



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:26 am GMT

PDB ID : 1Y1W
Title : Complete RNA Polymerase II elongation complex
Authors : Cramer, P.; Kettenberger, H.; Armache, K.-J.
Deposited on : 2004-11-19
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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

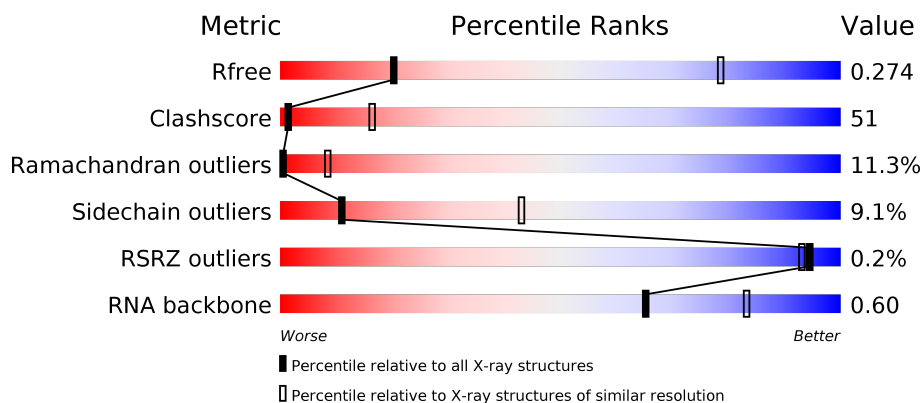
1 Overall quality at a glance

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}	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)
RNA backbone	2435	1026 (5.04-2.90)

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	T	19	<div> <div>5%</div> <div>32%</div> <div>68%</div> </div>
2	N	7	<div> <div>14%</div> <div>71%</div> <div>14%</div> </div>
3	P	10	<div> <div>80%</div> <div>10%</div> <div>10%</div> </div>
4	A	1733	<div> <div>25%</div> <div>45%</div> <div>10%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	D	221	
8	E	215	
9	F	155	
10	G	171	
11	H	146	
12	I	122	
13	J	70	
14	K	120	
15	L	70	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31802 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 DNA chain called 5'-D(P*AP*GP*TP*AP*CP*TP*TP*AP*CP*GP*CP*CP*TP*GP*GP*TP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	19	Total	C	N	O	P	21	0	0
			387	185	67	116	19			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*GP*TP*AP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	7	Total	C	N	O	P	20	0	0
			141	69	27	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			214	97	44	64	9			

- Molecule 4 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1112	Total	C	N	O	S	0	0	0
			8836	5594	1548	1639	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

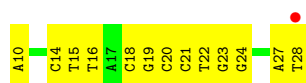
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

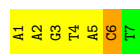
3 Residue-property plots

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

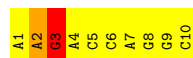
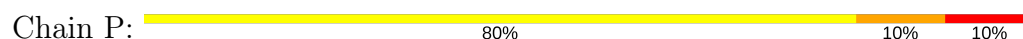
- Molecule 1: 5'-D(P*AP*GP*TP*AP*CP*TP*TP*AP*CP*GP*CP*CP*TP*GP*GP*TP*CP*AP*T)-3'



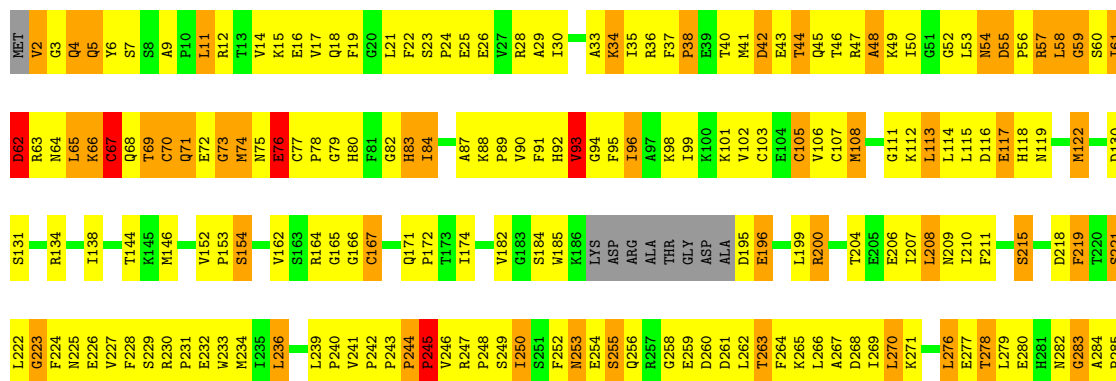
- Molecule 2: 5'-D(*AP*AP*GP*TP*AP*CP*T)-3'



- Molecule 3: 5'-R(*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'

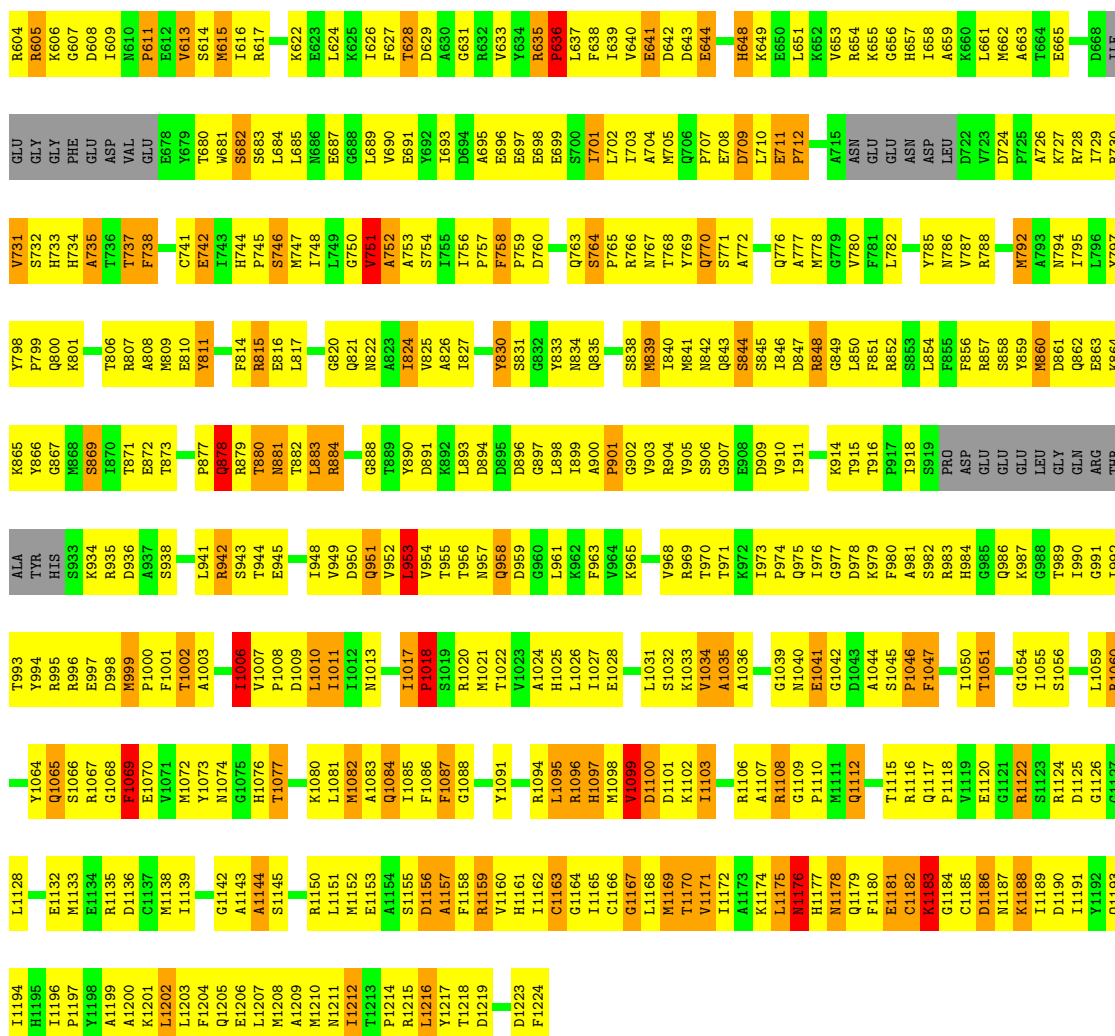


- Molecule 4: DNA-directed RNA polymerase II largest subunit

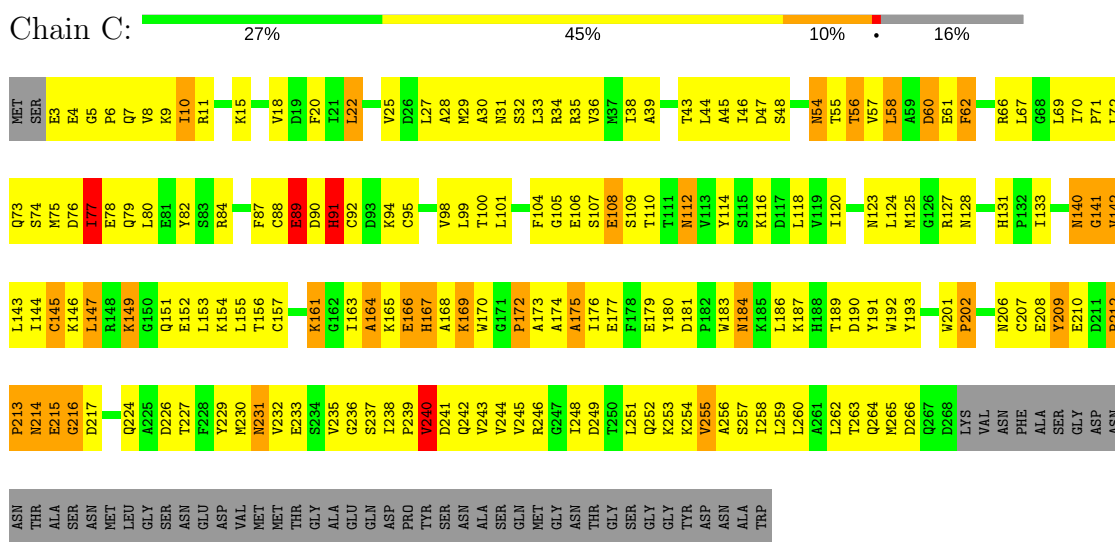


V1299	D1223	T1161	K1092	A1027	G887	E822	I756	A684	G615	V551	G484	D423	F347	H286
K1300	L1224	V1162	K1093	T1028	G888	G823	N757	E685	V616	W552	D485	I424	S348	H287
E1301		I1163	V1094	R1029	S889	L824	I758	A686	V617	W553	E486	Q425	A349	A288
P1302	I1227	P1164	T1095	R1030	R890	I825		K687	E618	P554	N487	L426	R350	L289
E1303	W1228	E1165	S1096	V1031	Q965	D826			G619	D555	N488	Q427	T351	E290
W1304		D1166	G1097	L1032	R966	T827			K620	W556	L489	Y428	V352	E291
V1305	D1231	E1167	V1098	Q1033	A967	A828			T621	D557	H490	G429	I353	A292
E1307		I1168	P1099	E1034	Q968	R829			V622	G558	V491	W430	S354	E293
L1236	L1236	I1169	R1100	E1035	G969	G830			G623	W559	P492	K431	G355	E294
T1308	I1237	L1170	R1101	R1036	V899	T831			S624	L560	Q493	E432	D356	L295
I1238	Q1171	Q1171	K1102	L1037	R971	A832			S625	P561		E433	P357	L296
R1239	L1172	L1172	L1105	T1038	R972	E833			G626	T562	T497	R434	N358	Q297
C1240	H1173	H1173	N1106	L1039	R973	T834			G627	P563	R498	H435		F298
R1241	F1174	F1174	N1106	L1040		G835			G628	A564	A499			F299
V1242	S1175	S1175	V1107	Q1040	N903	G836			L629	I566	E500	D438	V364	H299
V1243	L1176	L1176		A1041	T904	I837			I630	I565		N439	V366	V300
ARG		LEU	M1110	W1044	H906	Q838			H631	K567		D440		T302
ASP		ASP	M111	V1045	T907	R839			V632	P568		P441	S369	Y303
PRO		GLU	K1112		L908	R840			A506	C505		V442		K304
LYS		GLU	T1113	N1048	D909	L841			V507	P570		L443	K372	D305
SER		GLU	T1114	N1049	P910	L842			P508	L571		F444		D307
LEU		ALA	P1115	D985	S911	K843				W572		N445	Y376	I308
ASP		GLU	S1115	R986	L912	T782			C642	S573		R446		
ALA		GLN	L1116	V987	L913	A844				G574		Q447		
GLU		SER	T1117	Q1052	L914	L784			L645	K575		P448	T381	A309
PHE		PHE	V1118	Q1053	E914	E846			F646	Q576		S449	Y383	G310
ASP		ASP	V1119	L1054	D982	D847			G647	S513		P514	N384	Q311
GLU		GLU	L1120	R1055	L993	I848			N648	P514		L450	N384	P312
			L1121	R1056	Q994	E849			G649	Q515		H451	N385	I313
			P1122	E1255	E995	G921			L649	S516		K452	D386	A314
			G123	V1058	N996	D922			Q650	W580		N453	R387	L315
			H1124	H1059	L997				K651	K518		S454	L388	Q316
				H1059	L997				P652	P519		M455		K317
				L1192	L998				G520	C520		P456	V392	S318
				L1193	P999				N654	M521		A457		G319
				R1194	L1000							H458		R320
				L1195	R857				L658	V524		R459		P321
				L1196	L1001				H659	Q525		V460	H359	V322
				L1197	D930				N660	D526		K463	P400	X323
				L1198	L936				G661	P591		V462	G401	S324
				L1199	L936				F662	D592		P464	A402	I325
				L1200	Q935				L658	L588		Y465	K403	R326
				L1201	K934				H659	Q589		S465	Y404	A327
				L1202	K934				N660	L589		T467	W405	R328
				L1203	Q935				G667	L597		F468	R407	I406
				L1204	L943				D668	S599		R469	D408	K332
				L1205	F942				L670	P600		L470	S409	E333
				L1206	L943				A671	G601		N471	G410	G334
				L1207	L943				D672	D602		L472	D411	R335
				L1208	L943				G673	N603		S473	R412	I336
				L1209	L943				G673	G604		V474	I413	R337
				L1210	L943				G673	M605		T475	D414	G338
				L1211	L943				G673	L606		S476	L415	N339
				L1212	L943				G673	L607		P477	R416	L340
				L1213	L943				G673	L608		Y478	Y417	K341
				L1214	L943				G673	L609		Q545	S418	K342
				L1215	L943				G673	L610		L547	K419	K343
				L1216	L943				G673	L611		D481	R420	K344
				L1217	L943				G673	L612		F482	V345	V345
				L1218	L943				G673	L613		D483	G422	D346
				L1219	L943				G673	L614				
				L1220	L943				G673	L615				
				L1221	L943				G673	L616				
				L1222	L943				G673	L617				
				L1223	L943				G673	L618				
				L1224	L943				G673	L619				
				L1225	L943				G673	L620				
				L1226	L943				G673	L621				
				L1227	L943				G673	L622				
				L1228	L943				G673	L623				
				L1229	L943				G673	L624				
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				L1237	L943				G673	L632				
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				L1248	L943				G673	L643				
				L1249	L943				G673	L644				
				L1250	L943				G673	L645				
				L1251	L943				G673	L646				
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				L1277	L943				G673	L672				
				L1278	L943				G673	L673				
				L1279	L943				G673	L674				
				L1280	L943				G673	L675				
				L1281	L943				G673	L676				
				L1282	L943				G673	L677				
				L1283	L943				G673	L678				
				L1284	L943				G673	L679				
				L1285	L943				G673	L680				
				L1286	L943				G673	L681				
				L1287	L943				G673	L682				
				L1288	L943				G673	L683				
				L1289	L943				G673	L684				
				L1290	L943				G673	L685				
				L1291	L943				G673	L686				
				L1292	L943				G673	L687				
				L1293	L943				G673	L688				



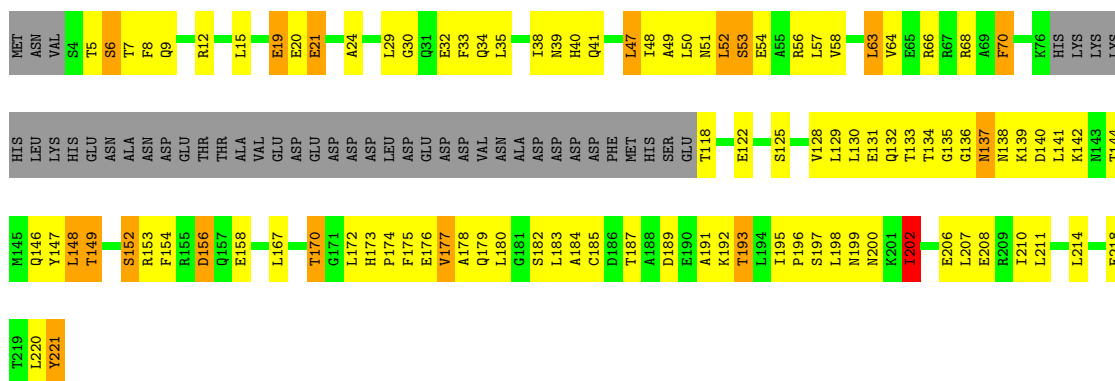


- Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide



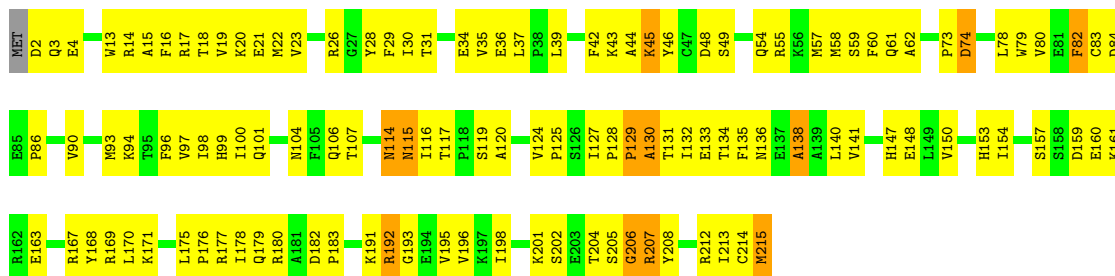
- Molecule 7: DNA-directed RNA polymerase II 32 kDa polypeptide

Chain D:



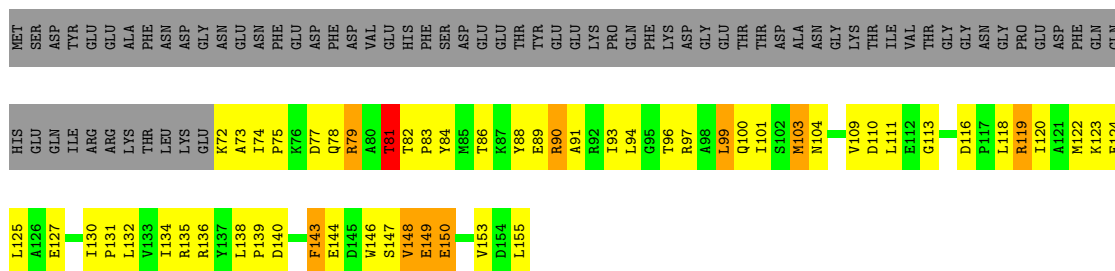
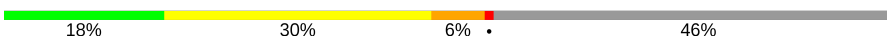
- Molecule 8: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:



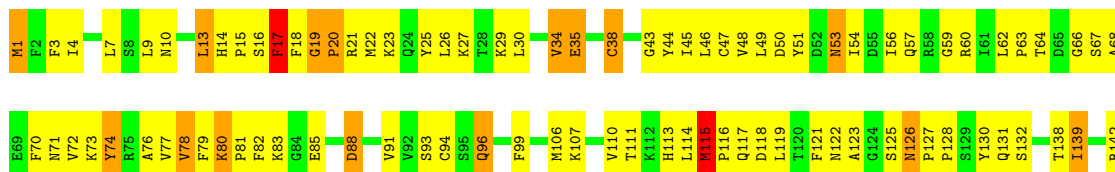
- Molecule 9: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:



- Molecule 10: DNA-directed RNA polymerase II 19 kDa polypeptide

Chain G:







4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.37Å 392.50Å 283.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 48.83 – 3.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 94.4 (48.83-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.10 (at 4.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.253 , 0.276 0.260 , 0.274	Depositor DCC
R_{free} test set	2054 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , -11.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.210 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.209 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	31802	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	T	1.15	1/432 (0.2%)	1.03	1/664 (0.2%)
2	N	1.74	1/158 (0.6%)	0.91	1/242 (0.4%)
3	P	1.17	2/240 (0.8%)	1.06	3/373 (0.8%)
4	A	0.50	0/11339	0.75	5/15334 (0.0%)
5	B	0.51	1/9008 (0.0%)	0.74	5/12146 (0.0%)
6	C	0.56	0/2133	0.76	0/2891
7	D	0.46	0/1365	0.71	0/1837
8	E	0.45	0/1788	0.64	0/2406
9	F	0.56	0/691	0.80	0/933
10	G	0.55	0/1368	0.76	0/1844
11	H	0.40	0/1086	0.65	0/1470
12	I	0.49	1/989 (0.1%)	0.72	0/1331
13	J	0.52	0/541	0.80	0/727
14	K	0.52	0/937	0.70	0/1265
15	L	0.47	0/365	0.74	0/485
All	All	0.54	6/32440 (0.0%)	0.75	15/43948 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	B	0	1
6	C	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	10	DA	O3'-P	-9.11	1.50	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	6	DC	O3'-P	7.11	1.69	1.61
12	I	78	CYS	CB-SG	-6.30	1.71	1.82
3	P	3	G	P-OP1	-6.03	1.38	1.49
5	B	503	GLY	CA-C	6.02	1.61	1.51
3	P	3	G	C2-N2	5.18	1.39	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	10	DA	OP1-P-O3'	7.38	121.44	105.20
3	P	3	G	O5'-P-OP1	-7.04	99.36	105.70
3	P	2	A	C2'-C3'-O3'	6.95	124.82	113.70
2	N	6	DC	P-O3'-C3'	6.32	127.28	119.70
5	B	1185	CYS	N-CA-C	-6.23	94.17	111.00
5	B	504	ARG	NE-CZ-NH2	-6.21	117.19	120.30
4	A	567	LYS	C-N-CD	5.73	140.42	128.40
5	B	503	GLY	C-N-CA	5.63	135.77	121.70
5	B	505	ASP	CB-CG-OD2	-5.58	113.28	118.30
4	A	452	LYS	N-CA-C	-5.58	95.94	111.00
3	P	3	G	N9-C1'-C2'	5.24	120.81	114.00
4	A	425	GLN	N-CA-C	-5.18	97.02	111.00
4	A	76	GLU	CB-CA-C	-5.18	100.05	110.40
5	B	508	LEU	CA-CB-CG	-5.16	103.43	115.30
4	A	466	SER	N-CA-C	5.09	124.75	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	503	GLY	Mainchain
6	C	82	TYR	Sidechain

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	T	387	0	216	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	141	0	81	8	0
3	P	214	0	111	13	0
4	A	11140	0	11217	1300	0
5	B	8836	0	8871	1003	0
6	C	2095	0	2051	255	0
7	D	1356	0	1319	117	0
8	E	1752	0	1776	148	0
9	F	679	0	701	86	0
10	G	1340	0	1357	157	0
11	H	1068	0	1040	110	0
12	I	971	0	930	105	0
13	J	532	0	542	94	0
14	K	919	0	929	93	0
15	L	363	0	387	45	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31802	0	31528	3238	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 51.

All (3238) 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)
7:D:40:HIS:HB3	10:G:73:LYS:NZ	1.61	1.14
14:K:47:ARG:HB3	14:K:47:ARG:HH11	1.00	1.14
4:A:53:LEU:HD23	4:A:54:ASN:H	1.08	1.12
4:A:76:GLU:O	4:A:76:GLU:HG3	1.53	1.08
4:A:53:LEU:HD23	4:A:54:ASN:N	1.70	1.07
7:D:48:ILE:HG21	10:G:4:ILE:HB	1.33	1.07
5:B:273:LEU:HB2	5:B:276:ILE:HD12	1.33	1.06
5:B:467:GLY:H	5:B:475:SER:HB3	1.18	1.06
5:B:824:ILE:HG22	5:B:1087:PHE:HE2	1.21	1.05
4:A:56:PRO:O	4:A:57:ARG:HG3	1.55	1.05
1:T:20:DC:H4'	4:A:447:GLN:NE2	1.70	1.05
4:A:779:PHE:HE1	4:A:785:PRO:HD3	1.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:43:THR:HG22	6:C:44:LEU:H	1.18	1.04
5:B:217:ARG:HE	5:B:405:ARG:HB2	1.20	1.04
4:A:1094:VAL:HG13	4:A:1113:THR:HG21	1.34	1.03
5:B:1072:MET:HE3	5:B:1085:ILE:HB	1.37	1.03
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.35	1.03
5:B:23:ALA:HB1	5:B:24:PRO:HD2	1.40	1.02
11:H:100:THR:HG23	11:H:138:GLU:HA	1.41	1.02
4:A:1017:LEU:HB2	8:E:206:GLY:H	1.25	1.01
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.23	1.01
4:A:855:THR:HG21	4:A:857:ARG:HE	1.22	1.00
6:C:142:VAL:H	13:J:16:ASP:HB3	1.28	0.99
4:A:963:ILE:HD11	4:A:1048:ASN:HB3	1.43	0.99
12:I:85:PHE:HD2	12:I:85:PHE:H	1.06	0.99
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.44	0.98
7:D:40:HIS:HB3	10:G:73:LYS:HZ3	1.13	0.97
4:A:901:LEU:H	4:A:926:GLN:NE2	1.63	0.97
5:B:467:GLY:N	5:B:475:SER:HB3	1.78	0.97
5:B:589:VAL:HG12	5:B:590:HIS:H	1.25	0.97
14:K:47:ARG:HB3	14:K:47:ARG:NH1	1.80	0.96
4:A:84:ILE:HD11	4:A:270:LEU:HD13	1.47	0.96
8:E:19:VAL:O	8:E:23:VAL:HG23	1.66	0.96
4:A:40:THR:HG22	4:A:41:MET:HG3	1.48	0.96
11:H:4:THR:HA	11:H:60:ALA:HB2	1.45	0.96
13:J:5:VAL:HG12	13:J:6:ARG:HG3	1.47	0.96
1:T:22:DT:H2"	1:T:23:DG:H5"	1.48	0.95
7:D:47:LEU:HD13	7:D:48:ILE:H	1.30	0.95
6:C:166:GLU:HG3	14:K:10:PHE:HZ	1.31	0.95
10:G:15:PRO:HA	10:G:18:PHE:CD1	2.01	0.95
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.30	0.95
10:G:1:MET:SD	10:G:79:PHE:HD1	1.89	0.95
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.49	0.94
4:A:563:PRO:HG3	4:A:572:TRP:CZ2	2.02	0.94
5:B:1065:GLN:HE21	5:B:1067:ARG:H	1.08	0.94
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.48	0.94
5:B:1072:MET:CE	5:B:1085:ILE:HB	1.98	0.94
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.50	0.93
4:A:535:THR:HG21	4:A:616:VAL:HA	1.50	0.93
14:K:65:HIS:HD2	14:K:67:PHE:H	1.17	0.93
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.49	0.93
5:B:65:GLU:HG3	5:B:66:ASP:H	1.33	0.93
5:B:847:ASP:HB3	6:C:167:HIS:NE2	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:754:SER:H	4:A:757:ASN:HD22	1.08	0.92
14:K:47:ARG:CB	14:K:47:ARG:HH11	1.82	0.92
4:A:829:VAL:HG21	5:B:508:LEU:HD13	1.50	0.92
5:B:189:LEU:HA	5:B:192:LEU:HD12	1.52	0.92
5:B:46:GLN:HG3	5:B:47:GLN:H	1.33	0.92
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.51	0.92
10:G:138:THR:HG22	10:G:139:ILE:H	1.32	0.92
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.05	0.91
6:C:262:LEU:HD11	14:K:87:LEU:HD23	1.53	0.91
8:E:198:ILE:HD11	8:E:212:ARG:HG3	1.52	0.91
5:B:1224:PHE:HE2	8:E:171:LYS:HG3	1.33	0.91
5:B:1065:GLN:HE21	5:B:1067:ARG:N	1.68	0.91
4:A:1445:ILE:H	4:A:1445:ILE:HD12	1.36	0.90
4:A:903:ASN:ND2	4:A:905:ASP:H	1.68	0.90
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.54	0.90
3:P:2:A:H2'	3:P:3:G:C8	2.05	0.90
6:C:57:VAL:HG11	13:J:60:PHE:HB3	1.52	0.90
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.02	0.89
6:C:47:ASP:HA	15:L:69:ALA:HB3	1.50	0.89
8:E:180:ARG:HH21	8:E:192:ARG:HB2	1.34	0.89
10:G:1:MET:SD	10:G:79:PHE:CD1	2.66	0.89
13:J:64:ASN:HB3	13:J:65:PRO:CD	2.03	0.89
8:E:94:LYS:HE2	8:E:98:ILE:HD11	1.54	0.89
13:J:36:LEU:HD12	13:J:47:ARG:NH1	1.88	0.89
5:B:1007:VAL:HG22	5:B:1008:PRO:HD2	1.53	0.88
5:B:918:ILE:HB	5:B:935:ARG:HD2	1.54	0.88
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.03	0.88
3:P:2:A:H2'	3:P:3:G:H8	1.37	0.88
4:A:858:ASN:ND2	4:A:860:LEU:H	1.72	0.88
5:B:579:ARG:HB2	5:B:586:TRP:HE1	1.39	0.88
6:C:44:LEU:HB2	6:C:77:ILE:HD11	1.54	0.88
10:G:23:LYS:HG3	10:G:56:ILE:HD11	1.54	0.88
4:A:1189:SER:O	4:A:1241:ARG:HD3	1.74	0.88
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.52	0.88
4:A:335:ARG:NH1	5:B:1202:LEU:HD13	1.89	0.87
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.40	0.87
4:A:356:ASP:HB2	4:A:469:ARG:NH1	1.90	0.87
7:D:144:THR:O	7:D:148:LEU:HB2	1.75	0.87
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.56	0.86
5:B:847:ASP:HB3	6:C:167:HIS:HE2	1.34	0.86
4:A:541:ILE:HG22	4:A:546:VAL:HG23	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:211:VAL:O	5:B:480:SER:HA	1.75	0.86
5:B:579:ARG:HB2	5:B:586:TRP:NE1	1.91	0.86
4:A:353:ILE:HG21	4:A:487:MET:HE3	1.56	0.86
1:T:20:DC:H4'	4:A:447:GLN:HE22	1.40	0.86
6:C:43:THR:HG22	6:C:44:LEU:N	1.88	0.86
10:G:7:LEU:HB2	10:G:74:TYR:CE2	2.10	0.86
4:A:709:THR:HG23	12:I:94:ASP:HA	1.57	0.86
5:B:549:THR:HG22	5:B:550:ASP:H	1.40	0.86
4:A:1341:ILE:HG23	4:A:1342:GLU:N	1.90	0.85
4:A:709:THR:HG22	4:A:711:ARG:H	1.38	0.85
4:A:825:ILE:HG22	5:B:508:LEU:HD11	1.59	0.85
5:B:466:TRP:O	5:B:468:GLU:N	2.08	0.85
6:C:32:SER:O	6:C:36:VAL:HG23	1.76	0.85
4:A:1329:THR:HG22	4:A:1331:SER:H	1.41	0.85
4:A:1444:MET:HE1	9:F:135:ARG:HB2	1.58	0.85
9:F:93:ILE:HD11	9:F:134:ILE:HD11	1.58	0.85
4:A:1312:ASN:O	4:A:1316:VAL:HG23	1.77	0.85
5:B:1197:PRO:HG2	5:B:1200:ALA:HB2	1.59	0.84
7:D:153:ARG:NH2	7:D:184:ALA:HA	1.92	0.84
11:H:81:PRO:HB2	11:H:82:PRO:HD2	1.58	0.84
5:B:800:GLN:HB3	13:J:52:THR:HG21	1.55	0.84
4:A:503:GLN:HE21	9:F:90:ARG:HH21	1.21	0.84
6:C:213:PRO:O	6:C:214:ASN:HB2	1.77	0.84
12:I:8:ARG:HG3	12:I:34:TYR:HE1	1.40	0.84
4:A:1329:THR:CG2	4:A:1331:SER:H	1.90	0.84
4:A:1242:VAL:HG12	4:A:1243:VAL:H	1.41	0.84
6:C:241:ASP:O	6:C:245:VAL:HG23	1.77	0.83
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.08	0.83
5:B:168:GLY:H	5:B:450:ALA:HB1	1.40	0.83
4:A:528:LEU:O	4:A:531:ILE:HG22	1.78	0.83
4:A:567:LYS:HG3	4:A:568:PRO:HD2	1.57	0.83
4:A:808:LEU:HD23	4:A:813:PHE:HA	1.60	0.83
5:B:521:LEU:HB3	5:B:633:VAL:HG11	1.60	0.83
6:C:56:THR:HG22	6:C:57:VAL:H	1.43	0.83
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.61	0.83
8:E:213:ILE:HG12	8:E:214:CYS:H	1.44	0.83
6:C:47:ASP:HA	15:L:69:ALA:CB	2.07	0.83
4:A:442:VAL:HB	4:A:489:LEU:HD11	1.61	0.83
4:A:741:ASN:HD22	4:A:744:LYS:H	1.27	0.82
5:B:882:THR:HG22	5:B:884:ARG:H	1.41	0.82
5:B:1096:ARG:O	5:B:1097:HIS:HB2	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:507:LYS:O	5:B:512:ARG:NE	2.10	0.82
5:B:25:ILE:HD11	5:B:653:VAL:O	1.77	0.82
5:B:806:THR:HG22	5:B:808:ALA:H	1.42	0.82
13:J:57:ILE:HA	13:J:60:PHE:HD2	1.44	0.82
4:A:475:THR:HG23	4:A:476:SER:H	1.42	0.82
5:B:770:GLN:OE1	5:B:983:ARG:HA	1.80	0.82
12:I:8:ARG:HG3	12:I:34:TYR:CE1	2.13	0.82
4:A:351:THR:HB	5:B:1103:ILE:HD12	1.62	0.82
6:C:232:VAL:HG21	6:C:244:VAL:HG22	1.60	0.82
5:B:217:ARG:NE	5:B:405:ARG:HB2	1.94	0.82
13:J:16:ASP:OD1	13:J:17:LYS:HD2	1.80	0.82
4:A:55:ASP:C	4:A:57:ARG:H	1.78	0.82
4:A:1329:THR:HG22	4:A:1331:SER:N	1.94	0.82
5:B:172:ILE:HD13	5:B:178:ASN:HB3	1.60	0.82
5:B:955:THR:HG22	5:B:956:THR:H	1.44	0.82
4:A:1444:MET:CE	9:F:135:ARG:HB2	2.08	0.82
5:B:955:THR:HG22	5:B:956:THR:N	1.95	0.82
4:A:794:PRO:HG2	4:A:795:GLU:OE2	1.80	0.81
8:E:175:LEU:HD23	8:E:176:PRO:HD2	1.60	0.81
11:H:102:TYR:OH	11:H:122:LEU:HD22	1.78	0.81
13:J:3:VAL:HG21	13:J:18:TRP:HB2	1.61	0.81
5:B:467:GLY:O	5:B:468:GLU:HB2	1.81	0.81
4:A:1341:ILE:HG23	4:A:1342:GLU:H	1.45	0.81
4:A:1420:ASP:HB3	4:A:1422:ARG:HG3	1.62	0.81
4:A:560:ILE:HG13	11:H:78:SER:HB2	1.62	0.81
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.63	0.81
5:B:955:THR:HG23	15:L:54:ARG:O	1.80	0.81
6:C:244:VAL:O	6:C:248:ILE:HG13	1.79	0.81
4:A:567:LYS:HB3	11:H:96:VAL:H	1.46	0.81
13:J:64:ASN:HB3	13:J:65:PRO:HD3	1.60	0.81
5:B:1065:GLN:NE2	5:B:1067:ARG:H	1.78	0.81
8:E:2:ASP:O	8:E:3:GLN:HG2	1.81	0.81
4:A:475:THR:HG23	4:A:476:SER:N	1.96	0.81
4:A:70:CYS:O	4:A:72:GLU:HG2	1.80	0.81
4:A:829:VAL:C	4:A:831:THR:H	1.82	0.80
5:B:516:ASN:N	5:B:516:ASN:HD22	1.76	0.80
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.61	0.80
4:A:106:VAL:HG13	4:A:112:LYS:O	1.81	0.80
5:B:515:HIS:HD2	5:B:517:THR:H	1.29	0.80
5:B:233:PRO:HG2	5:B:234:ILE:HD12	1.61	0.80
8:E:16:PHE:CZ	8:E:20:LYS:HE2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:78:PRO:HB3	5:B:1201:LYS:HE3	1.62	0.80
5:B:98:THR:O	5:B:126:SER:HB2	1.81	0.80
6:C:184:ASN:ND2	6:C:187:LYS:HA	1.97	0.80
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.17	0.80
4:A:310:GLY:O	4:A:312:PRO:HD2	1.81	0.80
4:A:567:LYS:NZ	11:H:46:LEU:HB2	1.97	0.80
5:B:1159:ARG:HB3	5:B:1159:ARG:HH11	1.47	0.80
5:B:952:VAL:HG12	5:B:953:LEU:H	1.46	0.80
12:I:71:SER:OG	12:I:83:ASN:HB2	1.82	0.80
4:A:768:GLN:CG	4:A:816:HIS:HA	2.11	0.80
5:B:824:ILE:HG22	5:B:1087:PHE:CE2	2.13	0.80
9:F:86:THR:HG23	9:F:89:GLU:OE1	1.82	0.79
12:I:26:LEU:HD23	12:I:37:GLU:HA	1.62	0.79
14:K:21:ILE:HG12	14:K:33:ILE:HG12	1.65	0.79
5:B:1099:VAL:O	5:B:1101:ASP:N	2.16	0.79
5:B:705:MET:H	5:B:710:LEU:HD12	1.47	0.79
6:C:186:LEU:HD21	6:C:224:GLN:O	1.82	0.79
11:H:59:ILE:HG22	11:H:60:ALA:N	1.97	0.79
13:J:12:LYS:O	13:J:14:VAL:HG23	1.83	0.79
4:A:76:GLU:O	4:A:76:GLU:CG	2.29	0.79
14:K:113:THR:O	14:K:114:LEU:HB2	1.81	0.79
4:A:903:ASN:C	4:A:903:ASN:HD22	1.86	0.79
10:G:13:LEU:HD21	10:G:17:PHE:HB2	1.61	0.79
4:A:253:ASN:HB3	5:B:935:ARG:NH2	1.98	0.79
11:H:4:THR:HA	11:H:60:ALA:CB	2.13	0.79
11:H:93:TYR:HB3	11:H:144:ILE:O	1.83	0.79
10:G:34:VAL:HG12	10:G:45:ILE:HG21	1.64	0.78
6:C:212:PRO:HB3	6:C:213:PRO:HD2	1.63	0.78
5:B:37:PHE:HE2	5:B:542:MET:HA	1.47	0.78
10:G:128:PRO:O	10:G:138:THR:HG23	1.83	0.78
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.65	0.78
5:B:508:LEU:O	5:B:509:ALA:HB2	1.82	0.78
11:H:23:VAL:HG22	11:H:43:ASN:HA	1.66	0.78
4:A:35:ILE:HG22	4:A:35:ILE:O	1.84	0.78
5:B:1183:LYS:HE3	5:B:1183:LYS:N	1.99	0.77
5:B:953:LEU:HD21	5:B:965:LYS:HB2	1.65	0.77
4:A:524:VAL:HG12	4:A:525:GLN:H	1.49	0.77
5:B:863:GLU:OE2	5:B:873:THR:HA	1.84	0.77
6:C:166:GLU:HG3	14:K:10:PHE:CZ	2.19	0.77
4:A:588:LEU:O	4:A:606:LEU:HA	1.85	0.77
4:A:798:GLY:HA2	4:A:815:PHE:CD1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:483:LEU:HD11	5:B:491:THR:HG23	1.67	0.77
8:E:117:THR:HG22	8:E:119:SER:H	1.47	0.77
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.66	0.77
4:A:754:SER:H	4:A:757:ASN:ND2	1.83	0.77
5:B:1159:ARG:HD3	5:B:1193:GLN:CG	2.13	0.77
4:A:321:PRO:O	4:A:322:VAL:HB	1.85	0.77
5:B:1162:ILE:HG22	5:B:1163:CYS:H	1.49	0.77
6:C:70:ILE:HG12	6:C:142:VAL:HG11	1.66	0.77
4:A:590:ARG:NH2	4:A:620:LYS:HB3	1.99	0.77
14:K:65:HIS:CD2	14:K:67:PHE:H	2.02	0.77
4:A:1116:LEU:HB2	4:A:1329:THR:OG1	1.83	0.77
4:A:567:LYS:HB3	11:H:95:TYR:HA	1.67	0.77
4:A:836:TYR:CE2	4:A:840:ARG:HD2	2.19	0.77
5:B:859:TYR:OH	5:B:941:LEU:HD12	1.85	0.76
5:B:102:VAL:HG23	5:B:112:LEU:HB2	1.66	0.76
5:B:1201:LYS:HE2	5:B:1205:GLN:OE1	1.85	0.76
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.15	0.76
5:B:503:GLY:HA3	5:B:507:LYS:HE3	1.67	0.76
8:E:22:MET:HE3	8:E:26:ARG:HE	1.50	0.76
8:E:29:PHE:O	8:E:30:ILE:HG13	1.85	0.76
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.66	0.76
5:B:1034:VAL:HG12	5:B:1035:ALA:N	1.99	0.76
5:B:53:GLN:HG2	5:B:547:VAL:HG22	1.66	0.76
5:B:39:ARG:NH2	5:B:665:GLU:HG2	2.01	0.76
6:C:43:THR:CG2	6:C:44:LEU:H	1.96	0.76
11:H:42:ILE:HG23	11:H:95:TYR:HE1	1.50	0.76
4:A:1291:VAL:HG13	4:A:1292:PRO:HD2	1.66	0.76
5:B:798:TYR:HE2	6:C:62:PHE:CE2	2.03	0.76
7:D:48:ILE:CG2	10:G:4:ILE:HB	2.12	0.76
12:I:8:ARG:CG	12:I:34:TYR:HE1	1.99	0.76
4:A:87:ALA:HB3	4:A:276:LEU:HD23	1.67	0.75
4:A:534:LEU:O	4:A:574:GLY:HA3	1.85	0.75
5:B:363:HIS:O	5:B:364:ILE:HB	1.85	0.75
5:B:1007:VAL:CG2	5:B:1008:PRO:HD2	2.16	0.75
4:A:152:VAL:CG1	4:A:153:PRO:HD2	2.17	0.75
4:A:225:ASN:HD22	4:A:228:PHE:H	1.32	0.75
5:B:1159:ARG:NH1	5:B:1159:ARG:HB3	2.01	0.75
6:C:179:GLU:HG2	6:C:180:TYR:N	1.99	0.75
4:A:1424:VAL:HG13	4:A:1436:ILE:CD1	2.15	0.75
5:B:200:GLY:HA2	5:B:202:TYR:CE2	2.22	0.75
4:A:1343:ALA:HB2	8:E:150:VAL:HG22	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:40:HIS:CB	10:G:73:LYS:NZ	2.46	0.75
4:A:590:ARG:NH1	4:A:590:ARG:HG3	2.02	0.75
5:B:37:PHE:CD1	5:B:41:LYS:HG3	2.22	0.75
5:B:995:ARG:HH12	6:C:165:LYS:HG2	1.52	0.75
4:A:855:THR:CG2	4:A:857:ARG:HE	1.99	0.75
5:B:351:TYR:CE1	5:B:355:ILE:HD11	2.21	0.75
5:B:577:ALA:HB1	5:B:589:VAL:HG11	1.68	0.75
5:B:613:VAL:HG13	5:B:627:PHE:O	1.87	0.75
7:D:170:THR:CG2	7:D:172:LEU:HG	2.17	0.75
4:A:899:VAL:HB	4:A:929:LEU:CD1	2.17	0.75
5:B:37:PHE:CE1	5:B:41:LYS:HG3	2.22	0.75
1:T:15:DT:H5"	4:A:1407:GLU:OE2	1.87	0.75
4:A:388:LEU:O	4:A:392:VAL:HG23	1.87	0.74
4:A:741:ASN:HD21	4:A:743:VAL:HB	1.50	0.74
4:A:670:ILE:HG23	4:A:805:LEU:HD21	1.68	0.74
4:A:92:HIS:O	4:A:94:GLY:N	2.19	0.74
4:A:1004:ASN:ND2	8:E:167:ARG:HD2	2.02	0.74
4:A:1116:LEU:N	4:A:1308:THR:HG22	2.02	0.74
4:A:993:LEU:HD23	4:A:1022:LEU:HD21	1.70	0.74
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.67	0.74
5:B:604:ARG:NH2	5:B:613:VAL:O	2.20	0.74
6:C:66:ARG:NH2	13:J:5:VAL:HG23	2.01	0.74
4:A:438:ASP:O	4:A:439:ASN:HB2	1.87	0.74
4:A:49:LYS:NZ	4:A:61:ILE:HG13	2.03	0.74
5:B:1099:VAL:CG1	5:B:1100:ASP:N	2.50	0.74
4:A:1332:PHE:HD2	4:A:1332:PHE:N	1.85	0.74
4:A:87:ALA:CB	4:A:276:LEU:HD23	2.18	0.74
5:B:359:GLU:O	5:B:362:PRO:HD3	1.87	0.74
5:B:378:LEU:O	5:B:378:LEU:HD12	1.86	0.74
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.02	0.74
5:B:223:VAL:HG11	5:B:381:MET:HG2	1.68	0.74
5:B:801:LYS:O	13:J:52:THR:HG23	1.88	0.74
5:B:642:ASP:O	5:B:644:GLU:N	2.20	0.74
9:F:81:THR:HG21	9:F:136:ARG:HD3	1.70	0.74
4:A:107:CYS:SG	4:A:171:GLN:HG2	2.28	0.74
4:A:646:PHE:O	4:A:650:GLN:HG3	1.88	0.74
4:A:858:ASN:HD22	4:A:858:ASN:C	1.89	0.74
5:B:996:ARG:NH1	6:C:38:ILE:HG23	2.01	0.74
4:A:69:THR:O	4:A:71:GLN:N	2.21	0.73
14:K:12:LEU:HD12	14:K:12:LEU:H	1.52	0.73
5:B:902:GLY:O	15:L:65:VAL:HG11	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:248:PRO:O	4:A:260:ASP:HB2	1.87	0.73
4:A:335:ARG:HA	4:A:339:ASN:HB2	1.68	0.73
10:G:80:LYS:HD3	10:G:80:LYS:N	2.03	0.73
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.69	0.73
5:B:906:SER:O	5:B:941:LEU:HD23	1.87	0.73
7:D:40:HIS:HB3	10:G:73:LYS:HZ2	1.51	0.73
5:B:1224:PHE:CE2	8:E:171:LYS:HG3	2.20	0.73
4:A:1121:GLU:HG2	4:A:1122:PRO:HD2	1.68	0.73
14:K:45:LEU:HG	14:K:94:ILE:HD13	1.69	0.73
4:A:783:THR:HG21	4:A:815:PHE:CZ	2.23	0.73
4:A:164:ARG:HG3	4:A:165:GLY:N	2.02	0.73
4:A:384:ASN:OD1	4:A:388:LEU:HD12	1.89	0.73
5:B:370:PHE:HE2	5:B:373:ARG:HH11	1.36	0.73
4:A:855:THR:HG21	4:A:857:ARG:NE	2.01	0.73
4:A:1422:ARG:HH22	5:B:1224:PHE:C	1.91	0.73
7:D:138:ASN:OD1	7:D:141:LEU:HB2	1.89	0.73
12:I:7:CYS:HB3	12:I:14:LEU:HD21	1.71	0.73
4:A:856:THR:HB	4:A:865:GLN:HB2	1.69	0.73
10:G:23:LYS:HG3	10:G:56:ILE:CD1	2.18	0.73
4:A:1348:LEU:HG	4:A:1372:VAL:CG2	2.18	0.73
5:B:295:GLY:H	5:B:298:LEU:HD23	1.53	0.73
4:A:903:ASN:HD22	4:A:904:THR:N	1.87	0.72
5:B:615:MET:HB3	5:B:626:ILE:HG12	1.71	0.72
5:B:975:GLN:O	5:B:990:ILE:HD12	1.89	0.72
7:D:29:LEU:HD22	10:G:82:PHE:CE2	2.24	0.72
4:A:302:THR:HA	4:A:305:ASP:O	1.89	0.72
4:A:382:PRO:HB3	4:A:428:TYR:HE2	1.53	0.72
4:A:567:LYS:CD	4:A:568:PRO:HD2	2.19	0.72
5:B:1017:ILE:HB	5:B:1018:PRO:HD3	1.71	0.72
5:B:507:LYS:H	5:B:512:ARG:HH21	1.35	0.72
5:B:603:LEU:HD13	5:B:608:ASP:HB2	1.71	0.72
4:A:347:PHE:H	5:B:1107:ALA:HA	1.55	0.72
5:B:171:PRO:HD2	5:B:457:LEU:HD13	1.71	0.72
7:D:176:GLU:O	7:D:178:ALA:N	2.18	0.72
9:F:119:ARG:HG3	9:F:119:ARG:HH11	1.53	0.72
6:C:165:LYS:O	14:K:6:ARG:NH1	2.22	0.72
4:A:1239:ARG:HH22	4:A:1241:ARG:NH2	1.87	0.72
5:B:1001:PHE:CE1	5:B:1073:TYR:HB2	2.24	0.72
5:B:281:PRO:HG2	5:B:284:ILE:HG13	1.69	0.72
5:B:879:ARG:HH11	5:B:883:LEU:HD22	1.54	0.72
5:B:365:THR:HG23	5:B:367:LEU:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:502:ILE:HG12	5:B:535:LEU:HD13	1.71	0.72
10:G:74:TYR:HD2	10:G:74:TYR:H	1.35	0.72
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.24	0.72
5:B:594:ALA:HA	5:B:617:ARG:NH1	2.05	0.72
7:D:134:THR:HG22	7:D:136:GLY:H	1.52	0.72
15:L:30:ILE:O	15:L:56:LEU:HA	1.88	0.72
5:B:589:VAL:HG12	5:B:590:HIS:N	2.04	0.72
5:B:112:LEU:HD12	5:B:113:TYR:H	1.54	0.72
5:B:953:LEU:O	5:B:953:LEU:HD23	1.89	0.72
4:A:67:CYS:O	4:A:70:CYS:HB3	1.90	0.72
5:B:1095:LEU:HD12	5:B:1095:LEU:H	1.54	0.72
5:B:847:ASP:HB3	6:C:167:HIS:CD2	2.24	0.72
6:C:98:VAL:C	6:C:99:LEU:HD23	2.09	0.72
11:H:40:LEU:HD13	11:H:123:MET:HB2	1.70	0.72
5:B:1099:VAL:HG12	5:B:1100:ASP:H	1.53	0.71
5:B:223:VAL:CG1	5:B:381:MET:HG2	2.19	0.71
5:B:601:ARG:O	5:B:605:ARG:HG3	1.89	0.71
7:D:33:PHE:CE1	10:G:80:LYS:HE3	2.24	0.71
12:I:50:THR:HG22	12:I:52:ILE:H	1.55	0.71
4:A:1437:GLY:O	4:A:1439:GLY:N	2.23	0.71
4:A:567:LYS:HZ1	11:H:46:LEU:HB2	1.53	0.71
5:B:23:ALA:HB1	5:B:24:PRO:CD	2.19	0.71
6:C:45:ALA:HA	6:C:72:LEU:CD1	2.19	0.71
4:A:897:TYR:HD2	4:A:936:LEU:HD13	1.55	0.71
5:B:562:GLY:HA3	5:B:590:HIS:CE1	2.26	0.71
5:B:411:PRO:O	5:B:414:ALA:HB3	1.89	0.71
5:B:800:GLN:HB3	13:J:52:THR:CG2	2.20	0.71
4:A:590:ARG:HB3	4:A:605:MET:N	2.05	0.71
6:C:183:TRP:CZ2	6:C:207:CYS:HB3	2.25	0.71
13:J:14:VAL:CG1	13:J:50:ILE:HD11	2.20	0.71
4:A:164:ARG:HG3	4:A:165:GLY:H	1.52	0.71
4:A:800:VAL:HG22	4:A:812:GLU:HB3	1.73	0.71
5:B:364:ILE:HG12	5:B:585:VAL:HG13	1.72	0.71
10:G:119:LEU:HD12	10:G:131:GLN:O	1.91	0.71
4:A:598:LEU:HA	11:H:122:LEU:HD13	1.71	0.71
4:A:1239:ARG:HH22	4:A:1241:ARG:HH22	1.39	0.71
4:A:1094:VAL:HG13	4:A:1113:THR:CG2	2.16	0.71
5:B:1069:PHE:HD1	5:B:1069:PHE:H	1.37	0.71
5:B:1085:ILE:HD12	5:B:1085:ILE:N	2.06	0.71
5:B:35:SER:HA	5:B:811:TYR:HE2	1.56	0.71
10:G:30:LEU:HD13	10:G:72:VAL:HG11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:728:ARG:HH12	5:B:1047:PHE:HB3	1.56	0.71
5:B:737:THR:HG21	12:I:66:PRO:HA	1.73	0.71
12:I:34:TYR:CD2	12:I:35:VAL:N	2.59	0.71
14:K:7:PHE:HA	14:K:10:PHE:CE2	2.26	0.71
4:A:1006:ILE:HD12	8:E:163:GLU:HG3	1.73	0.70
5:B:710:LEU:HA	5:B:733:HIS:HB3	1.74	0.70
4:A:1191:TRP:CD1	4:A:1256:GLU:HB2	2.27	0.70
5:B:882:THR:HG22	5:B:884:ARG:N	2.05	0.70
8:E:124:VAL:HG13	8:E:132:ILE:HB	1.71	0.70
12:I:111:THR:HG22	12:I:112:SER:N	2.06	0.70
4:A:1151:GLU:OE2	12:I:45:ARG:HD2	1.90	0.70
4:A:250:ILE:O	4:A:258:GLY:HA3	1.91	0.70
4:A:1332:PHE:N	4:A:1332:PHE:CD2	2.58	0.70
5:B:794:ASN:C	5:B:795:ILE:HD12	2.11	0.70
5:B:871:THR:HG22	5:B:872:GLU:O	1.90	0.70
11:H:81:PRO:CB	11:H:82:PRO:HD2	2.20	0.70
4:A:244:PRO:HB2	4:A:245:PRO:CD	2.20	0.70
4:A:63:ARG:HA	4:A:74:MET:SD	2.32	0.70
5:B:1163:CYS:SG	5:B:1165:ILE:HB	2.30	0.70
11:H:36:CYS:HA	11:H:126:GLU:O	1.91	0.70
5:B:365:THR:HG23	5:B:367:LEU:HG	1.74	0.70
5:B:827:ILE:HD12	5:B:1086:PHE:HD2	1.55	0.70
8:E:213:ILE:HG12	8:E:214:CYS:N	2.06	0.70
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.27	0.70
5:B:615:MET:C	5:B:616:ILE:HD12	2.11	0.70
6:C:20:PHE:HE1	6:C:22:LEU:HD12	1.56	0.70
4:A:903:ASN:HD22	4:A:905:ASP:H	1.37	0.70
4:A:346:ASP:HB3	5:B:1108:ARG:H	1.56	0.70
4:A:382:PRO:HD3	4:A:428:TYR:CD2	2.26	0.70
6:C:66:ARG:NH1	13:J:2:ILE:HG21	2.07	0.70
7:D:130:LEU:C	7:D:132:GLN:H	1.95	0.70
9:F:103:MET:O	9:F:104:ASN:HB2	1.91	0.70
14:K:50:LEU:HD11	14:K:75:ILE:HD13	1.72	0.70
4:A:1155:ASP:OD2	4:A:1161:THR:HG23	1.91	0.70
4:A:1341:ILE:CG2	4:A:1342:GLU:H	2.04	0.70
4:A:1394:THR:HG21	4:A:1398:MET:SD	2.32	0.70
10:G:15:PRO:HA	10:G:18:PHE:CE1	2.27	0.70
13:J:8:PHE:H	13:J:49:MET:CE	2.05	0.70
7:D:66:ARG:HD2	7:D:133:THR:HB	1.74	0.69
15:L:48:CYS:HB3	15:L:51:CYS:O	1.91	0.69
4:A:1450:LEU:HG	4:A:1450:LEU:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:56:PRO:O	4:A:57:ARG:CG	2.38	0.69
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.74	0.69
5:B:1002:THR:HG21	5:B:1006:ILE:HD12	1.74	0.69
14:K:31:VAL:HG12	14:K:32:VAL:N	2.07	0.69
4:A:79:GLY:HA3	4:A:243:PRO:CG	2.21	0.69
4:A:254:GLU:HB2	5:B:935:ARG:HH12	1.56	0.69
5:B:847:ASP:C	5:B:849:GLY:H	1.93	0.69
5:B:948:ILE:HG22	5:B:949:VAL:O	1.92	0.69
9:F:125:LEU:O	9:F:125:LEU:HG	1.91	0.69
4:A:450:LEU:N	4:A:450:LEU:HD12	2.07	0.69
4:A:722:LEU:O	4:A:725:ALA:HB3	1.91	0.69
4:A:816:HIS:CD2	5:B:764:SER:HB2	2.27	0.69
5:B:708:GLU:O	5:B:710:LEU:N	2.26	0.69
8:E:135:PHE:HD2	8:E:140:LEU:HD21	1.55	0.69
4:A:427:GLN:HG3	4:A:430:TRP:CZ2	2.27	0.69
4:A:49:LYS:HE2	4:A:61:ILE:HD12	1.73	0.69
5:B:701:ILE:HD11	5:B:703:ILE:HD11	1.74	0.69
11:H:59:ILE:HG22	11:H:60:ALA:H	1.58	0.69
4:A:1293:SER:OG	4:A:1294:PRO:HD2	1.93	0.69
5:B:1099:VAL:HG12	5:B:1100:ASP:N	2.07	0.69
13:J:48:ARG:HD2	13:J:49:MET:N	2.08	0.69
4:A:1030:ARG:HG3	4:A:1034:GLU:OE2	1.92	0.69
4:A:154:SER:HB3	4:A:162:VAL:HG21	1.74	0.69
4:A:665:GLY:O	4:A:667:GLY:N	2.26	0.69
7:D:47:LEU:HD13	7:D:48:ILE:N	2.05	0.69
15:L:38:LEU:O	15:L:39:SER:HB3	1.91	0.69
15:L:58:LYS:O	15:L:58:LYS:HG2	1.92	0.69
4:A:107:CYS:N	4:A:114:LEU:HD21	2.08	0.69
4:A:463:ILE:HB	4:A:464:PRO:HD2	1.75	0.69
5:B:496:ARG:HB3	5:B:496:ARG:HH11	1.57	0.69
7:D:34:GLN:O	7:D:47:LEU:HD23	1.92	0.69
8:E:22:MET:HE3	8:E:26:ARG:NE	2.07	0.69
4:A:55:ASP:C	4:A:57:ARG:N	2.47	0.69
4:A:853:ASP:OD1	4:A:855:THR:N	2.26	0.69
4:A:857:ARG:HD3	4:A:861:GLY:O	1.92	0.69
4:A:901:LEU:HG	4:A:926:GLN:NE2	2.08	0.69
6:C:239:PRO:HB2	6:C:241:ASP:OD1	1.92	0.69
6:C:263:THR:C	6:C:265:MET:H	1.96	0.69
6:C:5:GLY:O	6:C:7:GLN:HG3	1.93	0.69
8:E:135:PHE:HB3	8:E:140:LEU:HD11	1.75	0.69
3:P:10:C:H4'	4:A:485:ASP:OD1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:GLN:HE21	9:F:90:ARG:NH2	1.91	0.69
4:A:694:THR:O	4:A:698:GLN:HG3	1.90	0.69
4:A:886:ILE:HG22	4:A:887:GLY:N	2.08	0.69
4:A:107:CYS:H	4:A:114:LEU:HD21	1.56	0.68
5:B:831:SER:HB3	5:B:994:TYR:OH	1.93	0.68
7:D:52:LEU:HD21	7:D:147:TYR:HE2	1.57	0.68
14:K:46:ILE:O	14:K:50:LEU:HB2	1.92	0.68
4:A:88:LYS:HE3	4:A:280:GLU:OE2	1.94	0.68
4:A:853:ASP:O	4:A:854:ASN:HB2	1.92	0.68
5:B:1115:THR:O	5:B:1116:ARG:HB2	1.92	0.68
5:B:806:THR:HG22	5:B:808:ALA:N	2.08	0.68
10:G:7:LEU:HD11	10:G:45:ILE:HD11	1.76	0.68
1:T:15:DT:H1'	4:A:1386:ARG:NH1	2.09	0.68
4:A:1332:PHE:H	4:A:1332:PHE:HD2	1.40	0.68
4:A:285:PRO:HG2	4:A:288:ALA:HB3	1.74	0.68
4:A:591:PHE:HA	4:A:595:THR:HG21	1.76	0.68
4:A:672:ASP:HB2	4:A:736:ASN:OD1	1.92	0.68
4:A:866:PHE:O	4:A:867:ILE:HG13	1.94	0.68
4:A:885:THR:O	4:A:940:ARG:HD2	1.92	0.68
5:B:1165:ILE:HG22	5:B:1166:CYS:N	2.07	0.68
5:B:282:ILE:HD12	5:B:382:ILE:HD13	1.75	0.68
4:A:567:LYS:HD3	11:H:95:TYR:CD2	2.28	0.68
4:A:666:ILE:HD12	4:A:667:GLY:H	1.57	0.68
5:B:1180:PHE:HB3	5:B:1191:ILE:HD12	1.76	0.68
5:B:1223:ASP:O	5:B:1224:PHE:HB2	1.92	0.68
9:F:82:THR:HG22	9:F:84:TYR:H	1.56	0.68
11:H:99:GLY:HA3	11:H:118:PHE:HA	1.75	0.68
4:A:1348:LEU:HG	4:A:1372:VAL:HG23	1.74	0.68
4:A:547:LEU:HD22	14:K:58:PHE:CD1	2.29	0.68
5:B:824:ILE:CG2	5:B:1087:PHE:HE2	2.03	0.68
5:B:293:PRO:HG2	5:B:296:GLU:HB3	1.75	0.68
6:C:114:TYR:HB3	6:C:140:ASN:O	1.93	0.68
6:C:167:HIS:CE1	15:L:70:ARG:HB3	2.29	0.68
4:A:1152:ILE:HG13	12:I:44:TYR:HB3	1.76	0.68
4:A:763:ALA:O	4:A:803:SER:HB3	1.93	0.68
4:A:325:ILE:HG21	5:B:1210:MET:HG3	1.76	0.68
13:J:44:TYR:HA	13:J:47:ARG:HB2	1.74	0.68
3:P:1:A:H2'	3:P:2:A:C8	2.28	0.68
6:C:56:THR:HG22	6:C:57:VAL:N	2.09	0.68
15:L:40:LEU:HD13	15:L:44:ASP:HB3	1.76	0.68
4:A:152:VAL:HG12	4:A:153:PRO:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:198:ILE:CD1	8:E:212:ARG:HG3	2.23	0.68
5:B:502:ILE:HG22	5:B:507:LYS:HD2	1.76	0.68
5:B:745:PRO:O	5:B:748:ILE:HG12	1.94	0.68
9:F:130:ILE:O	9:F:148:VAL:HG21	1.93	0.68
4:A:1445:ILE:N	4:A:1445:ILE:HD12	2.06	0.67
4:A:475:THR:CG2	4:A:476:SER:H	2.07	0.67
4:A:800:VAL:HG13	4:A:812:GLU:OE1	1.94	0.67
6:C:253:LYS:O	6:C:256:ALA:HB3	1.95	0.67
6:C:73:GLN:NE2	6:C:74:SER:H	1.92	0.67
5:B:1208:MET:O	5:B:1211:ASN:N	2.23	0.67
6:C:179:GLU:HG2	6:C:180:TYR:H	1.59	0.67
9:F:90:ARG:HG3	9:F:91:ALA:N	2.09	0.67
4:A:567:LYS:CE	11:H:46:LEU:HB2	2.25	0.67
4:A:1341:ILE:CG2	4:A:1342:GLU:N	2.57	0.67
4:A:3:GLY:O	4:A:4:GLN:HB2	1.94	0.67
4:A:503:GLN:NE2	9:F:90:ARG:HH21	1.92	0.67
4:A:458:HIS:CE1	4:A:507:VAL:HG21	2.30	0.67
4:A:69:THR:C	4:A:71:GLN:H	1.95	0.67
5:B:653:VAL:CG2	5:B:689:LEU:HB3	2.24	0.67
7:D:170:THR:HG21	7:D:172:LEU:HG	1.75	0.67
2:N:3:DG:H2'	2:N:4:DT:OP2	1.93	0.67
4:A:55:ASP:CG	4:A:55:ASP:O	2.31	0.67
5:B:393:LYS:HE3	5:B:393:LYS:HA	1.77	0.67
7:D:198:LEU:O	7:D:200:ASN:N	2.27	0.67
13:J:44:TYR:HA	13:J:47:ARG:CB	2.24	0.67
1:T:23:DG:H2'	1:T:24:DG:C8	2.29	0.67
4:A:356:ASP:HB2	4:A:469:ARG:HH11	1.56	0.67
5:B:1045:SER:O	5:B:1046:PRO:O	2.12	0.67
10:G:138:THR:HG22	10:G:139:ILE:N	2.09	0.67
4:A:1017:LEU:HB2	8:E:206:GLY:N	2.06	0.67
4:A:399:HIS:HB3	4:A:400:PRO:CD	2.17	0.67
4:A:590:ARG:HH11	4:A:590:ARG:HG3	1.59	0.67
4:A:79:GLY:HA3	4:A:243:PRO:HG2	1.77	0.67
4:A:844:ALA:C	4:A:845:LEU:HD23	2.15	0.67
4:A:869:GLY:O	8:E:204:THR:HG21	1.94	0.67
7:D:40:HIS:CB	10:G:73:LYS:HZ2	2.07	0.67
5:B:758:PHE:CE1	5:B:1027:ILE:HG22	2.29	0.67
5:B:746:SER:HB2	5:B:1046:PRO:HG2	1.76	0.67
5:B:108:VAL:HG12	5:B:109:THR:H	1.58	0.67
5:B:955:THR:CG2	5:B:956:THR:H	2.08	0.67
8:E:48:ASP:CG	8:E:49:SER:H	1.99	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:90:VAL:HG23	8:E:120:ALA:HA	1.76	0.67
12:I:55:THR:CG2	12:I:58:VAL:HG21	2.25	0.67
4:A:450:LEU:H	4:A:450:LEU:HD12	1.60	0.67
5:B:860:MET:HG2	5:B:861:ASP:N	2.10	0.67
8:E:157:SER:OG	8:E:160:GLU:HG3	1.94	0.67
4:A:874:ASP:N	4:A:1058:VAL:HG22	2.10	0.66
4:A:1336:MET:CE	4:A:1381:LEU:HG	2.26	0.66
4:A:19:PHE:O	4:A:1416:ALA:HA	1.95	0.66
5:B:192:LEU:O	5:B:193:LYS:HB2	1.95	0.66
5:B:1065:GLN:NE2	5:B:1066:SER:N	2.42	0.66
5:B:125:SER:HA	5:B:171:PRO:HA	1.77	0.66
5:B:244:LEU:HD21	5:B:366:GLN:NE2	2.09	0.66
5:B:515:HIS:CD2	5:B:517:THR:H	2.12	0.66
5:B:563:MET:HE3	5:B:580:VAL:HB	1.76	0.66
4:A:1261:LYS:O	4:A:1264:GLU:HB3	1.95	0.66
4:A:351:THR:HG22	5:B:1103:ILE:HA	1.76	0.66
5:B:899:ILE:CD1	5:B:911:ILE:HA	2.26	0.66
5:B:95:ILE:HG13	5:B:130:VAL:HG22	1.77	0.66
5:B:975:GLN:HG2	5:B:976:ILE:H	1.60	0.66
11:H:17:PRO:HB3	11:H:24:CYS:SG	2.35	0.66
4:A:12:ARG:HD2	5:B:1218:THR:HB	1.76	0.66
4:A:503:GLN:C	4:A:504:LEU:HD12	2.16	0.66
5:B:376:PHE:CE2	5:B:569:TYR:HD2	2.12	0.66
5:B:508:LEU:O	5:B:509:ALA:CB	2.43	0.66
10:G:143:ILE:HG22	10:G:144:ARG:N	2.10	0.66
4:A:1444:MET:HG2	10:G:60:ARG:HA	1.75	0.66
4:A:567:LYS:HE3	11:H:46:LEU:HB2	1.78	0.66
4:A:335:ARG:HH12	5:B:1202:LEU:HD13	1.58	0.66
5:B:516:ASN:ND2	5:B:516:ASN:N	2.43	0.66
5:B:642:ASP:HB3	5:B:649:LYS:CD	2.26	0.66
6:C:39:ALA:CA	6:C:164:ALA:HB3	2.22	0.66
11:H:126:GLU:C	11:H:130:ARG:HH22	1.98	0.66
4:A:899:VAL:HB	4:A:929:LEU:HD11	1.77	0.66
5:B:852:ARG:HH22	15:L:70:ARG:C	1.99	0.66
6:C:66:ARG:HH21	13:J:5:VAL:HG23	1.61	0.66
4:A:666:ILE:HD11	5:B:1067:ARG:O	1.95	0.66
5:B:503:GLY:HA3	5:B:507:LYS:CE	2.25	0.66
5:B:952:VAL:HG12	5:B:953:LEU:N	2.11	0.66
12:I:32:CYS:SG	12:I:33:SER:N	2.69	0.66
4:A:1291:VAL:HG13	4:A:1292:PRO:CD	2.26	0.66
4:A:23:SER:HA	4:A:233:TRP:CD1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:701:LEU:HD21	12:I:114:GLN:HB2	1.78	0.66
5:B:859:TYR:CZ	5:B:941:LEU:HD12	2.31	0.66
1:T:20:DC:H4'	4:A:447:GLN:CD	2.16	0.66
4:A:590:ARG:HH21	4:A:620:LYS:HB3	1.60	0.66
5:B:229:ALA:HB1	5:B:231:PRO:HD2	1.77	0.66
5:B:357:GLN:O	5:B:366:GLN:HA	1.96	0.66
5:B:39:ARG:HH21	5:B:665:GLU:HG2	1.60	0.66
11:H:81:PRO:CB	11:H:82:PRO:CD	2.73	0.66
4:A:868:TYR:HD2	4:A:1058:VAL:HG21	1.59	0.65
5:B:1182:CYS:SG	5:B:1182:CYS:O	2.54	0.65
5:B:46:GLN:HG3	5:B:47:GLN:N	2.10	0.65
8:E:153:HIS:HB3	8:E:196:VAL:HG11	1.78	0.65
10:G:43:GLY:HA3	10:G:80:LYS:HB3	1.76	0.65
4:A:1120:LEU:O	4:A:1323:ASP:HB2	1.96	0.65
4:A:269:ILE:HD13	4:A:300:VAL:HG22	1.78	0.65
4:A:567:LYS:CB	11:H:95:TYR:HA	2.25	0.65
4:A:535:THR:CG2	4:A:616:VAL:HA	2.26	0.65
5:B:821:GLN:HE22	5:B:851:PHE:HA	1.60	0.65
6:C:147:LEU:HB2	6:C:151:GLN:HB2	1.78	0.65
7:D:56:ARG:HD3	7:D:149:THR:HA	1.77	0.65
9:F:79:ARG:HG3	9:F:144:GLU:OE1	1.96	0.65
10:G:59:GLY:HA3	10:G:70:PHE:CD2	2.32	0.65
5:B:995:ARG:NH1	6:C:165:LYS:HG2	2.10	0.65
11:H:100:THR:OG1	11:H:138:GLU:HG3	1.97	0.65
4:A:108:MET:N	4:A:108:MET:SD	2.69	0.65
4:A:2:VAL:HG21	5:B:1157:ALA:C	2.17	0.65
5:B:978:ASP:OD2	5:B:1098:MET:HG2	1.95	0.65
5:B:616:ILE:N	5:B:616:ILE:HD12	2.11	0.65
4:A:548:ASN:OD1	14:K:60:ALA:HB1	1.97	0.65
4:A:1115:SER:O	4:A:1116:LEU:HB3	1.94	0.65
5:B:179:CYS:SG	5:B:181:LEU:HB2	2.37	0.65
5:B:465:ASN:HD22	5:B:465:ASN:N	1.95	0.65
6:C:177:GLU:HG3	6:C:231:ASN:HD22	1.62	0.65
4:A:907:THR:CG2	4:A:908:LEU:N	2.58	0.65
7:D:134:THR:HG22	7:D:135:GLY:N	2.12	0.65
5:B:121:ASN:HA	5:B:207:GLY:HA2	1.79	0.65
8:E:202:SER:OG	8:E:204:THR:HG22	1.97	0.65
8:E:176:PRO:O	8:E:212:ARG:HA	1.96	0.65
5:B:766:ARG:HH22	5:B:1020:ARG:HH11	1.42	0.65
5:B:172:ILE:HD13	5:B:178:ASN:CB	2.27	0.65
5:B:557:PHE:CD2	5:B:557:PHE:C	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:642:ASP:HA	5:B:649:LYS:HA	1.77	0.65
11:H:56:THR:HB	11:H:145:ARG:HG2	1.79	0.65
4:A:1224:LEU:HD12	4:A:1241:ARG:O	1.97	0.65
4:A:385:ILE:HG22	4:A:386:ASP:N	2.11	0.65
6:C:252:GLN:HG3	14:K:95:ILE:HG23	1.79	0.65
4:A:18:GLN:HB2	5:B:1215:ARG:HB2	1.80	0.65
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.77	0.65
5:B:190:TYR:CE2	13:J:62:ARG:HB3	2.31	0.64
6:C:77:ILE:HG23	6:C:161:LYS:HE3	1.79	0.64
6:C:80:LEU:HD11	6:C:95:CYS:CA	2.28	0.64
7:D:130:LEU:O	7:D:132:GLN:N	2.29	0.64
7:D:202:ILE:HG21	7:D:207:LEU:HB2	1.78	0.64
2:N:1:DA:H1'	2:N:2:DA:O5'	1.96	0.64
3:P:9:G:H5''	5:B:776:GLN:HE22	1.62	0.64
4:A:1438:THR:HB	5:B:1144:ALA:HB3	1.80	0.64
7:D:5:THR:O	7:D:6:SER:O	2.15	0.64
4:A:332:LYS:HG3	4:A:333:GLU:HG2	1.77	0.64
4:A:618:GLU:O	4:A:620:LYS:N	2.30	0.64
4:A:630:ILE:HD13	4:A:646:PHE:CZ	2.32	0.64
5:B:604:ARG:HH22	5:B:614:SER:HA	1.63	0.64
8:E:84:ASP:O	8:E:86:PRO:HD3	1.97	0.64
4:A:1402:PHE:CE1	4:A:1403:GLU:HG3	2.33	0.64
4:A:33:ALA:O	4:A:83:HIS:HD2	1.81	0.64
4:A:68:GLN:C	4:A:70:CYS:H	2.00	0.64
4:A:901:LEU:CG	4:A:926:GLN:HE21	2.10	0.64
4:A:979:SER:OG	4:A:980:ASP:N	2.30	0.64
5:B:515:HIS:O	5:B:518:HIS:HB2	1.97	0.64
10:G:81:PRO:HG3	10:G:106:MET:SD	2.36	0.64
10:G:1:MET:HE3	10:G:80:LYS:C	2.17	0.64
11:H:4:THR:CA	11:H:60:ALA:HB2	2.22	0.64
4:A:1206:ASP:HB3	4:A:1274:ARG:HH12	1.61	0.64
5:B:999:MET:HE3	5:B:999:MET:HA	1.77	0.64
6:C:238:ILE:CG2	6:C:242:GLN:HB2	2.27	0.64
8:E:179:GLN:HB2	8:E:182:ASP:HB2	1.78	0.64
10:G:34:VAL:CG1	10:G:45:ILE:HG21	2.26	0.64
4:A:798:GLY:HA2	4:A:815:PHE:HD1	1.60	0.64
5:B:295:GLY:N	5:B:298:LEU:HD23	2.13	0.64
5:B:705:MET:H	5:B:710:LEU:CD1	2.11	0.64
8:E:93:MET:SD	8:E:97:VAL:HG23	2.37	0.64
8:E:192:ARG:HH11	8:E:192:ARG:HG3	1.62	0.64
11:H:99:GLY:N	11:H:118:PHE:HD2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1428:VAL:HG13	5:B:1151:LEU:CD2	2.27	0.64
5:B:777:ALA:HA	5:B:1095:LEU:HA	1.78	0.64
12:I:6:PHE:HB3	12:I:12:ASN:O	1.97	0.64
4:A:901:LEU:O	4:A:921:GLY:N	2.30	0.64
7:D:122:GLU:HA	7:D:125:SER:OG	1.98	0.64
8:E:15:ALA:O	8:E:19:VAL:HG23	1.98	0.64
4:A:1072:ILE:O	4:A:1075:PRO:HD2	1.98	0.64
4:A:863:VAL:HG11	4:A:866:PHE:CD2	2.33	0.64
5:B:911:ILE:HD11	5:B:941:LEU:HD13	1.78	0.64
6:C:172:PRO:O	6:C:235:VAL:HG23	1.97	0.64
10:G:88:ASP:HB3	10:G:144:ARG:HA	1.80	0.64
4:A:1107:VAL:HG12	4:A:1107:VAL:O	1.98	0.63
4:A:1116:LEU:HD11	4:A:1118:VAL:HG13	1.80	0.63
4:A:1166:ASP:OD2	4:A:1239:ARG:HD2	1.97	0.63
4:A:518:LYS:HE2	4:A:624:SER:O	1.97	0.63
5:B:1183:LYS:N	5:B:1183:LYS:CE	2.61	0.63
7:D:56:ARG:HB2	7:D:148:LEU:HD22	1.79	0.63
8:E:14:ARG:HH21	8:E:141:VAL:CG1	2.11	0.63
10:G:9:LEU:HD12	10:G:10:ASN:H	1.62	0.63
13:J:36:LEU:HD12	13:J:47:ARG:HH12	1.61	0.63
4:A:467:THR:O	4:A:469:ARG:HG3	1.99	0.63
5:B:635:ARG:NH2	5:B:742:GLU:OE2	2.32	0.63
6:C:22:LEU:HD13	6:C:230:MET:CE	2.28	0.63
4:A:1323:ASP:OD1	4:A:1325:THR:HB	1.98	0.63
5:B:880:THR:O	5:B:881:ASN:HB2	1.97	0.63
6:C:191:TYR:HD2	6:C:201:TRP:CD1	2.16	0.63
4:A:547:LEU:HB3	14:K:58:PHE:HE1	1.63	0.63
4:A:1341:ILE:HD12	4:A:1379:GLY:O	1.98	0.63
4:A:541:ILE:HD13	4:A:549:MET:CE	2.29	0.63
4:A:901:LEU:HD22	4:A:919:ILE:CG2	2.28	0.63
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.81	0.63
5:B:212:LEU:HD23	5:B:480:SER:HB2	1.80	0.63
5:B:798:TYR:HE2	6:C:62:PHE:CZ	2.17	0.63
5:B:1087:PHE:HD2	5:B:1088:GLY:N	1.97	0.63
5:B:549:THR:H	5:B:628:THR:HG23	1.63	0.63
4:A:1325:THR:O	8:E:148:GLU:HB2	1.98	0.63
4:A:84:ILE:HG23	4:A:84:ILE:O	1.97	0.63
5:B:121:ASN:HA	5:B:207:GLY:CA	2.28	0.63
7:D:173:HIS:O	7:D:177:VAL:HG23	1.98	0.63
5:B:622:LYS:HE2	12:I:59:VAL:HG22	1.79	0.63
4:A:265:LYS:NZ	4:A:322:VAL:HG22	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:567:LYS:HB3	11:H:96:VAL:N	2.12	0.63
10:G:1:MET:O	10:G:1:MET:SD	2.56	0.63
4:A:18:GLN:O	5:B:1215:ARG:HG2	1.98	0.63
4:A:265:LYS:HE2	4:A:322:VAL:CG1	2.29	0.63
4:A:728:LYS:O	4:A:732:LEU:HG	1.97	0.63
13:J:44:TYR:HD2	13:J:44:TYR:H	1.47	0.63
4:A:613:ILE:O	4:A:614:PHE:HB3	1.97	0.63
4:A:552:TRP:HE3	4:A:651:LYS:HB3	1.64	0.63
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.79	0.63
5:B:284:ILE:HD13	5:B:333:PHE:HD2	1.63	0.63
5:B:857:ARG:HD2	5:B:945:GLU:OE1	1.97	0.63
6:C:164:ALA:HA	6:C:167:HIS:O	1.98	0.63
4:A:504:LEU:HD11	9:F:91:ALA:HB1	1.79	0.63
5:B:237:VAL:HG22	5:B:257:LYS:HA	1.81	0.62
5:B:65:GLU:HG3	5:B:66:ASP:N	2.11	0.62
5:B:604:ARG:NH1	5:B:691:GLU:OE2	2.31	0.62
4:A:782:ARG:NH2	5:B:699:GLU:O	2.31	0.62
6:C:73:GLN:HB3	6:C:131:HIS:H	1.62	0.62
7:D:176:GLU:C	7:D:178:ALA:H	2.02	0.62
4:A:404:TYR:HB2	4:A:433:GLU:HB2	1.80	0.62
4:A:606:LEU:HB3	4:A:614:PHE:CE2	2.33	0.62
4:A:720:ARG:O	4:A:724:GLU:HB2	1.98	0.62
4:A:853:ASP:OD1	4:A:855:THR:HG22	1.98	0.62
5:B:1034:VAL:HG23	5:B:1059:LEU:HD13	1.81	0.62
5:B:205:ILE:O	5:B:207:GLY:N	2.33	0.62
6:C:73:GLN:HE21	6:C:74:SER:H	1.45	0.62
8:E:157:SER:C	8:E:159:ASP:H	2.03	0.62
10:G:18:PHE:HA	10:G:22:MET:CE	2.28	0.62
15:L:53:HIS:O	15:L:55:ILE:HG12	1.99	0.62
4:A:809:THR:OG1	4:A:812:GLU:HG3	1.98	0.62
4:A:665:GLY:HA2	5:B:1026:LEU:HD21	1.79	0.62
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.79	0.62
5:B:642:ASP:HB3	5:B:649:LYS:HG3	1.80	0.62
4:A:71:GLN:C	4:A:73:GLY:H	2.02	0.62
4:A:75:ASN:O	4:A:76:GLU:HB3	1.98	0.62
4:A:767:GLN:OE1	4:A:799:PHE:HB2	2.00	0.62
4:A:901:LEU:N	4:A:926:GLN:NE2	2.41	0.62
5:B:827:ILE:HD12	5:B:1086:PHE:CD2	2.34	0.62
5:B:233:PRO:HG2	5:B:234:ILE:CD1	2.28	0.62
5:B:293:PRO:HG2	5:B:296:GLU:CB	2.30	0.62
14:K:10:PHE:CD2	14:K:10:PHE:N	2.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1214:GLU:O	4:A:1218:GLN:HG2	1.99	0.62
4:A:93:VAL:HG22	4:A:301:ALA:HA	1.82	0.62
5:B:1082:MET:O	6:C:189:THR:HG23	1.99	0.62
5:B:36:ALA:HA	5:B:39:ARG:HD2	1.81	0.62
6:C:133:ILE:CD1	6:C:237:SER:HA	2.30	0.62
6:C:152:GLU:OE2	6:C:154:LYS:HE3	1.99	0.62
12:I:62:ILE:HG12	12:I:62:ILE:O	2.00	0.62
4:A:1019:CYS:O	4:A:1022:LEU:N	2.32	0.62
4:A:14:VAL:H	4:A:1432:GLN:HE22	1.48	0.62
4:A:23:SER:HB3	4:A:233:TRP:CE2	2.35	0.62
4:A:541:ILE:HD13	4:A:549:MET:HE1	1.81	0.62
4:A:699:ALA:HB3	4:A:701:LEU:HG	1.81	0.62
4:A:714:PHE:O	4:A:718:VAL:HG23	2.00	0.62
4:A:783:THR:HG21	4:A:815:PHE:CE2	2.35	0.62
4:A:899:VAL:HB	4:A:929:LEU:HD12	1.82	0.62
5:B:1107:ALA:O	5:B:1108:ARG:HG2	1.99	0.62
5:B:758:PHE:CE2	5:B:1044:ALA:HA	2.35	0.62
4:A:308:ILE:HG22	4:A:309:ALA:H	1.64	0.62
4:A:590:ARG:HB2	4:A:605:MET:HB3	1.81	0.62
4:A:855:THR:HG23	4:A:857:ARG:HG3	1.80	0.62
5:B:515:HIS:H	5:B:518:HIS:HD2	1.47	0.62
8:E:207:ARG:HH11	8:E:207:ARG:CB	2.12	0.62
4:A:1209:MET:HE1	4:A:1236:LEU:HB3	1.82	0.62
4:A:675:THR:O	4:A:679:ILE:HG13	1.98	0.62
4:A:897:TYR:CD2	4:A:936:LEU:HD13	2.35	0.62
11:H:113:ALA:HB2	11:H:126:GLU:HG3	1.81	0.62
13:J:2:ILE:H	13:J:57:ILE:CG2	2.13	0.62
5:B:43:LEU:HD11	5:B:811:TYR:O	2.00	0.62
7:D:53:SER:HB3	7:D:152:SER:CA	2.30	0.62
4:A:1017:LEU:HB3	8:E:205:SER:HA	1.80	0.62
4:A:1120:LEU:HD13	4:A:1304:TRP:O	2.00	0.62
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.30	0.62
4:A:262:LEU:O	4:A:264:PHE:N	2.33	0.62
5:B:611:PRO:HB3	5:B:685:LEU:HD11	1.80	0.62
5:B:737:THR:CG2	12:I:66:PRO:HA	2.30	0.62
7:D:134:THR:CG2	7:D:135:GLY:N	2.62	0.62
11:H:44:VAL:O	11:H:44:VAL:HG12	1.99	0.62
4:A:1007:ILE:C	4:A:1009:ASN:H	2.03	0.61
4:A:1057:VAL:HG12	4:A:1058:VAL:H	1.64	0.61
4:A:1227:ILE:HG22	4:A:1228:TRP:N	2.14	0.61
4:A:384:ASN:CG	4:A:388:LEU:HD12	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1162:ILE:HD11	5:B:1194:ILE:HD13	1.82	0.61
5:B:189:LEU:O	5:B:192:LEU:N	2.29	0.61
6:C:212:PRO:CB	6:C:213:PRO:HD2	2.30	0.61
7:D:53:SER:HB3	7:D:152:SER:HA	1.82	0.61
13:J:57:ILE:HA	13:J:60:PHE:CD2	2.32	0.61
4:A:340:LEU:HD21	5:B:1200:ALA:N	2.15	0.61
4:A:463:ILE:HD12	4:A:469:ARG:HD2	1.82	0.61
4:A:825:ILE:CG2	5:B:508:LEU:HD11	2.30	0.61
5:B:1169:MET:HE1	5:B:1201:LYS:HA	1.81	0.61
5:B:842:ASN:ND2	5:B:845:SER:H	1.98	0.61
8:E:23:VAL:HG13	8:E:78:LEU:HD13	1.82	0.61
13:J:14:VAL:HG12	13:J:14:VAL:O	2.00	0.61
4:A:1155:ASP:OD1	4:A:1161:THR:HA	2.00	0.61
4:A:263:THR:HG22	4:A:263:THR:O	2.00	0.61
4:A:319:GLY:HA3	5:B:471:LYS:HA	1.82	0.61
4:A:349:ALA:C	5:B:1128:LEU:HD11	2.20	0.61
4:A:471:ASN:OD1	4:A:472:LEU:N	2.34	0.61
4:A:738:LYS:HB2	4:A:740:LEU:HG	1.83	0.61
4:A:765:VAL:HG12	4:A:766:GLY:N	2.15	0.61
5:B:1065:GLN:HE21	5:B:1066:SER:N	1.97	0.61
5:B:770:GLN:CD	5:B:983:ARG:HA	2.20	0.61
7:D:47:LEU:HD11	10:G:3:PHE:CD2	2.35	0.61
11:H:89:LEU:C	11:H:91:ASP:H	2.04	0.61
4:A:1127:ASP:HB3	4:A:1130:GLN:CB	2.30	0.61
4:A:1305:VAL:HG12	4:A:1306:LEU:N	2.16	0.61
4:A:337:ARG:HD3	5:B:1132:GLU:OE1	2.01	0.61
5:B:705:MET:N	5:B:710:LEU:HD12	2.13	0.61
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.82	0.61
5:B:865:LYS:HE2	5:B:871:THR:OG1	2.01	0.61
6:C:98:VAL:O	6:C:99:LEU:HD23	2.00	0.61
10:G:1:MET:HG3	10:G:85:GLU:OE2	2.01	0.61
4:A:40:THR:HG22	4:A:41:MET:CG	2.28	0.61
4:A:730:GLY:O	4:A:732:LEU:N	2.34	0.61
5:B:496:ARG:NH1	5:B:539:LEU:HB2	2.16	0.61
5:B:825:VAL:CG1	5:B:826:ALA:N	2.63	0.61
9:F:89:GLU:OE2	9:F:134:ILE:HG21	2.01	0.61
14:K:65:HIS:HD2	14:K:67:PHE:N	1.94	0.61
4:A:49:LYS:HZ1	4:A:61:ILE:N	1.97	0.61
4:A:666:ILE:CD1	4:A:667:GLY:H	2.14	0.61
5:B:114:PRO:HG2	5:B:115:GLN:H	1.65	0.61
5:B:227:LYS:HB2	5:B:395:GLN:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.35	0.61
5:B:1006:ILE:HD13	13:J:44:TYR:CE2	2.35	0.61
8:E:180:ARG:HH21	8:E:192:ARG:CB	2.10	0.61
4:A:244:PRO:O	4:A:246:VAL:N	2.33	0.61
4:A:321:PRO:O	4:A:322:VAL:CB	2.49	0.61
4:A:981:LEU:CD2	4:A:1039:LYS:HA	2.31	0.61
4:A:351:THR:HB	5:B:1103:ILE:CD1	2.30	0.61
9:F:101:ILE:HD11	9:F:124:GLU:OE1	2.01	0.61
4:A:1410:PHE:HA	5:B:1212:ILE:HD11	1.83	0.61
5:B:496:ARG:NH1	5:B:496:ARG:HB3	2.15	0.61
3:P:8:G:O2'	3:P:9:G:H5'	2.00	0.61
4:A:1114:PRO:O	4:A:1115:SER:O	2.19	0.61
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.01	0.61
6:C:76:ASP:OD2	6:C:128:ASN:N	2.34	0.61
4:A:1149:ALA:HB2	12:I:47:GLU:HA	1.83	0.61
4:A:1002:GLY:HA3	4:A:1007:ILE:HG21	1.82	0.60
4:A:50:ILE:O	4:A:52:GLY:N	2.31	0.60
3:P:9:G:H5''	5:B:776:GLN:NE2	2.16	0.60
5:B:999:MET:HA	5:B:999:MET:CE	2.31	0.60
9:F:111:LEU:C	9:F:113:GLY:H	2.04	0.60
12:I:101:PHE:N	12:I:101:PHE:CD1	2.67	0.60
4:A:1313:LEU:O	4:A:1315:GLU:N	2.34	0.60
4:A:384:ASN:O	4:A:385:ILE:C	2.40	0.60
4:A:481:ASP:OD1	4:A:485:ASP:OD2	2.19	0.60
4:A:746:MET:HE3	5:B:1018:PRO:HG2	1.83	0.60
4:A:466:SER:O	5:B:1103:ILE:HD11	2.01	0.60
5:B:794:ASN:O	5:B:795:ILE:HD12	2.00	0.60
5:B:822:ASN:O	13:J:48:ARG:NH1	2.34	0.60
5:B:846:ILE:HG23	5:B:974:PRO:HG2	1.83	0.60
5:B:955:THR:CG2	5:B:956:THR:N	2.63	0.60
9:F:135:ARG:HD3	9:F:143:PHE:CD2	2.36	0.60
10:G:14:HIS:ND1	10:G:15:PRO:HD2	2.16	0.60
10:G:1:MET:C	10:G:1:MET:SD	2.80	0.60
4:A:598:LEU:HD22	11:H:25:ARG:NH1	2.16	0.60
4:A:1057:VAL:HG12	4:A:1058:VAL:N	2.16	0.60
4:A:265:LYS:HD2	4:A:265:LYS:N	2.16	0.60
5:B:1197:PRO:HG2	5:B:1200:ALA:CB	2.29	0.60
6:C:112:ASN:HB2	6:C:114:TYR:CE1	2.36	0.60
4:A:504:LEU:HD11	9:F:91:ALA:CB	2.31	0.60
5:B:213:ILE:HD12	5:B:497:ARG:HB3	1.83	0.60
5:B:230:ALA:N	5:B:231:PRO:HD2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:744:HIS:CG	5:B:745:PRO:HD2	2.36	0.60
5:B:850:LEU:HD12	5:B:851:PHE:N	2.16	0.60
6:C:124:LEU:O	6:C:127:ARG:HG2	2.02	0.60
4:A:1097:GLY:O	4:A:1100:ARG:HB3	2.01	0.60
4:A:114:LEU:HD13	4:A:171:GLN:OE1	2.02	0.60
4:A:341:MET:HE1	4:A:843:LYS:NZ	2.17	0.60
4:A:979:SER:OG	4:A:981:LEU:HG	2.01	0.60
11:H:89:LEU:HB3	11:H:91:ASP:OD1	2.02	0.60
6:C:66:ARG:NH2	13:J:3:VAL:O	2.34	0.60
4:A:1364:ASN:HD22	4:A:1365:TYR:N	1.99	0.60
4:A:366:VAL:HG21	4:A:460:VAL:HG22	1.84	0.60
4:A:475:THR:CG2	4:A:476:SER:N	2.64	0.60
1:T:18:DC:H5'	4:A:832:ALA:O	2.02	0.60
4:A:108:MET:SD	4:A:210:ILE:HD13	2.41	0.60
4:A:818:MET:HA	5:B:514:LEU:HB3	1.84	0.60
5:B:696:GLU:O	5:B:699:GLU:HB2	2.00	0.60
6:C:67:LEU:HD11	6:C:155:LEU:CD1	2.32	0.60
6:C:80:LEU:CD1	6:C:95:CYS:HA	2.32	0.60
4:A:1362:TYR:CD1	4:A:1363:VAL:N	2.70	0.60
4:A:783:THR:HG22	4:A:784:LEU:HG	1.82	0.60
5:B:118:ARG:HH22	5:B:194:GLU:CD	2.05	0.60
5:B:225:VAL:HG11	5:B:385:LEU:HA	1.84	0.60
14:K:49:GLU:HG3	14:K:94:ILE:CG1	2.32	0.60
4:A:1121:GLU:CG	4:A:1122:PRO:HD2	2.31	0.60
4:A:1373:ASP:HA	4:A:1376:THR:HG22	1.82	0.60
4:A:90:VAL:HG13	4:A:297:GLN:HA	1.82	0.60
4:A:965:GLN:O	4:A:968:GLN:HB2	2.02	0.60
12:I:13:MET:HG3	12:I:14:LEU:N	2.16	0.60
4:A:998:LEU:HD12	4:A:998:LEU:H	1.66	0.59
6:C:69:LEU:HD12	6:C:69:LEU:N	2.16	0.59
9:F:96:THR:O	9:F:99:LEU:HB3	2.02	0.59
4:A:265:LYS:HE2	4:A:322:VAL:HG13	1.83	0.59
4:A:289:ILE:C	4:A:291:GLU:H	2.05	0.59
5:B:1166:CYS:O	5:B:1166:CYS:SG	2.59	0.59
5:B:378:LEU:O	5:B:382:ILE:HG13	2.00	0.59
5:B:515:HIS:H	5:B:518:HIS:CD2	2.19	0.59
5:B:637:LEU:HD12	5:B:693:ILE:HD12	1.84	0.59
5:B:816:GLU:O	5:B:817:LEU:HD23	2.02	0.59
6:C:18:VAL:O	6:C:18:VAL:HG12	2.02	0.59
12:I:111:THR:HG22	12:I:112:SER:H	1.67	0.59
14:K:61:TYR:C	14:K:61:TYR:CD2	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:230:ARG:H	4:A:233:TRP:HE3	1.42	0.59
4:A:49:LYS:HZ3	4:A:61:ILE:HG13	1.66	0.59
4:A:741:ASN:ND2	4:A:743:VAL:HB	2.18	0.59
4:A:834:THR:HG22	4:A:835:GLY:N	2.17	0.59
5:B:642:ASP:HB3	5:B:649:LYS:CG	2.33	0.59
7:D:54:GLU:O	7:D:58:VAL:HG23	2.01	0.59
12:I:52:ILE:HG13	12:I:52:ILE:O	2.01	0.59
4:A:262:LEU:C	4:A:264:PHE:H	2.05	0.59
5:B:1162:ILE:HG22	5:B:1163:CYS:N	2.16	0.59
5:B:834:ASN:HA	5:B:838:SER:O	2.01	0.59
6:C:35:ARG:NH1	14:K:41:THR:OG1	2.34	0.59
4:A:1299:VAL:HG12	4:A:1300:LYS:N	2.16	0.59
4:A:1336:MET:HE3	4:A:1381:LEU:HG	1.84	0.59
4:A:663:SER:OG	4:A:664:THR:N	2.34	0.59
5:B:521:LEU:HB3	5:B:633:VAL:CG1	2.31	0.59
5:B:616:ILE:HG13	5:B:697:GLU:HG3	1.84	0.59
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.32	0.59
4:A:78:PRO:CB	5:B:1201:LYS:HE3	2.32	0.59
5:B:446:LEU:O	5:B:447:ALA:HB3	2.03	0.59
5:B:46:GLN:CG	5:B:47:GLN:H	2.11	0.59
6:C:18:VAL:HG23	6:C:240:VAL:HB	1.84	0.59
4:A:971:PHE:CE2	4:A:1040:GLN:HG2	2.37	0.59
4:A:264:PHE:O	4:A:267:ALA:HB3	2.01	0.59
4:A:69:THR:C	4:A:71:GLN:N	2.55	0.59
4:A:785:PRO:HG2	4:A:786:HIS:HD2	1.67	0.59
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.83	0.59
5:B:552:MET:HA	5:B:555:ILE:HB	1.84	0.59
1:T:24:DG:OP1	5:B:857:ARG:NH2	2.35	0.59
9:F:86:THR:OG1	9:F:89:GLU:HG3	2.03	0.59
11:H:27:GLU:HA	11:H:38:LEU:O	2.03	0.59
11:H:81:PRO:HB2	11:H:82:PRO:CD	2.31	0.59
12:I:82:GLU:HB3	12:I:104:LEU:HD12	1.84	0.59
13:J:47:ARG:HH11	13:J:47:ARG:HG2	1.66	0.59
4:A:23:SER:HB3	4:A:233:TRP:CZ2	2.38	0.59
4:A:47:ARG:HH12	4:A:254:GLU:HG2	1.68	0.59
5:B:408:LEU:HG	5:B:409:ALA:H	1.66	0.59
12:I:99:LEU:C	12:I:100:PHE:HD1	2.06	0.59
13:J:7:CYS:HB2	13:J:46:CYS:HB3	1.84	0.59
4:A:407:ARG:HG2	4:A:430:TRP:CH2	2.37	0.59
4:A:408:ASP:O	4:A:410:GLY:N	2.34	0.59
4:A:61:ILE:HG22	4:A:62:ASP:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:829:VAL:O	4:A:831:THR:N	2.36	0.59
5:B:1001:PHE:CE2	6:C:34:ARG:CZ	2.85	0.59
5:B:294:ASP:O	5:B:296:GLU:N	2.32	0.59
5:B:376:PHE:HE2	5:B:569:TYR:HD2	1.50	0.59
6:C:166:GLU:O	6:C:167:HIS:HB2	2.02	0.59
6:C:254:LYS:O	6:C:256:ALA:N	2.35	0.59
7:D:51:ASN:O	7:D:54:GLU:HB3	2.03	0.59
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.38	0.59
5:B:1084:GLN:NE2	5:B:1084:GLN:N	2.51	0.59
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.85	0.59
5:B:522:VAL:HG11	5:B:537:LYS:HB3	1.85	0.59
5:B:850:LEU:HD12	5:B:851:PHE:H	1.67	0.59
8:E:178:ILE:HG22	8:E:213:ILE:O	2.02	0.59
11:H:91:ASP:C	11:H:93:TYR:H	2.06	0.59
14:K:69:ALA:O	14:K:70:ARG:HB3	2.03	0.59
4:A:1010:ALA:HA	4:A:1013:ASP:OD2	2.02	0.58
4:A:364:VAL:O	4:A:364:VAL:HG13	2.03	0.58
5:B:1162:ILE:O	5:B:1171:VAL:HG21	2.03	0.58
6:C:18:VAL:O	6:C:20:PHE:HD2	1.85	0.58
6:C:238:ILE:HG23	6:C:242:GLN:HB2	1.85	0.58
4:A:537:ARG:NH1	11:H:120:GLY:O	2.36	0.58
11:H:143:LEU:N	11:H:143:LEU:HD12	2.18	0.58
4:A:1444:MET:HE1	9:F:135:ARG:CB	2.32	0.58
4:A:224:PHE:CE2	4:A:231:PRO:HG3	2.37	0.58
4:A:746:MET:CE	5:B:1018:PRO:HG2	2.34	0.58
5:B:731:VAL:HG12	5:B:732:SER:N	2.18	0.58
8:E:169:ARG:HH12	9:F:74:ILE:HD11	1.68	0.58
8:E:90:VAL:HA	8:E:120:ALA:HB2	1.84	0.58
7:D:47:LEU:HD11	10:G:3:PHE:HD2	1.68	0.58
13:J:21:TYR:HB2	13:J:39:LEU:HD13	1.85	0.58
4:A:1070:GLN:O	4:A:1072:ILE:N	2.37	0.58
4:A:225:ASN:ND2	4:A:228:PHE:H	2.00	0.58
4:A:567:LYS:CG	4:A:568:PRO:CD	2.79	0.58
10:G:1:MET:O	10:G:3:PHE:CE1	2.57	0.58
11:H:100:THR:HG22	11:H:101:ALA:N	2.18	0.58
4:A:119:ASN:O	4:A:122:MET:HB3	2.03	0.58
4:A:1299:VAL:HG12	4:A:1300:LYS:H	1.69	0.58
4:A:1454:MET:O	4:A:1454:MET:HG3	2.03	0.58
4:A:218:ASP:HA	4:A:221:SER:OG	2.03	0.58
4:A:269:ILE:HD11	4:A:300:VAL:HA	1.86	0.58
5:B:842:ASN:HD22	5:B:845:SER:CB	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1364:ASN:O	4:A:1365:TYR:C	2.42	0.58
7:D:51:ASN:O	7:D:52:LEU:O	2.22	0.58
9:F:77:ASP:C	9:F:79:ARG:H	2.05	0.58
11:H:18:GLY:O	11:H:19:ARG:HB2	2.04	0.58
4:A:1435:PRO:O	4:A:1436:ILE:HG13	2.03	0.58
4:A:843:LYS:HD3	4:A:846:GLU:OE2	2.04	0.58
7:D:56:ARG:NH2	7:D:57:LEU:HD21	2.18	0.58
9:F:73:ALA:HA	9:F:143:PHE:CE1	2.38	0.58
4:A:1035:TYR:O	4:A:1037:LEU:N	2.36	0.58
7:D:47:LEU:CD1	7:D:48:ILE:H	2.11	0.58
9:F:90:ARG:HD3	9:F:155:LEU:CD1	2.33	0.58
10:G:17:PHE:CD2	10:G:17:PHE:N	2.69	0.58
4:A:1445:ILE:HG12	10:G:18:PHE:CE2	2.38	0.58
4:A:35:ILE:HD12	4:A:241:VAL:HG21	1.86	0.58
4:A:382:PRO:HD3	4:A:428:TYR:HD2	1.67	0.58
4:A:50:ILE:C	4:A:52:GLY:H	2.06	0.58
4:A:658:LEU:HD23	4:A:659:HIS:CE1	2.38	0.58
4:A:982:THR:HB	4:A:985:ASP:H	1.68	0.58
5:B:1051:THR:HB	5:B:1054:GLY:H	1.68	0.58
5:B:57:TYR:CD1	5:B:57:TYR:N	2.70	0.58
5:B:606:LYS:HD2	5:B:608:ASP:OD2	2.04	0.58
4:A:541:ILE:CG2	4:A:546:VAL:HG23	2.32	0.58
5:B:118:ARG:HH11	5:B:204:ILE:HD11	1.68	0.58
5:B:798:TYR:CE2	6:C:62:PHE:CE2	2.90	0.58
15:L:40:LEU:HD22	15:L:44:ASP:CG	2.24	0.58
4:A:408:ASP:C	4:A:410:GLY:H	2.07	0.58
5:B:653:VAL:HG22	5:B:689:LEU:HB3	1.85	0.58
5:B:797:TYR:HE1	5:B:854:LEU:CD2	2.17	0.58
6:C:36:VAL:HG21	6:C:251:LEU:HD22	1.85	0.58
7:D:7:THR:O	7:D:9:GLN:N	2.37	0.58
10:G:1:MET:HE1	10:G:80:LYS:H	1.67	0.58
7:D:175:PHE:HZ	10:G:85:GLU:HG3	1.69	0.58
11:H:38:LEU:HD12	11:H:124:ARG:O	2.04	0.58
4:A:23:SER:HA	4:A:233:TRP:NE1	2.18	0.57
4:A:774:ARG:NH2	4:A:797:LYS:HB2	2.18	0.57
5:B:377:PHE:O	5:B:380:TYR:N	2.37	0.57
5:B:707:PRO:O	5:B:711:GLU:HG3	2.04	0.57
1:T:16:DT:H4'	4:A:1403:GLU:OE2	2.04	0.57
4:A:299:HIS:O	4:A:301:ALA:N	2.37	0.57
5:B:1099:VAL:C	5:B:1101:ASP:H	2.06	0.57
5:B:981:ALA:HB2	5:B:987:LYS:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:990:ILE:HG22	5:B:991:GLY:N	2.19	0.57
6:C:100:THR:HG22	6:C:101:LEU:N	2.18	0.57
6:C:112:ASN:HD22	6:C:112:ASN:N	2.02	0.57
8:E:114:ASN:O	8:E:115:ASN:HB3	2.03	0.57
4:A:254:GLU:O	4:A:256:GLN:N	2.37	0.57
4:A:500:GLU:OE2	5:B:1145:SER:HB2	2.04	0.57
5:B:1215:ARG:C	5:B:1216:LEU:HD23	2.24	0.57
6:C:66:ARG:NH2	13:J:5:VAL:CG2	2.68	0.57
7:D:35:LEU:HD23	7:D:174:PRO:HD2	1.86	0.57
4:A:1434:ALA:HB3	4:A:1436:ILE:HD12	1.86	0.57
4:A:670:ILE:HG23	4:A:805:LEU:CD2	2.35	0.57
5:B:351:TYR:O	5:B:355:ILE:HG13	2.04	0.57
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.70	0.57
5:B:879:ARG:NH1	5:B:883:LEU:HD22	2.18	0.57
5:B:1102:LYS:O	5:B:1103:ILE:C	2.41	0.57
4:A:836:TYR:O	4:A:839:ARG:N	2.38	0.57
5:B:63:ILE:O	5:B:67:SER:HB3	2.04	0.57
5:B:731:VAL:HG12	5:B:732:SER:H	1.69	0.57
13:J:1:MET:N	13:J:56:LEU:N	2.53	0.57
4:A:1242:VAL:HG12	4:A:1243:VAL:N	2.18	0.57
4:A:185:TRP:CZ3	4:A:200:ARG:HG2	2.39	0.57
4:A:743:VAL:O	4:A:747:VAL:HG23	2.04	0.57
5:B:1040:ASN:O	5:B:1041:GLU:C	2.43	0.57
5:B:838:SER:HB2	5:B:989:THR:O	2.04	0.57
5:B:957:ASN:O	5:B:959:ASP:N	2.38	0.57
4:A:1164:PRO:HG2	4:A:1165:GLU:H	1.68	0.57
4:A:1242:VAL:O	4:A:1243:VAL:HB	2.05	0.57
4:A:1365:TYR:O	4:A:1367:HIS:N	2.38	0.57
4:A:244:PRO:CB	4:A:245:PRO:CD	2.83	0.57
4:A:42:ASP:HB3	4:A:45:GLN:H	1.68	0.57
4:A:469:ARG:NH2	5:B:991:GLY:O	2.38	0.57
5:B:1011:ILE:O	5:B:1011:ILE:HG22	2.04	0.57
5:B:1107:ALA:O	5:B:1108:ARG:O	2.23	0.57
5:B:1115:THR:HG22	5:B:1117:GLN:HG3	1.87	0.57
5:B:167:ILE:HG22	5:B:453:ILE:HD12	1.86	0.57
5:B:321:GLY:O	5:B:323:VAL:N	2.37	0.57
5:B:953:LEU:CD2	5:B:965:LYS:HB2	2.35	0.57
5:B:999:MET:HB3	5:B:1007:VAL:HG21	1.87	0.57
4:A:55:ASP:N	4:A:56:PRO:HD3	2.20	0.57
4:A:982:THR:O	4:A:985:ASP:HB2	2.04	0.57
5:B:782:LEU:HD12	5:B:788:ARG:HH11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:18:PHE:HA	10:G:22:MET:HE2	1.85	0.57
4:A:1441:PHE:CZ	9:F:89:GLU:HA	2.40	0.57
4:A:63:ARG:HA	4:A:74:MET:CE	2.34	0.57
4:A:730:GLY:C	4:A:732:LEU:H	2.08	0.57
5:B:234:ILE:N	5:B:234:ILE:HD12	2.20	0.57
5:B:310:MET:O	5:B:313:MET:HB2	2.04	0.57
5:B:821:GLN:NE2	5:B:851:PHE:HA	2.19	0.57
6:C:22:LEU:HD23	6:C:25:VAL:HG21	1.85	0.57
5:B:39:ARG:HG2	5:B:39:ARG:HH11	1.70	0.56
5:B:806:THR:N	5:B:809:MET:HE3	2.20	0.56
5:B:950:ASP:O	5:B:951:GLN:HB2	2.05	0.56
6:C:258:ILE:N	6:C:258:ILE:HD12	2.19	0.56
8:E:94:LYS:CE	8:E:98:ILE:HD11	2.30	0.56
10:G:51:TYR:C	10:G:51:TYR:CD2	2.79	0.56
11:H:116:TYR:HB2	11:H:123:MET:HB3	1.85	0.56
14:K:31:VAL:CG1	14:K:32:VAL:N	2.68	0.56
14:K:6:ARG:O	14:K:9:LEU:HG	2.05	0.56
4:A:1199:ARG:O	4:A:1202:MET:HB2	2.05	0.56
4:A:1308:THR:HG23	4:A:1309:ASP:N	2.19	0.56
4:A:540:PHE:HB3	4:A:571:LEU:HD23	1.87	0.56
7:D:153:ARG:HH22	7:D:184:ALA:HA	1.67	0.56
11:H:15:VAL:HG22	11:H:26:ILE:HD11	1.86	0.56
12:I:111:THR:HG22	12:I:113:ASP:N	2.20	0.56
13:J:14:VAL:HG12	13:J:50:ILE:HD11	1.85	0.56
1:T:27:DA:C2	3:P:3:G:N2	2.74	0.56
4:A:35:ILE:CD1	4:A:241:VAL:HG21	2.35	0.56
4:A:265:LYS:HD2	4:A:265:LYS:H	1.71	0.56
4:A:858:ASN:ND2	4:A:858:ASN:C	2.55	0.56
5:B:1152:MET:SD	5:B:1197:PRO:HD3	2.45	0.56
5:B:27:ALA:O	5:B:29:ASP:N	2.38	0.56
5:B:315:LYS:N	5:B:316:PRO:HD2	2.21	0.56
5:B:582:VAL:HG23	5:B:626:ILE:HB	1.87	0.56
5:B:654:ARG:H	5:B:657:HIS:HD2	1.52	0.56
4:A:789:LYS:HE3	12:I:67:THR:CB	2.35	0.56
4:A:874:ASP:CA	4:A:1058:VAL:HG22	2.36	0.56
4:A:47:ARG:HH12	4:A:254:GLU:CG	2.18	0.56
4:A:311:GLN:O	4:A:312:PRO:C	2.44	0.56
4:A:416:ARG:C	4:A:417:TYR:HD2	2.09	0.56
5:B:980:PHE:HE2	5:B:1094:ARG:HG3	1.70	0.56
6:C:123:ASN:HD22	6:C:125:MET:HG2	1.68	0.56
6:C:3:GLU:HB3	14:K:104:ASN:HD21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:39:LEU:O	8:E:42:PHE:HB3	2.05	0.56
10:G:1:MET:CE	10:G:1:MET:O	2.53	0.56
12:I:34:TYR:HD2	12:I:35:VAL:N	2.03	0.56
4:A:331:GLY:O	4:A:332:LYS:HB3	2.04	0.56
4:A:49:LYS:HZ1	4:A:61:ILE:HG13	1.70	0.56
5:B:811:TYR:N	5:B:811:TYR:CD1	2.72	0.56
6:C:38:ILE:HA	6:C:173:ALA:HB2	1.88	0.56
13:J:43:ARG:HG3	13:J:45:CYS:SG	2.45	0.56
4:A:299:HIS:C	4:A:301:ALA:H	2.09	0.56
4:A:590:ARG:HH11	4:A:590:ARG:CG	2.18	0.56
4:A:901:LEU:H	4:A:926:GLN:HE21	1.48	0.56
4:A:909:ASP:O	4:A:911:SER:N	2.39	0.56
5:B:195:CYS:SG	5:B:197:PHE:HB2	2.46	0.56
6:C:22:LEU:HD13	6:C:230:MET:HE1	1.88	0.56
9:F:75:PRO:HG2	9:F:78:GLN:HB2	1.87	0.56
15:L:43:THR:O	15:L:43:THR:HG22	2.04	0.56
4:A:1007:ILE:O	4:A:1009:ASN:N	2.38	0.56
4:A:1319:VAL:HG13	4:A:1320:PRO:HD2	1.88	0.56
4:A:1364:ASN:HD22	4:A:1364:ASN:C	2.09	0.56
4:A:466:SER:HB2	5:B:1099:VAL:HG11	1.87	0.56
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.70	0.56
13:J:2:ILE:H	13:J:57:ILE:HG22	1.70	0.56
4:A:1335:ILE:HG23	4:A:1339:LEU:HD12	1.87	0.56
4:A:230:ARG:N	4:A:233:TRP:CE3	2.64	0.56
4:A:384:ASN:O	4:A:386:ASP:N	2.38	0.56
4:A:567:LYS:HD3	11:H:95:TYR:CG	2.40	0.56
4:A:68:GLN:O	4:A:70:CYS:N	2.38	0.56
5:B:217:ARG:C	5:B:217:ARG:HD2	2.26	0.56
9:F:109:VAL:HG21	9:F:124:GLU:HA	1.88	0.56
4:A:382:PRO:HD3	4:A:428:TYR:CE2	2.41	0.56
4:A:499:ALA:O	4:A:503:GLN:HB2	2.05	0.56
4:A:852:TYR:CD2	4:A:1060:PRO:HB2	2.41	0.56
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.39	0.56
5:B:265:SER:O	5:B:266:ALA:HB3	2.05	0.56
5:B:63:ILE:HD12	5:B:421:PHE:CE2	2.40	0.56
5:B:842:ASN:HD22	5:B:845:SER:HB3	1.71	0.56
7:D:63:LEU:HD13	7:D:133:THR:OG1	2.05	0.56
4:A:1343:ALA:HB2	8:E:150:VAL:CG2	2.35	0.56
4:A:548:ASN:HA	14:K:60:ALA:HB1	1.87	0.56
4:A:75:ASN:O	4:A:76:GLU:CB	2.53	0.56
5:B:197:PHE:HZ	5:B:816:GLU:HG2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:309:GLN:HG3	12:I:52:ILE:CD1	2.36	0.56
5:B:980:PHE:CD2	5:B:1094:ARG:HA	2.41	0.56
6:C:226:ASP:O	6:C:227:THR:HB	2.06	0.56
8:E:78:LEU:HD23	8:E:79:TRP:N	2.20	0.56
10:G:80:LYS:HG2	10:G:80:LYS:O	2.05	0.56
14:K:15:GLY:O	14:K:16:GLU:HG3	2.06	0.56
4:A:547:LEU:HD22	14:K:58:PHE:HD1	1.70	0.56
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.45	0.56
4:A:1283:VAL:HG12	4:A:1284:MET:H	1.71	0.56
4:A:907:THR:HG22	4:A:908:LEU:N	2.18	0.56
5:B:217:ARG:HE	5:B:405:ARG:CB	2.07	0.56
4:A:1441:PHE:HB2	9:F:135:ARG:O	2.05	0.56
14:K:63:VAL:HG23	14:K:63:VAL:O	2.06	0.56
2:N:5:DA:H2"	2:N:6:DC:OP2	2.05	0.56
4:A:1220:PHE:O	4:A:1221:LYS:HB2	2.05	0.55
4:A:1369:ALA:O	4:A:1372:VAL:HG12	2.06	0.55
4:A:546:VAL:O	4:A:550:LEU:HG	2.06	0.55
4:A:649:ILE:O	4:A:653:VAL:HG23	2.06	0.55
4:A:754:SER:N	4:A:757:ASN:HD22	1.92	0.55
4:A:913:LEU:HD12	4:A:914:GLU:N	2.21	0.55
4:A:757:ASN:HA	5:B:1021:MET:SD	2.46	0.55
6:C:252:GLN:CG	14:K:95:ILE:HG23	2.36	0.55
12:I:100:PHE:N	12:I:100:PHE:CD1	2.74	0.55
12:I:2:THR:O	12:I:3:THR:C	2.43	0.55
13:J:48:ARG:HE	13:J:49:MET:HE2	1.70	0.55
4:A:115:LEU:O	4:A:122:MET:HE2	2.07	0.55
4:A:1283:VAL:HG12	4:A:1284:MET:N	2.21	0.55
4:A:1430:LEU:HB2	4:A:1432:GLN:HG3	1.88	0.55
4:A:1436:ILE:O	4:A:1437:GLY:C	2.42	0.55
4:A:306:ASN:HB2	4:A:324:SER:HB3	1.88	0.55
4:A:929:LEU:CD2	4:A:983:ILE:HG21	2.36	0.55
5:B:1034:VAL:CG1	5:B:1035:ALA:N	2.69	0.55
5:B:358:LYS:HA	5:B:366:GLN:HB3	1.89	0.55
5:B:523:CYS:SG	5:B:524:PRO:HD2	2.46	0.55
5:B:197:PHE:CZ	5:B:816:GLU:HG2	2.41	0.55
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.42	0.55
8:E:35:VAL:C	8:E:37:LEU:H	2.10	0.55
14:K:49:GLU:HG3	14:K:94:ILE:HG12	1.88	0.55
4:A:1007:ILE:C	4:A:1009:ASN:N	2.59	0.55
4:A:356:ASP:O	4:A:358:ASN:N	2.39	0.55
4:A:673:GLY:O	4:A:676:MET:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:542:MET:HG2	5:B:747:MET:HB3	1.88	0.55
5:B:702:LEU:HD12	5:B:703:ILE:H	1.71	0.55
6:C:48:SER:O	6:C:157:CYS:HA	2.06	0.55
4:A:1444:MET:HE3	9:F:135:ARG:HB2	1.87	0.55
10:G:91:VAL:HB	10:G:139:ILE:O	2.06	0.55
4:A:628:GLY:O	4:A:632:VAL:HG23	2.06	0.55
5:B:980:PHE:CE2	5:B:1094:ARG:HG3	2.41	0.55
10:G:20:PRO:HG2	10:G:21:ARG:H	1.70	0.55
4:A:567:LYS:HZ2	11:H:47:PHE:HB2	1.71	0.55
4:A:1372:VAL:O	4:A:1376:THR:HG22	2.07	0.55
4:A:24:PRO:HD2	4:A:233:TRP:CD1	2.40	0.55
4:A:43:GLU:O	4:A:44:THR:HB	2.07	0.55
4:A:685:GLU:HG3	4:A:686:ALA:N	2.20	0.55
5:B:108:VAL:HG12	5:B:109:THR:N	2.22	0.55
5:B:240:ILE:CG2	5:B:254:LEU:HB3	2.36	0.55
5:B:579:ARG:HG2	5:B:579:ARG:HH11	1.71	0.55
5:B:57:TYR:HD1	5:B:57:TYR:N	2.04	0.55
10:G:79:PHE:CZ	10:G:106:MET:HE1	2.41	0.55
4:A:1290:LYS:O	4:A:1291:VAL:HG23	2.06	0.55
4:A:1428:VAL:HG13	5:B:1151:LEU:HD21	1.88	0.55
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.89	0.55
4:A:598:LEU:O	4:A:599:SER:C	2.45	0.55
5:B:1095:LEU:H	5:B:1095:LEU:CD1	2.14	0.55
5:B:1159:ARG:HD3	5:B:1193:GLN:HG2	1.87	0.55
5:B:918:ILE:HD12	5:B:935:ARG:HD3	1.89	0.55
12:I:106:CYS:O	12:I:107:SER:HB2	2.06	0.55
13:J:23:ASN:C	13:J:25:LEU:H	2.10	0.55
14:K:46:ILE:O	14:K:46:ILE:HG22	2.07	0.55
4:A:1377:THR:O	4:A:1379:GLY:N	2.40	0.55
4:A:341:MET:HE1	4:A:843:LYS:HZ3	1.71	0.55
4:A:828:ALA:HB1	5:B:530:GLY:HA2	1.85	0.55
5:B:763:GLN:C	5:B:765:PRO:HD2	2.27	0.55
4:A:667:GLY:HA3	6:C:192:TRP:CH2	2.41	0.55
8:E:177:ARG:HD3	8:E:215:MET:HG3	1.89	0.55
8:E:23:VAL:O	8:E:28:TYR:HB2	2.07	0.55
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.36	0.55
4:A:207:ILE:O	4:A:208:LEU:C	2.45	0.55
4:A:35:ILE:HG22	4:A:84:ILE:HD12	1.88	0.55
4:A:881:GLN:NE2	4:A:958:VAL:O	2.35	0.55
5:B:1180:PHE:O	5:B:1181:GLU:O	2.24	0.55
5:B:214:ALA:HB3	5:B:498:THR:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:502:ILE:HG12	5:B:535:LEU:CD1	2.35	0.55
6:C:31:ASN:O	6:C:32:SER:C	2.42	0.55
12:I:100:PHE:N	12:I:100:PHE:HD1	2.04	0.55
14:K:58:PHE:HB3	14:K:76:GLN:HB3	1.89	0.55
4:A:1209:MET:CE	4:A:1236:LEU:HB3	2.36	0.55
4:A:224:PHE:HD2	4:A:229:SER:O	1.90	0.55
4:A:524:VAL:HG12	4:A:525:GLN:N	2.19	0.55
4:A:528:LEU:HD23	4:A:751:SER:HA	1.89	0.55
5:B:843:GLN:O	5:B:844:SER:C	2.45	0.55
5:B:973:ILE:HG23	5:B:974:PRO:HD2	1.89	0.55
10:G:51:TYR:O	10:G:54:ILE:HG13	2.06	0.55
4:A:1027:ALA:O	4:A:1028:THR:C	2.43	0.55
4:A:414:ASP:OD1	4:A:416:ARG:HG3	2.07	0.55
5:B:520:GLY:HA2	5:B:748:ILE:HG22	1.89	0.55
5:B:847:ASP:C	5:B:849:GLY:N	2.60	0.55
4:A:870:GLU:HG2	8:E:208:TYR:CD2	2.42	0.55
9:F:130:ILE:O	9:F:148:VAL:CG2	2.55	0.55
10:G:15:PRO:O	10:G:16:SER:C	2.46	0.55
12:I:56:ALA:O	12:I:57:GLY:O	2.25	0.55
4:A:1279:ILE:HD11	4:A:1316:VAL:HG21	1.89	0.54
4:A:1385:THR:HG22	4:A:1386:ARG:N	2.22	0.54
4:A:679:ILE:O	4:A:682:THR:N	2.40	0.54
4:A:789:LYS:HE3	12:I:67:THR:HB	1.89	0.54
4:A:90:VAL:HG12	4:A:91:PHE:N	2.21	0.54
5:B:1197:PRO:O	5:B:1200:ALA:HB3	2.07	0.54
5:B:880:THR:HB	5:B:934:LYS:HD2	1.88	0.54
7:D:130:LEU:C	7:D:132:GLN:N	2.61	0.54
8:E:157:SER:C	8:E:159:ASP:N	2.61	0.54
11:H:127:GLY:O	11:H:128:ASN:HB2	2.07	0.54
12:I:34:TYR:HE2	12:I:36:GLU:HB3	1.71	0.54
4:A:366:VAL:CG2	4:A:460:VAL:HG22	2.37	0.54
4:A:418:SER:O	4:A:420:ARG:N	2.40	0.54
4:A:446:ARG:HB2	4:A:487:MET:SD	2.48	0.54
7:D:53:SER:CB	7:D:153:ARG:H	2.19	0.54
7:D:53:SER:HB3	7:D:152:SER:CB	2.37	0.54
8:E:14:ARG:HH21	8:E:141:VAL:HG12	1.72	0.54
10:G:106:MET:CG	10:G:107:LYS:N	2.70	0.54
10:G:56:ILE:O	10:G:57:GLN:HB2	2.06	0.54
15:L:32:ALA:HB3	15:L:55:ILE:HD12	1.88	0.54
4:A:1032:LEU:O	4:A:1036:ARG:HD3	2.07	0.54
5:B:1002:THR:HG23	5:B:1006:ILE:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1031:LEU:HD13	5:B:1055:ILE:HD11	1.89	0.54
5:B:472:ALA:HB1	5:B:474:SER:HB3	1.88	0.54
5:B:769:TYR:O	5:B:771:SER:N	2.40	0.54
6:C:145:CYS:HA	13:J:2:ILE:HD11	1.88	0.54
8:E:124:VAL:HG13	8:E:132:ILE:HD12	1.88	0.54
9:F:81:THR:HB	9:F:136:ARG:NH1	2.23	0.54
10:G:13:LEU:HD22	10:G:14:HIS:O	2.07	0.54
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.87	0.54
4:A:1208:THR:HG22	4:A:1210:GLY:H	1.73	0.54
4:A:1161:THR:OG1	4:A:1239:ARG:NH2	2.41	0.54
4:A:1100:ARG:HH21	4:A:1351:GLU:CG	2.21	0.54
4:A:146:MET:HA	4:A:171:GLN:HB2	1.90	0.54
5:B:1166:CYS:O	5:B:1168:LEU:N	2.39	0.54
5:B:278:GLN:HG2	5:B:279:ASP:H	1.72	0.54
5:B:39:ARG:HG2	5:B:39:ARG:NH1	2.23	0.54
5:B:830:TYR:O	5:B:831:SER:C	2.44	0.54
5:B:997:GLU:H	5:B:997:GLU:CD	2.11	0.54
8:E:207:ARG:HH11	8:E:207:ARG:HB3	1.72	0.54
8:E:22:MET:HE1	8:E:26:ARG:HH21	1.71	0.54
13:J:1:MET:H2	13:J:56:LEU:N	2.04	0.54
4:A:1118:VAL:O	4:A:1305:VAL:HG13	2.07	0.54
4:A:365:GLY:O	4:A:468:PHE:HA	2.08	0.54
4:A:590:ARG:HD2	4:A:605:MET:HB3	1.89	0.54
5:B:1034:VAL:C	5:B:1036:ALA:H	2.09	0.54
6:C:242:GLN:C	6:C:244:VAL:H	2.09	0.54
7:D:170:THR:HB	7:D:172:LEU:H	1.73	0.54
8:E:161:LYS:HD2	8:E:195:VAL:HG23	1.88	0.54
10:G:145:VAL:HG12	10:G:146:LYS:N	2.23	0.54
4:A:61:ILE:O	4:A:63:ARG:N	2.41	0.54
4:A:742:ASN:O	4:A:745:GLN:HB2	2.07	0.54
5:B:35:SER:O	5:B:39:ARG:HG3	2.07	0.54
5:B:710:LEU:O	5:B:711:GLU:HG2	2.07	0.54
6:C:120:ILE:HD13	6:C:124:LEU:HD21	1.90	0.54
11:H:4:THR:O	11:H:5:LEU:HD23	2.08	0.54
15:L:39:SER:O	15:L:40:LEU:HG	2.08	0.54
4:A:1401:SER:O	4:A:1402:PHE:HB2	2.07	0.54
4:A:341:MET:CE	4:A:843:LYS:NZ	2.71	0.54
4:A:986:ILE:HG22	4:A:987:VAL:N	2.23	0.54
5:B:224:GLN:O	5:B:238:ALA:HA	2.08	0.54
6:C:263:THR:C	6:C:265:MET:N	2.61	0.54
10:G:7:LEU:O	10:G:73:LYS:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:21:ILE:HG23	14:K:31:VAL:CG1	2.38	0.54
4:A:252:PHE:O	4:A:256:GLN:NE2	2.40	0.54
4:A:981:LEU:HD21	4:A:1038:THR:C	2.28	0.54
6:C:147:LEU:HD12	6:C:151:GLN:O	2.07	0.54
6:C:174:ALA:O	6:C:175:ALA:HB2	2.07	0.54
10:G:122:ASN:ND2	10:G:125:SER:HB3	2.23	0.54
4:A:105:CYS:O	4:A:114:LEU:HG	2.07	0.54
4:A:1127:ASP:HB3	4:A:1130:GLN:HB2	1.90	0.54
5:B:604:ARG:NH2	5:B:614:SER:HA	2.22	0.54
6:C:107:SER:C	6:C:109:SER:H	2.10	0.54
6:C:214:ASN:HB3	6:C:217:ASP:OD2	2.08	0.54
6:C:239:PRO:O	6:C:241:ASP:N	2.41	0.54
7:D:52:LEU:O	7:D:54:GLU:N	2.40	0.54
4:A:1017:LEU:CB	8:E:205:SER:HA	2.38	0.54
13:J:21:TYR:HB2	13:J:39:LEU:CD1	2.38	0.54
15:L:60:ARG:HG2	15:L:61:THR:H	1.73	0.54
4:A:134:ARG:O	4:A:138:ILE:HG13	2.07	0.54
4:A:244:PRO:CB	4:A:245:PRO:HD3	2.29	0.54
4:A:696:GLU:HG2	4:A:696:GLU:O	2.08	0.54
5:B:1106:ARG:NH1	5:B:1110:PRO:HD2	2.23	0.54
6:C:80:LEU:HD11	6:C:95:CYS:C	2.28	0.54
8:E:29:PHE:O	8:E:30:ILE:CG1	2.55	0.54
11:H:139:ASN:O	11:H:140:ALA:HB2	2.08	0.54
4:A:21:LEU:HG	4:A:1413:GLY:O	2.08	0.53
4:A:666:ILE:N	4:A:666:ILE:HD12	2.22	0.53
4:A:774:ARG:O	4:A:775:ILE:C	2.46	0.53
4:A:844:ALA:O	4:A:845:LEU:HD23	2.08	0.53
5:B:1159:ARG:HE	5:B:1193:GLN:HE21	1.56	0.53
6:C:256:ALA:O	6:C:259:LEU:N	2.41	0.53
10:G:88:ASP:OD2	10:G:88:ASP:N	2.40	0.53
12:I:111:THR:HG22	12:I:113:ASP:H	1.73	0.53
12:I:14:LEU:HA	12:I:28:GLU:O	2.08	0.53
5:B:309:GLN:HG3	12:I:52:ILE:HD11	1.89	0.53
4:A:1156:PRO:HA	4:A:1190:PRO:CB	2.38	0.53
4:A:42:ASP:HB3	4:A:45:GLN:HA	1.90	0.53
4:A:836:TYR:CD2	4:A:840:ARG:HD2	2.44	0.53
5:B:758:PHE:CE1	5:B:1027:ILE:CG2	2.91	0.53
5:B:466:TRP:C	5:B:468:GLU:H	2.09	0.53
5:B:53:GLN:HG2	5:B:547:VAL:CG2	2.36	0.53
8:E:3:GLN:HG3	8:E:4:GLU:N	2.22	0.53
9:F:119:ARG:NH1	9:F:119:ARG:HG3	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:109:VAL:HG11	9:F:123:LYS:HG2	1.90	0.53
13:J:8:PHE:H	13:J:49:MET:HE3	1.71	0.53
14:K:58:PHE:HE2	14:K:74:ARG:HE	1.53	0.53
4:A:761:MET:HA	4:A:804:TYR:HB2	1.89	0.53
4:A:868:TYR:CE1	4:A:1064:VAL:CG1	2.88	0.53
5:B:1022:THR:HG23	5:B:1022:THR:O	2.08	0.53
5:B:521:LEU:HD13	5:B:633:VAL:HB	1.90	0.53
5:B:980:PHE:HD2	5:B:1094:ARG:HA	1.72	0.53
7:D:35:LEU:H	7:D:35:LEU:HD12	1.72	0.53
7:D:49:ALA:HB2	7:D:174:PRO:HB3	1.90	0.53
10:G:110:VAL:HG22	10:G:161:GLY:O	2.08	0.53
4:A:1001:ARG:O	4:A:1002:GLY:O	2.26	0.53
4:A:195:ASP:O	4:A:196:GLU:HB3	2.08	0.53
4:A:265:LYS:HZ3	4:A:322:VAL:HG22	1.73	0.53
4:A:417:TYR:CD2	4:A:417:TYR:N	2.75	0.53
4:A:586:ILE:HG22	4:A:587:HIS:N	2.24	0.53
4:A:913:LEU:HD12	4:A:914:GLU:H	1.73	0.53
5:B:196:PRO:HG2	5:B:197:PHE:H	1.73	0.53
5:B:205:ILE:HD12	5:B:205:ILE:N	2.23	0.53
5:B:65:GLU:CG	5:B:66:ASP:H	2.16	0.53
5:B:952:VAL:O	5:B:953:LEU:HB3	2.08	0.53
5:B:986:GLN:OE1	5:B:986:GLN:HA	2.08	0.53
5:B:798:TYR:CE2	6:C:62:PHE:HE2	2.24	0.53
6:C:89:GLU:O	6:C:89:GLU:HG2	2.07	0.53
10:G:7:LEU:CD1	10:G:45:ILE:HD11	2.38	0.53
11:H:113:ALA:HB1	11:H:125:LEU:O	2.09	0.53
11:H:116:TYR:O	11:H:122:LEU:HA	2.08	0.53
4:A:399:HIS:O	4:A:401:GLY:N	2.41	0.53
5:B:1219:ASP:O	5:B:1219:ASP:OD1	2.27	0.53
5:B:225:VAL:HA	5:B:237:VAL:O	2.09	0.53
5:B:168:GLY:N	5:B:450:ALA:HB1	2.18	0.53
5:B:640:VAL:O	5:B:641:GLU:C	2.47	0.53
5:B:942:ARG:O	5:B:944:THR:N	2.42	0.53
6:C:189:THR:HG22	6:C:190:ASP:N	2.23	0.53
6:C:39:ALA:HA	6:C:164:ALA:CB	2.29	0.53
4:A:1116:LEU:HD12	4:A:1116:LEU:C	2.29	0.53
4:A:95:PHE:CD1	4:A:234:MET:HG2	2.44	0.53
4:A:534:LEU:O	4:A:534:LEU:HG	2.08	0.53
4:A:847:ASP:OD1	4:A:848:ILE:HG13	2.08	0.53
4:A:903:ASN:C	4:A:903:ASN:ND2	2.58	0.53
5:B:1001:PHE:CD2	6:C:34:ARG:NH2	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1410:PHE:HA	5:B:1212:ILE:CD1	2.39	0.53
5:B:750:GLY:O	5:B:751:VAL:C	2.46	0.53
12:I:50:THR:CG2	12:I:52:ILE:HG12	2.39	0.53
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.39	0.53
4:A:218:ASP:HA	4:A:221:SER:HG	1.74	0.53
4:A:401:GLY:C	4:A:435:HIS:HD2	2.12	0.53
4:A:829:VAL:C	4:A:831:THR:N	2.50	0.53
5:B:479:VAL:O	5:B:480:SER:HB3	2.09	0.53
11:H:83:GLN:C	11:H:85:GLY:H	2.12	0.53
4:A:1151:GLU:HA	12:I:44:TYR:O	2.09	0.53
4:A:152:VAL:HG12	4:A:153:PRO:CD	2.37	0.53
4:A:427:GLN:HB2	4:A:430:TRP:CD1	2.44	0.53
4:A:665:GLY:C	4:A:666:ILE:HD12	2.29	0.53
4:A:71:GLN:O	4:A:73:GLY:N	2.37	0.53
5:B:1050:ILE:HG22	5:B:1051:THR:N	2.24	0.53
5:B:872:GLU:HA	5:B:915:THR:O	2.09	0.53
6:C:168:ALA:O	6:C:170:TRP:N	2.42	0.53
9:F:103:MET:CE	10:G:66:GLY:H	2.22	0.53
10:G:14:HIS:CE1	10:G:15:PRO:HD2	2.43	0.53
4:A:1030:ARG:NH1	4:A:1035:TYR:OH	2.41	0.53
4:A:1434:ALA:CB	4:A:1436:ILE:HD12	2.39	0.53
4:A:401:GLY:C	4:A:435:HIS:CD2	2.82	0.53
4:A:497:THR:HG22	4:A:498:ARG:N	2.24	0.53
5:B:637:LEU:O	5:B:690:VAL:HG13	2.09	0.53
5:B:843:GLN:O	5:B:846:ILE:HB	2.09	0.53
6:C:184:ASN:HD21	6:C:187:LYS:HA	1.69	0.53
7:D:40:HIS:CE1	7:D:41:GLN:HG3	2.43	0.53
9:F:140:ASP:OD1	9:F:140:ASP:C	2.48	0.53
10:G:14:HIS:CD2	10:G:16:SER:H	2.27	0.53
4:A:241:VAL:HG13	4:A:266:LEU:HD13	1.90	0.53
4:A:601:LYS:HB2	4:A:603:ASN:ND2	2.24	0.53
5:B:118:ARG:HG2	5:B:204:ILE:HD13	1.91	0.53
6:C:175:ALA:O	6:C:176:ILE:HG13	2.09	0.53
6:C:20:PHE:CE1	6:C:22:LEU:HD12	2.42	0.53
7:D:185:CYS:HB2	7:D:211:LEU:HD22	1.89	0.53
10:G:1:MET:O	10:G:3:PHE:CD1	2.62	0.53
10:G:3:PHE:CE1	10:G:80:LYS:HE2	2.44	0.53
4:A:18:GLN:O	5:B:1215:ARG:CG	2.57	0.52
5:B:1189:ILE:HG22	5:B:1190:ASP:N	2.23	0.52
5:B:1216:LEU:N	5:B:1216:LEU:HD23	2.24	0.52
5:B:216:GLU:HA	5:B:406:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:558:LEU:C	5:B:560:GLU:H	2.13	0.52
8:E:29:PHE:C	8:E:30:ILE:HG13	2.28	0.52
10:G:111:THR:HB	10:G:114:LEU:HB2	1.91	0.52
10:G:49:LEU:HD21	10:G:77:VAL:HG23	1.89	0.52
11:H:95:TYR:HB3	11:H:144:ILE:HB	1.91	0.52
5:B:900:ALA:HB3	15:L:61:THR:OG1	2.09	0.52
4:A:382:PRO:CB	4:A:428:TYR:HE2	2.22	0.52
4:A:90:VAL:CG1	4:A:297:GLN:HA	2.39	0.52
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.72	0.52
5:B:467:GLY:O	5:B:468:GLU:CB	2.56	0.52
5:B:918:ILE:HG21	5:B:935:ARG:NH1	2.25	0.52
6:C:235:VAL:HG13	13:J:13:VAL:CG2	2.40	0.52
6:C:263:THR:O	6:C:265:MET:N	2.42	0.52
7:D:33:PHE:CZ	10:G:80:LYS:HE3	2.44	0.52
10:G:138:THR:CG2	10:G:139:ILE:H	2.13	0.52
10:G:80:LYS:HD3	10:G:80:LYS:H	1.73	0.52
15:L:52:GLY:O	15:L:53:HIS:C	2.48	0.52
4:A:1101:LEU:HB2	4:A:1355:VAL:HG11	1.91	0.52
4:A:249:SER:O	4:A:250:ILE:HG13	2.09	0.52
4:A:35:ILE:CG2	4:A:84:ILE:HD12	2.40	0.52
5:B:758:PHE:HE1	5:B:1027:ILE:HG22	1.73	0.52
5:B:1115:THR:HG21	5:B:1117:GLN:NE2	2.23	0.52
5:B:113:TYR:HB3	5:B:114:PRO:HD2	1.91	0.52
6:C:133:ILE:HD11	6:C:237:SER:HA	1.92	0.52
6:C:73:GLN:HE21	6:C:74:SER:N	2.07	0.52
10:G:34:VAL:HG12	10:G:45:ILE:CG2	2.35	0.52
11:H:31:THR:O	11:H:31:THR:HG22	2.10	0.52
1:T:27:DA:H2''	1:T:28:DT:OP2	2.08	0.52
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	1.90	0.52
4:A:152:VAL:HG13	4:A:153:PRO:HD2	1.89	0.52
4:A:399:HIS:CB	4:A:400:PRO:CD	2.79	0.52
4:A:765:VAL:HG23	4:A:802:ASN:O	2.10	0.52
4:A:946:VAL:HG22	8:E:201:LYS:HD2	1.90	0.52
5:B:980:PHE:HE2	5:B:1094:ARG:CG	2.21	0.52
5:B:1202:LEU:O	5:B:1206:GLU:HG3	2.09	0.52
5:B:745:PRO:C	5:B:747:MET:H	2.12	0.52
10:G:47:CYS:O	10:G:76:ALA:HB1	2.08	0.52
4:A:567:LYS:HB3	11:H:95:TYR:CA	2.38	0.52
4:A:1004:ASN:O	4:A:1008:GLN:HB2	2.10	0.52
4:A:621:THR:O	4:A:629:LEU:HB2	2.09	0.52
4:A:825:ILE:HG22	5:B:508:LEU:CD1	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:831:SER:CB	5:B:994:TYR:OH	2.58	0.52
6:C:31:ASN:O	6:C:34:ARG:N	2.42	0.52
8:E:55:ARG:HD2	8:E:83:CYS:O	2.09	0.52
9:F:147:SER:OG	9:F:150:GLU:HG3	2.09	0.52
10:G:26:LEU:O	10:G:27:LYS:C	2.47	0.52
10:G:96:GLN:HA	10:G:121:PHE:CE2	2.45	0.52
12:I:61:ASP:C	12:I:63:GLY:H	2.13	0.52
4:A:1336:MET:HE2	4:A:1381:LEU:HG	1.92	0.52
4:A:647:GLY:O	4:A:651:LYS:HG3	2.09	0.52
5:B:288:ALA:HA	5:B:331:LEU:HD12	1.92	0.52
5:B:429:PHE:HA	5:B:432:MET:HE3	1.92	0.52
5:B:579:ARG:CB	5:B:586:TRP:HE1	2.16	0.52
5:B:563:MET:HE1	5:B:587:HIS:HB2	1.92	0.52
5:B:758:PHE:N	5:B:759:PRO:CD	2.73	0.52
5:B:842:ASN:O	5:B:846:ILE:HG13	2.10	0.52
6:C:66:ARG:NH1	6:C:144:ILE:O	2.43	0.52
6:C:8:VAL:HG12	6:C:9:LYS:H	1.74	0.52
4:A:1153:TYR:CE1	12:I:42:LEU:HD13	2.45	0.52
4:A:92:HIS:HB2	4:A:236:LEU:HD21	1.90	0.52
4:A:35:ILE:HA	4:A:52:GLY:O	2.10	0.52
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.74	0.52
4:A:95:PHE:O	4:A:96:ILE:C	2.48	0.52
4:A:341:MET:CE	5:B:1135:ARG:NH1	2.73	0.52
5:B:225:VAL:O	5:B:226:PHE:CD2	2.63	0.52
5:B:282:ILE:CD1	5:B:382:ILE:HD13	2.40	0.52
6:C:22:LEU:HD13	6:C:230:MET:HE3	1.92	0.52
7:D:153:ARG:HB3	7:D:154:PHE:CE1	2.45	0.52
8:E:90:VAL:HG22	8:E:90:VAL:O	2.09	0.52
10:G:115:MET:CB	10:G:116:PRO:HD2	2.40	0.52
12:I:55:THR:HG22	12:I:58:VAL:HG21	1.91	0.52
13:J:45:CYS:O	13:J:48:ARG:HG3	2.08	0.52
15:L:61:THR:CG2	15:L:63:ARG:HG2	2.39	0.52
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.42	0.52
4:A:91:PHE:HB2	4:A:297:GLN:NE2	2.24	0.52
4:A:316:GLN:O	4:A:317:LYS:C	2.48	0.52
4:A:381:THR:CG2	4:A:383:TYR:H	2.23	0.52
4:A:353:ILE:HD12	4:A:487:MET:HE2	1.91	0.52
4:A:730:GLY:C	4:A:732:LEU:N	2.62	0.52
5:B:1132:GLU:O	5:B:1135:ARG:HB3	2.09	0.52
4:A:17:VAL:HA	5:B:1215:ARG:O	2.10	0.52
5:B:44:VAL:O	5:B:45:SER:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:847:ASP:O	5:B:849:GLY:N	2.43	0.52
6:C:80:LEU:HD11	6:C:95:CYS:HA	1.91	0.52
7:D:56:ARG:HD2	7:D:149:THR:OG1	2.09	0.52
8:E:78:LEU:C	8:E:78:LEU:HD23	2.29	0.52
12:I:13:MET:O	12:I:14:LEU:HD23	2.10	0.52
4:A:698:GLN:HA	12:I:97:MET:O	2.08	0.52
3:P:3:G:H2'	3:P:4:A:C8	2.45	0.52
4:A:337:ARG:NH2	4:A:839:ARG:HH12	2.08	0.52
4:A:840:ARG:O	4:A:841:LEU:C	2.48	0.52
5:B:557:PHE:C	5:B:557:PHE:HD2	2.12	0.52
6:C:146:LYS:C	6:C:147:LEU:HD23	2.29	0.52
6:C:206:ASN:OD1	6:C:229:TYR:CD2	2.63	0.52
8:E:198:ILE:HD11	8:E:212:ARG:CG	2.33	0.52
12:I:55:THR:HG21	12:I:109:ILE:HD13	1.92	0.52
5:B:954:VAL:O	15:L:55:ILE:O	2.27	0.52
4:A:1066:VAL:O	4:A:1069:ALA:HB3	2.09	0.52
4:A:1193:LEU:HD12	4:A:1194:ARG:N	2.24	0.52
4:A:166:GLY:O	4:A:167:CYS:SG	2.68	0.52
4:A:47:ARG:O	4:A:48:ALA:HB2	2.10	0.52
4:A:535:THR:HG23	4:A:575:LYS:HE2	1.91	0.52
5:B:400:HIS:ND1	5:B:517:THR:HG21	2.25	0.52
6:C:6:PRO:HB3	6:C:25:VAL:HG12	1.92	0.52
6:C:60:ASP:OD2	15:L:60:ARG:NH2	2.42	0.52
12:I:55:THR:O	12:I:55:THR:HG22	2.10	0.52
15:L:61:THR:HG22	15:L:63:ARG:HG2	1.91	0.52
4:A:1156:PRO:O	4:A:1158:PRO:HD3	2.10	0.51
4:A:41:MET:O	4:A:50:ILE:HG13	2.11	0.51
4:A:427:GLN:HG3	4:A:430:TRP:CE2	2.44	0.51
4:A:567:LYS:CB	4:A:568:PRO:CD	2.87	0.51
4:A:788:SER:O	4:A:789:LYS:O	2.29	0.51
5:B:324:ILE:HD13	5:B:330:ALA:HA	1.92	0.51
5:B:549:THR:HG22	5:B:550:ASP:N	2.17	0.51
6:C:215:GLU:O	6:C:216:GLY:C	2.48	0.51
14:K:53:ASP:OD1	14:K:55:LYS:HB2	2.10	0.51
4:A:1063:MET:SD	4:A:1436:ILE:HG12	2.50	0.51
4:A:244:PRO:O	4:A:247:ARG:N	2.38	0.51
4:A:444:PHE:CB	4:A:458:HIS:HD2	2.24	0.51
5:B:503:GLY:H	5:B:507:LYS:HD2	1.76	0.51
5:B:661:LEU:C	5:B:663:ALA:H	2.13	0.51
5:B:890:TYR:OH	5:B:936:ASP:OD2	2.27	0.51
8:E:153:HIS:HB3	8:E:196:VAL:CG1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:21:ILE:HG23	14:K:31:VAL:HG11	1.92	0.51
5:B:896:ASP:CG	15:L:58:LYS:HZ2	2.14	0.51
4:A:896:ARG:NH2	4:A:1030:ARG:NH2	2.58	0.51
4:A:167:CYS:SG	4:A:167:CYS:O	2.69	0.51
4:A:356:ASP:HB2	4:A:469:ARG:HH12	1.73	0.51
4:A:648:ASN:O	4:A:649:ILE:C	2.48	0.51
4:A:93:VAL:CG2	4:A:301:ALA:HA	2.40	0.51
5:B:205:ILE:O	5:B:206:ASN:C	2.49	0.51
5:B:603:LEU:HD13	5:B:608:ASP:CB	2.38	0.51
7:D:56:ARG:HA	7:D:148:LEU:HD13	1.93	0.51
7:D:50:LEU:HD11	10:G:4:ILE:HD11	1.93	0.51
13:J:7:CYS:CB	13:J:46:CYS:HB3	2.41	0.51
4:A:1197:LEU:HD12	4:A:1209:MET:HE1	1.93	0.51
4:A:1115:SER:C	4:A:1308:THR:HG22	2.31	0.51
5:B:20:ASP:O	5:B:22:SER:N	2.42	0.51
6:C:254:LYS:O	6:C:258:ILE:HD13	2.11	0.51
7:D:47:LEU:CD1	7:D:48:ILE:N	2.71	0.51
8:E:13:TRP:O	8:E:16:PHE:HB3	2.09	0.51
9:F:111:LEU:H	9:F:111:LEU:HD12	1.75	0.51
11:H:102:TYR:N	11:H:102:TYR:CD2	2.78	0.51
4:A:1279:ILE:HG23	4:A:1308:THR:OG1	2.11	0.51
4:A:98:LYS:O	4:A:99:ILE:C	2.49	0.51
5:B:1172:ILE:O	5:B:1172:ILE:HG22	2.11	0.51
5:B:469:GLN:O	5:B:470:LYS:HB2	2.10	0.51
5:B:603:LEU:HB3	5:B:609:ILE:CD1	2.41	0.51
5:B:785:TYR:CD1	5:B:785:TYR:C	2.83	0.51
6:C:116:LYS:HD3	6:C:140:ASN:HB3	1.93	0.51
6:C:35:ARG:NH1	14:K:41:THR:H	2.08	0.51
10:G:80:LYS:O	10:G:82:PHE:CE1	2.64	0.51
3:P:5:C:H2'	3:P:6:C:C6	2.45	0.51
4:A:1144:LYS:HB2	4:A:1268:LEU:O	2.10	0.51
4:A:567:LYS:HD2	4:A:568:PRO:HD2	1.90	0.51
4:A:600:PRO:C	4:A:602:ASP:H	2.12	0.51
5:B:230:ALA:N	5:B:231:PRO:CD	2.73	0.51
5:B:999:MET:HE2	5:B:1000:PRO:HD2	1.92	0.51
15:L:27:LEU:HD13	15:L:37:LYS:HE2	1.92	0.51
5:B:193:LYS:NZ	15:L:32:ALA:HB1	2.25	0.51
15:L:46:VAL:HG12	15:L:46:VAL:O	2.11	0.51
4:A:1327:ILE:HG22	8:E:147:HIS:CE1	2.45	0.51
4:A:1438:THR:HB	5:B:1144:ALA:CB	2.40	0.51
4:A:37:PHE:N	4:A:37:PHE:CD1	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1084:GLN:NE2	5:B:1084:GLN:H	2.07	0.51
5:B:115:GLN:HG2	5:B:193:LYS:CB	2.40	0.51
5:B:757:PRO:HD3	5:B:983:ARG:NH2	2.26	0.51
4:A:357:PRO:HD2	5:B:833:TYR:CE1	2.46	0.51
6:C:243:VAL:HG12	6:C:243:VAL:O	2.10	0.51
4:A:102:VAL:O	4:A:105:CYS:HB2	2.11	0.51
4:A:1116:LEU:HG	4:A:1308:THR:HB	1.92	0.51
4:A:89:PRO:HB2	4:A:204:THR:HG22	1.92	0.51
10:G:49:LEU:HD23	10:G:49:LEU:N	2.26	0.51
9:F:99:LEU:HD21	10:G:64:THR:O	2.10	0.51
12:I:25:LEU:HB3	12:I:38:ALA:HB2	1.93	0.51
12:I:50:THR:HG22	12:I:51:ASN:N	2.26	0.51
13:J:2:ILE:HG12	13:J:57:ILE:HD12	1.93	0.51
13:J:64:ASN:CB	13:J:65:PRO:CD	2.85	0.51
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.92	0.51
4:A:278:THR:O	4:A:282:ASN:HB2	2.11	0.51
4:A:82:GLY:O	4:A:241:VAL:N	2.38	0.51
5:B:298:LEU:N	5:B:298:LEU:CD2	2.74	0.51
6:C:76:ASP:O	6:C:79:GLN:HG2	2.11	0.51
7:D:52:LEU:C	7:D:54:GLU:H	2.14	0.51
8:E:22:MET:HE1	8:E:26:ARG:NH2	2.26	0.51
10:G:119:LEU:HD13	10:G:132:SER:HB2	1.93	0.51
10:G:74:TYR:N	10:G:74:TYR:CD2	2.79	0.51
4:A:1094:VAL:HG12	4:A:1095:THR:N	2.26	0.51
4:A:1101:LEU:O	4:A:1101:LEU:HD12	2.10	0.51
4:A:29:ALA:HB1	5:B:1184:GLY:HA2	1.91	0.51
5:B:361:LEU:N	5:B:362:PRO:CD	2.73	0.51
5:B:410:GLY:O	5:B:412:LEU:N	2.44	0.51
7:D:52:LEU:CD2	7:D:147:TYR:HE2	2.23	0.51
14:K:24:ASP:OD2	14:K:74:ARG:NH1	2.43	0.51
2:N:2:DA:H2"	2:N:3:DG:OP2	2.10	0.51
4:A:1333:ILE:HG22	4:A:1334:ASP:N	2.26	0.50
4:A:44:THR:O	4:A:45:GLN:HB2	2.12	0.50
4:A:666:ILE:H	5:B:1026:LEU:HD22	1.76	0.50
4:A:71:GLN:C	4:A:73:GLY:N	2.65	0.50
4:A:84:ILE:HD11	4:A:270:LEU:CD1	2.29	0.50
5:B:221:ASN:N	5:B:241:ARG:O	2.33	0.50
5:B:872:GLU:CD	5:B:914:LYS:HE2	2.32	0.50
8:E:61:GLN:HG2	8:E:62:ALA:N	2.26	0.50
9:F:103:MET:HE2	10:G:66:GLY:H	1.76	0.50
12:I:98:VAL:C	12:I:99:LEU:HD23	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:56:VAL:HA	14:K:77:THR:HG22	1.93	0.50
4:A:1451:VAL:O	4:A:1454:MET:HG2	2.11	0.50
4:A:353:ILE:CD1	4:A:487:MET:HE2	2.41	0.50
4:A:632:VAL:O	4:A:633:VAL:C	2.49	0.50
4:A:809:THR:H	4:A:812:GLU:HB2	1.76	0.50
4:A:817:ALA:HA	5:B:764:SER:OG	2.11	0.50
5:B:48:LEU:O	5:B:51:PHE:N	2.42	0.50
5:B:580:VAL:HG22	5:B:624:LEU:HB3	1.93	0.50
5:B:841:MET:SD	5:B:846:ILE:HD11	2.51	0.50
5:B:882:THR:CG2	5:B:884:ARG:HB2	2.40	0.50
9:F:81:THR:HG21	9:F:136:ARG:CD	2.41	0.50
13:J:1:MET:HE2	13:J:60:PHE:CE2	2.47	0.50
1:T:18:DC:OP1	1:T:18:DC:H3'	2.11	0.50
4:A:512:VAL:HA	4:A:519:PRO:HA	1.94	0.50
4:A:873:MET:HG2	4:A:957:PRO:HB3	1.92	0.50
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.94	0.50
9:F:116:ASP:C	9:F:116:ASP:OD1	2.49	0.50
10:G:99:PHE:HZ	10:G:163:ILE:HD13	1.76	0.50
13:J:44:TYR:N	13:J:44:TYR:CD2	2.79	0.50
13:J:7:CYS:HA	13:J:49:MET:HE3	1.92	0.50
4:A:79:GLY:HA3	4:A:243:PRO:HG3	1.93	0.50
5:B:1177:HIS:O	5:B:1179:GLN:N	2.45	0.50
5:B:770:GLN:OE1	5:B:983:ARG:CA	2.56	0.50
7:D:156:ASP:C	7:D:158:GLU:H	2.13	0.50
7:D:156:ASP:C	7:D:158:GLU:N	2.65	0.50
12:I:34:TYR:CE2	12:I:36:GLU:HB3	2.45	0.50
12:I:85:PHE:HD1	12:I:99:LEU:HD13	1.77	0.50
13:J:27:GLU:C	13:J:29:GLU:H	2.14	0.50
14:K:58:PHE:HB3	14:K:76:GLN:HE21	1.76	0.50
4:A:326:ARG:HH22	4:A:1407:GLU:HG3	1.76	0.50
4:A:446:ARG:HB2	4:A:487:MET:HG2	1.94	0.50
4:A:590:ARG:HD3	4:A:604:GLY:C	2.32	0.50
4:A:784:LEU:HB3	4:A:785:PRO:HD2	1.94	0.50
5:B:658:ILE:HG22	5:B:659:ALA:N	2.27	0.50
5:B:825:VAL:HG12	5:B:826:ALA:N	2.26	0.50
6:C:55:THR:O	6:C:55:THR:HG22	2.11	0.50
11:H:123:MET:HG2	11:H:124:ARG:N	2.26	0.50
12:I:111:THR:CG2	12:I:112:SER:N	2.74	0.50
12:I:33:SER:O	12:I:35:VAL:HG23	2.11	0.50
12:I:5:ARG:HD3	12:I:36:GLU:OE2	2.12	0.50
4:A:326:ARG:NH2	4:A:1407:GLU:HG3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:817:ALA:O	4:A:819:GLY:N	2.45	0.50
5:B:1095:LEU:HD12	5:B:1095:LEU:N	2.22	0.50
4:A:412:ARG:NH2	5:B:1108:ARG:NH1	2.60	0.50
4:A:1430:LEU:O	5:B:1197:PRO:HD2	2.11	0.50
5:B:205:ILE:CD1	5:B:205:ILE:N	2.74	0.50
5:B:745:PRO:O	5:B:747:MET:N	2.44	0.50
7:D:33:PHE:CZ	10:G:80:LYS:CE	2.95	0.50
8:E:124:VAL:CG1	8:E:132:ILE:HB	2.39	0.50
11:H:123:MET:HE1	11:H:142:LEU:HD11	1.93	0.50
12:I:85:PHE:HD2	12:I:85:PHE:N	1.89	0.50
4:A:1041:ALA:O	4:A:1044:TRP:HB3	2.12	0.50
4:A:573:SER:OG	4:A:576:GLN:HB2	2.11	0.50
4:A:608:ILE:HD12	4:A:613:ILE:CD1	2.42	0.50
4:A:768:GLN:HG2	4:A:816:HIS:CA	2.31	0.50
4:A:779:PHE:O	4:A:780:VAL:C	2.50	0.50
4:A:886:ILE:HG13	4:A:943:LEU:CD1	2.42	0.50
4:A:963:ILE:HD11	4:A:1048:ASN:CB	2.28	0.50
5:B:1072:MET:HE1	5:B:1085:ILE:HB	1.90	0.50
6:C:70:ILE:HD11	6:C:144:ILE:HG12	1.94	0.50
7:D:220:LEU:O	7:D:221:TYR:HD1	1.94	0.50
9:F:138:LEU:HB3	9:F:139:PRO:HD2	1.94	0.50
10:G:9:LEU:HG	10:G:10:ASN:N	2.27	0.50
11:H:27:GLU:HG2	11:H:39:THR:HG23	1.93	0.50
13:J:53:HIS:C	13:J:53:HIS:CD2	2.84	0.50
4:A:1334:ASP:O	4:A:1336:MET:N	2.45	0.50
4:A:420:ARG:O	4:A:421:ALA:C	2.50	0.50
4:A:464:PRO:HG2	4:A:465:TYR:HD1	1.77	0.50
4:A:942:PHE:C	4:A:942:PHE:CD2	2.85	0.50
4:A:1410:PHE:HD2	5:B:1212:ILE:HD12	1.77	0.50
5:B:26:THR:O	5:B:29:ASP:HB2	2.11	0.50
5:B:681:TRP:O	5:B:683:SER:N	2.45	0.50
5:B:882:THR:O	5:B:883:LEU:HB2	2.11	0.50
6:C:105:GLY:HA3	6:C:149:LYS:O	2.11	0.50
6:C:101:LEU:HD13	6:C:118:LEU:HD23	1.94	0.50
7:D:33:PHE:CE2	10:G:80:LYS:NZ	2.61	0.50
8:E:22:MET:CE	8:E:26:ARG:HH21	2.25	0.50
12:I:69:PRO:HG2	12:I:85:PHE:CD2	2.47	0.50
4:A:547:LEU:HB3	14:K:58:PHE:CE1	2.44	0.50
4:A:552:TRP:O	4:A:554:PRO:HD3	2.12	0.50
4:A:658:LEU:HD23	4:A:659:HIS:HE1	1.76	0.50
4:A:65:LEU:O	4:A:66:LYS:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:734:HIS:O	5:B:735:ALA:HB2	2.12	0.50
5:B:865:LYS:NZ	5:B:869:SER:HA	2.27	0.50
6:C:208:GLU:O	6:C:210:GLU:N	2.45	0.50
6:C:238:ILE:HG22	6:C:243:VAL:HG23	1.94	0.50
6:C:69:LEU:CD1	6:C:69:LEU:N	2.74	0.50
6:C:35:ARG:NH1	14:K:41:THR:N	2.59	0.50
4:A:1120:LEU:HD12	4:A:1120:LEU:N	2.26	0.49
4:A:268:ASP:O	4:A:269:ILE:C	2.50	0.49
4:A:30:ILE:HG23	5:B:1170:THR:HG23	1.94	0.49
4:A:442:VAL:CB	4:A:489:LEU:HD11	2.37	0.49
4:A:500:GLU:OE1	5:B:1143:ALA:C	2.50	0.49
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.93	0.49
4:A:18:GLN:H	5:B:1215:ARG:HB2	1.76	0.49
5:B:171:PRO:HD2	5:B:457:LEU:CD1	2.39	0.49
5:B:175:ARG:HH11	5:B:175:ARG:HG2	1.77	0.49
5:B:525:ALA:O	5:B:768:THR:HA	2.11	0.49
6:C:249:ASP:O	6:C:252:GLN:HB3	2.12	0.49
6:C:8:VAL:HG12	6:C:9:LYS:N	2.26	0.49
10:G:3:PHE:CD1	10:G:80:LYS:NZ	2.77	0.49
15:L:40:LEU:HD22	15:L:44:ASP:CB	2.42	0.49
4:A:1124:HIS:HB3	4:A:1130:GLN:HG2	1.93	0.49
4:A:1394:THR:O	4:A:1395:GLY:O	2.30	0.49
4:A:266:LEU:O	4:A:267:ALA:C	2.49	0.49
4:A:808:LEU:HD23	4:A:813:PHE:CA	2.37	0.49
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.12	0.49
4:A:947:PHE:CD2	4:A:954:TRP:CZ2	3.00	0.49
5:B:766:ARG:NH2	5:B:1020:ARG:HH11	2.10	0.49
4:A:2:VAL:HG21	5:B:1158:PHE:N	2.27	0.49
6:C:34:ARG:O	6:C:38:ILE:HG13	2.11	0.49
7:D:33:PHE:CZ	10:G:80:LYS:NZ	2.79	0.49
8:E:35:VAL:O	8:E:37:LEU:N	2.44	0.49
9:F:77:ASP:C	9:F:79:ARG:N	2.66	0.49
5:B:309:GLN:OE1	12:I:52:ILE:HD11	2.12	0.49
6:C:66:ARG:CZ	13:J:2:ILE:HG21	2.42	0.49
4:A:1059:HIS:O	4:A:1061:GLY:N	2.45	0.49
4:A:262:LEU:C	4:A:264:PHE:N	2.65	0.49
4:A:283:GLY:O	4:A:285:PRO:HD3	2.12	0.49
4:A:317:LYS:O	4:A:318:SER:CB	2.60	0.49
4:A:489:LEU:HD12	4:A:490:HIS:N	2.26	0.49
4:A:608:ILE:C	4:A:610:GLY:N	2.64	0.49
4:A:901:LEU:HA	4:A:907:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:909:ASP:C	4:A:911:SER:H	2.16	0.49
5:B:1106:ARG:NH1	5:B:1110:PRO:CD	2.76	0.49
5:B:32:ALA:O	5:B:35:SER:HB2	2.11	0.49
5:B:487:THR:O	5:B:490:SER:HB3	2.12	0.49
5:B:642:ASP:HB3	5:B:649:LYS:HD2	1.93	0.49
6:C:167:HIS:HD2	6:C:168:ALA:H	1.60	0.49
7:D:29:LEU:HD22	10:G:82:PHE:CD2	2.47	0.49
9:F:90:ARG:HD3	9:F:155:LEU:HD11	1.94	0.49
10:G:143:ILE:HG22	10:G:144:ARG:H	1.76	0.49
10:G:13:LEU:O	10:G:67:SER:HA	2.12	0.49
10:G:94:CYS:SG	10:G:99:PHE:HB3	2.51	0.49
11:H:41:ASP:O	11:H:42:ILE:HG13	2.13	0.49
13:J:45:CYS:SG	13:J:46:CYS:N	2.85	0.49
4:A:1019:CYS:O	4:A:1020:CYS:C	2.50	0.49
4:A:1369:ALA:O	4:A:1370:LEU:C	2.49	0.49
4:A:541:ILE:HG21	4:A:549:MET:HE3	1.93	0.49
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.43	0.49
4:A:863:VAL:HG11	4:A:866:PHE:CE2	2.48	0.49
6:C:91:HIS:HD2	6:C:91:HIS:O	1.94	0.49
11:H:142:LEU:C	11:H:143:LEU:HD12	2.32	0.49
4:A:113:LEU:O	4:A:114:LEU:HD23	2.13	0.49
4:A:1149:ALA:CB	12:I:47:GLU:HA	2.43	0.49
4:A:1329:THR:HG23	4:A:1331:SER:H	1.75	0.49
4:A:166:GLY:O	4:A:167:CYS:CB	2.61	0.49
4:A:219:PHE:CE2	4:A:231:PRO:HD2	2.47	0.49
4:A:381:THR:HG21	4:A:383:TYR:CD1	2.48	0.49
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.94	0.49
4:A:64:ASN:O	4:A:65:LEU:C	2.50	0.49
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.46	0.49
4:A:984:LYS:O	4:A:988:LEU:HB2	2.11	0.49
5:B:1084:GLN:C	5:B:1085:ILE:HD12	2.33	0.49
5:B:235:SER:O	5:B:236:HIS:HD2	1.94	0.49
5:B:327:ARG:O	5:B:331:LEU:HD13	2.12	0.49
5:B:744:HIS:HD2	5:B:746:SER:OG	1.94	0.49
5:B:765:PRO:O	5:B:768:THR:N	2.45	0.49
5:B:810:GLU:CB	5:B:815:ARG:HH22	2.26	0.49
5:B:860:MET:HG2	5:B:861:ASP:H	1.77	0.49
5:B:96:TYR:HB2	5:B:129:PHE:HB2	1.94	0.49
6:C:31:ASN:ND2	6:C:35:ARG:HD2	2.28	0.49
7:D:144:THR:HG21	10:G:46:LEU:HD13	1.95	0.49
14:K:53:ASP:HB3	14:K:56:VAL:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1130:GLN:O	4:A:1134:ILE:HG13	2.12	0.49
4:A:298:PHE:HD2	4:A:299:HIS:CD2	2.31	0.49
4:A:595:THR:O	4:A:596:THR:HG23	2.12	0.49
4:A:4:GLN:O	4:A:5:GLN:O	2.31	0.49
4:A:794:PRO:C	4:A:796:SER:H	2.14	0.49
5:B:728:ARG:NH1	5:B:1047:PHE:HB3	2.25	0.49
5:B:281:PRO:O	5:B:283:VAL:N	2.45	0.49
5:B:579:ARG:N	5:B:589:VAL:HG13	2.28	0.49
4:A:870:GLU:HG2	8:E:208:TYR:CG	2.47	0.49
8:E:55:ARG:C	8:E:57:MET:H	2.14	0.49
10:G:145:VAL:CG1	10:G:146:LYS:N	2.76	0.49
5:B:1039:GLY:HA2	13:J:51:LEU:CD2	2.42	0.49
14:K:107:THR:O	14:K:111:LEU:HG	2.12	0.49
4:A:1389:PHE:CD1	4:A:1389:PHE:C	2.85	0.49
4:A:381:THR:HG23	4:A:382:PRO:HD2	1.95	0.49
4:A:608:ILE:C	4:A:610:GLY:H	2.16	0.49
4:A:866:PHE:C	4:A:867:ILE:HG13	2.30	0.49
4:A:913:LEU:CD2	4:A:919:ILE:HD12	2.41	0.49
4:A:958:VAL:O	4:A:958:VAL:HG12	2.12	0.49
5:B:1065:GLN:NE2	5:B:1067:ARG:N	2.45	0.49
5:B:1106:ARG:HH12	5:B:1110:PRO:HG2	1.78	0.49
4:A:1431:GLY:HA3	5:B:1152:MET:SD	2.53	0.49
5:B:465:ASN:ND2	5:B:465:ASN:N	2.61	0.49
5:B:498:THR:HB	5:B:537:LYS:O	2.12	0.49
5:B:640:VAL:O	5:B:640:VAL:HG12	2.11	0.49
8:E:43:LYS:O	8:E:45:LYS:N	2.44	0.49
5:B:622:LYS:CE	12:I:59:VAL:HG22	2.43	0.49
13:J:3:VAL:HG21	13:J:18:TRP:CB	2.38	0.49
15:L:49:LYS:O	15:L:50:ASP:CB	2.60	0.49
4:A:215:SER:HB3	4:A:218:ASP:OD2	2.12	0.49
4:A:295:LEU:O	4:A:298:PHE:HB3	2.12	0.49
4:A:606:LEU:HB3	4:A:614:PHE:CD2	2.47	0.49
5:B:205:ILE:HG22	5:B:206:ASN:N	2.28	0.49
5:B:879:ARG:O	5:B:880:THR:HB	2.12	0.49
6:C:242:GLN:C	6:C:244:VAL:N	2.65	0.49
10:G:115:MET:HB3	10:G:116:PRO:HD2	1.94	0.49
13:J:34:THR:O	13:J:35:ALA:C	2.51	0.49
14:K:31:VAL:CG1	14:K:32:VAL:H	2.26	0.49
4:A:1036:ARG:HG2	4:A:1036:ARG:HH11	1.77	0.49
4:A:1280:GLU:O	4:A:1281:ARG:O	2.30	0.49
4:A:1349:TYR:CE1	4:A:1368:MET:HE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:372:LYS:HA	4:A:435:HIS:ND1	2.28	0.49
5:B:1032:SER:O	5:B:1036:ALA:HB2	2.12	0.49
5:B:1196:ILE:HG13	5:B:1196:ILE:O	2.11	0.49
5:B:307:ASP:O	5:B:309:GLN:N	2.46	0.49
5:B:460:ALA:HB1	5:B:466:TRP:CZ3	2.48	0.49
5:B:575:PRO:HG2	5:B:576:ASP:H	1.78	0.49
5:B:763:GLN:O	5:B:765:PRO:N	2.46	0.49
6:C:10:ILE:HA	6:C:20:PHE:HB2	1.93	0.49
7:D:134:THR:CG2	7:D:135:GLY:H	2.26	0.49
10:G:74:TYR:HD2	10:G:74:TYR:N	2.07	0.49
4:A:231:PRO:C	4:A:233:TRP:H	2.16	0.49
4:A:299:HIS:C	4:A:301:ALA:N	2.66	0.49
4:A:535:THR:CG2	4:A:575:LYS:HE2	2.42	0.49
4:A:590:ARG:HH21	4:A:620:LYS:CB	2.24	0.49
5:B:102:VAL:CG2	5:B:112:LEU:HD22	2.43	0.49
4:A:341:MET:HE3	5:B:1135:ARG:NH1	2.28	0.49
6:C:254:LYS:C	6:C:256:ALA:H	2.16	0.49
8:E:134:THR:C	8:E:135:PHE:HD1	2.16	0.49
8:E:175:LEU:HD23	8:E:176:PRO:CD	2.39	0.49
13:J:48:ARG:HE	13:J:49:MET:CE	2.26	0.49
13:J:57:ILE:O	13:J:60:PHE:HB2	2.13	0.49
14:K:12:LEU:CD1	14:K:12:LEU:H	2.24	0.49
4:A:18:GLN:HB3	5:B:1215:ARG:HG3	1.94	0.48
5:B:203:PHE:N	5:B:203:PHE:CD1	2.81	0.48
5:B:318:VAL:O	5:B:320:ASP:N	2.46	0.48
5:B:371:GLU:CD	5:B:371:GLU:H	2.17	0.48
4:A:253:ASN:HB3	5:B:935:ARG:CZ	2.42	0.48
6:C:154:LYS:O	6:C:155:LEU:HD23	2.12	0.48
7:D:167:LEU:HB3	7:D:177:VAL:HG13	1.95	0.48
8:E:46:TYR:CD2	8:E:58:MET:HG2	2.48	0.48
10:G:44:TYR:O	10:G:78:VAL:HA	2.13	0.48
4:A:164:ARG:CG	4:A:165:GLY:H	2.20	0.48
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.94	0.48
5:B:1187:ASN:O	5:B:1188:LYS:CB	2.61	0.48
4:A:18:GLN:CB	5:B:1215:ARG:HB2	2.42	0.48
5:B:844:SER:HB3	5:B:848:ARG:HH12	1.78	0.48
5:B:996:ARG:HH12	6:C:38:ILE:HG23	1.77	0.48
7:D:189:ASP:O	7:D:193:THR:HB	2.13	0.48
9:F:75:PRO:O	9:F:77:ASP:O	2.31	0.48
10:G:123:ALA:C	10:G:125:SER:H	2.16	0.48
12:I:85:PHE:CD2	12:I:85:PHE:N	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:53:HIS:CD2	13:J:54:VAL:N	2.81	0.48
14:K:65:HIS:CD2	14:K:67:PHE:HB2	2.48	0.48
14:K:82:ASP:OD1	14:K:84:LYS:N	2.45	0.48
4:A:1213:GLY:O	4:A:1216:ILE:N	2.46	0.48
4:A:1191:TRP:HB3	4:A:1260:LEU:HD23	1.96	0.48
4:A:1195:LEU:HD11	4:A:1267:MET:CE	2.44	0.48
4:A:382:PRO:HB3	4:A:428:TYR:CE2	2.41	0.48
5:B:240:ILE:HG23	5:B:240:ILE:O	2.13	0.48
5:B:595:ARG:O	5:B:596:LEU:C	2.51	0.48
6:C:258:ILE:CD1	6:C:258:ILE:N	2.75	0.48
8:E:55:ARG:C	8:E:57:MET:N	2.67	0.48
11:H:99:GLY:N	11:H:118:PHE:CD2	2.80	0.48
4:A:1102:LYS:HG2	4:A:1106:ASN:HD21	1.77	0.48
4:A:1162:VAL:O	4:A:1162:VAL:HG12	2.13	0.48
4:A:115:LEU:HB2	4:A:122:MET:CE	2.43	0.48
4:A:1373:ASP:HA	4:A:1376:THR:CG2	2.43	0.48
4:A:532:ARG:O	4:A:535:THR:HB	2.13	0.48
4:A:577:ILE:C	4:A:579:SER:N	2.64	0.48
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.94	0.48
4:A:809:THR:HG23	4:A:812:GLU:HG3	1.95	0.48
5:B:910:VAL:HG12	5:B:911:ILE:N	2.28	0.48
10:G:88:ASP:HA	10:G:144:ARG:HA	1.96	0.48
13:J:8:PHE:H	13:J:49:MET:HE1	1.79	0.48
4:A:1168:GLU:O	4:A:1172:LEU:HG	2.13	0.48
4:A:1291:VAL:HG13	4:A:1292:PRO:N	2.29	0.48
4:A:1279:ILE:HD11	4:A:1316:VAL:CG2	2.42	0.48
4:A:971:PHE:HE2	4:A:1040:GLN:HG2	1.79	0.48
4:A:466:SER:HB3	5:B:1103:ILE:HG12	1.94	0.48
4:A:14:VAL:HG21	5:B:1216:LEU:HD13	1.95	0.48
5:B:370:PHE:HE2	5:B:373:ARG:NH1	2.06	0.48
5:B:470:LYS:C	5:B:472:ALA:H	2.15	0.48
5:B:810:GLU:HB2	5:B:815:ARG:HH22	1.79	0.48
5:B:897:GLY:O	5:B:898:LEU:HD23	2.14	0.48
6:C:259:LEU:HD13	14:K:91:CYS:HB2	1.95	0.48
6:C:69:LEU:H	6:C:69:LEU:CD1	2.27	0.48
8:E:124:VAL:HG13	8:E:132:ILE:CB	2.40	0.48
10:G:20:PRO:HG2	10:G:21:ARG:N	2.28	0.48
11:H:23:VAL:HG13	11:H:42:ILE:O	2.14	0.48
4:A:313:GLN:O	4:A:314:ALA:HB3	2.13	0.48
4:A:381:THR:HG23	4:A:383:TYR:H	1.79	0.48
4:A:407:ARG:HB3	4:A:430:TRP:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:683:ILE:HD13	4:A:801:GLU:HG3	1.96	0.48
5:B:1084:GLN:HG2	6:C:201:TRP:CZ2	2.48	0.48
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.96	0.48
5:B:558:LEU:O	5:B:560:GLU:N	2.46	0.48
5:B:815:ARG:HD3	5:B:1041:GLU:OE2	2.14	0.48
6:C:255:VAL:HG12	14:K:91:CYS:HB3	1.94	0.48
8:E:117:THR:O	8:E:120:ALA:N	2.45	0.48
9:F:131:PRO:C	9:F:132:LEU:HD23	2.34	0.48
4:A:1116:LEU:CD1	4:A:1118:VAL:HG13	2.43	0.48
4:A:335:ARG:CA	4:A:339:ASN:HB2	2.41	0.48
4:A:775:ILE:HB	4:A:797:LYS:O	2.14	0.48
4:A:770:VAL:HA	4:A:822:GLU:OE1	2.14	0.48
5:B:333:PHE:O	5:B:334:ILE:HG13	2.14	0.48
5:B:345:LYS:O	5:B:347:LYS:HG2	2.13	0.48
5:B:834:ASN:HB3	5:B:840:ILE:HG13	1.95	0.48
6:C:254:LYS:C	6:C:256:ALA:N	2.64	0.48
7:D:53:SER:HB3	7:D:153:ARG:H	1.79	0.48
12:I:34:TYR:O	12:I:35:VAL:HG23	2.13	0.48
5:B:1039:GLY:HA2	13:J:51:LEU:HD21	1.95	0.48
5:B:129:PHE:HA	5:B:165:VAL:O	2.14	0.48
5:B:180:TYR:H	5:B:180:TYR:HD1	1.61	0.48
5:B:29:ASP:HB3	5:B:658:ILE:CD1	2.44	0.48
5:B:877:PRO:C	5:B:878:GLN:HG3	2.34	0.48
6:C:215:GLU:O	6:C:217:ASP:N	2.46	0.48
7:D:19:GLU:O	7:D:21:GLU:N	2.47	0.48
8:E:96:PHE:CZ	8:E:100:ILE:HD11	2.49	0.48
10:G:10:ASN:OD1	10:G:71:ASN:HA	2.13	0.48
10:G:143:ILE:CG2	10:G:144:ARG:N	2.77	0.48
10:G:20:PRO:CG	10:G:21:ARG:H	2.26	0.48
13:J:23:ASN:C	13:J:25:LEU:N	2.66	0.48
15:L:36:SER:O	15:L:37:LYS:C	2.51	0.48
3:P:5:C:H2'	3:P:6:C:H6	1.78	0.48
1:T:15:DT:H1'	4:A:1386:ARG:HH12	1.77	0.48
4:A:1396:ALA:O	4:A:1398:MET:N	2.47	0.48
4:A:1450:LEU:HD21	10:G:19:GLY:O	2.13	0.48
4:A:407:ARG:HG2	4:A:430:TRP:CZ3	2.49	0.48
4:A:388:LEU:HD22	4:A:432:VAL:HG21	1.96	0.48
4:A:565:ILE:O	4:A:570:PRO:HA	2.14	0.48
4:A:596:THR:C	4:A:598:LEU:N	2.67	0.48
4:A:626:ASN:O	4:A:631:HIS:CD2	2.67	0.48
4:A:95:PHE:O	4:A:98:LYS:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1187:ASN:O	5:B:1188:LYS:HB2	2.13	0.48
5:B:360:PHE:O	5:B:361:LEU:C	2.52	0.48
8:E:154:ILE:H	8:E:196:VAL:HG12	1.79	0.48
4:A:1441:PHE:CE2	9:F:89:GLU:HG2	2.49	0.48
10:G:150:CYS:C	10:G:151:ILE:HG13	2.33	0.48
11:H:100:THR:HG22	11:H:101:ALA:H	1.79	0.48
5:B:1077:THR:HG22	14:K:44:ASN:HD21	1.78	0.48
5:B:992:ILE:HD11	14:K:66:PRO:HB2	1.95	0.48
4:A:1341:ILE:O	4:A:1344:GLY:N	2.47	0.48
4:A:545:GLN:O	4:A:548:ASN:N	2.47	0.48
5:B:1033:LYS:NZ	5:B:1070:GLU:OE1	2.45	0.48
5:B:642:ASP:CB	5:B:649:LYS:HG3	2.43	0.48
5:B:661:LEU:C	5:B:663:ALA:N	2.67	0.48
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	1.96	0.48
6:C:3:GLU:HG2	6:C:4:GLU:N	2.29	0.48
11:H:62:SER:O	11:H:63:LEU:C	2.50	0.48
4:A:381:THR:O	4:A:384:ASN:N	2.43	0.47
4:A:577:ILE:O	4:A:580:VAL:HG23	2.14	0.47
4:A:608:ILE:HG13	4:A:613:ILE:HD12	1.95	0.47
5:B:1065:GLN:HG3	5:B:1067:ARG:H	1.78	0.47
5:B:95:ILE:CG1	5:B:130:VAL:HG22	2.41	0.47
5:B:205:ILE:CG2	5:B:206:ASN:N	2.76	0.47
5:B:63:ILE:HA	5:B:421:PHE:CE2	2.49	0.47
10:G:125:SER:OG	10:G:128:PRO:HA	2.14	0.47
4:A:1013:ASP:O	4:A:1015:VAL:N	2.46	0.47
4:A:172:PRO:HG3	4:A:185:TRP:CZ2	2.49	0.47
4:A:265:LYS:CE	4:A:322:VAL:HG13	2.44	0.47
4:A:53:LEU:CD2	4:A:54:ASN:N	2.60	0.47
4:A:853:ASP:O	4:A:854:ASN:CB	2.60	0.47
4:A:856:THR:HG22	4:A:864:ILE:HB	1.95	0.47
5:B:97:VAL:HG12	5:B:178:ASN:HD21	1.77	0.47
5:B:401:PHE:HD2	5:B:521:LEU:HD12	1.79	0.47
6:C:74:SER:HB2	6:C:77:ILE:HG12	1.94	0.47
9:F:81:THR:HG1	9:F:146:TRP:HE1	1.63	0.47
11:H:106:GLU:O	11:H:108:SER:N	2.46	0.47
13:J:56:LEU:O	13:J:59:LYS:N	2.47	0.47
15:L:40:LEU:HD13	15:L:44:ASP:CB	2.43	0.47
4:A:1025:ARG:O	4:A:1026:LEU:HD23	2.14	0.47
4:A:873:MET:C	4:A:1058:VAL:CG2	2.82	0.47
4:A:172:PRO:HB3	4:A:185:TRP:CE2	2.49	0.47
4:A:666:ILE:CD1	4:A:667:GLY:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1165:ILE:CG2	5:B:1166:CYS:N	2.76	0.47
5:B:446:LEU:HD23	5:B:446:LEU:N	2.29	0.47
5:B:522:VAL:HG12	5:B:523:CYS:N	2.27	0.47
7:D:184:ALA:O	7:D:185:CYS:SG	2.69	0.47
9:F:75:PRO:HG3	9:F:78:GLN:OE1	2.14	0.47
11:H:116:TYR:HE2	11:H:140:ALA:CB	2.27	0.47
11:H:91:ASP:O	11:H:93:TYR:N	2.47	0.47
4:A:369:SER:HB3	14:K:2:ASN:HD21	1.78	0.47
3:P:7:A:H2'	3:P:8:G:O4'	2.14	0.47
4:A:872:GLY:O	4:A:1058:VAL:HG23	2.14	0.47
5:B:1040:ASN:O	5:B:1042:GLY:N	2.47	0.47
5:B:1081:LEU:O	5:B:1083:ALA:O	2.33	0.47
5:B:102:VAL:CG2	5:B:112:LEU:HB2	2.41	0.47
5:B:258:LEU:O	5:B:259:TYR:O	2.33	0.47
5:B:386:LEU:O	5:B:388:CYS:N	2.48	0.47
5:B:435:THR:CG2	5:B:437:GLU:HB2	2.44	0.47
5:B:615:MET:CB	5:B:626:ILE:HG12	2.43	0.47
6:C:36:VAL:HG21	6:C:251:LEU:HB2	1.94	0.47
6:C:91:HIS:CD2	6:C:91:HIS:C	2.88	0.47
10:G:26:LEU:O	10:G:29:LYS:N	2.47	0.47
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	1.97	0.47
4:A:1445:ILE:HG12	10:G:18:PHE:HE2	1.77	0.47
4:A:277:GLU:C	4:A:279:LEU:H	2.18	0.47
4:A:67:CYS:O	4:A:68:GLN:HB2	2.14	0.47
4:A:817:ALA:O	4:A:818:MET:C	2.53	0.47
5:B:1084:GLN:HE21	5:B:1084:GLN:H	1.62	0.47
5:B:1214:PRO:HG2	5:B:1214:PRO:O	2.14	0.47
5:B:360:PHE:CD2	5:B:360:PHE:C	2.88	0.47
5:B:756:ILE:O	5:B:759:PRO:HD3	2.14	0.47
5:B:903:VAL:HG12	5:B:904:ARG:N	2.28	0.47
11:H:11:GLN:HA	11:H:53:ASP:O	2.15	0.47
11:H:82:PRO:C	11:H:84:ALA:H	2.13	0.47
4:A:1115:SER:OG	4:A:1116:LEU:N	2.47	0.47
4:A:277:GLU:O	4:A:279:LEU:N	2.47	0.47
4:A:58:LEU:O	4:A:59:GLY:O	2.32	0.47
5:B:1216:LEU:O	5:B:1217:TYR:HD1	1.96	0.47
5:B:54:PHE:HA	5:B:58:THR:HB	1.95	0.47
5:B:820:GLY:N	5:B:1091:TYR:OH	2.48	0.47
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.48	0.47
6:C:183:TRP:CE2	6:C:207:CYS:HB3	2.50	0.47
4:A:1059:HIS:ND1	9:F:86:THR:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:27:LYS:O	10:G:30:LEU:HB3	2.14	0.47
10:G:66:GLY:O	10:G:67:SER:C	2.52	0.47
15:L:58:LYS:O	15:L:59:ALA:O	2.31	0.47
4:A:1265:ASN:O	4:A:1268:LEU:N	2.41	0.47
4:A:1437:GLY:HA3	9:F:88:TYR:CD2	2.50	0.47
4:A:259:GLU:OE1	4:A:259:GLU:HA	2.14	0.47
4:A:43:GLU:O	4:A:44:THR:CB	2.63	0.47
4:A:545:GLN:O	4:A:546:VAL:C	2.52	0.47
4:A:726:ARG:HD2	4:A:765:VAL:O	2.15	0.47
5:B:1070:GLU:OE1	13:J:44:TYR:OH	2.33	0.47
5:B:1183:LYS:HA	5:B:1186:ASP:HA	1.96	0.47
5:B:711:GLU:H	5:B:712:PRO:HD2	1.79	0.47
5:B:787:VAL:O	5:B:787:VAL:HG12	2.15	0.47
6:C:27:LEU:O	6:C:28:ALA:C	2.52	0.47
6:C:76:ASP:O	6:C:77:ILE:C	2.52	0.47
7:D:176:GLU:C	7:D:178:ALA:N	2.64	0.47
8:E:78:LEU:HD21	8:E:80:VAL:HG23	1.97	0.47
4:A:1213:GLY:O	4:A:1214:GLU:C	2.52	0.47
4:A:471:ASN:O	4:A:474:VAL:HG12	2.15	0.47
4:A:567:LYS:HD2	4:A:568:PRO:CD	2.45	0.47
4:A:533:LYS:HE3	4:A:745:GLN:HE22	1.79	0.47
4:A:852:TYR:HA	4:A:1060:PRO:HB3	1.96	0.47
5:B:1085:ILE:CD1	5:B:1085:ILE:N	2.75	0.47
5:B:916:THR:O	5:B:935:ARG:HG3	2.14	0.47
6:C:236:GLY:C	6:C:238:ILE:N	2.68	0.47
7:D:195:ILE:O	7:D:197:SER:N	2.47	0.47
8:E:168:TYR:HB2	8:E:170:LEU:HG	1.97	0.47
10:G:149:GLY:O	10:G:159:ALA:HB1	2.15	0.47
10:G:14:HIS:HD2	10:G:16:SER:CB	2.27	0.47
7:D:24:ALA:HA	10:G:83:LYS:O	2.15	0.47
10:G:99:PHE:C	10:G:99:PHE:CD1	2.88	0.47
13:J:36:LEU:O	13:J:39:LEU:N	2.48	0.47
13:J:56:LEU:O	13:J:57:ILE:C	2.53	0.47
4:A:492:PRO:HB2	4:A:497:THR:HG22	1.96	0.47
4:A:60:SER:C	4:A:61:ILE:HG13	2.35	0.47
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.50	0.47
4:A:343:LYS:HE2	5:B:1156:ASP:OD2	2.15	0.47
5:B:1174:LYS:O	5:B:1176:ASN:HB2	2.14	0.47
5:B:593:PRO:HG2	5:B:617:ARG:NH2	2.29	0.47
6:C:46:ILE:HG13	6:C:72:LEU:HD11	1.97	0.47
6:C:89:GLU:O	6:C:90:ASP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:51:ASN:O	12:I:54:GLU:HG3	2.15	0.47
1:T:23:DG:H2'	1:T:24:DG:H8	1.78	0.47
4:A:1305:VAL:CG1	4:A:1306:LEU:N	2.77	0.47
4:A:1323:ASP:C	4:A:1325:THR:H	2.17	0.47
4:A:1342:GLU:CG	8:E:198:ILE:HD13	2.45	0.47
4:A:1453:TYR:O	4:A:1454:MET:HB3	2.15	0.47
4:A:300:VAL:O	4:A:300:VAL:HG12	2.13	0.47
4:A:350:ARG:HH11	4:A:350:ARG:HG3	1.80	0.47
5:B:798:TYR:HE2	6:C:62:PHE:HE2	1.52	0.47
5:B:838:SER:HA	5:B:989:THR:O	2.15	0.47
5:B:948:ILE:O	5:B:968:VAL:HG13	2.15	0.47
6:C:46:ILE:HG23	6:C:157:CYS:HB3	1.97	0.47
7:D:206:GLU:C	7:D:208:GLU:N	2.66	0.47
11:H:138:GLU:O	11:H:139:ASN:C	2.52	0.47
12:I:25:LEU:O	12:I:38:ALA:HB2	2.15	0.47
15:L:40:LEU:CD1	15:L:44:ASP:HB3	2.45	0.47
4:A:1018:PHE:O	4:A:1021:LEU:HB3	2.15	0.47
4:A:89:PRO:HB2	4:A:204:THR:CG2	2.45	0.47
4:A:406:ILE:HG13	4:A:431:LYS:HB2	1.97	0.47
4:A:352:VAL:O	4:A:467:THR:HB	2.15	0.47
4:A:630:ILE:HD13	4:A:646:PHE:HZ	1.79	0.47
4:A:996:ASN:O	4:A:998:LEU:HD12	2.15	0.47
5:B:1069:PHE:CD1	5:B:1069:PHE:N	2.80	0.47
5:B:1174:LYS:O	5:B:1176:ASN:N	2.47	0.47
5:B:366:GLN:O	5:B:367:LEU:O	2.33	0.47
5:B:39:ARG:HH21	5:B:665:GLU:CG	2.25	0.47
5:B:45:SER:O	5:B:46:GLN:C	2.53	0.47
5:B:487:THR:CG2	5:B:488:TYR:N	2.78	0.47
5:B:552:MET:C	5:B:554:ILE:H	2.17	0.47
5:B:582:VAL:HA	5:B:626:ILE:O	2.15	0.47
5:B:899:ILE:HD12	5:B:911:ILE:HG23	1.96	0.47
5:B:984:HIS:CG	5:B:1025:HIS:HB2	2.50	0.47
5:B:1001:PHE:HE2	6:C:34:ARG:CZ	2.27	0.47
11:H:127:GLY:HA3	11:H:130:ARG:NH2	2.29	0.47
4:A:1451:VAL:C	4:A:1453:TYR:H	2.18	0.46
4:A:231:PRO:HA	4:A:234:MET:HE2	1.98	0.46
4:A:231:PRO:O	4:A:233:TRP:N	2.48	0.46
4:A:308:ILE:HG22	4:A:309:ALA:N	2.29	0.46
4:A:939:ASP:OD1	4:A:1023:ARG:NH1	2.48	0.46
5:B:834:ASN:ND2	5:B:1013:ASN:HA	2.30	0.46
5:B:1034:VAL:O	5:B:1036:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:225:VAL:CG1	5:B:385:LEU:HA	2.44	0.46
5:B:570:VAL:HA	5:B:571:PRO:HD2	1.73	0.46
5:B:839:MET:HE1	5:B:980:PHE:HB3	1.96	0.46
5:B:94:LYS:HG2	5:B:95:ILE:N	2.30	0.46
6:C:140:ASN:O	6:C:141:GLY:O	2.32	0.46
6:C:229:TYR:CD1	6:C:229:TYR:N	2.83	0.46
7:D:51:ASN:C	7:D:52:LEU:O	2.52	0.46
8:E:192:ARG:NH1	8:E:192:ARG:HG3	2.28	0.46
9:F:132:LEU:O	9:F:148:VAL:HG22	2.15	0.46
11:H:58:THR:HG22	11:H:59:ILE:N	2.30	0.46
13:J:13:VAL:C	13:J:14:VAL:HG23	2.35	0.46
14:K:49:GLU:HG3	14:K:94:ILE:HG13	1.97	0.46
4:A:337:ARG:CZ	4:A:839:ARG:HH12	2.28	0.46
4:A:427:GLN:HB2	4:A:430:TRP:NE1	2.30	0.46
4:A:549:MET:SD	4:A:577:ILE:HD11	2.55	0.46
4:A:57:ARG:HB3	4:A:68:GLN:HG2	1.97	0.46
4:A:844:ALA:HB2	4:A:1389:PHE:CE2	2.49	0.46
5:B:293:PRO:C	5:B:294:ASP:O	2.52	0.46
5:B:838:SER:CA	5:B:989:THR:O	2.62	0.46
5:B:970:THR:HG22	5:B:971:THR:N	2.30	0.46
7:D:141:LEU:O	7:D:142:LYS:C	2.54	0.46
7:D:51:ASN:OD1	7:D:52:LEU:O	2.33	0.46
8:E:94:LYS:HG3	8:E:98:ILE:CD1	2.45	0.46
12:I:77:LYS:O	12:I:79:HIS:N	2.48	0.46
13:J:32:GLU:O	13:J:34:THR:N	2.48	0.46
14:K:59:ALA:HA	14:K:74:ARG:O	2.15	0.46
14:K:68:PHE:CD2	14:K:68:PHE:N	2.80	0.46
15:L:46:VAL:CG1	15:L:56:LEU:HD12	2.45	0.46
1:T:20:DC:H2''	1:T:21:DC:O5'	2.15	0.46
4:A:996:ASN:HB3	4:A:1050:GLU:OE2	2.16	0.46
4:A:1102:LYS:O	4:A:1106:ASN:ND2	2.48	0.46
4:A:1348:LEU:HG	4:A:1372:VAL:HG22	1.94	0.46
4:A:1405:THR:HB	4:A:1406:VAL:H	1.47	0.46
4:A:1447:GLU:OE2	10:G:23:LYS:HB2	2.15	0.46
4:A:270:LEU:O	4:A:271:LYS:C	2.53	0.46
4:A:574:GLY:O	4:A:575:LYS:C	2.53	0.46
4:A:693:VAL:HA	4:A:696:GLU:HB3	1.97	0.46
4:A:883:LEU:CD2	4:A:1021:LEU:HB2	2.45	0.46
5:B:108:VAL:CG1	5:B:109:THR:H	2.19	0.46
5:B:589:VAL:CG1	5:B:590:HIS:H	2.00	0.46
6:C:226:ASP:O	6:C:227:THR:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:116:TYR:HE2	11:H:140:ALA:HB1	1.81	0.46
11:H:98:TYR:C	11:H:118:PHE:HD2	2.18	0.46
14:K:47:ARG:HD3	14:K:59:ALA:O	2.15	0.46
14:K:93:SER:O	14:K:97:LYS:HG3	2.16	0.46
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.15	0.46
4:A:562:THR:HA	4:A:563:PRO:HD3	1.83	0.46
4:A:722:LEU:HD22	4:A:799:PHE:CD1	2.51	0.46
4:A:846:GLU:OE1	4:A:1425:SER:OG	2.33	0.46
5:B:1034:VAL:C	5:B:1036:ALA:N	2.69	0.46
5:B:189:LEU:HD23	5:B:192:LEU:HD12	1.97	0.46
5:B:364:ILE:HG22	5:B:365:THR:N	2.31	0.46
5:B:424:LEU:O	5:B:428:ILE:HG13	2.16	0.46
6:C:15:LYS:O	6:C:240:VAL:HG22	2.16	0.46
12:I:111:THR:CG2	12:I:112:SER:H	2.29	0.46
12:I:83:ASN:HA	12:I:102:VAL:O	2.16	0.46
12:I:99:LEU:C	12:I:100:PHE:CD1	2.89	0.46
13:J:1:MET:N	13:J:56:LEU:H	2.13	0.46
4:A:356:ASP:OD2	14:K:65:HIS:HE1	1.99	0.46
4:A:116:ASP:O	4:A:118:HIS:N	2.48	0.46
4:A:42:ASP:HB3	4:A:45:GLN:CA	2.46	0.46
4:A:785:PRO:HG2	4:A:786:HIS:CD2	2.47	0.46
4:A:500:GLU:OE2	5:B:1145:SER:CB	2.64	0.46
5:B:1177:HIS:C	5:B:1179:GLN:H	2.19	0.46
5:B:38:PHE:CD1	5:B:811:TYR:CD2	3.04	0.46
5:B:638:PHE:HD2	5:B:690:VAL:HG22	1.80	0.46
5:B:695:ALA:O	5:B:698:GLU:HB3	2.16	0.46
9:F:109:VAL:HG12	9:F:110:ASP:N	2.30	0.46
10:G:115:MET:CB	10:G:116:PRO:CD	2.94	0.46
2:N:3:DG:OP2	2:N:3:DG:H2'	2.16	0.46
4:A:1289:ARG:HD2	4:A:1303:GLU:OE2	2.16	0.46
4:A:1446:ASP:HB3	4:A:1449:SER:OG	2.16	0.46
5:B:758:PHE:HZ	5:B:1031:LEU:HD22	1.81	0.46
4:A:490:HIS:HB3	5:B:1150:ARG:NH1	2.31	0.46
5:B:329:THR:O	5:B:332:ASP:HB3	2.16	0.46
5:B:405:ARG:HA	5:B:631:GLY:O	2.16	0.46
7:D:35:LEU:HD21	7:D:173:HIS:HB3	1.97	0.46
8:E:54:GLN:O	8:E:57:MET:HB3	2.16	0.46
13:J:1:MET:HE2	13:J:60:PHE:HE2	1.81	0.46
4:A:1028:THR:O	4:A:1032:LEU:HD12	2.16	0.46
4:A:130:ASP:O	4:A:131:SER:C	2.54	0.46
4:A:684:ALA:O	4:A:687:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1072:MET:CE	5:B:1087:PHE:HD1	2.28	0.46
5:B:310:MET:HG3	5:B:386:LEU:CD1	2.46	0.46
5:B:455:SER:O	5:B:456:GLY:C	2.53	0.46
5:B:780:VAL:HG12	5:B:782:LEU:O	2.16	0.46
6:C:168:ALA:C	6:C:170:TRP:N	2.69	0.46
6:C:248:ILE:HD13	14:K:101:LEU:HD22	1.98	0.46
8:E:46:TYR:CE2	8:E:58:MET:HA	2.51	0.46
10:G:53:ASN:HD22	10:G:53:ASN:N	2.13	0.46
12:I:98:VAL:HG12	12:I:99:LEU:H	1.80	0.46
14:K:31:VAL:HG12	14:K:32:VAL:H	1.80	0.46
4:A:1153:TYR:CD2	4:A:1163:ILE:HD11	2.51	0.46
4:A:11:LEU:HB2	5:B:1193:GLN:OE1	2.16	0.46
4:A:41:MET:O	4:A:42:ASP:C	2.54	0.46
4:A:626:ASN:C	4:A:628:GLY:H	2.19	0.46
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.49	0.46
4:A:849:MET:HE1	4:A:1061:GLY:HA2	1.98	0.46
4:A:920:LEU:HD23	4:A:920:LEU:C	2.35	0.46
5:B:999:MET:HG2	5:B:1007:VAL:HG22	1.98	0.46
5:B:1183:LYS:HE3	5:B:1183:LYS:O	2.15	0.46
5:B:562:GLY:HA3	5:B:590:HIS:ND1	2.31	0.46
6:C:163:ILE:O	6:C:165:LYS:N	2.48	0.46
6:C:70:ILE:O	6:C:70:ILE:HG22	2.16	0.46
6:C:99:LEU:HD23	6:C:99:LEU:N	2.31	0.46
7:D:35:LEU:CD2	7:D:174:PRO:HD2	2.45	0.46
4:A:1327:ILE:HG22	8:E:147:HIS:HE1	1.81	0.46
9:F:109:VAL:HG13	9:F:127:GLU:OE1	2.16	0.46
11:H:22:LYS:O	11:H:23:VAL:HG23	2.15	0.46
12:I:82:GLU:O	12:I:104:LEU:HG	2.16	0.46
4:A:551:TYR:CE2	14:K:62:LYS:HE2	2.50	0.46
4:A:1237:ILE:HG22	4:A:1238:ILE:N	2.31	0.46
4:A:1265:ASN:C	4:A:1267:MET:N	2.68	0.46
4:A:404:TYR:CE2	4:A:414:ASP:HA	2.50	0.46
4:A:446:ARG:NH1	4:A:479:ASN:O	2.49	0.46
4:A:470:LEU:HD22	4:A:487:MET:CE	2.46	0.46
4:A:626:ASN:O	4:A:628:GLY:N	2.46	0.46
4:A:913:LEU:HD23	4:A:919:ILE:HD12	1.97	0.46
5:B:1096:ARG:O	5:B:1097:HIS:CB	2.54	0.46
5:B:303:TYR:N	5:B:303:TYR:CD2	2.82	0.46
5:B:210:LYS:HG3	5:B:461:LEU:O	2.15	0.46
5:B:814:PHE:O	5:B:816:GLU:N	2.49	0.46
6:C:9:LYS:O	6:C:10:ILE:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:75:MET:O	6:C:246:ARG:NH2	2.48	0.46
9:F:81:THR:HB	9:F:136:ARG:HH11	1.80	0.46
12:I:8:ARG:O	12:I:10:CYS:N	2.49	0.46
1:T:15:DT:H2''	1:T:16:DT:H5'	1.97	0.46
4:A:1001:ARG:HH11	4:A:1001:ARG:HG2	1.81	0.46
4:A:1222:ASN:O	4:A:1223:ASP:HB3	2.15	0.46
4:A:1451:VAL:C	4:A:1453:TYR:N	2.68	0.46
4:A:340:LEU:CD2	5:B:1199:ALA:HB3	2.45	0.46
4:A:596:THR:O	4:A:598:LEU:N	2.49	0.46
4:A:630:ILE:HG23	4:A:642:CYS:SG	2.56	0.46
4:A:874:ASP:N	4:A:1058:VAL:CG2	2.79	0.46
5:B:1060:ARG:HD2	5:B:1060:ARG:HA	1.48	0.46
5:B:1182:CYS:O	5:B:1183:LYS:O	2.34	0.46
5:B:283:VAL:O	5:B:286:PHE:N	2.49	0.46
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.96	0.46
5:B:377:PHE:C	5:B:379:GLY:N	2.67	0.46
5:B:48:LEU:O	5:B:49:ASP:C	2.52	0.46
6:C:70:ILE:HD11	6:C:144:ILE:CG1	2.46	0.46
8:E:17:ARG:O	8:E:20:LYS:HB2	2.16	0.46
9:F:111:LEU:N	9:F:111:LEU:HD12	2.29	0.46
9:F:143:PHE:C	9:F:143:PHE:CD1	2.90	0.46
10:G:121:PHE:HB2	10:G:130:TYR:CE2	2.51	0.46
11:H:93:TYR:CD1	11:H:93:TYR:N	2.83	0.46
14:K:42:LEU:HD21	14:K:46:ILE:HD11	1.98	0.46
4:A:103:CYS:O	4:A:106:VAL:O	2.34	0.45
4:A:563:PRO:HG3	4:A:572:TRP:CE2	2.50	0.45
4:A:774:ARG:O	4:A:775:ILE:O	2.34	0.45
4:A:854:ASN:HB3	4:A:1000:LEU:HD21	1.98	0.45
4:A:856:THR:HG22	4:A:856:THR:O	2.15	0.45
5:B:1065:GLN:NE2	5:B:1067:ARG:HG2	2.31	0.45
5:B:745:PRO:C	5:B:747:MET:N	2.70	0.45
5:B:842:ASN:ND2	5:B:845:SER:CB	2.78	0.45
5:B:882:THR:HB	5:B:934:LYS:O	2.15	0.45
6:C:181:ASP:OD2	6:C:184:ASN:HA	2.14	0.45
8:E:161:LYS:C	8:E:163:GLU:H	2.19	0.45
8:E:177:ARG:C	8:E:212:ARG:HD3	2.36	0.45
11:H:58:THR:HB	11:H:143:LEU:HD13	1.98	0.45
14:K:43:GLY:HA3	14:K:61:TYR:CE1	2.50	0.45
4:A:1011:GLN:NE2	4:A:1015:VAL:HG21	2.32	0.45
4:A:1045:VAL:O	4:A:1049:ILE:HG13	2.16	0.45
4:A:1435:PRO:HA	4:A:1439:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:337:ARG:CZ	4:A:839:ARG:NH1	2.79	0.45
4:A:418:SER:C	4:A:420:ARG:H	2.18	0.45
4:A:418:SER:C	4:A:420:ARG:N	2.68	0.45
5:B:114:PRO:O	5:B:116:GLU:N	2.49	0.45
4:A:1409:LEU:CD1	5:B:1207:LEU:HD21	2.36	0.45
5:B:38:PHE:HD1	5:B:811:TYR:CD2	2.34	0.45
5:B:581:PHE:N	5:B:624:LEU:O	2.39	0.45
6:C:179:GLU:CG	6:C:180:TYR:N	2.74	0.45
6:C:241:ASP:OD1	6:C:242:GLN:N	2.48	0.45
7:D:137:ASN:C	7:D:137:ASN:HD22	2.19	0.45
7:D:52:LEU:C	7:D:54:GLU:N	2.69	0.45
7:D:64:VAL:C	7:D:66:ARG:H	2.19	0.45
11:H:84:ALA:C	11:H:86:ASP:N	2.69	0.45
12:I:13:MET:HG3	12:I:14:LEU:H	1.80	0.45
4:A:1072:ILE:C	4:A:1075:PRO:HD2	2.36	0.45
4:A:1147:THR:HA	4:A:1197:LEU:HD23	1.98	0.45
4:A:1280:GLU:O	4:A:1281:ARG:C	2.54	0.45
4:A:1289:ARG:NH1	4:A:1326:ARG:NH1	2.63	0.45
4:A:1342:GLU:OE2	8:E:212:ARG:NH1	2.49	0.45
4:A:324:SER:O	4:A:325:ILE:C	2.53	0.45
4:A:415:LEU:HD23	4:A:415:LEU:HA	1.69	0.45
4:A:58:LEU:HD22	4:A:80:HIS:O	2.16	0.45
4:A:907:THR:HG23	4:A:908:LEU:H	1.81	0.45
5:B:1007:VAL:HG22	5:B:1008:PRO:CD	2.35	0.45
5:B:1115:THR:CG2	5:B:1117:GLN:HG3	2.46	0.45
5:B:769:TYR:O	5:B:772:ALA:N	2.49	0.45
6:C:10:ILE:HA	6:C:20:PHE:CB	2.46	0.45
7:D:153:ARG:C	7:D:154:PHE:CD1	2.89	0.45
7:D:68:ARG:C	7:D:70:PHE:H	2.20	0.45
8:E:114:ASN:O	8:E:115:ASN:CB	2.64	0.45
10:G:13:LEU:CD2	10:G:17:PHE:HB2	2.39	0.45
4:A:1118:VAL:O	4:A:1118:VAL:HG23	2.15	0.45
4:A:590:ARG:O	4:A:591:PHE:HB2	2.15	0.45
4:A:590:ARG:HD2	4:A:605:MET:CB	2.46	0.45
4:A:808:LEU:CD2	4:A:813:PHE:HA	2.38	0.45
5:B:1182:CYS:C	5:B:1183:LYS:HE3	2.35	0.45
5:B:199:MET:N	5:B:199:MET:SD	2.83	0.45
5:B:235:SER:C	5:B:236:HIS:HD2	2.19	0.45
5:B:69:LEU:HD22	5:B:429:PHE:CE1	2.51	0.45
5:B:765:PRO:O	5:B:766:ARG:C	2.53	0.45
5:B:864:LYS:N	5:B:872:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:918:ILE:HG21	5:B:935:ARG:HH11	1.81	0.45
7:D:64:VAL:C	7:D:66:ARG:N	2.68	0.45
4:A:185:TRP:HZ3	4:A:200:ARG:HG2	1.82	0.45
4:A:438:ASP:OD1	4:A:462:VAL:HG23	2.16	0.45
4:A:511:ILE:O	4:A:519:PRO:HA	2.16	0.45
4:A:477:PRO:CG	4:A:521:MET:HG2	2.47	0.45
4:A:526:ASP:OD1	5:B:1013:ASN:ND2	2.49	0.45
4:A:622:VAL:HG22	4:A:622:VAL:O	2.17	0.45
4:A:836:TYR:O	4:A:837:ILE:C	2.55	0.45
5:B:113:TYR:CD2	5:B:192:LEU:HD22	2.51	0.45
5:B:570:VAL:HG23	5:B:573:GLN:HB3	1.97	0.45
4:A:816:HIS:HE2	5:B:764:SER:H	1.64	0.45
6:C:88:CYS:SG	6:C:91:HIS:C	2.95	0.45
8:E:134:THR:C	8:E:135:PHE:CD1	2.89	0.45
8:E:157:SER:O	8:E:159:ASP:N	2.49	0.45
9:F:90:ARG:HD3	9:F:155:LEU:HD12	1.97	0.45
10:G:23:LYS:HG2	10:G:27:LYS:HE3	1.98	0.45
11:H:84:ALA:C	11:H:86:ASP:H	2.19	0.45
13:J:27:GLU:O	13:J:29:GLU:N	2.49	0.45
13:J:50:ILE:O	13:J:52:THR:N	2.49	0.45
15:L:32:ALA:HB3	15:L:55:ILE:CD1	2.47	0.45
4:A:1102:LYS:HG2	4:A:1106:ASN:ND2	2.30	0.45
4:A:1106:ASN:O	4:A:1107:VAL:HB	2.17	0.45
4:A:1370:LEU:O	4:A:1373:ASP:N	2.48	0.45
4:A:289:ILE:C	4:A:291:GLU:N	2.70	0.45
4:A:344:ARG:HD2	5:B:1118:PRO:O	2.17	0.45
4:A:575:LYS:NZ	4:A:615:GLY:H	2.15	0.45
4:A:709:THR:HB	4:A:712:GLU:HG3	1.99	0.45
4:A:784:LEU:HD11	4:A:815:PHE:CE2	2.51	0.45
4:A:841:LEU:O	4:A:845:LEU:HG	2.17	0.45
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.49	0.45
5:B:195:CYS:SG	5:B:196:PRO:HD2	2.56	0.45
5:B:221:ASN:OD1	5:B:242:SER:HA	2.15	0.45
5:B:918:ILE:HD12	5:B:935:ARG:CD	2.47	0.45
5:B:979:LYS:O	5:B:980:PHE:CD2	2.70	0.45
7:D:146:GLN:O	7:D:147:TYR:C	2.54	0.45
7:D:35:LEU:N	7:D:35:LEU:HD12	2.32	0.45
12:I:61:ASP:O	12:I:63:GLY:N	2.49	0.45
12:I:69:PRO:HG2	12:I:85:PHE:CE2	2.52	0.45
1:T:16:DT:C5'	4:A:1386:ARG:NH1	2.80	0.45
4:A:1074:GLU:HB3	4:A:1075:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1142:THR:O	4:A:1143:LEU:C	2.54	0.45
4:A:282:ASN:O	4:A:284:ALA:N	2.50	0.45
4:A:479:ASN:O	4:A:479:ASN:OD1	2.34	0.45
4:A:492:PRO:O	4:A:493:GLN:NE2	2.50	0.45
4:A:774:ARG:H	4:A:774:ARG:HG2	1.62	0.45
5:B:839:MET:HE3	5:B:1010:LEU:HD21	1.98	0.45
5:B:637:LEU:HD23	5:B:742:GLU:HA	1.97	0.45
5:B:732:SER:HB2	5:B:734:HIS:CD2	2.51	0.45
5:B:763:GLN:O	5:B:764:SER:C	2.55	0.45
5:B:766:ARG:NH2	5:B:1020:ARG:HD3	2.31	0.45
5:B:797:TYR:HE1	5:B:854:LEU:HD21	1.81	0.45
8:E:136:ASN:OD1	8:E:138:ALA:N	2.50	0.45
10:G:111:THR:HG22	10:G:113:HIS:H	1.82	0.45
10:G:20:PRO:CG	10:G:21:ARG:N	2.80	0.45
12:I:26:LEU:CD2	12:I:37:GLU:HA	2.41	0.45
14:K:5:ASP:O	14:K:6:ARG:C	2.55	0.45
4:A:1265:ASN:O	4:A:1267:MET:N	2.50	0.45
4:A:1348:LEU:O	4:A:1352:VAL:HG23	2.17	0.45
4:A:341:MET:CE	4:A:843:LYS:HZ1	2.29	0.45
5:B:596:LEU:O	5:B:600:LEU:HG	2.16	0.45
5:B:863:GLU:O	5:B:961:LEU:HD22	2.16	0.45
6:C:133:ILE:HD12	6:C:237:SER:HA	1.99	0.45
6:C:58:LEU:CD2	6:C:58:LEU:N	2.80	0.45
8:E:129:PRO:O	8:E:130:ALA:O	2.34	0.45
9:F:148:VAL:O	9:F:149:GLU:C	2.54	0.45
10:G:14:HIS:HD2	10:G:16:SER:HB2	1.82	0.45
14:K:88:LYS:O	14:K:89:ASN:C	2.55	0.45
4:A:1004:ASN:OD1	4:A:1005:GLU:N	2.50	0.45
4:A:1006:ILE:HD12	8:E:163:GLU:CG	2.46	0.45
4:A:1148:ILE:HB	4:A:1196:GLU:O	2.17	0.45
4:A:1206:ASP:HB3	4:A:1274:ARG:NH1	2.31	0.45
4:A:1100:ARG:NH2	4:A:1351:GLU:HG2	2.32	0.45
4:A:446:ARG:CD	4:A:480:ALA:HB2	2.47	0.45
4:A:477:PRO:HG2	4:A:521:MET:HG2	1.98	0.45
4:A:566:ILE:O	4:A:567:LYS:O	2.34	0.45
4:A:590:ARG:NH2	4:A:620:LYS:CB	2.75	0.45
4:A:7:SER:C	4:A:9:ALA:H	2.20	0.45
4:A:7:SER:OG	5:B:1193:GLN:NE2	2.50	0.45
5:B:980:PHE:HE2	5:B:1094:ARG:CB	2.30	0.45
5:B:318:VAL:C	5:B:320:ASP:N	2.71	0.45
5:B:594:ALA:HA	5:B:617:ARG:HH12	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:737:THR:O	5:B:738:PHE:C	2.55	0.45
5:B:1001:PHE:HD2	6:C:34:ARG:NH2	2.15	0.45
8:E:48:ASP:CG	8:E:49:SER:N	2.68	0.45
4:A:1111:MET:H	4:A:1111:MET:HG2	1.52	0.45
4:A:1118:VAL:HG12	4:A:1327:ILE:HG13	1.99	0.45
4:A:218:ASP:O	4:A:219:PHE:C	2.56	0.45
4:A:416:ARG:C	4:A:417:TYR:CD2	2.89	0.45
4:A:57:ARG:O	4:A:68:GLN:NE2	2.49	0.45
4:A:682:THR:HG23	4:A:728:LYS:HE3	1.99	0.45
4:A:846:GLU:HB2	4:A:847:ASP:H	1.64	0.45
4:A:960:ILE:O	4:A:961:ARG:C	2.55	0.45
5:B:1208:MET:HA	5:B:1212:ILE:O	2.17	0.45
5:B:189:LEU:O	5:B:190:TYR:C	2.55	0.45
5:B:25:ILE:HD11	5:B:653:VAL:C	2.37	0.45
5:B:708:GLU:O	5:B:709:ASP:C	2.56	0.45
7:D:202:ILE:CG2	7:D:207:LEU:HB2	2.44	0.45
8:E:202:SER:HB3	8:E:205:SER:O	2.15	0.45
13:J:13:VAL:O	13:J:14:VAL:CG2	2.65	0.45
13:J:2:ILE:HG22	13:J:3:VAL:O	2.17	0.45
4:A:1164:PRO:O	4:A:1166:ASP:N	2.50	0.44
4:A:42:ASP:HB3	4:A:45:GLN:N	2.30	0.44
4:A:504:LEU:HD12	4:A:504:LEU:N	2.31	0.44
4:A:577:ILE:O	4:A:578:LEU:C	2.51	0.44
4:A:65:LEU:O	4:A:66:LYS:C	2.55	0.44
4:A:839:ARG:O	4:A:840:ARG:C	2.54	0.44
5:B:1115:THR:HG21	5:B:1117:GLN:CD	2.38	0.44
5:B:1200:ALA:O	5:B:1203:LEU:HB3	2.17	0.44
5:B:351:TYR:CD1	5:B:355:ILE:HD11	2.52	0.44
5:B:785:TYR:CD1	5:B:786:ASN:N	2.85	0.44
5:B:843:GLN:HB2	5:B:993:THR:HB	1.98	0.44
6:C:112:ASN:CB	6:C:114:TYR:CE1	2.99	0.44
8:E:124:VAL:HA	8:E:132:ILE:HD12	1.99	0.44
4:A:871:ASP:HB3	8:E:204:THR:HG23	2.00	0.44
9:F:119:ARG:CG	9:F:119:ARG:NH1	2.80	0.44
11:H:33:GLN:C	11:H:35:GLN:H	2.21	0.44
15:L:28:LYS:HB2	15:L:39:SER:HA	1.98	0.44
4:A:1191:TRP:HD1	4:A:1256:GLU:HB2	1.81	0.44
4:A:1349:TYR:CA	4:A:1372:VAL:HG21	2.46	0.44
4:A:144:THR:O	4:A:146:MET:HG3	2.18	0.44
4:A:268:ASP:HB3	4:A:299:HIS:CE1	2.52	0.44
4:A:353:ILE:HB	4:A:470:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3:GLY:O	4:A:4:GLN:CB	2.64	0.44
5:B:1106:ARG:NH2	5:B:1109:GLY:H	2.14	0.44
4:A:7:SER:HB2	5:B:1175:LEU:HD22	1.99	0.44
5:B:181:LEU:HD22	5:B:189:LEU:HD22	1.99	0.44
5:B:436:VAL:HG12	5:B:436:VAL:O	2.17	0.44
5:B:687:GLU:O	5:B:689:LEU:HG	2.18	0.44
5:B:653:VAL:HG23	5:B:689:LEU:HB3	1.96	0.44
5:B:833:TYR:N	5:B:833:TYR:CD1	2.84	0.44
8:E:98:ILE:O	8:E:100:ILE:N	2.50	0.44
9:F:111:LEU:C	9:F:113:GLY:N	2.70	0.44
11:H:42:ILE:HG23	11:H:95:TYR:CE1	2.41	0.44
2:N:5:DA:H1'	2:N:6:DC:O5'	2.18	0.44
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.33	0.44
4:A:225:ASN:ND2	4:A:227:VAL:H	2.14	0.44
4:A:289:ILE:O	4:A:291:GLU:N	2.50	0.44
4:A:298:PHE:O	4:A:301:ALA:HB3	2.16	0.44
4:A:807:GLY:HA2	5:B:760:ASP:O	2.17	0.44
4:A:823:GLY:O	4:A:825:ILE:N	2.50	0.44
4:A:901:LEU:HD22	4:A:919:ILE:HG22	2.00	0.44
5:B:591:ARG:O	5:B:592:ASN:C	2.55	0.44
6:C:35:ARG:HH11	14:K:41:THR:CA	2.30	0.44
6:C:92:CYS:C	6:C:94:LYS:N	2.71	0.44
8:E:161:LYS:C	8:E:163:GLU:N	2.71	0.44
12:I:68:LEU:HB3	12:I:84:VAL:HG23	1.98	0.44
14:K:82:ASP:O	14:K:85:ASP:HB2	2.17	0.44
15:L:27:LEU:HD23	15:L:27:LEU:N	2.31	0.44
4:A:1070:GLN:O	4:A:1071:SER:C	2.55	0.44
4:A:1215:ARG:HD2	4:A:1215:ARG:HA	1.73	0.44
4:A:1239:ARG:HB3	4:A:1239:ARG:NH1	2.32	0.44
4:A:1450:LEU:O	4:A:1450:LEU:CG	2.64	0.44
4:A:441:PRO:HD2	4:A:498:ARG:NH2	2.33	0.44
4:A:50:ILE:C	4:A:52:GLY:N	2.67	0.44
4:A:666:ILE:HD12	4:A:667:GLY:N	2.31	0.44
4:A:673:GLY:N	4:A:674:PRO:HD2	2.32	0.44
4:A:84:ILE:O	4:A:84:ILE:CG2	2.64	0.44
4:A:901:LEU:HD22	4:A:919:ILE:HG21	2.00	0.44
5:B:1106:ARG:HD2	5:B:1125:ASP:O	2.18	0.44
5:B:217:ARG:HG3	5:B:405:ARG:O	2.18	0.44
5:B:603:LEU:HB3	5:B:609:ILE:HD11	1.99	0.44
5:B:882:THR:HG21	5:B:935:ARG:HA	1.98	0.44
6:C:123:ASN:ND2	6:C:125:MET:SD	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:74:SER:HB2	6:C:77:ILE:CG1	2.47	0.44
8:E:116:ILE:HG22	8:E:117:THR:N	2.32	0.44
10:G:127:PRO:HG2	10:G:138:THR:HG21	1.99	0.44
10:G:49:LEU:HG	10:G:76:ALA:HA	2.00	0.44
12:I:6:PHE:HA	12:I:14:LEU:HG	1.98	0.44
4:A:608:ILE:O	4:A:610:GLY:N	2.50	0.44
4:A:61:ILE:HG22	4:A:62:ASP:N	2.32	0.44
4:A:652:VAL:O	4:A:653:VAL:C	2.56	0.44
4:A:723:ASN:C	4:A:725:ALA:N	2.68	0.44
4:A:871:ASP:C	4:A:871:ASP:OD1	2.56	0.44
4:A:921:GLY:O	4:A:922:ASP:C	2.54	0.44
5:B:1031:LEU:HA	5:B:1055:ILE:HD13	2.00	0.44
5:B:507:LYS:N	5:B:512:ARG:HH21	2.11	0.44
5:B:376:PHE:O	5:B:586:TRP:HZ3	2.00	0.44
5:B:680:THR:O	5:B:684:LEU:HD12	2.18	0.44
5:B:753:ALA:O	5:B:756:ILE:HG13	2.17	0.44
5:B:842:ASN:ND2	5:B:845:SER:OG	2.50	0.44
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.51	0.44
8:E:129:PRO:O	8:E:130:ALA:C	2.56	0.44
10:G:38:CYS:SG	10:G:44:TYR:CE1	3.11	0.44
12:I:34:TYR:O	12:I:35:VAL:CG2	2.66	0.44
14:K:12:LEU:N	14:K:12:LEU:HD12	2.26	0.44
14:K:55:LYS:HB3	14:K:81:TYR:CD1	2.53	0.44
4:A:1356:ILE:HD12	4:A:1368:MET:SD	2.58	0.44
4:A:1430:LEU:O	5:B:1196:ILE:HG22	2.18	0.44
4:A:93:VAL:HG21	4:A:301:ALA:O	2.17	0.44
4:A:650:GLN:O	4:A:654:ASN:ND2	2.51	0.44
4:A:853:ASP:OD1	4:A:855:THR:CG2	2.63	0.44
5:B:1065:GLN:NE2	5:B:1066:SER:H	2.14	0.44
5:B:983:ARG:HD2	5:B:1091:TYR:HD2	1.83	0.44
11:H:110:ASP:O	11:H:128:ASN:ND2	2.49	0.44
12:I:85:PHE:CD1	12:I:99:LEU:HD13	2.53	0.44
4:A:547:LEU:HD22	14:K:58:PHE:CE1	2.52	0.44
4:A:224:PHE:CZ	4:A:231:PRO:HG3	2.52	0.44
4:A:336:ILE:HG22	4:A:337:ARG:N	2.32	0.44
4:A:668:ASP:HA	4:A:741:ASN:OD1	2.18	0.44
4:A:699:ALA:O	4:A:700:ASN:HB3	2.18	0.44
4:A:853:ASP:OD1	4:A:855:THR:CB	2.66	0.44
5:B:603:LEU:HB3	5:B:609:ILE:HG13	1.98	0.44
5:B:616:ILE:HG13	5:B:697:GLU:HA	2.00	0.44
5:B:893:LEU:HD22	5:B:897:GLY:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:255:SER:OG	5:B:918:ILE:HG23	2.17	0.44
13:J:8:PHE:N	13:J:49:MET:HE3	2.32	0.44
14:K:52:ASN:O	14:K:54:ARG:N	2.51	0.44
4:A:896:ARG:NH2	4:A:1030:ARG:HH21	2.16	0.44
4:A:1053:PHE:C	4:A:1055:ARG:H	2.21	0.44
4:A:1170:ILE:HG13	4:A:1170:ILE:H	1.61	0.44
4:A:1141:THR:OG1	4:A:1205:LYS:HD3	2.17	0.44
4:A:1227:ILE:CG2	4:A:1228:TRP:N	2.81	0.44
4:A:1420:ASP:O	4:A:1421:CYS:HB2	2.18	0.44
4:A:23:SER:O	4:A:26:GLU:N	2.50	0.44
4:A:340:LEU:HD21	5:B:1199:ALA:HB3	2.00	0.44
4:A:376:TYR:OH	4:A:498:ARG:HD2	2.18	0.44
4:A:711:ARG:NH1	12:I:95:THR:HB	2.33	0.44
5:B:1204:PHE:O	5:B:1207:LEU:HB2	2.18	0.44
5:B:1223:ASP:HB3	5:B:1224:PHE:H	1.68	0.44
5:B:29:ASP:OD1	5:B:658:ILE:HD13	2.18	0.44
5:B:368:GLU:O	5:B:370:PHE:N	2.49	0.44
5:B:882:THR:O	5:B:883:LEU:CB	2.64	0.44
7:D:130:LEU:HD22	7:D:134:THR:OG1	2.18	0.44
7:D:35:LEU:HD23	7:D:174:PRO:CD	2.47	0.44
8:E:82:PHE:N	8:E:82:PHE:CD1	2.86	0.44
9:F:101:ILE:HD13	9:F:120:ILE:CG2	2.47	0.44
10:G:14:HIS:CD2	10:G:16:SER:HB2	2.53	0.44
11:H:10:PHE:CD1	11:H:10:PHE:N	2.85	0.44
12:I:86:PHE:CE1	12:I:100:PHE:HB2	2.52	0.44
4:A:442:VAL:HB	4:A:489:LEU:CD1	2.42	0.44
4:A:567:LYS:HZ2	11:H:47:PHE:CB	2.31	0.44
4:A:68:GLN:C	4:A:70:CYS:N	2.70	0.44
4:A:774:ARG:CZ	4:A:797:LYS:CB	2.96	0.44
4:A:858:ASN:HD21	4:A:860:LEU:H	1.60	0.44
5:B:1202:LEU:O	5:B:1203:LEU:C	2.56	0.44
5:B:639:ILE:HD11	5:B:691:GLU:HB2	2.00	0.44
5:B:726:ALA:HB1	5:B:1051:THR:HG21	1.99	0.44
5:B:763:GLN:HG2	5:B:765:PRO:CD	2.47	0.44
8:E:124:VAL:N	8:E:125:PRO:HD2	2.33	0.44
8:E:207:ARG:CB	8:E:207:ARG:NH1	2.80	0.44
10:G:4:ILE:HG22	10:G:4:ILE:O	2.18	0.44
14:K:87:LEU:O	14:K:88:LYS:C	2.56	0.44
15:L:27:LEU:O	15:L:28:LYS:HG2	2.18	0.44
2:N:1:DA:C1'	2:N:2:DA:O5'	2.66	0.44
1:T:15:DT:H1'	1:T:16:DT:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1058:VAL:O	4:A:1060:PRO:HD3	2.18	0.43
4:A:15:LYS:O	4:A:1421:CYS:HB2	2.18	0.43
4:A:242:PRO:HD3	5:B:1209:ALA:CB	2.48	0.43
4:A:311:GLN:HB3	4:A:312:PRO:HD3	2.00	0.43
4:A:399:HIS:CG	4:A:400:PRO:N	2.82	0.43
4:A:508:PRO:O	4:A:511:ILE:HG13	2.18	0.43
4:A:567:LYS:HG3	4:A:568:PRO:CD	2.38	0.43
4:A:845:LEU:O	4:A:846:GLU:C	2.54	0.43
5:B:1163:CYS:SG	5:B:1166:CYS:N	2.83	0.43
5:B:879:ARG:HH11	5:B:883:LEU:CD2	2.27	0.43
6:C:91:HIS:CD2	6:C:91:HIS:O	2.70	0.43
7:D:211:LEU:HD23	7:D:214:LEU:HD12	1.99	0.43
8:E:168:TYR:CB	8:E:170:LEU:HG	2.47	0.43
10:G:117:GLN:O	10:G:119:LEU:N	2.51	0.43
10:G:1:MET:SD	10:G:79:PHE:CE1	3.10	0.43
4:A:1344:GLY:O	4:A:1345:ARG:C	2.56	0.43
4:A:230:ARG:N	4:A:233:TRP:CZ3	2.80	0.43
4:A:42:ASP:OD1	4:A:45:GLN:O	2.36	0.43
4:A:871:ASP:OD2	4:A:873:MET:HB2	2.18	0.43
5:B:1050:ILE:CG2	5:B:1051:THR:N	2.81	0.43
5:B:112:LEU:HD12	5:B:113:TYR:N	2.29	0.43
5:B:34:ILE:O	5:B:35:SER:C	2.57	0.43
5:B:484:ASN:ND2	5:B:486:TYR:CE1	2.86	0.43
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.18	0.43
5:B:558:LEU:C	5:B:560:GLU:N	2.72	0.43
5:B:579:ARG:HG2	5:B:579:ARG:NH1	2.32	0.43
4:A:254:GLU:HG3	5:B:935:ARG:HH22	1.82	0.43
6:C:186:LEU:HD12	6:C:186:LEU:N	2.33	0.43
6:C:232:VAL:HG21	6:C:244:VAL:CG2	2.41	0.43
6:C:6:PRO:HB3	6:C:25:VAL:CG1	2.49	0.43
8:E:101:GLN:NE2	8:E:127:ILE:HG21	2.33	0.43
11:H:15:VAL:HG22	11:H:26:ILE:CG1	2.48	0.43
11:H:5:LEU:O	11:H:6:PHE:HB2	2.16	0.43
11:H:59:ILE:CG2	11:H:60:ALA:N	2.68	0.43
1:T:19:DG:H2''	1:T:20:DC:O5'	2.18	0.43
4:A:114:LEU:O	4:A:115:LEU:HG	2.18	0.43
4:A:34:LYS:HD3	4:A:34:LYS:N	2.33	0.43
4:A:493:GLN:H	4:A:497:THR:HG21	1.82	0.43
4:A:779:PHE:CE1	4:A:785:PRO:CD	2.90	0.43
5:B:1135:ARG:O	5:B:1138:MET:N	2.51	0.43
5:B:20:ASP:C	5:B:22:SER:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:421:PHE:O	5:B:424:LEU:HB3	2.18	0.43
6:C:116:LYS:HD3	6:C:140:ASN:HA	2.01	0.43
6:C:56:THR:HG22	6:C:58:LEU:HD23	2.00	0.43
8:E:157:SER:HG	8:E:160:GLU:HG3	1.82	0.43
1:T:14:DC:C6	1:T:15:DT:H73	2.53	0.43
4:A:1385:THR:O	4:A:1387:HIS:N	2.51	0.43
4:A:184:SER:HB3	4:A:199:LEU:CD2	2.49	0.43
4:A:34:LYS:HB3	4:A:36:ARG:HE	1.83	0.43
4:A:660:ASN:O	4:A:661:GLY:O	2.36	0.43
4:A:852:TYR:CD2	4:A:1060:PRO:CB	3.02	0.43
5:B:464:GLY:HA2	5:B:479:VAL:O	2.19	0.43
5:B:642:ASP:CA	5:B:649:LYS:HG3	2.47	0.43
5:B:792:MET:HA	5:B:856:PHE:O	2.17	0.43
5:B:91:SER:OG	5:B:133:LYS:HB2	2.19	0.43
8:E:133:GLU:HB3	8:E:135:PHE:HE1	1.84	0.43
8:E:35:VAL:C	8:E:37:LEU:N	2.71	0.43
10:G:9:LEU:CG	10:G:10:ASN:N	2.82	0.43
4:A:113:LEU:HG	4:A:218:ASP:OD1	2.18	0.43
4:A:1211:GLN:O	4:A:1212:VAL:C	2.57	0.43
4:A:1239:ARG:HH11	4:A:1239:ARG:CB	2.32	0.43
4:A:1430:LEU:C	5:B:1197:PRO:HD2	2.39	0.43
4:A:174:ILE:HG23	4:A:182:VAL:O	2.18	0.43
4:A:243:PRO:O	4:A:244:PRO:C	2.57	0.43
4:A:535:THR:O	4:A:575:LYS:HG3	2.19	0.43
4:A:77:CYS:SG	4:A:77:CYS:O	2.76	0.43
4:A:786:HIS:CD2	4:A:786:HIS:N	2.86	0.43
5:B:859:TYR:CE1	5:B:941:LEU:HD12	2.53	0.43
5:B:957:ASN:O	5:B:958:GLN:C	2.57	0.43
10:G:88:ASP:CB	10:G:144:ARG:HA	2.47	0.43
12:I:15:TYR:N	12:I:15:TYR:CD1	2.86	0.43
13:J:28:ASP:O	13:J:29:GLU:C	2.57	0.43
14:K:10:PHE:HD2	14:K:10:PHE:N	2.16	0.43
14:K:85:ASP:O	14:K:88:LYS:HB2	2.19	0.43
4:A:264:PHE:O	4:A:267:ALA:N	2.51	0.43
4:A:335:ARG:HB3	4:A:336:ILE:H	1.70	0.43
4:A:41:MET:HB3	4:A:48:ALA:O	2.18	0.43
4:A:42:ASP:HA	4:A:46:THR:O	2.19	0.43
4:A:650:GLN:HB3	4:A:654:ASN:HD21	1.83	0.43
4:A:784:LEU:C	4:A:786:HIS:H	2.21	0.43
5:B:104:GLU:OE1	15:L:54:ARG:NH2	2.52	0.43
4:A:7:SER:CB	5:B:1175:LEU:HD22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:299:GLU:OE1	5:B:571:PRO:HG2	2.19	0.43
5:B:399:ASP:OD2	5:B:510:LYS:HB2	2.17	0.43
5:B:521:LEU:HD13	5:B:633:VAL:CG1	2.48	0.43
5:B:710:LEU:C	5:B:711:GLU:HG2	2.39	0.43
5:B:769:TYR:C	5:B:771:SER:N	2.69	0.43
4:A:857:ARG:CZ	9:F:139:PRO:HG3	2.48	0.43
10:G:35:GLU:OE2	10:G:48:VAL:HG23	2.19	0.43
11:H:123:MET:HE3	11:H:142:LEU:HD21	2.00	0.43
11:H:82:PRO:O	11:H:84:ALA:N	2.35	0.43
13:J:44:TYR:HA	13:J:47:ARG:HB3	1.98	0.43
14:K:83:PRO:O	14:K:84:LYS:C	2.56	0.43
4:A:106:VAL:HA	4:A:114:LEU:HD21	2.00	0.43
4:A:1156:PRO:HA	4:A:1190:PRO:HB3	2.00	0.43
4:A:474:VAL:HG13	4:A:474:VAL:O	2.18	0.43
4:A:667:GLY:HA3	6:C:192:TRP:HH2	1.83	0.43
4:A:907:THR:CG2	4:A:908:LEU:H	2.29	0.43
5:B:1001:PHE:C	5:B:1001:PHE:CD1	2.92	0.43
5:B:1142:GLY:HA3	9:F:88:TYR:HE2	1.84	0.43
5:B:1162:ILE:C	5:B:1171:VAL:HG21	2.38	0.43
5:B:23:ALA:O	5:B:654:ARG:HD2	2.18	0.43
5:B:294:ASP:N	5:B:294:ASP:OD2	2.48	0.43
5:B:653:VAL:O	5:B:654:ARG:HD3	2.19	0.43
5:B:520:GLY:H	5:B:748:ILE:HG22	1.82	0.43
6:C:69:LEU:HB3	13:J:6:ARG:HD3	2.01	0.43
7:D:210:ILE:O	7:D:214:LEU:HG	2.18	0.43
8:E:124:VAL:HG13	8:E:132:ILE:CG1	2.48	0.43
8:E:93:MET:SD	8:E:97:VAL:CG2	3.06	0.43
9:F:132:LEU:N	9:F:132:LEU:HD23	2.34	0.43
9:F:99:LEU:C	9:F:99:LEU:HD12	2.38	0.43
4:A:562:THR:HB	11:H:98:TYR:CD2	2.54	0.43
12:I:84:VAL:HG13	12:I:84:VAL:O	2.19	0.43
13:J:43:ARG:HG2	13:J:43:ARG:H	1.70	0.43
4:A:1074:GLU:HB3	4:A:1075:PRO:HD3	2.00	0.43
4:A:16:GLU:HB3	4:A:1418:LEU:HD11	1.99	0.43
4:A:21:LEU:HD11	4:A:1414:ALA:HA	2.00	0.43
4:A:23:SER:O	4:A:25:GLU:N	2.51	0.43
4:A:535:THR:HG21	4:A:616:VAL:CA	2.35	0.43
4:A:933:TYR:C	4:A:935:GLN:H	2.21	0.43
4:A:988:LEU:HA	4:A:988:LEU:HD23	1.91	0.43
5:B:1001:PHE:CE2	6:C:34:ARG:NE	2.86	0.43
5:B:1064:TYR:O	5:B:1065:GLN:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:31:TRP:CE3	5:B:34:ILE:HD12	2.54	0.43
5:B:34:ILE:O	5:B:37:PHE:HB3	2.19	0.43
5:B:616:ILE:CG1	5:B:697:GLU:HA	2.49	0.43
5:B:797:TYR:O	5:B:799:PRO:HD3	2.19	0.43
5:B:911:ILE:O	5:B:911:ILE:HG22	2.19	0.43
5:B:936:ASP:OD1	5:B:938:SER:N	2.45	0.43
5:B:97:VAL:HG12	5:B:178:ASN:ND2	2.34	0.43
4:A:871:ASP:HB3	8:E:204:THR:CG2	2.48	0.43
10:G:18:PHE:HA	10:G:22:MET:HE3	1.99	0.43
12:I:50:THR:HG22	12:I:52:ILE:N	2.30	0.43
4:A:1199:ARG:O	4:A:1202:MET:N	2.48	0.43
4:A:1261:LYS:HA	4:A:1264:GLU:HB3	2.00	0.43
4:A:1139:GLU:O	4:A:1275:GLY:HA3	2.18	0.43
4:A:79:GLY:CA	4:A:243:PRO:CG	2.96	0.43
4:A:966:ASN:O	4:A:967:ALA:C	2.57	0.43
5:B:310:MET:HG3	5:B:386:LEU:HD13	2.01	0.43
5:B:371:GLU:CD	5:B:371:GLU:N	2.70	0.43
5:B:563:MET:HA	5:B:589:VAL:O	2.19	0.43
5:B:959:ASP:HB2	5:B:961:LEU:HG	2.01	0.43
7:D:51:ASN:ND2	7:D:54:GLU:OE2	2.51	0.43
8:E:131:THR:HG21	8:E:191:LYS:NZ	2.33	0.43
4:A:562:THR:HB	11:H:98:TYR:CE2	2.54	0.43
14:K:19:LEU:HD22	14:K:33:ILE:CG2	2.49	0.43
4:A:350:ARG:HG3	4:A:350:ARG:NH1	2.34	0.43
4:A:356:ASP:C	4:A:358:ASN:H	2.22	0.43
4:A:767:GLN:NE2	4:A:774:ARG:CB	2.82	0.43
5:B:1201:LYS:O	5:B:1204:PHE:HB2	2.19	0.43
5:B:179:CYS:SG	5:B:181:LEU:CB	3.06	0.43
5:B:251:ILE:O	5:B:251:ILE:HG22	2.19	0.43
5:B:33:VAL:HG21	5:B:638:PHE:HZ	1.84	0.43
5:B:949:VAL:HG12	5:B:950:ASP:N	2.34	0.43
4:A:503:GLN:NE2	9:F:90:ARG:NH2	2.62	0.43
10:G:77:VAL:O	10:G:77:VAL:HG12	2.19	0.43
13:J:5:VAL:HG12	13:J:6:ARG:CG	2.33	0.43
14:K:83:PRO:O	14:K:86:ALA:N	2.52	0.43
15:L:30:ILE:HD11	15:L:59:ALA:HB2	2.00	0.43
4:A:939:ASP:OD2	4:A:1020:CYS:HA	2.19	0.42
4:A:365:GLY:HA3	4:A:463:ILE:HD13	2.01	0.42
4:A:392:VAL:CG1	4:A:415:LEU:HD11	2.39	0.42
4:A:556:TRP:CZ2	4:A:558:GLY:HA2	2.54	0.42
4:A:55:ASP:N	4:A:56:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:62:ASP:HB3	4:A:64:ASN:ND2	2.34	0.42
5:B:1115:THR:CG2	5:B:1117:GLN:NE2	2.82	0.42
4:A:1431:GLY:HA3	5:B:1197:PRO:HD3	2.01	0.42
5:B:259:TYR:H	5:B:259:TYR:HD1	1.67	0.42
5:B:593:PRO:O	5:B:594:ALA:C	2.57	0.42
6:C:173:ALA:O	6:C:174:ALA:HB3	2.19	0.42
6:C:179:GLU:CG	6:C:180:TYR:H	2.31	0.42
6:C:39:ALA:O	6:C:164:ALA:HB3	2.19	0.42
8:E:14:ARG:HH21	8:E:141:VAL:HG11	1.81	0.42
10:G:117:GLN:C	10:G:119:LEU:H	2.22	0.42
11:H:128:ASN:CG	11:H:128:ASN:O	2.57	0.42
15:L:55:ILE:HG12	15:L:55:ILE:H	1.46	0.42
4:A:1362:TYR:HD1	4:A:1363:VAL:N	2.16	0.42
4:A:306:ASN:ND2	4:A:322:VAL:HB	2.34	0.42
4:A:325:ILE:HG21	5:B:1210:MET:CG	2.46	0.42
4:A:767:GLN:HE21	4:A:774:ARG:HB3	1.84	0.42
4:A:825:ILE:CG2	5:B:508:LEU:CD1	2.95	0.42
6:C:88:CYS:SG	6:C:91:HIS:CA	3.07	0.42
9:F:77:ASP:O	9:F:79:ARG:N	2.53	0.42
10:G:126:ASN:HA	10:G:126:ASN:HD22	1.59	0.42
4:A:1406:VAL:O	4:A:1407:GLU:C	2.58	0.42
4:A:1434:ALA:HA	4:A:1435:PRO:HD3	1.88	0.42
4:A:332:LYS:O	4:A:334:GLY:N	2.52	0.42
4:A:355:GLY:N	4:A:482:PHE:CE1	2.87	0.42
5:B:1180:PHE:HB3	5:B:1191:ILE:CD1	2.48	0.42
5:B:552:MET:C	5:B:554:ILE:N	2.71	0.42
5:B:681:TRP:C	5:B:683:SER:N	2.73	0.42
6:C:248:ILE:HG13	6:C:248:ILE:H	1.55	0.42
6:C:90:ASP:O	6:C:91:HIS:CB	2.67	0.42
9:F:118:LEU:O	9:F:118:LEU:HD12	2.19	0.42
12:I:54:GLU:HB3	12:I:100:PHE:CE2	2.54	0.42
12:I:103:CYS:HB3	12:I:106:CYS:SG	2.59	0.42
2:N:2:DA:H1'	2:N:3:DG:O5'	2.19	0.42
4:A:1053:PHE:C	4:A:1055:ARG:N	2.73	0.42
4:A:1343:ALA:O	4:A:1346:ALA:HB3	2.19	0.42
4:A:1365:TYR:O	4:A:1366:ARG:C	2.57	0.42
4:A:1409:LEU:HD13	5:B:1207:LEU:CD2	2.37	0.42
4:A:90:VAL:HG13	4:A:297:GLN:CD	2.39	0.42
4:A:525:GLN:O	4:A:526:ASP:C	2.58	0.42
4:A:600:PRO:HG2	4:A:601:LYS:H	1.84	0.42
4:A:755:PHE:O	4:A:756:ILE:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:774:ARG:CZ	4:A:797:LYS:HG3	2.49	0.42
4:A:857:ARG:HG2	4:A:863:VAL:HA	2.02	0.42
4:A:870:GLU:HB2	8:E:204:THR:HG21	2.01	0.42
5:B:102:VAL:HG22	5:B:112:LEU:HD22	2.01	0.42
5:B:1143:ALA:O	5:B:1144:ALA:C	2.58	0.42
5:B:273:LEU:HD12	5:B:280:ILE:HD12	2.01	0.42
5:B:305:VAL:O	5:B:305:VAL:HG12	2.19	0.42
5:B:33:VAL:O	5:B:34:ILE:C	2.58	0.42
5:B:455:SER:O	5:B:458:LYS:N	2.52	0.42
5:B:470:LYS:HB3	5:B:471:LYS:H	1.65	0.42
5:B:862:GLN:HG2	5:B:963:PHE:CD1	2.51	0.42
5:B:999:MET:HE2	5:B:1000:PRO:CD	2.49	0.42
6:C:143:LEU:HD21	6:C:146:LYS:CE	2.48	0.42
6:C:70:ILE:HA	6:C:71:PRO:HD2	1.83	0.42
7:D:38:ILE:HG22	7:D:39:ASN:O	2.19	0.42
10:G:44:TYR:O	10:G:78:VAL:HG12	2.20	0.42
13:J:1:MET:HA	13:J:57:ILE:H	1.85	0.42
13:J:58:GLU:HA	13:J:61:LEU:HD12	2.02	0.42
3:P:4:A:O2'	3:P:5:C:H5'	2.18	0.42
4:A:1066:VAL:O	4:A:1067:LEU:C	2.58	0.42
4:A:117:GLU:H	4:A:117:GLU:CD	2.22	0.42
4:A:223:GLY:O	4:A:224:PHE:CD1	2.73	0.42
4:A:261:ASP:O	4:A:264:PHE:HB2	2.20	0.42
4:A:93:VAL:CG1	4:A:301:ALA:HB1	2.42	0.42
5:B:984:HIS:CD2	5:B:1025:HIS:HB2	2.54	0.42
5:B:1136:ASP:N	5:B:1136:ASP:OD1	2.52	0.42
5:B:496:ARG:HH12	5:B:539:LEU:HB2	1.82	0.42
5:B:581:PHE:HA	5:B:585:VAL:O	2.19	0.42
6:C:30:ALA:O	6:C:33:LEU:HB3	2.19	0.42
6:C:90:ASP:CG	6:C:90:ASP:O	2.58	0.42
10:G:9:LEU:HD12	10:G:10:ASN:N	2.32	0.42
11:H:101:ALA:HB2	11:H:116:TYR:CE1	2.54	0.42
12:I:29:CYS:SG	12:I:32:CYS:SG	3.17	0.42
4:A:789:LYS:HE3	12:I:67:THR:OG1	2.19	0.42
14:K:95:ILE:O	14:K:98:LEU:HB2	2.19	0.42
1:T:19:DG:H4'	5:B:1133:MET:SD	2.58	0.42
4:A:1118:VAL:HG23	4:A:1306:LEU:HB2	2.00	0.42
4:A:889:SER:C	4:A:891:ALA:N	2.69	0.42
5:B:1106:ARG:NH1	5:B:1110:PRO:HG2	2.33	0.42
5:B:259:TYR:HB2	5:B:268:THR:HG23	2.01	0.42
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:806:THR:CG2	5:B:808:ALA:HB3	2.49	0.42
5:B:975:GLN:HG2	5:B:976:ILE:N	2.32	0.42
6:C:240:VAL:O	6:C:244:VAL:HG23	2.19	0.42
6:C:80:LEU:HD12	6:C:95:CYS:HA	2.02	0.42
7:D:191:ALA:C	7:D:193:THR:H	2.23	0.42
9:F:72:LYS:O	9:F:73:ALA:HB3	2.19	0.42
10:G:25:TYR:O	10:G:26:LEU:C	2.58	0.42
10:G:47:CYS:SG	10:G:48:VAL:N	2.92	0.42
10:G:18:PHE:HZ	10:G:68:ALA:HB2	1.85	0.42
10:G:88:ASP:HB3	10:G:144:ARG:CA	2.49	0.42
11:H:123:MET:HE3	11:H:142:LEU:CD2	2.49	0.42
11:H:15:VAL:HG22	11:H:26:ILE:CD1	2.49	0.42
12:I:77:LYS:C	12:I:79:HIS:H	2.23	0.42
14:K:113:THR:O	14:K:114:LEU:CB	2.62	0.42
4:A:1329:THR:O	4:A:1335:ILE:HD12	2.20	0.42
4:A:1438:THR:HG22	4:A:1438:THR:O	2.18	0.42
4:A:67:CYS:O	4:A:68:GLN:CB	2.68	0.42
4:A:737:LEU:HD23	4:A:737:LEU:HA	1.75	0.42
4:A:78:PRO:HG3	5:B:1160:VAL:HG13	2.00	0.42
4:A:881:GLN:O	4:A:953:ASN:HA	2.19	0.42
5:B:1156:ASP:O	5:B:1157:ALA:O	2.37	0.42
5:B:1160:VAL:HG11	5:B:1169:MET:SD	2.59	0.42
5:B:235:SER:C	5:B:236:HIS:CD2	2.93	0.42
5:B:763:GLN:HG2	5:B:765:PRO:CG	2.50	0.42
5:B:872:GLU:HG2	5:B:916:THR:OG1	2.20	0.42
8:E:114:ASN:HA	8:E:114:ASN:HD22	1.63	0.42
9:F:99:LEU:HD12	9:F:99:LEU:O	2.19	0.42
12:I:110:PHE:N	12:I:110:PHE:CD2	2.88	0.42
4:A:1193:LEU:HD22	4:A:1260:LEU:HD11	2.02	0.42
4:A:1333:ILE:O	4:A:1337:GLU:HG3	2.19	0.42
4:A:1368:MET:O	4:A:1372:VAL:HB	2.19	0.42
4:A:860:LEU:HD11	4:A:1393:ASN:HB2	2.02	0.42
4:A:1423:GLY:H	4:A:1426:GLU:HG3	1.85	0.42
4:A:1444:MET:HG2	10:G:60:ARG:CA	2.48	0.42
4:A:810:PRO:HA	5:B:1047:PHE:CE2	2.54	0.42
4:A:514:PRO:HB2	4:A:875:ALA:HB3	2.01	0.42
4:A:896:ARG:HD3	4:A:897:TYR:HE1	1.84	0.42
5:B:1163:CYS:SG	5:B:1165:ILE:CB	3.04	0.42
5:B:287:ARG:NH1	5:B:324:ILE:O	2.53	0.42
5:B:311:LEU:O	5:B:312:GLU:C	2.58	0.42
5:B:520:GLY:CA	5:B:748:ILE:HG22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:758:PHE:CZ	5:B:1031:LEU:HD22	2.54	0.42
7:D:135:GLY:C	7:D:137:ASN:H	2.22	0.42
8:E:128:PRO:HA	8:E:129:PRO:C	2.40	0.42
11:H:76:THR:HG22	11:H:76:THR:O	2.19	0.42
4:A:1115:SER:C	4:A:1308:THR:CG2	2.88	0.42
4:A:1157:ASP:C	4:A:1159:ARG:H	2.23	0.42
4:A:1315:GLU:C	4:A:1317:MET:N	2.72	0.42
1:T:16:DT:H5"	4:A:1386:ARG:NH1	2.35	0.42
4:A:1426:GLU:H	4:A:1426:GLU:HG2	1.56	0.42
4:A:241:VAL:O	4:A:242:PRO:C	2.58	0.42
4:A:33:ALA:O	4:A:83:HIS:CD2	2.67	0.42
4:A:445:ASN:HB2	4:A:455:MET:HA	2.01	0.42
4:A:767:GLN:HE21	4:A:774:ARG:CB	2.33	0.42
4:A:971:PHE:O	4:A:972:HIS:C	2.58	0.42
5:B:1031:LEU:HD23	5:B:1044:ALA:HB2	2.02	0.42
5:B:1178:ASN:O	5:B:1179:GLN:C	2.58	0.42
7:D:128:VAL:O	7:D:132:GLN:HG3	2.20	0.42
9:F:109:VAL:HG11	9:F:123:LYS:CG	2.50	0.42
13:J:7:CYS:CA	13:J:49:MET:HE3	2.50	0.42
1:T:19:DG:OP2	4:A:332:LYS:NZ	2.42	0.42
4:A:1381:LEU:HD23	4:A:1381:LEU:HA	1.88	0.42
4:A:219:PHE:O	4:A:222:LEU:O	2.36	0.42
4:A:332:LYS:HG3	4:A:333:GLU:N	2.35	0.42
4:A:584:ASN:O	4:A:637:LYS:HE3	2.20	0.42
5:B:314:LEU:O	5:B:317:CYS:HB3	2.20	0.42
5:B:365:THR:HG23	5:B:367:LEU:N	2.31	0.42
5:B:510:LYS:N	5:B:511:PRO:HD3	2.35	0.42
5:B:566:LEU:O	5:B:567:GLU:C	2.58	0.42
6:C:259:LEU:CD1	14:K:91:CYS:HB2	2.50	0.42
6:C:56:THR:HG22	6:C:58:LEU:H	1.85	0.42
8:E:90:VAL:CA	8:E:120:ALA:HB2	2.47	0.42
10:G:142:ARG:O	10:G:171:ILE:HG13	2.20	0.42
11:H:143:LEU:C	11:H:144:ILE:HG13	2.40	0.42
4:A:1048:ASN:O	4:A:1049:ILE:C	2.58	0.41
4:A:1332:PHE:O	4:A:1333:ILE:C	2.57	0.41
4:A:218:ASP:O	4:A:219:PHE:O	2.38	0.41
4:A:782:ARG:HB3	4:A:789:LYS:HA	2.02	0.41
4:A:794:PRO:O	4:A:796:SER:N	2.53	0.41
4:A:909:ASP:C	4:A:911:SER:N	2.73	0.41
4:A:964:ILE:O	4:A:967:ALA:HB3	2.19	0.41
5:B:1065:GLN:HG3	5:B:1068:GLY:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1424:VAL:CG1	5:B:1139:ILE:HD13	2.45	0.41
5:B:324:ILE:CG2	5:B:325:GLN:N	2.82	0.41
5:B:563:MET:CE	5:B:580:VAL:HB	2.45	0.41
5:B:683:SER:O	5:B:687:GLU:HB2	2.20	0.41
5:B:766:ARG:HD3	5:B:766:ARG:HA	1.77	0.41
5:B:910:VAL:CG1	5:B:911:ILE:N	2.82	0.41
6:C:213:PRO:HG2	6:C:214:ASN:H	1.85	0.41
7:D:167:LEU:O	7:D:170:THR:OG1	2.31	0.41
7:D:191:ALA:O	7:D:193:THR:N	2.53	0.41
9:F:97:ARG:HA	9:F:97:ARG:HD2	1.76	0.41
12:I:101:PHE:HD1	12:I:101:PHE:N	2.18	0.41
4:A:1073:GLY:O	4:A:1076:ALA:HB3	2.20	0.41
4:A:417:TYR:O	4:A:418:SER:O	2.37	0.41
4:A:40:THR:CG2	4:A:41:MET:HG3	2.33	0.41
4:A:814:PHE:O	4:A:817:ALA:HB3	2.20	0.41
4:A:898:ARG:NH1	4:A:930:ASP:OD1	2.50	0.41
5:B:859:TYR:OH	5:B:941:LEU:CD1	2.62	0.41
5:B:971:THR:OG1	6:C:61:GLU:HG3	2.20	0.41
5:B:998:ASP:HB3	5:B:1076:HIS:HE1	1.85	0.41
6:C:107:SER:C	6:C:109:SER:N	2.74	0.41
6:C:262:LEU:HD23	6:C:262:LEU:HA	1.80	0.41
6:C:62:PHE:O	6:C:66:ARG:HG3	2.20	0.41
15:L:38:LEU:O	15:L:39:SER:CB	2.61	0.41
4:A:868:TYR:CD2	4:A:1058:VAL:HG21	2.48	0.41
4:A:1242:VAL:O	4:A:1243:VAL:CB	2.66	0.41
4:A:1111:MET:CE	4:A:1330:ASN:OD1	2.68	0.41
4:A:18:GLN:HG2	4:A:1418:LEU:HD13	2.01	0.41
4:A:381:THR:HG23	4:A:382:PRO:CD	2.50	0.41
4:A:452:LYS:HE2	4:A:452:LYS:HB3	1.85	0.41
4:A:933:TYR:C	4:A:935:GLN:N	2.74	0.41
5:B:1164:GLY:HA3	5:B:1190:ASP:OD2	2.20	0.41
4:A:29:ALA:HB1	5:B:1184:GLY:CA	2.50	0.41
5:B:125:SER:CA	5:B:171:PRO:HA	2.49	0.41
5:B:258:LEU:O	5:B:258:LEU:HG	2.19	0.41
5:B:651:LEU:HD11	5:B:707:PRO:CB	2.50	0.41
5:B:654:ARG:O	5:B:656:GLY:N	2.53	0.41
5:B:526:GLU:OE2	5:B:752:ALA:HB2	2.20	0.41
5:B:765:PRO:O	5:B:767:ASN:N	2.53	0.41
5:B:990:ILE:CG2	5:B:991:GLY:N	2.83	0.41
8:E:18:THR:O	8:E:19:VAL:C	2.57	0.41
8:E:16:PHE:CE2	8:E:20:LYS:HE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:22:MET:O	10:G:23:LYS:C	2.58	0.41
12:I:55:THR:HG23	12:I:58:VAL:HG21	2.01	0.41
13:J:23:ASN:O	13:J:25:LEU:N	2.52	0.41
4:A:1227:ILE:HG22	4:A:1228:TRP:H	1.80	0.41
4:A:1409:LEU:O	4:A:1412:ALA:HB3	2.21	0.41
4:A:254:GLU:HB2	5:B:935:ARG:NH1	2.29	0.41
4:A:278:THR:O	4:A:278:THR:HG22	2.19	0.41
4:A:279:LEU:O	4:A:284:ALA:HB2	2.20	0.41
4:A:629:LEU:O	4:A:633:VAL:HG23	2.21	0.41
4:A:676:MET:O	4:A:679:ILE:HB	2.21	0.41
4:A:341:MET:HE1	5:B:1135:ARG:NH1	2.35	0.41
5:B:121:ASN:OD1	5:B:963:PHE:HZ	2.04	0.41
5:B:170:LEU:HA	5:B:171:PRO:HD2	1.82	0.41
5:B:278:GLN:HG2	5:B:279:ASP:N	2.35	0.41
5:B:34:ILE:O	5:B:37:PHE:N	2.53	0.41
5:B:429:PHE:HA	5:B:432:MET:CE	2.49	0.41
5:B:468:GLU:HB3	5:B:469:GLN:H	1.49	0.41
5:B:376:PHE:HB3	5:B:586:TRP:CZ3	2.55	0.41
5:B:834:ASN:CA	5:B:838:SER:O	2.69	0.41
7:D:179:GLN:O	7:D:183:LEU:HB2	2.20	0.41
10:G:106:MET:HG2	10:G:107:LYS:N	2.36	0.41
10:G:138:THR:HG22	10:G:139:ILE:HG13	2.02	0.41
11:H:82:PRO:C	11:H:84:ALA:N	2.74	0.41
4:A:106:VAL:HG13	4:A:112:LYS:C	2.37	0.41
4:A:404:TYR:CD2	4:A:414:ASP:HA	2.55	0.41
4:A:402:ALA:CB	4:A:434:ARG:HA	2.51	0.41
4:A:463:ILE:HB	4:A:464:PRO:CD	2.49	0.41
4:A:853:ASP:C	4:A:853:ASP:OD1	2.59	0.41
4:A:970:THR:HG22	4:A:970:THR:O	2.20	0.41
5:B:842:ASN:HB3	5:B:1009:ASP:HA	2.03	0.41
5:B:1068:GLY:O	5:B:1069:PHE:O	2.39	0.41
5:B:1187:ASN:OD1	5:B:1188:LYS:N	2.45	0.41
5:B:365:THR:CG2	5:B:366:GLN:N	2.81	0.41
5:B:758:PHE:N	5:B:759:PRO:HD2	2.35	0.41
5:B:769:TYR:C	5:B:771:SER:H	2.24	0.41
5:B:980:PHE:CA	5:B:1095:LEU:HD11	2.50	0.41
6:C:154:LYS:C	6:C:155:LEU:HD23	2.40	0.41
6:C:168:ALA:C	6:C:170:TRP:H	2.24	0.41
7:D:63:LEU:HA	7:D:63:LEU:HD22	1.91	0.41
8:E:22:MET:CE	8:E:26:ARG:NH2	2.82	0.41
11:H:95:TYR:CE2	11:H:97:MET:CG	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:61:ASP:C	12:I:63:GLY:N	2.73	0.41
12:I:4:PHE:HE1	12:I:6:PHE:HE2	1.69	0.41
4:A:115:LEU:CB	4:A:122:MET:HE2	2.50	0.41
4:A:115:LEU:HB2	4:A:122:MET:HE2	2.02	0.41
4:A:116:ASP:C	4:A:118:HIS:N	2.74	0.41
4:A:1334:ASP:C	4:A:1336:MET:N	2.74	0.41
4:A:1388:GLY:O	4:A:1390:ASN:N	2.53	0.41
4:A:207:ILE:CG2	4:A:211:PHE:CE1	3.03	0.41
4:A:277:GLU:C	4:A:279:LEU:N	2.74	0.41
4:A:482:PHE:C	4:A:484:GLY:H	2.24	0.41
4:A:604:GLY:O	4:A:605:MET:HB2	2.21	0.41
4:A:680:THR:HG23	5:B:729:ILE:CD1	2.51	0.41
4:A:690:VAL:O	4:A:691:LEU:C	2.59	0.41
4:A:947:PHE:CD2	4:A:954:TRP:CE2	3.08	0.41
5:B:578:THR:O	5:B:578:THR:HG22	2.21	0.41
5:B:744:HIS:CD2	5:B:745:PRO:HD2	2.55	0.41
5:B:861:ASP:OD1	5:B:914:LYS:HD2	2.21	0.41
6:C:191:TYR:CD2	6:C:201:TRP:CD1	3.03	0.41
6:C:66:ARG:NH1	13:J:2:ILE:CG2	2.82	0.41
8:E:30:ILE:HG22	8:E:31:THR:N	2.35	0.41
9:F:123:LYS:O	9:F:124:GLU:C	2.57	0.41
12:I:4:PHE:HE1	12:I:6:PHE:CE2	2.39	0.41
14:K:45:LEU:C	14:K:47:ARG:H	2.23	0.41
4:A:206:GLU:O	4:A:207:ILE:C	2.59	0.41
4:A:262:LEU:HD12	4:A:328:ARG:NH2	2.35	0.41
4:A:349:ALA:CA	5:B:1128:LEU:HD11	2.51	0.41
4:A:527:THR:O	4:A:531:ILE:HB	2.21	0.41
4:A:723:ASN:O	4:A:724:GLU:C	2.59	0.41
4:A:768:GLN:HG3	4:A:816:HIS:HA	2.01	0.41
5:B:1065:GLN:HE21	5:B:1066:SER:CA	2.33	0.41
5:B:333:PHE:C	5:B:334:ILE:HG13	2.41	0.41
6:C:11:ARG:HD3	6:C:209:TYR:CE2	2.56	0.41
6:C:147:LEU:HD23	6:C:147:LEU:N	2.36	0.41
6:C:239:PRO:O	6:C:240:VAL:C	2.58	0.41
6:C:260:LEU:O	6:C:263:THR:HB	2.20	0.41
6:C:31:ASN:O	6:C:34:ARG:HB3	2.20	0.41
7:D:138:ASN:C	7:D:140:ASP:N	2.72	0.41
9:F:147:SER:O	9:F:148:VAL:C	2.59	0.41
9:F:97:ARG:NH1	9:F:100:GLN:OE1	2.53	0.41
12:I:101:PHE:HD1	12:I:101:PHE:H	1.67	0.41
14:K:38:GLU:HA	14:K:38:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:53:ASP:C	14:K:55:LYS:H	2.24	0.41
4:A:1373:ASP:CA	4:A:1376:THR:HG22	2.50	0.41
4:A:1425:SER:O	4:A:1426:GLU:C	2.59	0.41
4:A:146:MET:CA	4:A:171:GLN:HB2	2.50	0.41
4:A:306:ASN:HD22	4:A:322:VAL:HG12	1.86	0.41
4:A:403:LYS:O	4:A:404:TYR:CD2	2.74	0.41
4:A:408:ASP:C	4:A:410:GLY:N	2.72	0.41
4:A:574:GLY:O	4:A:577:ILE:N	2.51	0.41
4:A:608:ILE:CG1	4:A:613:ILE:HD12	2.51	0.41
4:A:964:ILE:O	4:A:967:ALA:N	2.54	0.41
4:A:343:LYS:NZ	5:B:1151:LEU:O	2.43	0.41
4:A:304:MET:HG2	5:B:1210:MET:HG2	2.03	0.41
5:B:314:LEU:O	5:B:315:LYS:C	2.59	0.41
5:B:388:CYS:O	5:B:391:ASP:N	2.50	0.41
5:B:604:ARG:O	5:B:607:GLY:N	2.54	0.41
5:B:730:ARG:O	5:B:731:VAL:O	2.39	0.41
6:C:54:ASN:HB2	6:C:153:LEU:HD12	2.03	0.41
7:D:180:LEU:HA	7:D:180:LEU:HD23	1.87	0.41
7:D:206:GLU:C	7:D:208:GLU:H	2.24	0.41
10:G:21:ARG:HD3	10:G:21:ARG:HA	1.85	0.41
12:I:98:VAL:HG12	12:I:99:LEU:N	2.36	0.41
13:J:44:TYR:HD2	13:J:44:TYR:N	2.13	0.41
14:K:31:VAL:O	14:K:74:ARG:HA	2.21	0.41
15:L:38:LEU:CD1	15:L:49:LYS:HE2	2.50	0.41
4:A:973:ILE:HD13	4:A:1037:LEU:HA	2.03	0.41
4:A:1041:ALA:O	4:A:1045:VAL:HG23	2.20	0.41
4:A:1070:GLN:C	4:A:1072:ILE:N	2.74	0.41
4:A:1127:ASP:O	4:A:1130:GLN:HB3	2.20	0.41
4:A:1445:ILE:CD1	4:A:1445:ILE:H	2.19	0.41
4:A:590:ARG:HD3	4:A:604:GLY:O	2.20	0.41
4:A:61:ILE:CG2	4:A:62:ASP:H	2.29	0.41
4:A:73:GLY:O	4:A:74:MET:C	2.59	0.41
4:A:954:TRP:HB3	4:A:955:PRO:HD2	2.02	0.41
4:A:93:VAL:HA	4:A:96:ILE:CD1	2.51	0.41
4:A:993:LEU:O	4:A:994:GLN:C	2.59	0.41
5:B:1110:PRO:HG3	5:B:1124:ARG:O	2.21	0.41
5:B:261:ARG:HB3	5:B:261:ARG:NH1	2.35	0.41
5:B:464:GLY:CA	5:B:479:VAL:O	2.68	0.41
5:B:492:LEU:HB2	5:B:751:VAL:HG11	2.03	0.41
5:B:60:GLN:O	5:B:63:ILE:HG22	2.21	0.41
5:B:865:LYS:C	5:B:866:TYR:CD1	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:873:THR:O	5:B:914:LYS:HA	2.20	0.41
5:B:899:ILE:CG2	5:B:903:VAL:HG21	2.50	0.41
6:C:181:ASP:OD1	6:C:186:LEU:HD13	2.21	0.41
6:C:67:LEU:HD11	6:C:155:LEU:HD12	2.01	0.41
8:E:191:LYS:O	8:E:193:GLY:N	2.54	0.41
8:E:78:LEU:HA	8:E:107:THR:HB	2.02	0.41
10:G:49:LEU:O	10:G:50:ASP:C	2.59	0.41
11:H:59:ILE:O	11:H:60:ALA:HB3	2.20	0.41
4:A:1349:TYR:O	4:A:1350:LYS:C	2.59	0.41
4:A:722:LEU:HD21	4:A:794:PRO:HB3	2.03	0.41
5:B:129:PHE:CD2	5:B:166:PHE:HA	2.56	0.41
5:B:285:ILE:O	5:B:288:ALA:HB3	2.21	0.41
5:B:298:LEU:N	5:B:298:LEU:HD22	2.35	0.41
5:B:516:ASN:ND2	5:B:516:ASN:H	2.16	0.41
5:B:62:ILE:HG23	5:B:418:LYS:HG2	2.03	0.41
5:B:704:ALA:HB3	5:B:741:CYS:SG	2.61	0.41
5:B:953:LEU:HD23	5:B:965:LYS:H	1.86	0.41
5:B:992:ILE:HG12	5:B:993:THR:N	2.36	0.41
5:B:840:ILE:CG2	5:B:994:TYR:HD1	2.34	0.41
6:C:100:THR:CG2	6:C:101:LEU:N	2.84	0.41
6:C:18:VAL:O	6:C:20:PHE:CD2	2.71	0.41
7:D:118:THR:HG22	7:D:118:THR:O	2.20	0.41
8:E:14:ARG:NH2	8:E:141:VAL:HG12	2.34	0.41
10:G:88:ASP:HB3	10:G:144:ARG:CB	2.51	0.41
11:H:25:ARG:HA	11:H:41:ASP:HA	2.03	0.41
11:H:62:SER:OG	11:H:63:LEU:N	2.53	0.41
12:I:54:GLU:OE2	12:I:118:ARG:NH1	2.53	0.41
13:J:32:GLU:O	13:J:35:ALA:N	2.54	0.41
13:J:3:VAL:HA	13:J:4:PRO:HD3	1.84	0.41
4:A:1062:GLU:OE2	9:F:88:TYR:OH	2.36	0.41
4:A:414:ASP:OD1	4:A:416:ARG:CG	2.69	0.41
4:A:817:ALA:O	4:A:820:GLY:N	2.54	0.41
5:B:1074:ASN:HB2	5:B:1081:LEU:HD21	2.03	0.41
5:B:1186:ASP:C	5:B:1186:ASP:OD1	2.59	0.41
5:B:1187:ASN:OD1	5:B:1189:ILE:N	2.53	0.41
5:B:807:ARG:HG2	5:B:1045:SER:OG	2.21	0.41
5:B:949:VAL:HG12	5:B:950:ASP:H	1.86	0.41
7:D:63:LEU:HD12	7:D:129:LEU:HG	2.03	0.41
8:E:94:LYS:HG3	8:E:98:ILE:HD11	2.01	0.41
4:A:1236:LEU:C	4:A:1237:ILE:HG13	2.42	0.40
4:A:1364:ASN:O	4:A:1366:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:231:PRO:C	4:A:233:TRP:N	2.74	0.40
4:A:79:GLY:CA	4:A:243:PRO:HG3	2.51	0.40
4:A:23:SER:O	4:A:24:PRO:C	2.59	0.40
4:A:690:VAL:O	4:A:693:VAL:N	2.54	0.40
4:A:791:ASP:OD1	4:A:791:ASP:C	2.59	0.40
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.35	0.40
5:B:33:VAL:O	5:B:36:ALA:N	2.55	0.40
5:B:753:ALA:HA	5:B:756:ILE:CD1	2.51	0.40
6:C:90:ASP:O	6:C:91:HIS:HB3	2.20	0.40
13:J:51:LEU:O	13:J:51:LEU:HD12	2.21	0.40
14:K:7:PHE:HA	14:K:10:PHE:HE2	1.78	0.40
4:A:1219:THR:HG21	4:A:1271:ILE:HG13	2.02	0.40
4:A:1339:LEU:O	8:E:150:VAL:HG21	2.21	0.40
4:A:1377:THR:O	4:A:1378:GLN:C	2.60	0.40
4:A:1409:LEU:HA	4:A:1409:LEU:HD23	1.85	0.40
4:A:239:LEU:CD1	4:A:240:PRO:HD2	2.46	0.40
4:A:241:VAL:HA	4:A:242:PRO:HD2	1.93	0.40
4:A:265:LYS:HZ3	4:A:322:VAL:HG13	1.87	0.40
4:A:577:ILE:O	4:A:579:SER:N	2.55	0.40
4:A:767:GLN:NE2	4:A:774:ARG:HB2	2.36	0.40
4:A:6:TYR:CD1	4:A:7:SER:N	2.89	0.40
4:A:857:ARG:NH1	9:F:139:PRO:HB2	2.36	0.40
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.45	0.40
5:B:257:LYS:O	5:B:258:LEU:HB2	2.21	0.40
5:B:446:LEU:O	5:B:447:ALA:CB	2.67	0.40
5:B:546:SER:OG	5:B:631:GLY:N	2.42	0.40
5:B:901:PRO:HD2	15:L:59:ALA:O	2.21	0.40
5:B:977:GLY:HA3	5:B:1099:VAL:CG2	2.52	0.40
6:C:246:ARG:HA	6:C:249:ASP:HB3	2.02	0.40
8:E:205:SER:O	8:E:206:GLY:C	2.60	0.40
11:H:40:LEU:CD1	11:H:123:MET:HB2	2.45	0.40
11:H:59:ILE:CG2	11:H:60:ALA:H	2.27	0.40
12:I:88:SER:HB3	12:I:95:THR:HG21	2.02	0.40
13:J:1:MET:HE2	13:J:56:LEU:HD12	2.03	0.40
4:A:1040:GLN:O	4:A:1041:ALA:C	2.59	0.40
4:A:1072:ILE:O	4:A:1075:PRO:CD	2.69	0.40
4:A:1339:LEU:HD13	8:E:147:HIS:CD2	2.56	0.40
4:A:28:ARG:O	4:A:29:ALA:C	2.60	0.40
4:A:432:VAL:O	4:A:433:GLU:C	2.59	0.40
4:A:49:LYS:NZ	4:A:61:ILE:CG1	2.79	0.40
4:A:524:VAL:HG12	4:A:525:GLN:HE21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.62	0.40
4:A:645:LEU:O	4:A:646:PHE:C	2.58	0.40
4:A:755:PHE:O	4:A:758:ILE:N	2.55	0.40
4:A:833:GLU:O	4:A:834:THR:C	2.59	0.40
5:B:1047:PHE:N	5:B:1047:PHE:CD1	2.81	0.40
5:B:635:ARG:HB2	5:B:636:PRO:HD2	2.03	0.40
5:B:648:HIS:CG	5:B:649:LYS:N	2.89	0.40
5:B:662:MET:HA	5:B:665:GLU:HB2	2.02	0.40
5:B:729:ILE:O	5:B:729:ILE:HG22	2.21	0.40
5:B:899:ILE:HD13	5:B:905:VAL:HG11	2.03	0.40
6:C:174:ALA:O	6:C:175:ALA:CB	2.69	0.40
6:C:177:GLU:CB	6:C:231:ASN:HB3	2.48	0.40
7:D:177:VAL:H	7:D:177:VAL:HG23	1.67	0.40
7:D:56:ARG:HH22	7:D:57:LEU:HD21	1.83	0.40
7:D:64:VAL:O	7:D:66:ARG:N	2.55	0.40
8:E:31:THR:OG1	8:E:34:GLU:N	2.50	0.40
8:E:79:TRP:CD1	8:E:96:PHE:HE1	2.38	0.40
9:F:103:MET:O	9:F:104:ASN:CB	2.61	0.40
10:G:45:ILE:HD13	10:G:45:ILE:HA	1.94	0.40
12:I:8:ARG:H	12:I:8:ARG:HG3	1.72	0.40
13:J:47:ARG:HH11	13:J:47:ARG:CG	2.34	0.40
4:A:1013:ASP:C	4:A:1015:VAL:N	2.75	0.40
4:A:1437:GLY:CA	9:F:88:TYR:CD2	3.04	0.40
4:A:350:ARG:NH1	4:A:488:ASN:OD1	2.49	0.40
4:A:543:LEU:HD12	4:A:547:LEU:HG	2.03	0.40
4:A:54:ASN:HA	4:A:58:LEU:HD12	2.04	0.40
4:A:809:THR:CG2	4:A:812:GLU:HG3	2.52	0.40
4:A:809:THR:O	4:A:810:PRO:C	2.60	0.40
4:A:815:PHE:O	4:A:816:HIS:C	2.60	0.40
5:B:1207:LEU:O	5:B:1210:MET:HB2	2.21	0.40
5:B:1167:GLY:O	5:B:1215:ARG:HA	2.22	0.40
5:B:27:ALA:O	5:B:30:SER:OG	2.36	0.40
5:B:386:LEU:C	5:B:388:CYS:N	2.74	0.40
5:B:168:GLY:HA2	5:B:454:THR:OG1	2.21	0.40
5:B:461:LEU:HD12	5:B:461:LEU:N	2.35	0.40
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.22	0.40
5:B:582:VAL:HG12	5:B:587:HIS:NE2	2.37	0.40
5:B:979:LYS:HG2	5:B:1095:LEU:CD1	2.51	0.40
4:A:1206:ASP:O	4:A:1274:ARG:NH1	2.52	0.40
4:A:1115:SER:O	4:A:1311:VAL:CG2	2.70	0.40
4:A:1335:ILE:O	4:A:1335:ILE:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:353:ILE:HD13	4:A:487:MET:HG3	2.04	0.40
4:A:596:THR:C	4:A:598:LEU:H	2.24	0.40
4:A:599:SER:HA	4:A:600:PRO:HD2	1.95	0.40
4:A:650:GLN:C	4:A:654:ASN:ND2	2.75	0.40
4:A:709:THR:HG22	4:A:710:LEU:N	2.37	0.40
4:A:794:PRO:C	4:A:796:SER:N	2.75	0.40
4:A:886:ILE:HG13	4:A:943:LEU:HD13	2.03	0.40
5:B:1008:PRO:HB2	5:B:1010:LEU:O	2.21	0.40
5:B:1027:ILE:O	5:B:1028:GLU:C	2.60	0.40
5:B:180:TYR:CD1	5:B:180:TYR:N	2.90	0.40
5:B:294:ASP:OD1	12:I:12:ASN:HB3	2.21	0.40
5:B:35:SER:HA	5:B:811:TYR:CE2	2.46	0.40
5:B:371:GLU:OE1	5:B:371:GLU:N	2.55	0.40
5:B:376:PHE:CE2	5:B:569:TYR:CD2	3.02	0.40
5:B:564:GLU:HA	5:B:565:PRO:HD2	1.91	0.40
5:B:637:LEU:CD2	5:B:742:GLU:HA	2.51	0.40
5:B:814:PHE:C	5:B:816:GLU:N	2.75	0.40
6:C:169:LYS:NZ	15:L:69:ALA:HB3	2.37	0.40
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.50	0.40
6:C:58:LEU:HD22	6:C:58:LEU:N	2.37	0.40
8:E:98:ILE:C	8:E:100:ILE:N	2.74	0.40
8:E:177:ARG:O	8:E:212:ARG:CD	2.70	0.40
8:E:17:ARG:O	8:E:21:GLU:HG3	2.22	0.40
9:F:82:THR:HA	9:F:83:PRO:HD3	1.81	0.40
9:F:94:LEU:HD21	9:F:122:MET:HA	2.03	0.40
11:H:41:ASP:HB2	11:H:121:LEU:HB3	2.02	0.40
11:H:58:THR:HG22	11:H:59:ILE:H	1.86	0.40
14:K:24:ASP:OD1	14:K:26:LYS:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1406/1733 (81%)	936 (67%)	311 (22%)	159 (11%)	0	8
5	B	1096/1224 (90%)	740 (68%)	215 (20%)	141 (13%)	0	6
6	C	264/318 (83%)	166 (63%)	64 (24%)	34 (13%)	0	6
7	D	173/221 (78%)	118 (68%)	38 (22%)	17 (10%)	1	12
8	E	212/215 (99%)	154 (73%)	44 (21%)	14 (7%)	1	23
9	F	82/155 (53%)	63 (77%)	16 (20%)	3 (4%)	4	36
10	G	169/171 (99%)	133 (79%)	24 (14%)	12 (7%)	1	20
11	H	129/146 (88%)	85 (66%)	28 (22%)	16 (12%)	0	7
12	I	117/122 (96%)	79 (68%)	27 (23%)	11 (9%)	1	14
13	J	63/70 (90%)	34 (54%)	15 (24%)	14 (22%)	0	1
14	K	112/120 (93%)	87 (78%)	17 (15%)	8 (7%)	1	20
15	L	44/70 (63%)	17 (39%)	18 (41%)	9 (20%)	0	2
All	All	3867/4565 (85%)	2612 (68%)	817 (21%)	438 (11%)	0	8

All (438) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	48	ALA
4	A	54	ASN
4	A	55	ASP
4	A	57	ARG
4	A	62	ASP
4	A	65	LEU
4	A	66	LYS
4	A	70	CYS
4	A	74	MET
4	A	76	GLU
4	A	93	VAL
4	A	154	SER
4	A	167	CYS
4	A	244	PRO
4	A	255	SER
4	A	286	HIS
4	A	311	GLN
4	A	318	SER
4	A	322	VAL
4	A	335	ARG
4	A	385	ILE

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Mol	Chain	Res	Type
4	A	409	SER
4	A	418	SER
4	A	423	ASP
4	A	536	LEU
4	A	567	LYS
4	A	619	LYS
4	A	626	ASN
4	A	666	ILE
4	A	765	VAL
4	A	775	ILE
4	A	780	VAL
4	A	789	LYS
4	A	847	ASP
4	A	968	GLN
4	A	1002	GLY
4	A	1016	THR
4	A	1036	ARG
4	A	1115	SER
4	A	1116	LEU
4	A	1122	PRO
4	A	1212	VAL
4	A	1223	ASP
4	A	1281	ARG
4	A	1314	SER
4	A	1341	ILE
4	A	1365	TYR
4	A	1366	ARG
4	A	1378	GLN
4	A	1403	GLU
4	A	1438	THR
5	B	28	GLU
5	B	45	SER
5	B	108	VAL
5	B	206	ASN
5	B	258	LEU
5	B	259	TYR
5	B	308	TRP
5	B	367	LEU
5	B	467	GLY
5	B	474	SER
5	B	504	ARG
5	B	509	ALA

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Mol	Chain	Res	Type
5	B	511	PRO
5	B	629	ASP
5	B	643	ASP
5	B	709	ASP
5	B	731	VAL
5	B	751	VAL
5	B	881	ASN
5	B	907	GLY
5	B	943	SER
5	B	958	GLN
5	B	1046	PRO
5	B	1100	ASP
5	B	1108	ARG
5	B	1157	ALA
5	B	1171	VAL
5	B	1175	LEU
5	B	1181	GLU
5	B	1182	CYS
5	B	1186	ASP
5	B	1188	LYS
6	C	91	HIS
6	C	110	THR
6	C	141	GLY
6	C	149	LYS
6	C	156	THR
6	C	161	LYS
6	C	184	ASN
6	C	213	PRO
6	C	214	ASN
6	C	215	GLU
6	C	231	ASN
7	D	6	SER
7	D	8	PHE
7	D	19	GLU
7	D	20	GLU
7	D	21	GLU
7	D	52	LEU
7	D	131	GLU
7	D	177	VAL
7	D	199	ASN
8	E	106	GLN
8	E	130	ALA

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Mol	Chain	Res	Type
9	F	81	THR
10	G	63	PRO
10	G	139	ILE
11	H	81	PRO
11	H	128	ASN
11	H	140	ALA
12	I	3	THR
12	I	9	ASP
12	I	57	GLY
12	I	79	HIS
13	J	2	ILE
13	J	6	ARG
13	J	32	GLU
13	J	64	ASN
15	L	50	ASP
15	L	53	HIS
15	L	59	ALA
4	A	42	ASP
4	A	44	THR
4	A	59	GLY
4	A	111	GLY
4	A	113	LEU
4	A	117	GLU
4	A	219	PHE
4	A	226	GLU
4	A	232	GLU
4	A	263	THR
4	A	278	THR
4	A	290	GLU
4	A	300	VAL
4	A	312	PRO
4	A	364	VAL
4	A	399	HIS
4	A	421	ALA
4	A	424	ILE
4	A	661	GLY
4	A	731	ARG
4	A	753	GLY
4	A	795	GLU
4	A	830	LYS
4	A	846	GLU
4	A	986	ILE

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Mol	Chain	Res	Type
4	A	1014	ALA
4	A	1071	SER
4	A	1165	GLU
4	A	1221	LYS
4	A	1386	ARG
4	A	1395	GLY
4	A	1397	LEU
4	A	1405	THR
5	B	21	GLU
5	B	27	ALA
5	B	46	GLN
5	B	114	PRO
5	B	115	GLN
5	B	186	GLU
5	B	229	ALA
5	B	257	LYS
5	B	260	GLY
5	B	282	ILE
5	B	322	PHE
5	B	334	ILE
5	B	369	GLY
5	B	468	GLU
5	B	470	LYS
5	B	513	GLN
5	B	540	SER
5	B	559	SER
5	B	682	SER
5	B	746	SER
5	B	770	GLN
5	B	848	ARG
5	B	869	SER
5	B	891	ASP
5	B	1006	ILE
5	B	1041	GLU
5	B	1069	PHE
5	B	1126	GLY
5	B	1156	ASP
5	B	1167	GLY
5	B	1178	ASN
5	B	1183	LYS
6	C	78	GLU
6	C	164	ALA

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Mol	Chain	Res	Type
6	C	167	HIS
6	C	175	ALA
6	C	202	PRO
6	C	209	TYR
6	C	216	GLY
6	C	240	VAL
6	C	264	GLN
7	D	12	ARG
7	D	53	SER
7	D	192	LYS
8	E	36	GLU
8	E	44	ALA
8	E	59	SER
8	E	73	PRO
8	E	74	ASP
8	E	192	ARG
8	E	206	GLY
10	G	35	GLU
10	G	53	ASN
10	G	154	VAL
11	H	21	ASN
11	H	32	THR
11	H	59	ILE
11	H	82	PRO
11	H	84	ALA
11	H	92	ASP
11	H	108	SER
12	I	78	CYS
12	I	106	CYS
13	J	8	PHE
13	J	14	VAL
13	J	18	TRP
13	J	28	ASP
13	J	29	GLU
13	J	33	GLY
13	J	51	LEU
14	K	7	PHE
14	K	15	GLY
14	K	29	ASN
14	K	53	ASP
14	K	88	LYS
4	A	4	GLN

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Mol	Chain	Res	Type
4	A	61	ILE
4	A	67	CYS
4	A	69	THR
4	A	71	GLN
4	A	223	GLY
4	A	245	PRO
4	A	253	ASN
4	A	317	LYS
4	A	357	PRO
4	A	419	LYS
4	A	439	ASN
4	A	517	ASN
4	A	525	GLN
4	A	534	LEU
4	A	817	ALA
4	A	818	MET
4	A	824	LEU
4	A	829	VAL
4	A	1008	GLN
4	A	1028	THR
4	A	1067	LEU
4	A	1114	PRO
4	A	1127	ASP
4	A	1133	LEU
4	A	1240	CYS
4	A	1242	VAL
4	A	1335	ILE
4	A	1389	PHE
5	B	48	LEU
5	B	58	THR
5	B	100	PRO
5	B	266	ALA
5	B	319	GLU
5	B	387	LEU
5	B	591	ARG
5	B	605	ARG
5	B	636	PRO
5	B	641	GLU
5	B	648	HIS
5	B	655	LYS
5	B	711	GLU
5	B	867	GLY

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Mol	Chain	Res	Type
5	B	878	GLN
5	B	951	GLN
5	B	1003	ALA
5	B	1017	ILE
5	B	1035	ALA
5	B	1097	HIS
5	B	1112	GLN
5	B	1144	ALA
5	B	1153	GLU
5	B	1155	SER
6	C	87	PHE
6	C	169	LYS
6	C	255	VAL
7	D	15	LEU
7	D	218	GLU
8	E	115	ASN
8	E	138	ALA
9	F	150	GLU
10	G	62	LEU
10	G	118	ASP
11	H	17	PRO
11	H	44	VAL
11	H	77	ARG
11	H	107	VAL
12	I	47	GLU
12	I	62	ILE
13	J	17	LYS
15	L	35	SER
15	L	40	LEU
15	L	43	THR
15	L	54	ARG
15	L	56	LEU
4	A	58	LEU
4	A	250	ILE
4	A	283	GLY
4	A	333	GLU
4	A	336	ILE
4	A	400	PRO
4	A	465	TYR
4	A	526	ASP
4	A	592	ASP
4	A	605	MET

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Mol	Chain	Res	Type
4	A	648	ASN
4	A	652	VAL
4	A	910	PRO
4	A	958	VAL
4	A	1231	ASP
4	A	1266	THR
4	A	1302	PRO
5	B	49	ASP
5	B	67	SER
5	B	364	ILE
5	B	418	LYS
5	B	466	TRP
5	B	590	HIS
5	B	727	LYS
5	B	735	ALA
5	B	738	PHE
5	B	752	ALA
5	B	754	SER
5	B	764	SER
5	B	792	MET
5	B	815	ARG
5	B	883	LEU
5	B	884	ARG
5	B	888	GLY
5	B	953	LEU
5	B	982	SER
5	B	1065	GLN
5	B	1103	ILE
5	B	1176	ASN
6	C	60	ASP
6	C	108	GLU
6	C	142	VAL
6	C	212	PRO
6	C	257	SER
7	D	30	GLY
8	E	45	LYS
8	E	99	HIS
10	G	115	MET
11	H	52	GLN
12	I	11	ASN
12	I	34	TYR
14	K	70	ARG

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Mol	Chain	Res	Type
14	K	79	GLU
14	K	104	ASN
4	A	101	LYS
4	A	386	ASP
4	A	599	SER
4	A	920	LEU
4	A	1120	LEU
4	A	1164	PRO
4	A	1370	LEU
5	B	30	SER
5	B	65	GLU
5	B	94	LYS
5	B	309	GLN
5	B	383	ASN
5	B	401	PHE
5	B	411	PRO
5	B	414	ALA
5	B	510	LYS
5	B	571	PRO
5	B	880	THR
5	B	942	ARG
5	B	1011	ILE
6	C	56	THR
6	C	84	ARG
7	D	196	PRO
9	F	149	GLU
10	G	17	PHE
10	G	20	PRO
11	H	135	LEU
13	J	24	LEU
13	J	27	GLU
4	A	276	LEU
4	A	492	PRO
4	A	598	LEU
4	A	649	ILE
4	A	756	ILE
4	A	1006	ILE
4	A	1057	VAL
4	A	1377	THR
5	B	261	ARG
5	B	844	SER
5	B	1082	MET

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Mol	Chain	Res	Type
6	C	89	GLU
10	G	34	VAL
12	I	32	CYS
4	A	38	PRO
4	A	96	ILE
5	B	23	ALA
5	B	295	GLY
5	B	410	GLY
5	B	478	GLY
5	B	520	GLY
5	B	551	PRO
5	B	1018	PRO
5	B	1099	VAL
6	C	77	ILE
4	A	84	ILE
4	A	196	GLU
4	A	1158	PRO
5	B	575	PRO
5	B	613	VAL
6	C	10	ILE
4	A	396	PRO
4	A	653	VAL
4	A	1384	VAL
4	A	1454	MET
5	B	283	VAL
5	B	712	PRO
5	B	824	ILE
6	C	172	PRO
10	G	19	GLY
15	L	46	VAL
4	A	1060	PRO
7	D	202	ILE
4	A	73	GLY
4	A	321	PRO
4	A	1406	VAL
5	B	611	PRO
5	B	758	PHE
8	E	129	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	
4	A	1239/1520 (82%)	1125 (91%)	114 (9%)	11	42
5	B	964/1061 (91%)	873 (91%)	91 (9%)	10	41
6	C	234/274 (85%)	213 (91%)	21 (9%)	11	43
7	D	140/200 (70%)	124 (89%)	16 (11%)	7	33
8	E	196/197 (100%)	188 (96%)	8 (4%)	35	69
9	F	74/137 (54%)	65 (88%)	9 (12%)	6	30
10	G	152/152 (100%)	139 (91%)	13 (9%)	12	46
11	H	117/128 (91%)	109 (93%)	8 (7%)	18	55
12	I	113/116 (97%)	98 (87%)	15 (13%)	4	28
13	J	60/65 (92%)	55 (92%)	5 (8%)	13	47
14	K	99/102 (97%)	90 (91%)	9 (9%)	11	43
15	L	40/57 (70%)	37 (92%)	3 (8%)	16	52
All	All	3428/4009 (86%)	3116 (91%)	312 (9%)	11	43

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	2	VAL
4	A	11	LEU
4	A	22	PHE
4	A	34	LYS
4	A	38	PRO
4	A	62	ASP
4	A	67	CYS
4	A	83	HIS
4	A	93	VAL
4	A	105	CYS
4	A	108	MET
4	A	122	MET
4	A	200	ARG
4	A	208	LEU

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Mol	Chain	Res	Type
4	A	209	ASN
4	A	215	SER
4	A	221	SER
4	A	236	LEU
4	A	245	PRO
4	A	270	LEU
4	A	293	GLU
4	A	302	THR
4	A	312	PRO
4	A	320	ARG
4	A	321	PRO
4	A	335	ARG
4	A	350	ARG
4	A	354	SER
4	A	381	THR
4	A	396	PRO
4	A	404	TYR
4	A	406	ILE
4	A	407	ARG
4	A	408	ASP
4	A	418	SER
4	A	425	GLN
4	A	443	LEU
4	A	445	ASN
4	A	449	SER
4	A	450	LEU
4	A	451	HIS
4	A	454	SER
4	A	462	VAL
4	A	470	LEU
4	A	481	ASP
4	A	493	GLN
4	A	497	THR
4	A	498	ARG
4	A	503	GLN
4	A	515	GLN
4	A	545	GLN
4	A	560	ILE
4	A	562	THR
4	A	598	LEU
4	A	618	GLU
4	A	626	ASN

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Mol	Chain	Res	Type
4	A	666	ILE
4	A	670	ILE
4	A	711	ARG
4	A	739	ASP
4	A	768	GLN
4	A	774	ARG
4	A	779	PHE
4	A	821	ARG
4	A	827	THR
4	A	831	THR
4	A	834	THR
4	A	845	LEU
4	A	858	ASN
4	A	871	ASP
4	A	890	ASP
4	A	903	ASN
4	A	929	LEU
4	A	940	ARG
4	A	949	ASP
4	A	992	ASP
4	A	1016	THR
4	A	1029	ARG
4	A	1030	ARG
4	A	1035	TYR
4	A	1052	GLN
4	A	1067	LEU
4	A	1110	ASN
4	A	1111	MET
4	A	1116	LEU
4	A	1122	PRO
4	A	1127	ASP
4	A	1152	ILE
4	A	1155	ASP
4	A	1170	ILE
4	A	1173	HIS
4	A	1193	LEU
4	A	1264	GLU
4	A	1271	ILE
4	A	1291	VAL
4	A	1295	THR
4	A	1298	TYR
4	A	1309	ASP

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Mol	Chain	Res	Type
4	A	1329	THR
4	A	1332	PHE
4	A	1333	ILE
4	A	1359	ASP
4	A	1364	ASN
4	A	1366	ARG
4	A	1372	VAL
4	A	1386	ARG
4	A	1389	PHE
4	A	1394	THR
4	A	1405	THR
4	A	1432	GLN
4	A	1442	ASP
4	A	1443	VAL
4	A	1445	ILE
4	A	1447	GLU
5	B	30	SER
5	B	44	VAL
5	B	57	TYR
5	B	61	ASP
5	B	175	ARG
5	B	188	ASP
5	B	194	GLU
5	B	199	MET
5	B	217	ARG
5	B	223	VAL
5	B	225	VAL
5	B	261	ARG
5	B	268	THR
5	B	286	PHE
5	B	294	ASP
5	B	298	LEU
5	B	365	THR
5	B	371	GLU
5	B	378	LEU
5	B	393	LYS
5	B	396	ASP
5	B	399	ASP
5	B	401	PHE
5	B	411	PRO
5	B	417	PHE
5	B	427	ASP

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Mol	Chain	Res	Type
5	B	429	PHE
5	B	463	THR
5	B	465	ASN
5	B	466	TRP
5	B	476	ARG
5	B	485	ARG
5	B	496	ARG
5	B	498	THR
5	B	502	ILE
5	B	516	ASN
5	B	557	PHE
5	B	570	VAL
5	B	582	VAL
5	B	593	PRO
5	B	603	LEU
5	B	615	MET
5	B	628	THR
5	B	635	ARG
5	B	636	PRO
5	B	644	GLU
5	B	682	SER
5	B	701	ILE
5	B	724	ASP
5	B	737	THR
5	B	742	GLU
5	B	751	VAL
5	B	811	TYR
5	B	830	TYR
5	B	835	GLN
5	B	839	MET
5	B	858	SER
5	B	860	MET
5	B	878	GLN
5	B	894	ASP
5	B	901	PRO
5	B	909	ASP
5	B	953	LEU
5	B	999	MET
5	B	1002	THR
5	B	1006	ILE
5	B	1010	LEU
5	B	1018	PRO

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Mol	Chain	Res	Type
5	B	1034	VAL
5	B	1047	PHE
5	B	1051	THR
5	B	1060	ARG
5	B	1069	PHE
5	B	1077	THR
5	B	1084	GLN
5	B	1087	PHE
5	B	1095	LEU
5	B	1096	ARG
5	B	1099	VAL
5	B	1112	GLN
5	B	1120	GLU
5	B	1122	ARG
5	B	1159	ARG
5	B	1163	CYS
5	B	1169	MET
5	B	1170	THR
5	B	1176	ASN
5	B	1183	LYS
5	B	1202	LEU
5	B	1212	ILE
5	B	1216	LEU
6	C	22	LEU
6	C	29	MET
6	C	54	ASN
6	C	58	LEU
6	C	62	PHE
6	C	77	ILE
6	C	89	GLU
6	C	91	HIS
6	C	104	PHE
6	C	106	GLU
6	C	108	GLU
6	C	112	ASN
6	C	140	ASN
6	C	145	CYS
6	C	147	LEU
6	C	166	GLU
6	C	193	TYR
6	C	202	PRO
6	C	233	GLU

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Mol	Chain	Res	Type
6	C	240	VAL
6	C	266	ASP
7	D	32	GLU
7	D	47	LEU
7	D	63	LEU
7	D	70	PHE
7	D	137	ASN
7	D	139	LYS
7	D	148	LEU
7	D	149	THR
7	D	152	SER
7	D	156	ASP
7	D	170	THR
7	D	182	SER
7	D	187	THR
7	D	193	THR
7	D	202	ILE
7	D	221	TYR
8	E	60	PHE
8	E	74	ASP
8	E	82	PHE
8	E	104	ASN
8	E	114	ASN
8	E	183	PRO
8	E	207	ARG
8	E	215	MET
9	F	79	ARG
9	F	81	THR
9	F	90	ARG
9	F	99	LEU
9	F	103	MET
9	F	119	ARG
9	F	143	PHE
9	F	148	VAL
9	F	153	VAL
10	G	1	MET
10	G	13	LEU
10	G	17	PHE
10	G	38	CYS
10	G	74	TYR
10	G	78	VAL
10	G	80	LYS

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Mol	Chain	Res	Type
10	G	88	ASP
10	G	93	SER
10	G	96	GLN
10	G	115	MET
10	G	126	ASN
10	G	171	ILE
11	H	7	ASP
11	H	62	SER
11	H	86	ASP
11	H	91	ASP
11	H	95	TYR
11	H	102	TYR
11	H	130	ARG
11	H	143	LEU
12	I	8	ARG
12	I	9	ASP
12	I	10	CYS
12	I	13	MET
12	I	15	TYR
12	I	31	THR
12	I	34	TYR
12	I	75	CYS
12	I	78	CYS
12	I	85	PHE
12	I	86	PHE
12	I	94	ASP
12	I	100	PHE
12	I	101	PHE
12	I	106	CYS
13	J	1	MET
13	J	9	SER
13	J	44	TYR
13	J	46	CYS
13	J	48	ARG
14	K	5	ASP
14	K	10	PHE
14	K	17	SER
14	K	25	THR
14	K	42	LEU
14	K	47	ARG
14	K	50	LEU
14	K	61	TYR

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Mol	Chain	Res	Type
14	K	78	THR
15	L	55	ILE
15	L	68	GLU
15	L	70	ARG

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

Mol	Chain	Res	Type
4	A	83	HIS
4	A	92	HIS
4	A	225	ASN
4	A	256	GLN
4	A	282	ASN
4	A	299	HIS
4	A	306	ASN
4	A	339	ASN
4	A	435	HIS
4	A	479	ASN
4	A	493	GLN
4	A	503	GLN
4	A	517	ASN
4	A	525	GLN
4	A	603	ASN
4	A	611	GLN
4	A	654	ASN
4	A	741	ASN
4	A	757	ASN
4	A	767	GLN
4	A	768	GLN
4	A	786	HIS
4	A	858	ASN
4	A	903	ASN
4	A	926	GLN
4	A	1130	GLN
4	A	1265	ASN
4	A	1364	ASN
4	A	1432	GLN
5	B	178	ASN
5	B	215	GLN
5	B	236	HIS
5	B	350	GLN
5	B	363	HIS

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Mol	Chain	Res	Type
5	B	366	GLN
5	B	383	ASN
5	B	465	ASN
5	B	484	ASN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	538	ASN
5	B	734	HIS
5	B	744	HIS
5	B	776	GLN
5	B	821	GLN
5	B	842	ASN
5	B	975	GLN
5	B	1015	HIS
5	B	1025	HIS
5	B	1065	GLN
5	B	1076	HIS
5	B	1084	GLN
5	B	1097	HIS
5	B	1117	GLN
5	B	1179	GLN
5	B	1193	GLN
6	C	24	ASN
6	C	73	GLN
6	C	91	HIS
6	C	112	ASN
6	C	123	ASN
6	C	231	ASN
6	C	252	GLN
7	D	40	HIS
7	D	137	ASN
7	D	179	GLN
8	E	8	ASN
8	E	101	GLN
8	E	104	ASN
8	E	114	ASN
8	E	147	HIS
10	G	14	HIS
10	G	53	ASN
10	G	97	HIS
10	G	122	ASN

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Mol	Chain	Res	Type
10	G	126	ASN
11	H	131	ASN
12	I	12	ASN
12	I	60	GLN
12	I	89	GLN
14	K	44	ASN
14	K	65	HIS
14	K	76	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	T	18/19 (94%)	0.23	1 (5%) 25 19	69, 103, 131, 137	0
2	N	6/7 (85%)	0.75	0 100 100	97, 99, 108, 108	0
3	P	10/10 (100%)	0.24	0 100 100	80, 94, 125, 127	0
4	A	1416/1733 (81%)	-0.76	4 (0%) 93 91	21, 75, 151, 195	0
5	B	1112/1224 (90%)	-0.71	3 (0%) 93 91	20, 87, 156, 186	0
6	C	266/318 (83%)	-0.79	0 100 100	34, 71, 130, 150	0
7	D	177/221 (80%)	-0.57	0 100 100	43, 99, 137, 155	0
8	E	214/215 (99%)	-0.56	0 100 100	47, 132, 177, 181	0
9	F	84/155 (54%)	-0.93	0 100 100	21, 49, 93, 113	0
10	G	171/171 (100%)	-0.77	0 100 100	47, 76, 106, 122	0
11	H	133/146 (91%)	-0.35	0 100 100	91, 130, 165, 175	0
12	I	119/122 (97%)	-0.40	0 100 100	63, 122, 153, 191	0
13	J	65/70 (92%)	-0.87	0 100 100	37, 69, 113, 118	0
14	K	114/120 (95%)	-0.80	0 100 100	37, 75, 104, 118	0
15	L	46/70 (65%)	-0.36	0 100 100	73, 127, 160, 168	0
All	All	3951/4601 (85%)	-0.70	8 (0%) 94 93	20, 84, 156, 195	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	4.7
5	B	471	LYS	3.3
1	T	28	DT	2.6
4	A	1175	SER	2.4
5	B	470	LYS	2.3
4	A	1455	PRO	2.2
5	B	504	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
4	A	1092	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
16	ZN	C	319	1/1	0.99	0.09	-0.80	28,28,28,28	0
16	ZN	A	1734	1/1	0.98	0.08	-1.00	73,73,73,73	0
16	ZN	I	204	1/1	0.98	0.10	-1.19	141,141,141,141	0
16	ZN	L	105	1/1	0.99	0.10	-1.41	90,90,90,90	0
16	ZN	B	1307	1/1	1.00	0.08	-1.50	31,31,31,31	0
16	ZN	A	1735	1/1	0.99	0.05	-1.80	36,36,36,36	0
16	ZN	J	101	1/1	0.99	0.06	-2.15	45,45,45,45	0
16	ZN	I	203	1/1	0.99	0.08	-2.40	80,80,80,80	0
17	MG	A	1736	1/1	0.99	0.07	-	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.