:TRP:NE1	3:A:655:PHE:CD1	2.77	0.53
4:B:875:GLU:O	4:B:877:PRO:HD3	2.09	0.53
4:B:916:THR:HG22	4:B:918:ILE:HG13	1.90	0.53
4:B:956:THR:CG2	4:B:960:GLY:HA2	2.38	0.53
6:E:28:TYR:CE1	6:E:78:LEU:HD12	2.44	0.53
3:A:407:ARG:HD2	3:A:413:ILE:HD11	1.91	0.53
4:B:234:ILE:HG21	4:B:257:LYS:HB3	1.91	0.53
4:B:484:ASN:ND2	4:B:486:TYR:CD1	2.76	0.53
6:E:17:ARG:O	6:E:21:GLU:HG3	2.09	0.53
8:H:38:LEU:CD1	8:H:125:LEU:HD13	2.38	0.53
9:I:29:CYS:C	9:I:31:THR:H	2.13	0.53
9:I:62:ILE:HG23	9:I:63:GLY:N	2.22	0.53
12:L:38:LEU:O	12:L:39:SER:CB	2.56	0.53
3:A:1111:MET:CE	3:A:1330:ASN:OD1	2.57	0.53
3:A:442:VAL:O	3:A:457:ALA:HA	2.09	0.53
3:A:444:PHE:HB3	3:A:458:HIS:CD2	2.43	0.53
3:A:696:GLU:OE2	3:A:702:LEU:HD23	2.08	0.53
3:A:928:LEU:O	3:A:931:GLU:N	2.43	0.53
4:B:287:ARG:HA	4:B:291:ILE:O	2.09	0.53
4:B:43:LEU:HD13	4:B:812:LEU:CD2	2.38	0.53
2:T:3:DG:H5'	3:A:836:TYR:HD1	1.70	0.53
3:A:337:ARG:CZ	3:A:839:ARG:HH12	2.22	0.52
4:B:463:THR:HG21	4:B:465:ASN:HD22	1.74	0.52
4:B:547:VAL:H	4:B:612:GLU:CD	2.12	0.52
4:B:898:LEU:CD2	4:B:964:VAL:HG11	2.38	0.52
5:C:93:ASP:OD1	5:C:122:SER:HB2	2.09	0.52
8:H:6:PHE:O	8:H:58:THR:HA	2.08	0.52
1:R:9:G:C5	1:R:10:A:N7	2.76	0.52
3:A:1299:VAL:CG1	3:A:1300:LYS:H	2.20	0.52
3:A:167:CYS:HB2	3:A:169:ASN:ND2	2.24	0.52
3:A:507:VAL:N	3:A:508:PRO:CD	2.72	0.52
4:B:248:SER:O	4:B:249:ARG:HB2	2.09	0.52
4:B:43:LEU:HD13	4:B:812:LEU:HD23	1.90	0.52
4:B:911:ILE:HD11	4:B:941:LEU:HD12	1.91	0.52
7:F:114:GLU:OE1	7:F:119:ARG:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.23	0.52
11:K:46:ILE:O	11:K:50:LEU:HB2	2.09	0.52
4:B:120:ARG:NH2	12:L:54:ARG:HD2	2.24	0.52
4:B:707:PRO:CG	4:B:708:GLU:H	2.21	0.52
4:B:999:MET:HE2	4:B:1011:ILE:HD11	1.91	0.52
5:C:164:ALA:HA	5:C:167:HIS:O	2.10	0.52
1:R:5:A:H2'	1:R:6:G:H8	1.70	0.52
3:A:261:ASP:OD2	3:A:323:LYS:HD2	2.10	0.52
3:A:675:THR:CG2	3:A:736:ASN:HD21	2.22	0.52
3:A:907:THR:HG22	3:A:908:LEU:N	2.25	0.52
4:B:287:ARG:HG2	4:B:292:ILE:CA	2.27	0.52
4:B:484:ASN:ND2	4:B:486:TYR:CE1	2.77	0.52
4:B:899:ILE:HD11	4:B:910:VAL:O	2.09	0.52
4:B:98:THR:OG1	4:B:127:GLY:HA3	2.09	0.52
6:E:12:LEU:HD22	6:E:55:ARG:CZ	2.39	0.52
6:E:124:VAL:HG22	6:E:132:ILE:CG2	2.39	0.52
7:F:132:LEU:O	7:F:148:VAL:HG23	2.09	0.52
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.73	0.52
3:A:451:HIS:CD2	3:A:1074:GLU:HG3	2.45	0.52
3:A:529:CYS:HB2	4:B:1015:HIS:CE1	2.43	0.52
4:B:1065:GLN:NE2	4:B:1067:ARG:HG2	2.24	0.52
4:B:271:ALA:HB3	4:B:285:ILE:CD1	2.40	0.52
4:B:857:ARG:HD2	4:B:945:GLU:OE1	2.08	0.52
4:B:293:PRO:HA	9:I:12:ASN:HD21	1.75	0.52
3:A:1147:THR:HA	3:A:1197:LEU:HD23	1.90	0.52
3:A:225:ASN:O	3:A:227:VAL:HG23	2.09	0.52
3:A:670:ILE:HD13	4:B:1067:ARG:CZ	2.39	0.52
4:B:100:PRO:HG3	4:B:172:ILE:HD12	1.92	0.52
4:B:118:ARG:NH2	4:B:194:GLU:CD	2.60	0.52
4:B:31:TRP:CD1	4:B:807:ARG:NH1	2.78	0.52
4:B:284:ILE:HD13	4:B:324:ILE:HD12	1.91	0.52
4:B:428:ILE:O	4:B:431:TYR:HB3	2.10	0.52
4:B:90:ILE:CD1	4:B:432:MET:SD	2.97	0.52
4:B:542:MET:HE1	4:B:743:ILE:CG2	2.39	0.52
6:E:35:VAL:C	6:E:37:LEU:H	2.12	0.52
8:H:84:ALA:C	8:H:86:ASP:H	2.13	0.52
1:R:10:A:N6	2:T:6:DC:H42	2.06	0.52
3:A:1319:VAL:CG1	3:A:1320:PRO:HD2	2.39	0.52
3:A:1359:ASP:C	3:A:1361:SER:H	2.13	0.52
3:A:470:LEU:HD21	3:A:487:MET:HE3	1.92	0.52
3:A:901:LEU:HD23	3:A:907:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:59:LEU:HD11	4:B:417:PHE:CZ	2.44	0.52
4:B:559:SER:HA	4:B:563:MET:HB3	1.91	0.52
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.10	0.52
3:A:1029:ARG:HG3	3:A:1029:ARG:HH11	1.74	0.52
3:A:1299:VAL:CG1	3:A:1300:LYS:N	2.72	0.52
3:A:134:ARG:NH1	3:A:220:THR:O	2.42	0.52
3:A:443:LEU:HD11	4:B:1138:MET:SD	2.50	0.52
3:A:596:THR:O	3:A:597:LEU:C	2.47	0.52
3:A:821:ARG:HG3	3:A:825:ILE:CD1	2.40	0.52
3:A:91:PHE:HB2	3:A:297:GLN:OE1	2.09	0.52
4:B:1084:GLN:HG2	5:C:201:TRP:CZ2	2.45	0.52
4:B:25:ILE:HG22	4:B:26:THR:N	2.24	0.52
4:B:614:SER:OG	4:B:627:PHE:HB2	2.09	0.52
9:I:73:ARG:O	9:I:81:ARG:HA	2.09	0.52
3:A:1116:LEU:N	3:A:1308:THR:HG22	2.25	0.52
3:A:1152:ILE:CG2	3:A:1260:LEU:HD23	2.38	0.52
3:A:817:ALA:HA	4:B:764:SER:OG	2.10	0.52
4:B:287:ARG:CG	4:B:292:ILE:HA	2.26	0.52
4:B:542:MET:HG3	4:B:747:MET:CE	2.38	0.52
4:B:552:MET:N	4:B:553:PRO:HD2	2.24	0.52
4:B:648:HIS:NE2	4:B:650:GLU:OE1	2.43	0.52
4:B:806:THR:C	4:B:808:ALA:H	2.12	0.52
3:A:49:LYS:HB3	3:A:55:ASP:HB2	1.92	0.52
4:B:825:VAL:HG12	4:B:826:ALA:N	2.24	0.52
7:F:77:ASP:O	7:F:78:GLN:HB2	2.09	0.52
3:A:1214:GLU:O	3:A:1218:GLN:HG2	2.10	0.51
3:A:326:ARG:HG2	3:A:1406:VAL:CG2	2.39	0.51
3:A:365:GLY:HA3	3:A:469:ARG:HB2	1.91	0.51
3:A:836:TYR:CE2	3:A:840:ARG:HD2	2.45	0.51
4:B:25:ILE:CG2	4:B:29:ASP:HB3	2.40	0.51
4:B:46:GLN:NE2	4:B:496:ARG:HA	2.25	0.51
4:B:640:VAL:O	4:B:641:GLU:C	2.46	0.51
4:B:864:LYS:HD3	4:B:871:THR:HA	1.91	0.51
12:L:38:LEU:HG	12:L:39:SER:N	2.25	0.51
1:R:9:G:C6	1:R:10:A:N7	2.78	0.51
2:T:1:DA:N6	2:T:2:DC:N4	2.58	0.51
3:A:1392:SER:O	3:A:1393:ASN:CB	2.58	0.51
3:A:13:THR:HG23	3:A:1432:GLN:NE2	2.24	0.51
3:A:50:ILE:HG22	3:A:51:GLY:N	2.24	0.51
3:A:568:PRO:HB2	5:C:221:TYR:CE1	2.45	0.51
4:B:827:ILE:HG12	4:B:1012:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:240:ILE:HG23	4:B:240:ILE:O	2.09	0.51
6:E:155:ARG:HD2	6:E:194:GLU:OE2	2.09	0.51
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.39	0.51
8:H:84:ALA:C	8:H:86:ASP:N	2.64	0.51
3:A:1269:GLU:OE2	4:B:263:GLY:HA3	2.10	0.51
3:A:384:ASN:OD1	3:A:388:LEU:HD12	2.10	0.51
3:A:41:MET:HG2	3:A:49:LYS:HG2	1.92	0.51
4:B:834:ASN:O	4:B:1013:ASN:HB2	2.10	0.51
1:R:5:A:N1	1:R:6:G:C5	2.74	0.51
3:A:1336:MET:HE1	3:A:1381:LEU:HG	1.92	0.51
3:A:737:LEU:HD11	3:A:758:ILE:HG21	1.92	0.51
6:E:121:MET:C	6:E:123:LEU:H	2.13	0.51
7:F:109:VAL:CG1	7:F:110:ASP:N	2.73	0.51
10:J:9:SER:CB	10:J:45:CYS:HB2	2.40	0.51
3:A:341:MET:CE	3:A:1401:SER:HB2	2.41	0.51
3:A:1436:ILE:CG2	3:A:1437:GLY:N	2.72	0.51
3:A:219:PHE:O	3:A:222:LEU:O	2.28	0.51
3:A:847:ASP:OD2	3:A:858:ASN:HB2	2.10	0.51
4:B:737:THR:CG2	9:I:66:PRO:HB2	2.40	0.51
3:A:357:PRO:HG2	4:B:833:TYR:CE1	2.45	0.51
4:B:846:ILE:HD13	4:B:974:PRO:HG2	1.91	0.51
11:K:65:HIS:HD2	11:K:67:PHE:HB2	1.74	0.51
1:R:9:G:C2	1:R:10:A:N7	2.79	0.51
3:A:511:ILE:HG12	3:A:521:MET:HE3	1.93	0.51
3:A:535:THR:HG23	3:A:575:LYS:HE2	1.93	0.51
3:A:61:ILE:HG22	3:A:62:ASP:N	2.16	0.51
3:A:722:LEU:HD11	3:A:794:PRO:HB3	1.91	0.51
3:A:898:ARG:HD2	3:A:899:VAL:N	2.26	0.51
4:B:1084:GLN:CD	4:B:1084:GLN:H	2.14	0.51
4:B:1106:ARG:HH12	4:B:1118:PRO:CB	2.24	0.51
3:A:1410:PHE:CE2	4:B:1212:ILE:HD11	2.45	0.51
4:B:751:VAL:HG12	4:B:752:ALA:N	2.26	0.51
4:B:864:LYS:HG2	4:B:871:THR:HG23	1.93	0.51
9:I:50:THR:HG22	9:I:52:ILE:H	1.75	0.51
9:I:75:CYS:O	9:I:77:LYS:N	2.44	0.51
3:A:1312:ASN:O	3:A:1316:VAL:HG23	2.11	0.51
3:A:340:LEU:HD21	4:B:1200:ALA:CB	2.40	0.51
3:A:567:LYS:HD2	3:A:568:PRO:HD2	1.92	0.51
3:A:810:PRO:O	3:A:813:PHE:HB3	2.11	0.51
3:A:929:LEU:H	3:A:929:LEU:CD2	2.23	0.51
3:A:1376:THR:HG23	6:E:212:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:23:VAL:HG13	6:E:28:TYR:CD1	2.45	0.51
7:F:101:ILE:HD13	7:F:120:ILE:HG22	1.92	0.51
1:R:9:G:N1	1:R:10:A:C5	2.79	0.51
3:A:96:ILE:O	3:A:100:LYS:HG3	2.10	0.51
3:A:649:ILE:O	3:A:653:VAL:HG23	2.11	0.51
3:A:715:GLU:OE2	3:A:774:ARG:NH1	2.43	0.51
3:A:751:SER:O	3:A:752:LYS:CG	2.59	0.51
3:A:753:GLY:HA2	3:A:757:ASN:HD22	1.74	0.51
4:B:130:VAL:CG2	4:B:167:ILE:HD12	2.33	0.51
4:B:563:MET:HG3	4:B:563:MET:O	2.10	0.51
10:J:7:CYS:SG	10:J:9:SER:HB2	2.50	0.51
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.26	0.51
12:L:40:LEU:HD13	12:L:44:ASP:OD1	2.11	0.51
3:A:1351:GLU:O	3:A:1352:VAL:C	2.49	0.51
4:B:1163:CYS:SG	4:B:1182:CYS:SG	3.08	0.51
3:A:329:LEU:HD22	4:B:1203:LEU:CD1	2.41	0.51
4:B:283:VAL:HG13	4:B:297:ILE:CD1	2.41	0.51
4:B:755:ILE:HG22	4:B:755:ILE:O	2.09	0.51
5:C:177:GLU:HG3	5:C:231:ASN:HB3	1.93	0.51
5:C:33:LEU:HG	5:C:37:MET:CE	2.41	0.51
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.92	0.51
10:J:54:VAL:O	10:J:56:LEU:N	2.43	0.51
11:K:101:LEU:HD23	11:K:101:LEU:O	2.11	0.51
11:K:91:CYS:O	11:K:95:ILE:HG13	2.11	0.51
12:L:27:LEU:HD13	12:L:37:LYS:CG	2.41	0.51
3:A:1384:VAL:HG12	3:A:1384:VAL:O	2.11	0.51
3:A:233:TRP:C	3:A:235:ILE:H	2.13	0.51
3:A:675:THR:HG21	3:A:736:ASN:HD21	1.76	0.51
4:B:195:CYS:SG	4:B:197:PHE:HB2	2.51	0.51
4:B:271:ALA:O	4:B:279:ASP:HA	2.11	0.51
3:A:795:GLU:HG2	4:B:731:VAL:HG21	1.93	0.51
6:E:46:TYR:HE2	6:E:58:MET:HA	1.76	0.51
7:F:109:VAL:CG2	7:F:124:GLU:HG2	2.40	0.51
9:I:25:LEU:HD12	9:I:26:LEU:H	1.76	0.51
10:J:36:LEU:HD13	10:J:47:ARG:HG2	1.92	0.51
2:T:8:DT:H73	2:T:8:DT:OP2	2.10	0.51
3:A:1364:ASN:ND2	3:A:1366:ARG:HH11	2.09	0.50
3:A:587:HIS:HA	3:A:607:ILE:O	2.11	0.50
4:B:1035:ALA:HB1	4:B:1040:ASN:O	2.10	0.50
4:B:1119:VAL:O	4:B:1126:GLY:HA3	2.11	0.50
4:B:1197:PRO:HG2	4:B:1200:ALA:CB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:130:VAL:CG1	4:B:131:ASP:N	2.74	0.50
4:B:234:ILE:H	4:B:234:ILE:CD1	2.16	0.50
10:J:48:ARG:NE	10:J:49:MET:HE2	2.26	0.50
11:K:24:ASP:HB3	11:K:30:ALA:HB3	1.93	0.50
3:A:107:CYS:HB2	3:A:114:LEU:HD23	1.93	0.50
3:A:1376:THR:HG23	3:A:1376:THR:O	2.12	0.50
3:A:346:ASP:CG	4:B:1108:ARG:HA	2.31	0.50
4:B:1096:ARG:O	4:B:1097:HIS:CB	2.59	0.50
4:B:292:ILE:N	4:B:293:PRO:HD2	2.25	0.50
4:B:642:ASP:HB3	4:B:649:LYS:CD	2.41	0.50
4:B:756:ILE:CG2	4:B:759:PRO:HB3	2.42	0.50
4:B:975:GLN:O	4:B:990:ILE:HD12	2.12	0.50
12:L:47:ARG:HG2	12:L:52:GLY:CA	2.39	0.50
1:R:5:A:C2'	1:R:6:G:O4'	2.60	0.50
3:A:1362:TYR:OH	3:A:1364:ASN:HA	2.11	0.50
3:A:105:CYS:SG	3:A:138:ILE:HG22	2.52	0.50
3:A:444:PHE:CB	3:A:458:HIS:HD2	2.24	0.50
3:A:754:SER:O	3:A:755:PHE:C	2.48	0.50
6:E:5:ASN:O	6:E:9:ILE:HG13	2.11	0.50
9:I:75:CYS:C	9:I:77:LYS:N	2.59	0.50
10:J:16:ASP:OD1	10:J:17:LYS:HE3	2.12	0.50
3:A:1349:TYR:CD2	3:A:1349:TYR:C	2.84	0.50
3:A:32:VAL:HG21	3:A:68:GLN:HE22	1.74	0.50
3:A:384:ASN:O	3:A:385:ILE:C	2.48	0.50
3:A:829:VAL:C	3:A:831:THR:H	2.15	0.50
4:B:185:THR:O	4:B:189:LEU:HG	2.11	0.50
4:B:514:LEU:HD12	4:B:515:HIS:H	1.74	0.50
4:B:577:ALA:HB1	4:B:589:VAL:HG11	1.91	0.50
5:C:254:LYS:HE2	11:K:42:LEU:HD13	1.94	0.50
3:A:167:CYS:O	3:A:169:ASN:N	2.45	0.50
3:A:27:VAL:HG13	3:A:240:PRO:HB3	1.92	0.50
3:A:893:PHE:CE1	3:A:940:ARG:HD2	2.46	0.50
4:B:581:PHE:HB2	4:B:625:LYS:HG2	1.93	0.50
4:B:911:ILE:HD11	4:B:941:LEU:HB2	1.94	0.50
3:A:738:LYS:NZ	5:C:194:GLU:HA	2.26	0.50
6:E:168:TYR:HB3	6:E:170:LEU:CG	2.41	0.50
8:H:31:THR:O	8:H:32:THR:HB	2.11	0.50
5:C:66:ARG:NH2	10:J:2:ILE:CG2	2.74	0.50
3:A:1142:THR:O	3:A:1273:LEU:HD22	2.12	0.50
3:A:683:ILE:HD11	3:A:764:CYS:CB	2.36	0.50
4:B:977:GLY:CA	4:B:1099:VAL:CG2	2.86	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:500:GLU:OE1	4:B:1143:ALA:HB1	2.11	0.50
4:B:35:SER:O	4:B:36:ALA:C	2.50	0.50
4:B:653:VAL:CG2	4:B:689:LEU:HB3	2.42	0.50
4:B:542:MET:CG	4:B:747:MET:HE3	2.38	0.50
4:B:858:SER:HA	4:B:966:VAL:O	2.11	0.50
9:I:101:PHE:O	9:I:109:ILE:HA	2.12	0.50
9:I:68:LEU:HB3	9:I:84:VAL:HG22	1.94	0.50
3:A:1134:ILE:O	3:A:1138:ILE:HG13	2.12	0.50
3:A:306:ASN:HD21	3:A:324:SER:N	2.08	0.50
4:B:1177:HIS:CB	4:B:1179:GLN:HE21	2.24	0.50
4:B:271:ALA:HB3	4:B:285:ILE:HD11	1.93	0.50
5:C:77:ILE:HG23	5:C:161:LYS:HE3	1.94	0.50
6:E:157:SER:C	6:E:159:ASP:N	2.64	0.50
8:H:47:PHE:HB2	8:H:95:TYR:HD1	1.76	0.50
3:A:100:LYS:NZ	3:A:176:LYS:HD2	2.27	0.50
3:A:573:SER:O	3:A:576:GLN:HB2	2.11	0.50
4:B:365:THR:HG23	4:B:367:LEU:HG	1.93	0.50
4:B:800:GLN:OE1	4:B:822:ASN:HB2	2.12	0.50
8:H:128:ASN:O	8:H:131:ASN:ND2	2.45	0.50
8:H:83:GLN:C	8:H:85:GLY:H	2.14	0.50
9:I:99:LEU:HB2	9:I:112:SER:HB3	1.94	0.50
1:R:10:A:C3'	14:R:3000:UTP:O1A	2.60	0.50
1:R:8:G:C2	2:T:8:DT:N3	2.79	0.50
3:A:135:PHE:HD1	3:A:222:LEU:HD22	1.76	0.50
3:A:376:TYR:OH	3:A:498:ARG:HD2	2.11	0.50
3:A:612:ILE:O	3:A:612:ILE:HG23	2.12	0.50
3:A:709:THR:CB	3:A:712:GLU:HG3	2.41	0.50
3:A:888:GLY:O	3:A:940:ARG:NH2	2.44	0.50
4:B:1159:ARG:CD	4:B:1193:GLN:HG3	2.31	0.50
4:B:260:GLY:O	4:B:267:ARG:HD3	2.12	0.50
5:C:11:ARG:NH2	5:C:229:TYR:CD2	2.68	0.50
6:E:54:GLN:O	6:E:57:MET:HB3	2.11	0.50
3:A:115:LEU:HB2	3:A:122:MET:CE	2.41	0.49
3:A:808:LEU:O	4:B:728:ARG:NH1	2.43	0.49
5:C:18:VAL:HG12	5:C:20:PHE:HD2	1.76	0.49
6:E:98:ILE:O	6:E:102:GLU:HG3	2.12	0.49
6:E:80:VAL:HG22	6:E:109:ILE:HD12	1.94	0.49
6:E:177:ARG:O	6:E:212:ARG:HD3	2.11	0.49
7:F:82:THR:HG22	7:F:84:TYR:N	2.27	0.49
8:H:6:PHE:HE1	8:H:130:ARG:NE	2.10	0.49
9:I:15:TYR:CD1	9:I:15:TYR:N	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:737:THR:CG2	9:I:66:PRO:CB	2.89	0.49
12:L:62:LYS:C	12:L:64:LEU:H	2.13	0.49
3:A:1189:SER:OG	3:A:1190:PRO:HD2	2.12	0.49
3:A:394:ASN:OD1	3:A:398:GLU:OE1	2.30	0.49
4:B:240:ILE:O	4:B:253:THR:HG23	2.11	0.49
4:B:269:ILE:CD1	4:B:386:LEU:HD21	2.39	0.49
4:B:579:ARG:HB2	4:B:586:TRP:NE1	2.27	0.49
4:B:844:SER:OG	4:B:996:ARG:N	2.33	0.49
4:B:873:THR:O	4:B:914:LYS:HA	2.13	0.49
4:B:896:ASP:OD2	12:L:58:LYS:HE3	2.13	0.49
7:F:133:VAL:HG22	7:F:147:SER:HA	1.95	0.49
12:L:62:LYS:O	12:L:64:LEU:HG	2.11	0.49
3:A:1150:SER:HB2	3:A:1195:LEU:HD23	1.92	0.49
3:A:185:TRP:HZ3	3:A:200:ARG:HG2	1.74	0.49
3:A:332:LYS:HG3	3:A:333:GLU:HG2	1.94	0.49
3:A:567:LYS:NZ	8:H:46:LEU:CB	2.67	0.49
3:A:741:ASN:ND2	3:A:743:VAL:N	2.61	0.49
3:A:74:MET:O	3:A:75:ASN:HB2	2.13	0.49
3:A:1410:PHE:HD2	4:B:1212:ILE:HD11	1.70	0.49
4:B:25:ILE:CG2	4:B:29:ASP:CB	2.90	0.49
5:C:43:THR:CG2	5:C:44:LEU:N	2.75	0.49
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.42	0.49
8:H:88:SER:O	8:H:89:LEU:HG	2.12	0.49
11:K:97:LYS:O	11:K:100:ALA:HB3	2.12	0.49
3:A:1284:MET:HG2	3:A:1306:LEU:CD2	2.43	0.49
3:A:538:ASP:OD1	8:H:22:LYS:HB2	2.13	0.49
4:B:1053:GLU:O	4:B:1054:GLY:C	2.50	0.49
3:A:15:LYS:CB	4:B:1220:ARG:HG2	2.33	0.49
4:B:283:VAL:O	4:B:286:PHE:HB2	2.11	0.49
4:B:660:LYS:O	4:B:663:ALA:HB3	2.13	0.49
12:L:52:GLY:O	12:L:54:ARG:HG3	2.12	0.49
3:A:418:SER:HB3	3:A:421:ALA:HB2	1.94	0.49
3:A:545:GLN:O	3:A:548:ASN:N	2.44	0.49
3:A:589:GLN:OE1	3:A:591:PHE:HE1	1.96	0.49
3:A:606:LEU:HB2	3:A:614:PHE:CE2	2.48	0.49
3:A:783:THR:HG21	3:A:815:PHE:CE2	2.48	0.49
3:A:834:THR:HG21	3:A:1077:THR:CA	2.43	0.49
4:B:635:ARG:NH1	4:B:742:GLU:OE2	2.46	0.49
8:H:76:THR:HG22	8:H:76:THR:O	2.11	0.49
3:A:466:SER:HB3	11:K:2:ASN:ND2	2.27	0.49
3:A:391:LEU:O	3:A:394:ASN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:108:VAL:CG1	4:B:109:THR:N	2.76	0.49
4:B:485:ARG:NH2	4:B:782:LEU:HD11	2.27	0.49
4:B:734:HIS:O	4:B:735:ALA:HB2	2.12	0.49
8:H:49:VAL:CG1	8:H:50:ALA:N	2.74	0.49
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.93	0.49
3:A:1001:ARG:HG2	3:A:1001:ARG:HH11	1.77	0.49
3:A:1153:TYR:HA	9:I:41:PRO:O	2.12	0.49
3:A:31:SER:HB2	3:A:83:HIS:HB2	1.91	0.49
3:A:474:VAL:HG13	3:A:478:TYR:CE1	2.48	0.49
3:A:491:VAL:O	3:A:493:GLN:NE2	2.46	0.49
3:A:511:ILE:HG12	3:A:521:MET:CE	2.42	0.49
3:A:69:THR:HG22	3:A:69:THR:O	2.12	0.49
3:A:857:ARG:HG2	3:A:863:VAL:HA	1.94	0.49
4:B:1043:ASP:O	4:B:1050:ILE:HD12	2.13	0.49
4:B:906:SER:O	4:B:907:GLY:C	2.50	0.49
7:F:82:THR:HG22	7:F:84:TYR:H	1.77	0.49
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.94	0.49
3:A:1364:ASN:HD21	3:A:1366:ARG:HH11	1.61	0.49
3:A:54:ASN:HA	3:A:58:LEU:HD12	1.95	0.49
3:A:61:ILE:HA	3:A:74:MET:SD	2.53	0.49
4:B:1208:MET:HA	4:B:1212:ILE:O	2.12	0.49
4:B:821:GLN:OE1	4:B:850:LEU:HD12	2.13	0.49
5:C:142:VAL:H	10:J:16:ASP:HB3	1.77	0.49
5:C:4:GLU:O	5:C:5:GLY:O	2.31	0.49
6:E:102:GLU:O	6:E:104:ASN:N	2.46	0.49
10:J:7:CYS:O	10:J:8:PHE:C	2.50	0.49
2:T:5:DT:H2''	2:T:6:DC:H5'	1.95	0.49
4:B:1077:THR:HG22	4:B:1079:LYS:HB2	1.94	0.49
4:B:1118:PRO:HD3	4:B:1155:SER:HA	1.95	0.49
4:B:351:TYR:O	4:B:355:ILE:HG13	2.13	0.49
4:B:653:VAL:HG12	4:B:654:ARG:N	2.28	0.49
4:B:890:TYR:O	4:B:892:LYS:N	2.46	0.49
5:C:67:LEU:HD11	5:C:155:LEU:HD13	1.95	0.49
8:H:59:ILE:O	8:H:60:ALA:HB3	2.12	0.49
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.94	0.49
1:R:2:U:C4	1:R:3:C:C4	3.01	0.49
2:T:10:DT:H2''	2:T:11:DC:H5'	1.93	0.49
3:A:418:SER:C	3:A:420:ARG:N	2.63	0.49
3:A:819:GLY:O	3:A:820:GLY:C	2.49	0.49
4:B:1106:ARG:HH21	4:B:1109:GLY:C	2.16	0.49
4:B:726:ALA:HB1	4:B:1051:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:87:LYS:HE2	7:F:88:TYR:CE1	2.48	0.49
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.95	0.49
3:A:1100:ARG:NH2	3:A:1330:ASN:HB2	2.28	0.48
3:A:1326:ARG:O	3:A:1327:ILE:C	2.49	0.48
3:A:1392:SER:O	3:A:1393:ASN:CG	2.51	0.48
3:A:1406:VAL:CG1	3:A:1410:PHE:HE1	2.26	0.48
3:A:89:PRO:C	3:A:204:THR:HG21	2.33	0.48
3:A:666:ILE:CD1	4:B:1030:LEU:HD22	2.41	0.48
4:B:726:ALA:HB1	4:B:1051:THR:CG2	2.43	0.48
4:B:1160:VAL:HG11	4:B:1169:MET:SD	2.53	0.48
1:R:5:A:N1	2:T:10:DT:O4	2.46	0.48
3:A:1066:VAL:O	3:A:1068:ALA:N	2.46	0.48
3:A:1099:PRO:O	3:A:1102:LYS:HB3	2.13	0.48
3:A:332:LYS:H	3:A:337:ARG:HD2	1.76	0.48
3:A:563:PRO:HG3	3:A:572:TRP:CH2	2.48	0.48
3:A:567:LYS:HZ2	8:H:46:LEU:CB	2.27	0.48
4:B:1054:GLY:O	4:B:1058:LEU:HG	2.13	0.48
4:B:284:ILE:CD1	4:B:324:ILE:HD12	2.43	0.48
7:F:81:THR:HG22	7:F:82:THR:H	1.78	0.48
8:H:36:CYS:HA	8:H:126:GLU:O	2.13	0.48
9:I:29:CYS:SG	9:I:31:THR:HG22	2.52	0.48
9:I:85:PHE:O	9:I:86:PHE:HB3	2.13	0.48
3:A:674:PRO:O	3:A:677:ARG:HB3	2.14	0.48
4:B:291:ILE:HD13	4:B:300:HIS:CD2	2.48	0.48
8:H:44:VAL:O	8:H:44:VAL:HG12	2.12	0.48
1:R:5:A:N3	1:R:6:G:C8	2.81	0.48
3:A:994:GLN:NE2	3:A:1019:CYS:HB3	2.27	0.48
3:A:890:ASP:H	3:A:1296:GLY:HA3	1.77	0.48
4:B:1053:GLU:O	4:B:1055:ILE:N	2.46	0.48
4:B:1106:ARG:NH2	4:B:1109:GLY:C	2.67	0.48
4:B:1156:ASP:HB3	4:B:1197:PRO:HA	1.95	0.48
4:B:225:VAL:HG11	4:B:388:CYS:HB3	1.95	0.48
4:B:570:VAL:HG11	4:B:573:GLN:OE1	2.13	0.48
4:B:781:PHE:O	4:B:782:LEU:HG	2.12	0.48
4:B:864:LYS:HB3	4:B:871:THR:HA	1.96	0.48
5:C:254:LYS:O	5:C:258:ILE:HD13	2.13	0.48
6:E:191:LYS:O	6:E:192:ARG:C	2.50	0.48
6:E:78:LEU:HD21	6:E:80:VAL:HG22	1.95	0.48
1:R:10:A:H2'	14:R:3000:UTP:O4'	2.13	0.48
3:A:18:GLN:O	4:B:1215:ARG:CG	2.62	0.48
3:A:68:GLN:NE2	3:A:80:HIS:CB	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:821:ARG:CG	3:A:825:ILE:HD11	2.41	0.48
3:A:918:GLU:O	3:A:918:GLU:HG3	2.12	0.48
3:A:994:GLN:HE21	3:A:1019:CYS:CB	2.26	0.48
4:B:1162:ILE:HD11	4:B:1194:ILE:CD1	2.41	0.48
4:B:227:LYS:HB2	4:B:395:GLN:OE1	2.14	0.48
4:B:488:TYR:CE2	4:B:813:LYS:HB2	2.48	0.48
4:B:825:VAL:CG1	4:B:826:ALA:N	2.76	0.48
8:H:33:GLN:OE1	8:H:129:TYR:CE2	2.67	0.48
11:K:83:PRO:HA	11:K:86:ALA:HB3	1.95	0.48
3:A:178:GLY:O	3:A:179:LEU:HD23	2.13	0.48
3:A:226:GLU:CG	3:A:227:VAL:N	2.75	0.48
3:A:549:MET:HE1	3:A:656:TRP:CD1	2.39	0.48
3:A:913:LEU:HD11	3:A:981:LEU:O	2.13	0.48
4:B:1182:CYS:O	4:B:1183:LYS:O	2.31	0.48
4:B:101:MET:HE2	4:B:169:ARG:HH12	1.78	0.48
4:B:171:PRO:HD2	4:B:457:LEU:CD1	2.43	0.48
4:B:380:TYR:CE1	4:B:384:ARG:HD3	2.48	0.48
5:C:212:PRO:HB3	5:C:213:PRO:HD2	1.95	0.48
5:C:75:MET:HG3	5:C:246:ARG:NH2	2.28	0.48
10:J:57:ILE:HG12	10:J:61:LEU:HD11	1.94	0.48
3:A:1386:ARG:HE	3:A:1387:HIS:CE1	2.32	0.48
3:A:874:ASP:HA	3:A:1058:VAL:HG22	1.95	0.48
4:B:806:THR:HG22	4:B:808:ALA:H	1.79	0.48
5:C:62:PHE:O	5:C:66:ARG:HG3	2.13	0.48
6:E:7:ARG:C	6:E:9:ILE:H	2.17	0.48
9:I:74:GLU:OE1	9:I:79:HIS:ND1	2.47	0.48
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.95	0.48
11:K:43:GLY:HA2	11:K:71:PHE:CZ	2.49	0.48
12:L:31:CYS:SG	12:L:34:CYS:SG	3.11	0.48
1:R:5:A:N1	1:R:6:G:O6	2.46	0.48
3:A:244:PRO:HG2	3:A:245:PRO:CD	2.33	0.48
3:A:376:TYR:CD2	3:A:376:TYR:C	2.87	0.48
3:A:378:GLU:HG2	3:A:388:LEU:HD11	1.94	0.48
3:A:929:LEU:HD21	3:A:983:ILE:HG21	1.94	0.48
4:B:108:VAL:CG1	4:B:109:THR:H	2.19	0.48
3:A:5:GLN:O	4:B:1159:ARG:NH2	2.47	0.48
4:B:55:VAL:HG12	4:B:56:ASP:N	2.27	0.48
4:B:956:THR:HG21	4:B:960:GLY:HA2	1.96	0.48
4:B:798:TYR:CD2	10:J:4:PRO:HG3	2.49	0.48
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.49	0.48
3:A:1195:LEU:HD11	3:A:1267:MET:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1412:ALA:HA	3:A:1417:GLU:OE2	2.14	0.48
3:A:365:GLY:O	3:A:468:PHE:HA	2.14	0.48
3:A:89:PRO:HG3	3:A:208:LEU:CD1	2.44	0.48
4:B:123:THR:O	4:B:125:SER:N	2.47	0.48
4:B:236:HIS:CE1	4:B:389:ALA:HA	2.49	0.48
8:H:125:LEU:HG	8:H:130:ARG:CZ	2.43	0.48
2:T:9:DC:O2	2:T:9:DC:C2'	2.56	0.48
3:A:116:ASP:HB2	3:A:118:HIS:CD2	2.49	0.48
3:A:1356:ILE:HD12	3:A:1368:MET:SD	2.54	0.48
3:A:1436:ILE:CG2	3:A:1437:GLY:H	2.22	0.48
3:A:515:GLN:HA	3:A:1367:HIS:NE2	2.29	0.48
3:A:738:LYS:HB3	8:H:19:ARG:HH22	1.79	0.48
3:A:742:ASN:O	3:A:745:GLN:HB2	2.13	0.48
4:B:46:GLN:HE21	4:B:496:ARG:HG2	1.78	0.48
3:A:817:ALA:HA	4:B:764:SER:HG	1.78	0.48
5:C:258:ILE:HG23	11:K:19:LEU:HD11	1.96	0.48
4:B:845:SER:HB2	10:J:8:PHE:HB3	1.96	0.48
1:R:10:A:H61	2:T:6:DC:H42	1.60	0.48
3:A:265:LYS:HZ1	3:A:323:LYS:H	1.62	0.47
3:A:954:TRP:O	3:A:956:LEU:HG	2.14	0.47
3:A:351:THR:CG2	4:B:1103:ILE:HA	2.36	0.47
4:B:1124:ARG:O	4:B:1125:ASP:HB3	2.14	0.47
4:B:174:LEU:O	4:B:175:ARG:CB	2.48	0.47
4:B:708:GLU:C	4:B:710:LEU:H	2.16	0.47
5:C:43:THR:HG22	5:C:44:LEU:N	2.29	0.47
6:E:135:PHE:HD2	6:E:140:LEU:HD21	1.79	0.47
9:I:50:THR:HG22	9:I:51:ASN:N	2.28	0.47
9:I:54:GLU:O	9:I:89:GLN:HG2	2.14	0.47
3:A:1017:LEU:O	3:A:1018:PHE:C	2.53	0.47
3:A:226:GLU:HG2	3:A:227:VAL:N	2.29	0.47
3:A:869:GLY:O	6:E:204:THR:HG21	2.14	0.47
4:B:773:MET:SD	4:B:987:LYS:HD2	2.54	0.47
7:F:98:ALA:O	7:F:117:PRO:HB2	2.14	0.47
8:H:47:PHE:CD1	8:H:95:TYR:HB2	2.49	0.47
3:A:1134:ILE:HD11	3:A:1321:GLY:HA3	1.96	0.47
3:A:1392:SER:O	3:A:1393:ASN:ND2	2.48	0.47
3:A:475:THR:CG2	3:A:476:SER:N	2.76	0.47
3:A:783:THR:CG2	3:A:815:PHE:CE2	2.97	0.47
4:B:51:PHE:CD2	4:B:173:MET:HB3	2.49	0.47
8:H:39:THR:O	8:H:123:MET:HA	2.14	0.47
8:H:49:VAL:CG1	8:H:50:ALA:H	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:66:ARG:CZ	10:J:2:ILE:HG21	2.44	0.47
3:A:1074:GLU:C	3:A:1076:ALA:N	2.67	0.47
3:A:332:LYS:N	3:A:337:ARG:HD2	2.29	0.47
6:E:56:LYS:HG3	6:E:84:ASP:CB	2.42	0.47
7:F:101:ILE:HD13	7:F:120:ILE:CG2	2.45	0.47
9:I:62:ILE:CG2	9:I:63:GLY:N	2.77	0.47
3:A:12:ARG:HD3	4:B:1218:THR:HB	1.97	0.47
3:A:14:VAL:H	3:A:1432:GLN:HE22	1.61	0.47
3:A:222:LEU:O	3:A:224:PHE:N	2.46	0.47
3:A:897:TYR:HD2	3:A:936:LEU:HD13	1.78	0.47
5:C:75:MET:HG3	5:C:246:ARG:HH22	1.77	0.47
6:E:100:ILE:CG2	6:E:105:PHE:HB2	2.42	0.47
12:L:30:ILE:CD1	12:L:59:ALA:HA	2.44	0.47
3:A:1074:GLU:C	3:A:1076:ALA:H	2.18	0.47
3:A:443:LEU:CD2	3:A:455:MET:HB3	2.42	0.47
3:A:890:ASP:N	3:A:1296:GLY:HA3	2.30	0.47
4:B:1177:HIS:C	4:B:1179:GLN:N	2.68	0.47
4:B:1169:MET:SD	4:B:1201:LYS:HG2	2.54	0.47
4:B:210:LYS:HE2	4:B:461:LEU:O	2.14	0.47
4:B:363:HIS:CD2	4:B:585:VAL:HG22	2.49	0.47
4:B:750:GLY:O	4:B:751:VAL:C	2.52	0.47
5:C:142:VAL:H	10:J:16:ASP:CB	2.26	0.47
7:F:79:ARG:HG2	7:F:146:TRP:CZ2	2.49	0.47
4:B:294:ASP:H	9:I:12:ASN:ND2	2.12	0.47
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.47
3:A:112:LYS:HG2	3:A:113:LEU:H	1.79	0.47
3:A:1237:ILE:CG2	3:A:1238:ILE:N	2.78	0.47
3:A:568:PRO:HB2	5:C:221:TYR:CZ	2.50	0.47
3:A:666:ILE:O	3:A:667:GLY:C	2.53	0.47
3:A:923:LEU:O	3:A:927:VAL:HG23	2.14	0.47
4:B:1013:ASN:OD1	4:B:1015:HIS:HB2	2.15	0.47
4:B:1065:GLN:HE22	4:B:1067:ARG:HG2	1.79	0.47
4:B:1104:HIS:HB2	4:B:1122:ARG:CD	2.44	0.47
4:B:1158:PHE:HE2	4:B:1201:LYS:HE3	1.80	0.47
3:A:22:PHE:HB2	4:B:1211:ASN:CG	2.35	0.47
4:B:800:GLN:HB3	10:J:52:THR:HG22	1.96	0.47
5:C:38:ILE:HG13	5:C:176:ILE:HD12	1.97	0.47
5:C:35:ARG:O	5:C:38:ILE:N	2.47	0.47
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.32	0.47
3:A:1074:GLU:HB3	3:A:1075:PRO:HD3	1.97	0.47
3:A:154:SER:HB3	3:A:162:VAL:HG21	1.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:531:ILE:CD1	3:A:617:VAL:HG11	2.44	0.47
3:A:804:TYR:HE1	4:B:1021:MET:CE	2.28	0.47
3:A:90:VAL:HG21	3:A:296:LEU:HG	1.96	0.47
4:B:1117:GLN:NE2	4:B:1156:ASP:OD2	2.48	0.47
4:B:230:ALA:C	4:B:232:SER:H	2.17	0.47
4:B:566:LEU:CD1	4:B:588:GLY:HA2	2.43	0.47
4:B:726:ALA:CB	4:B:1051:THR:HG21	2.45	0.47
4:B:763:GLN:CG	4:B:765:PRO:HD2	2.40	0.47
3:A:1327:ILE:O	6:E:147:HIS:HE1	1.98	0.47
4:B:1098:MET:O	4:B:1099:VAL:C	2.53	0.47
4:B:332:ASP:C	4:B:334:ILE:H	2.17	0.47
4:B:284:ILE:HD13	4:B:333:PHE:CD2	2.49	0.47
4:B:802:PRO:HA	4:B:822:ASN:HD21	1.79	0.47
6:E:58:MET:O	6:E:59:SER:C	2.53	0.47
7:F:101:ILE:HD11	7:F:124:GLU:OE1	2.15	0.47
7:F:147:SER:HG	7:F:150:GLU:HG3	1.77	0.47
3:A:1410:PHE:C	3:A:1412:ALA:N	2.68	0.47
4:B:100:PRO:O	4:B:180:TYR:OH	2.31	0.47
4:B:100:PRO:HD2	4:B:180:TYR:CE1	2.50	0.47
4:B:280:ILE:HD13	4:B:334:ILE:HG12	1.95	0.47
4:B:321:GLY:C	4:B:323:VAL:H	2.17	0.47
4:B:487:THR:HG22	4:B:489:SER:N	2.24	0.47
4:B:640:VAL:HG23	4:B:740:HIS:HA	1.97	0.47
5:C:258:ILE:N	5:C:258:ILE:HD12	2.30	0.47
5:C:263:THR:C	5:C:265:MET:H	2.18	0.47
9:I:2:THR:OG1	9:I:45:ARG:HB3	2.15	0.47
3:A:1227:ILE:HG22	3:A:1228:TRP:N	2.30	0.47
3:A:1237:ILE:HG22	3:A:1238:ILE:N	2.29	0.47
3:A:294:SER:HA	3:A:297:GLN:HB3	1.96	0.47
3:A:964:ILE:HD13	3:A:1035:TYR:CZ	2.50	0.47
4:B:1116:ARG:NH1	4:B:1198:TYR:CD1	2.83	0.47
4:B:291:ILE:HD13	4:B:300:HIS:NE2	2.30	0.47
4:B:780:VAL:HG21	10:J:56:LEU:HD11	1.97	0.47
6:E:179:GLN:OE1	6:E:179:GLN:HA	2.16	0.47
10:J:1:MET:O	10:J:2:ILE:O	2.33	0.47
11:K:83:PRO:O	11:K:87:LEU:N	2.46	0.47
3:A:1192:LEU:HD11	3:A:1239:ARG:CB	2.37	0.46
4:B:324:ILE:HG23	4:B:329:THR:HB	1.96	0.46
4:B:851:PHE:O	4:B:974:PRO:HD3	2.15	0.46
4:B:96:TYR:CD1	4:B:96:TYR:N	2.83	0.46
5:C:18:VAL:O	5:C:18:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:109:VAL:HG11	7:F:123:LYS:HG2	1.96	0.46
9:I:75:CYS:HG	9:I:106:CYS:HG	1.62	0.46
3:A:1173:HIS:CD2	3:A:1227:ILE:HG23	2.51	0.46
3:A:530:GLY:O	3:A:531:ILE:C	2.54	0.46
3:A:693:VAL:HG21	3:A:721:PHE:CE1	2.38	0.46
3:A:829:VAL:O	3:A:831:THR:N	2.48	0.46
3:A:881:GLN:OE1	3:A:959:ASN:HA	2.15	0.46
4:B:1106:ARG:CD	4:B:1126:GLY:O	2.62	0.46
4:B:298:LEU:N	4:B:298:LEU:HD23	2.29	0.46
4:B:821:GLN:HB2	4:B:851:PHE:CE2	2.49	0.46
5:C:62:PHE:CD2	5:C:62:PHE:C	2.89	0.46
1:R:8:G:C2	2:T:8:DT:C4	3.04	0.46
3:A:975:HIS:ND1	3:A:1036:ARG:HG3	2.30	0.46
3:A:352:VAL:HG12	3:A:353:ILE:N	2.29	0.46
3:A:679:ILE:HG23	3:A:729:ALA:CB	2.39	0.46
3:A:893:PHE:CD1	3:A:940:ARG:HD2	2.51	0.46
4:B:1072:MET:O	4:B:1081:LEU:HB2	2.15	0.46
4:B:1182:CYS:O	4:B:1183:LYS:HD2	2.15	0.46
4:B:315:LYS:O	4:B:318:VAL:N	2.46	0.46
4:B:300:HIS:ND1	4:B:376:PHE:CD2	2.81	0.46
4:B:842:ASN:HD22	4:B:845:SER:HB3	1.80	0.46
4:B:871:THR:HG22	4:B:872:GLU:O	2.14	0.46
4:B:906:SER:CB	4:B:946:ASN:HB2	2.46	0.46
6:E:96:PHE:CE1	6:E:100:ILE:HD11	2.50	0.46
9:I:34:TYR:O	9:I:35:VAL:HG23	2.16	0.46
3:A:112:LYS:HG2	3:A:113:LEU:N	2.31	0.46
3:A:1166:ASP:CG	3:A:1194:ARG:HH21	2.19	0.46
3:A:1140:HIS:HB2	3:A:1276:VAL:O	2.16	0.46
3:A:848:ILE:CD1	3:A:1374:VAL:HG21	2.45	0.46
3:A:1394:THR:HG21	3:A:1398:MET:SD	2.56	0.46
3:A:20:GLY:HA2	3:A:1413:GLY:O	2.14	0.46
3:A:381:THR:CG2	3:A:383:TYR:CD1	2.98	0.46
3:A:517:ASN:ND2	3:A:1362:TYR:CE2	2.83	0.46
3:A:709:THR:C	3:A:711:ARG:N	2.67	0.46
4:B:1051:THR:HG21	4:B:1053:GLU:HB2	1.97	0.46
4:B:167:ILE:HG22	4:B:167:ILE:O	2.14	0.46
4:B:653:VAL:C	4:B:654:ARG:HG2	2.36	0.46
4:B:830:TYR:CE2	4:B:1000:PRO:HD3	2.50	0.46
5:C:180:TYR:O	5:C:181:ASP:HB3	2.15	0.46
5:C:5:GLY:O	5:C:6:PRO:C	2.54	0.46
6:E:102:GLU:C	6:E:104:ASN:N	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:34:CYS:HG	12:L:51:CYS:HG	1.62	0.46
3:A:1037:LEU:HD13	3:A:1042:PHE:HA	1.98	0.46
3:A:849:MET:HB2	3:A:1063:MET:SD	2.55	0.46
3:A:1209:MET:CG	3:A:1236:LEU:HD22	2.45	0.46
3:A:1277:GLU:O	3:A:1278:ASN:HB2	2.14	0.46
4:B:282:ILE:HG13	4:B:283:VAL:N	2.31	0.46
4:B:332:ASP:C	4:B:334:ILE:N	2.68	0.46
4:B:640:VAL:HG12	4:B:640:VAL:O	2.15	0.46
3:A:446:ARG:HG2	3:A:446:ARG:NH1	2.28	0.46
3:A:50:ILE:HG22	3:A:51:GLY:H	1.81	0.46
3:A:567:LYS:CD	3:A:568:PRO:HD2	2.45	0.46
3:A:535:THR:HG22	3:A:616:VAL:HA	1.97	0.46
3:A:666:ILE:HG13	3:A:666:ILE:H	1.33	0.46
4:B:314:LEU:O	4:B:315:LYS:C	2.53	0.46
4:B:31:TRP:CE3	4:B:34:ILE:HD12	2.50	0.46
4:B:50:SER:O	4:B:53:GLN:HB3	2.16	0.46
4:B:574:SER:HB3	4:B:577:ALA:HB2	1.98	0.46
6:E:96:PHE:CE2	6:E:110:PHE:HB2	2.50	0.46
3:A:1208:THR:HG22	3:A:1210:GLY:H	1.81	0.46
3:A:223:GLY:HA3	3:A:1415:SER:HB3	1.98	0.46
3:A:573:SER:OG	3:A:576:GLN:HG3	2.15	0.46
3:A:658:LEU:HD13	4:B:831:SER:HA	1.98	0.46
3:A:87:ALA:HB3	3:A:276:LEU:CD2	2.45	0.46
4:B:1013:ASN:OD1	4:B:1015:HIS:N	2.44	0.46
4:B:260:GLY:HA3	4:B:267:ARG:HG2	1.98	0.46
4:B:62:ILE:HG21	4:B:417:PHE:HD2	1.80	0.46
4:B:519:TRP:HE1	4:B:635:ARG:HH22	1.64	0.46
4:B:737:THR:HG23	9:I:66:PRO:HB2	1.94	0.46
4:B:890:TYR:C	4:B:892:LYS:H	2.19	0.46
3:A:738:LYS:NZ	5:C:194:GLU:CA	2.79	0.46
5:C:262:LEU:O	5:C:265:MET:HB3	2.15	0.46
6:E:205:SER:O	6:E:206:GLY:C	2.54	0.46
8:H:113:ALA:HA	8:H:125:LEU:O	2.15	0.46
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.97	0.46
10:J:5:VAL:O	10:J:6:ARG:HB2	2.15	0.46
3:A:1242:VAL:CG1	3:A:1243:VAL:H	2.22	0.46
3:A:167:CYS:C	3:A:169:ASN:H	2.18	0.46
3:A:83:HIS:CE1	3:A:238:CYS:SG	3.08	0.46
3:A:858:ASN:ND2	3:A:858:ASN:C	2.68	0.46
4:B:295:GLY:O	4:B:299:GLU:HG3	2.16	0.46
4:B:316:PRO:HA	4:B:319:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:605:ARG:CZ	4:B:639:ILE:HD13	2.46	0.46
4:B:704:ALA:HB2	4:B:738:PHE:CE1	2.51	0.46
5:C:252:GLN:CG	11:K:95:ILE:HG23	2.46	0.46
8:H:138:GLU:O	8:H:139:ASN:C	2.53	0.46
4:B:800:GLN:CB	10:J:52:THR:CG2	2.89	0.46
3:A:1041:ALA:O	3:A:1044:TRP:HB3	2.15	0.46
3:A:53:LEU:HD13	3:A:263:THR:HG23	1.97	0.46
3:A:35:ILE:HD12	3:A:241:VAL:HG21	1.98	0.46
3:A:47:ARG:O	3:A:48:ALA:HB2	2.16	0.46
3:A:540:PHE:C	3:A:541:ILE:HD12	2.35	0.46
4:B:1017:ILE:HB	4:B:1018:PRO:HD3	1.98	0.46
4:B:1085:ILE:CG2	4:B:1086:PHE:N	2.78	0.46
4:B:230:ALA:N	4:B:231:PRO:HD2	2.31	0.46
4:B:702:LEU:HD21	4:B:735:ALA:HB1	1.98	0.46
4:B:893:LEU:HD22	4:B:897:GLY:O	2.16	0.46
6:E:94:LYS:O	6:E:98:ILE:HG13	2.16	0.46
11:K:12:LEU:CD1	11:K:12:LEU:H	2.23	0.46
11:K:61:TYR:CD1	11:K:61:TYR:C	2.89	0.46
3:A:1116:LEU:HD12	3:A:1329:THR:HG1	1.76	0.46
3:A:645:LEU:O	3:A:649:ILE:HG13	2.15	0.46
4:B:1154:ALA:O	4:B:1155:SER:CB	2.64	0.46
4:B:300:HIS:ND1	4:B:376:PHE:CE2	2.83	0.46
4:B:515:HIS:CD2	4:B:517:THR:OG1	2.66	0.46
4:B:758:PHE:C	4:B:760:ASP:N	2.68	0.46
4:B:860:MET:HB2	4:B:965:LYS:HG2	1.97	0.46
4:B:864:LYS:H	4:B:872:GLU:CG	2.28	0.46
4:B:914:LYS:H	4:B:938:SER:HB3	1.81	0.46
5:C:80:LEU:CD2	5:C:129:ILE:HD11	2.28	0.46
5:C:166:GLU:CG	11:K:10:PHE:CZ	2.96	0.46
7:F:117:PRO:O	7:F:120:ILE:HB	2.16	0.46
8:H:114:VAL:O	8:H:124:ARG:HA	2.16	0.46
8:H:40:LEU:HG	8:H:42:ILE:HG13	1.98	0.46
8:H:81:PRO:HD2	8:H:82:PRO:HD2	1.98	0.46
12:L:45:ALA:O	12:L:46:VAL:CG2	2.64	0.46
3:A:1208:THR:HG22	3:A:1210:GLY:N	2.32	0.45
3:A:477:PRO:HG2	3:A:521:MET:HG2	1.97	0.45
3:A:556:TRP:CZ3	3:A:558:GLY:HA2	2.51	0.45
3:A:573:SER:H	3:A:576:GLN:HG3	1.81	0.45
3:A:848:ILE:HD13	3:A:864:ILE:HD13	1.98	0.45
4:B:1120:GLU:HG2	4:B:1121:GLY:N	2.31	0.45
9:I:100:PHE:HZ	9:I:118:ARG:HH12	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:73:LEU:CD2	11:K:75:ILE:HD11	2.46	0.45
3:A:1225:PHE:O	3:A:1240:CYS:HA	2.14	0.45
4:B:1200:ALA:O	4:B:1201:LYS:C	2.54	0.45
4:B:345:LYS:O	4:B:347:LYS:N	2.49	0.45
4:B:839:MET:HE2	4:B:980:PHE:CD1	2.51	0.45
5:C:73:GLN:NE2	5:C:75:MET:H	1.97	0.45
6:E:112:TYR:CE2	6:E:134:THR:HB	2.51	0.45
6:E:10:SER:O	6:E:14:ARG:HG3	2.16	0.45
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.30	0.45
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.46	0.45
9:I:75:CYS:O	9:I:76:PRO:C	2.52	0.45
11:K:91:CYS:O	11:K:94:ILE:HB	2.16	0.45
3:A:103:CYS:O	3:A:106:VAL:O	2.35	0.45
3:A:889:SER:HB3	3:A:1297:GLU:HG3	1.97	0.45
3:A:152:VAL:CG1	3:A:153:PRO:HD2	2.45	0.45
3:A:388:LEU:O	3:A:392:VAL:HG23	2.17	0.45
4:B:824:ILE:CG2	4:B:1087:PHE:CE2	3.00	0.45
4:B:977:GLY:C	4:B:1099:VAL:HG23	2.37	0.45
4:B:201:GLY:H	4:B:202:TYR:HD2	1.63	0.45
4:B:361:LEU:N	4:B:362:PRO:HD2	2.31	0.45
4:B:589:VAL:HG12	4:B:590:HIS:H	1.81	0.45
3:A:567:LYS:NZ	8:H:95:TYR:CD1	2.80	0.45
10:J:48:ARG:HH21	10:J:49:MET:CE	2.24	0.45
11:K:55:LYS:CD	11:K:78:THR:HB	2.41	0.45
2:T:4:DA:H2'	2:T:5:DT:H72	1.98	0.45
3:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.45
3:A:1155:ASP:OD1	3:A:1162:VAL:HG23	2.17	0.45
3:A:418:SER:O	3:A:421:ALA:N	2.49	0.45
3:A:571:LEU:HD22	8:H:46:LEU:HD11	1.99	0.45
3:A:644:LYS:O	3:A:645:LEU:C	2.55	0.45
4:B:1106:ARG:HG2	4:B:1107:ALA:N	2.31	0.45
4:B:100:PRO:HA	4:B:125:SER:O	2.17	0.45
4:B:215:GLN:HB2	4:B:407:ASP:HB2	1.98	0.45
3:A:786:HIS:CE1	4:B:742:GLU:OE1	2.64	0.45
5:C:17:ASN:OD1	5:C:233:GLU:HG2	2.16	0.45
5:C:242:GLN:OE1	5:C:242:GLN:HA	2.16	0.45
8:H:109:LYS:HZ2	8:H:109:LYS:HB2	1.82	0.45
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.99	0.45
9:I:8:ARG:HG3	9:I:9:ASP:CG	2.37	0.45
3:A:1046:LEU:O	3:A:1047:SER:C	2.55	0.45
3:A:1209:MET:CE	3:A:1236:LEU:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542:GLU:C	3:A:546:VAL:HG23	2.36	0.45
4:B:1020:ARG:H	4:B:1020:ARG:HG2	1.51	0.45
5:C:62:PHE:C	5:C:62:PHE:HD2	2.20	0.45
9:I:34:TYR:O	9:I:35:VAL:CG2	2.65	0.45
9:I:75:CYS:C	9:I:77:LYS:H	2.20	0.45
14:R:3000:UTP:C6	14:R:3000:UTP:C3'	3.00	0.45
1:R:9:G:C2	1:R:10:A:C5	3.05	0.45
3:A:1114:PRO:O	3:A:1330:ASN:OD1	2.35	0.45
4:B:1158:PHE:CD2	4:B:1198:TYR:HD1	2.35	0.45
4:B:247:GLY:O	4:B:248:SER:HB3	2.17	0.45
4:B:549:THR:H	4:B:628:THR:HG22	1.81	0.45
8:H:101:ALA:HB2	8:H:116:TYR:CD2	2.51	0.45
3:A:1410:PHE:C	3:A:1412:ALA:H	2.19	0.45
3:A:210:ILE:O	3:A:214:ILE:HG13	2.17	0.45
3:A:420:ARG:O	3:A:424:ILE:HG13	2.16	0.45
3:A:55:ASP:HB3	3:A:56:PRO:HD3	1.98	0.45
3:A:592:ASP:N	3:A:595:THR:OG1	2.48	0.45
4:B:185:THR:H	4:B:188:ASP:HB2	1.81	0.45
4:B:322:PHE:CG	4:B:322:PHE:O	2.69	0.45
4:B:332:ASP:O	4:B:334:ILE:N	2.50	0.45
4:B:56:ASP:HB3	4:B:57:TYR:CD1	2.52	0.45
4:B:25:ILE:HD11	4:B:653:VAL:CB	2.46	0.45
6:E:102:GLU:C	6:E:104:ASN:H	2.20	0.45
3:A:1405:THR:O	3:A:1406:VAL:C	2.54	0.45
3:A:69:THR:O	4:B:1174:LYS:HG2	2.17	0.45
3:A:958:VAL:HG22	3:A:1052:GLN:HB3	1.98	0.45
4:B:1100:ASP:HA	4:B:1103:ILE:CG1	2.46	0.45
4:B:371:GLU:N	4:B:371:GLU:OE1	2.49	0.45
4:B:702:LEU:HD12	4:B:702:LEU:HA	1.76	0.45
4:B:744:HIS:CD2	4:B:746:SER:OG	2.70	0.45
4:B:963:PHE:HE2	4:B:965:LYS:HE3	1.81	0.45
4:B:980:PHE:HE1	4:B:990:ILE:CD1	2.30	0.45
9:I:29:CYS:O	9:I:31:THR:N	2.49	0.45
12:L:55:ILE:H	12:L:55:ILE:HG12	1.53	0.45
2:T:1:DA:N3	2:T:1:DA:C2'	2.77	0.45
3:A:329:LEU:HA	3:A:335:ARG:HB2	1.98	0.45
3:A:80:HIS:O	3:A:243:PRO:HB3	2.17	0.45
4:B:276:ILE:HD13	4:B:334:ILE:CG2	2.47	0.45
4:B:377:PHE:C	4:B:379:GLY:N	2.68	0.45
4:B:680:THR:O	4:B:683:SER:OG	2.34	0.45
4:B:686:ASN:C	4:B:688:GLY:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:839:MET:HE1	4:B:980:PHE:HB2	1.98	0.45
5:C:249:ASP:O	5:C:252:GLN:HB3	2.16	0.45
7:F:109:VAL:HG12	7:F:110:ASP:H	1.82	0.45
8:H:111:LEU:HA	8:H:127:GLY:O	2.17	0.45
3:A:974:ASP:CB	8:H:136:LYS:NZ	2.80	0.45
11:K:24:ASP:HB3	11:K:30:ALA:CB	2.47	0.45
3:A:219:PHE:CE2	3:A:231:PRO:HD2	2.52	0.45
3:A:517:ASN:OD1	3:A:517:ASN:O	2.34	0.45
4:B:238:ALA:HB3	4:B:256:VAL:HB	1.98	0.45
4:B:515:HIS:O	4:B:516:ASN:C	2.54	0.45
4:B:986:GLN:OE1	4:B:986:GLN:CA	2.64	0.45
5:C:120:ILE:HD11	5:C:130:GLY:O	2.17	0.45
5:C:39:ALA:HA	5:C:164:ALA:CB	2.46	0.45
9:I:92:ARG:CG	9:I:93:LYS:H	2.30	0.45
11:K:78:THR:O	11:K:79:GLU:C	2.56	0.45
1:R:2:U:C5	1:R:3:C:C4	3.05	0.45
3:A:1207:LEU:HA	3:A:1211:GLN:OE1	2.17	0.44
3:A:1336:MET:SD	3:A:1381:LEU:HG	2.56	0.44
4:B:1038:SER:HB3	4:B:1062:HIS:NE2	2.33	0.44
4:B:1169:MET:HE3	4:B:1205:GLN:HG2	2.00	0.44
4:B:426:LYS:O	4:B:430:ARG:HG3	2.17	0.44
4:B:864:LYS:HD3	4:B:871:THR:CA	2.47	0.44
6:E:147:HIS:CD2	6:E:149:LEU:H	2.35	0.44
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.47	0.44
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.98	0.44
3:A:1155:ASP:CG	3:A:1162:VAL:HG23	2.37	0.44
3:A:152:VAL:HG13	3:A:153:PRO:HD2	1.99	0.44
3:A:340:LEU:HD21	4:B:1200:ALA:CA	2.47	0.44
4:B:200:GLY:HA2	4:B:202:TYR:CD2	2.50	0.44
4:B:229:ALA:HB1	4:B:231:PRO:HD2	1.98	0.44
4:B:957:ASN:O	4:B:958:GLN:C	2.55	0.44
5:C:9:LYS:HB2	5:C:21:ILE:HB	1.98	0.44
6:E:190:LEU:HD11	6:E:196:VAL:HG11	1.98	0.44
8:H:5:LEU:O	8:H:133:ASN:HB3	2.17	0.44
9:I:99:LEU:HB2	9:I:112:SER:CB	2.46	0.44
9:I:7:CYS:HB2	9:I:14:LEU:CD2	2.34	0.44
12:L:62:LYS:O	12:L:64:LEU:N	2.37	0.44
3:A:541:ILE:HG12	3:A:549:MET:HE3	1.99	0.44
3:A:67:CYS:SG	3:A:77:CYS:SG	3.11	0.44
3:A:825:ILE:C	3:A:827:THR:N	2.70	0.44
4:B:1085:ILE:HG22	4:B:1086:PHE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:130:VAL:CG1	4:B:131:ASP:H	2.29	0.44
4:B:800:GLN:CB	10:J:52:THR:HG22	2.47	0.44
5:C:31:ASN:O	5:C:35:ARG:HG3	2.17	0.44
3:A:701:LEU:HA	9:I:115:LYS:HE3	1.98	0.44
3:A:1068:ALA:O	3:A:1069:ALA:C	2.55	0.44
3:A:1415:SER:O	3:A:1416:ALA:C	2.55	0.44
3:A:13:THR:HG23	3:A:1432:GLN:CD	2.38	0.44
3:A:456:MET:HB2	3:A:478:TYR:OH	2.17	0.44
3:A:756:ILE:CG2	3:A:757:ASN:N	2.80	0.44
3:A:78:PRO:O	3:A:79:GLY:C	2.56	0.44
3:A:21:LEU:HD21	3:A:95:PHE:CZ	2.53	0.44
4:B:1033:LYS:NZ	4:B:1070:GLU:OE1	2.46	0.44
4:B:216:GLU:OE1	4:B:537:LYS:CE	2.66	0.44
4:B:288:ALA:HA	4:B:331:LEU:HD13	1.99	0.44
4:B:276:ILE:HD13	4:B:334:ILE:HG23	1.99	0.44
4:B:365:THR:CG2	4:B:367:LEU:H	2.30	0.44
4:B:408:LEU:HA	4:B:408:LEU:HD12	1.71	0.44
4:B:446:LEU:HD23	4:B:446:LEU:N	2.33	0.44
4:B:664:THR:HG1	4:B:678:GLU:N	2.15	0.44
4:B:707:PRO:O	4:B:708:GLU:O	2.35	0.44
4:B:781:PHE:CE2	4:B:795:ILE:HD11	2.53	0.44
4:B:915:THR:HG21	4:B:934:LYS:HG2	1.99	0.44
4:B:958:GLN:C	4:B:960:GLY:H	2.20	0.44
5:C:69:LEU:HA	5:C:69:LEU:HD12	1.76	0.44
3:A:1441:PHE:HB2	7:F:134:ILE:CG2	2.47	0.44
8:H:98:TYR:O	8:H:118:PHE:HD2	1.99	0.44
2:T:6:DC:H4'	3:A:447:GLN:CD	2.37	0.44
3:A:1066:VAL:O	3:A:1067:LEU:C	2.56	0.44
3:A:233:TRP:O	3:A:235:ILE:N	2.50	0.44
3:A:50:ILE:C	3:A:52:GLY:N	2.69	0.44
3:A:741:ASN:HD22	3:A:743:VAL:N	2.16	0.44
3:A:815:PHE:O	3:A:818:MET:N	2.50	0.44
4:B:1002:THR:CG2	4:B:1004:GLU:HB2	2.47	0.44
4:B:1060:ARG:O	4:B:1063:GLY:N	2.45	0.44
4:B:361:LEU:O	4:B:363:HIS:O	2.35	0.44
4:B:709:ASP:C	4:B:710:LEU:HD23	2.38	0.44
4:B:526:GLU:CD	4:B:752:ALA:HB3	2.38	0.44
3:A:525:GLN:HB2	4:B:835:GLN:HG2	2.00	0.44
4:B:995:ARG:NH1	4:B:997:GLU:OE1	2.49	0.44
6:E:138:ALA:C	6:E:140:LEU:H	2.21	0.44
6:E:28:TYR:CE2	6:E:64:PRO:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:93:TYR:HA	8:H:145:ARG:CB	2.41	0.44
10:J:32:GLU:CD	10:J:32:GLU:H	2.19	0.44
11:K:24:ASP:OD1	11:K:26:LYS:N	2.51	0.44
3:A:1384:VAL:O	3:A:1389:PHE:HE2	2.01	0.44
3:A:243:PRO:HB2	3:A:245:PRO:HD2	1.99	0.44
3:A:388:LEU:HA	3:A:388:LEU:HD23	1.88	0.44
3:A:591:PHE:HD2	3:A:595:THR:HB	1.83	0.44
3:A:595:THR:HG22	3:A:596:THR:N	2.33	0.44
3:A:829:VAL:C	3:A:831:THR:N	2.70	0.44
3:A:760:GLN:OE1	4:B:1021:MET:HE2	2.16	0.44
4:B:168:GLY:H	4:B:450:ALA:HB1	1.82	0.44
4:B:214:ALA:HB2	4:B:408:LEU:CD1	2.48	0.44
4:B:65:GLU:HG3	4:B:66:ASP:N	2.27	0.44
4:B:640:VAL:HG23	4:B:740:HIS:CA	2.48	0.44
4:B:805:THR:HA	4:B:809:MET:HE1	2.00	0.44
4:B:864:LYS:HD3	4:B:871:THR:CB	2.47	0.44
4:B:995:ARG:HH11	4:B:995:ARG:HB2	1.81	0.44
5:C:236:GLY:C	5:C:238:ILE:N	2.69	0.44
6:E:185:ALA:CB	6:E:190:LEU:HD12	2.47	0.44
3:A:960:ILE:HD12	3:A:1021:LEU:HD21	1.99	0.44
3:A:494:SER:HB2	3:A:497:THR:OG1	2.18	0.44
3:A:679:ILE:O	3:A:682:THR:HB	2.18	0.44
4:B:487:THR:O	4:B:488:TYR:C	2.56	0.44
4:B:56:ASP:HB3	4:B:57:TYR:CE1	2.53	0.44
4:B:973:ILE:CG2	4:B:974:PRO:HD2	2.47	0.44
6:E:138:ALA:O	6:E:140:LEU:N	2.50	0.44
12:L:38:LEU:HG	12:L:39:SER:H	1.82	0.44
3:A:1118:VAL:O	3:A:1305:VAL:HG13	2.17	0.44
3:A:381:THR:O	3:A:384:ASN:N	2.41	0.44
3:A:458:HIS:ND1	3:A:507:VAL:HG21	2.33	0.44
3:A:845:LEU:O	3:A:848:ILE:HG13	2.17	0.44
4:B:102:VAL:HG21	4:B:112:LEU:HD13	1.99	0.44
4:B:370:PHE:N	4:B:371:GLU:OE1	2.50	0.44
4:B:912:ILE:O	4:B:938:SER:CB	2.59	0.44
4:B:847:ASP:O	5:C:65:HIS:HE1	2.01	0.44
9:I:50:THR:HG22	9:I:52:ILE:N	2.33	0.44
3:A:1094:VAL:HG12	3:A:1095:THR:N	2.32	0.44
3:A:1121:GLU:O	3:A:1122:PRO:C	2.56	0.44
3:A:1364:ASN:HD22	3:A:1365:TYR:N	2.13	0.44
3:A:84:ILE:CG2	3:A:239:LEU:HB3	2.48	0.44
3:A:366:VAL:HA	3:A:367:PRO:HD2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:567:LYS:HZ3	8:H:95:TYR:HE1	1.52	0.44
4:B:778:MET:HE1	4:B:1094:ARG:HD3	1.98	0.44
4:B:1185:CYS:O	4:B:1186:ASP:HB2	2.17	0.44
4:B:203:PHE:HE1	4:B:212:LEU:CD1	2.31	0.44
4:B:205:ILE:HG12	4:B:461:LEU:HB3	1.99	0.44
5:C:143:LEU:HD21	5:C:146:LYS:HE3	1.99	0.44
5:C:8:VAL:CG1	5:C:9:LYS:N	2.80	0.44
6:E:137:GLU:O	6:E:140:LEU:N	2.43	0.44
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.17	0.44
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.51	0.44
3:A:1349:TYR:O	3:A:1350:LYS:C	2.56	0.43
3:A:1364:ASN:HD22	3:A:1366:ARG:N	2.16	0.43
3:A:1441:PHE:HB2	7:F:134:ILE:HG23	2.00	0.43
3:A:326:ARG:HE	3:A:1406:VAL:HG11	1.82	0.43
3:A:404:TYR:HA	3:A:413:ILE:O	2.18	0.43
3:A:54:ASN:O	3:A:55:ASP:HB2	2.18	0.43
3:A:562:THR:HA	3:A:563:PRO:HD3	1.92	0.43
3:A:614:PHE:C	3:A:614:PHE:CD1	2.92	0.43
4:B:310:MET:O	4:B:313:MET:HB2	2.18	0.43
4:B:650:GLU:HG2	4:B:654:ARG:NH1	2.33	0.43
4:B:690:VAL:HG12	4:B:691:GLU:N	2.33	0.43
4:B:745:PRO:C	4:B:747:MET:N	2.70	0.43
5:C:135:GLN:C	5:C:136:ASP:O	2.56	0.43
5:C:46:ILE:HG23	5:C:157:CYS:HB3	2.00	0.43
5:C:77:ILE:CG2	5:C:161:LYS:HE3	2.48	0.43
8:H:5:LEU:O	8:H:6:PHE:HB2	2.18	0.43
9:I:91:ARG:HD3	9:I:91:ARG:HA	1.75	0.43
9:I:98:VAL:CG1	9:I:99:LEU:N	2.81	0.43
11:K:55:LYS:HD3	11:K:78:THR:OG1	2.18	0.43
3:A:1015:VAL:O	3:A:1015:VAL:HG12	2.18	0.43
3:A:535:THR:HG21	3:A:616:VAL:CA	2.43	0.43
3:A:533:LYS:C	3:A:535:THR:N	2.72	0.43
3:A:742:ASN:C	3:A:745:GLN:HB2	2.38	0.43
4:B:1002:THR:HG21	4:B:1006:ILE:HB	2.00	0.43
4:B:315:LYS:N	4:B:316:PRO:HD2	2.32	0.43
4:B:34:ILE:HG12	4:B:542:MET:HE1	2.00	0.43
6:E:133:GLU:HB3	6:E:135:PHE:HE1	1.83	0.43
6:E:82:PHE:CD1	6:E:82:PHE:N	2.85	0.43
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.48	0.43
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.49	0.43
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:2:U:H3'	1:R:3:C:C6	2.54	0.43
3:A:1049:ILE:O	3:A:1050:GLU:C	2.56	0.43
3:A:850:VAL:O	3:A:1060:PRO:HA	2.18	0.43
3:A:42:ASP:OD1	3:A:45:GLN:O	2.36	0.43
3:A:367:PRO:CB	3:A:466:SER:HA	2.47	0.43
3:A:629:LEU:CD1	3:A:645:LEU:HD21	2.48	0.43
4:B:1060:ARG:C	4:B:1062:HIS:N	2.69	0.43
4:B:189:LEU:O	4:B:190:TYR:C	2.57	0.43
4:B:212:LEU:HD13	4:B:409:ALA:HA	2.00	0.43
4:B:358:LYS:O	4:B:359:GLU:OE1	2.36	0.43
4:B:562:GLY:O	4:B:563:MET:C	2.56	0.43
4:B:781:PHE:HE2	4:B:795:ILE:HD11	1.83	0.43
4:B:850:LEU:CD2	4:B:1009:ASP:HB3	2.48	0.43
5:C:173:ALA:O	5:C:174:ALA:CB	2.64	0.43
6:E:113:GLN:HG2	6:E:137:GLU:OE1	2.19	0.43
6:E:7:ARG:C	6:E:9:ILE:N	2.71	0.43
9:I:84:VAL:CG1	9:I:84:VAL:O	2.65	0.43
11:K:92:ASN:O	11:K:93:SER:C	2.56	0.43
2:T:8:DT:H2'	2:T:9:DC:C6	2.53	0.43
3:A:1148:ILE:HD12	3:A:1196:GLU:HG2	2.01	0.43
3:A:1385:THR:HG22	3:A:1386:ARG:N	2.33	0.43
3:A:399:HIS:C	3:A:401:GLY:N	2.71	0.43
3:A:412:ARG:CZ	4:B:1108:ARG:NH2	2.81	0.43
3:A:778:GLY:HA3	4:B:516:ASN:CB	2.46	0.43
3:A:373:THR:HG21	4:B:1105:ALA:O	2.17	0.43
4:B:366:GLN:O	4:B:367:LEU:O	2.36	0.43
4:B:806:THR:C	4:B:808:ALA:N	2.70	0.43
5:C:123:ASN:ND2	5:C:125:MET:HG2	2.31	0.43
5:C:251:LEU:HG	11:K:98:LEU:HD11	2.01	0.43
5:C:264:GLN:H	5:C:264:GLN:HG3	1.61	0.43
5:C:31:ASN:O	5:C:32:SER:C	2.56	0.43
5:C:52:GLU:HB3	5:C:154:LYS:HB3	1.99	0.43
5:C:56:THR:CG2	5:C:57:VAL:N	2.69	0.43
8:H:57:VAL:HG12	8:H:58:THR:N	2.32	0.43
4:B:784:ASN:HB3	10:J:63:TYR:OH	2.18	0.43
12:L:27:LEU:HD13	12:L:37:LYS:CB	2.48	0.43
12:L:43:THR:HG22	12:L:43:THR:O	2.18	0.43
2:T:1:DA:N3	2:T:2:DC:C6	2.86	0.43
3:A:148:CYS:HB3	3:A:167:CYS:O	2.18	0.43
3:A:845:LEU:O	3:A:846:GLU:C	2.57	0.43
3:A:84:ILE:HG23	3:A:84:ILE:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:901:LEU:HD13	3:A:919:ILE:CG2	2.48	0.43
4:B:1171:VAL:HG13	4:B:1191:ILE:HD13	1.99	0.43
4:B:194:GLU:HA	4:B:194:GLU:OE1	2.18	0.43
4:B:202:TYR:CD2	4:B:202:TYR:N	2.87	0.43
4:B:904:ARG:CZ	4:B:948:ILE:HD11	2.48	0.43
4:B:831:SER:CB	4:B:994:TYR:OH	2.67	0.43
6:E:114:ASN:O	6:E:115:ASN:HB3	2.18	0.43
11:K:47:ARG:CB	11:K:47:ARG:HH11	2.23	0.43
3:A:968:GLN:NE2	3:A:1035:TYR:HB2	2.33	0.43
3:A:1424:VAL:HG11	4:B:1139:ILE:HD13	2.00	0.43
3:A:344:ARG:O	4:B:1118:PRO:HG2	2.19	0.43
3:A:565:ILE:HD13	3:A:567:LYS:HE2	2.01	0.43
3:A:774:ARG:O	3:A:775:ILE:C	2.57	0.43
3:A:99:ILE:O	3:A:102:VAL:HB	2.19	0.43
3:A:751:SER:OG	4:B:1015:HIS:CE1	2.71	0.43
4:B:1177:HIS:C	4:B:1179:GLN:H	2.22	0.43
4:B:1116:ARG:CZ	4:B:1198:TYR:CE1	3.01	0.43
4:B:280:ILE:CG2	4:B:285:ILE:HG13	2.47	0.43
4:B:295:GLY:H	4:B:298:LEU:HG	1.84	0.43
4:B:345:LYS:N	4:B:348:ARG:HE	2.15	0.43
4:B:758:PHE:CZ	4:B:1044:ALA:HA	2.53	0.43
4:B:955:THR:CG2	4:B:956:THR:N	2.49	0.43
4:B:955:THR:HA	12:L:54:ARG:O	2.19	0.43
5:C:148:ARG:HD3	5:C:149:LYS:H	1.83	0.43
5:C:39:ALA:CA	5:C:164:ALA:HB3	2.47	0.43
14:R:3000:UTP:C2	2:T:4:DA:N1	2.86	0.43
1:R:6:G:H2'	1:R:7:A:O5'	2.19	0.43
3:A:1097:GLY:C	3:A:1099:PRO:HD2	2.39	0.43
3:A:1336:MET:HE1	3:A:1381:LEU:N	2.33	0.43
3:A:1409:LEU:HD23	3:A:1409:LEU:HA	1.83	0.43
3:A:645:LEU:HD11	3:A:649:ILE:HD11	2.01	0.43
3:A:672:ASP:O	3:A:675:THR:HB	2.19	0.43
3:A:673:GLY:N	3:A:674:PRO:HD2	2.33	0.43
3:A:852:TYR:CE2	7:F:136:ARG:NE	2.86	0.43
4:B:1175:LEU:O	4:B:1176:ASN:CG	2.56	0.43
4:B:648:HIS:HB2	4:B:649:LYS:H	1.61	0.43
5:C:135:GLN:O	5:C:136:ASP:O	2.37	0.43
6:E:145:THR:HG21	6:E:187:TYR:CE2	2.53	0.43
6:E:9:ILE:C	6:E:11:ARG:N	2.71	0.43
12:L:40:LEU:HD23	12:L:40:LEU:HA	1.77	0.43
3:A:1194:ARG:HH22	3:A:1237:ILE:HD13	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:466:SER:HB3	11:K:2:ASN:HD22	1.83	0.43
3:A:457:ALA:O	3:A:507:VAL:HG23	2.19	0.43
3:A:545:GLN:O	3:A:546:VAL:C	2.55	0.43
3:A:709:THR:O	3:A:712:GLU:N	2.52	0.43
3:A:89:PRO:HG3	3:A:208:LEU:HD12	2.00	0.43
4:B:1108:ARG:O	4:B:1108:ARG:CG	2.67	0.43
4:B:128:LEU:HA	4:B:128:LEU:HD12	1.82	0.43
4:B:101:MET:HE3	4:B:169:ARG:HH22	1.84	0.43
4:B:126:SER:OG	4:B:172:ILE:HD11	2.18	0.43
4:B:642:ASP:O	4:B:643:ASP:C	2.56	0.43
4:B:705:MET:H	4:B:710:LEU:CD1	2.32	0.43
4:B:784:ASN:HD21	4:B:788:ARG:HD2	1.84	0.43
8:H:47:PHE:CB	8:H:95:TYR:HD1	2.31	0.43
9:I:106:CYS:O	9:I:107:SER:HB2	2.18	0.43
3:A:709:THR:HG23	9:I:94:ASP:HA	2.00	0.43
3:A:1004:ASN:O	3:A:1008:GLN:HB2	2.19	0.43
3:A:1300:LYS:HZ2	3:A:1300:LYS:HB3	1.84	0.43
3:A:1394:THR:HG22	3:A:1395:GLY:O	2.19	0.43
3:A:114:LEU:HD12	3:A:142:CYS:O	2.19	0.43
3:A:396:PRO:HG3	3:A:416:ARG:HB3	2.00	0.43
3:A:547:LEU:HD22	11:K:58:PHE:HD1	1.84	0.43
4:B:1103:ILE:O	4:B:1104:HIS:C	2.56	0.43
4:B:113:TYR:CD2	4:B:192:LEU:HD22	2.53	0.43
4:B:702:LEU:HD22	4:B:737:THR:CG2	2.49	0.43
6:E:16:PHE:CZ	6:E:20:LYS:HE2	2.54	0.43
6:E:69:ILE:O	6:E:73:PRO:HG3	2.19	0.43
7:F:140:ASP:OD1	7:F:141:GLY:N	2.52	0.43
8:H:111:LEU:HD23	8:H:127:GLY:O	2.18	0.43
3:A:306:ASN:OD1	3:A:313:GLN:NE2	2.51	0.43
3:A:337:ARG:CZ	3:A:839:ARG:CZ	2.97	0.43
3:A:815:PHE:C	3:A:817:ALA:N	2.72	0.43
3:A:907:THR:HG22	3:A:908:LEU:H	1.82	0.43
3:A:960:ILE:O	3:A:961:ARG:C	2.57	0.43
4:B:274:PRO:O	4:B:276:ILE:N	2.51	0.43
5:C:249:ASP:OD1	5:C:253:LYS:HE3	2.19	0.43
6:E:168:TYR:O	6:E:170:LEU:HD23	2.19	0.43
9:I:46:HIS:O	9:I:47:GLU:HB2	2.18	0.43
9:I:59:VAL:HG12	9:I:60:GLN:N	2.34	0.43
3:A:134:ARG:O	3:A:137:ALA:N	2.52	0.42
3:A:1428:VAL:HG13	4:B:1151:LEU:HD23	2.00	0.42
3:A:362:ASP:OD1	3:A:459:ARG:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:518:LYS:HB2	3:A:519:PRO:HD2	2.01	0.42
4:B:34:ILE:HG12	4:B:542:MET:CE	2.49	0.42
4:B:794:ASN:O	4:B:795:ILE:HD12	2.19	0.42
5:C:148:ARG:H	5:C:151:GLN:HG3	1.84	0.42
3:A:1366:ARG:HG2	3:A:1366:ARG:HH11	1.84	0.42
3:A:86:LEU:HB3	3:A:296:LEU:HD21	2.00	0.42
4:B:329:THR:O	4:B:332:ASP:HB3	2.19	0.42
4:B:601:ARG:O	4:B:605:ARG:HG3	2.19	0.42
4:B:708:GLU:C	4:B:710:LEU:N	2.72	0.42
4:B:806:THR:O	4:B:808:ALA:N	2.52	0.42
5:C:59:ALA:O	5:C:63:ILE:HG13	2.18	0.42
5:C:76:ASP:OD2	5:C:128:ASN:N	2.47	0.42
6:E:137:GLU:O	6:E:138:ALA:C	2.57	0.42
3:A:1027:ALA:O	3:A:1030:ARG:HB2	2.20	0.42
3:A:131:SER:OG	3:A:132:LYS:N	2.51	0.42
3:A:30:ILE:O	3:A:31:SER:O	2.37	0.42
3:A:451:HIS:HB2	3:A:454:SER:OG	2.19	0.42
3:A:753:GLY:HA2	3:A:757:ASN:ND2	2.34	0.42
3:A:80:HIS:N	3:A:243:PRO:HB3	2.34	0.42
3:A:962:ARG:O	3:A:963:ILE:C	2.57	0.42
4:B:1073:TYR:N	4:B:1073:TYR:CD1	2.87	0.42
4:B:1148:LYS:O	4:B:1152:MET:HB2	2.19	0.42
4:B:1177:HIS:O	4:B:1179:GLN:HG3	2.19	0.42
4:B:281:PRO:HG2	4:B:284:ILE:CD1	2.45	0.42
4:B:880:THR:O	4:B:881:ASN:HB2	2.20	0.42
5:C:8:VAL:HA	5:C:21:ILE:O	2.19	0.42
5:C:242:GLN:O	5:C:246:ARG:N	2.52	0.42
6:E:168:TYR:CB	6:E:170:LEU:HG	2.49	0.42
9:I:84:VAL:HG13	9:I:84:VAL:O	2.19	0.42
10:J:9:SER:HB2	10:J:45:CYS:HB2	2.00	0.42
11:K:95:ILE:O	11:K:98:LEU:HB2	2.19	0.42
4:B:955:THR:CG2	12:L:54:ARG:O	2.65	0.42
2:T:1:DA:H2''	2:T:2:DC:C5'	2.41	0.42
2:T:6:DC:C2'	2:T:7:DC:O5'	2.67	0.42
3:A:1152:ILE:HG23	3:A:1260:LEU:CD2	2.43	0.42
3:A:151:ASP:OD1	3:A:163:SER:HA	2.19	0.42
3:A:166:GLY:O	3:A:167:CYS:CB	2.67	0.42
3:A:223:GLY:O	3:A:1415:SER:CA	2.64	0.42
3:A:35:ILE:HD13	3:A:53:LEU:HD23	2.00	0.42
3:A:68:GLN:O	3:A:70:CYS:N	2.52	0.42
3:A:751:SER:O	3:A:752:LYS:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:7:SER:OG	4:B:1193:GLN:NE2	2.51	0.42
4:B:55:VAL:O	4:B:59:LEU:HB3	2.19	0.42
4:B:757:PRO:HG2	4:B:984:HIS:CE1	2.54	0.42
4:B:969:ARG:HG2	4:B:970:THR:N	2.33	0.42
4:B:994:TYR:HD1	4:B:999:MET:HE3	1.84	0.42
8:H:143:LEU:HD12	8:H:143:LEU:N	2.34	0.42
9:I:55:THR:HG21	9:I:109:ILE:CD1	2.49	0.42
10:J:21:TYR:CA	10:J:39:LEU:HD11	2.49	0.42
10:J:53:HIS:CE1	10:J:55:ASP:HA	2.54	0.42
4:B:115:GLN:HG2	4:B:193:LYS:HB2	2.01	0.42
4:B:1197:PRO:O	4:B:1200:ALA:HB3	2.19	0.42
4:B:1204:PHE:O	4:B:1207:LEU:HB2	2.19	0.42
4:B:39:ARG:HG2	4:B:39:ARG:HH11	1.85	0.42
6:E:72:PHE:CD2	6:E:155:ARG:NH2	2.83	0.42
3:A:1161:THR:OG1	3:A:1170:ILE:HD11	2.20	0.42
3:A:441:PRO:HG2	3:A:441:PRO:O	2.20	0.42
3:A:530:GLY:O	3:A:532:ARG:N	2.53	0.42
2:T:4:DA:C6	3:A:831:THR:HG21	2.54	0.42
3:A:984:LYS:O	3:A:988:LEU:HB2	2.19	0.42
4:B:1106:ARG:HH12	4:B:1118:PRO:CA	2.33	0.42
4:B:121:ASN:HA	4:B:207:GLY:CA	2.46	0.42
4:B:234:ILE:N	4:B:234:ILE:HD12	2.30	0.42
4:B:28:GLU:OE1	4:B:807:ARG:NH2	2.44	0.42
4:B:405:ARG:CZ	4:B:632:ARG:HG2	2.49	0.42
5:C:214:ASN:CB	5:C:217:ASP:OD2	2.68	0.42
6:E:59:SER:HA	6:E:80:VAL:O	2.19	0.42
3:A:1150:SER:HB2	3:A:1195:LEU:CD2	2.49	0.42
3:A:115:LEU:HB2	3:A:122:MET:HE2	2.02	0.42
3:A:1187:GLN:HA	3:A:1243:VAL:HG23	2.02	0.42
3:A:533:LYS:C	3:A:535:THR:H	2.23	0.42
3:A:76:GLU:O	3:A:78:PRO:CD	2.68	0.42
4:B:1182:CYS:SG	4:B:1185:CYS:HB2	2.60	0.42
4:B:101:MET:HE2	4:B:169:ARG:NH1	2.35	0.42
4:B:331:LEU:HA	4:B:331:LEU:HD12	1.87	0.42
4:B:640:VAL:HG22	4:B:651:LEU:HD23	2.01	0.42
4:B:758:PHE:CE2	4:B:1044:ALA:HA	2.53	0.42
4:B:834:ASN:HB2	4:B:838:SER:O	2.19	0.42
4:B:995:ARG:CB	4:B:995:ARG:HH11	2.33	0.42
5:C:252:GLN:NE2	11:K:99:GLY:N	2.68	0.42
6:E:100:ILE:O	6:E:101:GLN:C	2.58	0.42
3:A:873:MET:C	3:A:1058:VAL:HG23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:113:LEU:HG	3:A:218:ASP:OD1	2.19	0.42
3:A:401:GLY:H	3:A:435:HIS:HD2	1.66	0.42
3:A:639:PRO:HG2	3:A:640:GLN:H	1.84	0.42
3:A:683:ILE:CD1	3:A:764:CYS:HB2	2.42	0.42
3:A:908:LEU:O	3:A:909:ASP:C	2.58	0.42
4:B:105:SER:O	4:B:106:ASP:HB2	2.20	0.42
4:B:1072:MET:HE2	4:B:1087:PHE:HD1	1.85	0.42
4:B:203:PHE:HE1	4:B:212:LEU:HD12	1.85	0.42
4:B:346:GLU:O	4:B:347:LYS:C	2.58	0.42
4:B:435:THR:O	4:B:435:THR:HG22	2.20	0.42
4:B:484:ASN:CG	4:B:486:TYR:HE1	2.23	0.42
4:B:640:VAL:HG22	4:B:651:LEU:CD2	2.50	0.42
4:B:666:TYR:C	4:B:668:ASP:N	2.72	0.42
7:F:89:GLU:HB3	7:F:134:ILE:HD13	2.00	0.42
9:I:101:PHE:HD1	9:I:110:PHE:O	2.02	0.42
10:J:27:GLU:C	10:J:29:GLU:H	2.23	0.42
3:A:834:THR:HG21	3:A:1077:THR:HA	2.00	0.42
3:A:113:LEU:C	3:A:115:LEU:H	2.23	0.42
3:A:1168:GLU:O	3:A:1172:LEU:HG	2.19	0.42
3:A:1390:ASN:HD21	3:A:1399:ARG:HA	1.78	0.42
3:A:383:TYR:HB3	7:F:115:THR:CG2	2.44	0.42
3:A:637:LYS:HA	3:A:637:LYS:HD3	1.93	0.42
3:A:534:LEU:HD13	3:A:656:TRP:CD1	2.54	0.42
4:B:1152:MET:SD	4:B:1197:PRO:HD3	2.59	0.42
4:B:634:TYR:CD1	4:B:692:TYR:HB3	2.55	0.42
4:B:705:MET:N	4:B:710:LEU:HD12	2.34	0.42
4:B:749:LEU:HD22	4:B:753:ALA:CB	2.50	0.42
4:B:855:PHE:HZ	4:B:857:ARG:HH12	1.64	0.42
4:B:877:PRO:O	4:B:878:GLN:HG2	2.19	0.42
6:E:117:THR:C	6:E:119:SER:N	2.73	0.42
8:H:12:VAL:HG13	8:H:26:ILE:HG23	2.01	0.42
3:A:1342:GLU:HG2	6:E:212:ARG:HH11	1.83	0.42
3:A:1347:ALA:O	3:A:1348:LEU:C	2.55	0.42
3:A:407:ARG:HG2	3:A:430:TRP:CE2	2.54	0.42
3:A:474:VAL:HG13	3:A:474:VAL:O	2.20	0.42
3:A:633:VAL:HG11	3:A:645:LEU:HD22	2.01	0.42
3:A:68:GLN:C	3:A:70:CYS:N	2.73	0.42
3:A:725:ALA:HA	3:A:728:LYS:HE2	2.02	0.42
3:A:84:ILE:HG21	3:A:239:LEU:HD23	2.01	0.42
4:B:1106:ARG:HH12	4:B:1118:PRO:HA	1.85	0.42
4:B:546:SER:OG	4:B:631:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:5:GLY:O	5:C:6:PRO:O	2.37	0.42
6:E:19:VAL:O	6:E:19:VAL:HG12	2.20	0.42
8:H:31:THR:O	8:H:32:THR:OG1	2.37	0.42
11:K:93:SER:O	11:K:97:LYS:HG3	2.20	0.42
3:A:101:LYS:HG2	3:A:139:TRP:CZ2	2.55	0.41
3:A:1343:ALA:O	3:A:1346:ALA:HB3	2.20	0.41
3:A:1406:VAL:CG1	3:A:1410:PHE:CE1	3.03	0.41
3:A:1436:ILE:O	3:A:1437:GLY:C	2.56	0.41
3:A:38:PRO:CA	3:A:270:LEU:HD23	2.50	0.41
3:A:399:HIS:CB	3:A:400:PRO:HD3	2.45	0.41
3:A:59:GLY:HA2	3:A:67:CYS:SG	2.60	0.41
3:A:866:PHE:C	3:A:867:ILE:HG13	2.40	0.41
3:A:343:LYS:NZ	4:B:1156:ASP:OD2	2.49	0.41
4:B:230:ALA:O	4:B:232:SER:N	2.47	0.41
6:E:178:ILE:CG2	6:E:214:CYS:HA	2.48	0.41
7:F:111:LEU:C	7:F:113:GLY:N	2.71	0.41
8:H:57:VAL:CG1	8:H:58:THR:N	2.83	0.41
3:A:782:ARG:NH2	9:I:67:THR:HG22	2.35	0.41
5:C:14:SER:HA	11:K:114:LEU:HD22	2.02	0.41
11:K:71:PHE:CD1	11:K:71:PHE:C	2.93	0.41
3:A:1329:THR:HG22	3:A:1330:ASN:N	2.35	0.41
3:A:474:VAL:HG13	3:A:478:TYR:HE1	1.85	0.41
3:A:515:GLN:CG	3:A:516:SER:N	2.84	0.41
3:A:982:THR:HB	3:A:985:ASP:CG	2.40	0.41
4:B:350:GLN:O	4:B:351:TYR:C	2.58	0.41
4:B:368:GLU:O	4:B:371:GLU:OE1	2.37	0.41
4:B:56:ASP:CB	4:B:57:TYR:HD1	2.34	0.41
5:C:27:LEU:HD12	5:C:27:LEU:O	2.20	0.41
6:E:79:TRP:HD1	6:E:96:PHE:HE1	1.67	0.41
8:H:139:ASN:O	8:H:140:ALA:CB	2.68	0.41
1:R:2:U:C4	1:R:3:C:N4	2.88	0.41
3:A:1139:GLU:HG3	3:A:1280:GLU:O	2.20	0.41
3:A:1173:HIS:NE2	3:A:1227:ILE:HG23	2.35	0.41
3:A:1364:ASN:HD21	3:A:1366:ARG:NH1	2.19	0.41
3:A:88:LYS:HD2	3:A:293:GLU:OE1	2.20	0.41
3:A:683:ILE:O	3:A:686:ALA:N	2.53	0.41
3:A:881:GLN:NE2	3:A:958:VAL:O	2.46	0.41
4:B:1162:ILE:HG22	4:B:1163:CYS:N	2.34	0.41
4:B:1177:HIS:O	4:B:1179:GLN:N	2.52	0.41
4:B:1114:LEU:O	4:B:1198:TYR:HE2	2.04	0.41
4:B:315:LYS:O	4:B:317:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:797:TYR:HB3	4:B:798:TYR:CD1	2.55	0.41
4:B:879:ARG:O	4:B:880:THR:HB	2.20	0.41
8:H:4:THR:O	8:H:5:LEU:HD23	2.20	0.41
9:I:25:LEU:HD12	9:I:26:LEU:N	2.35	0.41
10:J:53:HIS:CD2	10:J:54:VAL:N	2.88	0.41
11:K:35:PHE:O	11:K:70:ARG:HB2	2.21	0.41
3:A:49:LYS:NZ	3:A:60:SER:HA	2.34	0.41
3:A:568:PRO:CB	5:C:221:TYR:CZ	3.03	0.41
3:A:542:GLU:OE1	3:A:569:LYS:HE2	2.20	0.41
3:A:783:THR:CG2	3:A:815:PHE:CZ	2.98	0.41
4:B:707:PRO:O	4:B:708:GLU:C	2.59	0.41
3:A:871:ASP:CB	6:E:204:THR:CG2	2.98	0.41
10:J:34:THR:O	10:J:35:ALA:C	2.58	0.41
11:K:82:ASP:O	11:K:85:ASP:HB2	2.20	0.41
12:L:41:SER:O	12:L:44:ASP:HB2	2.21	0.41
3:A:1126:ALA:O	3:A:1128:GLN:N	2.53	0.41
3:A:1254:ALA:O	3:A:1255:GLU:HB2	2.20	0.41
3:A:1317:MET:CA	3:A:1322:ILE:HD11	2.46	0.41
3:A:1402:PHE:O	3:A:1404:GLU:N	2.51	0.41
3:A:172:PRO:HB3	3:A:185:TRP:CZ2	2.55	0.41
3:A:339:ASN:HB3	4:B:1117:GLN:HE22	1.85	0.41
3:A:401:GLY:N	3:A:435:HIS:HD2	2.19	0.41
3:A:598:LEU:O	3:A:599:SER:C	2.59	0.41
3:A:885:THR:HG23	3:A:893:PHE:CE1	2.36	0.41
3:A:928:LEU:O	3:A:929:LEU:C	2.59	0.41
4:B:1020:ARG:O	4:B:1021:MET:C	2.58	0.41
4:B:1033:LYS:NZ	4:B:1087:PHE:O	2.51	0.41
4:B:240:ILE:C	4:B:253:THR:HG23	2.41	0.41
4:B:307:ASP:O	4:B:308:TRP:C	2.59	0.41
4:B:171:PRO:HD2	4:B:457:LEU:HD12	2.03	0.41
4:B:499:ASN:OD1	4:B:500:THR:N	2.53	0.41
4:B:54:PHE:HA	4:B:58:THR:CB	2.47	0.41
6:E:13:TRP:O	6:E:16:PHE:HB3	2.21	0.41
3:A:383:TYR:O	7:F:115:THR:HG22	2.20	0.41
8:H:83:GLN:C	8:H:85:GLY:N	2.73	0.41
3:A:980:ASP:OD2	3:A:1039:LYS:HB3	2.21	0.41
3:A:244:PRO:O	3:A:245:PRO:C	2.59	0.41
3:A:553:VAL:HG22	3:A:652:VAL:CG2	2.51	0.41
3:A:71:GLN:HB2	3:A:72:GLU:H	1.62	0.41
4:B:92:PHE:HD2	4:B:130:VAL:HG11	1.85	0.41
4:B:167:ILE:O	4:B:168:GLY:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:911:ILE:HD11	4:B:941:LEU:CB	2.50	0.41
3:A:568:PRO:HB3	5:C:221:TYR:OH	2.21	0.41
5:C:252:GLN:HG3	11:K:95:ILE:HG23	2.03	0.41
6:E:116:ILE:CG2	6:E:117:THR:N	2.84	0.41
6:E:72:PHE:CD1	6:E:72:PHE:N	2.89	0.41
9:I:63:GLY:O	9:I:70:ARG:NH2	2.53	0.41
9:I:85:PHE:HD1	9:I:99:LEU:HD22	1.83	0.41
10:J:3:VAL:CG2	10:J:18:TRP:CG	3.02	0.41
5:C:175:ALA:HB3	10:J:43:ARG:CZ	2.51	0.41
3:A:1155:ASP:O	3:A:1190:PRO:O	2.37	0.41
3:A:79:GLY:C	3:A:243:PRO:HG3	2.41	0.41
3:A:541:ILE:HD12	3:A:541:ILE:N	2.34	0.41
3:A:808:LEU:HD12	3:A:808:LEU:N	2.35	0.41
3:A:514:PRO:HB2	3:A:875:ALA:HB3	2.01	0.41
4:B:850:LEU:HD22	4:B:1009:ASP:HB3	2.02	0.41
4:B:1106:ARG:HH11	4:B:1118:PRO:HB3	1.82	0.41
4:B:120:ARG:HH12	12:L:54:ARG:NH1	2.18	0.41
4:B:269:ILE:HB	4:B:317:CYS:SG	2.60	0.41
4:B:53:GLN:HG2	4:B:547:VAL:HG13	2.02	0.41
5:C:186:LEU:HA	5:C:186:LEU:HD12	1.86	0.41
6:E:131:THR:HG21	6:E:191:LYS:HE2	2.02	0.41
6:E:71:LYS:C	6:E:73:PRO:HD3	2.40	0.41
3:A:1107:VAL:CG2	3:A:1383:SER:HA	2.51	0.41
3:A:14:VAL:HB	3:A:1430:LEU:HD13	2.02	0.41
3:A:332:LYS:H	3:A:337:ARG:CB	2.33	0.41
3:A:407:ARG:HG2	3:A:430:TRP:CZ2	2.56	0.41
3:A:481:ASP:C	3:A:481:ASP:OD1	2.58	0.41
3:A:556:TRP:CE2	3:A:558:GLY:HA2	2.56	0.41
3:A:648:ASN:O	3:A:649:ILE:C	2.59	0.41
4:B:205:ILE:HG21	4:B:462:ALA:HB2	2.03	0.41
4:B:244:LEU:HB2	4:B:249:ARG:HA	2.03	0.41
4:B:387:LEU:HD23	4:B:393:LYS:HD2	2.03	0.41
4:B:702:LEU:CD2	4:B:735:ALA:HB1	2.51	0.41
4:B:952:VAL:HG13	4:B:966:VAL:HG22	2.03	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41
11:K:106:GLU:O	11:K:110:ASN:ND2	2.54	0.41
3:A:1006:ILE:HG22	3:A:1007:ILE:N	2.36	0.41
3:A:1039:LYS:NZ	3:A:1043:ASP:OD1	2.47	0.41
3:A:574:GLY:O	3:A:577:ILE:HG12	2.21	0.41
4:B:1177:HIS:HB2	4:B:1179:GLN:HG3	2.03	0.41
4:B:51:PHE:O	4:B:54:PHE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:589:VAL:CG1	4:B:590:HIS:N	2.84	0.41
6:E:116:ILE:HG22	6:E:117:THR:N	2.36	0.41
7:F:109:VAL:CG1	7:F:110:ASP:H	2.34	0.41
9:I:6:PHE:HD2	9:I:13:MET:HA	1.86	0.41
9:I:99:LEU:HB2	9:I:112:SER:OG	2.21	0.41
9:I:98:VAL:HG12	9:I:99:LEU:N	2.36	0.41
2:T:9:DC:OP1	4:B:1123:SER:CB	2.61	0.41
3:A:1116:LEU:CD2	3:A:1316:VAL:HG21	2.51	0.41
3:A:134:ARG:O	3:A:136:ALA:N	2.54	0.41
3:A:14:VAL:O	3:A:15:LYS:HD3	2.20	0.41
3:A:432:VAL:O	3:A:434:ARG:N	2.54	0.41
3:A:843:LYS:HG3	3:A:1402:PHE:CD1	2.54	0.41
4:B:1115:THR:CG2	4:B:1199:ALA:HB2	2.50	0.41
4:B:1152:MET:O	4:B:1156:ASP:O	2.39	0.41
4:B:188:ASP:O	4:B:192:LEU:HG	2.21	0.41
4:B:205:ILE:CD1	4:B:205:ILE:N	2.84	0.41
4:B:418:LYS:O	4:B:420:LEU:N	2.54	0.41
4:B:577:ALA:HB1	4:B:589:VAL:HG12	2.00	0.41
4:B:579:ARG:HB2	4:B:586:TRP:HE1	1.84	0.41
4:B:737:THR:HG23	9:I:66:PRO:HB3	2.01	0.41
4:B:843:GLN:HB2	4:B:993:THR:OG1	2.20	0.41
5:C:114:TYR:CG	5:C:140:ASN:HB3	2.56	0.41
3:A:738:LYS:NZ	5:C:194:GLU:C	2.74	0.41
6:E:3:GLN:HG3	6:E:5:ASN:H	1.85	0.41
6:E:7:ARG:HG3	6:E:8:ASN:N	2.36	0.41
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.46	0.41
11:K:103:THR:O	11:K:106:GLU:N	2.53	0.41
11:K:65:HIS:HD2	11:K:67:PHE:CB	2.33	0.41
1:R:5:A:C5	1:R:6:G:N7	2.89	0.41
3:A:336:ILE:CD1	3:A:1405:THR:HG21	2.45	0.41
3:A:321:PRO:O	3:A:322:VAL:CB	2.63	0.41
3:A:535:THR:O	3:A:536:LEU:C	2.59	0.41
4:B:1149:GLU:HG3	4:B:1153:GLU:OE1	2.20	0.41
4:B:121:ASN:HD21	4:B:965:LYS:HE3	1.86	0.41
4:B:233:PRO:HG2	4:B:234:ILE:HG13	2.03	0.41
4:B:321:GLY:C	4:B:323:VAL:N	2.74	0.41
4:B:704:ALA:HB2	4:B:738:PHE:CD1	2.56	0.41
4:B:846:ILE:CG2	4:B:974:PRO:HG2	2.51	0.41
4:B:864:LYS:CG	4:B:865:LYS:N	2.80	0.41
4:B:992:ILE:CD1	4:B:994:TYR:CE2	3.04	0.41
3:A:1017:LEU:HB3	6:E:205:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:ALA:HA	8:H:87:ARG:CB	2.51	0.41
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.03	0.41
9:I:16:PRO:HA	9:I:26:LEU:O	2.20	0.41
3:A:1107:VAL:HG23	3:A:1383:SER:HA	2.03	0.40
3:A:205:GLU:O	3:A:208:LEU:HB2	2.22	0.40
3:A:530:GLY:O	3:A:533:LYS:N	2.53	0.40
3:A:650:GLN:O	3:A:651:LYS:C	2.58	0.40
3:A:909:ASP:OD1	3:A:910:PRO:HD2	2.22	0.40
3:A:960:ILE:HD12	3:A:1021:LEU:CD2	2.50	0.40
4:B:578:THR:HG23	4:B:622:LYS:C	2.42	0.40
4:B:627:PHE:O	4:B:632:ARG:NH1	2.54	0.40
4:B:941:LEU:HD21	4:B:946:ASN:HA	2.02	0.40
5:C:46:ILE:CG2	5:C:157:CYS:HB3	2.51	0.40
5:C:29:MET:O	5:C:30:ALA:C	2.59	0.40
5:C:51:VAL:HG22	5:C:155:LEU:CD2	2.47	0.40
6:E:63:ASN:HA	6:E:64:PRO:HD3	1.92	0.40
6:E:28:TYR:CE1	6:E:78:LEU:CD1	3.03	0.40
7:F:138:LEU:HD23	7:F:138:LEU:HA	1.83	0.40
8:H:126:GLU:N	8:H:130:ARG:HH12	2.19	0.40
10:J:48:ARG:HG2	10:J:48:ARG:HH11	1.86	0.40
11:K:47:ARG:HH11	11:K:48:ALA:N	2.19	0.40
3:A:1102:LYS:HG2	3:A:1106:ASN:ND2	2.36	0.40
3:A:1166:ASP:OD1	3:A:1194:ARG:NH2	2.49	0.40
3:A:203:SER:O	3:A:207:ILE:HG12	2.21	0.40
3:A:399:HIS:NE2	3:A:462:VAL:HG21	2.36	0.40
3:A:771:GLU:H	3:A:822:GLU:CD	2.25	0.40
4:B:1197:PRO:O	4:B:1200:ALA:N	2.52	0.40
4:B:175:ARG:HH11	4:B:175:ARG:HG2	1.87	0.40
4:B:803:LEU:CD1	4:B:1036:ALA:HB2	2.52	0.40
4:B:901:PRO:O	4:B:949:VAL:O	2.38	0.40
4:B:911:ILE:HG21	4:B:966:VAL:HG11	2.01	0.40
4:B:846:ILE:HG23	4:B:974:PRO:HG2	2.04	0.40
5:C:146:LYS:O	5:C:147:LEU:HD23	2.20	0.40
8:H:123:MET:HE1	8:H:142:LEU:HD11	2.03	0.40
8:H:96:VAL:HG13	8:H:143:LEU:HG	2.02	0.40
8:H:33:GLN:OE1	8:H:129:TYR:HE2	2.05	0.40
9:I:99:LEU:O	9:I:111:THR:HG23	2.21	0.40
2:T:7:DC:C5'	2:T:7:DC:P	3.05	0.40
3:A:1224:LEU:HD11	3:A:1240:CYS:HB3	2.03	0.40
3:A:1322:ILE:HD12	3:A:1327:ILE:HD12	2.03	0.40
3:A:18:GLN:O	4:B:1215:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:19:PHE:HA	4:B:1213:THR:O	2.22	0.40
3:A:331:GLY:O	3:A:332:LYS:O	2.39	0.40
3:A:445:ASN:HB3	3:A:455:MET:HG2	2.03	0.40
3:A:463:ILE:CD1	3:A:469:ARG:HG3	2.50	0.40
3:A:719:VAL:HG22	3:A:774:ARG:HD2	2.03	0.40
3:A:679:ILE:CG2	3:A:729:ALA:HB1	2.44	0.40
3:A:738:LYS:HA	8:H:19:ARG:NH2	2.36	0.40
3:A:751:SER:OG	4:B:1015:HIS:HE1	2.03	0.40
3:A:901:LEU:O	3:A:920:LEU:HD23	2.22	0.40
3:A:913:LEU:CD1	3:A:981:LEU:O	2.69	0.40
4:B:1104:HIS:HB2	4:B:1122:ARG:CB	2.51	0.40
4:B:175:ARG:HH11	4:B:175:ARG:CG	2.34	0.40
4:B:276:ILE:HD11	4:B:355:ILE:CD1	2.50	0.40
4:B:380:TYR:O	4:B:384:ARG:HG2	2.21	0.40
4:B:61:ASP:N	4:B:61:ASP:OD1	2.54	0.40
4:B:758:PHE:HB2	4:B:1024:ALA:HB1	2.03	0.40
4:B:840:ILE:HB	4:B:1011:ILE:HB	2.03	0.40
6:E:11:ARG:NH2	6:E:141:VAL:HG21	2.37	0.40
8:H:138:GLU:HG2	8:H:139:ASN:N	2.35	0.40
1:R:10:A:O3'	14:R:3000:UTP:O1A	2.37	0.40
3:A:270:LEU:O	3:A:274:ILE:HG13	2.22	0.40
3:A:894:GLU:C	3:A:896:ARG:N	2.74	0.40
4:B:1156:ASP:HB3	4:B:1197:PRO:CA	2.52	0.40
4:B:283:VAL:HG13	4:B:297:ILE:HD12	2.04	0.40
4:B:363:HIS:O	4:B:364:ILE:CG1	2.70	0.40
5:C:182:PRO:HB2	5:C:207:CYS:SG	2.61	0.40
6:E:182:ASP:O	6:E:186:LEU:HG	2.21	0.40
4:B:801:LYS:HE2	10:J:51:LEU:O	2.22	0.40
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.51	0.40
12:L:28:LYS:O	12:L:29:TYR:CG	2.74	0.40
3:A:1116:LEU:H	3:A:1308:THR:CG2	2.34	0.40
3:A:1220:PHE:O	3:A:1221:LYS:C	2.60	0.40
3:A:19:PHE:HB3	3:A:1413:GLY:HA2	2.03	0.40
3:A:302:THR:O	3:A:313:GLN:NE2	2.54	0.40
3:A:379:VAL:HG22	3:A:431:LYS:HG2	2.03	0.40
3:A:48:ALA:O	3:A:49:LYS:CG	2.65	0.40
3:A:531:ILE:CG2	3:A:532:ARG:N	2.84	0.40
4:B:1120:GLU:CG	4:B:1121:GLY:N	2.84	0.40
4:B:1159:ARG:NE	4:B:1193:GLN:NE2	2.33	0.40
4:B:1180:PHE:O	4:B:1181:GLU:CB	2.70	0.40
4:B:1198:TYR:HE1	4:B:1201:LYS:HZ2	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:288:ALA:O	4:B:331:LEU:CD1	2.69	0.40
4:B:484:ASN:ND2	4:B:486:TYR:HD1	2.19	0.40
4:B:616:ILE:HG12	4:B:696:GLU:HG3	2.03	0.40
4:B:849:GLY:O	4:B:850:LEU:C	2.59	0.40
4:B:1084:GLN:NE2	5:C:192:TRP:HB2	2.37	0.40
5:C:228:PHE:HB2	5:C:230:MET:HE2	2.02	0.40
5:C:66:ARG:HB3	10:J:5:VAL:HG21	2.04	0.40
6:E:90:VAL:HA	6:E:120:ALA:HB2	2.04	0.40
7:F:130:ILE:HA	7:F:131:PRO:HD2	1.94	0.40
7:F:138:LEU:HB3	7:F:139:PRO:CD	2.51	0.40
8:H:117:SER:HA	8:H:122:LEU:HD23	2.02	0.40
9:I:34:TYR:C	9:I:35:VAL:HG23	2.41	0.40
9:I:92:ARG:CG	9:I:93:LYS:N	2.84	0.40
4:B:120:ARG:HH22	12:L:54:ARG:HD2	1.86	0.40

All (59) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:736:THR:CB	9:I:79:HIS:CD2[2_556]	0.78	1.42
4:B:736:THR:OG1	9:I:79:HIS:NE2[2_556]	0.83	1.37
9:I:81:ARG:O	9:I:81:ARG:CB[2_556]	1.01	1.19
4:B:736:THR:OG1	9:I:79:HIS:CD2[2_556]	1.02	1.18
3:A:923:LEU:CD1	9:I:35:VAL:C[4_546]	1.06	1.14
3:A:918:GLU:CB	9:I:21:GLU:OE1[4_546]	1.09	1.11
9:I:81:ARG:CA	9:I:81:ARG:O[2_556]	1.16	1.04
4:B:736:THR:OG1	9:I:79:HIS:CE1[2_556]	1.24	0.96
9:I:81:ARG:CA	9:I:81:ARG:C[2_556]	1.27	0.93
9:I:81:ARG:C	9:I:81:ARG:CB[2_556]	1.30	0.90
4:B:736:THR:CB	9:I:79:HIS:NE2[2_556]	1.35	0.85
9:I:71:SER:O	9:I:81:ARG:NE[2_556]	1.40	0.80
4:B:736:THR:OG1	9:I:79:HIS:CG[2_556]	1.42	0.78
3:A:923:LEU:CD1	9:I:36:GLU:N[4_546]	1.50	0.70
4:B:736:THR:OG1	9:I:79:HIS:ND1[2_556]	1.51	0.69
3:A:923:LEU:CD2	9:I:35:VAL:CB[4_546]	1.54	0.66
9:I:80:SER:OG	9:I:82:GLU:OE1[2_556]	1.56	0.64
9:I:81:ARG:N	9:I:81:ARG:O[2_556]	1.57	0.63
3:A:918:GLU:CB	9:I:21:GLU:CD[4_546]	1.62	0.58
9:I:81:ARG:O	9:I:81:ARG:CG[2_556]	1.66	0.54
3:A:923:LEU:CG	9:I:35:VAL:CB[4_546]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:81:ARG:N	9:I:81:ARG:C[2_556]	1.73	0.47
3:A:923:LEU:CD1	9:I:35:VAL:O[4_546]	1.74	0.46
9:I:71:SER:N	9:I:81:ARG:NH2[2_556]	1.75	0.45
9:I:70:ARG:CA	9:I:81:ARG:NH2[2_556]	1.76	0.44
4:B:736:THR:CA	9:I:79:HIS:NE2[2_556]	1.77	0.43
9:I:80:SER:CB	9:I:82:GLU:CG[2_556]	1.79	0.41
9:I:70:ARG:C	9:I:81:ARG:NH2[2_556]	1.80	0.40
9:I:81:ARG:NH1	9:I:83:ASN:CB[2_556]	1.83	0.37
9:I:81:ARG:CA	9:I:81:ARG:CA[2_556]	1.83	0.37
3:A:918:GLU:CB	9:I:21:GLU:OE2[4_546]	1.85	0.35
9:I:81:ARG:NH1	9:I:83:ASN:CA[2_556]	1.89	0.31
9:I:81:ARG:NH1	9:I:83:ASN:C[2_556]	1.89	0.31
9:I:81:ARG:CA	9:I:81:ARG:CB[2_556]	1.91	0.29
9:I:81:ARG:C	9:I:81:ARG:C[2_556]	1.91	0.29
3:A:918:GLU:CA	9:I:21:GLU:OE1[4_546]	1.91	0.29
3:A:923:LEU:CD1	9:I:35:VAL:CA[4_546]	1.92	0.28
3:A:923:LEU:CD1	9:I:35:VAL:CG1[4_546]	1.92	0.28
3:A:923:LEU:CD2	9:I:35:VAL:CA[4_546]	1.93	0.27
4:B:736:THR:CG2	9:I:79:HIS:CD2[2_556]	1.96	0.24
9:I:71:SER:O	9:I:81:ARG:CD[2_556]	2.01	0.19
9:I:72:ASP:O	9:I:72:ASP:CB[2_556]	2.02	0.18
3:A:923:LEU:CD2	9:I:35:VAL:N[4_546]	2.04	0.16
3:A:923:LEU:CG	9:I:35:VAL:O[4_546]	2.07	0.13
3:A:923:LEU:CG	9:I:35:VAL:CG1[4_546]	2.07	0.13
3:A:923:LEU:CG	9:I:35:VAL:C[4_546]	2.07	0.13
3:A:923:LEU:CB	9:I:35:VAL:O[4_546]	2.09	0.11
9:I:80:SER:CB	9:I:82:GLU:CD[2_556]	2.09	0.11
9:I:81:ARG:NH1	9:I:83:ASN:O[2_556]	2.09	0.11
3:A:923:LEU:CD1	9:I:35:VAL:CB[4_546]	2.11	0.09
4:B:736:THR:CB	9:I:79:HIS:CG[2_556]	2.13	0.07
9:I:72:ASP:O	9:I:72:ASP:O[2_556]	2.15	0.05
9:I:82:GLU:OE2	9:I:105:SER:OG[2_556]	2.15	0.05
4:B:736:THR:CA	9:I:79:HIS:CD2[2_556]	2.15	0.05
4:B:736:THR:N	9:I:79:HIS:NE2[2_556]	2.15	0.05
4:B:715:ALA:CB	9:I:117:LYS:CD[2_556]	2.17	0.03
9:I:81:ARG:CD	9:I:83:ASN:ND2[2_556]	2.19	0.01
9:I:71:SER:C	9:I:81:ARG:NE[2_556]	2.19	0.01
9:I:80:SER:CB	9:I:82:GLU:OE1[2_556]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1365/1733 (79%)	1023 (75%)	252 (18%)	90 (7%)	1	18
4	B	1077/1224 (88%)	839 (78%)	169 (16%)	69 (6%)	1	19
5	C	264/318 (83%)	208 (79%)	40 (15%)	16 (6%)	1	19
6	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	3	25
7	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	3	28
8	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	6
9	I	117/122 (96%)	93 (80%)	15 (13%)	9 (8%)	1	15
10	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	19
11	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	17	56
12	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	1
All	All	3465/4173 (83%)	2656 (77%)	583 (17%)	226 (6%)	1	19

All (226) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	31	SER
3	A	48	ALA
3	A	55	ASP
3	A	56	PRO
3	A	74	MET
3	A	75	ASN
3	A	167	CYS
3	A	322	VAL
3	A	404	TYR
3	A	418	SER
3	A	543	LEU
3	A	567	LYS
3	A	597	LEU
3	A	598	LEU

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Mol	Chain	Res	Type
3	A	628	GLY
3	A	752	LYS
3	A	846	GLU
3	A	998	LEU
3	A	1036	ARG
3	A	1127	ASP
3	A	1206	ASP
3	A	1221	LYS
3	A	1223	ASP
3	A	1392	SER
3	A	1393	ASN
3	A	1403	GLU
3	A	1406	VAL
3	A	1416	ALA
4	B	65	GLU
4	B	124	TYR
4	B	174	LEU
4	B	175	ARG
4	B	200	GLY
4	B	229	ALA
4	B	364	ILE
4	B	367	LEU
4	B	531	GLN
4	B	708	GLU
4	B	709	ASP
4	B	731	VAL
4	B	751	VAL
4	B	958	GLN
4	B	959	ASP
4	B	1046	PRO
4	B	1103	ILE
4	B	1167	GLY
4	B	1176	ASN
4	B	1183	LYS
5	C	4	GLU
5	C	5	GLY
5	C	6	PRO
5	C	110	THR
5	C	142	VAL
5	C	215	GLU
7	F	73	ALA
8	H	32	THR

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Mol	Chain	Res	Type
8	H	81	PRO
8	H	140	ALA
9	I	8	ARG
10	J	2	ILE
10	J	55	ASP
12	L	27	LEU
12	L	38	LEU
12	L	64	LEU
3	A	35	ILE
3	A	54	ASN
3	A	62	ASP
3	A	87	ALA
3	A	109	HIS
3	A	135	PHE
3	A	168	GLY
3	A	332	LYS
3	A	385	ILE
3	A	419	LYS
3	A	534	LEU
3	A	568	PRO
3	A	790	ASP
3	A	986	ILE
3	A	1114	PRO
3	A	1365	TYR
3	A	1366	ARG
3	A	1379	GLY
4	B	55	VAL
4	B	168	GLY
4	B	275	TYR
4	B	346	GLU
4	B	410	GLY
4	B	480	SER
4	B	641	GLU
4	B	643	ASP
4	B	792	MET
4	B	864	LYS
4	B	866	TYR
4	B	884	ARG
4	B	891	ASP
4	B	992	ILE
4	B	1066	SER
4	B	1155	SER

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Mol	Chain	Res	Type
5	C	136	ASP
7	F	142	SER
8	H	61	SER
8	H	77	ARG
8	H	88	SER
8	H	128	ASN
9	I	30	ARG
9	I	79	HIS
12	L	39	SER
12	L	52	GLY
3	A	6	TYR
3	A	45	GLN
3	A	59	GLY
3	A	67	CYS
3	A	69	THR
3	A	335	ARG
3	A	433	GLU
3	A	596	THR
3	A	737	LEU
3	A	775	ILE
3	A	830	LYS
3	A	920	LEU
4	B	28	GLU
4	B	249	ARG
4	B	277	LYS
4	B	447	ALA
4	B	629	ASP
4	B	735	ALA
4	B	807	ARG
4	B	880	THR
4	B	1017	ILE
4	B	1099	VAL
4	B	1104	HIS
4	B	1178	ASN
5	C	48	SER
5	C	149	LYS
5	C	212	PRO
5	C	227	THR
6	E	31	THR
6	E	102	GLU
6	E	103	LYS
6	E	122	LYS

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Mol	Chain	Res	Type
6	E	139	ALA
6	E	206	GLY
7	F	128	LYS
8	H	8	ASP
8	H	17	PRO
8	H	82	PRO
8	H	135	LEU
8	H	139	ASN
9	I	9	ASP
9	I	33	SER
9	I	86	PHE
10	J	9	SER
12	L	63	ARG
3	A	101	LYS
3	A	134	ARG
3	A	139	TRP
3	A	223	GLY
3	A	424	ILE
3	A	599	SER
3	A	1067	LEU
3	A	1097	GLY
3	A	1115	SER
3	A	1122	PRO
3	A	1405	THR
4	B	304	ASP
4	B	436	VAL
4	B	501	PRO
4	B	667	GLN
4	B	791	THR
4	B	1054	GLY
4	B	1097	HIS
5	C	18	VAL
5	C	174	ALA
6	E	59	SER
10	J	6	ARG
12	L	50	ASP
12	L	56	LEU
3	A	58	LEU
3	A	399	HIS
3	A	400	PRO
3	A	958	VAL
3	A	972	HIS

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Mol	Chain	Res	Type
3	A	1098	VAL
3	A	1130	GLN
3	A	1282	VAL
3	A	1351	GLU
3	A	1378	GLN
4	B	248	SER
4	B	419	THR
4	B	619	ILE
4	B	648	HIS
4	B	687	GLU
4	B	707	PRO
4	B	712	PRO
4	B	764	SER
4	B	907	GLY
4	B	982	SER
4	B	1108	ARG
6	E	36	GLU
8	H	62	SER
8	H	89	LEU
9	I	47	GLU
9	I	88	SER
3	A	226	GLU
3	A	368	LYS
3	A	531	ILE
3	A	1014	ALA
3	A	1352	VAL
4	B	27	ALA
6	E	167	ARG
8	H	138	GLU
9	I	98	VAL
11	K	107	THR
12	L	59	ALA
4	B	247	GLY
3	A	336	ILE
3	A	1104	ILE
12	L	55	ILE
3	A	810	PRO
3	A	1075	PRO
3	A	1242	VAL
5	C	172	PRO
5	C	216	GLY
3	A	78	PRO

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Mol	Chain	Res	Type
4	B	511	PRO
5	C	218	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
3	A	1206/1520 (79%)	1128 (94%)	78 (6%)	17	44
4	B	952/1061 (90%)	886 (93%)	66 (7%)	15	43
5	C	234/274 (85%)	222 (95%)	12 (5%)	24	51
6	E	196/197 (100%)	189 (96%)	7 (4%)	35	60
7	F	74/137 (54%)	68 (92%)	6 (8%)	11	38
8	H	117/128 (91%)	112 (96%)	5 (4%)	29	55
9	I	113/116 (97%)	104 (92%)	9 (8%)	12	38
10	J	60/65 (92%)	56 (93%)	4 (7%)	16	43
11	K	99/102 (97%)	90 (91%)	9 (9%)	9	32
12	L	40/57 (70%)	35 (88%)	5 (12%)	4	22
All	All	3091/3657 (84%)	2890 (94%)	201 (6%)	17	44

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	GLN
3	A	22	PHE
3	A	31	SER
3	A	56	PRO
3	A	70	CYS
3	A	93	VAL
3	A	122	MET
3	A	247	ARG
3	A	269	ILE
3	A	302	THR
3	A	322	VAL

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Mol	Chain	Res	Type
3	A	326	ARG
3	A	351	THR
3	A	375	THR
3	A	381	THR
3	A	385	ILE
3	A	397	ASN
3	A	412	ARG
3	A	434	ARG
3	A	443	LEU
3	A	445	ASN
3	A	450	LEU
3	A	451	HIS
3	A	461	LYS
3	A	474	VAL
3	A	475	THR
3	A	493	GLN
3	A	503	GLN
3	A	524	VAL
3	A	538	ASP
3	A	590	ARG
3	A	596	THR
3	A	597	LEU
3	A	598	LEU
3	A	618	GLU
3	A	629	LEU
3	A	666	ILE
3	A	682	THR
3	A	740	LEU
3	A	741	ASN
3	A	745	GLN
3	A	756	ILE
3	A	768	GLN
3	A	774	ARG
3	A	821	ARG
3	A	845	LEU
3	A	849	MET
3	A	855	THR
3	A	858	ASN
3	A	920	LEU
3	A	929	LEU
3	A	948	VAL
3	A	949	ASP

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Mol	Chain	Res	Type
3	A	979	SER
3	A	1029	ARG
3	A	1035	TYR
3	A	1043	ASP
3	A	1057	VAL
3	A	1077	THR
3	A	1122	PRO
3	A	1128	GLN
3	A	1222	ASN
3	A	1232	ASN
3	A	1258	HIS
3	A	1264	GLU
3	A	1295	THR
3	A	1308	THR
3	A	1318	THR
3	A	1332	PHE
3	A	1335	ILE
3	A	1351	GLU
3	A	1359	ASP
3	A	1364	ASN
3	A	1366	ARG
3	A	1375	MET
3	A	1376	THR
3	A	1425	SER
3	A	1442	ASP
4	B	20	ASP
4	B	43	LEU
4	B	57	TYR
4	B	61	ASP
4	B	63	ILE
4	B	98	THR
4	B	109	THR
4	B	121	ASN
4	B	175	ARG
4	B	194	GLU
4	B	232	SER
4	B	234	ILE
4	B	261	ARG
4	B	268	THR
4	B	278	GLN
4	B	309	GLN
4	B	313	MET

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Mol	Chain	Res	Type
4	B	317	CYS
4	B	320	ASP
4	B	331	LEU
4	B	376	PHE
4	B	387	LEU
4	B	396	ASP
4	B	408	LEU
4	B	466	TRP
4	B	485	ARG
4	B	513	GLN
4	B	514	LEU
4	B	538	ASN
4	B	547	VAL
4	B	570	VAL
4	B	576	ASP
4	B	624	LEU
4	B	629	ASP
4	B	644	GLU
4	B	680	THR
4	B	723	VAL
4	B	732	SER
4	B	762	ASN
4	B	764	SER
4	B	780	VAL
4	B	791	THR
4	B	835	GLN
4	B	901	PRO
4	B	909	ASP
4	B	915	THR
4	B	944	THR
4	B	951	GLN
4	B	953	LEU
4	B	976	ILE
4	B	986	GLN
4	B	987	LYS
4	B	996	ARG
4	B	999	MET
4	B	1007	VAL
4	B	1021	MET
4	B	1049	ASP
4	B	1103	ILE
4	B	1111	MET

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Mol	Chain	Res	Type
4	B	1118	PRO
4	B	1132	GLU
4	B	1147	LEU
4	B	1150	ARG
4	B	1151	LEU
4	B	1183	LYS
4	B	1185	CYS
5	C	22	LEU
5	C	25	VAL
5	C	26	ASP
5	C	62	PHE
5	C	69	LEU
5	C	77	ILE
5	C	133	ILE
5	C	148	ARG
5	C	229	TYR
5	C	233	GLU
5	C	240	VAL
5	C	264	GLN
6	E	40	GLU
6	E	60	PHE
6	E	74	ASP
6	E	84	ASP
6	E	92	THR
6	E	104	ASN
6	E	183	PRO
7	F	79	ARG
7	F	90	ARG
7	F	103	MET
7	F	111	LEU
7	F	115	THR
7	F	133	VAL
8	H	21	ASN
8	H	27	GLU
8	H	109	LYS
8	H	110	ASP
8	H	134	ASN
9	I	7	CYS
9	I	12	ASN
9	I	29	CYS
9	I	31	THR
9	I	52	ILE

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Mol	Chain	Res	Type
9	I	75	CYS
9	I	76	PRO
9	I	87	GLN
9	I	103	CYS
10	J	2	ILE
10	J	7	CYS
10	J	47	ARG
10	J	48	ARG
11	K	20	LYS
11	K	25	THR
11	K	31	VAL
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	77	THR
11	K	81	TYR
11	K	114	LEU
12	L	50	ASP
12	L	54	ARG
12	L	55	ILE
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
3	A	92	HIS
3	A	118	HIS
3	A	169	ASN
3	A	225	ASN
3	A	339	ASN
3	A	358	ASN
3	A	435	HIS
3	A	445	ASN
3	A	447	GLN
3	A	493	GLN
3	A	503	GLN
3	A	517	ASN
3	A	631	HIS
3	A	723	ASN
3	A	736	ASN

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Mol	Chain	Res	Type
3	A	741	ASN
3	A	757	ASN
3	A	768	GLN
3	A	786	HIS
3	A	858	ASN
3	A	926	GLN
3	A	965	GLN
3	A	968	GLN
3	A	994	GLN
3	A	1364	ASN
3	A	1387	HIS
3	A	1390	ASN
3	A	1393	ASN
3	A	1432	GLN
4	B	46	GLN
4	B	53	GLN
4	B	178	ASN
4	B	215	GLN
4	B	236	HIS
4	B	325	GLN
4	B	363	HIS
4	B	465	ASN
4	B	484	ASN
4	B	513	GLN
4	B	515	HIS
4	B	516	ASN
4	B	518	HIS
4	B	538	ASN
4	B	657	HIS
4	B	744	HIS
4	B	822	ASN
4	B	842	ASN
4	B	862	GLN
4	B	957	ASN
4	B	975	GLN
4	B	1015	HIS
4	B	1065	GLN
4	B	1117	GLN
4	B	1179	GLN
4	B	1193	GLN
5	C	65	HIS
5	C	73	GLN

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Mol	Chain	Res	Type
5	C	112	ASN
5	C	123	ASN
5	C	167	HIS
5	C	242	GLN
5	C	252	GLN
6	E	5	ASN
6	E	32	GLN
6	E	101	GLN
6	E	104	ASN
6	E	114	ASN
6	E	147	HIS
8	H	33	GLN
9	I	12	ASN
10	J	53	HIS
11	K	52	ASN
11	K	65	HIS
11	K	76	GLN
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/10 (100%)	3 (30%)	3 (30%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A
1	R	6	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A
1	R	4	G
1	R	5	A

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](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	UTP	R	3000	1,13	26,30,30	3.30	11 (42%)	34,47,47	3.24	9 (26%)

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
14	UTP	R	3000	1,13	1/1/7/7	4/22/38/38	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	R	3000	UTP	C1'-N1	7.74	1.61	1.46
14	R	3000	UTP	C6-C5	-6.77	1.34	1.52
14	R	3000	UTP	C3'-C4'	-5.50	1.38	1.53
14	R	3000	UTP	C5'-C4'	5.26	1.68	1.51
14	R	3000	UTP	O2'-C2'	5.17	1.55	1.43
14	R	3000	UTP	C6-N1	-5.08	1.38	1.47
14	R	3000	UTP	O3'-C3'	-4.34	1.32	1.43
14	R	3000	UTP	O4'-C4'	-4.29	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	R	3000	UTP	C5-C4	-2.63	1.44	1.50
14	R	3000	UTP	C2-N1	2.53	1.39	1.35
14	R	3000	UTP	PB-O1B	-2.01	1.45	1.55

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	3000	UTP	O4'-C4'-C5'	13.11	152.51	109.37
14	R	3000	UTP	O5'-C5'-C4'	6.78	132.33	108.99
14	R	3000	UTP	C5'-C4'-C3'	-6.59	90.48	115.18
14	R	3000	UTP	O3'-C3'-C2'	-4.56	97.06	111.82
14	R	3000	UTP	O4'-C4'-C3'	4.34	113.69	105.11
14	R	3000	UTP	C5-C6-N1	3.38	122.75	111.61
14	R	3000	UTP	O2'-C2'-C1'	-2.80	100.68	110.02
14	R	3000	UTP	O2'-C2'-C3'	-2.09	105.06	111.82
14	R	3000	UTP	C4'-O4'-C1'	-2.03	105.00	109.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	R	3000	UTP	C4'

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	R	3000	UTP	C5'-O5'-PA-O2A
14	R	3000	UTP	C5'-O5'-PA-O3A
14	R	3000	UTP	C4'-C5'-O5'-PA
14	R	3000	UTP	O4'-C4'-C5'-O5'

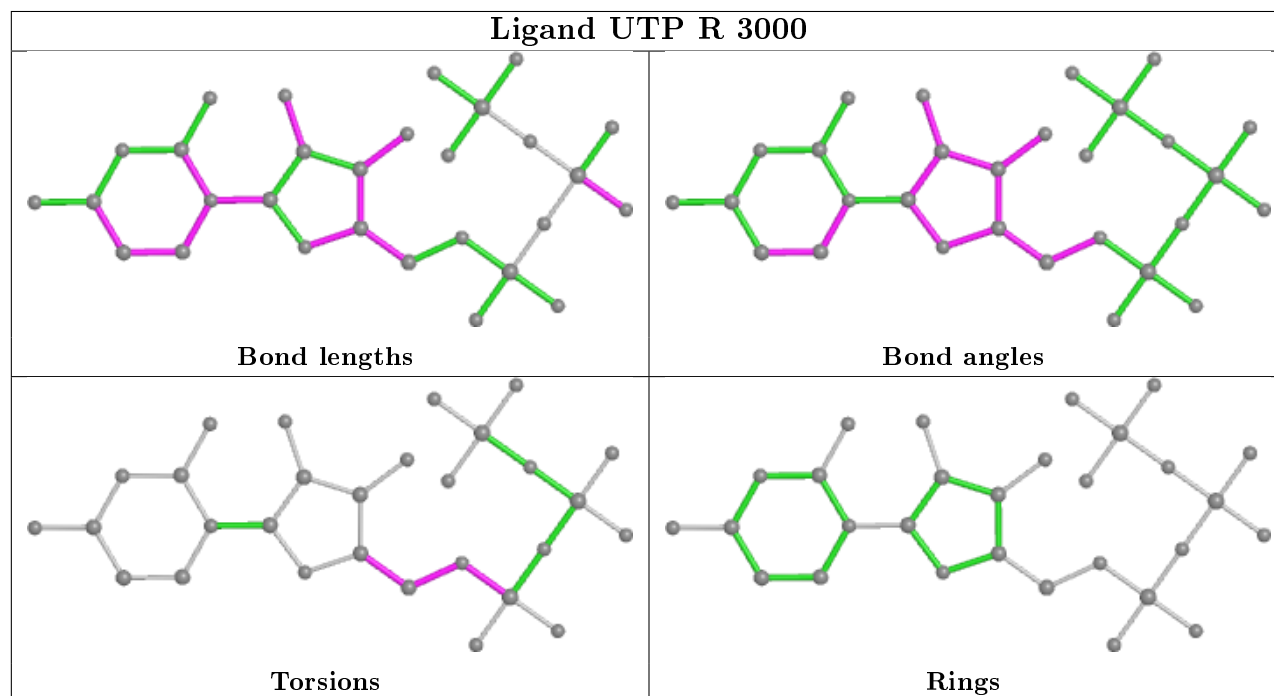
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	R	3000	UTP	8	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	T	3
1	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	7:DC	O3'	8:DT	P	1.39
1	R	5:A	O3'	6:G	P	1.33
1	T	4:DA	O3'	5:DT	P	1.24

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	3:DG	O3'	4:DA	P	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

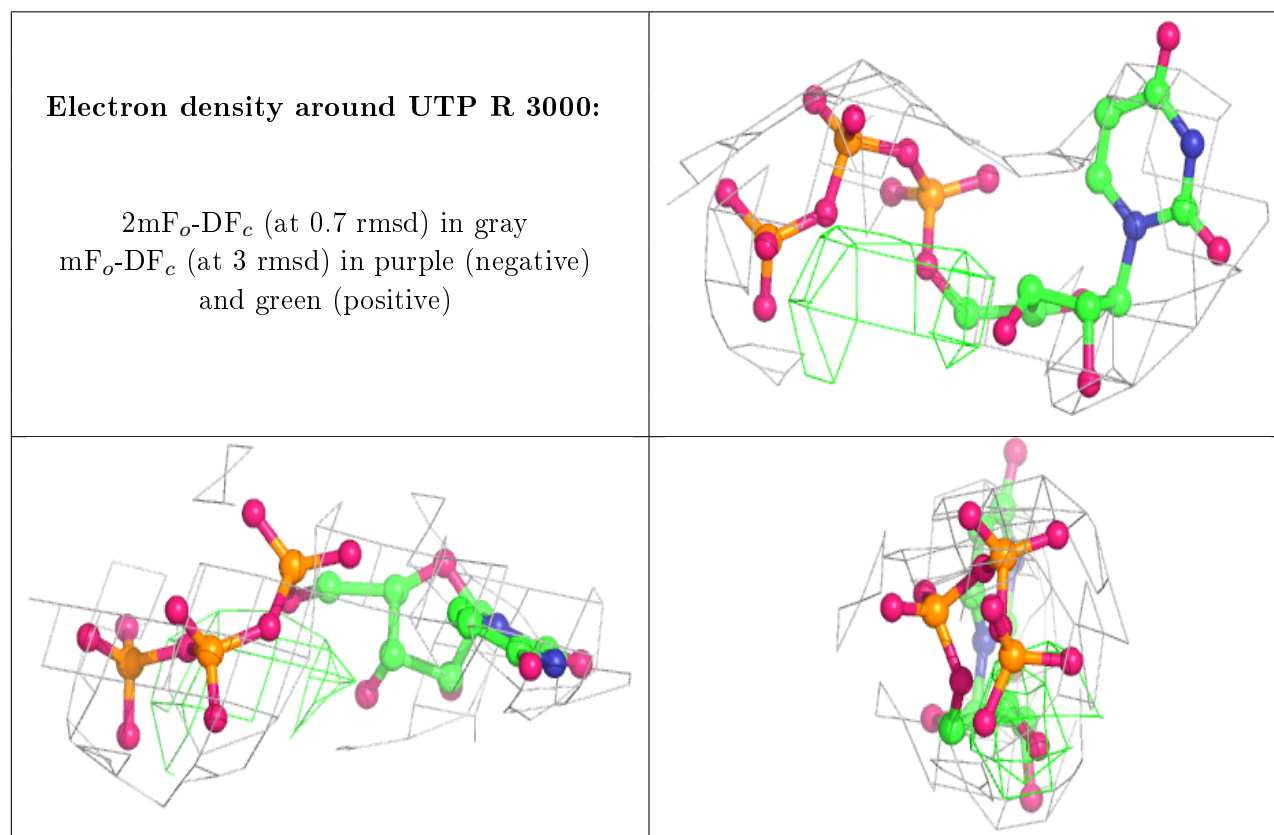
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.