



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:01 AM GMT

PDB ID : 3GTO
Title : Backtracked RNA polymerase II complex with 15mer RNA
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 4.00 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

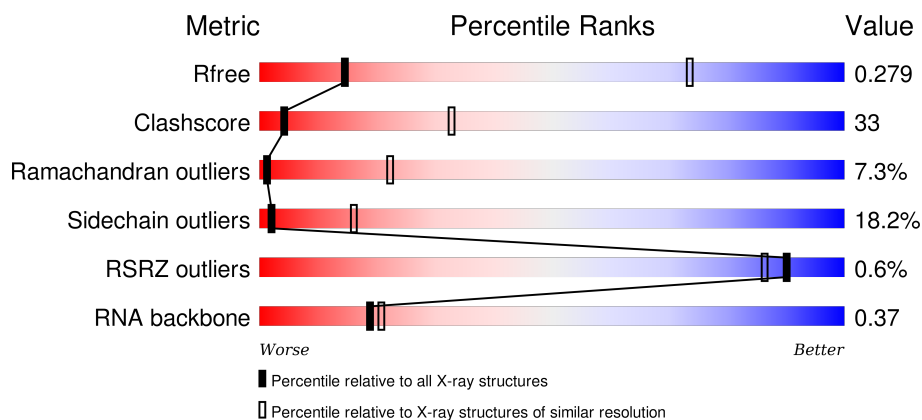
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)
RNA backbone	2183	1079 (5.04-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 32%, green 35%, orange 12%, grey 20%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 32% 35% 12% 20% </div> </div>
2	B	1224	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 36%, yellow 42%, orange 11%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 36% 42% 11% 10% </div> </div>
3	C	318	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 34%, yellow 39%, orange 9%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 34% 39% 9% 16% </div> </div>
4	E	215	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 47%, yellow 40%, orange 10%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 47% 40% 10% </div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	15	
12	T	28	
13	N	14	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29259 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	12	Total	C	N	O	P	0	0	0
			260	117	52	80	11			

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 13 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

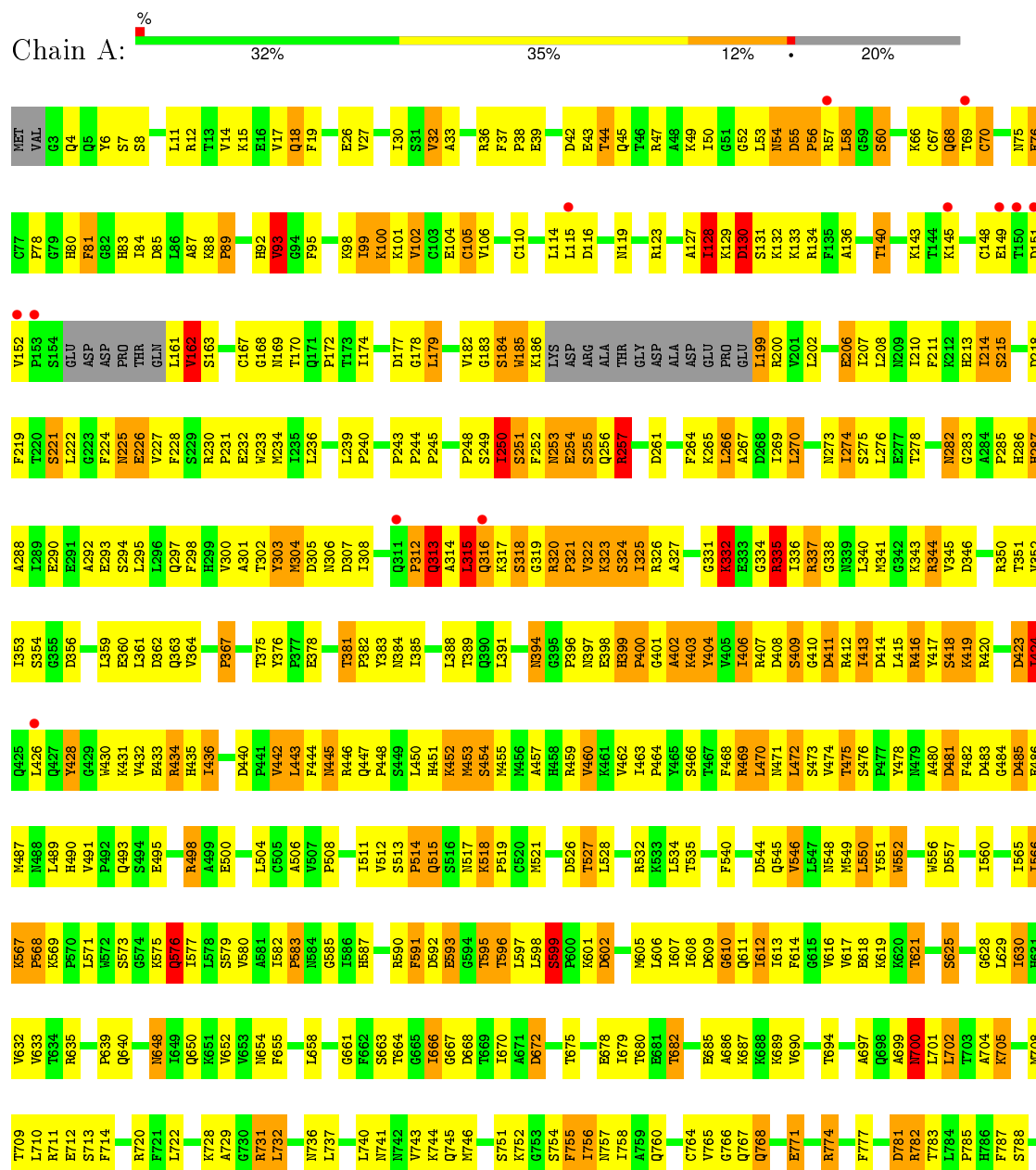
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



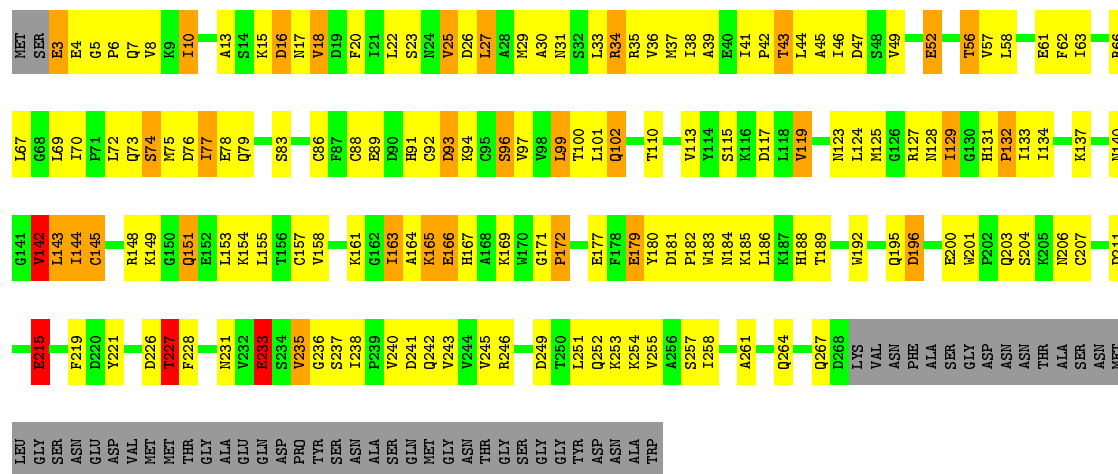


E1134	E1061	G991	GLU	R848	T783	D642	Y569	R497	M432	R363	I291	I204	GLU
R1136	H1062	I992	GLU	G849	M784	D643	W570	T498	Q433	I364	I292	I205	GLN
D1137		T993	LEU	F851		E644			R434	T365	P293	M206	ALA
M1138	Q1065	Y994	GLY	R788	ASN	A715	Q573	P501	T435	Q366	D294	M205	ILE
I1139	S1066	R995	GLN	M789	GLU	GLU	P574	I502	T436	S208	G295	E209	ASP
A1140	R1067	R956	ARG	D790	GLU	G647	P575	GLY	V436	E368	E296	K210	VAL
H1141	G1068	R957	THR	T791	ASN	G648	P576	ARG	E437	G369	K211	V211	THR
G1142	F1069	D998	THR	M792	ASP	G649	A577	ASP	GLU	F370	I297		GLY
A1143	R999	R999	ALA	A793	LEU	L651		ASP	ALA	E371	C302	L212	ARG
A1144	Y1073	F1001	TYR	M794	LEU	K652	F581	GLY	HIS				GLU
S1145	M1074	T1002	HIS	R795	LEU	K653	V582	LEU	ASP	R372	W308	M221	LEU
G1075	G1075	A1003	ASP	R796	LEU	R654		LEU	PHE	K374	Q309	I222	LYS
L1147	T1077	R935	ASP	Y797	THR	K655	V585	ASP	MET	A375	M310	V225	TYR
K1148	G1078	D936	ASP	Y798	THR	I658	M586	ASP	LYS	F376	L311		GLU
R1150	K1079	A937	ASP	P799	THR	L661	H587	LEU	L446	F377	E312		LEU
L1151	K1080	S938	ASP	K801	THR	L662	G588	LEU	A447	L378	M312	A229	ILE
M1152	L1081	P1008	GLY	P802	GLY	Y666	V589	GLY	T448	G379	L314	A230	ALA
E1153	A1082	I1009	GLY	L803	GLY	Q667	H590	GLY	H449	K385	K315	P231	GLU
A1154	G1083	L1010	GLY	G804	GLY	Q668	R591	GLY	A450	V381	P316		GLU
S1155	Q1083	I1011	GLY	T805	GLY	I668	M592	GLY	K451	I382	E319	S235	SER
D1156	T944	T944	GLY	A735	GLY	I669	P593	GLY	L452	L383	H236		GLY
L1157	F1085	E945	GLY	T806	GLY	I670	A594	GLY	T453	R384	G321	S242	ASP
F1087	F1087	E945	GLY	R807	GLY	I671	R595	GLY	T454	L385	G321		ASP
G1088	F1087	E945	GLY	F738	GLY	I672	L596	GLY	L457	L386	F322	A243	SER
P1089	P1089	E945	GLY	T739	GLY	I673	V597	GLY	K458	L387	V323	L244	GLU
T1090	T1090	E945	GLY	H740	GLY	I674	E598	GLY	K459	L388	I324	E245	GLY
Y1091	Y1091	E945	GLY	C741	GLY	I675	T599	GLY	L460	A399	G325	G247	GLY
I1092	I1092	E945	GLY	E742	GLY	I676	L600	GLY	A461	L390	D326	K247	GLY
Q1093	Q1093	E945	GLY	I743	GLY	I677	V599	GLY	L462	L391	D327	E259	GLY
R1094	R1094	E945	GLY	H744	GLY	I678	L603	GLY	T463	D391	R328	R249	GLY
L1095	L1095	E945	GLY	P745	GLY	I679	B604	GLY	L464	K393	T329	E250	GLY
H1096	H1096	E945	GLY	S746	GLY	I680		GLY	L465	D394	A330		GLY
M1097	M1097	E945	GLY	I746	GLY	I681	D608	GLY	L466	R398	L331	V256	GLY
Y1098	Y1098	E945	GLY	I747	GLY	I682	T609	GLY	Q467	L399	D332	K257	GLY
L1099	L1099	E945	GLY	I748	GLY	I683	M610	GLY	L468	L408	F332	L258	GLY
H1100	H1100	E945	GLY	I749	GLY	I684	P611	GLY	L471	L412	I334	Y259	GLY
L1101	L1101	E945	GLY	I750	GLY	I685	B612	GLY	L472	L413	G345	G260	GLY
M1102	M1102	E945	GLY	I751	GLY	I686	V613	GLY	L473	L414	ARG	R261	GLY
L1103	L1103	E945	GLY	I752	GLY	I687	S614	GLY	L474	L415	ARG	S264	GLY
R1104	R1104	E945	GLY	I753	GLY	I688	P615	GLY	L475	L416	THR	S265	GLY
L1105	L1105	E945	GLY	I754	GLY	I689	B621	GLY	L476	L417	ALA	A266	GLY
H1106	H1106	E945	GLY	I755	GLY	I690	E622	GLY	L477	L418	LEU	R267	GLY
L1107	L1107	E945	GLY	I756	GLY	I691	K625	GLY	L478	L419	ILE	T268	GLY
M1108	M1108	E945	GLY	I757	GLY	I692	E631	GLY	L479	L420	LYS	I269	GLY
L1109	L1109	E945	GLY	I758	GLY	I693	R632	GLY	L480	L421	LYS	L273	GLY
H1110	H1110	E945	GLY	I759	GLY	I694	V634	GLY	L481	L422	K345	P274	GLY
L1111	L1111	E945	GLY	I760	GLY	I695	R635	GLY	L482	L423	E346	P275	GLY
M1112	M1112	E945	GLY	I761	GLY	I696	R636	GLY	L483	L424	K347	I276	GLY
L1113	L1113	E945	GLY	I762	GLY	I697	E632	GLY	L484	L425	R348	K277	GLY
H1114	H1114	E945	GLY	I763	GLY	I698	K633	GLY	L485	L426	Y351	Q278	GLY
L1115	L1115	E945	GLY	I764	GLY	I699	R634	GLY	L486	L427	C195	G127	GLY
M1116	M1116	E945	GLY	I765	GLY	I700	R635	GLY	L487	L428	D128	F129	GLY
L1117	L1117	E945	GLY	I766	GLY	I701	R636	GLY	L488	L429	K355	I284	GLY
H1118	H1118	E945	GLY	I767	GLY	I702	R637	GLY	L489	L430	K356	I285	GLY
L1119	L1119	E945	GLY	I768	GLY	I703	R638	GLY	L490	L431	K357	F286	GLY
M1120	M1120	E945	GLY	I769	GLY	I704	R639	GLY	L491	L432	G200	R287	GLY
L1121	L1121	E945	GLY	I770	GLY	I705	R640	GLY	L492	L433	G201	A288	GLY
H1122	H1122	E945	GLY	I771	GLY	I706	R641	GLY	L493	L434	F203		GLY
L1123	L1123	E945	GLY	I772	GLY	I707	R642	GLY	L494	L435			GLY
M1124	M1124	E945	GLY	I773	GLY	I708	R643	GLY	L495	L436			GLY
L1125	L1125	E945	GLY	I774	GLY	I709	R644	GLY	L496	L437			GLY
H1126	H1126	E945	GLY	I775	GLY	I710	R645	GLY	L497	L438			GLY
L1127	L1127	E945	GLY	I776	GLY	I711	R646	GLY	L498	L439			GLY
M1128	M1128	E945	GLY	I777	GLY	I712	R647	GLY	L499	L440			GLY
L1129	L1129	E945	GLY	I778	GLY	I713	R648	GLY	L500	L441			GLY
H1130	H1130	E945	GLY	I779	GLY	I714	R649	GLY	L501	L442			GLY
L1131	L1131	E945	GLY	I780	GLY	I715	R650	GLY	L502	L443			GLY
M1132	M1132	E945	GLY	I781	GLY	I716	R651	GLY	L503	L444			GLY
L1133	L1133	E945	GLY	I782	GLY	I717	R652	GLY	L504	L445			GLY
H1134	H1134	E945	GLY	I783	GLY	I718	R653	GLY	L505	L446			GLY
L1135	L1135	E945	GLY	I784	GLY	I719	R654	GLY	L506	L447			GLY
M1136	M1136	E945	GLY	I785	GLY	I720	R655	GLY	L507	L448			GLY
L1137	L1137	E945	GLY	I786	GLY	I721	R656	GLY	L508	L449			GLY
H1138	H1138	E945	GLY	I787	GLY	I722	R657	GLY	L509	L450			GLY
L1139	L1139	E945	GLY	I788	GLY	I723	R658	GLY	L510	L451			GLY
M1140	M1140	E945	GLY	I789	GLY	I724	R659	GLY	L511	L452			GLY
L1141	L1141	E945	GLY	I790	GLY	I725	R660	GLY	L512	L453			GLY
H1142	H1142	E945	GLY	I791	GLY	I726	R661	GLY	L513	L454			GLY
L1143	L1143	E945	GLY	I792	GLY	I727	R662	GLY	L514	L455			GLY
M1144	M1144	E945	GLY	I793	GLY	I728	R663	GLY	L515	L456			GLY
L1145	L1145	E945	GLY	I794	GLY	I729	R664	GLY	L516	L457			GLY
H1146	H1146	E945	GLY	I795	GLY	I730	R665	GLY	L517	L458			GLY
L1147	L1147	E945	GLY	I796	GLY	I731	R666	GLY	L518	L459			GLY
M1148	M1148	E945	GLY	I797	GLY	I732	R667	GLY	L519	L460			GLY
L1149	L1149	E945	GLY	I798	GLY	I733	R668	GLY	L520	L461			GLY
H1150	H1150	E945	GLY	I799	GLY	I734	R669	GLY	L521	L462			GLY
L1151	L1151	E945	GLY	I800	GLY	I735	R670	GLY	L522	L463			GLY
M1152	M1152	E945	GLY	I801	GLY	I736	R671	GLY	L523	L464			GLY
L1153	L1153	E945	GLY	I802	GLY	I737	R672	GLY	L524	L465			GLY
H1154	H1154	E945	GLY	I803	GLY	I738	R673	GLY	L525	L466			GLY
L1155	L1155	E945	GLY	I804	GLY	I739	R674	GLY	L526	L467			GLY
M1156	M1156	E945	GLY	I805	GLY	I740	R675	GLY	L527	L468			GLY
L1157	L1157	E945	GLY	I806	GLY	I741	R676	GLY	L528	L469			GLY
H1158	H1158	E945	GLY	I807	GLY	I742	R677	GLY	L529	L470			GLY
L1159	L1159	E945	GLY	I808	GLY	I743	R678	GLY	L530	L471			GLY
M1160	M1160	E945	GLY	I809	GLY	I744	R679	GLY	L531	L472			GLY
L1161	L1161	E945	GLY	I810	GLY	I745	R680	GLY	L532	L473			GLY
H1162	H1162	E945	GLY	I811	GLY	I746	R681	GLY	L533	L474			GLY
L1163	L1163	E945	GLY	I812	GLY	I747	R682	GLY	L534	L475			GLY
M1164	M1164	E945	GLY	I813	GLY	I748	R683	GLY	L535	L476			GLY
L1165	L1165	E945	GLY	I814	GLY	I749	R684	GLY	L536	L477			GLY
H1166	H1166	E945	GLY	I815	GLY	I750	R685	GLY	L537	L478			GLY
L1167	L1167	E945	GLY	I816	GLY	I751	R686	GLY	L538	L479			GLY
M1168	M1168	E945	GLY	I817	GLY	I752	R687	GLY	L539	L480			GLY
L1169	L1169	E945	GLY	I818	GLY	I753	R688	GLY	L540	L481			GLY
H1170	H1170	E945	GLY	I819	GLY	I754	R689	GLY	L541	L482			GLY
L1171	L1171	E945	GLY	I820	GLY	I755	R690	GLY	L542	L483			GLY
M1172	M1172	E945	GLY	I821	GLY	I756	R691	GLY	L543	L484			GLY
L1173	L1173	E945	GLY	I822	GLY	I757	R692	GLY	L544	L485			GLY
H1174	H1174	E945	GLY	I823	GLY	I758	R693	GLY	L545	L486			GLY



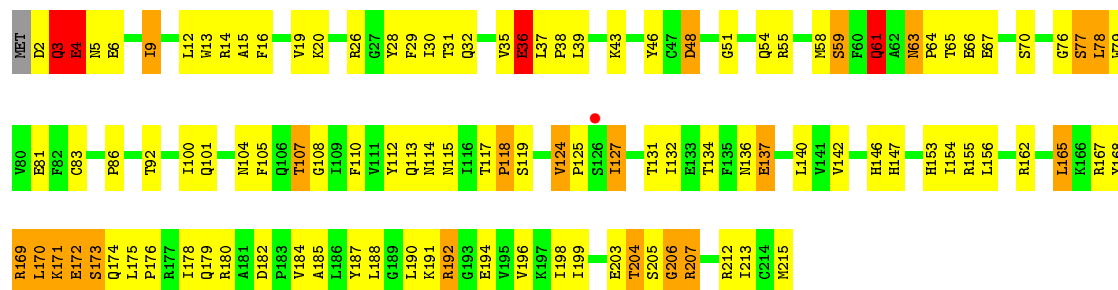
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 34% 39% 9% 16%



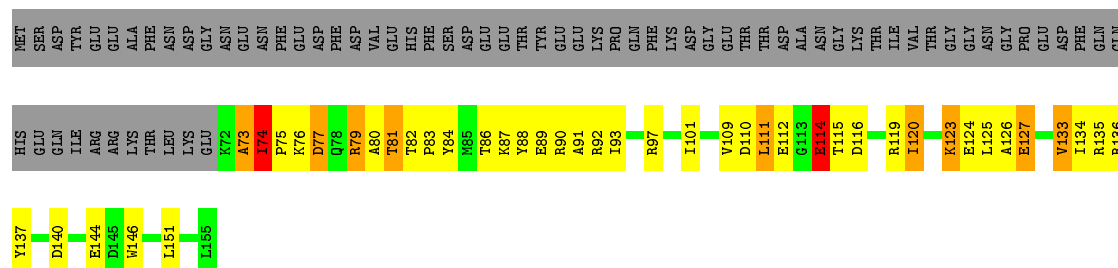
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 47% 40% 10%



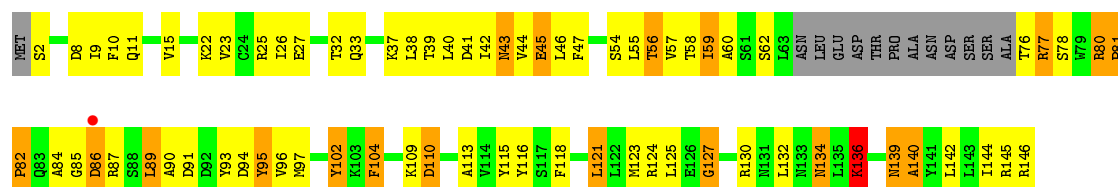
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 26% 21% 6% 46%

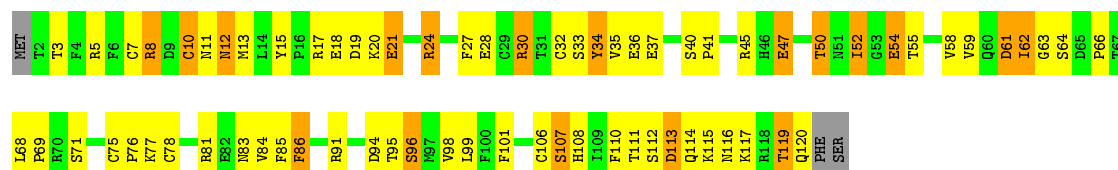


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

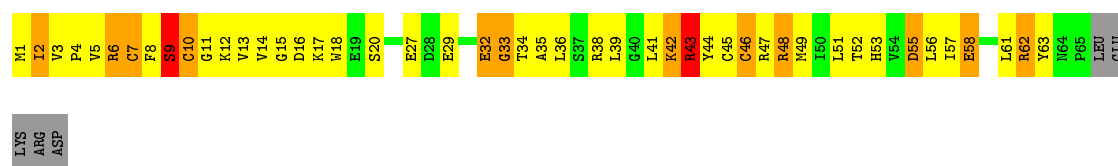
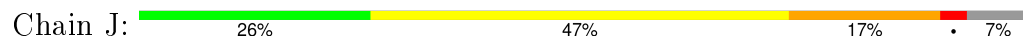
Chain H: 41% 36% 13% 9%



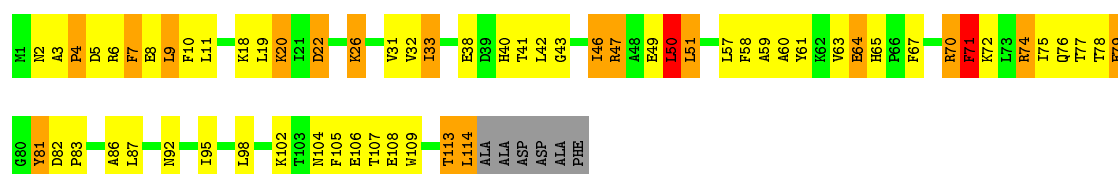
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9



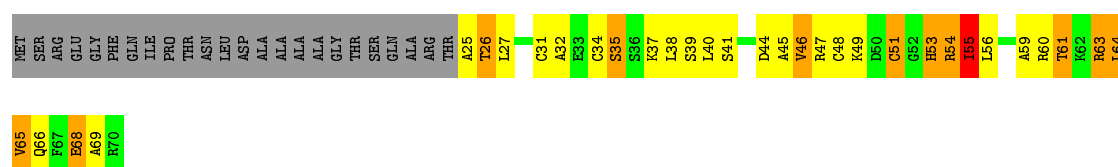
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



• Molecule 9: DNA-directed RNA polymerase II subunit RPB11



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



• Molecule 11: RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*CP*AP*C)-3')

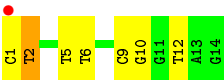




● Molecule 12: DNA (28-MER)



● Molecule 13: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.85Å 222.80Å 194.98Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 49.45 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-4.00) 93.6 (49.45-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.269 , 0.290 0.264 , 0.279	Depositor DCC
R_{free} test set	2847 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 66.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 56200 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29259	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	43/11163 (0.4%)	0.81	10/15091 (0.1%)
2	B	1.13	48/8963 (0.5%)	0.88	19/12086 (0.2%)
3	C	1.16	11/2133 (0.5%)	0.84	0/2891
4	E	1.12	9/1788 (0.5%)	0.80	3/2406 (0.1%)
5	F	1.14	3/691 (0.4%)	0.87	0/933
6	H	1.01	3/1086 (0.3%)	0.84	0/1470
7	I	1.26	9/989 (0.9%)	0.95	5/1331 (0.4%)
8	J	1.28	9/541 (1.7%)	0.97	3/727 (0.4%)
9	K	1.08	3/937 (0.3%)	0.80	1/1265 (0.1%)
10	L	1.09	0/365	0.93	0/485
11	R	1.25	1/292 (0.3%)	1.79	5/455 (1.1%)
12	T	1.39	1/634 (0.2%)	1.90	22/975 (2.3%)
13	N	1.83	8/317 (2.5%)	1.67	6/488 (1.2%)
All	All	1.11	148/29899 (0.5%)	0.91	74/40603 (0.2%)

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
3	C	0	1
6	H	0	1
7	I	0	1
All	All	0	3

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	574	SER	CB-OG	12.89	1.59	1.42
4	E	137	GLU	CD-OE1	11.71	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	54	GLU	CD-OE1	11.17	1.38	1.25
1	A	1426	GLU	CD-OE1	10.61	1.37	1.25
2	B	598	GLU	CD-OE2	10.45	1.37	1.25
1	A	1426	GLU	CD-OE2	10.34	1.37	1.25
13	N	2	DT	P-O5'	9.68	1.69	1.59
2	B	742	GLU	CD-OE1	9.61	1.36	1.25
13	N	1	DC	N1-C6	9.32	1.42	1.37
4	E	4	GLU	CD-OE1	9.29	1.35	1.25
3	C	74	SER	CB-OG	9.28	1.54	1.42
9	K	38	GLU	CD-OE1	9.15	1.35	1.25
8	J	29	GLU	CD-OE2	9.08	1.35	1.25
2	B	1070	GLU	CB-CG	8.96	1.69	1.52
1	A	1165	GLU	CD-OE1	8.68	1.35	1.25
4	E	155	ARG	CZ-NH1	8.58	1.44	1.33
4	E	137	GLU	CD-OE2	8.55	1.35	1.25
1	A	1194	ARG	CZ-NH1	8.40	1.44	1.33
8	J	29	GLU	CD-OE1	8.40	1.34	1.25
2	B	116	GLU	CD-OE1	8.33	1.34	1.25
8	J	9	SER	CB-OG	8.29	1.53	1.42
11	R	10	A	P-O5'	8.03	1.67	1.59
13	N	1	DC	N3-C4	7.91	1.39	1.33
8	J	58	GLU	CD-OE1	7.78	1.34	1.25
1	A	1293	SER	CB-OG	7.58	1.52	1.42
8	J	20	SER	CB-OG	7.55	1.52	1.42
5	F	114	GLU	CD-OE1	7.47	1.33	1.25
8	J	33	GLY	C-O	7.43	1.35	1.23
5	F	127	GLU	CD-OE1	7.43	1.33	1.25
1	A	1277	GLU	CD-OE1	7.38	1.33	1.25
3	C	52	GLU	CD-OE1	7.33	1.33	1.25
1	A	593	GLU	CD-OE1	7.32	1.33	1.25
2	B	844	SER	CB-OG	7.25	1.51	1.42
8	J	58	GLU	CD-OE2	7.15	1.33	1.25
1	A	43	GLU	CD-OE2	7.07	1.33	1.25
12	T	3	DA	O5'-C5'	6.95	1.59	1.42
3	C	233	GLU	CD-OE2	6.87	1.33	1.25
1	A	846	GLU	CD-OE2	6.85	1.33	1.25
1	A	678	GLU	CD-OE1	6.83	1.33	1.25
2	B	935	ARG	CZ-NH1	6.77	1.41	1.33
2	B	1061	GLU	CD-OE1	6.71	1.33	1.25
9	K	64	GLU	CD-OE1	6.70	1.33	1.25
2	B	368	GLU	CD-OE2	6.70	1.33	1.25
5	F	127	GLU	CD-OE2	6.59	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	327	ARG	CZ-NH2	6.56	1.41	1.33
1	A	678	GLU	CD-OE2	6.55	1.32	1.25
2	B	986	GLN	CG-CD	6.53	1.66	1.51
4	E	207	ARG	CZ-NH1	6.49	1.41	1.33
2	B	39	ARG	CZ-NH1	6.46	1.41	1.33
13	N	6	DT	C5-C7	6.42	1.53	1.50
4	E	36	GLU	CD-OE2	6.40	1.32	1.25
2	B	543	SER	CB-OG	6.40	1.50	1.42
3	C	86	CYS	CB-SG	6.39	1.93	1.82
1	A	625	SER	CB-OG	6.38	1.50	1.42
1	A	1196	GLU	CD-OE1	6.34	1.32	1.25
3	C	204	SER	CB-OG	6.34	1.50	1.42
1	A	1165	GLU	CG-CD	6.33	1.61	1.51
2	B	635	ARG	CZ-NH1	6.31	1.41	1.33
2	B	731	VAL	C-O	6.31	1.35	1.23
3	C	257	SER	CB-OG	6.30	1.50	1.42
3	C	179	GLU	CB-CG	6.30	1.64	1.52
4	E	81	GLU	CD-OE1	6.29	1.32	1.25
3	C	52	GLU	CD-OE2	6.24	1.32	1.25
2	B	182	SER	CB-OG	6.20	1.50	1.42
2	B	384	ARG	CZ-NH1	6.18	1.41	1.33
1	A	1117	THR	CB-OG1	6.15	1.55	1.43
2	B	967	ARG	CZ-NH1	6.09	1.41	1.33
7	I	96	SER	CB-OG	6.08	1.50	1.42
2	B	480	SER	CB-OG	6.06	1.50	1.42
1	A	771	GLU	CD-OE1	6.05	1.32	1.25
1	A	66	LYS	CE-NZ	6.04	1.64	1.49
13	N	12	DT	O5'-C5'	6.00	1.57	1.42
1	A	43	GLU	CD-OE1	5.98	1.32	1.25
2	B	245	GLU	CG-CD	5.97	1.60	1.51
13	N	6	DT	N1-C6	5.96	1.42	1.38
2	B	823	ALA	C-O	5.93	1.34	1.23
2	B	696	GLU	CD-OE1	5.92	1.32	1.25
2	B	742	GLU	CD-OE2	5.88	1.32	1.25
2	B	1183	LYS	CD-CE	5.87	1.66	1.51
1	A	36	ARG	CZ-NH1	5.83	1.40	1.33
1	A	1415	SER	CB-OG	5.83	1.49	1.42
1	A	350	ARG	CZ-NH1	5.82	1.40	1.33
4	E	81	GLU	CD-OE2	5.80	1.32	1.25
2	B	372	SER	CB-OG	5.75	1.49	1.42
1	A	682	THR	C-O	5.75	1.34	1.23
13	N	1	DC	C4-C5	5.72	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	43	ARG	CZ-NH1	5.72	1.40	1.33
2	B	1117	GLN	CD-NE2	5.70	1.47	1.32
1	A	332	LYS	CE-NZ	5.70	1.63	1.49
2	B	696	GLU	CD-OE2	5.70	1.31	1.25
1	A	1151	GLU	CD-OE1	5.69	1.31	1.25
1	A	870	GLU	C-O	5.68	1.34	1.23
1	A	934	LYS	CE-NZ	5.67	1.63	1.49
6	H	136	LYS	CE-NZ	-5.67	1.34	1.49
1	A	1074	GLU	CD-OE1	5.65	1.31	1.25
13	N	1	DC	N1-C2	5.65	1.45	1.40
2	B	797	TYR	CE1-CZ	5.63	1.45	1.38
2	B	486	TYR	CE1-CZ	5.63	1.45	1.38
6	H	45	GLU	CD-OE1	5.63	1.31	1.25
2	B	430	ARG	CZ-NH1	5.60	1.40	1.33
3	C	215	GLU	CD-OE2	5.58	1.31	1.25
2	B	700	SER	CB-OG	5.55	1.49	1.42
3	C	96	SER	CA-CB	5.55	1.61	1.52
7	I	61	ASP	CG-OD1	5.52	1.38	1.25
1	A	1301	GLU	CD-OE1	5.51	1.31	1.25
1	A	1297	GLU	CD-OE1	5.50	1.31	1.25
1	A	1423	GLY	C-O	5.49	1.32	1.23
7	I	24	ARG	CZ-NH1	5.47	1.40	1.33
2	B	368	GLU	CD-OE1	5.45	1.31	1.25
1	A	354	SER	CB-OG	5.43	1.49	1.42
1	A	1301	GLU	CD-OE2	5.43	1.31	1.25
2	B	1061	GLU	CD-OE2	5.40	1.31	1.25
7	I	45	ARG	CZ-NH1	5.36	1.40	1.33
2	B	1009	ASP	CB-CG	5.33	1.62	1.51
1	A	226	GLU	CD-OE2	5.31	1.31	1.25
1	A	85	ASP	CG-OD1	5.29	1.37	1.25
7	I	81	ARG	CZ-NH1	5.29	1.40	1.33
2	B	797	TYR	CG-CD2	5.28	1.46	1.39
1	A	599	SER	CB-OG	5.27	1.49	1.42
2	B	187	SER	CB-OG	5.26	1.49	1.42
7	I	47	GLU	CG-CD	5.21	1.59	1.51
2	B	906	SER	CB-OG	5.19	1.49	1.42
1	A	1404	GLU	CD-OE1	5.19	1.31	1.25
1	A	149	GLU	CD-OE2	5.17	1.31	1.25
1	A	179	LEU	C-O	5.17	1.33	1.23
2	B	641	GLU	CD-OE2	5.17	1.31	1.25
2	B	468	GLU	CG-CD	5.14	1.59	1.51
2	B	598	GLU	CD-OE1	5.13	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1148	LYS	CD-CE	5.10	1.64	1.51
7	I	115	LYS	CD-CE	5.10	1.64	1.51
2	B	1028	GLU	CG-CD	5.09	1.59	1.51
1	A	900	ASP	C-O	5.07	1.32	1.23
1	A	593	GLU	CD-OE2	5.07	1.31	1.25
9	K	26	LYS	CE-NZ	5.07	1.61	1.49
2	B	1181	GLU	CD-OE2	5.07	1.31	1.25
2	B	678	GLU	CD-OE2	5.05	1.31	1.25
2	B	531	GLN	CD-NE2	5.05	1.45	1.32
2	B	666	TYR	CE1-CZ	5.04	1.45	1.38
3	C	166	GLU	CD-OE1	5.04	1.31	1.25
6	H	127	GLY	C-O	5.04	1.31	1.23
2	B	957	ASN	CG-OD1	5.03	1.35	1.24
4	E	61	GLN	CD-NE2	5.03	1.45	1.32
7	I	12	ASN	CG-ND2	5.02	1.45	1.32
1	A	177	ASP	CG-OD1	5.02	1.36	1.25
1	A	700	ASN	CG-OD1	5.02	1.34	1.24
8	J	46	CYS	C-O	5.01	1.32	1.23
1	A	1025	ARG	NE-CZ	5.01	1.39	1.33
2	B	486	TYR	CG-CD2	5.00	1.45	1.39

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	16	DC	O4'-C4'-C3'	-10.87	99.48	106.00
1	A	1173	HIS	N-CA-C	9.95	137.86	111.00
1	A	1172	LEU	N-CA-C	9.54	136.75	111.00
12	T	16	DC	O4'-C1'-N1	8.87	114.21	108.00
12	T	27	DA	O4'-C4'-C3'	-8.83	100.70	106.00
4	E	155	ARG	NE-CZ-NH2	-8.09	116.25	120.30
2	B	327	ARG	NE-CZ-NH2	-7.92	116.34	120.30
4	E	207	ARG	NE-CZ-NH2	-7.74	116.43	120.30
2	B	1222	ARG	NE-CZ-NH2	7.53	124.06	120.30
12	T	21	DC	C4'-C3'-C2'	-7.51	96.34	103.10
2	B	39	ARG	NE-CZ-NH2	-7.50	116.55	120.30
12	T	11	DG	O4'-C1'-N9	7.46	113.22	108.00
2	B	635	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	36	ARG	NE-CZ-NH1	7.39	124.00	120.30
11	R	10	A	O4'-C1'-N9	-7.37	102.30	108.20
13	N	10	DG	P-O3'-C3'	7.36	128.53	119.70
1	A	731	ARG	NE-CZ-NH1	7.31	123.96	120.30
2	B	852	ARG	NE-CZ-NH2	-7.15	116.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1172	LEU	CB-CA-C	-7.14	96.63	110.20
11	R	3	C	O4'-C1'-N1	6.97	113.78	108.20
8	J	43	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	1173	HIS	N-CA-CB	-6.90	98.17	110.60
13	N	6	DT	O4'-C1'-N1	6.90	112.83	108.00
2	B	935	ARG	NE-CZ-NH2	-6.88	116.86	120.30
12	T	25	DC	O4'-C1'-N1	6.88	112.81	108.00
12	T	19	DT	N3-C2-O2	-6.84	118.20	122.30
13	N	9	DC	O4'-C1'-N1	6.83	112.78	108.00
8	J	10	CYS	CA-CB-SG	6.78	126.20	114.00
11	R	12	G	C3'-C2'-C1'	6.50	106.70	101.50
12	T	6	DG	P-O3'-C3'	6.47	127.46	119.70
12	T	19	DT	C4-C5-C7	6.28	122.77	119.00
12	T	15	DA	P-O3'-C3'	6.21	127.16	119.70
12	T	3	DA	C5'-C4'-C3'	6.19	125.25	114.10
12	T	4	DC	O4'-C1'-N1	6.19	112.33	108.00
12	T	23	DC	O4'-C4'-C3'	-6.15	102.04	104.50
4	E	155	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	B	967	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	731	ARG	NE-CZ-NH2	-6.07	117.26	120.30
2	B	39	ARG	NE-CZ-NH1	5.95	123.28	120.30
13	N	2	DT	P-O3'-C3'	5.88	126.75	119.70
7	I	10	CYS	CA-CB-SG	5.83	124.49	114.00
12	T	22	DT	C4'-C3'-C2'	-5.82	97.86	103.10
2	B	1096	ARG	NE-CZ-NH1	5.82	123.21	120.30
12	T	20	DC	N1-C2-O2	5.75	122.35	118.90
7	I	81	ARG	NE-CZ-NH2	-5.71	117.45	120.30
12	T	27	DA	C4'-C3'-C2'	-5.71	97.96	103.10
2	B	1010	LEU	CB-CG-CD1	-5.69	101.32	111.00
2	B	384	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	B	637	LEU	CA-CB-CG	5.56	128.09	115.30
11	R	12	G	C8-N9-C4	-5.50	104.20	106.40
12	T	1	DC	N3-C4-N4	-5.50	114.15	118.00
2	B	967	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	36	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	1098	MET	CG-SD-CE	5.40	108.84	100.20
1	A	1194	ARG	NE-CZ-NH2	-5.40	117.60	120.30
8	J	43	ARG	NE-CZ-NH1	5.37	122.98	120.30
12	T	27	DA	O4'-C1'-N9	5.36	111.75	108.00
12	T	16	DC	C4'-C3'-C2'	-5.34	98.30	103.10
7	I	113	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	1116	LEU	CA-CB-CG	5.31	127.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	539	LEU	CA-CB-CG	5.29	127.47	115.30
2	B	430	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	B	1011	ILE	CB-CA-C	-5.26	101.08	111.60
7	I	24	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	B	782	LEU	CA-CB-CG	5.24	127.35	115.30
9	K	74	ARG	NE-CZ-NH2	-5.22	117.69	120.30
12	T	3	DA	O4'-C4'-C3'	-5.21	102.42	104.50
11	R	8	G	C5'-C4'-O4'	5.21	115.35	109.10
7	I	81	ARG	NE-CZ-NH1	5.17	122.89	120.30
13	N	6	DT	C4-C5-C7	5.11	122.07	119.00
12	T	10	DA	O4'-C1'-N9	5.02	111.52	108.00
12	T	1	DC	C5-C4-N4	5.02	123.71	120.20
2	B	1098	MET	CB-CG-SD	-5.01	97.36	112.40
13	N	1	DC	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	172	PRO	Peptide
6	H	136	LYS	Peptide
7	I	77	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10969	0	11071	924	0
2	B	8792	0	8824	632	0
3	C	2095	0	2052	131	0
4	E	1752	0	1776	91	0
5	F	679	0	701	45	0
6	H	1068	0	1040	64	0
7	I	971	0	928	46	0
8	J	532	0	544	65	0
9	K	919	0	929	64	0
10	L	363	0	387	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	R	260	0	132	15	0
12	T	566	0	316	21	0
13	N	284	0	161	5	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	1	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	1	0
15	A	1	0	0	0	0
All	All	29259	0	28861	1940	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1940) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CG	1:A:400:PRO:HD3	1.44	1.48
1:A:315:LEU:HB2	1:A:316:GLN:C	1.39	1.43
1:A:315:LEU:HB2	1:A:316:GLN:CA	1.51	1.38
1:A:256:GLN:CA	1:A:257:ARG:HB3	1.59	1.30
1:A:1111:MET:CG	1:A:1114:PRO:HG3	1.64	1.27
2:B:865:LYS:HG2	2:B:866:TYR:N	1.44	1.24
1:A:1116:LEU:HD23	1:A:1329:THR:CG2	1.68	1.22
1:A:256:GLN:HA	1:A:257:ARG:CB	1.60	1.21
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.76	1.21
1:A:320:ARG:N	1:A:320:ARG:HD2	1.45	1.19
2:B:864:LYS:HG3	2:B:865:LYS:N	1.59	1.18
1:A:399:HIS:CD2	1:A:400:PRO:HD3	1.81	1.16
1:A:399:HIS:CG	1:A:400:PRO:CD	2.29	1.16
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.26	1.15
1:A:399:HIS:CB	1:A:400:PRO:HD3	1.75	1.15
1:A:315:LEU:CD2	1:A:316:GLN:HA	1.77	1.14
1:A:323:LYS:HD3	1:A:323:LYS:N	1.50	1.14
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.29	1.14
2:B:865:LYS:CG	2:B:866:TYR:H	1.61	1.14
1:A:1116:LEU:HD23	1:A:1329:THR:HG22	1.30	1.12
1:A:129:LYS:O	1:A:130:ASP:HB2	1.45	1.12
1:A:253:ASN:HA	1:A:256:GLN:O	1.48	1.11
1:A:590:ARG:HH11	1:A:590:ARG:HG3	0.99	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:796:LEU:HB3	2:B:799:PRO:HD3	1.29	1.11
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.12	1.11
1:A:399:HIS:CB	1:A:400:PRO:CD	2.29	1.10
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.12	1.10
1:A:399:HIS:HB3	1:A:400:PRO:CD	1.83	1.08
2:B:882:THR:HG21	2:B:935:ARG:HA	1.30	1.08
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.27	1.08
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.31	1.07
1:A:315:LEU:H	1:A:315:LEU:HD13	1.20	1.07
1:A:573:SER:O	1:A:576:GLN:HB2	1.52	1.07
1:A:315:LEU:HB2	1:A:317:LYS:N	1.68	1.07
11:R:4:G:H2'	11:R:5:A:H8	1.07	1.07
1:A:315:LEU:CB	1:A:316:GLN:CA	2.30	1.06
11:R:4:G:H2'	11:R:5:A:C8	1.89	1.06
2:B:976:ILE:O	2:B:990:ILE:HB	1.56	1.06
1:A:765:VAL:CG2	1:A:800:VAL:HB	1.84	1.06
1:A:213:HIS:O	1:A:214:ILE:O	1.72	1.06
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.32	1.06
1:A:49:LYS:HD3	1:A:55:ASP:OD1	1.54	1.05
1:A:315:LEU:CB	1:A:316:GLN:HA	1.84	1.05
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.87	1.05
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	1.71	1.04
1:A:315:LEU:HB3	1:A:318:SER:N	1.71	1.04
1:A:855:THR:HG21	1:A:857:ARG:HE	1.23	1.04
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.36	1.03
2:B:634:TYR:HE1	2:B:692:TYR:CD1	1.75	1.03
1:A:805:LEU:HD13	1:A:805:LEU:C	1.78	1.03
3:C:102:GLN:HG2	3:C:154:LYS:HD3	1.39	1.03
1:A:630:ILE:H	1:A:630:ILE:HD12	1.19	1.03
1:A:67:CYS:HB3	1:A:70:CYS:SG	1.97	1.02
1:A:805:LEU:O	1:A:805:LEU:HD13	1.60	1.02
1:A:320:ARG:CD	1:A:320:ARG:H	1.62	1.02
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.88	1.02
1:A:315:LEU:HB3	1:A:318:SER:H	0.85	1.01
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	0.85	1.01
1:A:351:THR:CG2	2:B:1103:ILE:HD12	1.89	1.00
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.25	1.00
1:A:319:GLY:CA	1:A:320:ARG:HH11	1.75	1.00
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.40	1.00
1:A:446:ARG:NE	1:A:480:ALA:HB2	1.77	0.99
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:HB3	1:A:257:ARG:N	1.77	0.99
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.78	0.99
1:A:351:THR:HG23	2:B:1103:ILE:CD1	1.93	0.98
1:A:1111:MET:SD	1:A:1114:PRO:HG3	2.02	0.98
2:B:636:PRO:HB3	2:B:743:ILE:HG13	1.41	0.98
1:A:320:ARG:H	1:A:320:ARG:HD2	0.84	0.98
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.05	0.98
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.28	0.98
1:A:315:LEU:CB	1:A:316:GLN:C	2.33	0.97
1:A:573:SER:H	1:A:576:GLN:HG3	1.23	0.97
2:B:1149:GLU:HG3	2:B:1153:GLU:HG2	1.47	0.96
1:A:322:VAL:C	1:A:323:LYS:HD3	1.85	0.96
4:E:86:PRO:CB	4:E:114:ASN:HD22	1.77	0.96
2:B:1096:ARG:HG2	2:B:1096:ARG:HH11	1.26	0.96
1:A:590:ARG:NH1	1:A:590:ARG:HG3	1.79	0.96
2:B:864:LYS:HG3	2:B:865:LYS:H	1.27	0.95
1:A:765:VAL:HG23	1:A:800:VAL:HB	1.48	0.95
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.46	0.95
2:B:363:HIS:O	2:B:364:ILE:HB	1.67	0.94
1:A:567:LYS:HB3	6:H:96:VAL:H	1.32	0.94
1:A:253:ASN:CB	1:A:257:ARG:N	2.30	0.94
2:B:1076:HIS:ND1	9:K:40:HIS:CD2	2.35	0.93
1:A:401:GLY:N	1:A:435:HIS:HD2	1.65	0.93
1:A:315:LEU:HD12	1:A:319:GLY:HA2	1.49	0.93
2:B:864:LYS:HZ3	2:B:867:GLY:N	1.67	0.93
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.51	0.93
2:B:955:THR:HG22	2:B:956:THR:H	1.34	0.92
1:A:315:LEU:CB	1:A:318:SER:H	1.81	0.92
1:A:315:LEU:HD23	1:A:316:GLN:HA	1.49	0.92
2:B:98:THR:O	2:B:126:SER:HB3	1.70	0.92
3:C:56:THR:HG21	3:C:145:CYS:SG	2.10	0.91
1:A:256:GLN:CB	1:A:257:ARG:HB3	2.00	0.91
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.68	0.91
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.00	0.91
1:A:741:ASN:HD22	1:A:744:LYS:H	1.13	0.91
2:B:864:LYS:CG	2:B:865:LYS:H	1.83	0.91
1:A:630:ILE:HD12	1:A:630:ILE:N	1.85	0.91
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.69	0.91
1:A:1111:MET:HG2	1:A:1114:PRO:HG3	1.53	0.90
1:A:315:LEU:CB	1:A:317:LYS:N	2.33	0.90
1:A:319:GLY:CA	1:A:320:ARG:NH1	2.33	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:H	1:A:435:HIS:HD2	1.19	0.90
3:C:70:ILE:HD11	3:C:144:ILE:CD1	2.01	0.90
1:A:855:THR:CG2	1:A:857:ARG:HE	1.85	0.90
2:B:913:GLY:HA2	2:B:938:SER:CB	2.01	0.90
1:A:805:LEU:C	1:A:805:LEU:CD1	2.39	0.90
1:A:315:LEU:CD1	1:A:319:GLY:HA2	2.02	0.90
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.35	0.90
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.38	0.89
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.50	0.89
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.13	0.89
5:F:109:VAL:HG12	5:F:110:ASP:H	1.37	0.88
1:A:351:THR:HG22	1:A:352:VAL:N	1.88	0.88
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.09	0.88
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.56	0.87
8:J:7:CYS:SG	8:J:10:CYS:N	2.46	0.87
3:C:142:VAL:HG13	3:C:143:LEU:N	1.89	0.87
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.61	0.87
1:A:1404:GLU:O	1:A:1408:ILE:HG12	1.75	0.87
2:B:955:THR:HG22	2:B:956:THR:N	1.88	0.86
7:I:111:THR:HG22	7:I:113:ASP:H	1.37	0.86
1:A:406:ILE:N	1:A:406:ILE:HD12	1.91	0.86
1:A:751:SER:HB2	2:B:1015:HIS:HE1	1.39	0.86
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.74	0.85
1:A:315:LEU:HD12	1:A:319:GLY:CA	2.05	0.85
2:B:635:ARG:O	2:B:636:PRO:O	1.93	0.85
2:B:864:LYS:HE2	2:B:870:ILE:O	1.76	0.85
1:A:630:ILE:H	1:A:630:ILE:CD1	1.89	0.85
2:B:293:PRO:O	2:B:297:ILE:HG12	1.75	0.85
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.59	0.84
2:B:807:ARG:HG3	2:B:807:ARG:HH11	1.40	0.84
1:A:253:ASN:CB	1:A:256:GLN:C	2.46	0.84
8:J:42:LYS:O	8:J:47:ARG:HD2	1.78	0.84
1:A:320:ARG:CD	1:A:320:ARG:N	2.30	0.84
1:A:323:LYS:O	1:A:324:SER:HB3	1.76	0.84
2:B:899:ILE:HD11	2:B:911:ILE:HG12	1.58	0.84
7:I:17:ARG:HG2	7:I:18:GLU:H	1.43	0.84
1:A:399:HIS:HB3	1:A:400:PRO:HD2	1.57	0.84
1:A:830:LYS:HD3	1:A:1079:MET:O	1.78	0.84
1:A:315:LEU:HD13	1:A:315:LEU:N	1.91	0.83
2:B:975:GLN:HG2	2:B:976:ILE:H	1.43	0.83
2:B:542:MET:HB3	2:B:636:PRO:HD3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:HH11	1:A:590:ARG:CG	1.85	0.83
2:B:880:THR:O	2:B:881:ASN:HB2	1.75	0.83
2:B:37:PHE:O	2:B:38:PHE:HB2	1.75	0.83
1:A:319:GLY:HA3	1:A:320:ARG:NH1	1.93	0.83
1:A:257:ARG:HG2	1:A:257:ARG:O	1.78	0.83
9:K:113:THR:O	9:K:114:LEU:HB2	1.78	0.83
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.13	0.83
7:I:7:CYS:SG	7:I:8:ARG:O	2.36	0.83
1:A:590:ARG:O	1:A:591:PHE:CD1	2.31	0.82
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.08	0.82
9:K:65:HIS:HD2	9:K:67:PHE:H	1.23	0.82
1:A:518:LYS:HG3	1:A:519:PRO:HD2	1.61	0.82
1:A:265:LYS:C	1:A:267:ALA:H	1.83	0.82
1:A:1111:MET:SD	1:A:1114:PRO:CG	2.68	0.82
1:A:889:SER:HB2	1:A:892:ALA:H	1.42	0.82
1:A:777:PHE:CE2	1:A:781:ASP:O	2.33	0.82
4:E:61:GLN:HB3	4:E:79:TRP:HE3	1.45	0.81
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.60	0.81
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.09	0.81
11:R:3:C:H42	12:T:26:DG:H1	1.29	0.81
1:A:55:ASP:H	1:A:56:PRO:HD2	1.44	0.81
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.63	0.81
1:A:1215:ARG:HH12	1:A:1272:THR:HG22	1.45	0.81
1:A:239:LEU:HD12	1:A:240:PRO:CD	2.08	0.81
2:B:803:LEU:N	2:B:822:ASN:HD21	1.78	0.81
1:A:253:ASN:HB2	1:A:256:GLN:C	2.01	0.81
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.44	0.81
1:A:276:LEU:HD11	1:A:292:ALA:HB3	1.61	0.81
1:A:344:ARG:HG3	1:A:344:ARG:NH1	1.93	0.80
2:B:875:GLU:O	2:B:877:PRO:HD3	1.81	0.80
9:K:70:ARG:O	9:K:71:PHE:HB3	1.81	0.80
2:B:351:TYR:O	2:B:355:ILE:HG13	1.82	0.80
2:B:636:PRO:HB3	2:B:743:ILE:CG1	2.10	0.80
1:A:765:VAL:HG21	1:A:800:VAL:HB	1.63	0.80
1:A:67:CYS:CB	1:A:70:CYS:SG	2.70	0.80
2:B:1076:HIS:ND1	9:K:40:HIS:HD2	1.80	0.80
2:B:635:ARG:CB	2:B:636:PRO:HD2	2.12	0.80
1:A:351:THR:HG22	1:A:352:VAL:H	1.47	0.80
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.63	0.80
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.64	0.80
3:C:102:GLN:HG2	3:C:154:LYS:CD	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:992:ILE:HD11	9:K:67:PHE:CE2	2.17	0.79
1:A:1101:LEU:HD13	1:A:1355:VAL:HG11	1.63	0.79
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.46	0.79
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.48	0.79
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.17	0.79
1:A:249:SER:O	1:A:250:ILE:CG1	2.30	0.79
1:A:346:ASP:H	2:B:1154:ALA:HB1	1.47	0.79
2:B:706:GLN:O	2:B:710:LEU:HB2	1.82	0.79
1:A:316:GLN:O	1:A:316:GLN:CG	2.31	0.78
1:A:319:GLY:HA2	1:A:320:ARG:NH1	1.97	0.78
2:B:708:GLU:HG3	2:B:709:ASP:H	1.48	0.78
2:B:864:LYS:HE3	2:B:871:THR:HG23	1.66	0.78
1:A:913:LEU:HD11	1:A:981:LEU:O	1.84	0.78
1:A:283:GLY:O	1:A:285:PRO:HD3	1.84	0.78
1:A:261:ASP:HB3	1:A:323:LYS:HE3	1.64	0.78
2:B:64:CYS:HA	2:B:67:SER:HB2	1.65	0.78
1:A:401:GLY:H	1:A:435:HIS:CD2	2.01	0.78
2:B:552:MET:HG3	2:B:553:PRO:HD3	1.65	0.78
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.66	0.77
1:A:315:LEU:HD23	1:A:316:GLN:CA	2.14	0.77
2:B:567:GLU:CD	2:B:567:GLU:H	1.86	0.77
1:A:319:GLY:HA3	1:A:320:ARG:HH11	1.49	0.77
1:A:182:VAL:HG12	1:A:183:GLY:H	1.48	0.77
1:A:323:LYS:O	1:A:324:SER:CB	2.32	0.77
12:T:15:DA:H2''	12:T:16:DC:O5'	1.85	0.77
1:A:344:ARG:HH11	1:A:344:ARG:CG	1.95	0.77
3:C:91:HIS:HB2	3:C:96:SER:OG	1.84	0.77
1:A:323:LYS:N	1:A:323:LYS:CD	2.34	0.76
2:B:980:PHE:O	2:B:981:ALA:HB2	1.85	0.76
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.68	0.76
4:E:86:PRO:HB3	4:E:114:ASN:ND2	2.00	0.76
1:A:1111:MET:CG	1:A:1114:PRO:CG	2.57	0.76
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.41	0.76
1:A:182:VAL:HG12	1:A:183:GLY:N	1.99	0.76
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.67	0.76
1:A:590:ARG:O	1:A:591:PHE:HB2	1.84	0.76
3:C:101:LEU:HD12	3:C:117:ASP:O	1.84	0.76
1:A:590:ARG:O	1:A:591:PHE:CB	2.32	0.76
3:C:133:ILE:HD13	3:C:236:GLY:O	1.86	0.76
1:A:315:LEU:CG	1:A:316:GLN:HA	2.16	0.76
2:B:471:LYS:HG3	2:B:472:ALA:N	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.66	0.75
6:H:145:ARG:O	6:H:146:ARG:OXT	2.04	0.75
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.02	0.75
1:A:255:SER:O	1:A:256:GLN:HG3	1.87	0.75
2:B:1096:ARG:HG3	2:B:1097:HIS:CD2	2.20	0.75
2:B:1148:LYS:O	2:B:1152:MET:HB2	1.87	0.75
5:F:82:THR:HG22	5:F:84:TYR:HB2	1.67	0.75
9:K:92:ASN:HA	9:K:95:ILE:HD12	1.68	0.75
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.68	0.74
1:A:315:LEU:HD12	1:A:318:SER:C	2.08	0.74
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.45	0.74
8:J:7:CYS:HG	8:J:10:CYS:H	1.35	0.74
2:B:744:HIS:HD2	2:B:746:SER:OG	1.71	0.74
4:E:86:PRO:CB	4:E:114:ASN:ND2	2.50	0.74
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.70	0.74
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.68	0.74
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.69	0.74
2:B:64:CYS:HA	2:B:67:SER:CB	2.18	0.74
1:A:151:ASP:CG	1:A:163:SER:HA	2.08	0.74
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.68	0.74
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.69	0.74
1:A:1111:MET:SD	1:A:1114:PRO:CB	2.75	0.74
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.13	0.74
8:J:35:ALA:O	8:J:39:LEU:HD12	1.88	0.74
1:A:532:ARG:HH22	1:A:745:GLN:HE21	1.36	0.74
4:E:86:PRO:HB3	4:E:114:ASN:HD22	1.52	0.73
1:A:255:SER:C	1:A:256:GLN:HG3	2.08	0.73
2:B:956:THR:HA	2:B:961:LEU:O	1.87	0.73
1:A:249:SER:O	1:A:250:ILE:HG12	1.87	0.73
4:E:15:ALA:HA	4:E:140:LEU:O	1.88	0.73
1:A:446:ARG:HE	1:A:480:ALA:HB2	1.51	0.73
2:B:494:HIS:HD2	2:B:497:ARG:NH1	1.86	0.73
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	1.70	0.73
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.24	0.73
2:B:973:ILE:HG22	2:B:974:PRO:HD2	1.70	0.73
2:B:95:ILE:HD12	2:B:130:VAL:HG22	1.71	0.72
1:A:253:ASN:CA	1:A:256:GLN:O	2.32	0.72
11:R:4:G:C2'	11:R:5:A:H8	1.95	0.72
1:A:446:ARG:HD2	1:A:480:ALA:CB	2.19	0.72
2:B:1004:GLU:O	3:C:177:GLU:HG2	1.88	0.72
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:77:SER:HB2	4:E:105:PHE:HA	1.70	0.72
3:C:74:SER:O	3:C:77:ILE:HB	1.88	0.72
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.71	0.72
8:J:45:CYS:SG	8:J:46:CYS:N	2.62	0.72
12:T:26:DG:N3	12:T:27:DA:H1'	2.04	0.72
2:B:955:THR:CG2	2:B:956:THR:H	2.02	0.72
1:A:802:ASN:HD21	2:B:729:ILE:H	1.35	0.72
1:A:1407:GLU:H	1:A:1407:GLU:CD	1.93	0.72
2:B:649:LYS:O	2:B:650:GLU:HB2	1.90	0.72
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.53	0.72
2:B:31:TRP:CZ2	2:B:744:HIS:CD2	2.78	0.72
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.70	0.72
1:A:1348:LEU:HD23	1:A:1372:VAL:HG22	1.71	0.72
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.24	0.72
1:A:151:ASP:OD1	1:A:163:SER:HB2	1.90	0.72
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.30	0.72
1:A:249:SER:C	1:A:250:ILE:HG23	2.09	0.71
10:L:51:CYS:HG	14:L:105:ZN:ZN	1.04	0.71
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.89	0.71
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.72	0.71
2:B:591:ARG:O	2:B:592:ASN:HB3	1.89	0.71
1:A:485:ASP:N	1:A:485:ASP:OD1	2.21	0.71
2:B:980:PHE:O	2:B:981:ALA:CB	2.37	0.71
1:A:364:VAL:HG12	1:A:459:ARG:O	1.89	0.71
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.72	0.71
6:H:44:VAL:O	6:H:44:VAL:HG12	1.91	0.71
2:B:636:PRO:CB	2:B:637:LEU:HA	2.21	0.71
1:A:1342:GLU:HG2	4:E:212:ARG:HH12	1.54	0.71
1:A:413:ILE:CD1	1:A:413:ILE:N	2.54	0.71
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.72	0.71
1:A:814:PHE:CE1	2:B:514:LEU:HD21	2.25	0.71
1:A:1111:MET:SD	1:A:1114:PRO:CA	2.79	0.71
9:K:18:LYS:O	9:K:19:LEU:HD23	1.90	0.71
1:A:1116:LEU:H	1:A:1308:THR:HB	1.55	0.71
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.73	0.71
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.54	0.71
1:A:667:GLY:HA2	1:A:670:ILE:HG13	1.73	0.71
1:A:315:LEU:HD12	1:A:319:GLY:N	2.04	0.70
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.23	0.70
1:A:315:LEU:H	1:A:315:LEU:CD1	1.93	0.70
1:A:276:LEU:CD1	1:A:292:ALA:HB3	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.27	0.70
2:B:744:HIS:CD2	2:B:746:SER:OG	2.44	0.70
2:B:1094:ARG:HH22	2:B:1098:MET:HG2	1.53	0.70
12:T:13:DA:H61	13:N:2:DT:C7	2.04	0.70
2:B:485:ARG:HG2	2:B:485:ARG:HH11	1.56	0.70
2:B:634:TYR:CE1	2:B:692:TYR:HD1	2.08	0.70
2:B:881:ASN:HB2	2:B:933:SER:N	2.06	0.70
4:E:61:GLN:HB3	4:E:79:TRP:CE3	2.26	0.70
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.74	0.70
3:C:142:VAL:HG13	3:C:143:LEU:H	1.57	0.70
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.74	0.70
2:B:610:ASN:OD1	2:B:612:GLU:HB2	1.92	0.70
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.74	0.70
1:A:316:GLN:HG3	1:A:316:GLN:O	1.91	0.70
1:A:855:THR:HG21	1:A:857:ARG:NE	2.02	0.70
8:J:48:ARG:HH21	8:J:49:MET:CE	2.04	0.69
2:B:302:CYS:SG	2:B:310:MET:HG2	2.32	0.69
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.73	0.69
2:B:972:LYS:HD3	2:B:1098:MET:SD	2.32	0.69
1:A:250:ILE:O	1:A:251:SER:HB3	1.93	0.69
10:L:40:LEU:HD22	10:L:44:ASP:OD2	1.93	0.69
3:C:219:PHE:CD2	6:H:45:GLU:HG2	2.27	0.69
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.75	0.69
1:A:401:GLY:O	1:A:402:ALA:HB2	1.91	0.69
2:B:1099:VAL:HG12	2:B:1103:ILE:CD1	2.16	0.69
8:J:6:ARG:HB3	8:J:11:GLY:O	1.92	0.69
1:A:413:ILE:HD13	1:A:413:ILE:N	2.06	0.69
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.08	0.69
4:E:77:SER:CB	4:E:105:PHE:HA	2.23	0.69
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.74	0.69
1:A:925:LEU:O	1:A:929:LEU:HB2	1.93	0.69
1:A:304:MET:HG3	2:B:1210:MET:HG3	1.74	0.69
4:E:173:SER:O	4:E:174:GLN:HG2	1.92	0.69
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.08	0.69
3:C:124:LEU:O	3:C:127:ARG:HG2	1.93	0.69
1:A:445:ASN:HB2	1:A:454:SER:O	1.92	0.69
1:A:381:THR:HG22	1:A:384:ASN:ND2	2.09	0.68
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.74	0.68
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.74	0.68
1:A:1132:LYS:O	1:A:1135:ARG:HB3	1.91	0.68
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:H	1:A:926:GLN:NE2	1.91	0.68
2:B:859:TYR:OH	2:B:941:LEU:HD22	1.92	0.68
2:B:955:THR:HG23	10:L:54:ARG:O	1.93	0.68
2:B:1027:ILE:O	2:B:1029:CYS:N	2.26	0.68
1:A:256:GLN:HB3	1:A:257:ARG:HB3	1.75	0.68
3:C:142:VAL:CG1	3:C:143:LEU:N	2.57	0.68
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.23	0.68
1:A:152:VAL:O	1:A:162:VAL:HG23	1.94	0.68
1:A:128:ILE:HG22	1:A:134:ARG:HG3	1.75	0.68
1:A:27:VAL:O	1:A:30:ILE:HG22	1.94	0.68
3:C:167:HIS:HD2	3:C:169:LYS:H	1.39	0.68
3:C:3:GLU:HA	9:K:104:ASN:HD21	1.58	0.68
1:A:1101:LEU:O	1:A:1105:LEU:HD12	1.94	0.68
1:A:249:SER:O	1:A:250:ILE:HG23	1.94	0.68
1:A:1025:ARG:HG2	1:A:1025:ARG:HH11	1.59	0.68
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.28	0.67
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.76	0.67
4:E:199:ILE:O	4:E:199:ILE:HG22	1.94	0.67
1:A:302:THR:HG21	1:A:313:GLN:NE2	2.08	0.67
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.59	0.67
1:A:413:ILE:HD13	1:A:413:ILE:H	1.59	0.67
2:B:628:THR:O	2:B:628:THR:HG22	1.95	0.67
2:B:975:GLN:HG2	2:B:976:ILE:N	2.10	0.67
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.42	0.67
5:F:109:VAL:HG12	5:F:110:ASP:N	2.09	0.67
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.59	0.67
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.77	0.67
1:A:1116:LEU:CD2	1:A:1329:THR:HG22	2.18	0.67
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.24	0.67
2:B:589:VAL:HG12	2:B:590:HIS:N	2.08	0.67
1:A:590:ARG:O	1:A:591:PHE:CG	2.47	0.67
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.82	0.67
2:B:494:HIS:CD2	2:B:497:ARG:NH1	2.63	0.67
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.60	0.67
4:E:46:TYR:CE2	4:E:58:MET:HA	2.30	0.67
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.10	0.67
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.25	0.67
2:B:549:THR:HG22	2:B:550:ASP:H	1.59	0.67
4:E:14:ARG:HH12	4:E:142:VAL:HG22	1.60	0.67
1:A:629:LEU:HD23	1:A:633:VAL:HG23	1.77	0.67
2:B:825:VAL:HG23	2:B:1010:LEU:HG	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:32:GLU:H	8:J:32:GLU:CD	1.96	0.67
1:A:315:LEU:HD22	1:A:316:GLN:HA	1.76	0.66
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.26	0.66
2:B:865:LYS:CG	2:B:866:TYR:N	2.31	0.66
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.76	0.66
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.76	0.66
1:A:58:LEU:HD22	1:A:244:PRO:HD2	1.75	0.66
4:E:29:PHE:O	4:E:30:ILE:HG13	1.95	0.66
2:B:560:GLU:O	2:B:561:TRP:CD1	2.48	0.66
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.77	0.66
2:B:101:MET:HE3	2:B:169:ARG:HH12	1.58	0.66
6:H:22:LYS:O	6:H:23:VAL:HG23	1.95	0.66
1:A:1398:MET:O	1:A:1400:CYS:N	2.29	0.66
2:B:108:VAL:HG12	2:B:109:THR:H	1.60	0.66
3:C:172:PRO:O	3:C:235:VAL:HG23	1.96	0.66
2:B:884:ARG:O	2:B:936:ASP:HB3	1.96	0.66
1:A:115:LEU:HD11	1:A:145:LYS:HE3	1.77	0.66
1:A:565:ILE:HD13	6:H:46:LEU:CD1	2.26	0.66
2:B:980:PHE:O	2:B:1095:LEU:HD12	1.93	0.66
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.34	0.66
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.30	0.66
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.29	0.66
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.78	0.66
6:H:26:ILE:HG22	6:H:40:LEU:O	1.96	0.66
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.78	0.66
3:C:88:CYS:SG	14:C:319:ZN:ZN	1.84	0.66
2:B:766:ARG:NH1	2:B:769:TYR:CE1	2.64	0.66
1:A:590:ARG:NH1	1:A:590:ARG:CG	2.52	0.66
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.04	0.66
1:A:401:GLY:N	1:A:435:HIS:CD2	2.57	0.66
2:B:591:ARG:O	2:B:592:ASN:CB	2.42	0.66
1:A:629:LEU:HD23	1:A:633:VAL:CG2	2.26	0.66
1:A:1400:CYS:O	1:A:1405:THR:HG23	1.96	0.66
1:A:628:GLY:O	1:A:632:VAL:HG23	1.95	0.66
2:B:474:SER:C	2:B:476:ARG:H	1.98	0.66
1:A:53:LEU:O	1:A:56:PRO:CD	2.44	0.66
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.43	0.66
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.78	0.65
1:A:1215:ARG:NH1	1:A:1272:THR:HG22	2.10	0.65
6:H:89:LEU:O	6:H:91:ASP:N	2.27	0.65
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.60	0.65
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.60	0.65
2:B:899:ILE:CD1	2:B:911:ILE:HG12	2.25	0.65
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.12	0.65
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.32	0.65
1:A:901:LEU:HA	1:A:907:THR:HG23	1.79	0.65
1:A:408:ASP:O	1:A:410:GLY:N	2.30	0.65
2:B:649:LYS:O	2:B:650:GLU:CB	2.45	0.65
1:A:1386:ARG:HD3	1:A:1403:GLU:HG2	1.79	0.65
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.27	0.65
2:B:816:GLU:OE1	2:B:816:GLU:N	2.30	0.65
6:H:43:ASN:CG	6:H:46:LEU:HD12	2.17	0.65
1:A:406:ILE:HD13	1:A:431:LYS:HB2	1.79	0.65
4:E:172:GLU:O	4:E:174:GLN:N	2.30	0.65
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.11	0.65
2:B:1106:ARG:HD3	2:B:1126:GLY:O	1.97	0.65
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.77	0.64
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.79	0.64
1:A:751:SER:CB	2:B:1015:HIS:HE1	2.08	0.64
2:B:711:GLU:H	2:B:712:PRO:HD3	1.62	0.64
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.96	0.64
2:B:345:LYS:O	2:B:348:ARG:HG2	1.96	0.64
4:E:171:LYS:O	4:E:173:SER:N	2.30	0.64
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.78	0.64
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.80	0.64
2:B:378:LEU:O	2:B:382:ILE:HG12	1.97	0.64
6:H:58:THR:HG22	6:H:59:ILE:N	2.11	0.64
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.26	0.64
1:A:675:THR:HG22	1:A:679:ILE:HD11	1.78	0.64
2:B:522:VAL:HG13	2:B:538:ASN:O	1.97	0.64
1:A:404:TYR:HA	1:A:413:ILE:O	1.98	0.64
1:A:672:ASP:CB	1:A:736:ASN:HD21	2.09	0.64
1:A:896:ARG:HD2	1:A:897:TYR:HE1	1.62	0.64
4:E:63:ASN:HB3	4:E:64:PRO:CD	2.27	0.64
2:B:635:ARG:O	2:B:636:PRO:C	2.36	0.64
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.33	0.64
1:A:406:ILE:HD12	1:A:406:ILE:H	1.62	0.64
2:B:550:ASP:OD2	2:B:552:MET:CG	2.46	0.64
2:B:108:VAL:HG12	2:B:109:THR:N	2.12	0.64
3:C:58:LEU:HD21	8:J:57:ILE:HD13	1.78	0.64
1:A:388:LEU:HD22	1:A:432:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:830:TYR:O	2:B:832:GLY:N	2.30	0.64
1:A:464:PRO:HG2	9:K:67:PHE:CD1	2.33	0.64
2:B:986:GLN:NE2	2:B:1016:ALA:HB1	2.13	0.64
5:F:109:VAL:HG23	5:F:124:GLU:HG2	1.79	0.64
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.79	0.64
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.97	0.64
2:B:1103:ILE:N	2:B:1103:ILE:HD13	2.11	0.64
4:E:3:GLN:HG3	4:E:4:GLU:N	2.12	0.64
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.80	0.64
6:H:84:ALA:O	6:H:86:ASP:N	2.30	0.64
2:B:451:LYS:HA	2:B:454:THR:HB	1.79	0.64
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.28	0.64
1:A:105:CYS:O	1:A:114:LEU:HG	1.98	0.64
1:A:55:ASP:O	1:A:57:ARG:N	2.31	0.64
8:J:1:MET:N	8:J:56:LEU:H	1.96	0.64
1:A:777:PHE:CD2	1:A:781:ASP:O	2.52	0.63
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.80	0.63
7:I:35:VAL:HG12	7:I:36:GLU:N	2.13	0.63
2:B:276:ILE:HG22	2:B:278:GLN:H	1.63	0.63
2:B:168:GLY:H	2:B:450:ALA:HB1	1.63	0.63
1:A:324:SER:O	1:A:326:ARG:N	2.32	0.63
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.63
1:A:475:THR:HG22	1:A:476:SER:N	2.13	0.63
1:A:802:ASN:ND2	2:B:729:ILE:H	1.95	0.63
1:A:1067:LEU:HD12	1:A:1067:LEU:O	1.99	0.63
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.79	0.63
1:A:265:LYS:O	1:A:267:ALA:N	2.31	0.63
1:A:440:ASP:H	1:A:460:VAL:HG23	1.63	0.63
3:C:184:ASN:HD21	3:C:189:THR:H	1.46	0.63
1:A:351:THR:CG2	1:A:352:VAL:N	2.60	0.63
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.11	0.63
1:A:955:PRO:O	1:A:956:LEU:HG	1.99	0.63
2:B:864:LYS:NZ	2:B:867:GLY:N	2.45	0.63
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.34	0.63
2:B:879:ARG:CZ	2:B:879:ARG:H	2.11	0.63
2:B:1148:LYS:O	2:B:1152:MET:N	2.31	0.63
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.80	0.63
1:A:264:PHE:CE1	1:A:317:LYS:HB3	2.34	0.63
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.14	0.63
1:A:1154:TYR:CE2	1:A:1156:PRO:HG3	2.34	0.63
1:A:1116:LEU:HD23	1:A:1329:THR:HG21	1.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:GLY:HA2	2:B:454:THR:OG1	1.99	0.62
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.81	0.62
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.80	0.62
2:B:1084:GLN:HE21	3:C:192:TRP:HB2	1.64	0.62
4:E:28:TYR:HE1	4:E:78:LEU:HD13	1.63	0.62
6:H:113:ALA:HA	6:H:125:LEU:O	1.99	0.62
2:B:420:LEU:O	2:B:423:LYS:HB3	1.99	0.62
1:A:302:THR:HG21	1:A:313:GLN:HE22	1.63	0.62
3:C:73:GLN:HE21	3:C:75:MET:H	1.47	0.62
1:A:821:ARG:O	1:A:825:ILE:HG12	2.00	0.62
1:A:577:ILE:O	1:A:580:VAL:HG23	2.00	0.62
3:C:100:THR:HB	3:C:119:VAL:HG12	1.81	0.62
2:B:803:LEU:H	2:B:822:ASN:HD21	1.47	0.62
2:B:552:MET:HG3	2:B:553:PRO:CD	2.29	0.62
1:A:324:SER:O	1:A:325:ILE:C	2.38	0.62
2:B:865:LYS:HG2	2:B:866:TYR:H	0.66	0.62
1:A:1025:ARG:HG2	1:A:1025:ARG:NH1	2.14	0.62
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.00	0.62
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.81	0.62
1:A:55:ASP:N	1:A:56:PRO:CD	2.62	0.62
2:B:851:PHE:HB3	2:B:1094:ARG:HD2	1.82	0.62
1:A:518:LYS:CG	1:A:519:PRO:HD2	2.30	0.62
1:A:253:ASN:HA	1:A:256:GLN:C	2.19	0.62
1:A:53:LEU:O	1:A:56:PRO:HD3	2.00	0.62
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.15	0.62
1:A:320:ARG:CB	1:A:321:PRO:HA	2.30	0.62
2:B:1082:MET:HA	3:C:189:THR:HA	1.81	0.62
1:A:845:LEU:O	1:A:848:ILE:HG12	1.99	0.62
1:A:787:PHE:CZ	1:A:796:SER:HB2	2.35	0.62
1:A:261:ASP:HB3	1:A:323:LYS:CE	2.30	0.61
1:A:253:ASN:HB2	1:A:257:ARG:N	2.10	0.61
1:A:253:ASN:HB3	1:A:257:ARG:H	1.61	0.61
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.83	0.61
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.82	0.61
2:B:211:VAL:O	2:B:480:SER:HA	2.00	0.61
1:A:754:SER:H	1:A:757:ASN:HD22	1.46	0.61
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.82	0.61
1:A:332:LYS:C	1:A:334:GLY:H	2.04	0.61
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.64	0.61
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.67	0.61
5:F:82:THR:CG2	5:F:84:TYR:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.82	0.61
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.15	0.61
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.40	0.61
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.83	0.61
5:F:111:LEU:H	5:F:111:LEU:HD13	1.65	0.61
2:B:1096:ARG:HG2	2:B:1096:ARG:NH1	2.04	0.61
8:J:44:TYR:CA	8:J:47:ARG:HB2	2.18	0.61
1:A:568:PRO:HB3	3:C:221:TYR:CZ	2.36	0.61
1:A:1025:ARG:CG	1:A:1025:ARG:HH11	2.14	0.61
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.83	0.61
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.52	0.61
1:A:1111:MET:SD	1:A:1114:PRO:HA	2.41	0.61
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.83	0.61
1:A:765:VAL:HG21	1:A:800:VAL:CB	2.30	0.61
1:A:833:GLU:HG2	1:A:1102:LYS:HE3	1.83	0.61
1:A:98:LYS:O	1:A:101:LYS:N	2.33	0.61
2:B:589:VAL:CG1	2:B:590:HIS:N	2.64	0.60
3:C:172:PRO:C	3:C:235:VAL:HG23	2.21	0.60
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.01	0.60
2:B:766:ARG:HH21	2:B:1020:ARG:HB3	1.65	0.60
2:B:322:PHE:CD1	2:B:322:PHE:O	2.55	0.60
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.40	0.60
1:A:1161:THR:HG22	1:A:1162:VAL:H	1.66	0.60
2:B:622:LYS:HE2	7:I:59:VAL:HG22	1.82	0.60
2:B:640:VAL:HG12	2:B:640:VAL:O	2.00	0.60
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.83	0.60
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.00	0.60
3:C:185:LYS:HE3	3:C:211:ASP:O	2.01	0.60
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.01	0.60
1:A:648:ASN:O	1:A:652:VAL:HG23	2.02	0.60
2:B:475:SER:C	2:B:477:ALA:N	2.53	0.60
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.02	0.60
2:B:1096:ARG:HG3	2:B:1097:HIS:CG	2.37	0.60
1:A:672:ASP:H	1:A:736:ASN:ND2	1.99	0.60
1:A:129:LYS:O	1:A:130:ASP:CB	2.32	0.60
6:H:44:VAL:CG1	6:H:44:VAL:O	2.49	0.60
1:A:442:VAL:HG11	1:A:489:LEU:HD21	1.83	0.60
2:B:273:LEU:HD11	2:B:285:ILE:CD1	2.31	0.60
2:B:802:PRO:HA	2:B:1091:TYR:CD1	2.36	0.60
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.16	0.60
1:A:55:ASP:H	1:A:56:PRO:CD	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:LYS:O	8:J:52:THR:CG2	2.50	0.60
2:B:1012:ILE:HD13	2:B:1092:TYR:OH	2.02	0.60
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.60	0.60
1:A:567:LYS:O	1:A:569:LYS:N	2.34	0.60
10:L:41:SER:O	10:L:44:ASP:HB2	2.02	0.60
1:A:883:LEU:HD11	1:A:1017:LEU:HD21	1.84	0.60
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.36	0.60
2:B:288:ALA:CB	2:B:331:LEU:HD12	2.32	0.60
1:A:1437:GLY:HA3	5:F:88:TYR:CD2	2.36	0.60
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.67	0.60
9:K:20:LYS:HD3	9:K:22:ASP:OD2	2.02	0.60
4:E:171:LYS:O	4:E:172:GLU:C	2.40	0.59
2:B:322:PHE:HZ	7:I:30:ARG:HH11	1.48	0.59
2:B:1153:GLU:N	2:B:1153:GLU:OE2	2.35	0.59
2:B:957:ASN:HD22	2:B:959:ASP:H	1.49	0.59
1:A:754:SER:N	1:A:757:ASN:HD22	1.99	0.59
1:A:949:ASP:N	1:A:949:ASP:OD1	2.26	0.59
1:A:182:VAL:CG1	1:A:183:GLY:H	2.14	0.59
4:E:2:ASP:O	4:E:3:GLN:HB3	2.02	0.59
3:C:73:GLN:NE2	3:C:237:SER:O	2.35	0.59
1:A:685:GLU:O	1:A:689:LYS:HB2	2.02	0.59
1:A:675:THR:HG22	1:A:679:ILE:CD1	2.33	0.59
3:C:41:ILE:HG13	3:C:172:PRO:HG3	1.84	0.59
1:A:303:TYR:CG	1:A:303:TYR:O	2.56	0.59
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.85	0.59
1:A:58:LEU:HD21	1:A:243:PRO:HB3	1.84	0.59
2:B:315:LYS:N	2:B:316:PRO:HD2	2.18	0.59
6:H:139:ASN:O	6:H:140:ALA:HB2	2.03	0.59
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.02	0.59
1:A:557:ASP:HA	9:K:26:LYS:HE3	1.84	0.59
2:B:1027:ILE:O	2:B:1030:LEU:N	2.36	0.59
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.68	0.59
2:B:501:PRO:O	2:B:502:ILE:HB	2.03	0.59
2:B:779:GLY:O	2:B:795:ILE:HG23	2.02	0.59
1:A:315:LEU:CD1	1:A:319:GLY:CA	2.72	0.59
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.68	0.59
2:B:976:ILE:HD11	2:B:992:ILE:HD12	1.85	0.59
4:E:86:PRO:CA	4:E:114:ASN:HD22	2.14	0.59
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.83	0.59
1:A:996:ASN:HA	1:A:998:LEU:HD23	1.83	0.59
1:A:399:HIS:CD2	1:A:400:PRO:CD	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	1.85	0.59
2:B:1131:GLY:O	2:B:1134:GLU:N	2.34	0.59
3:C:13:ALA:HA	3:C:17:ASN:O	2.02	0.59
1:A:265:LYS:HD2	1:A:303:TYR:HB2	1.85	0.59
4:E:77:SER:HB2	4:E:105:PHE:CA	2.33	0.59
2:B:789:MET:CE	2:B:965:LYS:HB3	2.32	0.59
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.84	0.59
2:B:830:TYR:O	2:B:831:SER:C	2.40	0.59
6:H:139:ASN:O	6:H:140:ALA:CB	2.51	0.59
1:A:567:LYS:CB	6:H:95:TYR:HA	2.33	0.58
1:A:470:LEU:HD21	1:A:487:MET:CE	2.32	0.58
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.85	0.58
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.85	0.58
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.84	0.58
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.38	0.58
1:A:1398:MET:C	1:A:1400:CYS:H	2.05	0.58
1:A:787:PHE:CE1	1:A:796:SER:HB2	2.38	0.58
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.85	0.58
2:B:1103:ILE:HD13	2:B:1103:ILE:H	1.68	0.58
8:J:9:SER:OG	8:J:48:ARG:NH2	2.36	0.58
2:B:550:ASP:OD2	2:B:552:MET:HG3	2.03	0.58
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.85	0.58
1:A:253:ASN:CA	1:A:256:GLN:C	2.70	0.58
3:C:93:ASP:O	3:C:127:ARG:NH2	2.36	0.58
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.85	0.58
2:B:986:GLN:OE1	2:B:986:GLN:CA	2.49	0.58
8:J:7:CYS:HB3	8:J:46:CYS:SG	2.43	0.58
2:B:179:CYS:SG	2:B:180:TYR:N	2.76	0.58
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.85	0.58
2:B:975:GLN:CG	2:B:976:ILE:H	2.16	0.58
1:A:1105:LEU:HD23	1:A:1384:VAL:HG21	1.86	0.58
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.69	0.58
6:H:127:GLY:HA3	6:H:130:ARG:NH2	2.19	0.58
2:B:515:HIS:H	2:B:518:HIS:CD2	2.22	0.58
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.50	0.58
2:B:383:ASN:O	2:B:387:LEU:HB2	2.03	0.58
1:A:399:HIS:CG	1:A:400:PRO:N	2.72	0.58
2:B:98:THR:O	2:B:126:SER:CB	2.49	0.58
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.03	0.58
1:A:95:PHE:O	1:A:99:ILE:HG13	2.03	0.58
1:A:869:GLY:O	4:E:204:THR:HG21	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:HZ3	2:B:867:GLY:CA	2.15	0.58
2:B:864:LYS:CE	2:B:870:ILE:O	2.51	0.58
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.16	0.58
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.85	0.58
1:A:151:ASP:OD2	1:A:163:SER:HA	2.04	0.58
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.03	0.58
2:B:128:LEU:HB2	2:B:167:ILE:O	2.04	0.58
2:B:703:ILE:HA	2:B:740:HIS:O	2.04	0.58
2:B:766:ARG:HA	2:B:769:TYR:HD1	1.69	0.58
1:A:352:VAL:CG2	2:B:1099:VAL:HG13	2.32	0.58
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.34	0.57
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.85	0.57
2:B:474:SER:C	2:B:476:ARG:N	2.57	0.57
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.85	0.57
2:B:733:HIS:O	2:B:735:ALA:N	2.35	0.57
4:E:153:HIS:O	4:E:154:ILE:HD13	2.04	0.57
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.68	0.57
1:A:256:GLN:HB3	1:A:257:ARG:CD	2.33	0.57
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.33	0.57
8:J:7:CYS:SG	8:J:9:SER:N	2.77	0.57
1:A:182:VAL:CG1	1:A:183:GLY:N	2.67	0.57
1:A:99:ILE:HA	1:A:102:VAL:HG23	1.87	0.57
3:C:43:THR:HG23	3:C:44:LEU:N	2.19	0.57
3:C:144:ILE:HG22	3:C:145:CYS:HB3	1.87	0.57
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.68	0.57
1:A:1436:ILE:O	1:A:1437:GLY:C	2.43	0.57
1:A:490:HIS:HB3	2:B:1150:ARG:CZ	2.34	0.57
1:A:807:GLY:O	2:B:728:ARG:HD3	2.04	0.57
2:B:596:LEU:O	2:B:600:LEU:HD23	2.05	0.57
5:F:74:ILE:HG21	5:F:144:GLU:HG2	1.86	0.57
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.85	0.57
1:A:777:PHE:CD2	1:A:781:ASP:C	2.78	0.57
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.69	0.57
1:A:335:ARG:HH11	2:B:1202:LEU:HD12	1.68	0.57
1:A:323:LYS:HD3	1:A:323:LYS:H	1.60	0.57
1:A:256:GLN:HA	1:A:257:ARG:HB2	1.74	0.57
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.86	0.57
1:A:1342:GLU:CG	4:E:212:ARG:NH1	2.62	0.57
2:B:384:ARG:HH22	2:B:621:GLU:HG3	1.69	0.57
2:B:638:PHE:O	2:B:740:HIS:HB3	2.05	0.57
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:7:PHE:C	9:K:9:LEU:H	2.08	0.57
1:A:11:LEU:HA	2:B:1193:GLN:O	2.04	0.57
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.58	0.57
11:R:9:G:O2'	11:R:10:A:H5'	2.04	0.57
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.86	0.57
2:B:636:PRO:CB	2:B:637:LEU:CA	2.83	0.57
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.20	0.57
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.87	0.57
1:A:119:ASN:O	1:A:123:ARG:HG3	2.04	0.57
2:B:736:THR:O	2:B:736:THR:HG22	2.05	0.57
1:A:635:ARG:HE	1:A:877:HIS:HA	1.70	0.57
2:B:34:ILE:HD13	2:B:542:MET:HE1	1.87	0.56
2:B:1096:ARG:HH11	2:B:1096:ARG:CG	2.09	0.56
11:R:9:G:C2'	11:R:10:A:H5'	2.33	0.56
2:B:519:TRP:O	2:B:519:TRP:CD1	2.58	0.56
1:A:249:SER:O	1:A:250:ILE:HD13	2.04	0.56
1:A:814:PHE:O	1:A:817:ALA:HB3	2.06	0.56
3:C:79:GLN:HE21	3:C:127:ARG:HB3	1.68	0.56
1:A:1115:SER:HB3	1:A:1330:ASN:ND2	2.19	0.56
1:A:567:LYS:HB3	6:H:96:VAL:N	2.12	0.56
12:T:27:DA:N3	12:T:27:DA:H2'	2.19	0.56
2:B:650:GLU:HG3	2:B:651:LEU:N	2.20	0.56
1:A:32:VAL:HB	1:A:57:ARG:CB	2.34	0.56
3:C:69:LEU:O	8:J:6:ARG:NH1	2.32	0.56
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.66	0.56
1:A:172:PRO:HB2	1:A:174:ILE:HG12	1.87	0.56
2:B:778:MET:CE	2:B:853:SER:HB3	2.34	0.56
1:A:408:ASP:O	1:A:409:SER:C	2.44	0.56
2:B:65:GLU:OE1	2:B:65:GLU:N	2.38	0.56
3:C:39:ALA:O	3:C:164:ALA:HB3	2.05	0.56
2:B:541:LEU:HB2	2:B:747:MET:CE	2.35	0.56
1:A:185:TRP:O	1:A:186:LYS:HB2	2.05	0.56
1:A:55:ASP:N	1:A:56:PRO:HD2	2.15	0.56
2:B:1060:ARG:C	2:B:1062:HIS:H	2.07	0.56
1:A:361:LEU:HD21	1:A:521:MET:HE1	1.88	0.56
1:A:402:ALA:O	1:A:415:LEU:CD1	2.53	0.56
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.87	0.56
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.36	0.56
1:A:567:LYS:CB	1:A:568:PRO:CD	2.59	0.56
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.40	0.56
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.69	0.56
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.40	0.56
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.35	0.56
1:A:1277:GLU:O	1:A:1279:ILE:HD12	2.05	0.56
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.24	0.56
1:A:320:ARG:CB	1:A:321:PRO:CA	2.84	0.56
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.36	0.56
1:A:962:ARG:O	1:A:964:ILE:N	2.39	0.56
2:B:863:GLU:O	2:B:864:LYS:C	2.43	0.56
12:T:26:DG:C2	12:T:27:DA:H1'	2.39	0.56
1:A:809:THR:HB	1:A:810:PRO:HD2	1.87	0.56
1:A:596:THR:C	1:A:598:LEU:H	2.08	0.56
2:B:976:ILE:HG23	2:B:977:GLY:N	2.21	0.55
1:A:302:THR:HA	1:A:305:ASP:O	2.05	0.55
1:A:705:LYS:HE3	1:A:713:SER:HB2	1.87	0.55
1:A:179:LEU:HD11	1:A:298:PHE:HD1	1.70	0.55
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.87	0.55
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.40	0.55
6:H:130:ARG:HB3	6:H:134:ASN:HD22	1.72	0.55
1:A:791:ASP:OD1	1:A:791:ASP:C	2.44	0.55
4:E:171:LYS:H	4:E:174:GLN:HG3	1.70	0.55
3:C:167:HIS:CD2	3:C:169:LYS:H	2.22	0.55
4:E:3:GLN:CG	4:E:5:ASN:H	2.18	0.55
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.18	0.55
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.87	0.55
1:A:213:HIS:O	1:A:214:ILE:C	2.40	0.55
2:B:175:ARG:CG	2:B:175:ARG:HH11	2.20	0.55
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.88	0.55
1:A:463:ILE:CB	1:A:464:PRO:HD2	2.36	0.55
3:C:186:LEU:CB	3:C:188:HIS:HD2	2.20	0.55
1:A:929:LEU:HD21	1:A:983:ILE:CG2	2.36	0.55
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.89	0.55
2:B:983:ARG:C	2:B:984:HIS:CG	2.80	0.55
2:B:1017:ILE:H	2:B:1018:PRO:HD3	1.71	0.55
1:A:130:ASP:C	1:A:132:LYS:H	2.09	0.55
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.60	0.55
1:A:249:SER:O	1:A:250:ILE:CD1	2.54	0.55
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.36	0.55
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.22	0.55
1:A:661:GLY:N	2:B:1081:LEU:HD22	2.21	0.55
3:C:99:LEU:HD23	3:C:99:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:HB2	1:A:321:PRO:CA	2.36	0.55
1:A:352:VAL:HG12	1:A:353:ILE:N	2.22	0.55
1:A:765:VAL:CG2	1:A:800:VAL:CB	2.73	0.55
1:A:406:ILE:N	1:A:406:ILE:CD1	2.62	0.55
2:B:1027:ILE:O	2:B:1028:GLU:C	2.45	0.55
1:A:376:TYR:CD2	1:A:376:TYR:C	2.80	0.55
1:A:446:ARG:HG3	1:A:487:MET:HG2	1.89	0.55
2:B:169:ARG:O	2:B:171:PRO:HD3	2.07	0.55
7:I:85:PHE:O	7:I:86:PHE:HB3	2.07	0.55
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.88	0.55
1:A:315:LEU:HD12	1:A:318:SER:O	2.06	0.55
11:R:5:A:C2	11:R:6:G:C5	2.95	0.55
2:B:95:ILE:CD1	2:B:130:VAL:HG22	2.36	0.55
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.72	0.55
1:A:33:ALA:HB3	1:A:83:HIS:H	1.72	0.55
1:A:694:THR:HA	1:A:714:PHE:HE1	1.70	0.55
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.87	0.55
2:B:203:PHE:C	2:B:204:ILE:HD12	2.27	0.55
1:A:472:LEU:HD21	2:B:835:GLN:CB	2.37	0.55
1:A:1111:MET:HG3	1:A:1114:PRO:CG	2.30	0.54
1:A:344:ARG:O	2:B:1155:SER:HB2	2.06	0.54
7:I:71:SER:HB3	7:I:85:PHE:CE2	2.43	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.46	0.54
2:B:426:LYS:HD2	2:B:430:ARG:HH22	1.71	0.54
3:C:251:LEU:O	3:C:255:VAL:HG23	2.06	0.54
2:B:780:VAL:O	2:B:817:LEU:HD23	2.07	0.54
2:B:364:ILE:O	2:B:365:THR:HB	2.07	0.54
1:A:903:ASN:O	1:A:907:THR:OG1	2.26	0.54
8:J:7:CYS:HA	8:J:49:MET:HG2	1.89	0.54
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.89	0.54
1:A:320:ARG:HB2	1:A:321:PRO:HB3	1.89	0.54
3:C:66:ARG:NH2	8:J:3:VAL:O	2.40	0.54
1:A:947:PHE:CD2	1:A:954:TRP:CE2	2.96	0.54
2:B:992:ILE:CD1	9:K:67:PHE:HE2	2.12	0.54
2:B:101:MET:CE	2:B:169:ARG:HH12	2.19	0.54
5:F:86:THR:OG1	5:F:89:GLU:HG3	2.07	0.54
2:B:604:ARG:HA	2:B:609:ILE:O	2.07	0.54
1:A:352:VAL:HG21	2:B:1099:VAL:HG13	1.89	0.54
1:A:568:PRO:HD3	6:H:94:ASP:O	2.06	0.54
2:B:1094:ARG:NH2	2:B:1098:MET:HG2	2.21	0.54
7:I:27:PHE:O	7:I:35:VAL:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:168:TYR:O	4:E:170:LEU:HG	2.06	0.54
5:F:76:LYS:O	5:F:79:ARG:HD2	2.07	0.54
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.07	0.54
9:K:65:HIS:HD2	9:K:67:PHE:N	2.01	0.54
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.88	0.54
4:E:168:TYR:HB3	4:E:170:LEU:HD11	1.90	0.54
4:E:36:GLU:O	4:E:38:PRO:HD3	2.07	0.54
3:C:165:LYS:O	9:K:6:ARG:NH1	2.40	0.54
2:B:792:MET:HE1	2:B:857:ARG:NH2	2.22	0.54
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.89	0.54
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.90	0.54
9:K:49:GLU:C	9:K:51:LEU:H	2.09	0.54
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.90	0.54
1:A:805:LEU:CD2	2:B:1052:VAL:HG21	2.38	0.54
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.43	0.54
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.88	0.54
4:E:191:LYS:H	4:E:194:GLU:HB2	1.72	0.54
1:A:383:TYR:HB3	5:F:115:THR:HB	1.89	0.54
4:E:127:ILE:HG12	4:E:127:ILE:O	2.08	0.54
3:C:143:LEU:C	3:C:143:LEU:HD12	2.28	0.54
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.89	0.54
2:B:273:LEU:HD11	2:B:285:ILE:HD11	1.90	0.54
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.89	0.53
1:A:402:ALA:O	1:A:415:LEU:HD12	2.08	0.53
1:A:332:LYS:H	1:A:337:ARG:HB3	1.71	0.53
1:A:709:THR:HG23	7:I:94:ASP:HA	1.90	0.53
1:A:893:PHE:C	1:A:893:PHE:CD2	2.81	0.53
1:A:257:ARG:CG	1:A:257:ARG:O	2.51	0.53
1:A:471:ASN:O	1:A:472:LEU:C	2.47	0.53
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.90	0.53
2:B:329:THR:HA	2:B:332:ASP:CB	2.38	0.53
3:C:242:GLN:O	3:C:246:ARG:HG3	2.08	0.53
1:A:351:THR:HG21	1:A:466:SER:O	2.08	0.53
9:K:40:HIS:HE1	9:K:63:VAL:CG2	2.21	0.53
1:A:1398:MET:C	1:A:1400:CYS:N	2.61	0.53
1:A:335:ARG:NH1	2:B:1202:LEU:HD12	2.24	0.53
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.44	0.53
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.08	0.53
9:K:65:HIS:CD2	9:K:67:PHE:H	2.14	0.53
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.23	0.53
1:A:482:PHE:HD1	2:B:835:GLN:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ASP:OD2	2:B:829:CYS:CB	2.57	0.53
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.90	0.53
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.91	0.53
2:B:361:LEU:O	2:B:363:HIS:O	2.26	0.53
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.72	0.53
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.29	0.53
1:A:599:SER:C	1:A:601:LYS:H	2.12	0.53
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.48	0.53
1:A:822:GLU:O	1:A:826:ASP:OD2	2.27	0.53
2:B:521:LEU:HD22	2:B:633:VAL:HB	1.89	0.53
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.42	0.53
1:A:401:GLY:O	1:A:402:ALA:CB	2.56	0.53
4:E:15:ALA:O	4:E:19:VAL:HG23	2.08	0.53
9:K:46:ILE:O	9:K:50:LEU:HB2	2.08	0.53
1:A:590:ARG:HH21	1:A:621:THR:HA	1.74	0.53
2:B:913:GLY:HA2	2:B:938:SER:HB2	1.87	0.53
1:A:528:LEU:HD23	1:A:751:SER:HA	1.91	0.53
1:A:1410:PHE:O	1:A:1413:GLY:N	2.41	0.53
8:J:7:CYS:CB	8:J:46:CYS:SG	2.97	0.53
2:B:778:MET:O	2:B:819:ALA:HB1	2.08	0.53
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.49	0.53
3:C:43:THR:CG2	3:C:44:LEU:N	2.72	0.53
3:C:5:GLY:O	3:C:7:GLN:HG2	2.09	0.53
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.17	0.53
8:J:7:CYS:CA	8:J:49:MET:HE3	2.38	0.53
8:J:2:ILE:O	8:J:2:ILE:HG23	2.09	0.53
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.91	0.53
4:E:153:HIS:CD2	4:E:198:ILE:HG12	2.43	0.52
2:B:592:ASN:N	2:B:593:PRO:CD	2.71	0.52
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.74	0.52
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.09	0.52
1:A:765:VAL:HG23	1:A:766:GLY:H	1.74	0.52
2:B:954:VAL:O	10:L:55:ILE:O	2.27	0.52
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.91	0.52
1:A:49:LYS:HD3	1:A:55:ASP:CG	2.28	0.52
3:C:66:ARG:HH21	8:J:4:PRO:HA	1.74	0.52
1:A:252:PHE:O	1:A:252:PHE:HD1	1.91	0.52
1:A:361:LEU:HD21	1:A:521:MET:CE	2.39	0.52
1:A:880:LYS:CG	1:A:880:LYS:O	2.57	0.52
1:A:464:PRO:CG	9:K:67:PHE:CD1	2.92	0.52
2:B:983:ARG:O	2:B:984:HIS:CG	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:THR:HG22	1:A:616:VAL:HA	1.91	0.52
1:A:894:GLU:C	1:A:896:ARG:H	2.13	0.52
1:A:312:PRO:O	1:A:313:GLN:HB2	2.10	0.52
1:A:858:ASN:HD22	1:A:858:ASN:C	2.12	0.52
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.39	0.52
4:E:6:GLU:O	4:E:9:ILE:HG22	2.09	0.52
2:B:981:ALA:HB3	2:B:1095:LEU:HD11	1.92	0.52
1:A:403:LYS:HA	1:A:415:LEU:HB2	1.91	0.52
1:A:885:THR:O	1:A:940:ARG:HG3	2.09	0.52
6:H:58:THR:HG22	6:H:59:ILE:H	1.74	0.52
3:C:58:LEU:HD21	8:J:57:ILE:CD1	2.40	0.52
5:F:111:LEU:H	5:F:111:LEU:CD1	2.22	0.52
1:A:639:PRO:HG2	1:A:640:GLN:HG2	1.92	0.52
2:B:737:THR:HG21	7:I:66:PRO:HA	1.91	0.52
2:B:864:LYS:HD3	2:B:870:ILE:O	2.10	0.52
1:A:15:LYS:HE2	2:B:1220:ARG:HG2	1.91	0.52
7:I:99:LEU:O	7:I:111:THR:HG23	2.09	0.52
1:A:127:ALA:O	1:A:128:ILE:C	2.48	0.52
4:E:30:ILE:HG22	4:E:31:THR:O	2.09	0.52
4:E:2:ASP:O	4:E:3:GLN:CB	2.57	0.52
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.25	0.52
3:C:241:ASP:O	3:C:245:VAL:HG23	2.09	0.52
1:A:265:LYS:NZ	1:A:323:LYS:HE2	2.25	0.52
1:A:1118:VAL:HA	1:A:1327:ILE:HG13	1.90	0.52
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.92	0.52
1:A:161:LEU:O	1:A:162:VAL:O	2.27	0.52
1:A:648:ASN:OD1	1:A:648:ASN:N	2.43	0.52
3:C:16:ASP:O	3:C:233:GLU:HA	2.10	0.52
2:B:176:SER:O	2:B:182:SER:HB2	2.10	0.52
2:B:363:HIS:O	2:B:364:ILE:CB	2.47	0.52
1:A:1021:LEU:O	1:A:1024:SER:N	2.43	0.52
1:A:417:TYR:O	1:A:418:SER:HB3	2.10	0.52
1:A:1341:ILE:HB	4:E:182:ASP:OD2	2.09	0.52
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.10	0.52
2:B:516:ASN:H	2:B:516:ASN:HD22	1.56	0.52
2:B:912:ILE:O	2:B:938:SER:HB2	2.10	0.51
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.74	0.51
2:B:882:THR:CG2	2:B:935:ARG:HA	2.22	0.51
2:B:204:ILE:N	2:B:204:ILE:HD12	2.25	0.51
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.91	0.51
1:A:575:LYS:HB3	1:A:612:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HD2	1:A:221:SER:O	2.11	0.51
8:J:1:MET:N	8:J:56:LEU:N	2.58	0.51
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.91	0.51
1:A:863:VAL:O	1:A:864:ILE:HD13	2.10	0.51
6:H:84:ALA:C	6:H:86:ASP:N	2.64	0.51
1:A:265:LYS:HZ1	1:A:323:LYS:HE2	1.75	0.51
1:A:39:GLU:O	1:A:53:LEU:HB2	2.09	0.51
1:A:803:SER:OG	1:A:806:ARG:HD2	2.10	0.51
1:A:471:ASN:O	1:A:473:SER:N	2.44	0.51
1:A:251:SER:OG	1:A:252:PHE:N	2.42	0.51
2:B:475:SER:C	2:B:477:ALA:H	2.14	0.51
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.91	0.51
2:B:323:VAL:O	2:B:324:ILE:HG13	2.10	0.51
2:B:428:ILE:HD11	2:B:448:ILE:HD13	1.91	0.51
1:A:256:GLN:HB3	1:A:257:ARG:HD3	1.90	0.51
2:B:64:CYS:HA	2:B:67:SER:HB3	1.92	0.51
1:A:1437:GLY:CA	5:F:88:TYR:CD2	2.93	0.51
6:H:15:VAL:HA	6:H:26:ILE:HD12	1.92	0.51
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.76	0.51
1:A:1161:THR:HG23	1:A:1239:ARG:NH2	2.25	0.51
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.75	0.51
1:A:705:LYS:HG3	1:A:713:SER:HB3	1.92	0.51
1:A:608:ILE:HG12	1:A:613:ILE:HG13	1.93	0.51
1:A:514:PRO:O	1:A:515:GLN:C	2.49	0.51
3:C:226:ASP:O	3:C:227:THR:O	2.29	0.51
2:B:978:ASP:OD1	2:B:1099:VAL:HG23	2.11	0.51
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.08	0.51
1:A:401:GLY:CA	1:A:435:HIS:CD2	2.94	0.51
1:A:575:LYS:HB3	1:A:612:ILE:CG1	2.40	0.51
1:A:802:ASN:HD21	2:B:729:ILE:N	2.05	0.51
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.10	0.51
1:A:1438:THR:HG23	5:F:92:ARG:HB2	1.92	0.51
7:I:106:CYS:O	7:I:107:SER:C	2.49	0.51
1:A:321:PRO:O	1:A:322:VAL:HG22	2.10	0.51
3:C:102:GLN:CG	3:C:154:LYS:HD3	2.26	0.51
6:H:115:TYR:CE2	6:H:124:ARG:HG3	2.45	0.51
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.46	0.51
2:B:498:THR:O	2:B:536:VAL:HA	2.09	0.51
1:A:319:GLY:HA2	1:A:320:ARG:HH11	1.57	0.51
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.17	0.51
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ASP:OD2	2:B:829:CYS:HB2	2.10	0.51
2:B:778:MET:CE	2:B:1094:ARG:HH11	2.24	0.51
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.44	0.51
1:A:92:HIS:ND1	1:A:236:LEU:HD21	2.25	0.51
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.93	0.51
1:A:475:THR:CG2	1:A:476:SER:N	2.74	0.51
3:C:3:GLU:HA	9:K:104:ASN:ND2	2.25	0.51
2:B:696:GLU:O	2:B:699:GLU:HB2	2.11	0.51
3:C:42:PRO:HA	3:C:163:ILE:HG23	1.92	0.51
1:A:857:ARG:HB3	1:A:862:ASN:O	2.11	0.51
1:A:1021:LEU:O	1:A:1022:LEU:C	2.48	0.51
1:A:249:SER:O	1:A:250:ILE:CB	2.59	0.51
1:A:1434:ALA:O	1:A:1436:ILE:N	2.44	0.51
2:B:814:PHE:C	2:B:816:GLU:H	2.14	0.51
1:A:794:PRO:O	1:A:797:LYS:N	2.41	0.51
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.75	0.51
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.93	0.50
2:B:1065:GLN:HE21	2:B:1069:PHE:H	1.59	0.50
3:C:66:ARG:NH2	8:J:4:PRO:HA	2.26	0.50
6:H:41:ASP:HB3	6:H:121:LEU:HD22	1.93	0.50
1:A:705:LYS:HE3	1:A:713:SER:CB	2.41	0.50
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.41	0.50
1:A:49:LYS:NZ	1:A:60:SER:HA	2.26	0.50
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.44	0.50
2:B:902:GLY:O	10:L:65:VAL:HG11	2.11	0.50
1:A:965:GLN:HA	1:A:968:GLN:HG2	1.93	0.50
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.44	0.50
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.41	0.50
2:B:313:MET:HG3	2:B:390:LEU:HD21	1.94	0.50
1:A:794:PRO:HA	1:A:797:LYS:HB2	1.93	0.50
10:L:34:CYS:O	10:L:35:SER:HB2	2.10	0.50
1:A:351:THR:CG2	1:A:352:VAL:H	2.18	0.50
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.77	0.50
2:B:957:ASN:HB3	2:B:961:LEU:HB2	1.92	0.50
1:A:76:GLU:CD	2:B:1159:ARG:HH12	2.15	0.50
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.41	0.50
1:A:658:LEU:HD22	2:B:831:SER:HA	1.92	0.50
9:K:32:VAL:HB	9:K:74:ARG:HG3	1.93	0.50
4:E:113:GLN:HB3	4:E:137:GLU:OE1	2.11	0.50
1:A:1116:LEU:CD2	1:A:1329:THR:CG2	2.64	0.50
1:A:285:PRO:O	1:A:286:HIS:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ILE:HD11	1:A:428:TYR:CE2	2.47	0.50
1:A:99:ILE:HG12	1:A:234:MET:SD	2.51	0.50
1:A:1061:GLY:O	1:A:1062:GLU:C	2.50	0.50
2:B:62:ILE:HD12	2:B:418:LYS:HE2	1.94	0.50
2:B:647:GLY:O	2:B:648:HIS:O	2.30	0.50
1:A:1166:ASP:CG	1:A:1194:ARG:HH21	2.15	0.50
4:E:3:GLN:HG2	4:E:5:ASN:H	1.76	0.50
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.11	0.50
2:B:176:SER:O	2:B:182:SER:CB	2.60	0.50
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.93	0.50
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.12	0.50
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.12	0.50
4:E:165:LEU:HD13	4:E:170:LEU:O	2.11	0.50
9:K:6:ARG:O	9:K:8:GLU:N	2.45	0.50
1:A:880:LYS:O	1:A:880:LYS:HG2	2.12	0.50
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.94	0.50
2:B:864:LYS:CG	2:B:865:LYS:N	2.36	0.50
1:A:590:ARG:HG2	1:A:591:PHE:H	1.77	0.50
11:R:3:C:H2'	11:R:4:G:C8	2.46	0.50
1:A:765:VAL:HG21	1:A:800:VAL:CG1	2.41	0.50
2:B:648:HIS:O	2:B:649:LYS:O	2.30	0.50
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.10	0.50
1:A:184:SER:HA	1:A:199:LEU:HD13	1.93	0.50
1:A:100:LYS:O	1:A:104:GLU:HG3	2.12	0.50
2:B:863:GLU:O	2:B:864:LYS:O	2.30	0.49
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.42	0.49
2:B:840:ILE:HB	2:B:1011:ILE:HD12	1.93	0.49
2:B:1168:LEU:HD21	2:B:1214:PRO:HD2	1.93	0.49
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.12	0.49
1:A:909:ASP:OD1	1:A:911:SER:HB3	2.11	0.49
6:H:109:LYS:HB3	6:H:110:ASP:C	2.31	0.49
1:A:666:ILE:HG23	2:B:1026:LEU:HD12	1.94	0.49
1:A:672:ASP:N	1:A:736:ASN:HD21	2.11	0.49
6:H:59:ILE:O	6:H:60:ALA:HB3	2.12	0.49
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.43	0.49
2:B:982:SER:O	2:B:1093:GLN:HG3	2.12	0.49
1:A:273:ASN:C	1:A:275:SER:H	2.15	0.49
2:B:1074:ASN:OD1	2:B:1076:HIS:N	2.45	0.49
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.93	0.49
5:F:83:PRO:HG2	5:F:84:TYR:HD1	1.77	0.49
1:A:902:LEU:CG	1:A:926:GLN:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1060:ARG:C	2:B:1062:HIS:N	2.65	0.49
1:A:527:THR:HG21	1:A:650:GLN:HG2	1.92	0.49
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.94	0.49
2:B:565:PRO:HB2	2:B:567:GLU:OE2	2.13	0.49
1:A:1134:ILE:O	1:A:1138:ILE:CG1	2.61	0.49
1:A:100:LYS:HD3	1:A:104:GLU:OE1	2.12	0.49
1:A:314:ALA:HA	1:A:320:ARG:HA	1.95	0.49
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.13	0.49
1:A:605:MET:HE3	1:A:606:LEU:H	1.77	0.49
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.27	0.49
2:B:807:ARG:CG	2:B:807:ARG:HH11	2.17	0.49
1:A:777:PHE:HD2	1:A:782:ARG:CA	2.25	0.49
2:B:515:HIS:H	2:B:518:HIS:HD2	1.58	0.49
1:A:500:GLU:HG2	2:B:1143:ALA:HB1	1.94	0.49
1:A:711:ARG:HH12	7:I:95:THR:HB	1.77	0.49
5:F:114:GLU:OE2	5:F:119:ARG:HG2	2.12	0.49
1:A:290:GLU:HA	1:A:293:GLU:HG3	1.93	0.49
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.95	0.49
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.77	0.49
7:I:35:VAL:CG1	7:I:36:GLU:N	2.76	0.49
2:B:745:PRO:O	2:B:747:MET:N	2.46	0.49
1:A:962:ARG:O	1:A:963:ILE:C	2.51	0.49
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.93	0.49
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.48	0.49
1:A:1111:MET:SD	1:A:1114:PRO:HB3	2.50	0.49
1:A:406:ILE:HD13	1:A:431:LYS:CB	2.42	0.49
12:T:16:DC:C6	12:T:17:DG:C8	3.01	0.49
2:B:211:VAL:HG12	2:B:212:LEU:N	2.27	0.49
6:H:80:ARG:O	6:H:81:PRO:O	2.30	0.49
1:A:991:LYS:O	1:A:994:GLN:HB3	2.11	0.49
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.94	0.49
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.95	0.49
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.95	0.49
1:A:316:GLN:O	1:A:316:GLN:HG2	2.11	0.49
1:A:1364:ASN:HD22	1:A:1364:ASN:C	2.15	0.49
2:B:1149:GLU:HG3	2:B:1153:GLU:CG	2.30	0.49
8:J:7:CYS:CB	8:J:49:MET:HE3	2.43	0.49
2:B:566:LEU:HD22	2:B:586:TRP:O	2.13	0.49
2:B:310:MET:O	2:B:313:MET:HB2	2.13	0.49
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.95	0.49
1:A:672:ASP:N	1:A:736:ASN:ND2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	1.95	0.49
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.77	0.49
1:A:579:SER:HB3	1:A:611:GLN:HA	1.94	0.49
1:A:18:GLN:HG3	1:A:228:PHE:HE1	1.78	0.49
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.48	0.49
8:J:45:CYS:O	8:J:48:ARG:HG3	2.13	0.49
1:A:252:PHE:CD1	1:A:252:PHE:C	2.85	0.49
2:B:592:ASN:H	2:B:593:PRO:HD3	1.78	0.49
1:A:544:ASP:N	1:A:544:ASP:OD1	2.46	0.49
2:B:174:LEU:O	2:B:175:ARG:CB	2.60	0.49
4:E:78:LEU:HD12	4:E:107:THR:HB	1.95	0.49
1:A:472:LEU:CD2	2:B:835:GLN:HB3	2.41	0.49
1:A:1397:LEU:O	1:A:1400:CYS:HB2	2.12	0.49
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.13	0.49
1:A:822:GLU:O	1:A:826:ASP:CG	2.51	0.49
1:A:451:HIS:HB3	1:A:453:MET:N	2.28	0.49
1:A:483:ASP:OD1	11:R:11:U:P	2.71	0.49
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.35	0.48
1:A:249:SER:O	1:A:250:ILE:CG2	2.60	0.48
1:A:791:ASP:OD1	1:A:793:SER:OG	2.30	0.48
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.95	0.48
7:I:19:ASP:HB3	7:I:24:ARG:H	1.78	0.48
8:J:15:GLY:C	8:J:17:LYS:H	2.16	0.48
1:A:32:VAL:HB	1:A:57:ARG:HB3	1.95	0.48
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.32	0.48
5:F:80:ALA:O	5:F:81:THR:C	2.51	0.48
1:A:947:PHE:CZ	4:E:203:GLU:HA	2.48	0.48
1:A:755:PHE:O	1:A:758:ILE:N	2.46	0.48
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.43	0.48
1:A:206:GLU:O	1:A:210:ILE:HG12	2.13	0.48
2:B:292:ILE:HD11	2:B:327:ARG:HG2	1.95	0.48
2:B:864:LYS:NZ	2:B:867:GLY:CA	2.75	0.48
1:A:367:PRO:HG3	1:A:466:SER:C	2.34	0.48
2:B:483:LEU:O	2:B:484:ASN:HB2	2.13	0.48
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.48	0.48
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.13	0.48
2:B:209:GLU:OE2	2:B:485:ARG:HD2	2.14	0.48
1:A:410:GLY:O	1:A:411:ASP:O	2.30	0.48
2:B:124:TYR:HH	2:B:179:CYS:HG	1.60	0.48
6:H:109:LYS:HB3	6:H:110:ASP:CA	2.43	0.48
1:A:396:PRO:O	1:A:397:ASN:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HD23	1:A:316:GLN:CB	2.43	0.48
2:B:639:ILE:HG22	2:B:640:VAL:N	2.27	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.96	0.48
10:L:48:CYS:SG	10:L:49:LYS:N	2.85	0.48
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.96	0.48
1:A:464:PRO:HG2	9:K:67:PHE:CE1	2.49	0.48
1:A:446:ARG:HE	1:A:480:ALA:CB	2.24	0.48
4:E:205:SER:O	4:E:207:ARG:N	2.47	0.48
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.96	0.48
1:A:18:GLN:HE21	1:A:1418:LEU:HD13	1.78	0.48
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.12	0.48
4:E:35:VAL:C	4:E:37:LEU:H	2.17	0.48
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.48	0.48
1:A:815:PHE:O	1:A:818:MET:N	2.46	0.48
3:C:31:ASN:O	3:C:33:LEU:N	2.47	0.48
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.96	0.48
1:A:53:LEU:O	1:A:56:PRO:HD2	2.13	0.48
7:I:71:SER:HB3	7:I:85:PHE:HE2	1.78	0.48
1:A:364:VAL:O	1:A:364:VAL:HG13	2.13	0.48
6:H:38:LEU:HD12	6:H:124:ARG:O	2.14	0.48
2:B:476:ARG:O	2:B:478:GLY:N	2.47	0.48
1:A:787:PHE:CE2	1:A:796:SER:HB2	2.48	0.48
2:B:329:THR:HA	2:B:332:ASP:HB2	1.96	0.48
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.48	0.48
2:B:235:SER:OG	2:B:236:HIS:CD2	2.66	0.48
4:E:108:GLY:HA3	4:E:132:ILE:HG12	1.96	0.48
4:E:12:LEU:HG	4:E:12:LEU:O	2.13	0.48
3:C:249:ASP:O	3:C:253:LYS:HG3	2.12	0.48
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.96	0.48
1:A:545:GLN:O	1:A:546:VAL:C	2.52	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.95	0.48
1:A:320:ARG:HB2	1:A:321:PRO:CB	2.43	0.48
1:A:254:GLU:HA	1:A:255:SER:HA	1.64	0.48
1:A:1215:ARG:O	1:A:1218:GLN:HB2	2.14	0.48
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.96	0.48
1:A:596:THR:C	1:A:598:LEU:N	2.67	0.48
1:A:650:GLN:HB3	1:A:654:ASN:ND2	2.29	0.48
1:A:928:LEU:HA	1:A:931:GLU:HB3	1.96	0.48
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.78	0.48
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.48	0.48
11:R:3:C:H2'	11:R:4:G:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:3:VAL:CG2	8:J:18:TRP:CG	2.97	0.47
2:B:485:ARG:NH1	2:B:485:ARG:HG2	2.27	0.47
1:A:455:MET:HE1	2:B:1130:PHE:HE1	1.78	0.47
3:C:167:HIS:HD2	3:C:169:LYS:N	2.09	0.47
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.29	0.47
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.49	0.47
2:B:745:PRO:C	2:B:747:MET:N	2.64	0.47
2:B:745:PRO:C	2:B:747:MET:H	2.16	0.47
1:A:608:ILE:CG1	1:A:613:ILE:HG13	2.44	0.47
7:I:106:CYS:O	7:I:108:HIS:N	2.47	0.47
4:E:112:TYR:O	4:E:137:GLU:HG3	2.14	0.47
6:H:80:ARG:HB3	6:H:81:PRO:HD2	1.95	0.47
1:A:1100:ARG:HH21	1:A:1351:GLU:HG3	1.79	0.47
3:C:148:ARG:O	3:C:151:GLN:HG3	2.14	0.47
2:B:361:LEU:CD2	2:B:377:PHE:HD2	2.27	0.47
1:A:518:LYS:CB	1:A:519:PRO:HD2	2.44	0.47
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.44	0.47
1:A:445:ASN:HD21	1:A:447:GLN:HE21	1.62	0.47
1:A:755:PHE:O	1:A:757:ASN:N	2.48	0.47
2:B:633:VAL:O	2:B:694:ASP:HB2	2.14	0.47
2:B:773:MET:C	2:B:775:LYS:N	2.66	0.47
3:C:196:ASP:O	3:C:200:GLU:HB2	2.14	0.47
2:B:416:LEU:CD2	2:B:457:LEU:HD23	2.43	0.47
3:C:18:VAL:O	3:C:231:ASN:HA	2.15	0.47
6:H:104:PHE:N	6:H:104:PHE:CD1	2.82	0.47
6:H:43:ASN:ND2	6:H:46:LEU:HD12	2.30	0.47
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.96	0.47
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.45	0.47
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.78	0.47
2:B:424:LEU:O	2:B:428:ILE:HG12	2.13	0.47
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.96	0.47
5:F:125:LEU:C	5:F:127:GLU:H	2.16	0.47
2:B:563:MET:HG3	2:B:563:MET:O	2.13	0.47
1:A:367:PRO:HB3	1:A:466:SER:HA	1.96	0.47
1:A:567:LYS:NZ	6:H:97:MET:HG2	2.29	0.47
2:B:777:ALA:HA	2:B:1095:LEU:HD23	1.97	0.47
1:A:385:ILE:HD11	1:A:428:TYR:CZ	2.49	0.47
2:B:779:GLY:O	2:B:795:ILE:HA	2.15	0.47
1:A:294:SER:O	1:A:298:PHE:HB2	2.15	0.47
9:K:49:GLU:C	9:K:51:LEU:N	2.68	0.47
1:A:556:TRP:CZ2	1:A:560:ILE:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CE1	1:A:462:VAL:HG21	2.49	0.47
1:A:130:ASP:O	1:A:132:LYS:N	2.48	0.47
2:B:365:THR:OG1	2:B:367:LEU:HG	2.14	0.47
5:F:109:VAL:CG1	5:F:110:ASP:H	2.17	0.47
1:A:1059:HIS:CE1	5:F:87:LYS:H	2.32	0.47
8:J:53:HIS:HE1	8:J:55:ASP:OD1	1.96	0.47
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.14	0.47
1:A:1111:MET:HG3	1:A:1114:PRO:CD	2.44	0.47
1:A:1407:GLU:O	1:A:1411:GLU:HG2	2.15	0.47
1:A:535:THR:CG2	1:A:616:VAL:HA	2.44	0.47
2:B:577:ALA:HB1	2:B:589:VAL:HG13	1.96	0.47
2:B:260:GLY:O	2:B:267:ARG:HD3	2.14	0.47
1:A:1104:ILE:HD13	1:A:1332:PHE:CE2	2.50	0.47
2:B:957:ASN:ND2	2:B:958:GLN:N	2.63	0.47
1:A:276:LEU:CD1	1:A:292:ALA:CB	2.91	0.47
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.50	0.47
6:H:84:ALA:C	6:H:86:ASP:H	2.18	0.47
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.28	0.47
2:B:805:THR:HG21	2:B:815:ARG:HD3	1.96	0.47
1:A:700:ASN:ND2	7:I:116:ASN:HD21	2.13	0.47
7:I:32:CYS:SG	7:I:34:TYR:CB	3.03	0.47
9:K:92:ASN:O	9:K:95:ILE:N	2.47	0.47
1:A:929:LEU:HD21	1:A:983:ILE:HG23	1.95	0.47
1:A:1025:ARG:HG3	1:A:1030:ARG:NH1	2.30	0.47
1:A:1072:ILE:HG22	1:A:1072:ILE:O	2.14	0.47
1:A:947:PHE:CD2	1:A:954:TRP:NE1	2.82	0.47
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.12	0.47
1:A:951:GLU:OE2	1:A:951:GLU:HA	2.14	0.47
2:B:708:GLU:HG3	2:B:709:ASP:N	2.24	0.47
2:B:552:MET:O	2:B:555:ILE:HB	2.15	0.47
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.96	0.47
1:A:848:ILE:O	1:A:1065:GLY:N	2.37	0.47
3:C:185:LYS:CE	3:C:211:ASP:O	2.63	0.47
4:E:168:TYR:CB	4:E:170:LEU:HD11	2.45	0.47
2:B:45:SER:OG	2:B:46:GLN:N	2.48	0.47
1:A:133:LYS:HA	1:A:136:ALA:HB3	1.97	0.47
1:A:590:ARG:O	1:A:591:PHE:HD1	1.95	0.47
1:A:446:ARG:HH12	1:A:448:PRO:HD2	1.79	0.47
2:B:1013:ASN:C	2:B:1015:HIS:H	2.19	0.47
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.29	0.47
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1039:GLY:HA2	8:J:51:LEU:HD22	1.96	0.47
6:H:76:THR:O	6:H:77:ARG:O	2.33	0.47
1:A:809:THR:H	1:A:812:GLU:HB2	1.81	0.46
1:A:805:LEU:HD21	2:B:1052:VAL:HG21	1.96	0.46
1:A:947:PHE:CE2	1:A:954:TRP:CE2	3.04	0.46
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.51	0.46
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.45	0.46
1:A:700:ASN:HD22	7:I:116:ASN:HD21	1.64	0.46
9:K:102:LYS:O	9:K:106:GLU:HG2	2.15	0.46
1:A:583:PRO:O	1:A:610:GLY:HA2	2.15	0.46
1:A:320:ARG:N	1:A:320:ARG:HH11	2.13	0.46
1:A:407:ARG:HA	1:A:430:TRP:CD1	2.50	0.46
1:A:286:HIS:O	1:A:288:ALA:N	2.42	0.46
2:B:592:ASN:H	2:B:593:PRO:CD	2.27	0.46
2:B:769:TYR:O	2:B:772:ALA:N	2.49	0.46
2:B:814:PHE:C	2:B:816:GLU:N	2.67	0.46
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.61	0.46
2:B:519:TRP:C	2:B:519:TRP:CD1	2.88	0.46
2:B:490:SER:OG	2:B:491:THR:N	2.48	0.46
12:T:27:DA:N3	12:T:28:DT:H5'	2.31	0.46
1:A:55:ASP:O	1:A:56:PRO:C	2.52	0.46
9:K:40:HIS:HE1	9:K:63:VAL:HG22	1.78	0.46
1:A:741:ASN:ND2	1:A:744:LYS:H	1.95	0.46
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.81	0.46
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.96	0.46
2:B:586:TRP:NE1	2:B:588:GLY:O	2.48	0.46
2:B:573:GLN:O	2:B:575:PRO:HD3	2.16	0.46
2:B:541:LEU:HB2	2:B:747:MET:HE1	1.97	0.46
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.28	0.46
1:A:591:PHE:HD2	1:A:595:THR:HB	1.80	0.46
3:C:102:GLN:HA	3:C:153:LEU:O	2.16	0.46
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.46
6:H:22:LYS:HD3	6:H:45:GLU:OE1	2.16	0.46
2:B:451:LYS:O	2:B:452:THR:C	2.53	0.46
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.64	0.46
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.98	0.46
1:A:549:MET:O	1:A:552:TRP:HB2	2.16	0.46
1:A:609:ASP:C	1:A:611:GLN:H	2.19	0.46
1:A:1325:THR:HA	4:E:147:HIS:HA	1.97	0.46
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.97	0.46
4:E:175:LEU:HB2	4:E:213:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.53	0.46
7:I:40:SER:HB2	7:I:41:PRO:CD	2.45	0.46
1:A:68:GLN:C	1:A:70:CYS:H	2.18	0.46
1:A:252:PHE:CD1	1:A:252:PHE:O	2.69	0.46
1:A:37:PHE:HB2	1:A:52:GLY:CA	2.44	0.46
1:A:93:VAL:HG21	1:A:304:MET:HB3	1.97	0.46
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.81	0.46
1:A:793:SER:O	1:A:794:PRO:C	2.54	0.46
1:A:360:GLU:O	1:A:363:GLN:HB2	2.16	0.46
2:B:199:MET:N	2:B:199:MET:SD	2.82	0.46
8:J:6:ARG:HG2	8:J:13:VAL:HA	1.98	0.46
1:A:403:LYS:HB2	1:A:404:TYR:CD1	2.50	0.46
12:T:13:DA:H61	13:N:2:DT:H71	1.79	0.46
1:A:755:PHE:O	1:A:756:ILE:C	2.54	0.46
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.80	0.46
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.13	0.46
1:A:997:LEU:O	1:A:1053:PHE:CE2	2.68	0.46
2:B:221:ASN:OD1	2:B:242:SER:HA	2.16	0.46
1:A:573:SER:N	1:A:576:GLN:HG3	2.07	0.46
1:A:857:ARG:HA	1:A:864:ILE:HG12	1.97	0.46
2:B:862:GLN:HE21	2:B:961:LEU:HD13	1.81	0.46
1:A:239:LEU:CD1	1:A:240:PRO:HD2	2.35	0.46
2:B:555:ILE:CD1	2:B:587:HIS:CE1	2.99	0.46
5:F:83:PRO:O	5:F:151:LEU:HD23	2.16	0.46
8:J:32:GLU:CD	8:J:32:GLU:N	2.68	0.46
2:B:600:LEU:HD12	2:B:615:MET:SD	2.56	0.46
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.51	0.46
2:B:1023:VAL:O	2:B:1024:ALA:C	2.54	0.46
1:A:322:VAL:CA	1:A:323:LYS:HD3	2.46	0.46
2:B:34:ILE:HD13	2:B:542:MET:CE	2.45	0.46
1:A:67:CYS:O	1:A:70:CYS:SG	2.74	0.46
2:B:681:TRP:O	2:B:684:LEU:HB2	2.16	0.46
1:A:442:VAL:CG1	1:A:491:VAL:HG22	2.45	0.46
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.79	0.46
3:C:33:LEU:HG	3:C:37:MET:CE	2.46	0.46
1:A:839:ARG:O	1:A:843:LYS:HB2	2.16	0.46
2:B:603:LEU:O	2:B:608:ASP:N	2.48	0.46
1:A:303:TYR:CD1	1:A:303:TYR:O	2.68	0.46
1:A:251:SER:HB2	11:R:1:A:N3	2.31	0.46
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.98	0.46
1:A:774:ARG:NH2	1:A:794:PRO:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:O	1:A:598:LEU:N	2.48	0.46
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.36	0.46
3:C:101:LEU:HD21	3:C:113:VAL:HG11	1.98	0.46
2:B:370:PHE:CD2	2:B:373:ARG:HG3	2.51	0.46
1:A:629:LEU:CD2	1:A:633:VAL:HG21	2.46	0.46
1:A:332:LYS:O	1:A:334:GLY:N	2.48	0.46
3:C:43:THR:HG23	3:C:44:LEU:H	1.80	0.46
2:B:615:MET:HG2	2:B:626:ILE:HG23	1.98	0.46
1:A:968:GLN:O	1:A:968:GLN:HG3	2.16	0.46
10:L:60:ARG:HG3	10:L:61:THR:N	2.31	0.46
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.80	0.46
10:L:26:THR:O	10:L:26:THR:HG22	2.16	0.46
1:A:1362:TYR:C	1:A:1362:TYR:CD1	2.87	0.46
8:J:6:ARG:HA	8:J:12:LYS:O	2.15	0.45
2:B:175:ARG:CG	2:B:175:ARG:NH1	2.77	0.45
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.16	0.45
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.31	0.45
2:B:288:ALA:O	2:B:331:LEU:HD11	2.16	0.45
1:A:694:THR:HA	1:A:714:PHE:CE1	2.50	0.45
1:A:412:ARG:HH22	2:B:1108:ARG:NH2	2.13	0.45
1:A:585:GLY:N	1:A:609:ASP:OD1	2.40	0.45
1:A:396:PRO:O	1:A:398:GLU:O	2.34	0.45
1:A:140:THR:HA	1:A:143:LYS:HE3	1.98	0.45
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.98	0.45
1:A:315:LEU:CB	1:A:317:LYS:H	2.26	0.45
1:A:590:ARG:HG2	1:A:591:PHE:N	2.31	0.45
2:B:955:THR:CG2	2:B:956:THR:N	2.58	0.45
8:J:8:PHE:H	8:J:49:MET:HE3	1.80	0.45
1:A:185:TRP:HZ3	1:A:200:ARG:HB3	1.81	0.45
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.16	0.45
7:I:40:SER:HB2	7:I:41:PRO:HD3	1.97	0.45
2:B:208:SER:OG	2:B:210:LYS:HE2	2.16	0.45
1:A:922:ASP:OD1	1:A:923:LEU:N	2.46	0.45
2:B:274:PRO:O	2:B:275:TYR:HB2	2.16	0.45
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.76	0.45
1:A:482:PHE:HB2	2:B:836:GLU:O	2.17	0.45
10:L:38:LEU:HD21	10:L:49:LYS:HG2	1.98	0.45
2:B:95:ILE:HG13	2:B:129:PHE:O	2.16	0.45
1:A:1235:LYS:HG2	1:A:1237:ILE:HD11	1.98	0.45
6:H:26:ILE:N	6:H:40:LEU:O	2.50	0.45
2:B:763:GLN:O	2:B:766:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:GLN:O	1:A:839:ARG:C	2.55	0.45
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.17	0.45
4:E:67:GLU:O	4:E:70:SER:HB3	2.17	0.45
4:E:169:ARG:HG3	5:F:140:ASP:HB3	1.97	0.45
2:B:190:TYR:CD2	8:J:62:ARG:HB3	2.52	0.45
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.49	0.45
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.98	0.45
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.98	0.45
7:I:111:THR:HG22	7:I:112:SER:N	2.32	0.45
2:B:515:HIS:CD2	2:B:517:THR:H	2.34	0.45
2:B:589:VAL:CG1	2:B:590:HIS:H	2.30	0.45
2:B:800:GLN:HG2	8:J:52:THR:HG22	1.98	0.45
2:B:430:ARG:CD	2:B:434:ARG:HH22	2.29	0.45
7:I:32:CYS:SG	7:I:34:TYR:HB2	2.57	0.45
1:A:1392:SER:O	1:A:1394:THR:N	2.48	0.45
1:A:495:GLU:O	1:A:498:ARG:HG3	2.17	0.45
1:A:320:ARG:H	1:A:320:ARG:HH11	1.64	0.45
2:B:796:LEU:HB3	2:B:799:PRO:CD	2.22	0.45
1:A:575:LYS:CG	1:A:612:ILE:HD11	2.47	0.45
1:A:99:ILE:HG13	1:A:99:ILE:H	1.49	0.45
1:A:661:GLY:CA	2:B:1081:LEU:HD22	2.46	0.45
10:L:61:THR:HG21	10:L:63:ARG:HG3	1.98	0.45
4:E:48:ASP:HB3	4:E:54:GLN:HB2	1.97	0.45
2:B:48:LEU:O	2:B:49:ASP:C	2.55	0.45
1:A:699:ALA:O	1:A:701:LEU:N	2.49	0.45
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.98	0.45
2:B:1148:LYS:O	2:B:1152:MET:CB	2.62	0.45
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.43	0.45
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.98	0.45
2:B:575:PRO:C	2:B:577:ALA:H	2.19	0.45
2:B:779:GLY:C	2:B:795:ILE:HG23	2.37	0.45
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.98	0.45
1:A:550:LEU:HD13	1:A:550:LEU:HA	1.79	0.45
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.16	0.45
7:I:62:ILE:C	7:I:64:SER:H	2.19	0.45
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.32	0.45
1:A:391:LEU:O	1:A:394:ASN:N	2.49	0.45
2:B:1149:GLU:CG	2:B:1153:GLU:HG2	2.33	0.45
2:B:361:LEU:N	2:B:362:PRO:HD3	2.32	0.45
1:A:672:ASP:HB2	1:A:736:ASN:ND2	2.28	0.45
1:A:545:GLN:HB3	1:A:549:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ARG:O	2:B:984:HIS:CD2	2.70	0.45
1:A:412:ARG:NH2	2:B:1108:ARG:NH2	2.65	0.45
2:B:737:THR:O	2:B:738:PHE:C	2.56	0.45
2:B:319:GLU:C	2:B:321:GLY:H	2.19	0.45
12:T:26:DG:C2	12:T:27:DA:C8	3.05	0.45
12:T:13:DA:H61	13:N:2:DT:H73	1.77	0.45
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.99	0.45
3:C:99:LEU:CD2	3:C:99:LEU:N	2.79	0.45
1:A:1117:THR:N	1:A:1328:TYR:O	2.50	0.45
12:T:9:DA:C5	12:T:10:DA:C6	3.05	0.45
1:A:324:SER:O	1:A:327:ALA:N	2.49	0.45
2:B:647:GLY:O	2:B:648:HIS:C	2.55	0.45
1:A:68:GLN:O	1:A:70:CYS:N	2.50	0.45
1:A:1342:GLU:CG	4:E:212:ARG:HH11	2.25	0.45
1:A:239:LEU:HD12	1:A:240:PRO:N	2.31	0.45
1:A:746:MET:HG2	1:A:751:SER:OG	2.17	0.45
1:A:557:ASP:HA	9:K:26:LYS:CE	2.45	0.45
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.34	0.45
2:B:321:GLY:C	2:B:323:VAL:H	2.21	0.45
1:A:219:PHE:CE1	1:A:230:ARG:HG2	2.52	0.45
10:L:25:ALA:N	10:L:27:LEU:HD22	2.32	0.45
3:C:56:THR:CG2	3:C:145:CYS:SG	2.95	0.45
2:B:1006:ILE:HG22	2:B:1087:PHE:HZ	1.82	0.45
2:B:845:SER:HB2	8:J:8:PHE:HB3	1.99	0.45
2:B:1027:ILE:C	2:B:1029:CYS:N	2.69	0.45
1:A:587:HIS:HA	1:A:607:ILE:O	2.17	0.45
5:F:111:LEU:N	5:F:111:LEU:CD1	2.79	0.45
2:B:202:TYR:H	2:B:202:TYR:HD2	1.63	0.45
1:A:768:GLN:CG	1:A:816:HIS:HA	2.47	0.45
2:B:773:MET:C	2:B:775:LYS:H	2.20	0.45
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.17	0.45
2:B:870:ILE:O	2:B:870:ILE:HG22	2.16	0.44
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.38	0.44
1:A:382:PRO:N	1:A:428:TYR:HE2	2.14	0.44
1:A:629:LEU:HD23	1:A:633:VAL:HG21	1.99	0.44
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.98	0.44
4:E:108:GLY:O	4:E:132:ILE:HG23	2.17	0.44
12:T:9:DA:C6	12:T:10:DA:N1	2.85	0.44
12:T:18:DA:H2'	12:T:19:DT:C6	2.52	0.44
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.34	0.44
11:R:3:C:N4	12:T:26:DG:H1	2.08	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.32	0.44
1:A:81:PHE:HE2	1:A:240:PRO:HB2	1.83	0.44
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.33	0.44
1:A:550:LEU:HD12	1:A:556:TRP:CD1	2.52	0.44
1:A:881:GLN:CD	1:A:959:ASN:HA	2.37	0.44
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.52	0.44
6:H:97:MET:HB2	6:H:118:PHE:CD2	2.52	0.44
5:F:81:THR:O	5:F:82:THR:C	2.55	0.44
1:A:575:LYS:HG2	1:A:612:ILE:HD11	1.99	0.44
1:A:445:ASN:CB	1:A:455:MET:HG2	2.46	0.44
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.99	0.44
2:B:859:TYR:CD1	2:B:859:TYR:N	2.86	0.44
1:A:1067:LEU:HD12	1:A:1071:SER:OG	2.18	0.44
3:C:251:LEU:HG	9:K:98:LEU:HD11	1.99	0.44
2:B:329:THR:HA	2:B:332:ASP:HB3	1.98	0.44
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.83	0.44
2:B:405:ARG:HA	2:B:631:GLY:O	2.16	0.44
6:H:57:VAL:HG22	6:H:144:ILE:HG12	1.99	0.44
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.15	0.44
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.98	0.44
1:A:774:ARG:NH1	1:A:797:LYS:HD2	2.32	0.44
1:A:599:SER:OG	1:A:614:PHE:CD1	2.66	0.44
1:A:423:ASP:C	1:A:424:ILE:HG13	2.37	0.44
2:B:552:MET:N	2:B:553:PRO:HD2	2.33	0.44
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.62	0.44
1:A:1030:ARG:O	1:A:1031:VAL:C	2.55	0.44
1:A:947:PHE:HD2	1:A:954:TRP:CE2	2.36	0.44
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.98	0.44
3:C:29:MET:O	3:C:30:ALA:C	2.55	0.44
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.99	0.44
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.00	0.44
11:R:6:G:H2'	11:R:7:A:H8	1.83	0.44
1:A:343:LYS:NZ	2:B:1156:ASP:OD2	2.50	0.44
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.45	0.44
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.53	0.44
2:B:44:VAL:O	2:B:45:SER:C	2.55	0.44
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.00	0.44
8:J:36:LEU:HD23	8:J:36:LEU:HA	1.85	0.44
4:E:184:VAL:O	4:E:187:TYR:N	2.50	0.44
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.47	0.44
1:A:1340:GLY:O	1:A:1342:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.99	0.44
2:B:273:LEU:HD11	2:B:285:ILE:HD12	2.00	0.44
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.98	0.44
5:F:116:ASP:HB3	5:F:119:ARG:CB	2.47	0.44
9:K:83:PRO:O	9:K:86:ALA:HB3	2.18	0.44
1:A:315:LEU:N	1:A:315:LEU:HD22	2.33	0.44
1:A:466:SER:HB3	9:K:2:ASN:ND2	2.33	0.44
1:A:32:VAL:HB	1:A:57:ARG:HB2	2.00	0.44
4:E:176:PRO:O	4:E:212:ARG:HA	2.18	0.44
1:A:341:MET:HE1	1:A:843:LYS:HZ1	1.82	0.44
1:A:336:ILE:HA	1:A:340:LEU:HD12	2.00	0.44
3:C:131:HIS:HA	3:C:132:PRO:HD2	1.92	0.44
1:A:353:ILE:HD11	1:A:481:ASP:O	2.18	0.44
2:B:843:GLN:N	2:B:994:TYR:O	2.43	0.44
1:A:809:THR:O	1:A:812:GLU:HB2	2.18	0.44
1:A:53:LEU:HB3	1:A:54:ASN:H	1.52	0.44
1:A:474:VAL:HG22	1:A:478:TYR:CE1	2.53	0.44
2:B:881:ASN:CB	2:B:933:SER:N	2.80	0.44
2:B:999:MET:HG2	2:B:1008:PRO:HD2	2.00	0.44
2:B:791:THR:O	2:B:792:MET:CB	2.66	0.44
1:A:219:PHE:CZ	1:A:230:ARG:HG2	2.53	0.44
1:A:1080:THR:HG22	1:A:1081:LEU:N	2.33	0.44
1:A:265:LYS:HD2	1:A:303:TYR:CB	2.48	0.43
1:A:352:VAL:CG1	1:A:353:ILE:N	2.81	0.43
1:A:463:ILE:HB	1:A:464:PRO:CD	2.47	0.43
2:B:956:THR:CA	2:B:961:LEU:O	2.63	0.43
1:A:526:ASP:OD2	2:B:829:CYS:HB3	2.18	0.43
2:B:1051:THR:HB	2:B:1054:GLY:H	1.82	0.43
4:E:199:ILE:CG2	4:E:199:ILE:O	2.65	0.43
2:B:806:THR:H	2:B:809:MET:HG3	1.83	0.43
2:B:542:MET:SD	2:B:636:PRO:HG3	2.58	0.43
2:B:1103:ILE:H	2:B:1103:ILE:CD1	2.29	0.43
12:T:25:DC:H2'	12:T:26:DG:H8	1.83	0.43
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.53	0.43
2:B:766:ARG:HA	2:B:769:TYR:CD1	2.52	0.43
8:J:56:LEU:O	8:J:57:ILE:C	2.54	0.43
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.17	0.43
1:A:962:ARG:C	1:A:964:ILE:N	2.69	0.43
1:A:315:LEU:N	1:A:315:LEU:CD1	2.63	0.43
1:A:256:GLN:CA	1:A:257:ARG:CB	2.38	0.43
2:B:1118:PRO:HD3	2:B:1155:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:LEU:HD11	1:A:758:ILE:HG21	2.01	0.43
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.18	0.43
1:A:102:VAL:HB	1:A:211:PHE:HZ	1.83	0.43
1:A:815:PHE:O	1:A:816:HIS:C	2.56	0.43
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.53	0.43
7:I:96:SER:HB2	7:I:98:VAL:HG23	2.00	0.43
2:B:1033:LYS:O	2:B:1036:ALA:HB3	2.18	0.43
1:A:809:THR:CB	1:A:810:PRO:HD2	2.47	0.43
1:A:402:ALA:O	1:A:415:LEU:HD13	2.19	0.43
8:J:7:CYS:HA	8:J:49:MET:HE3	2.00	0.43
1:A:250:ILE:O	1:A:251:SER:CB	2.64	0.43
1:A:667:GLY:HA2	1:A:670:ILE:HG12	2.00	0.43
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.84	0.43
5:F:76:LYS:O	5:F:79:ARG:CD	2.67	0.43
1:A:709:THR:HB	1:A:712:GLU:HG3	2.00	0.43
1:A:1379:GLY:O	4:E:179:GLN:HG2	2.18	0.43
2:B:202:TYR:N	2:B:202:TYR:CD2	2.84	0.43
7:I:75:CYS:HB3	7:I:110:PHE:HE2	1.82	0.43
5:F:125:LEU:O	5:F:127:GLU:N	2.51	0.43
1:A:1261:LYS:C	1:A:1263:ILE:N	2.72	0.43
1:A:389:THR:OG1	1:A:426:LEU:HD12	2.19	0.43
2:B:333:PHE:O	2:B:333:PHE:CG	2.72	0.43
2:B:701:ILE:HG12	2:B:702:LEU:N	2.34	0.43
1:A:729:ALA:HA	1:A:732:LEU:HB2	2.01	0.43
1:A:152:VAL:O	1:A:162:VAL:CG2	2.65	0.43
6:H:58:THR:CG2	6:H:59:ILE:N	2.79	0.43
1:A:1161:THR:CG2	1:A:1163:ILE:H	2.31	0.43
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.82	0.43
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.33	0.43
8:J:15:GLY:O	8:J:17:LYS:N	2.50	0.43
1:A:315:LEU:HB3	1:A:317:LYS:N	2.22	0.43
2:B:637:LEU:HD22	2:B:741:CYS:O	2.17	0.43
12:T:26:DG:N2	12:T:27:DA:H1'	2.34	0.43
3:C:41:ILE:HD11	3:C:243:VAL:HG13	2.01	0.43
2:B:763:GLN:HG2	2:B:764:SER:N	2.33	0.43
4:E:3:GLN:HG3	4:E:5:ASN:H	1.82	0.43
1:A:598:LEU:O	1:A:599:SER:C	2.57	0.43
4:E:136:ASN:OD1	4:E:137:GLU:N	2.50	0.43
7:I:32:CYS:SG	7:I:33:SER:N	2.91	0.43
2:B:697:GLU:O	2:B:698:GLU:C	2.56	0.43
2:B:1056:SER:CB	2:B:1066:SER:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:755:ILE:HA	2:B:755:ILE:HD13	1.86	0.43
1:A:924:LYS:HB2	1:A:924:LYS:NZ	2.33	0.43
1:A:130:ASP:C	1:A:132:LYS:N	2.71	0.43
2:B:981:ALA:CB	2:B:1095:LEU:HD11	2.49	0.43
7:I:99:LEU:HB2	7:I:101:PHE:CE1	2.53	0.43
2:B:108:VAL:CG1	2:B:109:THR:N	2.81	0.43
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.84	0.43
1:A:796:SER:O	1:A:796:SER:OG	2.31	0.43
1:A:943:LEU:C	1:A:945:GLU:N	2.72	0.43
2:B:1056:SER:HB3	2:B:1066:SER:O	2.18	0.43
7:I:50:THR:HG22	7:I:52:ILE:HG22	2.00	0.43
4:E:26:ARG:HD3	4:E:188:LEU:HA	2.01	0.43
1:A:508:PRO:O	1:A:511:ILE:HG13	2.18	0.43
6:H:102:TYR:HE2	6:H:116:TYR:C	2.22	0.43
1:A:686:ALA:O	1:A:690:VAL:HG23	2.18	0.43
1:A:590:ARG:HB3	1:A:605:MET:N	2.34	0.43
11:R:5:A:N3	11:R:6:G:C8	2.87	0.43
1:A:1364:ASN:ND2	1:A:1366:ARG:N	2.55	0.43
2:B:126:SER:O	2:B:169:ARG:HA	2.19	0.43
9:K:43:GLY:HA3	9:K:71:PHE:CE1	2.54	0.43
1:A:172:PRO:HB3	1:A:183:GLY:HA3	2.01	0.43
2:B:481:GLN:HB2	2:B:494:HIS:HE1	1.83	0.43
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.33	0.43
1:A:787:PHE:CD1	1:A:796:SER:HB2	2.53	0.43
2:B:394:ASP:OD2	7:I:91:ARG:HB3	2.18	0.43
6:H:9:ILE:HG12	6:H:56:THR:HG23	2.01	0.43
10:L:68:GLU:HG3	10:L:68:GLU:H	1.57	0.43
1:A:343:LYS:NZ	2:B:1156:ASP:HB2	2.34	0.43
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.19	0.43
10:L:46:VAL:HG12	10:L:47:ARG:H	1.83	0.43
7:I:17:ARG:HG2	7:I:18:GLU:N	2.21	0.43
2:B:40:GLU:OE2	2:B:681:TRP:HB3	2.19	0.43
2:B:95:ILE:HA	2:B:129:PHE:O	2.19	0.43
1:A:1072:ILE:HD11	1:A:1368:MET:CA	2.47	0.43
2:B:1084:GLN:N	2:B:1084:GLN:CD	2.72	0.43
1:A:700:ASN:HD22	7:I:116:ASN:ND2	2.16	0.43
2:B:104:GLU:HG2	2:B:104:GLU:H	1.66	0.43
2:B:637:LEU:O	2:B:690:VAL:HG13	2.19	0.43
7:I:69:PRO:HG2	7:I:85:PHE:CE1	2.53	0.43
1:A:1059:HIS:CE1	5:F:86:THR:HA	2.53	0.43
2:B:1168:LEU:HB3	2:B:1169:MET:H	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:ARG:HD3	2:B:566:LEU:HD23	2.01	0.43
3:C:182:PRO:HG3	3:C:206:ASN:O	2.18	0.43
1:A:1398:MET:O	1:A:1401:SER:N	2.44	0.43
3:C:30:ALA:O	3:C:33:LEU:HB3	2.19	0.43
1:A:922:ASP:O	1:A:923:LEU:HG	2.19	0.43
12:T:19:DT:H2'	12:T:20:DC:O4'	2.19	0.43
1:A:982:THR:C	1:A:984:LYS:N	2.71	0.43
1:A:106:VAL:HG11	1:A:214:ILE:HD11	2.00	0.42
2:B:1149:GLU:HG2	2:B:1153:GLU:HB2	2.01	0.42
2:B:555:ILE:HD12	2:B:587:HIS:CE1	2.53	0.42
1:A:902:LEU:H	1:A:902:LEU:HG	1.69	0.42
3:C:76:ASP:OD2	3:C:128:ASN:HB3	2.19	0.42
9:K:78:THR:HG22	9:K:79:GLU:N	2.34	0.42
7:I:21:GLU:H	7:I:21:GLU:HG3	1.62	0.42
2:B:637:LEU:HD23	2:B:742:GLU:OE2	2.18	0.42
3:C:115:SER:HB3	3:C:142:VAL:HG12	2.01	0.42
1:A:282:ASN:HB3	1:A:283:GLY:H	1.60	0.42
4:E:16:PHE:O	4:E:19:VAL:N	2.51	0.42
3:C:180:TYR:O	3:C:181:ASP:HB3	2.19	0.42
2:B:92:PHE:HB3	2:B:130:VAL:HG11	2.01	0.42
2:B:195:CYS:CB	2:B:782:LEU:HD22	2.49	0.42
8:J:1:MET:O	8:J:2:ILE:O	2.37	0.42
1:A:1134:ILE:H	1:A:1134:ILE:HG13	1.51	0.42
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.84	0.42
4:E:12:LEU:HD22	4:E:55:ARG:NH2	2.34	0.42
9:K:102:LYS:O	9:K:106:GLU:CG	2.67	0.42
1:A:1146:VAL:O	1:A:1197:LEU:HD23	2.19	0.42
2:B:458:LYS:O	2:B:462:ALA:HB2	2.18	0.42
2:B:976:ILE:HD11	2:B:992:ILE:HA	2.02	0.42
1:A:805:LEU:HD12	1:A:806:ARG:N	2.35	0.42
8:J:7:CYS:HB2	8:J:49:MET:HE3	2.01	0.42
1:A:913:LEU:HG	1:A:915:SER:H	1.84	0.42
1:A:416:ARG:H	1:A:416:ARG:HG2	1.52	0.42
1:A:1025:ARG:CG	1:A:1025:ARG:NH1	2.77	0.42
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.54	0.42
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.35	0.42
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.54	0.42
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.83	0.42
2:B:551:PRO:O	2:B:554:ILE:HB	2.20	0.42
1:A:919:ILE:O	1:A:920:LEU:C	2.57	0.42
2:B:1207:LEU:HD23	2:B:1207:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:GLY:HA2	3:C:172:PRO:HD3	1.73	0.42
1:A:332:LYS:H	1:A:337:ARG:CB	2.33	0.42
2:B:332:ASP:C	2:B:334:ILE:H	2.22	0.42
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.02	0.42
9:K:61:TYR:HA	9:K:72:LYS:O	2.19	0.42
1:A:44:THR:O	1:A:45:GLN:HB2	2.20	0.42
1:A:1336:MET:CE	1:A:1380:GLY:HA2	2.49	0.42
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.51	0.42
4:E:114:ASN:O	4:E:115:ASN:HB3	2.19	0.42
1:A:1390:ASN:ND2	1:A:1402:PHE:HB3	2.35	0.42
1:A:535:THR:HG21	1:A:617:VAL:H	1.84	0.42
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.02	0.42
6:H:26:ILE:CG2	6:H:40:LEU:HB3	2.49	0.42
1:A:332:LYS:C	1:A:334:GLY:N	2.71	0.42
9:K:57:LEU:HD12	9:K:76:GLN:HG2	2.01	0.42
1:A:219:PHE:HB3	1:A:224:PHE:HB2	2.00	0.42
2:B:840:ILE:HG23	2:B:992:ILE:HG22	2.02	0.42
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.19	0.42
1:A:885:THR:OG1	1:A:1024:SER:HB3	2.20	0.42
1:A:1072:ILE:HD11	1:A:1368:MET:HG2	2.01	0.42
2:B:1020:ARG:HG2	2:B:1020:ARG:H	1.64	0.42
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.78	0.42
1:A:954:TRP:HE3	1:A:955:PRO:HD2	1.84	0.42
1:A:756:ILE:O	1:A:760:GLN:HG3	2.19	0.42
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	2.01	0.42
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.34	0.42
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.84	0.42
9:K:63:VAL:HG23	9:K:63:VAL:O	2.19	0.42
1:A:442:VAL:HG12	1:A:491:VAL:HG22	2.01	0.42
2:B:276:ILE:CG2	2:B:277:LYS:N	2.83	0.42
1:A:1067:LEU:HD12	1:A:1067:LEU:C	2.40	0.42
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.54	0.42
2:B:461:LEU:HD12	2:B:461:LEU:HA	1.97	0.42
1:A:253:ASN:HB2	1:A:256:GLN:CA	2.48	0.42
1:A:346:ASP:N	2:B:1154:ALA:HB1	2.24	0.42
2:B:534:GLY:O	2:B:537:LYS:HD3	2.20	0.42
1:A:848:ILE:HD13	1:A:858:ASN:HB3	2.01	0.42
2:B:58:THR:O	2:B:62:ILE:HG12	2.20	0.42
2:B:594:ALA:HB2	7:I:61:ASP:OD1	2.20	0.42
2:B:874:PHE:CD2	2:B:914:LYS:HB3	2.55	0.42
2:B:43:LEU:HD11	2:B:811:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:LEU:O	1:A:1315:GLU:N	2.53	0.42
1:A:602:ASP:HB3	1:A:616:VAL:HG23	2.01	0.42
4:E:100:ILE:HG12	4:E:105:PHE:HD1	1.83	0.42
1:A:408:ASP:C	1:A:410:GLY:N	2.73	0.42
1:A:833:GLU:O	1:A:834:THR:C	2.58	0.42
2:B:801:LYS:O	8:J:52:THR:HG23	2.20	0.42
1:A:996:ASN:C	1:A:998:LEU:N	2.73	0.42
9:K:7:PHE:C	9:K:9:LEU:N	2.74	0.42
10:L:34:CYS:O	10:L:35:SER:CB	2.68	0.42
6:H:77:ARG:O	6:H:78:SER:C	2.57	0.42
3:C:131:HIS:O	3:C:132:PRO:C	2.57	0.42
9:K:3:ALA:HA	9:K:4:PRO:HD3	1.93	0.42
9:K:4:PRO:HG2	9:K:4:PRO:O	2.20	0.42
12:T:11:DG:N2	13:N:5:DT:O2	2.53	0.42
1:A:1271:ILE:HG22	1:A:1273:LEU:HD12	2.01	0.42
1:A:884:ASP:OD2	1:A:884:ASP:N	2.50	0.42
2:B:708:GLU:O	2:B:710:LEU:N	2.53	0.42
2:B:762:ASN:HD21	2:B:1022:THR:HA	1.85	0.42
1:A:841:LEU:O	1:A:845:LEU:HG	2.20	0.42
3:C:10:ILE:HG21	3:C:13:ALA:HB2	2.01	0.42
10:L:32:ALA:HB3	10:L:55:ILE:HD12	2.02	0.42
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.85	0.42
1:A:582:ILE:HA	1:A:583:PRO:HD3	1.75	0.42
1:A:1191:TRP:HB3	1:A:1260:LEU:HD22	2.01	0.42
2:B:1099:VAL:H	2:B:1099:VAL:HG23	1.55	0.41
1:A:566:ILE:O	1:A:567:LYS:O	2.37	0.41
2:B:899:ILE:HD11	2:B:911:ILE:CG1	2.40	0.41
2:B:1096:ARG:HG3	2:B:1097:HIS:N	2.35	0.41
2:B:1147:LEU:O	2:B:1151:LEU:HB2	2.20	0.41
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.48	0.41
1:A:675:THR:C	1:A:679:ILE:HD12	2.40	0.41
6:H:23:VAL:HG21	6:H:121:LEU:HD21	2.01	0.41
2:B:1138:MET:HG3	2:B:1146:PHE:CE2	2.55	0.41
2:B:430:ARG:HD3	2:B:434:ARG:NH2	2.34	0.41
3:C:78:GLU:OE1	3:C:246:ARG:HD3	2.19	0.41
1:A:1238:ILE:HG22	1:A:1240:CYS:SG	2.60	0.41
6:H:39:THR:O	6:H:123:MET:HA	2.20	0.41
1:A:512:VAL:HG13	1:A:512:VAL:O	2.20	0.41
1:A:215:SER:HB3	1:A:218:ASP:OD2	2.20	0.41
2:B:37:PHE:HD1	2:B:681:TRP:CE2	2.38	0.41
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:74:ILE:HA	5:F:74:ILE:HD13	1.90	0.41
2:B:65:GLU:CD	2:B:66:ASP:H	2.24	0.41
1:A:185:TRP:CZ3	1:A:200:ARG:HB3	2.55	0.41
1:A:826:ASP:N	1:A:826:ASP:OD2	2.45	0.41
6:H:123:MET:HE1	6:H:142:LEU:HD13	2.02	0.41
1:A:225:ASN:O	1:A:227:VAL:N	2.53	0.41
1:A:567:LYS:HB3	6:H:95:TYR:HA	2.01	0.41
2:B:377:PHE:O	2:B:380:TYR:N	2.51	0.41
2:B:956:THR:HB	10:L:46:VAL:HG21	2.03	0.41
1:A:518:LYS:CB	1:A:519:PRO:CD	2.99	0.41
1:A:1059:HIS:ND1	5:F:87:LYS:HG2	2.35	0.41
2:B:778:MET:HE1	2:B:853:SER:HB3	2.01	0.41
1:A:1166:ASP:OD1	1:A:1194:ARG:NH2	2.44	0.41
3:C:41:ILE:HG13	3:C:172:PRO:CG	2.48	0.41
2:B:99:LYS:HA	2:B:100:PRO:HD2	1.76	0.41
4:E:191:LYS:HE3	4:E:191:LYS:HB2	1.84	0.41
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.41
1:A:551:TYR:OH	9:K:32:VAL:HG21	2.21	0.41
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.20	0.41
12:T:9:DA:C6	12:T:10:DA:C6	3.08	0.41
2:B:412:LEU:O	2:B:413:LEU:C	2.57	0.41
2:B:639:ILE:CG2	2:B:640:VAL:N	2.83	0.41
2:B:911:ILE:O	2:B:912:ILE:HG13	2.20	0.41
1:A:1021:LEU:O	1:A:1023:ARG:N	2.54	0.41
2:B:710:LEU:O	2:B:711:GLU:HB3	2.21	0.41
2:B:554:ILE:O	2:B:555:ILE:C	2.59	0.41
1:A:794:PRO:O	1:A:796:SER:N	2.54	0.41
2:B:658:ILE:O	2:B:661:LEU:HB2	2.20	0.41
2:B:386:LEU:C	2:B:388:CYS:N	2.74	0.41
2:B:516:ASN:ND2	2:B:516:ASN:H	2.17	0.41
1:A:423:ASP:HB3	1:A:424:ILE:H	1.26	0.41
2:B:1033:LYS:N	2:B:1089:PRO:HG2	2.35	0.41
4:E:124:VAL:H	4:E:125:PRO:CD	2.34	0.41
2:B:1200:ALA:O	2:B:1201:LYS:C	2.57	0.41
6:H:93:TYR:CD2	6:H:145:ARG:HD3	2.56	0.41
2:B:384:ARG:HH22	2:B:621:GLU:CG	2.32	0.41
4:E:165:LEU:HD22	4:E:165:LEU:HA	1.90	0.41
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.68	0.41
1:A:609:ASP:O	1:A:611:GLN:N	2.53	0.41
1:A:232:GLU:HG2	1:A:233:TRP:CD1	2.56	0.41
1:A:278:THR:HG22	1:A:278:THR:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.21	0.41
1:A:353:ILE:HG13	1:A:485:ASP:O	2.20	0.41
1:A:809:THR:HB	1:A:810:PRO:CD	2.51	0.41
4:E:59:SER:O	4:E:79:TRP:CH2	2.73	0.41
2:B:129:PHE:HE2	2:B:166:PHE:HB2	1.79	0.41
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.91	0.41
4:E:63:ASN:HB3	4:E:64:PRO:HD3	1.99	0.41
5:F:93:ILE:HD11	5:F:134:ILE:HD11	2.03	0.41
3:C:31:ASN:C	3:C:33:LEU:N	2.73	0.41
8:J:36:LEU:O	8:J:41:LEU:HB2	2.21	0.41
1:A:1080:THR:HG22	1:A:1081:LEU:H	1.84	0.41
2:B:309:GLN:OE1	7:I:52:ILE:HG23	2.21	0.41
1:A:1414:ALA:C	1:A:1416:ALA:H	2.24	0.41
1:A:345:VAL:HA	2:B:1118:PRO:HG2	2.02	0.41
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.79	0.41
1:A:446:ARG:HD3	1:A:478:TYR:O	2.20	0.41
1:A:406:ILE:HG22	1:A:407:ARG:N	2.36	0.41
2:B:879:ARG:HB2	2:B:880:THR:H	1.33	0.41
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.02	0.41
8:J:2:ILE:O	8:J:2:ILE:CG2	2.69	0.41
2:B:276:ILE:HG22	2:B:277:LYS:N	2.36	0.41
1:A:911:SER:O	1:A:978:PRO:HB3	2.21	0.41
5:F:125:LEU:C	5:F:127:GLU:N	2.74	0.41
7:I:33:SER:O	7:I:34:TYR:C	2.59	0.41
2:B:60:GLN:O	2:B:63:ILE:HG22	2.20	0.41
1:A:274:ILE:HG22	1:A:274:ILE:O	2.21	0.41
2:B:638:PHE:CD1	2:B:743:ILE:HD13	2.56	0.41
1:A:805:LEU:CD1	1:A:806:ARG:N	2.82	0.41
1:A:68:GLN:O	1:A:68:GLN:CD	2.59	0.41
1:A:1349:TYR:O	1:A:1350:LYS:C	2.59	0.41
4:E:179:GLN:O	4:E:182:ASP:HB2	2.21	0.41
1:A:1261:LYS:C	1:A:1263:ILE:H	2.24	0.41
2:B:248:SER:HB3	2:B:249:ARG:H	1.65	0.41
1:A:844:ALA:HB2	1:A:1389:PHE:CZ	2.56	0.41
2:B:520:GLY:HA3	2:B:635:ARG:CD	2.51	0.41
1:A:214:ILE:HA	1:A:214:ILE:HD13	1.84	0.41
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.56	0.41
2:B:1158:PHE:CD2	2:B:1198:TYR:HD1	2.38	0.41
1:A:1408:ILE:O	1:A:1412:ALA:HB2	2.20	0.41
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.56	0.41
2:B:999:MET:HB3	2:B:1007:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:PRO:C	1:A:956:LEU:HG	2.41	0.41
2:B:1131:GLY:O	2:B:1132:GLU:C	2.58	0.41
1:A:335:ARG:HE	1:A:335:ARG:HA	1.86	0.41
2:B:519:TRP:O	2:B:519:TRP:HD1	2.02	0.41
3:C:33:LEU:HG	3:C:37:MET:HE3	2.03	0.41
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	2.02	0.41
2:B:1053:GLU:HB3	2:B:1057:LYS:HE3	2.02	0.41
2:B:1055:ILE:HD13	2:B:1055:ILE:HA	1.94	0.41
2:B:975:GLN:CG	2:B:976:ILE:N	2.78	0.41
2:B:1155:SER:OG	2:B:1156:ASP:N	2.53	0.41
9:K:40:HIS:CE1	9:K:63:VAL:CG2	3.03	0.41
7:I:111:THR:CG2	7:I:112:SER:N	2.84	0.41
1:A:384:ASN:O	1:A:385:ILE:C	2.59	0.41
2:B:762:ASN:HD22	2:B:763:GLN:H	1.69	0.41
6:H:91:ASP:CG	6:H:91:ASP:O	2.59	0.41
2:B:655:LYS:O	2:B:658:ILE:HG22	2.21	0.41
5:F:73:ALA:O	5:F:74:ILE:HG12	2.21	0.41
1:A:965:GLN:HG3	1:A:965:GLN:H	1.65	0.41
2:B:62:ILE:HG23	2:B:418:LYS:HG2	2.03	0.41
5:F:75:PRO:O	5:F:77:ASP:O	2.39	0.41
1:A:590:ARG:CG	1:A:591:PHE:H	2.33	0.40
11:R:6:G:N3	11:R:7:A:C8	2.90	0.40
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.67	0.40
1:A:532:ARG:O	1:A:535:THR:N	2.50	0.40
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.20	0.40
1:A:929:LEU:CD2	1:A:983:ILE:CG2	2.99	0.40
1:A:381:THR:HG22	1:A:384:ASN:CG	2.41	0.40
1:A:491:VAL:O	1:A:493:GLN:NE2	2.54	0.40
6:H:82:PRO:C	6:H:84:ALA:H	2.25	0.40
1:A:598:LEU:HD13	6:H:25:ARG:HH12	1.86	0.40
10:L:53:HIS:O	10:L:55:ILE:N	2.50	0.40
9:K:108:GLU:O	9:K:109:TRP:C	2.59	0.40
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.03	0.40
7:I:119:THR:O	7:I:120:GLN:HG2	2.21	0.40
1:A:214:ILE:HG22	1:A:215:SER:O	2.22	0.40
1:A:32:VAL:HB	1:A:57:ARG:HD2	2.02	0.40
12:T:17:DG:N3	12:T:17:DG:H2'	2.36	0.40
3:C:46:ILE:CD1	3:C:72:LEU:HD11	2.51	0.40
2:B:859:TYR:CZ	2:B:941:LEU:HD22	2.55	0.40
1:A:794:PRO:O	1:A:795:GLU:C	2.59	0.40
3:C:31:ASN:O	3:C:34:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:OG	2:B:236:HIS:HD2	2.03	0.40
1:A:1053:PHE:O	1:A:1055:ARG:N	2.53	0.40
2:B:205:ILE:O	2:B:208:SER:N	2.48	0.40
2:B:487:THR:O	2:B:488:TYR:C	2.59	0.40
1:A:664:THR:OG1	2:B:1014:PRO:HB2	2.21	0.40
1:A:444:PHE:O	1:A:478:TYR:CE2	2.75	0.40
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.90	0.40
1:A:666:ILE:HG23	2:B:1026:LEU:CD1	2.52	0.40
13:N:2:DT:O2	13:N:2:DT:H2'	2.22	0.40
3:C:76:ASP:O	3:C:79:GLN:HG2	2.22	0.40
2:B:99:LYS:HB3	2:B:180:TYR:CE2	2.56	0.40
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.56	0.40
7:I:15:TYR:N	7:I:15:TYR:CD1	2.89	0.40
1:A:265:LYS:C	1:A:267:ALA:N	2.53	0.40
2:B:839:MET:O	2:B:990:ILE:HA	2.21	0.40
2:B:992:ILE:HG21	2:B:994:TYR:CE2	2.56	0.40
2:B:291:ILE:CG2	2:B:297:ILE:HD13	2.50	0.40
1:A:442:VAL:O	1:A:457:ALA:HA	2.21	0.40
2:B:115:GLN:O	2:B:119:LEU:HD12	2.21	0.40
1:A:1048:ASN:O	1:A:1049:ILE:C	2.60	0.40
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.55	0.40
1:A:1404:GLU:HB3	1:A:1407:GLU:HG2	2.02	0.40
2:B:287:ARG:HA	2:B:291:ILE:O	2.20	0.40
3:C:46:ILE:H	3:C:46:ILE:HG12	1.58	0.40
3:C:46:ILE:HD12	3:C:157:CYS:HB3	2.02	0.40
8:J:35:ALA:O	8:J:39:LEU:CD1	2.62	0.40
2:B:821:GLN:HE22	2:B:851:PHE:H	1.69	0.40
2:B:745:PRO:O	2:B:748:ILE:HG12	2.22	0.40
2:B:426:LYS:HG3	2:B:430:ARG:HH12	1.87	0.40
1:A:1049:ILE:O	1:A:1050:GLU:C	2.60	0.40
4:E:117:THR:HA	4:E:118:PRO:HD2	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1383/1733 (80%)	1038 (75%)	233 (17%)	112 (8%)	1	19
2	B	1088/1224 (89%)	822 (76%)	188 (17%)	78 (7%)	1	23
3	C	264/318 (83%)	209 (79%)	48 (18%)	7 (3%)	6	47
4	E	212/215 (99%)	162 (76%)	39 (18%)	11 (5%)	2	31
5	F	82/155 (53%)	65 (79%)	13 (16%)	4 (5%)	3	32
6	H	129/146 (88%)	97 (75%)	21 (16%)	11 (8%)	1	17
7	I	117/122 (96%)	83 (71%)	25 (21%)	9 (8%)	1	20
8	J	63/70 (90%)	45 (71%)	14 (22%)	4 (6%)	2	27
9	K	112/120 (93%)	89 (80%)	16 (14%)	7 (6%)	2	27
10	L	44/70 (63%)	24 (54%)	9 (20%)	11 (25%)	0	1
All	All	3494/4173 (84%)	2634 (75%)	606 (17%)	254 (7%)	1	22

All (254) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	54	ASN
1	A	55	ASP
1	A	56	PRO
1	A	93	VAL
1	A	130	ASP
1	A	162	VAL
1	A	214	ILE
1	A	248	PRO
1	A	250	ILE
1	A	251	SER
1	A	253	ASN
1	A	257	ARG
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	325	ILE
1	A	331	GLY
1	A	399	HIS
1	A	402	ALA
1	A	411	ASP
1	A	428	TYR

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Mol	Chain	Res	Type
1	A	567	LYS
1	A	568	PRO
1	A	591	PHE
1	A	700	ASN
1	A	846	GLU
1	A	998	LEU
1	A	1036	ARG
1	A	1255	GLU
1	A	1393	ASN
2	B	100	PRO
2	B	176	SER
2	B	229	ALA
2	B	249	ARG
2	B	436	VAL
2	B	466	TRP
2	B	477	ALA
2	B	484	ASN
2	B	531	GLN
2	B	592	ASN
2	B	636	PRO
2	B	648	HIS
2	B	649	LYS
2	B	650	GLU
2	B	711	GLU
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	831	SER
2	B	864	LYS
2	B	865	LYS
2	B	981	ALA
2	B	1046	PRO
2	B	1157	ALA
2	B	1181	GLU
3	C	142	VAL
3	C	149	LYS
3	C	227	THR
4	E	3	GLN
4	E	59	SER
4	E	172	GLU
4	E	173	SER
5	F	74	ILE

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Mol	Chain	Res	Type
6	H	77	ARG
6	H	81	PRO
6	H	140	ALA
7	I	20	LYS
7	I	47	GLU
7	I	107	SER
8	J	2	ILE
8	J	6	ARG
9	K	71	PHE
10	L	26	THR
10	L	35	SER
1	A	50	ILE
1	A	68	GLN
1	A	226	GLU
1	A	266	LEU
1	A	312	PRO
1	A	313	GLN
1	A	409	SER
1	A	472	LEU
1	A	515	GLN
1	A	517	ASN
1	A	592	ASP
1	A	597	LEU
1	A	610	GLY
1	A	756	ILE
1	A	972	HIS
1	A	986	ILE
1	A	1048	ASN
1	A	1054	LEU
1	A	1341	ILE
1	A	1388	GLY
1	A	1399	ARG
2	B	53	GLN
2	B	58	THR
2	B	475	SER
2	B	516	ASN
2	B	540	SER
2	B	708	GLU
2	B	709	ASP
2	B	1028	GLU
2	B	1166	CYS
2	B	1176	ASN

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Mol	Chain	Res	Type
3	C	110	THR
4	E	192	ARG
4	E	206	GLY
5	F	81	THR
6	H	32	THR
6	H	82	PRO
6	H	85	GLY
6	H	134	ASN
7	I	21	GLU
7	I	34	TYR
7	I	86	PHE
8	J	16	ASP
9	K	81	TYR
10	L	54	ARG
10	L	55	ILE
10	L	64	LEU
1	A	69	THR
1	A	76	GLU
1	A	89	PRO
1	A	128	ILE
1	A	131	SER
1	A	167	CYS
1	A	178	GLY
1	A	282	ASN
1	A	424	ILE
1	A	593	GLU
1	A	708	MET
1	A	755	PHE
1	A	810	PRO
1	A	895	LYS
1	A	903	ASN
1	A	922	ASP
1	A	957	PRO
1	A	963	ILE
1	A	1022	LEU
1	A	1062	GLU
1	A	1188	GLN
1	A	1223	ASP
1	A	1261	LYS
1	A	1270	ASN
1	A	1274	ARG
1	A	1314	SER

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Mol	Chain	Res	Type
1	A	1327	ILE
1	A	1398	MET
1	A	1435	PRO
2	B	21	GLU
2	B	67	SER
2	B	248	SER
2	B	333	PHE
2	B	555	ILE
2	B	563	MET
2	B	738	PHE
2	B	879	ARG
2	B	881	ASN
2	B	958	GLN
2	B	1047	PHE
2	B	1156	ASP
2	B	1167	GLY
2	B	1201	LYS
3	C	215	GLU
4	E	36	GLU
5	F	73	ALA
5	F	126	ALA
6	H	62	SER
7	I	54	GLU
9	K	5	ASP
9	K	46	ILE
10	L	45	ALA
1	A	287	HIS
1	A	318	SER
1	A	404	TYR
1	A	484	GLY
1	A	923	LEU
1	A	994	GLN
1	A	1021	LEU
1	A	1221	LYS
1	A	1438	THR
2	B	45	SER
2	B	266	ALA
2	B	367	LEU
2	B	418	LYS
2	B	712	PRO
2	B	746	SER
2	B	876	LYS

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Mol	Chain	Res	Type
2	B	878	GLN
2	B	891	ASP
2	B	997	GLU
2	B	1186	ASP
2	B	1222	ARG
2	B	1223	ASP
4	E	124	VAL
6	H	43	ASN
6	H	90	ALA
9	K	7	PHE
10	L	37	LYS
10	L	59	ALA
1	A	87	ALA
1	A	274	ILE
1	A	332	LYS
1	A	335	ARG
1	A	418	SER
1	A	514	PRO
1	A	576	GLN
1	A	958	VAL
2	B	365	THR
2	B	483	LEU
2	B	488	TYR
2	B	791	THR
2	B	792	MET
2	B	799	PRO
2	B	1021	MET
2	B	1061	GLU
3	C	6	PRO
3	C	144	ILE
10	L	39	SER
10	L	56	LEU
1	A	367	PRO
1	A	546	VAL
1	A	583	PRO
1	A	795	GLU
1	A	1122	PRO
1	A	1424	VAL
2	B	575	PRO
2	B	613	VAL
2	B	647	GLY
2	B	1027	ILE

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Mol	Chain	Res	Type
2	B	1178	ASN
4	E	76	GLY
7	I	63	GLY
9	K	4	PRO
9	K	50	LEU
10	L	53	HIS
1	A	400	PRO
2	B	1017	ILE
4	E	51	GLY
8	J	33	GLY
1	A	829	VAL
1	A	1437	GLY
4	E	118	PRO
6	H	59	ILE
1	A	916	GLY
2	B	1103	ILE
2	B	1165	ILE
7	I	76	PRO
1	A	599	SER
1	A	1049	ILE
1	A	1107	VAL
1	A	321	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	
1	A	1218/1520 (80%)	987 (81%)	231 (19%)	2	14
2	B	960/1061 (90%)	790 (82%)	170 (18%)	2	18
3	C	234/274 (85%)	188 (80%)	46 (20%)	1	13
4	E	196/197 (100%)	164 (84%)	32 (16%)	3	22
5	F	74/137 (54%)	63 (85%)	11 (15%)	4	26
6	H	117/128 (91%)	97 (83%)	20 (17%)	2	19
7	I	113/116 (97%)	95 (84%)	18 (16%)	3	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	13
9	K	99/102 (97%)	81 (82%)	18 (18%)	2	16
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	9
All	All	3111/3657 (85%)	2544 (82%)	567 (18%)	2	16

All (567) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	8	SER
1	A	12	ARG
1	A	18	GLN
1	A	26	GLU
1	A	32	VAL
1	A	44	THR
1	A	47	ARG
1	A	58	LEU
1	A	60	SER
1	A	70	CYS
1	A	80	HIS
1	A	81	PHE
1	A	84	ILE
1	A	93	VAL
1	A	99	ILE
1	A	100	LYS
1	A	102	VAL
1	A	105	CYS
1	A	110	CYS
1	A	116	ASP
1	A	128	ILE
1	A	130	ASP
1	A	140	THR
1	A	162	VAL
1	A	169	ASN
1	A	170	THR
1	A	184	SER
1	A	185	TRP
1	A	199	LEU
1	A	206	GLU
1	A	208	LEU
1	A	215	SER

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Mol	Chain	Res	Type
1	A	221	SER
1	A	222	LEU
1	A	225	ASN
1	A	250	ILE
1	A	254	GLU
1	A	255	SER
1	A	257	ARG
1	A	266	LEU
1	A	270	LEU
1	A	287	HIS
1	A	295	LEU
1	A	297	GLN
1	A	303	TYR
1	A	304	MET
1	A	306	ASN
1	A	307	ASP
1	A	308	ILE
1	A	313	GLN
1	A	315	LEU
1	A	316	GLN
1	A	320	ARG
1	A	323	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	381	THR
1	A	394	ASN
1	A	403	LYS
1	A	406	ILE
1	A	413	ILE
1	A	416	ARG
1	A	419	LYS
1	A	423	ASP
1	A	424	ILE
1	A	434	ARG
1	A	436	ILE
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	453	MET

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Mol	Chain	Res	Type
1	A	454	SER
1	A	460	VAL
1	A	469	ARG
1	A	470	LEU
1	A	475	THR
1	A	481	ASP
1	A	485	ASP
1	A	486	GLU
1	A	498	ARG
1	A	513	SER
1	A	518	LYS
1	A	527	THR
1	A	534	LEU
1	A	550	LEU
1	A	552	TRP
1	A	566	ILE
1	A	576	GLN
1	A	595	THR
1	A	596	THR
1	A	599	SER
1	A	602	ASP
1	A	612	ILE
1	A	618	GLU
1	A	619	LYS
1	A	621	THR
1	A	625	SER
1	A	630	ILE
1	A	648	ASN
1	A	663	SER
1	A	666	ILE
1	A	672	ASP
1	A	680	THR
1	A	682	THR
1	A	687	LYS
1	A	702	LEU
1	A	705	LYS
1	A	720	ARG
1	A	728	LYS
1	A	732	LEU
1	A	740	LEU
1	A	752	LYS
1	A	764	CYS

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Mol	Chain	Res	Type
1	A	768	GLN
1	A	771	GLU
1	A	774	ARG
1	A	781	ASP
1	A	782	ARG
1	A	783	THR
1	A	788	SER
1	A	796	SER
1	A	797	LYS
1	A	801	GLU
1	A	803	SER
1	A	805	LEU
1	A	821	ARG
1	A	826	ASP
1	A	829	VAL
1	A	830	LYS
1	A	831	THR
1	A	838	GLN
1	A	855	THR
1	A	858	ASN
1	A	867	ILE
1	A	879	GLU
1	A	880	LYS
1	A	885	THR
1	A	886	ILE
1	A	895	LYS
1	A	896	ARG
1	A	897	TYR
1	A	902	LEU
1	A	905	ASP
1	A	907	THR
1	A	911	SER
1	A	918	GLU
1	A	924	LYS
1	A	929	LEU
1	A	949	ASP
1	A	969	GLN
1	A	982	THR
1	A	988	LEU
1	A	990	VAL
1	A	996	ASN
1	A	998	LEU

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Mol	Chain	Res	Type
1	A	1006	ILE
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1037	LEU
1	A	1048	ASN
1	A	1058	VAL
1	A	1067	LEU
1	A	1074	GLU
1	A	1081	LEU
1	A	1094	VAL
1	A	1095	THR
1	A	1110	ASN
1	A	1111	MET
1	A	1118	VAL
1	A	1120	LEU
1	A	1127	ASP
1	A	1128	GLN
1	A	1134	ILE
1	A	1135	ARG
1	A	1146	VAL
1	A	1160	SER
1	A	1161	THR
1	A	1165	GLU
1	A	1172	LEU
1	A	1173	HIS
1	A	1187	GLN
1	A	1193	LEU
1	A	1199	ARG
1	A	1217	LYS
1	A	1219	THR
1	A	1222	ASN
1	A	1231	ASP
1	A	1232	ASN
1	A	1235	LYS
1	A	1262	LYS
1	A	1264	GLU
1	A	1273	LEU
1	A	1274	ARG
1	A	1276	VAL
1	A	1280	GLU

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Mol	Chain	Res	Type
1	A	1281	ARG
1	A	1285	MET
1	A	1291	VAL
1	A	1299	VAL
1	A	1300	LYS
1	A	1301	GLU
1	A	1312	ASN
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1336	MET
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1355	VAL
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1394	THR
1	A	1398	MET
1	A	1400	CYS
1	A	1403	GLU
1	A	1405	THR
1	A	1407	GLU
1	A	1420	ASP
1	A	1425	SER
1	A	1428	VAL
2	B	28	GLU
2	B	40	GLU
2	B	66	ASP
2	B	67	SER
2	B	95	ILE
2	B	98	THR
2	B	104	GLU
2	B	106	ASP
2	B	109	THR
2	B	119	LEU
2	B	120	ARG
2	B	126	SER

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Mol	Chain	Res	Type
2	B	175	ARG
2	B	177	LYS
2	B	187	SER
2	B	188	ASP
2	B	199	MET
2	B	202	TYR
2	B	222	ILE
2	B	225	VAL
2	B	244	LEU
2	B	246	LYS
2	B	248	SER
2	B	249	ARG
2	B	261	ARG
2	B	264	SER
2	B	268	THR
2	B	283	VAL
2	B	313	MET
2	B	319	GLU
2	B	327	ARG
2	B	347	LYS
2	B	348	ARG
2	B	354	ASP
2	B	387	LEU
2	B	391	ASP
2	B	393	LYS
2	B	398	ARG
2	B	404	LYS
2	B	408	LEU
2	B	416	LEU
2	B	424	LEU
2	B	425	THR
2	B	426	LYS
2	B	427	ASP
2	B	429	PHE
2	B	432	MET
2	B	437	GLU
2	B	459	TYR
2	B	461	LEU
2	B	463	THR
2	B	468	GLU
2	B	473	MET
2	B	479	VAL

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Mol	Chain	Res	Type
2	B	482	VAL
2	B	483	LEU
2	B	487	THR
2	B	489	SER
2	B	490	SER
2	B	513	GLN
2	B	527	THR
2	B	537	LYS
2	B	542	MET
2	B	549	THR
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	582	VAL
2	B	591	ARG
2	B	595	ARG
2	B	600	LEU
2	B	614	SER
2	B	633	VAL
2	B	637	LEU
2	B	641	GLU
2	B	644	GLU
2	B	651	LEU
2	B	668	ASP
2	B	682	SER
2	B	694	ASP
2	B	701	ILE
2	B	705	MET
2	B	728	ARG
2	B	737	THR
2	B	740	HIS
2	B	742	GLU
2	B	751	VAL
2	B	762	ASN
2	B	764	SER
2	B	790	ASP
2	B	791	THR
2	B	794	ASN
2	B	800	GLN
2	B	807	ARG
2	B	812	LEU
2	B	822	ASN

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Mol	Chain	Res	Type
2	B	825	VAL
2	B	829	CYS
2	B	830	TYR
2	B	847	ASP
2	B	861	ASP
2	B	864	LYS
2	B	865	LYS
2	B	866	TYR
2	B	868	MET
2	B	869	SER
2	B	872	GLU
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	882	THR
2	B	883	LEU
2	B	886	LYS
2	B	892	LYS
2	B	895	ASP
2	B	899	ILE
2	B	905	VAL
2	B	906	SER
2	B	911	ILE
2	B	944	THR
2	B	951	GLN
2	B	953	LEU
2	B	957	ASN
2	B	959	ASP
2	B	971	THR
2	B	973	ILE
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	998	ASP
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1020	ARG
2	B	1022	THR
2	B	1028	GLU

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Mol	Chain	Res	Type
2	B	1050	ILE
2	B	1051	THR
2	B	1062	HIS
2	B	1077	THR
2	B	1082	MET
2	B	1090	THR
2	B	1093	GLN
2	B	1096	ARG
2	B	1098	MET
2	B	1099	VAL
2	B	1103	ILE
2	B	1113	VAL
2	B	1115	THR
2	B	1124	ARG
2	B	1132	GLU
2	B	1141	HIS
2	B	1145	SER
2	B	1147	LEU
2	B	1153	GLU
2	B	1159	ARG
2	B	1165	ILE
2	B	1166	CYS
2	B	1178	ASN
2	B	1183	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1218	THR
2	B	1219	ASP
2	B	1223	ASP
3	C	3	GLU
3	C	4	GLU
3	C	10	ILE
3	C	15	LYS
3	C	16	ASP
3	C	18	VAL
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG

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Mol	Chain	Res	Type
3	C	36	VAL
3	C	38	ILE
3	C	43	THR
3	C	49	VAL
3	C	56	THR
3	C	62	PHE
3	C	77	ILE
3	C	83	SER
3	C	89	GLU
3	C	93	ASP
3	C	99	LEU
3	C	102	GLN
3	C	119	VAL
3	C	129	ILE
3	C	132	PRO
3	C	134	ILE
3	C	137	LYS
3	C	140	ASN
3	C	142	VAL
3	C	143	LEU
3	C	145	CYS
3	C	151	GLN
3	C	163	ILE
3	C	165	LYS
3	C	166	GLU
3	C	183	TRP
3	C	195	GLN
3	C	196	ASP
3	C	203	GLN
3	C	215	GLU
3	C	227	THR
3	C	233	GLU
3	C	235	VAL
3	C	240	VAL
3	C	254	LYS
3	C	267	GLN
4	E	3	GLN
4	E	4	GLU
4	E	9	ILE
4	E	32	GLN
4	E	43	LYS
4	E	48	ASP

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Mol	Chain	Res	Type
4	E	61	GLN
4	E	63	ASN
4	E	65	THR
4	E	66	GLU
4	E	77	SER
4	E	78	LEU
4	E	83	CYS
4	E	92	THR
4	E	101	GLN
4	E	104	ASN
4	E	107	THR
4	E	110	PHE
4	E	119	SER
4	E	127	ILE
4	E	131	THR
4	E	134	THR
4	E	146	HIS
4	E	156	LEU
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	170	LEU
4	E	171	LYS
4	E	192	ARG
4	E	196	VAL
4	E	204	THR
5	F	74	ILE
5	F	77	ASP
5	F	79	ARG
5	F	90	ARG
5	F	97	ARG
5	F	111	LEU
5	F	112	GLU
5	F	114	GLU
5	F	120	ILE
5	F	123	LYS
5	F	133	VAL
6	H	2	SER
6	H	11	GLN
6	H	27	GLU
6	H	33	GLN
6	H	37	LYS

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Mol	Chain	Res	Type
6	H	54	SER
6	H	55	LEU
6	H	56	THR
6	H	80	ARG
6	H	86	ASP
6	H	87	ARG
6	H	89	LEU
6	H	95	TYR
6	H	102	TYR
6	H	104	PHE
6	H	110	ASP
6	H	121	LEU
6	H	132	LEU
6	H	136	LYS
6	H	139	ASN
7	I	3	THR
7	I	5	ARG
7	I	8	ARG
7	I	10	CYS
7	I	11	ASN
7	I	12	ASN
7	I	13	MET
7	I	28	GLU
7	I	30	ARG
7	I	37	GLU
7	I	50	THR
7	I	52	ILE
7	I	62	ILE
7	I	78	CYS
7	I	83	ASN
7	I	114	GLN
7	I	117	LYS
7	I	119	THR
8	J	7	CYS
8	J	9	SER
8	J	14	VAL
8	J	27	GLU
8	J	32	GLU
8	J	34	THR
8	J	38	ARG
8	J	42	LYS
8	J	43	ARG

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Mol	Chain	Res	Type
8	J	48	ARG
8	J	55	ASP
8	J	62	ARG
9	K	9	LEU
9	K	20	LYS
9	K	22	ASP
9	K	31	VAL
9	K	33	ILE
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	64	GLU
9	K	70	ARG
9	K	71	PHE
9	K	75	ILE
9	K	77	THR
9	K	79	GLU
9	K	81	TYR
9	K	107	THR
9	K	113	THR
9	K	114	LEU
10	L	31	CYS
10	L	46	VAL
10	L	51	CYS
10	L	55	ILE
10	L	61	THR
10	L	63	ARG
10	L	65	VAL
10	L	66	GLN
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	75	ASN
1	A	80	HIS
1	A	169	ASN
1	A	171	GLN
1	A	282	ASN
1	A	313	GLN
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	435	HIS
1	A	445	ASN
1	A	451	HIS
1	A	493	GLN
1	A	517	ASN
1	A	654	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	858	ASN
1	A	926	GLN
1	A	965	GLN
1	A	966	ASN
1	A	968	GLN
1	A	1033	GLN
1	A	1171	GLN
1	A	1173	HIS
1	A	1278	ASN
1	A	1312	ASN
1	A	1330	ASN
1	A	1364	ASN
1	A	1390	ASN
1	A	1432	GLN
2	B	47	GLN
2	B	121	ASN
2	B	236	HIS
2	B	433	GLN
2	B	465	ASN
2	B	484	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	734	HIS
2	B	744	HIS
2	B	762	ASN
2	B	794	ASN
2	B	822	ASN
2	B	834	ASN
2	B	862	GLN

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Mol	Chain	Res	Type
2	B	957	ASN
2	B	1015	HIS
2	B	1040	ASN
2	B	1065	GLN
2	B	1084	GLN
2	B	1179	GLN
2	B	1193	GLN
2	B	1211	ASN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	188	HIS
3	C	203	GLN
4	E	32	GLN
4	E	61	GLN
4	E	63	ASN
4	E	114	ASN
4	E	147	HIS
6	H	11	GLN
6	H	33	GLN
6	H	134	ASN
6	H	137	GLN
7	I	11	ASN
7	I	60	GLN
7	I	83	ASN
7	I	116	ASN
8	J	53	HIS
9	K	40	HIS
9	K	65	HIS
9	K	92	ASN
10	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/15 (73%)	3 (27%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	10	A
11	R	12	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1395/1733 (80%)	-0.34	13 (0%) 85 80	76, 116, 186, 214	0
2	B	1106/1224 (90%)	-0.37	3 (0%) 94 92	72, 109, 156, 180	0
3	C	266/318 (83%)	-0.50	0 100 100	83, 106, 145, 154	0
4	E	214/215 (99%)	-0.41	1 (0%) 91 88	104, 151, 192, 196	0
5	F	84/155 (54%)	-0.47	0 100 100	99, 123, 142, 147	0
6	H	133/146 (91%)	-0.21	1 (0%) 87 82	123, 143, 165, 167	0
7	I	119/122 (97%)	-0.43	0 100 100	113, 132, 150, 160	0
8	J	65/70 (92%)	-0.62	0 100 100	77, 94, 126, 131	0
9	K	114/120 (95%)	-0.45	0 100 100	87, 108, 124, 131	0
10	L	46/70 (65%)	-0.22	0 100 100	100, 161, 179, 181	0
11	R	12/15 (80%)	0.19	0 100 100	100, 128, 185, 192	0
12	T	28/28 (100%)	0.10	1 (3%) 46 36	102, 210, 322, 325	0
13	N	14/14 (100%)	0.48	1 (7%) 19 13	287, 311, 317, 318	0
All	All	3596/4230 (85%)	-0.37	20 (0%) 90 86	72, 116, 181, 325	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	5.2
1	A	1176	LEU	4.3
1	A	150	THR	3.9
1	A	153	PRO	3.2
12	T	3	DA	3.1
1	A	152	VAL	3.0
1	A	316	GLN	2.9
13	N	1	DC	2.9
1	A	151	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	2.7
2	B	250	PHE	2.5
2	B	1223	ASP	2.5
1	A	57	ARG	2.5
1	A	426	LEU	2.4
6	H	86	ASP	2.4
4	E	126	SER	2.4
1	A	145	LYS	2.3
1	A	115	LEU	2.2
1	A	311	GLN	2.2
2	B	865	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	ZN	C	319	1/1	1.00	0.05	-1.34	97,97,97,97	0
14	ZN	A	1735	1/1	0.97	0.07	-1.39	155,155,155,155	0
14	ZN	I	203	1/1	0.99	0.05	-1.44	123,123,123,123	0
14	ZN	B	1307	1/1	0.99	0.07	-1.51	158,158,158,158	0
14	ZN	I	204	1/1	0.99	0.05	-1.58	131,131,131,131	0
15	MG	A	1736	1/1	0.80	0.15	-1.85	92,92,92,92	0
14	ZN	A	1734	1/1	0.90	0.05	-2.28	212,212,212,212	0
14	ZN	J	101	1/1	0.99	0.12	-2.38	93,93,93,93	0
14	ZN	L	105	1/1	0.98	0.05	-	169,169,169,169	0

6.5 Other polymers [i](#)

There are no such residues in this entry.