



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:53 AM UTC

PDB ID : 1I6H / pdb_00001i6h
Title : RNA POLYMERASE II ELONGATION COMPLEX
Authors : Gnatt, A.L.; Cramer, P.; Kornberg, R.D.
Deposited on : 2001-03-02
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

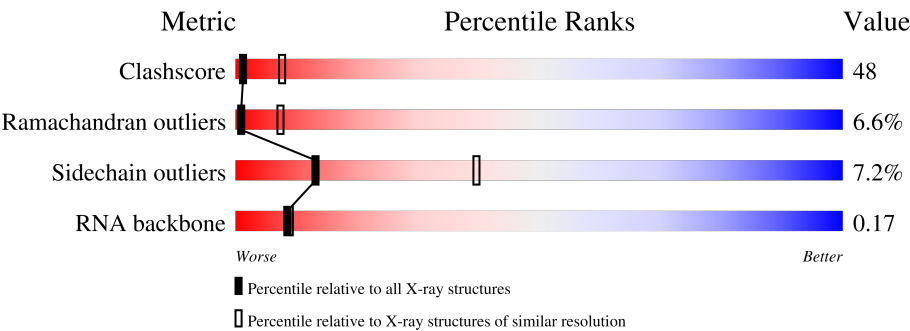
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	13	15% 69% 15%
2	R	9	11% 56% 11% 22%
3	A	1733	27% 43% 9% 20%
4	B	1224	28% 51% 10% 10%
5	C	318	33% 40% 10% 16%
6	E	215	39% 56% 5%

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

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28430 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*AP*AP*TP*GP*CP*CP*TP*GP*GP*TP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	13	Total	C	N	O	P	0	0	0
			267	127	47	80	13			

- Molecule 2 is a RNA chain called 5'-R(P*GP*AP*CP*CP*AP*GP*GP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	9	Total	C	N	O	P	0	0	0
			196	87	39	61	9			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1097	Total	C	N	O	S	0	0	0
			8721	5526	1523	1618	54			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

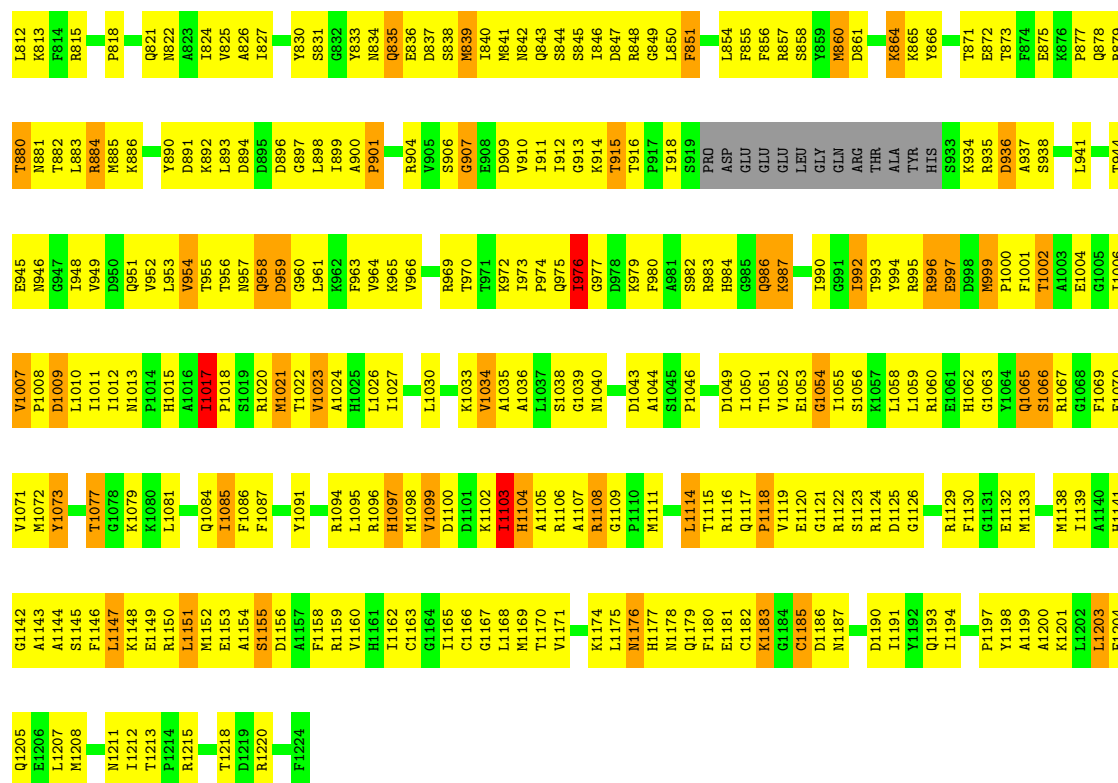
- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

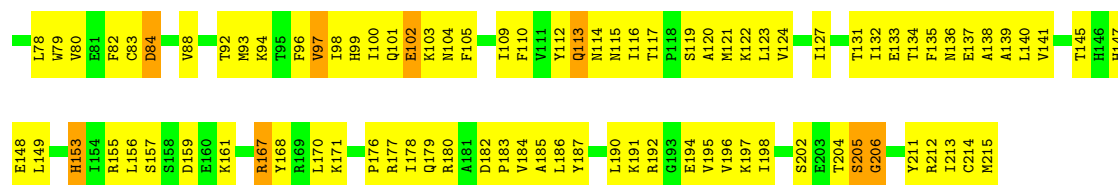
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	R	1	Total	Mg	0	0
			1	1		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

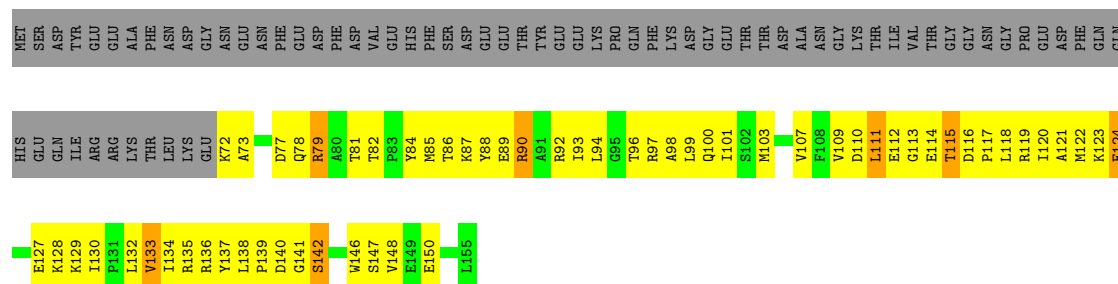
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	THR	THR	THR	THR	GLU	THR	H1387	P1324	THR	ASP	GLU	V1118	L1054	L983	S914	R849	G778	Q698	G623	V491
	THR	THR	THR	VAL	GLU	GLU	T1325	T1325	GLU		GLU		R1055	K984	S915	R850	F779	Q698	G623	V491
	GLY	THR	THR	LVS	VAL	E1255	F1389	R1327	E1255	S1189	E1255	P1122	S1056	D985		H851		L701	G628	Q493
	GLY	GLY	GLY	THR	THR	E1255	R1391	V1328	E1255	P1190	V1328		V1058	V987	R919	D853	T783	T703	L629	Q493
	ALA	ALA	ALA	MET	MET	H1288	T1329	T1329	MET	H1191	T1329	A1126	H1059	L988	L920	R854	L784	A704	V633	E495
	ASP	ASP	ASP	PRO	PRO	M1289	M1330	M1330	PRO	L1192	L1192	D1127	P1060		G921	R855	F785			T62
	ASP	ASP	ASP	PRO	PRO	M1289	M1330	M1330	PRO	L1192	L1192	D1127	P1060		G921	R855	F785			T62
	THR	THR	THR	GLN	GLN	T1394	T1394	F1331	GLN	R1193	R1193	Q1128	G1081	D992	L922	R856	H786	T709	P663	T497
	GLY	GLY	GLY	GLN	GLN	G1395	F1331	F1331	GLN	R1194	R1194	Q1128	G1081	D992	L922	R856	H786	T709	P663	T497
ALA	ALA	ALA	ALA	LVS	LVS	L1262	A1396	I1333	L1262	L1195	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
	ALA	ALA	ALA	LVS	LVS	L1263	A1396	I1333	L1263	L1196	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
	ALA	ALA	ALA	LVS	LVS	L1263	A1396	I1333	L1263	L1196	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
	ALA	ALA	ALA	LVS	LVS	L1263	A1396	I1333	L1263	L1196	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
	ALA	ALA	ALA	LVS	LVS	L1263	A1396	I1333	L1263	L1196	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
	ALA	ALA	ALA	LVS	LVS	L1263	A1396	I1333	L1263	L1196	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
	ALA	ALA	ALA	LVS	LVS	L1263	A1396	I1333	L1263	L1196	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
	ALA	ALA	ALA	LVS	LVS	L1263	A1396	I1333	L1263	L1196	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
	ALA	ALA	ALA	LVS	LVS	L1263	A1396	I1333	L1263	L1196	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
	ALA	ALA	ALA	LVS	LVS	L1263	A1396	I1333	L1263	L1196	Q1130	M1063	M1063	Q994	L923	R857	K789	R711	P639	A498
PHE	THR	THR	THR	GLN	GLN	GLN	E1403	G1340	GLN	K1205	L1206	A1137			E931	R865		S713	Q640	Q503
	THR	THR	THR	GLN	GLN	GLN	E1404	G1340	GLN	K1206	L1206	A1137			E931	R865		S713	Q640	Q503
	GLY	GLY	GLY	ASP	ASP	ASP	T1405	E1342	ASP	L1207	L1207	L1138	G1073	L1006	E932	R866	F794	F721	M648	K575
	GLY	GLY	GLY	GLY	GLY	GLY	A1406	G1343	GLY	T1208	L1208	L1138	G1073	L1006	E932	R866	F794	F721	M648	K575
	ALA	ALA	ALA	GLY	GLY	GLY	E1407	G1344	GLY	M1209	E1139	L1139	E1074	L1007	E933	R867	F794	F721	M648	K575
	PRO	PRO	PRO	GLY	GLY	GLY	A1407	G1344	GLY	G1210	H1140	L1140	A1076	Q1008	R868					Q576
	PRO	PRO	PRO	VAL	VAL	VAL	I1408	R1345	VAL	Q1211	T1141	L1141	A1076	Q1008	R868					Q576
	THR	THR	THR	VAL	VAL	VAL	L1408	R1345	VAL	Q1211	T1141	L1141	A1076	Q1008	R868					Q576
	THR	THR	THR	VAL	VAL	VAL	L1409	A1346	THR	Q1212	T1142	L1142	Q1077	A1010	E936	R870	T809	P810	V652	L578
	SER	SER	SER	PRO	PRO	PRO	F1410	A1347	PRO	G1213	L1143	L1143	M1079			G672	A729	K728	V653	S516
PHE	PRO	PRO	PRO	GLY	GLY	GLY	E4411	E1277	GLY	E1214	L1278				E932	R873	E812	N736	P655	A581
	PRO	PRO	PRO	GLY	GLY	GLY	E4411	E1277	GLY	E1214	L1278				E932	R873	E812	N736	P655	A581
	GLY	GLY	GLY	SER	SER	SER	A1412	V1349	SER	R1215	L1147	L1081	V1015	R940	R874	F813	F814	L737	L657	N584
	GLY	GLY	GLY	ASN	ASN	ASN	G1413	G1344	ASN	L1216	T1148	ASN	L1017	R941	D874	F814	L737	L657	N584	
	GLY	GLY	GLY	ASN	ASN	ASN	G1413	G1344	ASN	L1216	T1148	ASN	L1017	R941	D874	F814	L737	L657	N584	
	GLY	GLY	GLY	ASN	ASN	ASN	G1413	G1344	ASN	L1216	T1148	ASN	L1017	R941	D874	F814	L737	L657	N584	
	GLY	GLY	GLY	ASN	ASN	ASN	G1413	G1344	ASN	L1216	T1148	ASN	L1017	R941	D874	F814	L737	L657	N584	
	GLY	GLY	GLY	ASN	ASN	ASN	G1413	G1344	ASN	L1216	T1148	ASN	L1017	R941	D874	F814	L737	L657	N584	
	GLY	GLY	GLY	ASN	ASN	ASN	G1413	G1344	ASN	L1216	T1148	ASN	L1017	R941	D874	F814	L737	L657	N584	
	GLY	GLY	GLY	ASN	ASN	ASN	G1413	G1344	ASN	L1216	T1148	ASN	L1017	R941	D874	F814	L737	L657	N584	
PHE	VAL	VAL	VAL	SER	SER	SER	S1415	V1352	SER	Q1218	S1150	PHE	C1019			R878	H816	D739	H587	M521
	VAL	VAL	VAL	SER	SER	SER	S1415	V1352	SER	Q1218	S1150	PHE	C1019			R878	H816	D739	H587	M521
	SER	SER	SER	GLY	GLY	GLY	A1416	V1283	GLY	T1219	E1151	HIS	G1020	V948	R879	L740		L740	S663	G522
	SER	SER	SER	GLY	GLY	GLY	A1416	V1283	GLY	T1219	E1151	HIS	G1020	V948	R879	L740		L740	S663	G522
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	SER	SER	SER	GLY	GLY	GLY	A1416	V1283	GLY	T1219	E1151	HIS	G1020	V948	R879	L740		L740	S663	G522
	SER	SER	SER	GLY	GLY	GLY	A1416	V1283	GLY	T1219	E1151	HIS	G1020	V948	R879	L740		L740	S663	G522
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	GLY	GLY	GLY	VAL	VAL	VAL	V1355	E1366	VAL	F1220	V1152	PHE	C1019			R881	H816	D739	H587	M521
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	GLY	GLY	GLY	VAL	VAL	VAL	V1355	E1366	VAL	F1220	V1152	PHE	C1019			R881	H816	D739	H587	M521
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PHE	GLY	GLY	GLY	VAL	VAL	VAL	V1355	E1366	VAL	F1220	V1152	PHE	C1019			R881	H816	D739	H587	M521
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	GLY	GLY	GLY	VAL	VAL	VAL	V1355	E1366	VAL	F1220	V1152	PHE	C1019			R881	H816	D739	H587	M521
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	GLY	GLY	GLY	VAL	VAL	VAL	V1355	E1366	VAL	F1220	V1152	PHE	C1019			R881	H816	D739	H587	M521
	GLY	GLY	GLY	VAL	VAL	VAL	V1355	E1366	VAL	F1220	V1152	PHE	C1019			R881	H816	D739	H587	M521
	GLY	GLY	GLY	VAL	VAL	VAL	V1355	E1366	VAL	F1220	V1152	PHE	C1019			R881	H816	D739	H587	M521
PHE	GLY	GLY	GLY	VAL	VAL	VAL	V1355	E1366	VAL	F1220	V1152	PHE	C1019							





• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

Chain F: 15% 34% 5% 46%



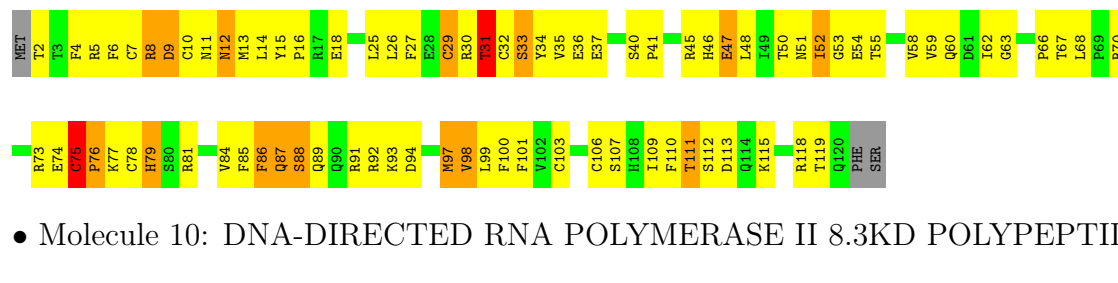
• Molecule 8: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

Chain H: 27% 52% 12% 9%



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I: 30% 53% 12%



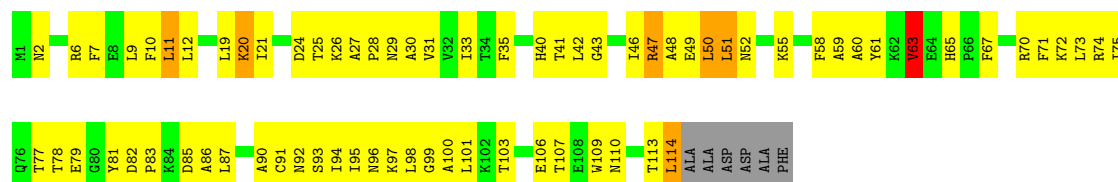
• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

Chain J: 26% 51% 14% 7%

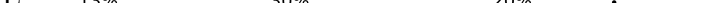


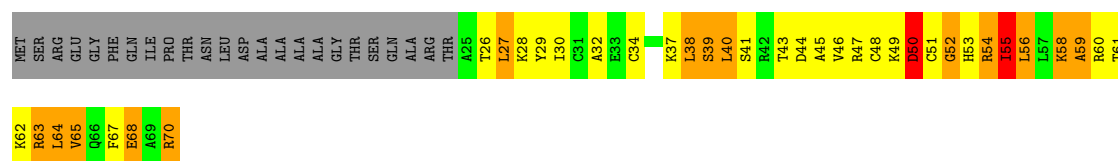
● Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE

Chain K: 34% 55% 5% • 5%



- Molecule 12: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE

Chain L:  13% 30% 20% 1% 34%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.30Å 220.70Å 191.30Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28430	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.61	0/298	1.01	1/456 (0.2%)
2	R	1.28	2/219 (0.9%)	1.73	8/338 (2.4%)
3	A	0.53	0/11048	1.07	74/14936 (0.5%)
4	B	0.56	0/8891	1.07	58/11990 (0.5%)
5	C	0.59	0/2133	1.19	27/2891 (0.9%)
6	E	0.42	0/1788	1.03	12/2406 (0.5%)
7	F	0.48	0/691	0.99	4/933 (0.4%)
8	H	0.46	0/1086	1.11	11/1470 (0.7%)
9	I	0.53	0/989	1.10	7/1331 (0.5%)
10	J	0.67	0/541	1.09	4/727 (0.6%)
11	K	0.53	0/937	0.95	3/1265 (0.2%)
12	L	0.54	0/366	1.10	5/485 (1.0%)
All	All	0.55	2/28987 (0.0%)	1.08	214/39228 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	9	A	P-OP2	6.72	1.62	1.49
2	R	9	A	P-OP1	5.43	1.59	1.49

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	296	GLU	N-CA-C	-12.31	97.62	112.89
5	C	173	ALA	N-CA-C	11.19	123.48	111.28
2	R	9	A	N9-C1'-C2'	-11.15	95.27	112.00
3	A	452	LYS	N-CA-C	-10.91	97.29	112.45
3	A	474	VAL	N-CA-C	-10.76	102.57	112.90
2	R	9	A	C2'-C3'-O3'	-10.53	97.91	113.70
2	R	8	C	C2'-C3'-O3'	-9.99	98.71	113.70
9	I	75	CYS	N-CA-C	-9.96	97.10	109.65
5	C	39	ALA	N-CA-C	9.54	127.37	114.12
5	C	183	TRP	N-CA-C	-9.10	95.85	110.32
3	A	1311	VAL	N-CA-C	8.83	121.20	108.48
4	B	976	ILE	N-CA-C	8.81	118.88	110.42
2	R	9	A	C1'-C2'-O2'	-8.61	95.49	108.40
8	H	85	GLY	N-CA-C	-8.43	105.05	114.40
4	B	736	THR	N-CA-C	-8.40	100.07	110.65
8	H	80	ARG	CA-C-N	-8.23	111.91	120.38
8	H	80	ARG	C-N-CA	-8.23	111.91	120.38
3	A	1392	SER	N-CA-C	8.12	128.11	110.80
3	A	693	VAL	N-CA-C	-7.84	103.60	110.74
3	A	950	GLY	N-CA-C	-7.60	104.56	115.27
4	B	606	LYS	N-CA-C	-7.60	103.27	112.54
6	E	171	LYS	N-CA-C	-7.59	100.73	110.53
3	A	241	VAL	N-CA-C	7.57	115.05	107.55
4	B	392	ARG	N-CA-C	-7.50	104.28	113.50
3	A	398	GLU	N-CA-C	-7.49	95.43	108.69
4	B	514	LEU	N-CA-C	-7.48	98.74	109.96
8	H	81	PRO	N-CA-C	7.47	119.81	110.70
4	B	591	ARG	N-CA-C	-7.43	101.27	110.41
3	A	1215	ARG	N-CA-C	-7.39	102.60	111.69
3	A	564	ALA	N-CA-C	-7.32	103.33	111.82
3	A	481	ASP	N-CA-C	-7.27	97.66	108.79
3	A	417	TYR	N-CA-C	-7.21	98.10	109.50
4	B	851	PHE	N-CA-C	7.20	121.32	111.39
6	E	5	ASN	N-CA-C	-7.12	102.93	111.69
12	L	58	LYS	N-CA-C	7.01	121.56	110.70
4	B	1077	THR	N-CA-C	6.96	121.01	112.23
3	A	1440	ALA	N-CA-C	-6.96	104.67	113.43
5	C	137	LYS	N-CA-C	-6.92	103.47	112.68
3	A	1338	VAL	N-CA-C	6.92	117.89	111.45
9	I	119	THR	N-CA-C	-6.91	104.88	113.38
7	F	112	GLU	N-CA-C	-6.89	104.95	113.15
5	C	233	GLU	N-CA-C	-6.87	100.35	110.52
6	E	202	SER	N-CA-C	6.86	119.86	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	351	TYR	N-CA-C	-6.84	102.90	111.11
4	B	363	HIS	N-CA-C	-6.83	101.52	110.33
3	A	296	LEU	N-CA-C	-6.79	103.81	111.07
6	E	65	THR	N-CA-C	-6.76	102.09	110.41
3	A	71	GLN	CB-CA-C	-6.75	108.77	116.54
1	D	3	DA	C4'-C3'-O3'	-6.70	99.95	110.00
3	A	1403	GLU	N-CA-C	6.69	125.06	110.80
8	H	122	LEU	N-CA-C	6.68	120.77	110.42
4	B	1130	PHE	N-CA-C	-6.64	102.45	111.55
3	A	797	LYS	N-CA-C	6.61	120.04	112.57
5	C	89	GLU	N-CA-C	-6.59	98.48	108.96
3	A	1269	GLU	N-CA-C	6.58	122.40	113.97
4	B	703	ILE	N-CA-C	6.51	117.26	107.75
12	L	65	VAL	N-CA-C	6.51	117.95	108.58
4	B	712	PRO	N-CA-C	-6.50	99.09	112.47
5	C	194	GLU	N-CA-C	-6.46	105.97	114.31
3	A	466	SER	N-CA-C	6.43	124.50	110.80
10	J	2	ILE	N-CA-C	6.40	122.65	109.34
4	B	761	HIS	N-CA-C	-6.38	102.90	112.54
3	A	643	ALA	N-CA-C	-6.38	104.25	111.07
4	B	99	LYS	N-CA-C	-6.37	101.82	110.36
3	A	491	VAL	N-CA-C	6.36	114.82	107.89
3	A	729	ALA	N-CA-C	-6.35	104.36	111.28
3	A	1262	LYS	N-CA-C	-6.34	104.80	112.54
3	A	1010	ALA	N-CA-C	-6.34	104.00	111.03
6	E	97	VAL	N-CA-C	-6.33	104.17	110.62
9	I	111	THR	N-CA-C	6.31	119.92	110.14
12	L	67	PHE	N-CA-C	6.31	119.78	109.24
3	A	776	ALA	N-CA-C	6.29	119.03	110.35
4	B	56	ASP	N-CA-C	6.28	118.68	111.02
5	C	41	ILE	CA-C-N	6.25	126.22	120.03
5	C	41	ILE	C-N-CA	6.25	126.22	120.03
4	B	1085	ILE	N-CA-C	6.23	118.44	108.85
6	E	153	HIS	N-CA-C	-6.22	100.43	110.32
3	A	399	HIS	N-CA-C	6.19	123.48	109.81
4	B	801	LYS	N-CA-C	-6.16	102.00	109.83
4	B	681	TRP	N-CA-C	-6.16	104.83	112.90
4	B	1009	ASP	N-CA-C	-6.15	105.61	113.23
3	A	602	ASP	N-CA-C	-6.14	102.92	111.39
3	A	1021	LEU	N-CA-C	-6.12	103.55	111.02
5	C	166	GLU	N-CA-C	-6.12	104.72	111.82
8	H	50	ALA	N-CA-C	6.11	115.92	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	ILE	N-CA-C	6.10	122.03	109.34
3	A	938	LYS	N-CA-C	-6.08	104.73	111.36
3	A	1148	ILE	N-CA-C	-6.00	105.28	110.74
3	A	496	GLU	N-CA-C	-5.95	104.43	111.03
2	R	9	A	C4'-C3'-O3'	-5.90	104.15	113.00
3	A	1170	ILE	N-CA-C	5.87	116.05	110.53
4	B	706	GLN	N-CA-C	-5.87	102.21	110.31
9	I	31	THR	N-CA-C	-5.86	106.27	113.41
2	R	3	C	O5'-P-OP2	5.85	125.55	108.00
3	A	749	ALA	N-CA-C	-5.83	105.00	111.36
4	B	599	THR	N-CA-C	-5.83	104.55	111.03
8	H	36	CYS	N-CA-C	5.83	119.02	109.76
5	C	108	GLU	N-CA-C	-5.81	106.00	112.57
4	B	541	LEU	N-CA-C	5.79	117.40	111.14
3	A	325	ILE	N-CA-C	-5.78	107.22	111.90
3	A	710	LEU	N-CA-C	-5.78	104.35	111.75
2	R	9	A	C5'-C4'-C3'	5.74	124.62	116.00
9	I	11	ASN	N-CA-C	5.74	119.48	111.90
3	A	266	LEU	N-CA-C	-5.73	106.12	113.23
5	C	237	SER	N-CA-C	-5.72	105.41	112.38
3	A	553	VAL	CA-C-N	5.71	125.39	119.05
3	A	553	VAL	C-N-CA	5.71	125.39	119.05
4	B	172	ILE	N-CA-C	5.71	116.80	108.58
4	B	165	VAL	N-CA-C	5.68	116.48	108.36
5	C	259	LEU	N-CA-C	-5.67	105.01	111.14
4	B	900	ALA	CA-C-N	5.67	126.92	119.84
4	B	900	ALA	C-N-CA	5.67	126.92	119.84
3	A	399	HIS	CA-C-N	-5.66	112.77	119.84
3	A	399	HIS	C-N-CA	-5.66	112.77	119.84
3	A	524	VAL	N-CA-C	5.65	121.09	109.34
3	A	468	PHE	N-CA-C	-5.65	101.92	110.28
3	A	395	GLY	CA-C-N	5.64	126.89	119.84
3	A	395	GLY	C-N-CA	5.64	126.89	119.84
4	B	109	THR	N-CA-C	-5.62	100.08	109.24
4	B	294	ASP	N-CA-C	-5.62	98.84	110.80
4	B	640	VAL	N-CA-C	5.58	119.00	113.53
11	K	63	VAL	N-CA-C	-5.58	98.40	106.88
10	J	45	CYS	N-CA-C	-5.57	105.21	111.28
3	A	44	THR	N-CA-C	-5.56	105.12	112.24
5	C	62	PHE	N-CA-C	-5.56	105.14	111.14
4	B	413	LEU	N-CA-C	-5.54	105.24	111.28
3	A	1162	VAL	N-CA-C	-5.54	105.53	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1391	ARG	N-CA-C	-5.53	104.89	111.69
3	A	330	LYS	N-CA-C	5.52	118.02	110.24
3	A	750	GLY	N-CA-C	-5.51	100.11	113.18
5	C	8	VAL	N-CA-C	5.51	117.06	109.46
4	B	894	ASP	N-CA-C	-5.51	101.85	110.17
8	H	3	ASN	N-CA-C	5.51	115.55	108.34
7	F	124	GLU	N-CA-C	-5.50	106.06	112.89
5	C	41	ILE	N-CA-C	-5.50	103.90	108.63
4	B	936	ASP	N-CA-C	5.50	118.42	110.28
6	E	161	LYS	N-CA-C	-5.50	105.29	111.28
5	C	94	LYS	N-CA-C	-5.49	106.94	113.97
3	A	827	THR	N-CA-C	-5.49	105.21	111.14
6	E	180	ARG	N-CA-C	-5.48	105.31	111.28
3	A	666	ILE	CB-CA-C	-5.47	104.96	111.97
4	B	647	GLY	N-CA-C	5.47	126.15	113.18
5	C	118	LEU	N-CA-C	-5.46	102.92	110.35
5	C	225	ALA	N-CA-C	5.46	117.13	108.67
5	C	37	MET	N-CA-C	-5.45	105.24	111.07
6	E	63	ASN	CA-C-N	5.43	125.36	119.76
6	E	63	ASN	C-N-CA	5.43	125.36	119.76
3	A	1307	GLU	N-CA-C	-5.43	101.43	110.17
11	K	52	ASN	N-CA-C	-5.43	106.82	113.50
6	E	113	GLN	N-CA-C	5.42	119.89	113.12
12	L	68	GLU	N-CA-C	-5.42	101.83	109.96
3	A	143	LYS	N-CA-C	-5.41	107.05	113.97
3	A	288	ALA	N-CA-C	-5.38	105.39	113.89
4	B	693	ILE	N-CA-C	5.37	115.69	108.17
4	B	112	LEU	N-CA-C	5.35	118.33	109.46
4	B	1023	VAL	N-CA-C	5.34	116.07	110.62
3	A	847	ASP	N-CA-C	5.34	119.50	113.15
3	A	1389	PHE	N-CA-C	5.33	119.63	113.18
4	B	1114	LEU	N-CA-C	5.33	117.17	111.36
5	C	56	THR	N-CA-C	5.33	116.79	110.19
8	H	103	LYS	N-CA-C	5.32	117.58	108.90
3	A	562	THR	CA-C-N	5.31	125.31	119.89
3	A	562	THR	C-N-CA	5.31	125.31	119.89
9	I	18	GLU	N-CA-C	5.31	117.89	109.24
4	B	648	HIS	N-CA-C	5.30	122.10	110.80
4	B	253	THR	N-CA-C	5.28	118.16	109.76
8	H	16	ASP	N-CA-C	5.28	117.97	109.15
4	B	1123	SER	N-CA-C	-5.26	105.97	112.38
5	C	80	LEU	N-CA-C	-5.25	100.48	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1216	ILE	CB-CA-C	-5.24	104.98	112.22
4	B	739	THR	N-CA-C	-5.24	107.55	114.31
4	B	1203	LEU	N-CA-C	-5.24	105.26	110.97
4	B	756	ILE	CB-CA-C	-5.22	106.09	110.94
8	H	107	VAL	N-CA-C	-5.22	106.13	112.76
3	A	693	VAL	CB-CA-C	-5.22	105.05	111.94
10	J	5	VAL	N-CA-C	-5.21	101.97	108.84
5	C	258	ILE	N-CA-C	-5.21	105.33	111.00
3	A	861	GLY	N-CA-C	-5.19	107.37	114.64
3	A	1188	GLN	N-CA-C	5.19	117.87	110.24
4	B	69	LEU	N-CA-C	5.19	118.05	109.85
4	B	278	GLN	N-CA-C	5.19	116.08	107.73
3	A	628	GLY	N-CA-C	5.18	125.46	113.18
5	C	193	TYR	N-CA-C	5.18	117.29	109.41
5	C	240	VAL	N-CA-C	5.18	115.80	110.36
6	E	205	SER	N-CA-C	-5.17	99.68	108.26
3	A	580	VAL	N-CA-C	-5.16	105.51	110.72
4	B	107	GLY	N-CA-C	5.16	118.51	110.88
4	B	317	CYS	N-CA-C	-5.16	105.35	111.69
2	R	3	C	O4'-C4'-C3'	-5.16	98.84	104.00
3	A	1113	THR	CA-C-N	5.16	126.29	119.84
3	A	1113	THR	C-N-CA	5.16	126.29	119.84
4	B	743	ILE	N-CA-C	-5.14	105.48	110.42
9	I	10	CYS	N-CA-C	5.13	119.17	113.01
4	B	110	HIS	N-CA-C	5.13	118.10	109.95
4	B	66	ASP	N-CA-C	-5.12	106.78	112.57
3	A	696	GLU	N-CA-C	-5.12	105.39	110.97
4	B	886	LYS	N-CA-C	5.10	117.43	109.52
12	L	40	LEU	N-CA-C	5.10	116.56	108.96
4	B	604	ARG	N-CA-C	-5.09	106.92	113.23
3	A	12	ARG	N-CA-C	5.08	116.54	108.96
4	B	659	ALA	N-CA-C	-5.07	105.88	111.71
3	A	415	LEU	N-CA-C	5.07	121.60	110.80
5	C	129	ILE	N-CA-C	5.06	114.53	108.06
11	K	20	LYS	N-CA-C	-5.06	99.74	108.69
10	J	10	CYS	N-CA-C	5.05	119.71	113.50
3	A	1078	GLN	N-CA-C	-5.05	106.04	113.61
4	B	293	PRO	N-CA-C	5.04	118.80	111.03
3	A	337	ARG	N-CA-C	5.04	116.58	111.14
3	A	886	ILE	N-CA-C	5.03	116.12	111.45
4	B	854	LEU	N-CA-C	-5.01	102.65	110.42
5	C	38	ILE	N-CA-C	5.01	115.73	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	445	ASN	N-CA-C	5.00	116.98	109.23
7	F	130	ILE	CA-C-N	5.00	126.09	119.84
7	F	130	ILE	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2	DA	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	267	0	148	31	0
2	R	196	0	100	25	0
3	A	10857	0	10959	1110	0
4	B	8721	0	8746	938	0
5	C	2095	0	2052	175	0
6	E	1752	0	1776	143	0
7	F	679	0	701	68	0
8	H	1068	0	1040	134	0
9	I	971	0	933	108	0
10	J	532	0	544	78	0
11	K	919	0	929	93	0
12	L	364	0	388	57	0
13	R	1	0	0	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	1	0
14	J	1	0	0	1	0
14	L	1	0	0	0	0
All	All	28430	0	28316	2692	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 48.

All (2692) 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)
3:A:567:LYS:HB2	3:A:568:PRO:HD2	1.18	1.17
12:L:60:ARG:HG3	12:L:61:THR:H	1.05	1.15
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.13
4:B:345:LYS:HA	4:B:348:ARG:HE	1.11	1.13
3:A:353:ILE:HD13	3:A:487:MET:HE3	1.23	1.12
3:A:1364:ASN:ND2	3:A:1366:ARG:HG2	1.65	1.11
6:E:124:VAL:HG13	6:E:132:ILE:HB	1.33	1.09
4:B:1051:THR:HG22	4:B:1053:GLU:H	1.00	1.09
1:D:1:DA:H1'	3:A:1386:ARG:HH12	1.02	1.09
3:A:855:THR:HG21	3:A:857:ARG:HE	1.12	1.09
3:A:93:VAL:HG13	3:A:301:ALA:HB1	1.33	1.08
3:A:704:ALA:HB2	3:A:710:LEU:HG	1.34	1.07
3:A:1329:THR:HG22	3:A:1331:SER:H	1.15	1.07
4:B:512:ARG:HH21	4:B:535:LEU:HD11	1.17	1.07
3:A:666:ILE:HD11	4:B:1030:LEU:HD13	1.27	1.05
4:B:287:ARG:HG2	4:B:292:ILE:HA	1.38	1.04
7:F:81:THR:HG21	7:F:136:ARG:HD3	1.38	1.04
4:B:570:VAL:HB	4:B:573:GLN:HB3	1.36	1.04
3:A:1161:THR:HG22	3:A:1163:ILE:H	1.18	1.04
4:B:708:GLU:HG3	4:B:709:ASP:H	1.17	1.04
4:B:1159:ARG:HE	4:B:1193:GLN:NE2	1.56	1.03
3:A:902:LEU:HG	3:A:926:GLN:HG3	1.39	1.02
4:B:977:GLY:HA3	4:B:1099:VAL:HG21	1.41	1.02
5:C:80:LEU:HD22	5:C:129:ILE:HD11	1.41	1.02
4:B:120:ARG:HG2	4:B:955:THR:HG21	1.40	1.01
3:A:913:LEU:HD12	3:A:914:GLU:H	1.25	1.01
3:A:567:LYS:CB	3:A:568:PRO:HD2	1.91	1.01
3:A:567:LYS:HB3	8:H:96:VAL:H	1.26	1.01
4:B:1002:THR:HG22	4:B:1006:ILE:H	1.22	1.01
4:B:1159:ARG:NE	4:B:1193:GLN:HE21	1.57	1.01
3:A:1111:MET:HE2	3:A:1114:PRO:HA	1.39	1.00
5:C:57:VAL:HG11	10:J:60:PHE:HB3	1.44	0.99
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.39	0.98
3:A:115:LEU:HB2	3:A:122:MET:HE2	1.45	0.98
4:B:1100:ASP:HA	4:B:1103:ILE:HD11	1.46	0.98
11:K:113:THR:O	11:K:114:LEU:HB2	1.60	0.97
3:A:244:PRO:HG2	3:A:245:PRO:HD3	1.46	0.97
1:D:1:DA:H1'	3:A:1386:ARG:NH1	1.80	0.96
4:B:639:ILE:HD11	4:B:691:GLU:HG3	1.47	0.96
4:B:842:ASN:ND2	4:B:845:SER:H	1.62	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:135:PHE:HB3	6:E:140:LEU:HD11	1.45	0.96
4:B:174:LEU:O	4:B:175:ARG:HB2	1.64	0.96
5:C:56:THR:HG22	5:C:57:VAL:H	1.28	0.95
9:I:75:CYS:HG	14:I:204:ZN:ZN	0.68	0.95
3:A:1116:LEU:HD12	3:A:1329:THR:OG1	1.67	0.95
5:C:167:HIS:CD2	5:C:169:LYS:H	1.83	0.95
4:B:955:THR:HG22	4:B:956:THR:H	1.31	0.95
4:B:1051:THR:HG22	4:B:1053:GLU:N	1.81	0.95
4:B:200:GLY:HA2	4:B:202:TYR:CE2	2.02	0.94
3:A:783:THR:HG22	3:A:784:LEU:HG	1.49	0.94
4:B:392:ARG:HH21	9:I:52:ILE:HD11	1.30	0.94
3:A:1281:ARG:HD2	3:A:1309:ASP:OD2	1.68	0.93
4:B:1159:ARG:HD3	4:B:1193:GLN:HG3	1.48	0.93
4:B:842:ASN:HD22	4:B:845:SER:H	1.17	0.93
4:B:737:THR:HG21	9:I:66:PRO:O	1.68	0.93
3:A:338:GLY:HA2	4:B:1129:ARG:HH22	1.33	0.93
4:B:824:ILE:HG12	10:J:48:ARG:HH12	1.32	0.92
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.47	0.92
10:J:1:MET:H1	10:J:56:LEU:HB2	1.35	0.92
3:A:1399:ARG:HB3	3:A:1408:ILE:HD13	1.50	0.92
12:L:60:ARG:HG3	12:L:61:THR:N	1.85	0.91
3:A:1435:PRO:HA	3:A:1439:GLY:O	1.69	0.91
4:B:1002:THR:HG22	4:B:1006:ILE:N	1.84	0.91
5:C:73:GLN:HE21	5:C:75:MET:H	1.14	0.91
7:F:93:ILE:HD11	7:F:134:ILE:HD11	1.53	0.90
9:I:111:THR:HG22	9:I:113:ASP:N	1.86	0.90
3:A:351:THR:HG23	4:B:1103:ILE:HA	1.53	0.90
5:C:22:LEU:HD22	5:C:25:VAL:HG21	1.53	0.90
6:E:5:ASN:HD21	6:E:52:ARG:HG2	1.34	0.90
3:A:15:LYS:HB3	4:B:1220:ARG:HG2	1.51	0.90
3:A:1194:ARG:NH2	3:A:1237:ILE:HD13	1.87	0.90
3:A:381:THR:HG22	3:A:383:TYR:H	1.35	0.90
3:A:590:ARG:HG3	3:A:590:ARG:NH1	1.86	0.89
4:B:956:THR:HA	4:B:961:LEU:O	1.71	0.89
4:B:955:THR:HG22	4:B:956:THR:N	1.85	0.89
3:A:868:TYR:HD2	3:A:1058:VAL:HG21	1.38	0.89
3:A:1105:LEU:HD22	3:A:1384:VAL:HG21	1.53	0.89
3:A:1410:PHE:CD2	4:B:1212:ILE:HD11	2.08	0.89
4:B:519:TRP:HZ2	4:B:705:MET:HE1	1.37	0.89
3:A:61:ILE:HG22	3:A:62:ASP:H	1.37	0.88
3:A:666:ILE:CD1	4:B:1030:LEU:HD13	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:57:VAL:HG11	10:J:60:PHE:CB	2.03	0.88
3:A:567:LYS:NZ	8:H:46:LEU:HB2	1.87	0.88
3:A:567:LYS:HB2	3:A:568:PRO:CD	2.01	0.88
4:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.88
4:B:955:THR:CG2	4:B:956:THR:H	1.87	0.88
3:A:549:MET:SD	3:A:577:ILE:HD12	2.12	0.88
5:C:167:HIS:HD2	5:C:169:LYS:H	0.90	0.88
5:C:44:LEU:HB2	5:C:77:ILE:HD11	1.55	0.88
3:A:962:ARG:HA	3:A:965:GLN:HE21	1.37	0.88
3:A:1192:LEU:HD11	3:A:1239:ARG:HB3	1.56	0.88
4:B:512:ARG:HH21	4:B:535:LEU:CD1	1.88	0.87
3:A:667:GLY:HA2	3:A:670:ILE:HD12	1.56	0.87
4:B:345:LYS:CA	4:B:348:ARG:HE	1.87	0.87
3:A:590:ARG:HG3	3:A:590:ARG:HH11	1.37	0.87
4:B:1077:THR:HG22	4:B:1079:LYS:H	1.35	0.87
4:B:1065:GLN:HE21	4:B:1067:ARG:N	1.72	0.87
4:B:1159:ARG:HE	4:B:1193:GLN:HE21	0.93	0.87
10:J:46:CYS:HG	14:J:101:ZN:ZN	0.84	0.86
3:A:337:ARG:NH1	3:A:839:ARG:HH12	1.72	0.86
4:B:228:LYS:HD3	4:B:234:ILE:HD13	1.57	0.86
3:A:804:TYR:HE1	4:B:1021:MET:HE3	1.40	0.86
3:A:886:ILE:HD11	3:A:943:LEU:HB3	1.56	0.86
3:A:269:ILE:HD11	3:A:300:VAL:HA	1.57	0.86
3:A:443:LEU:HD22	3:A:455:MET:HE2	1.58	0.86
4:B:130:VAL:HG21	4:B:167:ILE:HD12	1.56	0.86
4:B:977:GLY:HA3	4:B:1099:VAL:CG2	2.04	0.86
3:A:1039:LYS:O	3:A:1043:ASP:HB2	1.76	0.86
4:B:801:LYS:O	10:J:52:THR:HG23	1.76	0.86
1:D:1:DA:C1'	3:A:1386:ARG:HH12	1.87	0.85
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.11	0.85
4:B:519:TRP:CZ2	4:B:705:MET:HE1	2.11	0.85
4:B:744:HIS:HD2	4:B:746:SER:H	1.23	0.85
4:B:912:ILE:O	4:B:938:SER:HB2	1.76	0.85
3:A:417:TYR:O	3:A:418:SER:HB2	1.75	0.85
3:A:1242:VAL:HG12	3:A:1243:VAL:H	1.40	0.85
8:H:125:LEU:HG	8:H:130:ARG:NH1	1.92	0.85
3:A:1348:LEU:HD23	3:A:1372:VAL:HG13	1.59	0.84
3:A:535:THR:HG21	3:A:617:VAL:H	1.43	0.84
6:E:177:ARG:HD3	6:E:215:MET:SD	2.18	0.84
4:B:1106:ARG:NH1	4:B:1118:PRO:HB3	1.91	0.84
3:A:709:THR:HG21	9:I:93:LYS:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:147:SER:OG	7:F:150:GLU:HG3	1.78	0.84
2:R:2:A:C2'	2:R:3:C:H5'	2.07	0.83
3:A:683:ILE:HD11	3:A:764:CYS:HB2	1.60	0.83
4:B:345:LYS:HA	4:B:348:ARG:NE	1.91	0.83
4:B:1106:ARG:HH21	4:B:1109:GLY:H	1.23	0.83
3:A:353:ILE:CD1	3:A:487:MET:HE3	2.07	0.83
3:A:1118:VAL:CG2	3:A:1306:LEU:HB2	2.08	0.83
3:A:1390:ASN:ND2	3:A:1399:ARG:HA	1.93	0.83
11:K:12:LEU:H	11:K:12:LEU:HD12	1.42	0.83
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.61	0.83
4:B:108:VAL:HG12	4:B:109:THR:H	1.42	0.83
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.42	0.83
4:B:999:MET:HG3	4:B:1000:PRO:HD2	1.61	0.83
3:A:605:MET:HE3	3:A:614:PHE:O	1.78	0.83
5:C:11:ARG:NH2	5:C:229:TYR:HD2	1.77	0.83
6:E:2:ASP:O	6:E:3:GLN:HG2	1.78	0.82
3:A:1017:LEU:HB2	6:E:206:GLY:H	1.44	0.82
4:B:1002:THR:CG2	4:B:1006:ILE:H	1.91	0.82
3:A:1111:MET:HE1	3:A:1330:ASN:OD1	1.79	0.82
3:A:565:ILE:HG23	3:A:567:LYS:HG2	1.62	0.82
3:A:511:ILE:HG12	3:A:521:MET:HE3	1.62	0.82
5:C:37:MET:HG2	5:C:243:VAL:HG12	1.62	0.81
3:A:885:THR:HG23	3:A:893:PHE:HE1	1.43	0.81
4:B:1106:ARG:HE	4:B:1109:GLY:N	1.79	0.81
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.61	0.81
8:H:93:TYR:HB3	8:H:144:ILE:O	1.80	0.81
3:A:406:ILE:HB	3:A:431:LYS:HB2	1.61	0.81
3:A:563:PRO:HG3	3:A:572:TRP:CZ2	2.15	0.81
4:B:269:ILE:HD11	4:B:386:LEU:HD21	1.62	0.81
9:I:50:THR:CG2	9:I:52:ILE:HG23	2.11	0.81
3:A:742:ASN:HA	3:A:745:GLN:HB2	1.63	0.81
4:B:244:LEU:O	4:B:249:ARG:HG2	1.81	0.81
3:A:337:ARG:NH1	3:A:839:ARG:NH1	2.29	0.81
4:B:637:LEU:HD12	4:B:693:ILE:HD12	1.60	0.81
8:H:5:LEU:HD11	8:H:135:LEU:HG	1.63	0.80
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.11	0.80
4:B:121:ASN:N	4:B:121:ASN:HD22	1.79	0.80
4:B:800:GLN:HB3	10:J:52:THR:CG2	2.11	0.80
4:B:899:ILE:HD11	4:B:911:ILE:HA	1.63	0.80
3:A:93:VAL:CG1	3:A:301:ALA:HB1	2.11	0.80
3:A:208:LEU:HD22	3:A:212:LYS:HE3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1106:ARG:HH21	4:B:1109:GLY:N	1.78	0.80
3:A:472:LEU:O	3:A:475:THR:HB	1.81	0.80
4:B:834:ASN:HB3	4:B:840:ILE:HG13	1.63	0.80
4:B:200:GLY:HA2	4:B:202:TYR:HE2	1.43	0.80
4:B:293:PRO:HG2	4:B:296:GLU:CB	2.12	0.80
3:A:679:ILE:HG23	3:A:729:ALA:HB1	1.63	0.80
4:B:1100:ASP:HA	4:B:1103:ILE:CD1	2.12	0.80
5:C:148:ARG:NH1	10:J:64:ASN:HA	1.96	0.80
9:I:75:CYS:SG	9:I:78:CYS:SG	2.80	0.80
3:A:868:TYR:CE1	3:A:1064:VAL:HG11	2.17	0.80
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.63	0.80
3:A:313:GLN:HB2	3:A:322:VAL:HG23	1.64	0.80
4:B:1065:GLN:HE21	4:B:1067:ARG:H	1.28	0.80
4:B:118:ARG:HH22	4:B:194:GLU:CD	1.90	0.79
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.12	0.79
3:A:32:VAL:HG21	3:A:68:GLN:NE2	1.97	0.79
3:A:523:ILE:HD12	3:A:622:VAL:CG2	2.12	0.79
3:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.46	0.79
4:B:1106:ARG:NH2	4:B:1109:GLY:H	1.79	0.79
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.62	0.79
4:B:842:ASN:ND2	4:B:845:SER:N	2.31	0.79
5:C:56:THR:HG22	5:C:57:VAL:N	1.97	0.79
3:A:666:ILE:HD13	4:B:1030:LEU:HD22	1.65	0.79
4:B:487:THR:HG22	4:B:489:SER:H	1.48	0.79
8:H:89:LEU:C	8:H:91:ASP:H	1.90	0.79
4:B:542:MET:HE3	4:B:747:MET:HG3	1.63	0.78
3:A:913:LEU:HD12	3:A:914:GLU:N	1.99	0.78
4:B:102:VAL:CG2	4:B:112:LEU:HB2	2.13	0.78
3:A:40:THR:HG22	3:A:41:MET:HG3	1.64	0.78
3:A:783:THR:HG21	3:A:815:PHE:CZ	2.19	0.78
3:A:1438:THR:HB	4:B:1144:ALA:HB3	1.66	0.78
4:B:796:LEU:HB3	4:B:799:PRO:HG3	1.63	0.78
1:D:1:DA:H2'	1:D:2:DA:C8	2.18	0.78
3:A:768:GLN:CG	3:A:816:HIS:HA	2.13	0.78
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.66	0.78
3:A:298:PHE:O	3:A:302:THR:HB	1.83	0.78
3:A:399:HIS:O	3:A:401:GLY:N	2.17	0.78
3:A:901:LEU:H	3:A:926:GLN:NE2	1.82	0.78
3:A:1118:VAL:HG22	3:A:1306:LEU:HB2	1.64	0.78
3:A:23:SER:HB3	3:A:233:TRP:CZ2	2.19	0.78
3:A:1281:ARG:O	3:A:1282:VAL:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1299:VAL:HG12	3:A:1300:LYS:H	1.47	0.78
4:B:392:ARG:NH2	9:I:52:ILE:HD11	1.98	0.78
4:B:1100:ASP:OD1	4:B:1103:ILE:HD11	1.84	0.78
3:A:58:LEU:HD22	3:A:80:HIS:O	1.83	0.77
3:A:313:GLN:HB2	3:A:322:VAL:CG2	2.14	0.77
3:A:855:THR:HG21	3:A:857:ARG:NE	1.95	0.77
4:B:855:PHE:HZ	4:B:857:ARG:NH1	1.81	0.77
5:C:165:LYS:O	11:K:6:ARG:NH1	2.17	0.77
3:A:541:ILE:HG12	3:A:549:MET:HE1	1.66	0.77
2:R:3:C:H2'	2:R:4:C:C6	2.19	0.77
3:A:1094:VAL:HG13	3:A:1113:THR:HG21	1.66	0.77
4:B:542:MET:HG3	4:B:747:MET:HE3	1.66	0.77
3:A:849:MET:HE3	3:A:1061:GLY:HA2	1.67	0.77
3:A:1076:ALA:HA	3:A:1079:MET:HE2	1.65	0.77
3:A:1345:ARG:HD2	3:A:1373:ASP:OD1	1.84	0.77
4:B:496:ARG:NH1	4:B:539:LEU:HB2	1.99	0.77
3:A:70:CYS:O	3:A:72:GLU:HG2	1.84	0.77
3:A:24:PRO:HB3	3:A:237:THR:HB	1.67	0.77
4:B:211:VAL:HG21	4:B:483:LEU:HD13	1.68	0.77
12:L:38:LEU:O	12:L:39:SER:HB3	1.85	0.77
4:B:102:VAL:HG23	4:B:112:LEU:HB2	1.65	0.76
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.49	0.76
10:J:10:CYS:SG	10:J:46:CYS:SG	2.83	0.76
4:B:232:SER:OG	4:B:234:ILE:HD12	1.84	0.76
4:B:707:PRO:HG2	4:B:708:GLU:H	1.49	0.76
5:C:166:GLU:HG3	11:K:10:PHE:HZ	1.51	0.76
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.50	0.76
3:A:336:ILE:HD12	3:A:1405:THR:HG21	1.68	0.76
3:A:341:MET:HE1	3:A:1401:SER:HB2	1.68	0.76
3:A:896:ARG:HD3	3:A:897:TYR:CE1	2.21	0.76
4:B:882:THR:HG22	4:B:884:ARG:H	1.50	0.76
4:B:996:ARG:NH2	5:C:174:ALA:O	2.19	0.76
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.68	0.76
5:C:124:LEU:O	5:C:127:ARG:HG2	1.85	0.76
10:J:12:LYS:O	10:J:14:VAL:HG23	1.85	0.76
1:D:3:DA:H5'	3:A:836:TYR:CE1	2.21	0.76
3:A:31:SER:CB	3:A:83:HIS:HB2	2.15	0.76
3:A:265:LYS:NZ	3:A:323:LYS:H	1.84	0.76
3:A:1323:ASP:OD1	3:A:1325:THR:HB	1.86	0.76
4:B:1106:ARG:HE	4:B:1109:GLY:H	1.29	0.76
4:B:1166:CYS:O	4:B:1168:LEU:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:223:GLY:O	3:A:1415:SER:HA	1.86	0.76
4:B:583:ASN:HD21	4:B:628:THR:HB	1.49	0.76
4:B:1096:ARG:O	4:B:1097:HIS:HB2	1.85	0.76
3:A:95:PHE:O	3:A:99:ILE:HG13	1.85	0.75
3:A:469:ARG:HH21	4:B:976:ILE:HD13	1.51	0.75
3:A:41:MET:HA	3:A:49:LYS:HA	1.68	0.75
4:B:423:LYS:HA	4:B:426:LYS:HE2	1.68	0.75
4:B:899:ILE:CD1	4:B:911:ILE:HA	2.16	0.75
5:C:57:VAL:CG1	10:J:60:PHE:HB3	2.15	0.75
4:B:62:ILE:HG23	4:B:418:LYS:HG2	1.69	0.75
4:B:842:ASN:HD22	4:B:845:SER:N	1.83	0.75
4:B:313:MET:HE3	4:B:386:LEU:HD22	1.68	0.75
6:E:69:ILE:HG23	6:E:73:PRO:HA	1.67	0.75
3:A:326:ARG:HG2	3:A:1406:VAL:HG21	1.67	0.75
4:B:770:GLN:HG2	4:B:983:ARG:O	1.86	0.75
2:R:8:C:O2'	2:R:9:A:H5'	1.87	0.75
3:A:575:LYS:HB3	3:A:612:ILE:CG2	2.17	0.74
3:A:1146:VAL:HG11	3:A:1202:MET:SD	2.27	0.74
4:B:711:GLU:N	4:B:712:PRO:HD3	2.02	0.74
2:R:1:G:H2'	2:R:2:A:C8	2.22	0.74
3:A:535:THR:CG2	3:A:616:VAL:HA	2.18	0.74
11:K:65:HIS:HD2	11:K:67:PHE:H	1.35	0.74
3:A:804:TYR:CE1	4:B:1021:MET:HE3	2.21	0.74
4:B:651:LEU:HD11	4:B:707:PRO:HB3	1.69	0.74
7:F:111:LEU:HD12	7:F:111:LEU:N	2.02	0.74
3:A:321:PRO:O	3:A:322:VAL:HB	1.87	0.74
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.16	0.74
3:A:268:ASP:HB3	3:A:299:HIS:CE1	2.23	0.74
6:E:61:GLN:HE21	6:E:105:PHE:HE2	1.33	0.74
3:A:1436:ILE:HG22	3:A:1437:GLY:H	1.52	0.74
3:A:1436:ILE:HG22	3:A:1437:GLY:N	2.03	0.74
3:A:1299:VAL:HG12	3:A:1300:LYS:N	2.02	0.74
8:H:123:MET:HE1	8:H:142:LEU:HD13	1.69	0.74
3:A:458:HIS:CE1	3:A:507:VAL:HG21	2.22	0.74
4:B:570:VAL:HB	4:B:573:GLN:CB	2.17	0.74
4:B:1106:ARG:NE	4:B:1109:GLY:H	1.85	0.74
3:A:857:ARG:HD3	3:A:861:GLY:O	1.88	0.74
8:H:5:LEU:HB3	8:H:133:ASN:O	1.88	0.74
3:A:853:ASP:OD1	3:A:855:THR:HB	1.88	0.74
3:A:500:GLU:OE2	4:B:1145:SER:HB2	1.88	0.73
3:A:925:LEU:O	3:A:929:LEU:HD23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:118:ARG:HG3	4:B:204:ILE:HD13	1.68	0.73
4:B:172:ILE:HD13	4:B:178:ASN:HB3	1.70	0.73
3:A:567:LYS:HB3	8:H:96:VAL:N	2.02	0.73
3:A:693:VAL:HG21	3:A:721:PHE:HE1	1.51	0.73
3:A:858:ASN:C	3:A:858:ASN:HD22	1.96	0.73
6:E:61:GLN:NE2	6:E:105:PHE:HE2	1.86	0.73
3:A:399:HIS:HB3	3:A:400:PRO:HD3	1.69	0.73
3:A:691:LEU:HD11	3:A:695:LYS:HE3	1.71	0.73
3:A:828:ALA:HB2	4:B:530:GLY:HA2	1.70	0.73
3:A:1436:ILE:CG2	4:B:1142:GLY:HA2	2.17	0.73
4:B:363:HIS:O	4:B:364:ILE:HB	1.88	0.73
4:B:999:MET:HE2	4:B:1011:ILE:HD11	1.71	0.73
3:A:443:LEU:HD21	3:A:455:MET:HB3	1.70	0.73
3:A:1441:PHE:CZ	7:F:89:GLU:HA	2.23	0.73
3:A:445:ASN:CB	3:A:455:MET:HG2	2.19	0.73
6:E:124:VAL:HA	6:E:132:ILE:HD12	1.70	0.73
3:A:75:ASN:O	3:A:76:GLU:HB3	1.88	0.73
11:K:65:HIS:CD2	11:K:67:PHE:H	2.06	0.73
3:A:154:SER:HB3	3:A:162:VAL:CG2	2.17	0.73
3:A:445:ASN:HB2	3:A:455:MET:HG2	1.70	0.73
4:B:58:THR:O	4:B:62:ILE:HG13	1.89	0.73
4:B:745:PRO:O	4:B:748:ILE:HG12	1.88	0.73
4:B:879:ARG:HB3	4:B:883:LEU:HD23	1.70	0.73
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.88	0.73
4:B:313:MET:CE	4:B:386:LEU:HD22	2.19	0.72
4:B:1007:VAL:HG22	4:B:1008:PRO:HD2	1.71	0.72
3:A:598:LEU:HD22	8:H:25:ARG:NH1	2.05	0.72
3:A:710:LEU:H	3:A:710:LEU:HD12	1.52	0.72
4:B:521:LEU:HD22	4:B:633:VAL:HG12	1.69	0.72
9:I:74:GLU:HB3	9:I:79:HIS:HA	1.70	0.72
3:A:353:ILE:HD13	3:A:487:MET:CE	2.14	0.72
3:A:417:TYR:O	3:A:418:SER:CB	2.36	0.72
4:B:234:ILE:HD12	4:B:234:ILE:H	1.54	0.72
4:B:980:PHE:CE2	4:B:1094:ARG:HG3	2.23	0.72
3:A:48:ALA:O	3:A:49:LYS:HG3	1.89	0.72
3:A:868:TYR:CD2	3:A:1058:VAL:HG21	2.23	0.72
5:C:167:HIS:HD2	5:C:169:LYS:N	1.76	0.72
3:A:337:ARG:NE	3:A:839:ARG:HH22	1.88	0.72
3:A:567:LYS:HD3	8:H:95:TYR:CD1	2.25	0.72
3:A:1258:HIS:ND1	3:A:1262:LYS:HE3	2.04	0.72
4:B:542:MET:HE1	4:B:743:ILE:HG21	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:570:VAL:HG21	4:B:573:GLN:NE2	2.04	0.72
3:A:351:THR:HG21	4:B:1103:ILE:HG23	1.71	0.72
3:A:534:LEU:O	3:A:574:GLY:HA3	1.88	0.72
4:B:193:LYS:HD3	4:B:787:VAL:HG11	1.70	0.72
8:H:35:GLN:HB3	8:H:111:LEU:HD21	1.70	0.72
3:A:32:VAL:HB	3:A:57:ARG:HD2	1.71	0.72
3:A:1397:LEU:O	3:A:1400:CYS:HB2	1.89	0.72
3:A:901:LEU:HG	3:A:926:GLN:HE21	1.54	0.72
4:B:1066:SER:O	4:B:1067:ARG:HD3	1.90	0.72
2:R:1:G:H2'	2:R:2:A:H8	1.54	0.72
4:B:708:GLU:O	4:B:710:LEU:N	2.22	0.71
4:B:737:THR:HG23	9:I:66:PRO:CB	2.20	0.71
1:D:12:DC:N3	2:R:1:G:N2	2.32	0.71
3:A:899:VAL:HB	3:A:929:LEU:HD12	1.71	0.71
3:A:575:LYS:HB3	3:A:612:ILE:HG23	1.71	0.71
3:A:1152:ILE:HG23	3:A:1260:LEU:HD23	1.71	0.71
3:A:1399:ARG:HB2	3:A:1408:ILE:HG21	1.70	0.71
3:A:1332:PHE:H	3:A:1332:PHE:HD2	1.38	0.71
4:B:637:LEU:CD1	4:B:693:ILE:HD12	2.20	0.71
4:B:1072:MET:HE3	4:B:1085:ILE:HD12	1.70	0.71
5:C:98:VAL:C	5:C:99:LEU:HD23	2.16	0.71
6:E:168:TYR:HB3	6:E:170:LEU:HD21	1.72	0.71
4:B:46:GLN:HG3	4:B:47:GLN:N	2.03	0.71
11:K:55:LYS:HD3	11:K:78:THR:CB	2.20	0.71
3:A:340:LEU:HD21	4:B:1200:ALA:HB2	1.72	0.71
3:A:900:ASP:OD2	3:A:903:ASN:HB2	1.90	0.71
3:A:1209:MET:SD	3:A:1236:LEU:HB3	2.30	0.71
3:A:675:THR:CB	3:A:736:ASN:HD21	2.04	0.71
4:B:555:ILE:HD13	4:B:587:HIS:CE1	2.26	0.71
7:F:81:THR:HG21	7:F:136:ARG:CD	2.20	0.71
11:K:55:LYS:HD3	11:K:78:THR:HB	1.72	0.71
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.71	0.71
4:B:708:GLU:HG3	4:B:709:ASP:N	1.98	0.70
3:A:451:HIS:NE2	3:A:1074:GLU:HG3	2.06	0.70
3:A:1015:VAL:HG12	3:A:1019:CYS:SG	2.31	0.70
4:B:309:GLN:HG3	9:I:52:ILE:HD13	1.72	0.70
12:L:47:ARG:HG2	12:L:52:GLY:HA2	1.72	0.70
3:A:672:ASP:HB2	3:A:736:ASN:OD1	1.90	0.70
3:A:675:THR:HG21	3:A:736:ASN:ND2	2.06	0.70
4:B:108:VAL:HG12	4:B:109:THR:N	2.06	0.70
3:A:974:ASP:HB2	8:H:136:LYS:HZ1	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:792:MET:HA	4:B:856:PHE:O	1.91	0.70
4:B:1056:SER:HB3	4:B:1066:SER:HB2	1.74	0.70
3:A:503:GLN:HE21	7:F:90:ARG:NH2	1.88	0.70
3:A:741:ASN:HD22	3:A:741:ASN:C	1.99	0.70
3:A:335:ARG:HA	3:A:339:ASN:HD22	1.57	0.70
3:A:343:LYS:HE3	4:B:1151:LEU:O	1.92	0.70
3:A:383:TYR:HB3	7:F:115:THR:HG22	1.73	0.70
3:A:567:LYS:HE3	8:H:46:LEU:HD12	1.71	0.70
5:C:18:VAL:HG23	5:C:240:VAL:HG11	1.72	0.70
3:A:463:ILE:HB	3:A:464:PRO:HD2	1.74	0.70
3:A:855:THR:HG23	3:A:857:ARG:HG3	1.72	0.70
4:B:638:PHE:CE1	4:B:743:ILE:HA	2.26	0.70
4:B:955:THR:HG23	12:L:54:ARG:O	1.91	0.70
6:E:56:LYS:HG3	6:E:84:ASP:HB2	1.73	0.70
4:B:636:PRO:O	4:B:637:LEU:HG	1.90	0.70
3:A:225:ASN:O	3:A:227:VAL:N	2.21	0.70
3:A:367:PRO:HB3	3:A:466:SER:HA	1.73	0.70
3:A:1095:THR:HG22	3:A:1100:ARG:HB2	1.74	0.70
4:B:293:PRO:HG2	4:B:296:GLU:HB3	1.74	0.70
3:A:584:ASN:O	3:A:637:LYS:HE3	1.92	0.69
4:B:130:VAL:HG12	4:B:131:ASP:N	2.07	0.69
3:A:1394:THR:HG23	3:A:1398:MET:HE3	1.73	0.69
4:B:463:THR:CG2	4:B:465:ASN:HD22	2.05	0.69
6:E:83:CYS:SG	6:E:88:VAL:HG22	2.32	0.69
8:H:36:CYS:SG	8:H:130:ARG:NH2	2.65	0.69
1:D:4:DT:H2'	1:D:5:DG:C8	2.27	0.69
3:A:1208:THR:HB	3:A:1211:GLN:HG3	1.74	0.69
4:B:314:LEU:O	4:B:317:CYS:HB2	1.92	0.69
4:B:378:LEU:O	4:B:382:ILE:HG13	1.92	0.69
3:A:472:LEU:HD11	4:B:835:GLN:NE2	2.07	0.69
4:B:957:ASN:HD22	4:B:961:LEU:HD12	1.57	0.69
8:H:49:VAL:HG12	8:H:50:ALA:N	2.07	0.69
3:A:392:VAL:HG13	3:A:415:LEU:HD11	1.74	0.69
4:B:281:PRO:HG2	4:B:284:ILE:HD12	1.73	0.69
5:C:39:ALA:HA	5:C:164:ALA:HB3	1.75	0.69
3:A:340:LEU:HD13	3:A:1429:ILE:HG23	1.74	0.69
3:A:414:ASP:OD1	3:A:416:ARG:HG2	1.93	0.69
3:A:763:ALA:O	3:A:803:SER:HB3	1.92	0.69
3:A:786:HIS:HE1	4:B:742:GLU:OE1	1.76	0.69
4:B:954:VAL:O	12:L:55:ILE:O	2.11	0.69
3:A:391:LEU:HD22	3:A:400:PRO:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:280:ILE:CD1	4:B:334:ILE:HG12	2.23	0.68
2:R:2:A:H2'	2:R:3:C:O4'	1.93	0.68
3:A:567:LYS:HE3	8:H:46:LEU:CD1	2.22	0.68
3:A:693:VAL:CG2	3:A:721:PHE:HE1	2.07	0.68
4:B:22:SER:O	4:B:654:ARG:HD2	1.94	0.68
4:B:46:GLN:HG3	4:B:47:GLN:H	1.58	0.68
4:B:65:GLU:HG3	4:B:66:ASP:H	1.56	0.68
4:B:884:ARG:O	4:B:936:ASP:HB3	1.93	0.68
4:B:986:GLN:OE1	4:B:986:GLN:HA	1.92	0.68
5:C:51:VAL:HG22	5:C:155:LEU:HD22	1.76	0.68
9:I:75:CYS:SG	9:I:103:CYS:SG	2.91	0.68
3:A:768:GLN:HG2	3:A:816:HIS:HA	1.75	0.68
4:B:976:ILE:O	4:B:990:ILE:HB	1.94	0.68
8:H:7:ASP:O	8:H:8:ASP:HB2	1.92	0.68
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.76	0.68
3:A:44:THR:O	3:A:45:GLN:HB2	1.91	0.68
3:A:72:GLU:OE2	4:B:1175:LEU:HD12	1.92	0.68
3:A:535:THR:HG21	3:A:617:VAL:N	2.08	0.68
4:B:542:MET:CE	4:B:747:MET:HG3	2.22	0.68
3:A:563:PRO:HB2	3:A:565:ILE:O	1.94	0.68
3:A:599:SER:HB2	3:A:603:ASN:H	1.58	0.68
4:B:562:GLY:HA3	4:B:590:HIS:CE1	2.29	0.68
2:R:2:A:O2'	2:R:3:C:H5'	1.93	0.68
3:A:446:ARG:HG2	3:A:446:ARG:HH11	1.59	0.68
3:A:453:MET:HB3	3:A:477:PRO:HB3	1.76	0.68
4:B:864:LYS:HB3	4:B:872:GLU:H	1.59	0.68
9:I:55:THR:HG23	9:I:58:VAL:HG21	1.76	0.68
3:A:994:GLN:HE22	3:A:1023:ARG:HE	1.38	0.67
3:A:1390:ASN:HD22	3:A:1399:ARG:HA	1.57	0.67
4:B:54:PHE:HA	4:B:58:THR:HB	1.74	0.67
4:B:514:LEU:HD12	4:B:515:HIS:N	2.09	0.67
4:B:709:ASP:O	4:B:710:LEU:HD23	1.94	0.67
4:B:839:MET:HE3	4:B:1010:LEU:HD11	1.74	0.67
5:C:93:ASP:O	5:C:127:ARG:NH2	2.27	0.67
5:C:166:GLU:HG3	11:K:10:PHE:CZ	2.29	0.67
12:L:40:LEU:HD13	12:L:44:ASP:CG	2.19	0.67
3:A:535:THR:HG21	3:A:616:VAL:HA	1.75	0.67
3:A:694:THR:O	3:A:698:GLN:HG3	1.94	0.67
9:I:53:GLY:O	9:I:89:GLN:HB2	1.94	0.67
5:C:56:THR:HG21	5:C:145:CYS:SG	2.35	0.67
3:A:450:LEU:HD13	3:A:1074:GLU:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:288:ALA:HB1	4:B:331:LEU:HD12	1.75	0.67
4:B:842:ASN:ND2	4:B:844:SER:HB2	2.09	0.67
6:E:127:ILE:O	6:E:127:ILE:HG13	1.93	0.67
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.76	0.67
12:L:60:ARG:CG	12:L:61:THR:H	1.94	0.67
5:C:5:GLY:O	5:C:7:GLN:HG3	1.95	0.67
5:C:8:VAL:HG12	5:C:9:LYS:N	2.09	0.67
5:C:80:LEU:HD22	5:C:129:ILE:CD1	2.21	0.67
4:B:121:ASN:HA	4:B:207:GLY:HA3	1.77	0.67
4:B:280:ILE:HG22	4:B:285:ILE:HG13	1.76	0.67
4:B:1147:LEU:HD22	4:B:1151:LEU:HD22	1.77	0.67
3:A:16:GLU:HB3	3:A:1418:LEU:HD11	1.77	0.67
3:A:76:GLU:OE2	4:B:1159:ARG:NH1	2.28	0.67
3:A:736:ASN:O	3:A:737:LEU:C	2.38	0.67
3:A:994:GLN:HE21	3:A:1019:CYS:HB3	1.59	0.67
3:A:351:THR:CG2	4:B:1103:ILE:HG23	2.24	0.67
3:A:1348:LEU:HD21	3:A:1375:MET:SD	2.35	0.67
4:B:128:LEU:HB3	4:B:167:ILE:O	1.95	0.67
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.76	0.67
12:L:45:ALA:O	12:L:46:VAL:HG23	1.95	0.67
12:L:51:CYS:O	12:L:53:HIS:N	2.28	0.67
3:A:828:ALA:CB	4:B:530:GLY:HA2	2.25	0.67
7:F:109:VAL:HG12	7:F:110:ASP:N	2.10	0.67
8:H:97:MET:HE2	8:H:142:LEU:HD23	1.76	0.67
3:A:1193:LEU:HD21	3:A:1267:MET:HE2	1.77	0.66
3:A:1364:ASN:ND2	3:A:1365:TYR:N	2.43	0.66
4:B:566:LEU:HD13	4:B:588:GLY:HA2	1.77	0.66
4:B:882:THR:HG21	4:B:935:ARG:HA	1.75	0.66
4:B:957:ASN:O	4:B:959:ASP:N	2.28	0.66
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.30	0.66
3:A:88:LYS:HD2	3:A:293:GLU:CD	2.20	0.66
4:B:363:HIS:O	4:B:364:ILE:CB	2.44	0.66
3:A:897:TYR:CD2	3:A:936:LEU:HD13	2.30	0.66
4:B:711:GLU:N	4:B:712:PRO:CD	2.57	0.66
4:B:986:GLN:HE22	4:B:1020:ARG:CZ	2.08	0.66
5:C:254:LYS:HB3	11:K:42:LEU:HD11	1.76	0.66
3:A:306:ASN:HD21	3:A:324:SER:H	1.43	0.66
3:A:381:THR:HG22	3:A:383:TYR:N	2.09	0.66
5:C:260:LEU:O	5:C:264:GLN:HG3	1.95	0.66
3:A:305:ASP:HB3	3:A:308:ILE:HD11	1.77	0.66
3:A:590:ARG:HH11	3:A:590:ARG:CG	2.06	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:751:SER:O	3:A:752:LYS:HG2	1.96	0.66
4:B:1002:THR:HG23	4:B:1004:GLU:N	2.10	0.66
8:H:106:GLU:C	8:H:108:SER:H	2.02	0.66
3:A:90:VAL:CG1	3:A:297:GLN:HA	2.26	0.66
3:A:525:GLN:CB	4:B:835:GLN:HG2	2.25	0.66
3:A:1267:MET:HA	3:A:1271:ILE:HD12	1.77	0.66
3:A:1333:ILE:O	3:A:1336:MET:HB3	1.96	0.66
4:B:603:LEU:HB3	4:B:609:ILE:HG13	1.76	0.66
9:I:32:CYS:SG	9:I:33:SER:N	2.69	0.66
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.09	0.66
2:R:1:G:O2'	2:R:2:A:H5'	1.95	0.66
2:R:3:C:H2'	2:R:4:C:H6	1.59	0.66
3:A:914:GLU:HB2	3:A:979:SER:O	1.95	0.66
4:B:287:ARG:NH2	4:B:294:ASP:OD2	2.28	0.66
4:B:349:ILE:O	4:B:352:ALA:HB3	1.96	0.66
4:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.77	0.66
6:E:78:LEU:HD23	6:E:78:LEU:C	2.20	0.66
3:A:541:ILE:HG21	3:A:549:MET:HE3	1.78	0.66
4:B:1106:ARG:CZ	4:B:1109:GLY:H	2.07	0.66
3:A:590:ARG:HB3	3:A:605:MET:N	2.10	0.66
3:A:715:GLU:O	3:A:719:VAL:HG23	1.96	0.66
3:A:816:HIS:CE1	4:B:764:SER:HB2	2.31	0.66
3:A:1115:SER:HA	3:A:1308:THR:HG22	1.77	0.66
4:B:311:LEU:HB3	9:I:4:PHE:CZ	2.30	0.66
4:B:1162:ILE:HD11	4:B:1194:ILE:HD13	1.77	0.66
3:A:102:VAL:HG21	3:A:234:MET:HE1	1.77	0.66
3:A:1042:PHE:CE2	3:A:1046:LEU:HD11	2.31	0.66
4:B:1001:PHE:CZ	4:B:1073:TYR:HB2	2.30	0.66
3:A:95:PHE:HE2	3:A:1414:ALA:HB2	1.62	0.65
3:A:1193:LEU:HB2	3:A:1260:LEU:HD11	1.78	0.65
4:B:751:VAL:O	4:B:754:SER:HB2	1.95	0.65
4:B:911:ILE:CG2	4:B:966:VAL:HG11	2.26	0.65
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.77	0.65
3:A:814:PHE:O	3:A:817:ALA:HB3	1.95	0.65
3:A:1319:VAL:HG13	3:A:1320:PRO:HD2	1.79	0.65
3:A:1342:GLU:OE2	6:E:212:ARG:NH1	2.28	0.65
4:B:824:ILE:CG1	10:J:48:ARG:HH12	2.08	0.65
5:C:8:VAL:HG12	5:C:9:LYS:H	1.60	0.65
3:A:1364:ASN:HD22	3:A:1364:ASN:C	2.04	0.65
5:C:22:LEU:HD22	5:C:25:VAL:CG2	2.25	0.65
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:87:ALA:HB3	3:A:276:LEU:HD23	1.79	0.65
4:B:649:LYS:HE2	4:B:738:PHE:O	1.96	0.65
4:B:711:GLU:H	4:B:712:PRO:HD3	1.60	0.65
4:B:114:PRO:HG3	4:B:181:LEU:HD11	1.79	0.65
4:B:120:ARG:CG	4:B:955:THR:HG21	2.23	0.65
4:B:211:VAL:HG23	4:B:483:LEU:HB2	1.78	0.65
4:B:293:PRO:HG2	4:B:296:GLU:HB2	1.78	0.65
6:E:176:PRO:O	6:E:212:ARG:HA	1.95	0.65
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.27	0.65
3:A:381:THR:CG2	3:A:383:TYR:H	2.09	0.65
3:A:1161:THR:HG22	3:A:1163:ILE:N	2.03	0.65
4:B:805:THR:HG21	4:B:815:ARG:HE	1.62	0.65
4:B:1197:PRO:HG2	4:B:1200:ALA:HB2	1.79	0.65
3:A:381:THR:HG21	3:A:383:TYR:CD1	2.31	0.65
3:A:443:LEU:CD2	3:A:455:MET:HE2	2.27	0.65
4:B:101:MET:HE3	4:B:169:ARG:HH22	1.62	0.65
4:B:879:ARG:HB3	4:B:883:LEU:CD2	2.26	0.65
8:H:107:VAL:HG21	8:H:126:GLU:HG3	1.79	0.65
3:A:512:VAL:HA	3:A:519:PRO:HA	1.79	0.65
3:A:1224:LEU:HD12	3:A:1241:ARG:O	1.97	0.65
3:A:1394:THR:CG2	3:A:1395:GLY:N	2.60	0.65
7:F:111:LEU:HD12	7:F:111:LEU:H	1.61	0.65
10:J:9:SER:OG	10:J:48:ARG:NH2	2.30	0.65
4:B:686:ASN:C	4:B:688:GLY:H	2.04	0.64
6:E:124:VAL:HG22	6:E:132:ILE:HG21	1.79	0.64
7:F:96:THR:O	7:F:100:GLN:HG3	1.97	0.64
8:H:89:LEU:C	8:H:91:ASP:N	2.55	0.64
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.78	0.64
3:A:329:LEU:HD23	3:A:335:ARG:HG3	1.78	0.64
3:A:1035:TYR:O	3:A:1037:LEU:N	2.30	0.64
4:B:788:ARG:NH1	4:B:790:ASP:OD1	2.31	0.64
4:B:1051:THR:CG2	4:B:1053:GLU:H	1.93	0.64
5:C:11:ARG:HH21	5:C:229:TYR:HD2	1.44	0.64
5:C:114:TYR:CD2	5:C:140:ASN:HB3	2.32	0.64
6:E:96:PHE:CZ	6:E:100:ILE:HD11	2.32	0.64
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.79	0.64
3:A:579:SER:OG	3:A:612:ILE:HG22	1.97	0.64
4:B:46:GLN:HE22	4:B:496:ARG:HA	1.62	0.64
4:B:446:LEU:O	4:B:447:ALA:HB3	1.97	0.64
4:B:1170:THR:O	4:B:1170:THR:HG22	1.97	0.64
3:A:901:LEU:HA	3:A:907:THR:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:994:GLN:HE22	3:A:1023:ARG:NE	1.95	0.64
4:B:577:ALA:HB1	4:B:589:VAL:CG1	2.27	0.64
4:B:666:TYR:C	4:B:668:ASP:H	2.06	0.64
3:A:523:ILE:HD12	3:A:622:VAL:HG21	1.80	0.64
3:A:629:LEU:HD13	3:A:645:LEU:HD21	1.79	0.64
4:B:604:ARG:HG2	4:B:604:ARG:O	1.98	0.64
3:A:1436:ILE:HB	4:B:1144:ALA:HB2	1.80	0.64
4:B:25:ILE:HG22	4:B:29:ASP:HB2	1.79	0.64
4:B:1034:VAL:HG23	4:B:1059:LEU:HB2	1.80	0.64
3:A:475:THR:HG22	3:A:476:SER:N	2.12	0.64
3:A:1242:VAL:HG12	3:A:1243:VAL:N	2.12	0.64
3:A:523:ILE:HD12	3:A:622:VAL:HG22	1.79	0.64
3:A:1402:PHE:CD2	3:A:1403:GLU:HG3	2.33	0.64
4:B:1001:PHE:CE1	4:B:1073:TYR:HB2	2.33	0.64
4:B:1072:MET:CE	4:B:1085:ILE:HB	2.28	0.64
5:C:241:ASP:HB3	11:K:109:TRP:CE2	2.32	0.64
6:E:50:MET:HE3	6:E:50:MET:O	1.98	0.64
7:F:109:VAL:HG21	7:F:124:GLU:HA	1.79	0.64
3:A:84:ILE:HG23	3:A:239:LEU:HB3	1.80	0.63
4:B:515:HIS:HD2	4:B:517:THR:OG1	1.81	0.63
4:B:1104:HIS:HB2	4:B:1122:ARG:HD2	1.80	0.63
3:A:225:ASN:O	3:A:226:GLU:HG2	1.99	0.63
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.33	0.63
12:L:48:CYS:SG	12:L:49:LYS:N	2.70	0.63
4:B:914:LYS:HB3	4:B:937:ALA:O	1.98	0.63
4:B:373:ARG:NE	4:B:567:GLU:OE2	2.29	0.63
4:B:519:TRP:C	4:B:519:TRP:CD1	2.76	0.63
7:F:86:THR:OG1	7:F:89:GLU:HG3	1.98	0.63
3:A:33:ALA:O	3:A:83:HIS:HB3	1.99	0.63
3:A:268:ASP:HB3	3:A:299:HIS:ND1	2.14	0.63
3:A:328:ARG:O	3:A:335:ARG:HG2	1.99	0.63
3:A:354:SER:HA	3:A:482:PHE:CD2	2.34	0.63
3:A:1074:GLU:HB3	3:A:1075:PRO:CD	2.29	0.63
12:L:55:ILE:HG13	12:L:56:LEU:H	1.63	0.63
3:A:418:SER:O	3:A:420:ARG:N	2.32	0.63
4:B:221:ASN:OD1	4:B:242:SER:HA	1.98	0.63
4:B:525:ALA:O	4:B:527:THR:HG22	1.98	0.63
6:E:100:ILE:HG23	6:E:105:PHE:HB2	1.80	0.63
8:H:12:VAL:HA	8:H:28:ALA:CB	2.28	0.63
8:H:31:THR:O	8:H:32:THR:CB	2.47	0.63
4:B:512:ARG:NH2	4:B:535:LEU:HD11	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:780:VAL:HG21	10:J:56:LEU:CD1	2.29	0.63
3:A:418:SER:O	3:A:419:LYS:C	2.39	0.63
4:B:1201:LYS:O	4:B:1205:GLN:HG3	1.97	0.63
3:A:244:PRO:CG	3:A:245:PRO:HD3	2.27	0.63
3:A:1212:VAL:O	3:A:1216:ILE:HG13	1.99	0.63
6:E:93:MET:HE3	6:E:120:ALA:O	1.98	0.63
6:E:157:SER:C	6:E:159:ASP:H	2.07	0.63
3:A:1317:MET:HA	3:A:1322:ILE:HD11	1.81	0.62
3:A:1364:ASN:ND2	3:A:1364:ASN:C	2.56	0.62
4:B:496:ARG:HH11	4:B:539:LEU:HB2	1.62	0.62
6:E:156:LEU:HD12	6:E:195:VAL:HG12	1.81	0.62
6:E:178:ILE:HG23	6:E:214:CYS:HA	1.81	0.62
7:F:111:LEU:H	7:F:111:LEU:CD1	2.12	0.62
3:A:689:LYS:O	3:A:693:VAL:HG23	2.00	0.62
3:A:821:ARG:HG3	3:A:825:ILE:HD11	1.81	0.62
3:A:1054:LEU:O	3:A:1057:VAL:HG23	1.99	0.62
4:B:913:GLY:HA2	4:B:938:SER:HB3	1.81	0.62
4:B:1106:ARG:HD2	4:B:1126:GLY:O	1.99	0.62
4:B:1187:ASN:OD1	4:B:1190:ASP:HB3	1.99	0.62
3:A:590:ARG:HB3	3:A:605:MET:H	1.64	0.62
3:A:108:MET:O	3:A:109:HIS:HB2	1.99	0.62
3:A:672:ASP:OD1	3:A:674:PRO:HD2	2.00	0.62
3:A:778:GLY:HA3	4:B:516:ASN:HB2	1.80	0.62
3:A:871:ASP:HB3	6:E:204:THR:CG2	2.30	0.62
3:A:915:SER:O	3:A:919:ILE:HG13	2.00	0.62
4:B:1072:MET:HE3	4:B:1085:ILE:CD1	2.30	0.62
4:B:208:SER:OG	4:B:210:LYS:HD3	1.99	0.62
4:B:1002:THR:HG23	4:B:1004:GLU:H	1.64	0.62
3:A:871:ASP:HB3	6:E:204:THR:HG22	1.82	0.62
3:A:1021:LEU:O	3:A:1025:ARG:HG2	2.00	0.62
4:B:195:CYS:HB3	4:B:782:LEU:HD22	1.81	0.62
5:C:46:ILE:HA	5:C:159:ALA:HA	1.82	0.62
5:C:173:ALA:O	5:C:174:ALA:HB3	2.00	0.62
7:F:109:VAL:HG23	7:F:124:GLU:HG2	1.82	0.62
8:H:49:VAL:HG12	8:H:50:ALA:H	1.62	0.62
3:A:148:CYS:O	3:A:168:GLY:HA2	1.99	0.62
3:A:709:THR:HB	3:A:712:GLU:H	1.64	0.62
3:A:871:ASP:OD2	6:E:204:THR:HG23	1.99	0.62
5:C:166:GLU:HA	11:K:6:ARG:HB3	1.82	0.62
7:F:97:ARG:O	7:F:101:ILE:HG13	1.99	0.62
3:A:1444:MET:HE1	7:F:135:ARG:CZ	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:111:LEU:C	7:F:113:GLY:H	2.07	0.62
4:B:25:ILE:HG22	4:B:26:THR:H	1.65	0.61
4:B:842:ASN:HD21	4:B:844:SER:HB2	1.63	0.61
8:H:89:LEU:HD22	8:H:91:ASP:CG	2.25	0.61
11:K:63:VAL:CG2	11:K:63:VAL:O	2.48	0.61
3:A:401:GLY:C	3:A:435:HIS:CD2	2.79	0.61
4:B:29:ASP:HB3	4:B:658:ILE:CD1	2.30	0.61
4:B:114:PRO:HB3	4:B:174:LEU:HD11	1.82	0.61
5:C:49:VAL:HG21	5:C:67:LEU:HD12	1.83	0.61
5:C:123:ASN:HD22	5:C:125:MET:HG2	1.65	0.61
5:C:235:VAL:HG21	10:J:6:ARG:HH21	1.65	0.61
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.34	0.61
3:A:898:ARG:HB2	3:A:933:TYR:CE1	2.34	0.61
4:B:101:MET:HE3	4:B:169:ARG:NH2	2.15	0.61
12:L:51:CYS:HB2	12:L:53:HIS:CD2	2.35	0.61
3:A:855:THR:CG2	3:A:857:ARG:HG3	2.30	0.61
4:B:39:ARG:HE	4:B:665:GLU:HG2	1.64	0.61
4:B:616:ILE:HD12	4:B:616:ILE:N	2.15	0.61
9:I:7:CYS:HB2	9:I:29:CYS:HB2	1.81	0.61
12:L:34:CYS:SG	12:L:51:CYS:SG	2.98	0.61
3:A:503:GLN:HE21	7:F:90:ARG:HH21	1.47	0.61
3:A:1437:GLY:HA3	7:F:88:TYR:CD2	2.36	0.61
4:B:549:THR:HB	4:B:628:THR:CG2	2.30	0.61
4:B:787:VAL:O	4:B:787:VAL:HG12	2.00	0.61
6:E:96:PHE:O	6:E:100:ILE:HG13	1.99	0.61
3:A:961:ARG:O	3:A:965:GLN:HG3	2.00	0.61
6:E:93:MET:O	6:E:97:VAL:HG23	2.00	0.61
7:F:135:ARG:HG2	7:F:137:TYR:CE1	2.34	0.61
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.83	0.61
3:A:506:ALA:HB1	3:A:508:PRO:HD2	1.83	0.61
3:A:567:LYS:CG	3:A:568:PRO:HD2	2.31	0.61
3:A:1293:SER:OG	3:A:1294:PRO:HD2	2.01	0.61
4:B:299:GLU:OE1	4:B:571:PRO:HG2	2.01	0.61
4:B:809:MET:HE1	4:B:983:ARG:NH2	2.16	0.61
4:B:839:MET:HE3	4:B:1010:LEU:CD1	2.30	0.61
7:F:138:LEU:HB3	7:F:139:PRO:HD2	1.83	0.61
9:I:8:ARG:HG3	9:I:9:ASP:N	2.16	0.61
1:D:6:DC:H4'	3:A:447:GLN:NE2	2.16	0.61
3:A:73:GLY:O	3:A:75:ASN:N	2.32	0.61
3:A:709:THR:OG1	3:A:712:GLU:HG3	2.00	0.61
12:L:26:THR:O	12:L:27:LEU:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:789:LYS:HG3	9:I:67:THR:HB	1.83	0.61
5:C:131:HIS:O	5:C:132:PRO:C	2.43	0.61
8:H:106:GLU:C	8:H:108:SER:N	2.57	0.61
3:A:982:THR:HG22	3:A:984:LYS:H	1.64	0.60
3:A:1132:LYS:O	3:A:1135:ARG:HB3	2.01	0.60
3:A:1208:THR:O	3:A:1212:VAL:HG23	2.01	0.60
4:B:446:LEU:O	4:B:447:ALA:CB	2.48	0.60
4:B:1138:MET:HE2	4:B:1146:PHE:CD2	2.36	0.60
3:A:338:GLY:HA2	4:B:1129:ARG:NH2	2.10	0.60
3:A:445:ASN:HB2	3:A:454:SER:O	2.00	0.60
4:B:57:TYR:CD1	4:B:57:TYR:N	2.68	0.60
4:B:429:PHE:HA	4:B:432:MET:HE3	1.82	0.60
7:F:101:ILE:HD12	7:F:121:ALA:HB2	1.82	0.60
3:A:528:LEU:O	3:A:531:ILE:HG22	2.01	0.60
4:B:211:VAL:O	4:B:480:SER:HA	2.01	0.60
4:B:999:MET:HE2	4:B:1011:ILE:CD1	2.30	0.60
3:A:824:LEU:O	3:A:827:THR:HB	2.00	0.60
3:A:1115:SER:O	3:A:1329:THR:HG23	2.02	0.60
4:B:582:VAL:HG22	4:B:626:ILE:HB	1.82	0.60
4:B:913:GLY:HA2	4:B:938:SER:CB	2.32	0.60
11:K:90:ALA:O	11:K:94:ILE:HG13	2.01	0.60
1:D:2:DA:H2'	1:D:3:DA:C8	2.37	0.60
3:A:86:LEU:HA	3:A:273:ASN:OD1	2.02	0.60
3:A:337:ARG:CZ	3:A:839:ARG:NH1	2.64	0.60
3:A:567:LYS:O	3:A:569:LYS:N	2.35	0.60
3:A:1402:PHE:CE2	3:A:1403:GLU:HG3	2.37	0.60
4:B:90:ILE:HD12	4:B:432:MET:SD	2.42	0.60
4:B:1169:MET:HE1	4:B:1201:LYS:O	2.00	0.60
6:E:47:CYS:HA	6:E:53:PRO:HA	1.83	0.60
2:R:8:C:H2'	2:R:9:A:O4'	2.02	0.60
3:A:322:VAL:O	3:A:323:LYS:HG3	2.01	0.60
4:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.31	0.60
3:A:306:ASN:OD1	3:A:324:SER:HB3	2.01	0.60
9:I:85:PHE:CD1	9:I:99:LEU:HD22	2.37	0.60
3:A:896:ARG:NH2	3:A:1030:ARG:HH21	2.00	0.60
4:B:185:THR:HG23	4:B:188:ASP:OD2	2.01	0.60
3:A:1192:LEU:HD22	3:A:1239:ARG:NH2	2.16	0.60
4:B:794:ASN:C	4:B:795:ILE:HD12	2.26	0.60
4:B:1117:GLN:HG3	4:B:1156:ASP:OD1	2.02	0.60
3:A:76:GLU:HG3	3:A:76:GLU:O	2.02	0.60
3:A:756:ILE:HG22	3:A:757:ASN:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:463:THR:HG22	4:B:465:ASN:HD22	1.66	0.60
9:I:15:TYR:O	9:I:27:PHE:HA	2.02	0.60
3:A:1394:THR:HG22	3:A:1395:GLY:N	2.17	0.59
4:B:217:ARG:NH1	4:B:407:ASP:OD1	2.35	0.59
4:B:778:MET:CE	4:B:1094:ARG:HD3	2.32	0.59
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.66	0.59
3:A:68:GLN:HE22	3:A:80:HIS:HB3	1.67	0.59
4:B:803:LEU:H	4:B:822:ASN:HD21	1.48	0.59
5:C:244:VAL:O	5:C:248:ILE:HG13	2.03	0.59
3:A:44:THR:O	3:A:44:THR:HG22	2.02	0.59
3:A:107:CYS:HB2	3:A:114:LEU:CD2	2.33	0.59
3:A:151:ASP:HA	3:A:162:VAL:O	2.02	0.59
3:A:549:MET:SD	3:A:577:ILE:CD1	2.87	0.59
3:A:704:ALA:HB2	3:A:710:LEU:CG	2.23	0.59
3:A:809:THR:O	3:A:810:PRO:C	2.46	0.59
3:A:901:LEU:N	3:A:926:GLN:NE2	2.50	0.59
4:B:778:MET:HE3	4:B:1094:ARG:HD3	1.84	0.59
4:B:912:ILE:HD11	4:B:966:VAL:HG23	1.84	0.59
4:B:1102:LYS:O	4:B:1104:HIS:N	2.32	0.59
4:B:1159:ARG:CD	4:B:1193:GLN:HE21	2.15	0.59
4:B:1171:VAL:CG1	4:B:1191:ILE:HD13	2.32	0.59
4:B:1174:LYS:HB2	4:B:1179:GLN:O	2.02	0.59
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.01	0.59
3:A:1018:PHE:O	3:A:1021:LEU:HB3	2.03	0.59
3:A:1158:PRO:HB3	3:A:1241:ARG:NH1	2.17	0.59
4:B:708:GLU:CG	4:B:709:ASP:H	1.97	0.59
4:B:975:GLN:HG2	4:B:976:ILE:H	1.67	0.59
5:C:166:GLU:CG	11:K:10:PHE:HZ	2.14	0.59
3:A:1042:PHE:HE2	3:A:1046:LEU:HD11	1.66	0.59
5:C:18:VAL:HG23	5:C:240:VAL:CG1	2.33	0.59
6:E:29:PHE:HB2	6:E:65:THR:HG22	1.83	0.59
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.29	0.59
3:A:239:LEU:HD12	3:A:240:PRO:HD2	1.84	0.59
3:A:1223:ASP:HA	3:A:1243:VAL:CG1	2.32	0.59
4:B:198:ASP:OD1	4:B:485:ARG:NH2	2.33	0.59
4:B:995:ARG:NH1	4:B:995:ARG:HB2	2.16	0.59
6:E:5:ASN:ND2	6:E:52:ARG:HG2	2.12	0.59
3:A:50:ILE:C	3:A:52:GLY:H	2.09	0.59
3:A:225:ASN:ND2	3:A:227:VAL:HB	2.18	0.59
3:A:779:PHE:CZ	4:B:517:THR:HA	2.37	0.59
3:A:1365:TYR:O	3:A:1366:ARG:C	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1444:MET:HE1	7:F:135:ARG:NE	2.18	0.59
4:B:405:ARG:NH1	4:B:632:ARG:HG2	2.17	0.59
4:B:512:ARG:NH2	4:B:535:LEU:CD1	2.62	0.59
4:B:642:ASP:O	4:B:644:GLU:N	2.36	0.59
8:H:139:ASN:O	8:H:140:ALA:HB2	2.02	0.59
3:A:31:SER:OG	3:A:83:HIS:HB2	2.02	0.59
3:A:90:VAL:HG11	3:A:297:GLN:HA	1.84	0.59
3:A:1341:ILE:HD12	3:A:1379:GLY:C	2.28	0.59
4:B:479:VAL:HG12	4:B:480:SER:N	2.17	0.59
4:B:779:GLY:HA2	4:B:796:LEU:HB2	1.85	0.59
5:C:148:ARG:HG3	10:J:61:LEU:O	2.03	0.59
6:E:78:LEU:HD23	6:E:79:TRP:N	2.16	0.59
8:H:109:LYS:HB2	8:H:109:LYS:NZ	2.18	0.59
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.33	0.59
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.83	0.59
3:A:840:ARG:HB3	3:A:1384:VAL:HG12	1.85	0.59
6:E:61:GLN:HB2	6:E:79:TRP:CE3	2.38	0.59
8:H:84:ALA:HA	8:H:87:ARG:CG	2.32	0.59
3:A:596:THR:O	3:A:598:LEU:N	2.36	0.58
3:A:738:LYS:HZ1	5:C:194:GLU:C	2.11	0.58
3:A:1295:THR:HG23	3:A:1297:GLU:OE1	2.03	0.58
4:B:28:GLU:CD	4:B:807:ARG:HH22	2.10	0.58
4:B:642:ASP:HB3	4:B:649:LYS:HD2	1.85	0.58
4:B:744:HIS:CD2	4:B:746:SER:H	2.14	0.58
4:B:758:PHE:C	4:B:760:ASP:H	2.11	0.58
7:F:85:MET:HE1	7:F:148:VAL:HG13	1.84	0.58
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.33	0.58
3:A:68:GLN:HE22	3:A:80:HIS:CB	2.15	0.58
3:A:469:ARG:NH2	4:B:976:ILE:HD13	2.18	0.58
3:A:1004:ASN:ND2	6:E:167:ARG:HD2	2.18	0.58
4:B:46:GLN:O	4:B:408:LEU:HD23	2.03	0.58
4:B:640:VAL:O	4:B:641:GLU:C	2.46	0.58
7:F:127:GLU:O	7:F:129:LYS:HG3	2.03	0.58
12:L:51:CYS:C	12:L:53:HIS:H	2.12	0.58
3:A:399:HIS:C	3:A:401:GLY:H	2.10	0.58
3:A:1336:MET:CE	3:A:1381:LEU:HG	2.33	0.58
4:B:589:VAL:HG12	4:B:590:HIS:N	2.18	0.58
4:B:806:THR:HB	4:B:809:MET:HG3	1.85	0.58
6:E:156:LEU:HD12	6:E:195:VAL:CG1	2.33	0.58
3:A:714:PHE:HB2	9:I:97:MET:HE1	1.86	0.58
4:B:653:VAL:HG22	4:B:689:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:860:MET:HG2	4:B:861:ASP:N	2.18	0.58
9:I:7:CYS:C	9:I:8:ARG:O	2.43	0.58
3:A:97:ALA:HA	3:A:100:LYS:HE3	1.84	0.58
4:B:118:ARG:NH2	4:B:194:GLU:CD	2.60	0.58
9:I:75:CYS:C	9:I:77:LYS:N	2.59	0.58
3:A:93:VAL:HG11	3:A:308:ILE:CD1	2.33	0.58
3:A:567:LYS:CB	3:A:568:PRO:CD	2.67	0.58
3:A:821:ARG:O	3:A:822:GLU:C	2.46	0.58
3:A:896:ARG:HD3	3:A:897:TYR:HE1	1.67	0.58
3:A:1308:THR:HG21	3:A:1310:GLY:O	2.04	0.58
3:A:57:ARG:O	3:A:68:GLN:HG3	2.03	0.58
3:A:524:VAL:HG12	3:A:525:GLN:H	1.69	0.58
3:A:1332:PHE:CD2	3:A:1332:PHE:N	2.72	0.58
4:B:803:LEU:N	4:B:822:ASN:HD21	2.02	0.58
4:B:1201:LYS:HE2	4:B:1205:GLN:NE2	2.18	0.58
7:F:111:LEU:N	7:F:111:LEU:CD1	2.67	0.58
9:I:47:GLU:OE1	9:I:50:THR:HG23	2.04	0.58
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.85	0.58
3:A:219:PHE:O	3:A:222:LEU:N	2.33	0.58
3:A:444:PHE:HB3	3:A:458:HIS:HD2	1.68	0.58
3:A:1385:THR:HG22	3:A:1386:ARG:H	1.68	0.58
4:B:23:ALA:O	4:B:654:ARG:HB3	2.04	0.58
4:B:23:ALA:HB1	4:B:24:PRO:HD2	1.85	0.58
4:B:101:MET:HB2	4:B:169:ARG:HH12	1.69	0.58
4:B:855:PHE:HZ	4:B:857:ARG:HH11	1.52	0.58
3:A:28:ARG:HG2	3:A:83:HIS:CE1	2.39	0.58
3:A:101:LYS:O	3:A:105:CYS:HB2	2.04	0.58
3:A:166:GLY:O	3:A:167:CYS:HB3	2.03	0.58
3:A:260:ASP:OD1	3:A:261:ASP:N	2.37	0.58
3:A:567:LYS:HZ3	8:H:95:TYR:HE1	1.50	0.58
3:A:1074:GLU:O	3:A:1076:ALA:N	2.37	0.58
3:A:1149:ALA:HB2	9:I:47:GLU:HA	1.84	0.58
3:A:1325:THR:O	6:E:148:GLU:HB2	2.04	0.58
4:B:25:ILE:HG22	4:B:29:ASP:CB	2.34	0.58
4:B:701:ILE:HD11	4:B:703:ILE:HD11	1.86	0.58
6:E:61:GLN:HB2	6:E:79:TRP:HE3	1.69	0.58
3:A:385:ILE:HG22	3:A:386:ASP:N	2.18	0.58
3:A:1143:LEU:HD23	3:A:1267:MET:HB3	1.86	0.58
3:A:1281:ARG:HB2	3:A:1309:ASP:HB2	1.86	0.58
3:A:1400:CYS:SG	3:A:1409:LEU:HG	2.44	0.58
4:B:1077:THR:CG2	4:B:1079:LYS:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:ARG:HE	10:J:49:MET:CE	2.16	0.58
3:A:41:MET:HB3	3:A:48:ALA:O	2.04	0.57
3:A:482:PHE:CD1	4:B:836:GLU:HB2	2.38	0.57
3:A:742:ASN:CA	3:A:745:GLN:HB2	2.33	0.57
3:A:1155:ASP:OD2	3:A:1161:THR:HG23	2.04	0.57
4:B:130:VAL:HG12	4:B:131:ASP:H	1.68	0.57
4:B:980:PHE:CE1	4:B:990:ILE:HD11	2.39	0.57
5:C:175:ALA:HB3	10:J:43:ARG:NH2	2.19	0.57
7:F:81:THR:HG22	7:F:82:THR:N	2.18	0.57
11:K:47:ARG:HD3	11:K:59:ALA:O	2.03	0.57
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.39	0.57
12:L:49:LYS:O	12:L:50:ASP:HB2	2.03	0.57
3:A:40:THR:HG21	3:A:259:GLU:OE2	2.04	0.57
4:B:1077:THR:HG22	4:B:1079:LYS:N	2.13	0.57
6:E:213:ILE:HG23	6:E:213:ILE:O	2.04	0.57
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.85	0.57
3:A:93:VAL:HG22	3:A:301:ALA:HA	1.86	0.57
3:A:337:ARG:CD	3:A:839:ARG:HH22	2.17	0.57
3:A:414:ASP:O	3:A:417:TYR:O	2.22	0.57
4:B:205:ILE:N	4:B:205:ILE:HD12	2.19	0.57
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.84	0.57
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.38	0.57
3:A:596:THR:O	3:A:597:LEU:C	2.47	0.57
3:A:886:ILE:CD1	3:A:943:LEU:HB3	2.31	0.57
4:B:287:ARG:NH1	4:B:324:ILE:O	2.37	0.57
4:B:547:VAL:H	4:B:612:GLU:CD	2.13	0.57
4:B:1168:LEU:HD13	4:B:1208:MET:HE3	1.86	0.57
5:C:251:LEU:O	5:C:255:VAL:HG23	2.04	0.57
6:E:35:VAL:C	6:E:37:LEU:H	2.12	0.57
8:H:81:PRO:CB	8:H:82:PRO:CD	2.81	0.57
3:A:98:LYS:O	3:A:102:VAL:HG23	2.05	0.57
3:A:225:ASN:HD22	3:A:227:VAL:HB	1.68	0.57
3:A:663:SER:OG	3:A:664:THR:N	2.34	0.57
3:A:879:GLU:OE2	3:A:962:ARG:NH2	2.37	0.57
3:A:901:LEU:H	3:A:926:GLN:HE21	1.50	0.57
3:A:1315:GLU:O	3:A:1318:THR:HG23	2.04	0.57
4:B:756:ILE:O	4:B:759:PRO:HD3	2.04	0.57
4:B:1079:LYS:HA	5:C:27:LEU:HD21	1.87	0.57
7:F:87:LYS:HE2	7:F:88:TYR:CZ	2.39	0.57
3:A:577:ILE:O	3:A:580:VAL:HG23	2.04	0.57
3:A:741:ASN:C	3:A:741:ASN:ND2	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:46:TYR:HA	6:E:57:MET:SD	2.43	0.57
8:H:97:MET:CE	8:H:142:LEU:HD23	2.35	0.57
3:A:353:ILE:HG22	3:A:468:PHE:HB2	1.85	0.57
3:A:619:LYS:O	3:A:623:GLY:N	2.38	0.57
3:A:1300:LYS:NZ	3:A:1300:LYS:HB3	2.20	0.57
4:B:130:VAL:CG2	4:B:167:ILE:HD12	2.34	0.57
4:B:983:ARG:HD2	4:B:1091:TYR:HB3	1.86	0.57
5:C:37:MET:HG2	5:C:243:VAL:CG1	2.34	0.57
5:C:56:THR:CG2	5:C:57:VAL:H	2.09	0.57
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.45	0.57
9:I:29:CYS:C	9:I:31:THR:H	2.13	0.57
11:K:50:LEU:CD1	11:K:73:LEU:HD21	2.35	0.57
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.86	0.57
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.36	0.57
12:L:62:LYS:C	12:L:64:LEU:H	2.13	0.57
3:A:63:ARG:HA	3:A:74:MET:HE2	1.86	0.57
3:A:225:ASN:C	3:A:227:VAL:H	2.10	0.57
3:A:567:LYS:NZ	8:H:95:TYR:CE1	2.71	0.57
4:B:806:THR:C	4:B:808:ALA:H	2.12	0.57
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.69	0.57
3:A:69:THR:HB	4:B:1174:LYS:HE2	1.87	0.57
3:A:1342:GLU:HG3	6:E:198:ILE:HG21	1.86	0.57
4:B:211:VAL:CG2	4:B:483:LEU:HD13	2.32	0.57
4:B:973:ILE:HG23	4:B:974:PRO:HD2	1.87	0.57
4:B:1051:THR:HG22	4:B:1052:VAL:N	2.17	0.57
4:B:1106:ARG:HH12	4:B:1118:PRO:HB3	1.67	0.57
3:A:399:HIS:O	3:A:435:HIS:HD2	1.87	0.57
3:A:565:ILE:CG2	3:A:567:LYS:HG2	2.31	0.57
3:A:1420:ASP:O	3:A:1421:CYS:HB2	2.04	0.57
4:B:704:ALA:HB1	4:B:710:LEU:HD12	1.87	0.57
4:B:1147:LEU:HD22	4:B:1151:LEU:CD2	2.34	0.57
3:A:1436:ILE:HG22	4:B:1142:GLY:HA2	1.87	0.56
4:B:955:THR:OG1	12:L:55:ILE:HA	2.04	0.56
4:B:984:HIS:HB3	4:B:1022:THR:OG1	2.05	0.56
4:B:1072:MET:HE3	4:B:1085:ILE:HB	1.86	0.56
5:C:258:ILE:O	5:C:261:ALA:HB3	2.04	0.56
11:K:46:ILE:HG22	11:K:50:LEU:HD12	1.86	0.56
3:A:185:TRP:CZ3	3:A:200:ARG:HG2	2.40	0.56
3:A:401:GLY:O	3:A:435:HIS:CD2	2.58	0.56
3:A:537:ARG:HB2	8:H:20:TYR:CE2	2.39	0.56
4:B:429:PHE:HA	4:B:432:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:384:ASN:O	3:A:385:ILE:C	2.48	0.56
3:A:672:ASP:HB3	3:A:675:THR:OG1	2.05	0.56
3:A:882:SER:HA	3:A:952:ALA:O	2.04	0.56
3:A:1364:ASN:ND2	3:A:1366:ARG:N	2.53	0.56
3:A:1364:ASN:HD21	3:A:1366:ARG:HG2	1.68	0.56
6:E:22:MET:HE1	6:E:135:PHE:CE2	2.40	0.56
8:H:89:LEU:HD22	8:H:91:ASP:OD2	2.05	0.56
9:I:7:CYS:O	9:I:8:ARG:O	2.24	0.56
9:I:78:CYS:SG	9:I:106:CYS:SG	3.02	0.56
3:A:35:ILE:HG12	3:A:52:GLY:O	2.06	0.56
4:B:57:TYR:N	4:B:57:TYR:HD1	2.03	0.56
4:B:121:ASN:N	4:B:121:ASN:ND2	2.50	0.56
4:B:311:LEU:HB3	9:I:4:PHE:CE2	2.40	0.56
4:B:522:VAL:HG11	4:B:537:LYS:HB3	1.86	0.56
4:B:566:LEU:HD22	4:B:586:TRP:O	2.06	0.56
4:B:979:LYS:HG2	4:B:1095:LEU:HD12	1.86	0.56
8:H:6:PHE:HE1	8:H:130:ARG:HE	1.53	0.56
1:D:8:DT:H2'	1:D:9:DG:O4'	2.04	0.56
3:A:547:LEU:HD22	11:K:58:PHE:CD1	2.41	0.56
3:A:1193:LEU:CD2	3:A:1267:MET:HE2	2.35	0.56
3:A:1342:GLU:HG2	6:E:212:ARG:NH1	2.20	0.56
4:B:243:ALA:HA	4:B:250:PHE:O	2.05	0.56
3:A:452:LYS:HB3	4:B:1141:HIS:CE1	2.40	0.56
3:A:1017:LEU:HD23	6:E:204:THR:O	2.05	0.56
4:B:1022:THR:HG23	4:B:1022:THR:O	2.05	0.56
6:E:46:TYR:CE2	6:E:58:MET:HA	2.40	0.56
3:A:76:GLU:O	3:A:76:GLU:CG	2.52	0.56
5:C:55:THR:HB	5:C:152:GLU:H	1.70	0.56
5:C:99:LEU:HD23	5:C:99:LEU:N	2.20	0.56
8:H:82:PRO:O	8:H:83:GLN:HB2	2.04	0.56
11:K:65:HIS:HD2	11:K:67:PHE:N	2.02	0.56
2:R:3:C:H2'	2:R:4:C:O4'	2.06	0.56
3:A:838:GLN:O	3:A:842:VAL:HG23	2.06	0.56
4:B:120:ARG:NH1	12:L:54:ARG:NH1	2.54	0.56
4:B:1116:ARG:HD2	4:B:1198:TYR:CG	2.40	0.56
3:A:92:HIS:HD2	3:A:94:GLY:H	1.53	0.56
3:A:233:TRP:C	3:A:235:ILE:H	2.13	0.56
3:A:1096:SER:O	3:A:1099:PRO:HG2	2.05	0.56
3:A:1261:LYS:HA	3:A:1264:GLU:HB3	1.88	0.56
3:A:1359:ASP:C	3:A:1361:SER:H	2.13	0.56
5:C:145:CYS:SG	5:C:146:LYS:N	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.88	0.56
3:A:216:VAL:O	3:A:219:PHE:HB2	2.06	0.56
3:A:1349:TYR:C	3:A:1349:TYR:CD2	2.84	0.56
4:B:958:GLN:O	4:B:960:GLY:N	2.33	0.56
4:B:1171:VAL:HG11	4:B:1191:ILE:HD13	1.88	0.56
5:C:248:ILE:CD1	11:K:101:LEU:HD22	2.35	0.56
3:A:346:ASP:CG	4:B:1108:ARG:HA	2.31	0.55
3:A:849:MET:HE3	3:A:1061:GLY:CA	2.35	0.55
3:A:1351:GLU:O	3:A:1352:VAL:C	2.49	0.55
3:A:1399:ARG:CB	3:A:1408:ILE:HD13	2.28	0.55
4:B:556:THR:HG22	4:B:557:PHE:N	2.20	0.55
7:F:99:LEU:HD12	7:F:99:LEU:O	2.05	0.55
12:L:26:THR:HG22	12:L:27:LEU:N	2.21	0.55
3:A:1308:THR:CG2	3:A:1310:GLY:O	2.55	0.55
3:A:1329:THR:HG22	3:A:1331:SER:N	2.01	0.55
3:A:1389:PHE:O	3:A:1392:SER:HB3	2.05	0.55
4:B:361:LEU:N	4:B:362:PRO:CD	2.69	0.55
5:C:70:ILE:HD11	5:C:144:ILE:HG12	1.88	0.55
5:C:242:GLN:NE2	5:C:246:ARG:HE	2.02	0.55
1:D:4:DT:H2'	1:D:5:DG:H8	1.72	0.55
4:B:864:LYS:HD3	4:B:871:THR:OG1	2.05	0.55
4:B:898:LEU:HD22	4:B:964:VAL:HG11	1.89	0.55
5:C:101:LEU:HD13	5:C:118:LEU:HD23	1.88	0.55
5:C:242:GLN:HE21	5:C:246:ARG:HE	1.54	0.55
6:E:195:VAL:HG22	6:E:213:ILE:HB	1.88	0.55
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.89	0.55
3:A:754:SER:O	3:A:755:PHE:C	2.48	0.55
3:A:825:ILE:HD12	4:B:513:GLN:NE2	2.21	0.55
4:B:120:ARG:HE	4:B:955:THR:CG2	2.20	0.55
4:B:839:MET:CE	4:B:980:PHE:HB2	2.35	0.55
4:B:839:MET:HE1	4:B:980:PHE:HB2	1.89	0.55
8:H:83:GLN:C	8:H:85:GLY:H	2.14	0.55
4:B:479:VAL:HG12	4:B:480:SER:H	1.72	0.55
4:B:801:LYS:O	10:J:52:THR:CG2	2.52	0.55
4:B:980:PHE:HE1	4:B:990:ILE:HD11	1.70	0.55
4:B:1051:THR:CG2	4:B:1052:VAL:N	2.70	0.55
5:C:229:TYR:N	5:C:229:TYR:CD1	2.74	0.55
6:E:121:MET:C	6:E:123:LEU:H	2.13	0.55
11:K:61:TYR:HA	11:K:72:LYS:O	2.06	0.55
3:A:463:ILE:HD11	3:A:469:ARG:HG3	1.89	0.55
3:A:517:ASN:ND2	3:A:1362:TYR:HE2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:548:ASN:HA	11:K:60:ALA:HB1	1.87	0.55
4:B:25:ILE:HD11	4:B:653:VAL:HB	1.89	0.55
4:B:172:ILE:HD13	4:B:178:ASN:CB	2.37	0.55
4:B:864:LYS:HG3	4:B:865:LYS:N	2.21	0.55
3:A:556:TRP:CE3	3:A:558:GLY:HA2	2.41	0.55
3:A:683:ILE:HD11	3:A:764:CYS:CB	2.35	0.55
3:A:1116:LEU:O	3:A:1308:THR:HB	2.07	0.55
4:B:1084:GLN:H	4:B:1084:GLN:CD	2.14	0.55
6:E:195:VAL:HG22	6:E:213:ILE:CB	2.36	0.55
3:A:337:ARG:NE	3:A:839:ARG:NH2	2.55	0.55
3:A:738:LYS:HB2	3:A:740:LEU:HG	1.89	0.55
3:A:875:ALA:HB2	3:A:1366:ARG:HD2	1.88	0.55
3:A:885:THR:HG22	3:A:885:THR:O	2.05	0.55
3:A:1326:ARG:O	3:A:1327:ILE:C	2.49	0.55
4:B:515:HIS:H	4:B:518:HIS:CD2	2.24	0.55
7:F:72:LYS:N	7:F:142:SER:HA	2.22	0.55
7:F:94:LEU:HD21	7:F:122:MET:HA	1.89	0.55
3:A:693:VAL:HG21	3:A:721:PHE:CE1	2.39	0.55
3:A:867:ILE:HG22	3:A:872:GLY:N	2.22	0.55
3:A:885:THR:O	3:A:940:ARG:HG3	2.07	0.55
3:A:1073:GLY:O	3:A:1076:ALA:HB3	2.07	0.55
4:B:35:SER:O	4:B:36:ALA:C	2.50	0.55
4:B:864:LYS:N	4:B:872:GLU:OE1	2.39	0.55
4:B:1180:PHE:O	4:B:1181:GLU:HB2	2.05	0.55
6:E:61:GLN:NE2	6:E:105:PHE:CE2	2.71	0.55
7:F:109:VAL:HG13	7:F:127:GLU:OE1	2.07	0.55
9:I:111:THR:HG22	9:I:112:SER:N	2.19	0.55
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.22	0.55
3:A:233:TRP:C	3:A:235:ILE:N	2.60	0.55
3:A:533:LYS:O	3:A:535:THR:N	2.40	0.55
3:A:665:GLY:HA3	4:B:1086:PHE:CD1	2.41	0.55
3:A:1222:ASN:O	3:A:1223:ASP:HB3	2.06	0.55
3:A:1328:TYR:CG	3:A:1329:THR:N	2.74	0.55
3:A:1341:ILE:HD12	3:A:1379:GLY:O	2.07	0.55
4:B:549:THR:HB	4:B:628:THR:HG23	1.89	0.55
4:B:906:SER:O	4:B:907:GLY:C	2.50	0.55
5:C:238:ILE:HG23	5:C:242:GLN:HB2	1.89	0.55
6:E:46:TYR:CD2	6:E:58:MET:HG2	2.42	0.55
6:E:157:SER:C	6:E:159:ASP:N	2.64	0.55
6:E:176:PRO:HD2	6:E:211:TYR:O	2.07	0.55
9:I:111:THR:CG2	9:I:112:SER:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:63:ARG:O	12:L:64:LEU:O	2.24	0.55
3:A:710:LEU:HD12	3:A:710:LEU:N	2.20	0.54
4:B:566:LEU:HD13	4:B:588:GLY:CA	2.37	0.54
4:B:783:THR:HA	10:J:60:PHE:HE1	1.72	0.54
4:B:911:ILE:HD11	4:B:941:LEU:CD1	2.37	0.54
5:C:162:GLY:HA3	5:C:170:TRP:CE2	2.41	0.54
6:E:16:PHE:CD1	6:E:58:MET:HE2	2.42	0.54
3:A:23:SER:HB3	3:A:233:TRP:CE2	2.41	0.54
3:A:843:LYS:HG3	3:A:1402:PHE:HD1	1.72	0.54
4:B:287:ARG:HG2	4:B:292:ILE:CA	2.27	0.54
4:B:515:HIS:H	4:B:518:HIS:HD2	1.55	0.54
3:A:1339:LEU:HD13	6:E:147:HIS:CD2	2.41	0.54
4:B:63:ILE:HA	4:B:421:PHE:CE2	2.42	0.54
4:B:308:TRP:CH2	9:I:45:ARG:HG2	2.43	0.54
4:B:680:THR:HG22	4:B:681:TRP:H	1.72	0.54
4:B:780:VAL:HG21	10:J:56:LEU:HD13	1.88	0.54
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.47	0.54
10:J:32:GLU:O	10:J:36:LEU:HG	2.07	0.54
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.26	0.54
3:A:646:PHE:O	3:A:650:GLN:HG3	2.08	0.54
3:A:845:LEU:N	3:A:845:LEU:HD23	2.22	0.54
4:B:93:GLY:N	4:B:131:ASP:O	2.37	0.54
4:B:108:VAL:CG1	4:B:109:THR:H	2.18	0.54
6:E:191:LYS:O	6:E:192:ARG:C	2.50	0.54
9:I:62:ILE:HG23	9:I:63:GLY:N	2.22	0.54
3:A:399:HIS:O	3:A:435:HIS:CD2	2.60	0.54
3:A:451:HIS:CE1	3:A:1074:GLU:HG3	2.42	0.54
3:A:741:ASN:ND2	3:A:743:VAL:H	2.05	0.54
3:A:1116:LEU:H	3:A:1308:THR:HG22	1.72	0.54
4:B:756:ILE:HG21	4:B:759:PRO:HB3	1.90	0.54
4:B:784:ASN:ND2	4:B:788:ARG:HD2	2.23	0.54
4:B:837:ASP:OD1	4:B:1020:ARG:NH2	2.41	0.54
7:F:107:VAL:HG12	7:F:109:VAL:H	1.72	0.54
9:I:2:THR:HG22	9:I:2:THR:O	2.07	0.54
3:A:15:LYS:HD2	4:B:1220:ARG:HE	1.72	0.54
3:A:350:ARG:HB2	3:A:488:ASN:OD1	2.08	0.54
3:A:356:ASP:OD2	11:K:65:HIS:HE1	1.90	0.54
3:A:819:GLY:O	3:A:820:GLY:C	2.49	0.54
3:A:902:LEU:HD21	3:A:923:LEU:HD23	1.90	0.54
3:A:1205:LYS:O	3:A:1207:LEU:N	2.41	0.54
3:A:1366:ARG:O	3:A:1369:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:406:LEU:HD12	4:B:545:ILE:HD11	1.89	0.54
6:E:153:HIS:CE1	6:E:184:VAL:HG11	2.43	0.54
12:L:27:LEU:HD13	12:L:37:LYS:HB3	1.90	0.54
3:A:515:GLN:HG3	3:A:516:SER:N	2.22	0.54
3:A:563:PRO:HG3	3:A:572:TRP:CE2	2.42	0.54
3:A:849:MET:CE	3:A:1061:GLY:HA2	2.36	0.54
4:B:179:CYS:SG	4:B:181:LEU:HB2	2.47	0.54
4:B:195:CYS:CB	4:B:782:LEU:HD22	2.37	0.54
5:C:13:ALA:O	11:K:114:LEU:HD13	2.08	0.54
8:H:84:ALA:C	8:H:86:ASP:H	2.13	0.54
3:A:89:PRO:O	3:A:204:THR:HG21	2.07	0.54
4:B:34:ILE:O	4:B:37:PHE:HB3	2.06	0.54
4:B:292:ILE:H	4:B:293:PRO:HD2	1.73	0.54
4:B:484:ASN:ND2	4:B:486:TYR:CD1	2.76	0.54
8:H:59:ILE:HG22	8:H:60:ALA:N	2.21	0.54
8:H:84:ALA:C	8:H:86:ASP:N	2.64	0.54
3:A:122:MET:O	3:A:126:LEU:HG	2.07	0.54
3:A:339:ASN:O	3:A:343:LYS:HG2	2.07	0.54
3:A:556:TRP:CD2	3:A:558:GLY:HA2	2.42	0.54
3:A:768:GLN:HG2	3:A:816:HIS:CA	2.38	0.54
3:A:974:ASP:HB2	8:H:136:LYS:NZ	2.20	0.54
3:A:1194:ARG:HH22	3:A:1237:ILE:HD13	1.73	0.54
4:B:205:ILE:HD11	4:B:461:LEU:HD23	1.90	0.54
4:B:542:MET:HE1	4:B:743:ILE:CG2	2.37	0.54
4:B:708:GLU:C	4:B:710:LEU:H	2.16	0.54
4:B:755:ILE:CG2	4:B:755:ILE:O	2.55	0.54
3:A:226:GLU:HG2	3:A:227:VAL:HG23	1.90	0.54
3:A:1094:VAL:HG13	3:A:1113:THR:CG2	2.37	0.54
4:B:288:ALA:HB1	4:B:331:LEU:CD1	2.38	0.54
5:C:11:ARG:NH2	5:C:229:TYR:CD2	2.68	0.54
5:C:183:TRP:CZ2	5:C:207:CYS:HB3	2.42	0.54
6:E:168:TYR:HB3	6:E:170:LEU:CD2	2.36	0.54
3:A:92:HIS:CD2	3:A:94:GLY:H	2.26	0.53
3:A:367:PRO:HB3	3:A:465:TYR:O	2.08	0.53
3:A:444:PHE:HB3	3:A:458:HIS:CD2	2.43	0.53
3:A:608:ILE:HD12	3:A:613:ILE:CD1	2.38	0.53
3:A:898:ARG:HD2	3:A:899:VAL:H	1.73	0.53
5:C:241:ASP:O	5:C:245:VAL:HG23	2.08	0.53
3:A:38:PRO:N	3:A:270:LEU:HD23	2.22	0.53
3:A:557:ASP:OD2	3:A:559:VAL:HB	2.08	0.53
4:B:102:VAL:HG22	4:B:112:LEU:HD22	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:644:GLU:HG3	4:B:654:ARG:HH22	1.74	0.53
4:B:916:THR:HG22	4:B:918:ILE:HG13	1.90	0.53
6:E:23:VAL:HG12	6:E:28:TYR:HB2	1.89	0.53
10:J:52:THR:O	10:J:52:THR:HG22	2.08	0.53
1:D:10:DG:OP1	4:B:792:MET:HE2	2.08	0.53
3:A:225:ASN:O	3:A:227:VAL:HG23	2.09	0.53
3:A:829:VAL:C	3:A:831:THR:H	2.15	0.53
3:A:1147:THR:HA	3:A:1197:LEU:HD23	1.90	0.53
3:A:1220:PHE:O	3:A:1222:ASN:N	2.42	0.53
3:A:1225:PHE:CE2	3:A:1227:ILE:HD11	2.43	0.53
4:B:235:SER:OG	4:B:236:HIS:HD2	1.91	0.53
4:B:899:ILE:HD11	4:B:910:VAL:O	2.09	0.53
8:H:6:PHE:O	8:H:58:THR:HA	2.08	0.53
10:J:7:CYS:O	10:J:8:PHE:C	2.50	0.53
3:A:696:GLU:OE2	3:A:702:LEU:HD23	2.08	0.53
3:A:963:ILE:HD12	3:A:1049:ILE:HG12	1.88	0.53
4:B:43:LEU:HD13	4:B:812:LEU:CD2	2.38	0.53
4:B:405:ARG:HA	4:B:631:GLY:O	2.09	0.53
4:B:842:ASN:HD22	4:B:845:SER:CB	2.21	0.53
4:B:848:ARG:NH1	10:J:8:PHE:O	2.35	0.53
4:B:1106:ARG:HH21	4:B:1109:GLY:C	2.16	0.53
5:C:189:THR:HG22	5:C:190:ASP:N	2.24	0.53
8:H:5:LEU:CD1	8:H:135:LEU:HG	2.34	0.53
8:H:32:THR:HG22	8:H:33:GLN:HG3	1.90	0.53
12:L:38:LEU:O	12:L:39:SER:CB	2.56	0.53
3:A:154:SER:HB3	3:A:162:VAL:HG23	1.89	0.53
3:A:760:GLN:HB2	4:B:1021:MET:HE1	1.89	0.53
3:A:852:TYR:CE2	7:F:136:ARG:HG2	2.42	0.53
3:A:1116:LEU:HD12	3:A:1329:THR:HG1	1.72	0.53
3:A:1375:MET:HG2	3:A:1382:THR:O	2.08	0.53
3:A:1410:PHE:HD2	4:B:1212:ILE:HD11	1.70	0.53
4:B:287:ARG:CG	4:B:292:ILE:HA	2.26	0.53
5:C:248:ILE:HD13	11:K:101:LEU:HD22	1.89	0.53
6:E:17:ARG:O	6:E:21:GLU:HG3	2.09	0.53
6:E:28:TYR:CE1	6:E:78:LEU:HD12	2.44	0.53
6:E:197:LYS:HG3	6:E:211:TYR:CE2	2.42	0.53
3:A:90:VAL:HG13	3:A:297:GLN:HA	1.90	0.53
3:A:337:ARG:CZ	3:A:839:ARG:HH12	2.22	0.53
4:B:43:LEU:HD13	4:B:812:LEU:HD23	1.90	0.53
5:C:46:ILE:HD13	5:C:157:CYS:CB	2.38	0.53
3:A:134:ARG:HH12	3:A:220:THR:HG22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:552:TRP:NE1	3:A:655:PHE:CD1	2.77	0.53
4:B:463:THR:HG21	4:B:465:ASN:HD22	1.74	0.53
4:B:542:MET:CG	4:B:747:MET:HE3	2.36	0.53
4:B:911:ILE:HD11	4:B:941:LEU:HD12	1.91	0.53
7:F:114:GLU:OE1	7:F:119:ARG:HG3	2.08	0.53
8:H:89:LEU:O	8:H:91:ASP:N	2.37	0.53
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.23	0.53
3:A:384:ASN:OD1	3:A:385:ILE:N	2.42	0.53
4:B:90:ILE:CD1	4:B:432:MET:SD	2.97	0.53
4:B:428:ILE:HG22	4:B:432:MET:HE2	1.91	0.53
4:B:1065:GLN:NE2	4:B:1067:ARG:HG2	2.24	0.53
6:E:78:LEU:HD21	6:E:109:ILE:HD12	1.90	0.53
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.67	0.53
3:A:89:PRO:C	3:A:204:THR:HG21	2.33	0.53
3:A:1375:MET:HE3	3:A:1384:VAL:HG23	1.91	0.53
3:A:1392:SER:O	3:A:1393:ASN:CG	2.52	0.53
8:H:38:LEU:CD1	8:H:125:LEU:HD13	2.38	0.53
9:I:46:HIS:CD2	9:I:48:LEU:HD21	2.44	0.53
3:A:134:ARG:NH1	3:A:220:THR:O	2.42	0.53
3:A:376:TYR:C	3:A:376:TYR:CD2	2.87	0.53
3:A:418:SER:C	3:A:420:ARG:N	2.63	0.53
3:A:529:CYS:HB2	4:B:1015:HIS:CE1	2.43	0.53
3:A:675:THR:CG2	3:A:736:ASN:HD21	2.22	0.53
4:B:234:ILE:HG21	4:B:257:LYS:HB3	1.91	0.53
4:B:284:ILE:HD13	4:B:324:ILE:HD12	1.91	0.53
4:B:844:SER:OG	4:B:996:ARG:N	2.33	0.53
4:B:875:GLU:O	4:B:877:PRO:HD3	2.09	0.53
4:B:898:LEU:CD2	4:B:964:VAL:HG11	2.38	0.53
7:F:118:LEU:O	7:F:122:MET:HG3	2.08	0.53
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.39	0.53
3:A:114:LEU:HD22	3:A:171:GLN:NE2	2.23	0.52
3:A:261:ASP:OD2	3:A:323:LYS:HD2	2.09	0.52
3:A:710:LEU:H	3:A:710:LEU:CD1	2.19	0.52
3:A:852:TYR:CZ	7:F:136:ARG:HG2	2.44	0.52
3:A:1299:VAL:CG1	3:A:1300:LYS:N	2.72	0.52
4:B:293:PRO:HA	9:I:12:ASN:HD21	1.74	0.52
4:B:750:GLY:O	4:B:751:VAL:C	2.53	0.52
4:B:956:THR:CG2	4:B:960:GLY:HA2	2.38	0.52
6:E:124:VAL:HG22	6:E:132:ILE:CG2	2.39	0.52
11:K:46:ILE:O	11:K:50:LEU:HB2	2.09	0.52
3:A:219:PHE:O	3:A:222:LEU:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:271:ALA:HB3	4:B:285:ILE:CD1	2.40	0.52
4:B:857:ARG:HD2	4:B:945:GLU:OE1	2.08	0.52
5:C:80:LEU:CD2	5:C:129:ILE:HD11	2.28	0.52
7:F:132:LEU:O	7:F:148:VAL:HG23	2.09	0.52
3:A:590:ARG:O	3:A:591:PHE:HB2	2.08	0.52
3:A:670:ILE:HD13	4:B:1067:ARG:CZ	2.39	0.52
3:A:714:PHE:CB	9:I:97:MET:HE1	2.40	0.52
4:B:287:ARG:HA	4:B:291:ILE:O	2.09	0.52
7:F:109:VAL:CG1	7:F:110:ASP:N	2.73	0.52
3:A:442:VAL:O	3:A:457:ALA:HA	2.09	0.52
3:A:1017:LEU:O	3:A:1018:PHE:C	2.53	0.52
3:A:1161:THR:HG22	3:A:1162:VAL:N	2.24	0.52
3:A:1365:TYR:O	3:A:1367:HIS:N	2.42	0.52
4:B:31:TRP:CD1	4:B:807:ARG:NH1	2.78	0.52
4:B:120:ARG:NH2	12:L:54:ARG:HD2	2.24	0.52
4:B:559:SER:HA	4:B:563:MET:HB3	1.91	0.52
4:B:1053:GLU:O	4:B:1054:GLY:C	2.50	0.52
5:C:57:VAL:HG11	10:J:60:PHE:HB2	1.88	0.52
5:C:164:ALA:HA	5:C:167:HIS:O	2.10	0.52
6:E:7:ARG:C	6:E:9:ILE:H	2.17	0.52
6:E:12:LEU:HD22	6:E:55:ARG:CZ	2.39	0.52
9:I:29:CYS:SG	9:I:29:CYS:O	2.66	0.52
11:K:63:VAL:O	11:K:63:VAL:HG23	2.08	0.52
12:L:47:ARG:HG2	12:L:52:GLY:CA	2.39	0.52
3:A:50:ILE:HG22	3:A:51:GLY:N	2.24	0.52
3:A:91:PHE:HB2	3:A:297:GLN:OE1	2.09	0.52
3:A:568:PRO:HB2	5:C:221:TYR:CE1	2.45	0.52
3:A:722:LEU:HD11	3:A:794:PRO:HB3	1.91	0.52
3:A:907:THR:HG22	3:A:908:LEU:N	2.25	0.52
3:A:1116:LEU:N	3:A:1308:THR:HG22	2.25	0.52
4:B:240:ILE:HG23	4:B:240:ILE:O	2.09	0.52
4:B:321:GLY:C	4:B:323:VAL:H	2.17	0.52
4:B:484:ASN:ND2	4:B:486:TYR:CE1	2.77	0.52
4:B:1177:HIS:HB3	4:B:1179:GLN:HE21	1.74	0.52
7:F:97:ARG:NE	7:F:124:GLU:OE1	2.31	0.52
11:K:65:HIS:HD2	11:K:67:PHE:HB2	1.74	0.52
3:A:32:VAL:HG21	3:A:68:GLN:HE22	1.74	0.52
3:A:357:PRO:HG2	4:B:833:TYR:CE1	2.45	0.52
3:A:1029:ARG:HH11	3:A:1029:ARG:HG3	1.74	0.52
4:B:1069:PHE:HA	4:B:1085:ILE:O	2.08	0.52
4:B:1106:ARG:NH2	4:B:1109:GLY:C	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:155:ARG:HD2	6:E:194:GLU:OE2	2.09	0.52
7:F:101:ILE:HD13	7:F:120:ILE:HG22	1.91	0.52
9:I:73:ARG:O	9:I:81:ARG:HA	2.09	0.52
3:A:27:VAL:HG13	3:A:240:PRO:HB3	1.91	0.52
3:A:387:ARG:O	3:A:391:LEU:HG	2.09	0.52
3:A:451:HIS:CD2	3:A:1074:GLU:HG3	2.45	0.52
3:A:808:LEU:O	4:B:728:ARG:NH1	2.43	0.52
3:A:859:SER:OG	3:A:1398:MET:HE1	2.10	0.52
3:A:928:LEU:O	3:A:931:GLU:N	2.42	0.52
3:A:1152:ILE:CG2	3:A:1260:LEU:HD23	2.38	0.52
3:A:1392:SER:O	3:A:1393:ASN:CB	2.58	0.52
4:B:248:SER:O	4:B:249:ARG:HB2	2.09	0.52
4:B:332:ASP:C	4:B:334:ILE:H	2.17	0.52
4:B:614:SER:OG	4:B:627:PHE:HB2	2.09	0.52
12:L:38:LEU:HG	12:L:39:SER:N	2.24	0.52
3:A:365:GLY:HA3	3:A:469:ARG:HB2	1.91	0.52
3:A:507:VAL:N	3:A:508:PRO:CD	2.72	0.52
3:A:847:ASP:OD2	3:A:858:ASN:HB2	2.10	0.52
4:B:120:ARG:HB2	4:B:122:LEU:HG	1.91	0.52
4:B:737:THR:CG2	9:I:66:PRO:HB2	2.40	0.52
4:B:825:VAL:HG12	4:B:826:ALA:N	2.24	0.52
4:B:864:LYS:HD3	4:B:871:THR:HA	1.91	0.52
10:J:7:CYS:SG	10:J:9:SER:HB2	2.50	0.52
3:A:96:ILE:O	3:A:100:LYS:HG3	2.10	0.52
3:A:817:ALA:HA	4:B:764:SER:OG	2.10	0.52
4:B:292:ILE:N	4:B:293:PRO:HD2	2.25	0.52
4:B:552:MET:N	4:B:553:PRO:HD2	2.24	0.52
6:E:58:MET:O	6:E:59:SER:C	2.53	0.52
3:A:167:CYS:HB2	3:A:169:ASN:ND2	2.24	0.52
3:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.73	0.52
3:A:836:TYR:CE2	3:A:840:ARG:HD2	2.45	0.52
3:A:1394:THR:CG2	3:A:1398:MET:HE3	2.40	0.52
4:B:1084:GLN:HG2	5:C:201:TRP:CZ2	2.45	0.52
4:B:1197:PRO:HG2	4:B:1200:ALA:CB	2.40	0.52
1:D:2:DA:OP1	3:A:1403:GLU:O	2.29	0.51
3:A:929:LEU:H	3:A:929:LEU:CD2	2.23	0.51
3:A:1269:GLU:OE2	4:B:263:GLY:HA3	2.10	0.51
4:B:98:THR:OG1	4:B:127:GLY:HA3	2.09	0.51
4:B:230:ALA:C	4:B:232:SER:H	2.17	0.51
4:B:577:ALA:HB1	4:B:589:VAL:HG11	1.91	0.51
4:B:834:ASN:O	4:B:1013:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:93:ASP:OD1	5:C:122:SER:HB2	2.09	0.51
6:E:23:VAL:HG13	6:E:28:TYR:CD1	2.45	0.51
6:E:102:GLU:C	6:E:104:ASN:N	2.67	0.51
8:H:138:GLU:O	8:H:139:ASN:C	2.53	0.51
10:J:9:SER:CB	10:J:45:CYS:HB2	2.40	0.51
1:D:1:DA:H2'	1:D:2:DA:H8	1.70	0.51
3:A:22:PHE:HB2	4:B:1211:ASN:CG	2.35	0.51
3:A:49:LYS:HB3	3:A:55:ASP:HB2	1.92	0.51
3:A:167:CYS:C	3:A:169:ASN:H	2.18	0.51
3:A:407:ARG:HD2	3:A:413:ILE:HD11	1.91	0.51
3:A:540:PHE:C	3:A:541:ILE:HD12	2.35	0.51
3:A:666:ILE:O	3:A:667:GLY:C	2.53	0.51
4:B:563:MET:HE2	4:B:588:GLY:HA3	1.92	0.51
4:B:846:ILE:HD13	4:B:974:PRO:HG2	1.91	0.51
4:B:1034:VAL:HG12	4:B:1035:ALA:N	2.23	0.51
6:E:5:ASN:O	6:E:9:ILE:HG13	2.10	0.51
10:J:54:VAL:O	10:J:56:LEU:N	2.43	0.51
3:A:530:GLY:O	3:A:531:ILE:C	2.54	0.51
3:A:753:GLY:HA2	3:A:757:ASN:HD22	1.74	0.51
3:A:1074:GLU:C	3:A:1076:ALA:H	2.18	0.51
4:B:25:ILE:HG22	4:B:26:THR:N	2.24	0.51
7:F:109:VAL:CG2	7:F:124:GLU:HG2	2.40	0.51
3:A:384:ASN:OD1	3:A:388:LEU:HD12	2.10	0.51
3:A:737:LEU:HD11	3:A:758:ILE:HG21	1.92	0.51
3:A:1299:VAL:CG1	3:A:1300:LYS:H	2.20	0.51
4:B:271:ALA:O	4:B:279:ASP:HA	2.11	0.51
4:B:755:ILE:O	4:B:755:ILE:HG22	2.09	0.51
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.10	0.51
3:A:1319:VAL:CG1	3:A:1320:PRO:HD2	2.39	0.51
3:A:1364:ASN:ND2	3:A:1366:ARG:HH11	2.09	0.51
4:B:59:LEU:HD11	4:B:417:PHE:CZ	2.44	0.51
4:B:737:THR:CG2	9:I:66:PRO:CB	2.89	0.51
4:B:1169:MET:HE3	4:B:1205:GLN:HG2	1.93	0.51
4:B:1200:ALA:O	4:B:1201:LYS:C	2.54	0.51
5:C:263:THR:C	5:C:265:MET:H	2.18	0.51
3:A:13:THR:HG23	3:A:1432:GLN:NE2	2.24	0.51
3:A:443:LEU:HD11	4:B:1138:MET:SD	2.50	0.51
3:A:715:GLU:OE2	3:A:774:ARG:NH1	2.43	0.51
3:A:898:ARG:HD2	3:A:899:VAL:N	2.26	0.51
3:A:901:LEU:HD23	3:A:907:THR:HG23	1.92	0.51
3:A:1376:THR:HG23	6:E:212:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:46:GLN:NE2	4:B:496:ARG:HA	2.25	0.51
4:B:271:ALA:HB3	4:B:285:ILE:HD11	1.93	0.51
4:B:648:HIS:NE2	4:B:650:GLU:OE1	2.43	0.51
4:B:827:ILE:HG12	4:B:1012:ILE:HD11	1.93	0.51
5:C:177:GLU:HG3	5:C:231:ASN:HB3	1.93	0.51
7:F:77:ASP:O	7:F:78:GLN:HB2	2.09	0.51
1:D:10:DG:OP1	4:B:857:ARG:NH2	2.44	0.51
1:D:12:DC:C2	2:R:1:G:N2	2.75	0.51
3:A:795:GLU:HG2	4:B:731:VAL:HG21	1.93	0.51
4:B:130:VAL:CG1	4:B:131:ASP:N	2.74	0.51
4:B:563:MET:HG3	4:B:563:MET:O	2.10	0.51
4:B:707:PRO:CG	4:B:708:GLU:H	2.21	0.51
4:B:890:TYR:C	4:B:892:LYS:H	2.19	0.51
4:B:1162:ILE:HD11	4:B:1194:ILE:CD1	2.41	0.51
5:C:5:GLY:O	5:C:6:PRO:C	2.54	0.51
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.73	0.51
9:I:50:THR:HG22	9:I:52:ILE:H	1.75	0.51
3:A:340:LEU:HD21	4:B:1200:ALA:CB	2.40	0.51
3:A:535:THR:HG23	3:A:575:LYS:HE2	1.93	0.51
3:A:587:HIS:HA	3:A:607:ILE:O	2.11	0.51
3:A:821:ARG:HG3	3:A:825:ILE:CD1	2.40	0.51
3:A:1444:MET:HE2	7:F:135:ARG:HB2	1.92	0.51
4:B:25:ILE:CG2	4:B:29:ASP:HB3	2.40	0.51
4:B:283:VAL:HG13	4:B:297:ILE:CD1	2.41	0.51
4:B:879:ARG:HD3	4:B:885:MET:HE2	1.92	0.51
4:B:1035:ALA:HB1	4:B:1040:ASN:O	2.10	0.51
4:B:1098:MET:O	4:B:1099:VAL:C	2.53	0.51
4:B:1106:ARG:HH12	4:B:1118:PRO:CB	2.24	0.51
4:B:1177:HIS:C	4:B:1179:GLN:N	2.68	0.51
5:C:62:PHE:C	5:C:62:PHE:CD2	2.89	0.51
9:I:25:LEU:HD12	9:I:26:LEU:H	1.76	0.51
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.92	0.51
3:A:326:ARG:HG2	3:A:1406:VAL:CG2	2.39	0.51
3:A:542:GLU:C	3:A:546:VAL:HG23	2.36	0.51
3:A:1362:TYR:OH	3:A:1364:ASN:HA	2.11	0.51
3:A:1410:PHE:C	3:A:1412:ALA:N	2.68	0.51
4:B:428:ILE:O	4:B:431:TYR:HB3	2.10	0.51
4:B:542:MET:HE2	4:B:747:MET:HE2	1.93	0.51
4:B:642:ASP:HB3	4:B:649:LYS:CD	2.41	0.51
4:B:1163:CYS:SG	4:B:1182:CYS:SG	3.08	0.51
5:C:66:ARG:NH2	10:J:2:ILE:CG2	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:751:SER:O	3:A:752:LYS:CG	2.59	0.51
3:A:810:PRO:O	3:A:813:PHE:HB3	2.11	0.51
3:A:888:GLY:O	3:A:940:ARG:NH2	2.44	0.51
3:A:893:PHE:CE1	3:A:940:ARG:HD2	2.46	0.51
3:A:1214:GLU:O	3:A:1218:GLN:HG2	2.10	0.51
4:B:283:VAL:O	4:B:286:PHE:HB2	2.11	0.51
4:B:653:VAL:C	4:B:654:ARG:HG2	2.36	0.51
4:B:1159:ARG:CD	4:B:1193:GLN:HG3	2.31	0.51
5:C:33:LEU:HG	5:C:37:MET:CE	2.41	0.51
11:K:24:ASP:HB3	11:K:30:ALA:HB3	1.93	0.51
3:A:41:MET:HG2	3:A:49:LYS:HG2	1.92	0.50
3:A:135:PHE:HD1	3:A:222:LEU:HD22	1.76	0.50
3:A:185:TRP:HZ3	3:A:200:ARG:HG2	1.74	0.50
3:A:329:LEU:HD22	4:B:1203:LEU:CD1	2.41	0.50
3:A:1405:THR:O	3:A:1406:VAL:C	2.54	0.50
3:A:1410:PHE:CE2	4:B:1212:ILE:HD11	2.45	0.50
11:K:55:LYS:CD	11:K:78:THR:HB	2.41	0.50
3:A:15:LYS:CB	4:B:1220:ARG:HG2	2.33	0.50
3:A:376:TYR:OH	3:A:498:ARG:HD2	2.11	0.50
3:A:567:LYS:NZ	8:H:46:LEU:CB	2.67	0.50
3:A:1166:ASP:CG	3:A:1194:ARG:HH21	2.19	0.50
3:A:1384:VAL:HG12	3:A:1384:VAL:O	2.11	0.50
4:B:100:PRO:HG3	4:B:172:ILE:HD12	1.92	0.50
5:C:18:VAL:HG12	5:C:20:PHE:HD2	1.76	0.50
12:L:27:LEU:HD13	12:L:37:LYS:CG	2.41	0.50
3:A:50:ILE:C	3:A:52:GLY:N	2.69	0.50
3:A:394:ASN:OD1	3:A:398:GLU:OE1	2.30	0.50
3:A:1312:ASN:O	3:A:1316:VAL:HG23	2.11	0.50
4:B:195:CYS:SG	4:B:197:PHE:HB2	2.51	0.50
4:B:514:LEU:HD12	4:B:515:HIS:H	1.74	0.50
5:C:254:LYS:HE2	11:K:42:LEU:HD13	1.94	0.50
11:K:91:CYS:O	11:K:95:ILE:HG13	2.11	0.50
12:L:62:LYS:O	12:L:64:LEU:HG	2.11	0.50
3:A:500:GLU:OE1	4:B:1143:ALA:HB1	2.11	0.50
3:A:573:SER:O	3:A:576:GLN:HB2	2.11	0.50
4:B:542:MET:HG3	4:B:747:MET:CE	2.38	0.50
4:B:1060:ARG:C	4:B:1062:HIS:N	2.69	0.50
9:I:29:CYS:SG	9:I:31:THR:HG22	2.52	0.50
9:I:68:LEU:HB3	9:I:84:VAL:HG22	1.94	0.50
3:A:341:MET:CE	3:A:1401:SER:HB2	2.41	0.50
4:B:485:ARG:NH2	4:B:782:LEU:HD11	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:864:LYS:HG2	4:B:871:THR:HG23	1.93	0.50
6:E:168:TYR:HB3	6:E:170:LEU:CG	2.41	0.50
8:H:31:THR:O	8:H:32:THR:HB	2.11	0.50
9:I:75:CYS:O	9:I:77:LYS:N	2.44	0.50
11:K:101:LEU:O	11:K:101:LEU:HD23	2.11	0.50
3:A:105:CYS:SG	3:A:138:ILE:HG22	2.52	0.50
3:A:107:CYS:HB2	3:A:114:LEU:HD23	1.93	0.50
3:A:649:ILE:O	3:A:653:VAL:HG23	2.11	0.50
3:A:1376:THR:HG23	3:A:1376:THR:O	2.12	0.50
4:B:240:ILE:O	4:B:253:THR:HG23	2.11	0.50
4:B:751:VAL:HG12	4:B:752:ALA:N	2.26	0.50
8:H:128:ASN:O	8:H:131:ASN:ND2	2.45	0.50
10:J:32:GLU:CD	10:J:32:GLU:H	2.20	0.50
3:A:31:SER:HB2	3:A:83:HIS:HB2	1.91	0.50
3:A:444:PHE:CB	3:A:458:HIS:HD2	2.24	0.50
3:A:612:ILE:HG23	3:A:612:ILE:O	2.12	0.50
4:B:653:VAL:CG2	4:B:689:LEU:HB3	2.42	0.50
4:B:975:GLN:O	4:B:990:ILE:HD12	2.12	0.50
4:B:1119:VAL:O	4:B:1126:GLY:HA3	2.11	0.50
5:C:77:ILE:HG23	5:C:161:LYS:HE3	1.94	0.50
10:J:36:LEU:HD13	10:J:47:ARG:HG2	1.92	0.50
3:A:100:LYS:NZ	3:A:176:LYS:HD2	2.27	0.50
3:A:1189:SER:OG	3:A:1190:PRO:HD2	2.12	0.50
4:B:314:LEU:O	4:B:315:LYS:C	2.53	0.50
4:B:579:ARG:HB2	4:B:586:TRP:NE1	2.27	0.50
6:E:177:ARG:O	6:E:212:ARG:HD3	2.11	0.50
8:H:44:VAL:O	8:H:44:VAL:HG12	2.12	0.50
8:H:59:ILE:O	8:H:60:ALA:HB3	2.12	0.50
9:I:8:ARG:HG3	9:I:9:ASP:CG	2.37	0.50
9:I:15:TYR:N	9:I:15:TYR:CD1	2.79	0.50
9:I:75:CYS:C	9:I:77:LYS:H	2.20	0.50
12:L:40:LEU:HD13	12:L:44:ASP:OD1	2.11	0.50
3:A:167:CYS:O	3:A:169:ASN:N	2.45	0.50
3:A:332:LYS:HG3	3:A:333:GLU:HG2	1.94	0.50
3:A:545:GLN:O	3:A:548:ASN:N	2.44	0.50
3:A:567:LYS:HD2	3:A:568:PRO:HD2	1.92	0.50
3:A:644:LYS:O	3:A:645:LEU:C	2.55	0.50
3:A:1436:ILE:CG2	3:A:1437:GLY:N	2.72	0.50
4:B:581:PHE:HB2	4:B:625:LYS:HG2	1.93	0.50
4:B:758:PHE:C	4:B:760:ASP:N	2.68	0.50
5:C:43:THR:CG2	5:C:44:LEU:N	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:306:ASN:HD21	3:A:324:SER:N	2.08	0.49
3:A:821:ARG:CG	3:A:825:ILE:HD11	2.41	0.49
3:A:1001:ARG:HG2	3:A:1001:ARG:HH11	1.77	0.49
4:B:377:PHE:C	4:B:379:GLY:N	2.68	0.49
4:B:977:GLY:C	4:B:1099:VAL:HG23	2.37	0.49
6:E:98:ILE:O	6:E:102:GLU:HG3	2.12	0.49
7:F:82:THR:HG22	7:F:84:TYR:H	1.77	0.49
9:I:75:CYS:O	9:I:76:PRO:C	2.52	0.49
10:J:16:ASP:OD1	10:J:17:LYS:HE3	2.12	0.49
12:L:52:GLY:O	12:L:54:ARG:HG3	2.12	0.49
3:A:54:ASN:HA	3:A:58:LEU:HD12	1.95	0.49
3:A:466:SER:HB3	11:K:2:ASN:ND2	2.28	0.49
3:A:666:ILE:CD1	4:B:1030:LEU:HD22	2.41	0.49
3:A:857:ARG:HG2	3:A:863:VAL:HA	1.94	0.49
3:A:1134:ILE:O	3:A:1138:ILE:HG13	2.12	0.49
4:B:635:ARG:NH1	4:B:742:GLU:OE2	2.45	0.49
4:B:858:SER:HA	4:B:966:VAL:O	2.11	0.49
4:B:911:ILE:HD11	4:B:941:LEU:HB2	1.94	0.49
6:E:54:GLN:O	6:E:57:MET:HB3	2.11	0.49
8:H:76:THR:O	8:H:76:THR:HG22	2.11	0.49
8:H:88:SER:O	8:H:89:LEU:HG	2.12	0.49
11:K:61:TYR:CD1	11:K:61:TYR:C	2.89	0.49
1:D:2:DA:H4'	3:A:1403:GLU:OE2	2.12	0.49
3:A:78:PRO:O	3:A:79:GLY:C	2.56	0.49
3:A:709:THR:CB	3:A:712:GLU:HG3	2.41	0.49
3:A:1142:THR:O	3:A:1273:LEU:HD22	2.12	0.49
3:A:1153:TYR:HA	9:I:41:PRO:O	2.12	0.49
4:B:260:GLY:O	4:B:267:ARG:HD3	2.12	0.49
4:B:269:ILE:CD1	4:B:386:LEU:HD21	2.39	0.49
4:B:734:HIS:O	4:B:735:ALA:HB2	2.12	0.49
5:C:62:PHE:C	5:C:62:PHE:HD2	2.20	0.49
8:H:49:VAL:CG1	8:H:50:ALA:N	2.74	0.49
11:K:97:LYS:O	11:K:100:ALA:HB3	2.12	0.49
3:A:61:ILE:HA	3:A:74:MET:SD	2.53	0.49
3:A:74:MET:O	3:A:75:ASN:HB2	2.13	0.49
3:A:738:LYS:NZ	5:C:194:GLU:HA	2.26	0.49
3:A:1155:ASP:CG	3:A:1162:VAL:HG23	2.37	0.49
3:A:1410:PHE:C	3:A:1412:ALA:H	2.19	0.49
4:B:332:ASP:C	4:B:334:ILE:N	2.68	0.49
4:B:351:TYR:O	4:B:355:ILE:HG13	2.13	0.49
4:B:365:THR:HG23	4:B:367:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:763:GLN:CG	4:B:765:PRO:HD2	2.40	0.49
4:B:873:THR:O	4:B:914:LYS:HA	2.12	0.49
6:E:7:ARG:C	6:E:9:ILE:N	2.71	0.49
3:A:332:LYS:H	3:A:337:ARG:HD2	1.76	0.49
3:A:606:LEU:HB2	3:A:614:PHE:CE2	2.47	0.49
3:A:741:ASN:ND2	3:A:743:VAL:N	2.60	0.49
3:A:834:THR:HG21	3:A:1077:THR:CA	2.43	0.49
4:B:570:VAL:HG11	4:B:573:GLN:OE1	2.13	0.49
4:B:660:LYS:O	4:B:663:ALA:HB3	2.13	0.49
4:B:958:GLN:C	4:B:960:GLY:H	2.20	0.49
4:B:1043:ASP:O	4:B:1050:ILE:HD12	2.12	0.49
5:C:4:GLU:O	5:C:5:GLY:O	2.31	0.49
5:C:22:LEU:CD1	5:C:230:MET:HE1	2.42	0.49
5:C:236:GLY:C	5:C:238:ILE:N	2.69	0.49
6:E:46:TYR:HE2	6:E:58:MET:HA	1.76	0.49
7:F:133:VAL:HG22	7:F:147:SER:HA	1.95	0.49
8:H:47:PHE:HB2	8:H:95:TYR:HD1	1.76	0.49
9:I:101:PHE:O	9:I:109:ILE:HA	2.12	0.49
11:K:78:THR:O	11:K:79:GLU:C	2.56	0.49
1:D:2:DA:H5'	3:A:1403:GLU:HB3	1.95	0.49
3:A:1436:ILE:O	3:A:1437:GLY:C	2.56	0.49
4:B:55:VAL:HG12	4:B:56:ASP:N	2.27	0.49
4:B:291:ILE:HD13	4:B:300:HIS:CD2	2.48	0.49
4:B:756:ILE:CG2	4:B:759:PRO:HB3	2.42	0.49
4:B:896:ASP:OD2	12:L:58:LYS:HE3	2.13	0.49
4:B:1208:MET:HA	4:B:1212:ILE:O	2.12	0.49
5:C:31:ASN:O	5:C:32:SER:C	2.56	0.49
3:A:918:GLU:O	3:A:918:GLU:HG3	2.12	0.49
3:A:1046:LEU:O	3:A:1047:SER:C	2.55	0.49
3:A:1364:ASN:HD21	3:A:1366:ARG:HH11	1.60	0.49
4:B:488:TYR:CE2	4:B:813:LYS:HB2	2.48	0.49
4:B:709:ASP:C	4:B:710:LEU:HD23	2.38	0.49
4:B:800:GLN:OE1	4:B:822:ASN:HB2	2.12	0.49
4:B:957:ASN:O	4:B:958:GLN:C	2.55	0.49
10:J:1:MET:N	10:J:56:LEU:HB2	2.17	0.49
1:D:2:DA:C5'	3:A:1403:GLU:HB3	2.43	0.49
3:A:378:GLU:HG2	3:A:388:LEU:HD11	1.95	0.49
3:A:874:ASP:HA	3:A:1058:VAL:HG22	1.95	0.49
3:A:890:ASP:H	3:A:1296:GLY:HA3	1.77	0.49
3:A:1066:VAL:O	3:A:1068:ALA:N	2.46	0.49
3:A:1074:GLU:C	3:A:1076:ALA:N	2.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1121:GLU:O	3:A:1122:PRO:C	2.56	0.49
4:B:185:THR:O	4:B:189:LEU:HG	2.11	0.49
4:B:1054:GLY:O	4:B:1058:LEU:HG	2.13	0.49
5:C:212:PRO:HB3	5:C:213:PRO:HD2	1.95	0.49
5:C:254:LYS:O	5:C:258:ILE:HD13	2.13	0.49
6:E:102:GLU:O	6:E:104:ASN:N	2.46	0.49
8:H:36:CYS:HA	8:H:126:GLU:O	2.13	0.49
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.95	0.49
10:J:48:ARG:NH2	10:J:49:MET:HE1	2.20	0.49
1:D:6:DC:H4'	3:A:447:GLN:HE22	1.78	0.49
3:A:69:THR:O	3:A:69:THR:HG22	2.12	0.49
3:A:475:THR:CG2	3:A:476:SER:N	2.76	0.49
3:A:873:MET:HE3	3:A:957:PRO:HG3	1.94	0.49
3:A:1150:SER:HB2	3:A:1195:LEU:HD23	1.93	0.49
4:B:171:PRO:HD2	4:B:457:LEU:CD1	2.43	0.49
4:B:781:PHE:O	4:B:782:LEU:HG	2.12	0.49
4:B:821:GLN:OE1	4:B:850:LEU:HD12	2.13	0.49
4:B:977:GLY:CA	4:B:1099:VAL:CG2	2.86	0.49
4:B:1118:PRO:HD3	4:B:1155:SER:HA	1.94	0.49
4:B:1182:CYS:O	4:B:1183:LYS:O	2.31	0.49
6:E:80:VAL:HG22	6:E:109:ILE:HD12	1.94	0.49
7:F:82:THR:HG22	7:F:84:TYR:N	2.27	0.49
8:H:6:PHE:HE1	8:H:130:ARG:NE	2.10	0.49
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.93	0.49
3:A:1348:LEU:CD2	3:A:1372:VAL:HG13	2.39	0.49
4:B:1160:VAL:HG11	4:B:1169:MET:SD	2.53	0.49
5:C:142:VAL:H	10:J:16:ASP:HB3	1.77	0.49
6:E:102:GLU:C	6:E:104:ASN:H	2.20	0.49
9:I:85:PHE:O	9:I:86:PHE:HB3	2.13	0.49
11:K:83:PRO:HA	11:K:86:ALA:HB3	1.95	0.49
3:A:5:GLN:O	4:B:1159:ARG:NH2	2.46	0.48
3:A:13:THR:HG23	3:A:1432:GLN:CD	2.38	0.48
3:A:474:VAL:HG13	3:A:478:TYR:CE1	2.48	0.48
3:A:491:VAL:O	3:A:493:GLN:NE2	2.46	0.48
3:A:538:ASP:OD1	8:H:22:LYS:HB2	2.12	0.48
3:A:994:GLN:NE2	3:A:1019:CYS:HB3	2.27	0.48
3:A:1099:PRO:O	3:A:1102:LYS:HB3	2.13	0.48
3:A:1347:ALA:O	3:A:1348:LEU:C	2.56	0.48
3:A:1349:TYR:O	3:A:1350:LYS:C	2.56	0.48
4:B:1053:GLU:O	4:B:1055:ILE:N	2.46	0.48
4:B:1177:HIS:CB	4:B:1179:GLN:HE21	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:111:LEU:C	7:F:113:GLY:N	2.71	0.48
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.32	0.48
3:A:589:GLN:OE1	3:A:591:PHE:HE1	1.96	0.48
3:A:1284:MET:HG2	3:A:1306:LEU:CD2	2.43	0.48
3:A:1386:ARG:HE	3:A:1387:HIS:CE1	2.32	0.48
3:A:1415:SER:O	3:A:1416:ALA:C	2.56	0.48
4:B:487:THR:HG22	4:B:489:SER:N	2.24	0.48
4:B:737:THR:HG23	9:I:66:PRO:HB2	1.93	0.48
4:B:1060:ARG:O	4:B:1063:GLY:N	2.45	0.48
6:E:205:SER:O	6:E:206:GLY:C	2.54	0.48
8:H:39:THR:O	8:H:123:MET:HA	2.14	0.48
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.94	0.48
11:K:92:ASN:O	11:K:93:SER:C	2.56	0.48
2:R:6:G:O2'	2:R:7:G:H5'	2.13	0.48
2:R:9:A:C8	2:R:9:A:C3'	2.96	0.48
3:A:226:GLU:CG	3:A:227:VAL:N	2.75	0.48
3:A:365:GLY:O	3:A:468:PHE:HA	2.14	0.48
3:A:742:ASN:C	3:A:745:GLN:HB2	2.38	0.48
3:A:783:THR:HG21	3:A:815:PHE:CE2	2.48	0.48
3:A:954:TRP:O	3:A:956:LEU:HG	2.14	0.48
3:A:1049:ILE:O	3:A:1050:GLU:C	2.56	0.48
3:A:1406:VAL:CG1	3:A:1410:PHE:HE1	2.26	0.48
4:B:25:ILE:CG2	4:B:29:ASP:CB	2.90	0.48
4:B:227:LYS:HB2	4:B:395:GLN:OE1	2.14	0.48
4:B:515:HIS:O	4:B:516:ASN:C	2.54	0.48
5:C:142:VAL:H	10:J:16:ASP:CB	2.26	0.48
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.94	0.48
9:I:99:LEU:HB2	9:I:112:SER:HB3	1.94	0.48
3:A:154:SER:HB3	3:A:162:VAL:HG21	1.92	0.48
3:A:178:GLY:O	3:A:179:LEU:HD23	2.13	0.48
3:A:674:PRO:O	3:A:677:ARG:HB3	2.14	0.48
3:A:845:LEU:O	3:A:846:GLU:C	2.57	0.48
3:A:1066:VAL:O	3:A:1067:LEU:C	2.55	0.48
3:A:1068:ALA:O	3:A:1069:ALA:C	2.55	0.48
3:A:1097:GLY:C	3:A:1099:PRO:HD2	2.39	0.48
4:B:380:TYR:CE1	4:B:384:ARG:HD3	2.48	0.48
4:B:526:GLU:CD	4:B:752:ALA:HB3	2.38	0.48
4:B:653:VAL:HG12	4:B:654:ARG:N	2.28	0.48
4:B:726:ALA:HB1	4:B:1051:THR:CG2	2.43	0.48
3:A:226:GLU:HG2	3:A:227:VAL:N	2.29	0.48
3:A:418:SER:HB3	3:A:421:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1152:ILE:HG23	3:A:1260:LEU:CD2	2.43	0.48
4:B:806:THR:C	4:B:808:ALA:N	2.70	0.48
5:C:135:GLN:C	5:C:136:ASP:O	2.56	0.48
3:A:381:THR:O	3:A:384:ASN:N	2.41	0.48
3:A:994:GLN:HE21	3:A:1019:CYS:CB	2.26	0.48
3:A:1100:ARG:NH2	3:A:1330:ASN:HB2	2.28	0.48
4:B:284:ILE:CD1	4:B:324:ILE:HD12	2.43	0.48
4:B:806:THR:HG22	4:B:808:ALA:H	1.79	0.48
4:B:1175:LEU:O	4:B:1176:ASN:CG	2.56	0.48
5:C:43:THR:HG22	5:C:44:LEU:N	2.29	0.48
5:C:62:PHE:O	5:C:66:ARG:HG3	2.13	0.48
5:C:75:MET:HG3	5:C:246:ARG:NH2	2.28	0.48
6:E:78:LEU:HD21	6:E:80:VAL:HG22	1.95	0.48
7:F:87:LYS:HE2	7:F:88:TYR:CE1	2.48	0.48
10:J:57:ILE:HG12	10:J:61:LEU:HD11	1.94	0.48
1:D:5:DG:N2	2:R:8:C:N3	2.61	0.48
3:A:391:LEU:O	3:A:394:ASN:N	2.46	0.48
3:A:774:ARG:O	3:A:775:ILE:C	2.57	0.48
4:B:280:ILE:HD13	4:B:334:ILE:HG12	1.95	0.48
4:B:642:ASP:O	4:B:643:ASP:C	2.56	0.48
4:B:845:SER:HB2	10:J:8:PHE:HB3	1.96	0.48
4:B:890:TYR:O	4:B:892:LYS:N	2.46	0.48
7:F:81:THR:HG22	7:F:82:THR:H	1.78	0.48
9:I:62:ILE:CG2	9:I:63:GLY:N	2.77	0.48
3:A:89:PRO:HG3	3:A:208:LEU:CD1	2.44	0.48
3:A:112:LYS:HG2	3:A:113:LEU:H	1.79	0.48
4:B:51:PHE:CD2	4:B:173:MET:HB3	2.49	0.48
4:B:708:GLU:C	4:B:710:LEU:N	2.72	0.48
6:E:135:PHE:HD2	6:E:140:LEU:HD21	1.79	0.48
6:E:138:ALA:C	6:E:140:LEU:H	2.21	0.48
9:I:50:THR:HG22	9:I:51:ASN:N	2.28	0.48
11:K:83:PRO:O	11:K:87:LEU:N	2.46	0.48
3:A:18:GLN:O	4:B:1215:ARG:CG	2.62	0.48
3:A:869:GLY:O	6:E:204:THR:HG21	2.14	0.48
3:A:1412:ALA:HA	3:A:1417:GLU:OE2	2.14	0.48
4:B:363:HIS:CD2	4:B:585:VAL:HG22	2.49	0.48
5:C:67:LEU:HD11	5:C:155:LEU:HD13	1.95	0.48
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.49	0.48
3:A:14:VAL:H	3:A:1432:GLN:HE22	1.61	0.48
3:A:90:VAL:HG21	3:A:296:LEU:HG	1.95	0.48
3:A:913:LEU:HD11	3:A:981:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1300:LYS:HB3	3:A:1300:LYS:HZ3	1.79	0.48
3:A:1356:ILE:HD12	3:A:1368:MET:SD	2.54	0.48
4:B:46:GLN:HE21	4:B:496:ARG:HG2	1.78	0.48
4:B:956:THR:HG21	4:B:960:GLY:HA2	1.96	0.48
4:B:1065:GLN:HE22	4:B:1067:ARG:HG2	1.79	0.48
6:E:100:ILE:CG2	6:E:105:PHE:HB2	2.42	0.48
8:H:93:TYR:HA	8:H:145:ARG:CB	2.41	0.48
9:I:54:GLU:O	9:I:89:GLN:HG2	2.14	0.48
1:D:9:DG:H1	2:R:4:C:H42	1.62	0.47
3:A:68:GLN:NE2	3:A:80:HIS:CB	2.76	0.47
3:A:443:LEU:CD2	3:A:455:MET:HB3	2.42	0.47
3:A:545:GLN:O	3:A:546:VAL:C	2.55	0.47
3:A:929:LEU:HD21	3:A:983:ILE:HG21	1.94	0.47
4:B:210:LYS:HE2	4:B:461:LEU:O	2.14	0.47
4:B:236:HIS:CE1	4:B:389:ALA:HA	2.49	0.47
4:B:284:ILE:HD13	4:B:333:PHE:CD2	2.49	0.47
4:B:291:ILE:HD13	4:B:300:HIS:NE2	2.29	0.47
4:B:1103:ILE:O	4:B:1104:HIS:C	2.56	0.47
5:C:35:ARG:O	5:C:38:ILE:N	2.47	0.47
8:H:33:GLN:OE1	8:H:129:TYR:CE2	2.67	0.47
3:A:786:HIS:CE1	4:B:742:GLU:OE1	2.64	0.47
3:A:1134:ILE:HD11	3:A:1321:GLY:HA3	1.96	0.47
4:B:825:VAL:CG1	4:B:826:ALA:N	2.76	0.47
4:B:864:LYS:HB3	4:B:871:THR:HA	1.96	0.47
7:F:109:VAL:HG11	7:F:123:LYS:HG2	1.96	0.47
3:A:61:ILE:HG22	3:A:62:ASP:N	2.16	0.47
3:A:742:ASN:O	3:A:745:GLN:HB2	2.13	0.47
3:A:1237:ILE:HG22	3:A:1238:ILE:N	2.29	0.47
3:A:1336:MET:HE1	3:A:1380:GLY:C	2.40	0.47
4:B:294:ASP:H	9:I:12:ASN:ND2	2.13	0.47
4:B:726:ALA:HB1	4:B:1051:THR:HG21	1.95	0.47
4:B:745:PRO:C	4:B:747:MET:N	2.70	0.47
4:B:773:MET:SD	4:B:987:LYS:HD2	2.54	0.47
5:C:66:ARG:CZ	10:J:2:ILE:HG21	2.44	0.47
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.47
3:A:332:LYS:N	3:A:337:ARG:HD2	2.28	0.47
3:A:614:PHE:CD1	3:A:614:PHE:C	2.92	0.47
3:A:783:THR:CG2	3:A:815:PHE:CE2	2.97	0.47
3:A:885:THR:HG23	3:A:893:PHE:CE1	2.36	0.47
4:B:189:LEU:O	4:B:190:TYR:C	2.57	0.47
4:B:300:HIS:ND1	4:B:376:PHE:CD2	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:666:TYR:C	4:B:668:ASP:N	2.72	0.47
4:B:821:GLN:HB2	4:B:851:PHE:CE2	2.49	0.47
4:B:1020:ARG:H	4:B:1020:ARG:HG2	1.51	0.47
4:B:1077:THR:HG22	4:B:1079:LYS:HB2	1.95	0.47
4:B:1124:ARG:O	4:B:1125:ASP:HB3	2.14	0.47
4:B:1156:ASP:HB3	4:B:1197:PRO:HA	1.95	0.47
7:F:79:ARG:HG2	7:F:146:TRP:CZ2	2.49	0.47
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.95	0.47
11:K:43:GLY:HA2	11:K:71:PHE:CZ	2.49	0.47
3:A:545:GLN:OE1	3:A:549:MET:HE2	2.14	0.47
3:A:829:VAL:O	3:A:831:THR:N	2.48	0.47
3:A:1074:GLU:HB3	3:A:1075:PRO:HD3	1.97	0.47
4:B:408:LEU:HD12	4:B:408:LEU:HA	1.71	0.47
4:B:562:GLY:O	4:B:563:MET:C	2.56	0.47
4:B:798:TYR:CD2	10:J:4:PRO:HG3	2.49	0.47
4:B:1177:HIS:C	4:B:1179:GLN:H	2.22	0.47
5:C:258:ILE:HD12	5:C:258:ILE:N	2.30	0.47
6:E:56:LYS:HG3	6:E:84:ASP:CB	2.42	0.47
6:E:117:THR:C	6:E:119:SER:N	2.73	0.47
6:E:137:GLU:O	6:E:138:ALA:C	2.57	0.47
8:H:83:GLN:C	8:H:85:GLY:N	2.73	0.47
3:A:20:GLY:HA2	3:A:1413:GLY:O	2.14	0.47
3:A:533:LYS:C	3:A:535:THR:H	2.23	0.47
4:B:123:THR:O	4:B:125:SER:N	2.47	0.47
9:I:100:PHE:HZ	9:I:118:ARG:HH12	1.62	0.47
1:D:3:DA:H5'	3:A:836:TYR:HE1	1.77	0.47
3:A:12:ARG:HD3	4:B:1218:THR:HB	1.97	0.47
3:A:383:TYR:HB3	7:F:115:THR:CG2	2.44	0.47
3:A:709:THR:C	3:A:711:ARG:N	2.67	0.47
3:A:738:LYS:HB3	8:H:19:ARG:HH22	1.78	0.47
3:A:829:VAL:C	3:A:831:THR:N	2.70	0.47
3:A:1327:ILE:O	6:E:147:HIS:HE1	1.98	0.47
3:A:1436:ILE:CG2	3:A:1437:GLY:H	2.22	0.47
4:B:100:PRO:HD2	4:B:180:TYR:CE1	2.50	0.47
4:B:298:LEU:N	4:B:298:LEU:HD23	2.29	0.47
4:B:566:LEU:CD1	4:B:588:GLY:HA2	2.44	0.47
4:B:726:ALA:CB	4:B:1051:THR:HG21	2.45	0.47
4:B:1013:ASN:OD1	4:B:1015:HIS:HB2	2.15	0.47
4:B:1020:ARG:O	4:B:1021:MET:C	2.58	0.47
4:B:1104:HIS:HB2	4:B:1122:ARG:CD	2.44	0.47
4:B:1158:PHE:HE2	4:B:1201:LYS:HE3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:125:LEU:HG	8:H:130:ARG:CZ	2.43	0.47
12:L:62:LYS:O	12:L:64:LEU:N	2.37	0.47
3:A:515:GLN:HA	3:A:1367:HIS:NE2	2.29	0.47
3:A:679:ILE:HG23	3:A:729:ALA:CB	2.39	0.47
3:A:890:ASP:N	3:A:1296:GLY:HA3	2.30	0.47
3:A:1225:PHE:O	3:A:1240:CYS:HA	2.14	0.47
4:B:830:TYR:CE2	4:B:1000:PRO:HD3	2.50	0.47
4:B:851:PHE:O	4:B:974:PRO:HD3	2.15	0.47
4:B:1033:LYS:NZ	4:B:1070:GLU:OE1	2.46	0.47
4:B:1116:ARG:NH1	4:B:1198:TYR:CD1	2.83	0.47
5:C:75:MET:HG3	5:C:246:ARG:HH22	1.77	0.47
7:F:101:ILE:HD13	7:F:120:ILE:CG2	2.45	0.47
7:F:101:ILE:HD11	7:F:124:GLU:OE1	2.15	0.47
12:L:30:ILE:CD1	12:L:59:ALA:HA	2.44	0.47
3:A:116:ASP:HB2	3:A:118:HIS:CD2	2.49	0.47
3:A:352:VAL:HG12	3:A:353:ILE:N	2.29	0.47
3:A:533:LYS:C	3:A:535:THR:N	2.72	0.47
3:A:567:LYS:NZ	8:H:95:TYR:CD1	2.80	0.47
3:A:568:PRO:HB2	5:C:221:TYR:CZ	2.50	0.47
3:A:881:GLN:OE1	3:A:959:ASN:HA	2.15	0.47
4:B:842:ASN:HD22	4:B:845:SER:HB3	1.80	0.47
4:B:1117:GLN:NE2	4:B:1156:ASP:OD2	2.48	0.47
7:F:98:ALA:O	7:F:117:PRO:HB2	2.14	0.47
10:J:5:VAL:O	10:J:6:ARG:HB2	2.15	0.47
11:K:71:PHE:CD1	11:K:71:PHE:C	2.93	0.47
1:D:6:DC:H2'	1:D:7:DC:C6	2.50	0.47
3:A:83:HIS:CE1	3:A:238:CYS:SG	3.08	0.47
3:A:113:LEU:C	3:A:115:LEU:H	2.23	0.47
3:A:381:THR:CG2	3:A:383:TYR:CD1	2.98	0.47
3:A:573:SER:OG	3:A:576:GLN:HG3	2.15	0.47
3:A:1227:ILE:HG22	3:A:1228:TRP:N	2.30	0.47
3:A:1392:SER:O	3:A:1393:ASN:ND2	2.48	0.47
4:B:96:TYR:N	4:B:96:TYR:CD1	2.83	0.47
4:B:167:ILE:O	4:B:167:ILE:HG22	2.14	0.47
3:A:351:THR:CG2	4:B:1103:ILE:HA	2.36	0.46
3:A:849:MET:HB2	3:A:1063:MET:SD	2.55	0.46
3:A:1209:MET:CG	3:A:1236:LEU:HD22	2.45	0.46
4:B:346:GLU:O	4:B:347:LYS:C	2.58	0.46
4:B:780:VAL:HG21	10:J:56:LEU:HD11	1.97	0.46
4:B:800:GLN:CB	10:J:52:THR:CG2	2.89	0.46
4:B:906:SER:CB	4:B:946:ASN:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1169:MET:SD	4:B:1201:LYS:HG2	2.54	0.46
4:B:1182:CYS:O	4:B:1183:LYS:HD2	2.15	0.46
5:C:18:VAL:HG12	5:C:18:VAL:O	2.15	0.46
5:C:180:TYR:O	5:C:181:ASP:HB3	2.15	0.46
6:E:9:ILE:C	6:E:11:ARG:N	2.71	0.46
6:E:96:PHE:CE2	6:E:110:PHE:HB2	2.50	0.46
8:H:113:ALA:HA	8:H:125:LEU:O	2.15	0.46
9:I:74:GLU:OE1	9:I:79:HIS:ND1	2.47	0.46
3:A:962:ARG:O	3:A:963:ILE:C	2.57	0.46
3:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.46
4:B:31:TRP:CE3	4:B:34:ILE:HD12	2.50	0.46
4:B:225:VAL:HG11	4:B:388:CYS:HB3	1.95	0.46
4:B:300:HIS:ND1	4:B:376:PHE:CE2	2.83	0.46
4:B:871:THR:HG22	4:B:872:GLU:O	2.14	0.46
9:I:34:TYR:O	9:I:35:VAL:HG23	2.16	0.46
3:A:481:ASP:C	3:A:481:ASP:OD1	2.58	0.46
3:A:531:ILE:CD1	3:A:617:VAL:HG11	2.44	0.46
3:A:650:GLN:O	3:A:651:LYS:C	2.58	0.46
3:A:848:ILE:CD1	3:A:1374:VAL:HG21	2.45	0.46
3:A:893:PHE:CD1	3:A:940:ARG:HD2	2.50	0.46
3:A:964:ILE:HD13	3:A:1035:TYR:CZ	2.50	0.46
3:A:975:HIS:ND1	3:A:1036:ARG:HG3	2.30	0.46
4:B:324:ILE:HG23	4:B:329:THR:HB	1.96	0.46
4:B:686:ASN:C	4:B:688:GLY:N	2.70	0.46
5:C:258:ILE:HG23	11:K:19:LEU:HD11	1.96	0.46
6:E:71:LYS:C	6:E:73:PRO:HD3	2.41	0.46
11:K:98:LEU:O	11:K:99:GLY:C	2.58	0.46
3:A:563:PRO:HG3	3:A:572:TRP:CH2	2.48	0.46
3:A:897:TYR:HD2	3:A:936:LEU:HD13	1.78	0.46
3:A:1277:GLU:O	3:A:1278:ASN:HB2	2.14	0.46
3:A:1394:THR:HG21	3:A:1398:MET:SD	2.56	0.46
4:B:802:PRO:HA	4:B:822:ASN:HD21	1.79	0.46
4:B:806:THR:OG1	4:B:809:MET:HE3	2.15	0.46
4:B:1072:MET:O	4:B:1081:LEU:HB2	2.15	0.46
6:E:96:PHE:CE1	6:E:100:ILE:HD11	2.50	0.46
6:E:179:GLN:HA	6:E:179:GLN:OE1	2.16	0.46
10:J:27:GLU:C	10:J:29:GLU:H	2.23	0.46
3:A:152:VAL:CG1	3:A:153:PRO:HD2	2.45	0.46
3:A:1140:HIS:HB2	3:A:1276:VAL:O	2.16	0.46
3:A:1237:ILE:CG2	3:A:1238:ILE:N	2.78	0.46
4:B:282:ILE:HG13	4:B:283:VAL:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:800:GLN:HB3	10:J:52:THR:HG22	1.97	0.46
4:B:1120:GLU:HG2	4:B:1121:GLY:N	2.31	0.46
5:C:252:GLN:CG	11:K:95:ILE:HG23	2.46	0.46
9:I:2:THR:OG1	9:I:45:ARG:HB3	2.15	0.46
3:A:67:CYS:SG	3:A:77:CYS:SG	3.11	0.46
3:A:517:ASN:OD1	3:A:517:ASN:O	2.34	0.46
3:A:535:THR:HG21	3:A:616:VAL:CA	2.43	0.46
3:A:815:PHE:C	3:A:817:ALA:N	2.72	0.46
3:A:894:GLU:C	3:A:896:ARG:N	2.74	0.46
3:A:960:ILE:O	3:A:961:ARG:C	2.57	0.46
3:A:1336:MET:HE1	3:A:1381:LEU:N	2.31	0.46
4:B:62:ILE:HG21	4:B:417:PHE:HD2	1.80	0.46
4:B:199:MET:SD	4:B:199:MET:N	2.87	0.46
4:B:350:GLN:O	4:B:351:TYR:C	2.59	0.46
4:B:860:MET:HB2	4:B:965:LYS:HG2	1.97	0.46
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.97	0.46
12:L:55:ILE:H	12:L:55:ILE:HG12	1.53	0.46
2:R:2:A:H2'	2:R:3:C:H5'	1.91	0.46
3:A:222:LEU:O	3:A:224:PHE:N	2.46	0.46
3:A:294:SER:HA	3:A:297:GLN:HB3	1.96	0.46
3:A:645:LEU:O	3:A:649:ILE:HG13	2.15	0.46
4:B:519:TRP:HE1	4:B:635:ARG:HH22	1.64	0.46
4:B:1017:ILE:HB	4:B:1018:PRO:HD3	1.98	0.46
3:A:50:ILE:HG22	3:A:51:GLY:H	1.81	0.46
3:A:53:LEU:HD13	3:A:263:THR:HG23	1.97	0.46
3:A:418:SER:O	3:A:421:ALA:N	2.49	0.46
3:A:556:TRP:CZ3	3:A:558:GLY:HA2	2.51	0.46
3:A:1041:ALA:O	3:A:1044:TRP:HB3	2.15	0.46
4:B:238:ALA:HB3	4:B:256:VAL:HB	1.98	0.46
4:B:361:LEU:N	4:B:362:PRO:HD2	2.31	0.46
4:B:574:SER:HB3	4:B:577:ALA:HB2	1.98	0.46
5:C:38:ILE:HG13	5:C:176:ILE:HD12	1.97	0.46
5:C:249:ASP:O	5:C:252:GLN:HB3	2.16	0.46
8:H:47:PHE:CD1	8:H:95:TYR:HB2	2.50	0.46
3:A:35:ILE:HD12	3:A:241:VAL:HG21	1.98	0.46
3:A:477:PRO:HG2	3:A:521:MET:HG2	1.97	0.46
3:A:908:LEU:O	3:A:909:ASP:C	2.58	0.46
3:A:1111:MET:CE	3:A:1330:ASN:OD1	2.57	0.46
3:A:1173:HIS:CD2	3:A:1227:ILE:HG23	2.51	0.46
3:A:1208:THR:HG22	3:A:1210:GLY:H	1.81	0.46
4:B:704:ALA:HB2	4:B:738:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:707:PRO:O	4:B:708:GLU:C	2.59	0.46
5:C:242:GLN:OE1	5:C:242:GLN:HA	2.16	0.46
3:A:79:GLY:C	3:A:243:PRO:HG3	2.41	0.46
3:A:446:ARG:HG2	3:A:446:ARG:NH1	2.28	0.46
3:A:517:ASN:ND2	3:A:1362:TYR:CE2	2.83	0.46
3:A:738:LYS:NZ	5:C:194:GLU:CA	2.79	0.46
4:B:25:ILE:HD11	4:B:653:VAL:CB	2.46	0.46
4:B:185:THR:H	4:B:188:ASP:HB2	1.81	0.46
4:B:276:ILE:HD13	4:B:334:ILE:CG2	2.47	0.46
4:B:345:LYS:O	4:B:347:LYS:N	2.49	0.46
4:B:589:VAL:HG12	4:B:590:HIS:H	1.81	0.46
4:B:864:LYS:H	4:B:872:GLU:CG	2.28	0.46
4:B:892:LYS:NZ	4:B:909:ASP:OD2	2.47	0.46
4:B:914:LYS:H	4:B:938:SER:HB3	1.81	0.46
4:B:1100:ASP:HA	4:B:1103:ILE:CG1	2.46	0.46
5:C:29:MET:O	5:C:30:ALA:C	2.58	0.46
6:E:100:ILE:O	6:E:101:GLN:C	2.58	0.46
11:K:73:LEU:CD2	11:K:75:ILE:HD11	2.46	0.46
3:A:112:LYS:HG2	3:A:113:LEU:N	2.31	0.45
3:A:873:MET:C	3:A:1058:VAL:HG23	2.40	0.45
3:A:923:LEU:O	3:A:927:VAL:HG23	2.14	0.45
3:A:982:THR:HB	3:A:985:ASP:CG	2.40	0.45
4:B:215:GLN:HB2	4:B:407:ASP:HB2	1.97	0.45
4:B:230:ALA:N	4:B:231:PRO:HD2	2.31	0.45
4:B:322:PHE:O	4:B:322:PHE:CG	2.69	0.45
4:B:348:ARG:O	4:B:349:ILE:C	2.60	0.45
4:B:605:ARG:CZ	4:B:639:ILE:HD13	2.46	0.45
4:B:995:ARG:NH1	4:B:997:GLU:OE1	2.49	0.45
4:B:1070:GLU:O	4:B:1071:VAL:C	2.59	0.45
4:B:1154:ALA:O	4:B:1155:SER:CB	2.64	0.45
6:E:10:SER:O	6:E:14:ARG:HG3	2.16	0.45
3:A:223:GLY:HA3	3:A:1415:SER:HB3	1.98	0.45
3:A:825:ILE:C	3:A:827:THR:N	2.70	0.45
3:A:1317:MET:CA	3:A:1322:ILE:HD11	2.46	0.45
4:B:201:GLY:H	4:B:202:TYR:HD2	1.63	0.45
4:B:640:VAL:O	4:B:640:VAL:HG12	2.15	0.45
4:B:640:VAL:HG23	4:B:740:HIS:HA	1.97	0.45
4:B:1106:ARG:CD	4:B:1126:GLY:O	2.62	0.45
5:C:262:LEU:O	5:C:265:MET:HB3	2.15	0.45
3:A:47:ARG:O	3:A:48:ALA:HB2	2.16	0.45
3:A:399:HIS:C	3:A:401:GLY:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:658:LEU:HD13	4:B:831:SER:HA	1.98	0.45
3:A:889:SER:HB3	3:A:1297:GLU:HG3	1.97	0.45
3:A:1037:LEU:HD13	3:A:1042:PHE:HA	1.98	0.45
3:A:1098:VAL:O	3:A:1099:PRO:C	2.59	0.45
3:A:1208:THR:HG22	3:A:1210:GLY:N	2.31	0.45
3:A:1336:MET:SD	3:A:1381:LEU:HG	2.56	0.45
4:B:295:GLY:O	4:B:299:GLU:HG3	2.16	0.45
4:B:708:GLU:CG	4:B:709:ASP:N	2.69	0.45
4:B:1085:ILE:CG2	4:B:1086:PHE:N	2.78	0.45
8:H:49:VAL:CG1	8:H:50:ALA:H	2.27	0.45
8:H:114:VAL:O	8:H:124:ARG:HA	2.16	0.45
10:J:1:MET:O	10:J:2:ILE:O	2.33	0.45
3:A:573:SER:H	3:A:576:GLN:HG3	1.81	0.45
3:A:701:LEU:HA	9:I:115:LYS:HE3	1.98	0.45
3:A:866:PHE:C	3:A:867:ILE:HG13	2.40	0.45
3:A:1155:ASP:OD1	3:A:1162:VAL:HG23	2.17	0.45
3:A:1208:THR:N	3:A:1211:GLN:OE1	2.49	0.45
3:A:1433:MET:HE1	7:F:92:ARG:CZ	2.47	0.45
4:B:229:ALA:HB1	4:B:231:PRO:HD2	1.98	0.45
4:B:371:GLU:OE1	4:B:371:GLU:N	2.49	0.45
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.46	0.45
8:H:101:ALA:HB2	8:H:116:TYR:CD2	2.51	0.45
10:J:34:THR:O	10:J:35:ALA:C	2.58	0.45
3:A:567:LYS:CD	3:A:568:PRO:HD2	2.45	0.45
3:A:648:ASN:O	3:A:649:ILE:C	2.59	0.45
3:A:1209:MET:CE	3:A:1236:LEU:HB3	2.47	0.45
4:B:370:PHE:N	4:B:371:GLU:OE1	2.50	0.45
4:B:549:THR:H	4:B:628:THR:HG22	1.81	0.45
4:B:893:LEU:HD22	4:B:897:GLY:O	2.16	0.45
4:B:980:PHE:HE1	4:B:990:ILE:CD1	2.30	0.45
4:B:1085:ILE:HG22	4:B:1086:PHE:N	2.31	0.45
4:B:1158:PHE:CD2	4:B:1198:TYR:HD1	2.35	0.45
6:E:78:LEU:C	6:E:78:LEU:CD2	2.89	0.45
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.30	0.45
11:K:91:CYS:O	11:K:94:ILE:HB	2.16	0.45
3:A:329:LEU:HA	3:A:335:ARG:HB2	1.98	0.45
3:A:420:ARG:O	3:A:424:ILE:HG13	2.16	0.45
3:A:738:LYS:NZ	5:C:194:GLU:C	2.74	0.45
3:A:958:VAL:HG22	3:A:1052:GLN:HB3	1.98	0.45
4:B:240:ILE:C	4:B:253:THR:HG23	2.41	0.45
4:B:484:ASN:CG	4:B:486:TYR:HE1	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:578:THR:HG23	4:B:622:LYS:C	2.42	0.45
4:B:707:PRO:O	4:B:708:GLU:O	2.35	0.45
4:B:824:ILE:CG2	4:B:1087:PHE:CE2	3.00	0.45
5:C:8:VAL:CG1	5:C:9:LYS:N	2.80	0.45
5:C:17:ASN:OD1	5:C:233:GLU:HG2	2.16	0.45
5:C:120:ILE:HD11	5:C:130:GLY:O	2.17	0.45
6:E:136:ASN:C	6:E:136:ASN:OD1	2.60	0.45
6:E:147:HIS:CD2	6:E:149:LEU:H	2.35	0.45
9:I:34:TYR:O	9:I:35:VAL:CG2	2.65	0.45
3:A:69:THR:O	4:B:1174:LYS:HG2	2.17	0.45
3:A:388:LEU:O	3:A:392:VAL:HG23	2.17	0.45
3:A:1220:PHE:O	3:A:1221:LYS:C	2.60	0.45
4:B:50:SER:O	4:B:53:GLN:HB3	2.16	0.45
4:B:365:THR:CG2	4:B:367:LEU:H	2.30	0.45
4:B:1051:THR:HG21	4:B:1053:GLU:HB2	1.97	0.45
5:C:9:LYS:HB2	5:C:21:ILE:HB	1.98	0.45
6:E:112:TYR:CE2	6:E:134:THR:HB	2.51	0.45
7:F:117:PRO:O	7:F:120:ILE:HB	2.16	0.45
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.98	0.45
8:H:111:LEU:HA	8:H:127:GLY:O	2.17	0.45
9:I:99:LEU:HB2	9:I:112:SER:CB	2.46	0.45
3:A:55:ASP:HB3	3:A:56:PRO:HD3	1.98	0.45
3:A:666:ILE:H	3:A:666:ILE:HG13	1.33	0.45
3:A:778:GLY:HA3	4:B:516:ASN:CB	2.46	0.45
3:A:1192:LEU:HD11	3:A:1239:ARG:CB	2.37	0.45
4:B:168:GLY:H	4:B:450:ALA:HB1	1.82	0.45
4:B:702:LEU:HD21	4:B:735:ALA:HB1	1.98	0.45
4:B:737:THR:O	4:B:738:PHE:C	2.60	0.45
4:B:744:HIS:CD2	4:B:746:SER:OG	2.70	0.45
4:B:864:LYS:HD3	4:B:871:THR:CA	2.47	0.45
8:H:40:LEU:HG	8:H:42:ILE:HG13	1.98	0.45
11:K:12:LEU:H	11:K:12:LEU:CD1	2.23	0.45
12:L:45:ALA:O	12:L:46:VAL:CG2	2.64	0.45
3:A:233:TRP:O	3:A:235:ILE:N	2.50	0.45
3:A:340:LEU:HD21	4:B:1200:ALA:CA	2.47	0.45
3:A:456:MET:HB2	3:A:478:TYR:OH	2.17	0.45
3:A:598:LEU:O	3:A:599:SER:C	2.59	0.45
4:B:56:ASP:HB3	4:B:57:TYR:CD1	2.52	0.45
4:B:276:ILE:HD13	4:B:334:ILE:HG23	1.99	0.45
4:B:515:HIS:CD2	4:B:517:THR:OG1	2.66	0.45
4:B:680:THR:O	4:B:683:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:963:PHE:HE2	4:B:965:LYS:HE3	1.81	0.45
4:B:1106:ARG:HG2	4:B:1107:ALA:N	2.31	0.45
5:C:166:GLU:CG	11:K:10:PHE:CZ	2.96	0.45
5:C:186:LEU:HA	5:C:186:LEU:HD12	1.86	0.45
6:E:190:LEU:HD11	6:E:196:VAL:HG11	1.98	0.45
8:H:57:VAL:HG12	8:H:58:THR:N	2.32	0.45
8:H:81:PRO:HD2	8:H:82:PRO:HD2	1.98	0.45
12:L:38:LEU:HG	12:L:39:SER:H	1.82	0.45
3:A:152:VAL:HG13	3:A:153:PRO:HD2	1.99	0.45
3:A:921:GLY:O	3:A:922:ASP:C	2.59	0.45
3:A:974:ASP:CB	8:H:136:LYS:NZ	2.80	0.45
4:B:200:GLY:HA2	4:B:202:TYR:CD2	2.50	0.45
4:B:426:LYS:O	4:B:430:ARG:HG3	2.17	0.45
8:H:11:GLN:C	8:H:28:ALA:HB1	2.42	0.45
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.99	0.45
9:I:7:CYS:HB2	9:I:14:LEU:CD2	2.34	0.45
9:I:92:ARG:CG	9:I:93:LYS:H	2.30	0.45
3:A:210:ILE:O	3:A:214:ILE:HG13	2.17	0.44
3:A:771:GLU:H	3:A:822:GLU:CD	2.25	0.44
4:B:216:GLU:OE1	4:B:537:LYS:CE	2.66	0.44
4:B:260:GLY:HA3	4:B:267:ARG:HG2	1.98	0.44
4:B:316:PRO:HA	4:B:319:GLU:HG2	1.98	0.44
4:B:664:THR:HG1	4:B:678:GLU:N	2.14	0.44
4:B:912:ILE:O	4:B:938:SER:CB	2.59	0.44
4:B:973:ILE:CG2	4:B:974:PRO:HD2	2.47	0.44
6:E:82:PHE:CD1	6:E:82:PHE:N	2.85	0.44
6:E:94:LYS:O	6:E:98:ILE:HG13	2.16	0.44
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.47	0.44
3:A:243:PRO:HB2	3:A:245:PRO:HD2	1.99	0.44
3:A:535:THR:O	3:A:536:LEU:C	2.59	0.44
3:A:1409:LEU:HD23	3:A:1409:LEU:HA	1.83	0.44
3:A:1441:PHE:HB2	7:F:134:ILE:CG2	2.47	0.44
4:B:362:PRO:C	4:B:363:HIS:O	2.58	0.44
4:B:640:VAL:HG23	4:B:740:HIS:CA	2.48	0.44
4:B:847:ASP:O	5:C:65:HIS:HE1	2.01	0.44
4:B:1185:CYS:O	4:B:1186:ASP:HB2	2.17	0.44
5:C:22:LEU:HD12	5:C:230:MET:HE1	1.99	0.44
5:C:39:ALA:HA	5:C:164:ALA:CB	2.46	0.44
9:I:34:TYR:C	9:I:35:VAL:HG23	2.41	0.44
3:A:54:ASN:O	3:A:55:ASP:HB2	2.18	0.44
3:A:466:SER:HB3	11:K:2:ASN:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:494:SER:HB2	3:A:497:THR:OG1	2.18	0.44
3:A:848:ILE:HD13	3:A:864:ILE:HD13	1.98	0.44
3:A:901:LEU:HD13	3:A:919:ILE:CG2	2.48	0.44
3:A:928:LEU:O	3:A:929:LEU:C	2.59	0.44
3:A:1048:ASN:O	3:A:1049:ILE:C	2.61	0.44
4:B:247:GLY:O	4:B:248:SER:HB3	2.17	0.44
4:B:800:GLN:CB	10:J:52:THR:HG22	2.47	0.44
5:C:31:ASN:O	5:C:35:ARG:HG3	2.17	0.44
5:C:123:ASN:ND2	5:C:125:MET:HG2	2.31	0.44
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.17	0.44
11:K:24:ASP:HB3	11:K:30:ALA:CB	2.47	0.44
12:L:43:THR:HG22	12:L:43:THR:O	2.18	0.44
3:A:103:CYS:O	3:A:106:VAL:O	2.35	0.44
3:A:458:HIS:ND1	3:A:507:VAL:HG21	2.33	0.44
4:B:65:GLU:HG3	4:B:66:ASP:N	2.27	0.44
4:B:100:PRO:HA	4:B:125:SER:O	2.16	0.44
4:B:205:ILE:HG12	4:B:461:LEU:HB3	1.99	0.44
4:B:332:ASP:O	4:B:334:ILE:N	2.50	0.44
4:B:690:VAL:HG12	4:B:691:GLU:N	2.33	0.44
4:B:864:LYS:HD3	4:B:871:THR:CB	2.47	0.44
4:B:1038:SER:HB3	4:B:1062:HIS:NE2	2.32	0.44
4:B:1163:CYS:C	4:B:1165:ILE:H	2.25	0.44
5:C:52:GLU:HB3	5:C:154:LYS:HB3	1.99	0.44
5:C:173:ALA:O	5:C:174:ALA:CB	2.64	0.44
7:F:109:VAL:HG12	7:F:110:ASP:H	1.82	0.44
8:H:5:LEU:O	8:H:133:ASN:HB3	2.17	0.44
9:I:98:VAL:CG1	9:I:99:LEU:N	2.81	0.44
2:R:8:C:H2'	2:R:9:A:C8	2.52	0.44
3:A:219:PHE:CE2	3:A:231:PRO:HD2	2.52	0.44
3:A:525:GLN:HB2	4:B:835:GLN:HG2	2.00	0.44
3:A:571:LEU:HD22	8:H:46:LEU:HD11	1.99	0.44
3:A:968:GLN:NE2	3:A:1035:TYR:HB2	2.33	0.44
3:A:1114:PRO:O	3:A:1330:ASN:OD1	2.35	0.44
3:A:1377:THR:C	3:A:1379:GLY:H	2.25	0.44
4:B:100:PRO:O	4:B:180:TYR:OH	2.31	0.44
4:B:904:ARG:CZ	4:B:948:ILE:HD11	2.48	0.44
6:E:133:GLU:HB3	6:E:135:PHE:HE1	1.83	0.44
3:A:783:THR:CG2	3:A:815:PHE:CZ	2.98	0.44
3:A:1118:VAL:O	3:A:1305:VAL:HG13	2.17	0.44
4:B:214:ALA:HB2	4:B:408:LEU:CD1	2.48	0.44
4:B:315:LYS:O	4:B:318:VAL:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:650:GLU:HG2	4:B:654:ARG:NH1	2.33	0.44
4:B:972:LYS:CD	4:B:1098:MET:HE1	2.48	0.44
4:B:1171:VAL:HG13	4:B:1191:ILE:HD13	1.99	0.44
6:E:28:TYR:CE2	6:E:64:PRO:HG3	2.53	0.44
6:E:185:ALA:CB	6:E:190:LEU:HD12	2.47	0.44
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.23	0.44
3:A:21:LEU:HD21	3:A:95:PHE:CZ	2.53	0.44
3:A:92:HIS:CD2	3:A:92:HIS:C	2.96	0.44
3:A:373:THR:HG21	4:B:1105:ALA:O	2.18	0.44
3:A:381:THR:O	3:A:382:PRO:C	2.60	0.44
3:A:591:PHE:HD2	3:A:595:THR:HB	1.83	0.44
3:A:845:LEU:O	3:A:848:ILE:HG13	2.17	0.44
3:A:1207:LEU:HA	3:A:1211:GLN:OE1	2.17	0.44
4:B:194:GLU:OE1	4:B:194:GLU:HA	2.18	0.44
4:B:487:THR:O	4:B:488:TYR:C	2.56	0.44
4:B:986:GLN:OE1	4:B:986:GLN:CA	2.64	0.44
5:C:69:LEU:HD12	5:C:69:LEU:HA	1.76	0.44
5:C:77:ILE:CG2	5:C:161:LYS:HE3	2.48	0.44
5:C:148:ARG:HD3	5:C:149:LYS:H	1.83	0.44
9:I:106:CYS:O	9:I:107:SER:HB2	2.18	0.44
11:K:92:ASN:C	11:K:94:ILE:N	2.75	0.44
3:A:31:SER:HB2	3:A:82:GLY:C	2.43	0.44
3:A:84:ILE:HG23	3:A:84:ILE:O	2.17	0.44
3:A:595:THR:HG22	3:A:596:THR:N	2.33	0.44
3:A:679:ILE:O	3:A:682:THR:HB	2.18	0.44
3:A:741:ASN:HD22	3:A:743:VAL:N	2.16	0.44
3:A:1384:VAL:O	3:A:1389:PHE:HE2	2.01	0.44
4:B:56:ASP:HB3	4:B:57:TYR:CE1	2.53	0.44
4:B:126:SER:OG	4:B:172:ILE:HD11	2.18	0.44
4:B:806:THR:N	4:B:809:MET:HE3	2.33	0.44
4:B:1002:THR:CG2	4:B:1004:GLU:HB2	2.47	0.44
4:B:1072:MET:HE2	4:B:1085:ILE:HB	1.96	0.44
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.48	0.44
8:H:98:TYR:O	8:H:118:PHE:HD2	1.99	0.44
11:K:40:HIS:O	11:K:41:THR:C	2.60	0.44
1:D:1:DA:C1'	3:A:1386:ARG:NH1	2.62	0.44
3:A:709:THR:HG23	9:I:94:ASP:HA	2.00	0.44
4:B:57:TYR:O	4:B:58:THR:C	2.60	0.44
5:C:143:LEU:HD21	5:C:146:LYS:HE3	1.99	0.44
9:I:84:VAL:O	9:I:84:VAL:CG1	2.65	0.44
11:K:24:ASP:OD1	11:K:26:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:496:GLU:O	3:A:497:THR:C	2.60	0.43
3:A:592:ASP:N	3:A:595:THR:OG1	2.48	0.43
3:A:815:PHE:O	3:A:818:MET:N	2.50	0.43
5:C:46:ILE:HG23	5:C:157:CYS:HB3	2.00	0.43
6:E:113:GLN:HG2	6:E:137:GLU:OE1	2.19	0.43
8:H:5:LEU:O	8:H:6:PHE:HB2	2.18	0.43
3:A:53:LEU:O	3:A:54:ASN:C	2.60	0.43
3:A:68:GLN:C	3:A:70:CYS:N	2.73	0.43
3:A:362:ASP:OD1	3:A:459:ARG:HD3	2.18	0.43
3:A:399:HIS:CB	3:A:400:PRO:HD3	2.45	0.43
3:A:404:TYR:HA	3:A:413:ILE:O	2.18	0.43
3:A:1166:ASP:OD1	3:A:1194:ARG:NH2	2.49	0.43
4:B:274:PRO:O	4:B:276:ILE:N	2.51	0.43
4:B:315:LYS:N	4:B:316:PRO:HD2	2.32	0.43
4:B:321:GLY:C	4:B:323:VAL:N	2.74	0.43
4:B:345:LYS:N	4:B:348:ARG:HE	2.16	0.43
4:B:781:PHE:CE2	4:B:795:ILE:HD11	2.53	0.43
4:B:1116:ARG:CZ	4:B:1198:TYR:CE1	3.01	0.43
6:E:16:PHE:O	6:E:17:ARG:C	2.60	0.43
9:I:50:THR:HG22	9:I:52:ILE:N	2.33	0.43
3:A:326:ARG:HE	3:A:1406:VAL:HG11	1.82	0.43
3:A:344:ARG:O	4:B:1118:PRO:HG2	2.19	0.43
3:A:457:ALA:O	3:A:507:VAL:HG23	2.19	0.43
3:A:547:LEU:HD22	11:K:58:PHE:HD1	1.84	0.43
3:A:751:SER:OG	4:B:1015:HIS:CE1	2.71	0.43
3:A:922:ASP:CG	3:A:925:LEU:HG	2.43	0.43
3:A:960:ILE:HD12	3:A:1021:LEU:HD21	1.99	0.43
3:A:1428:VAL:HG13	4:B:1151:LEU:HD23	2.00	0.43
4:B:446:LEU:N	4:B:446:LEU:HD23	2.33	0.43
4:B:745:PRO:C	4:B:747:MET:H	2.27	0.43
5:C:73:GLN:NE2	5:C:75:MET:H	1.97	0.43
5:C:249:ASP:OD1	5:C:253:LYS:HE3	2.19	0.43
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.49	0.43
9:I:29:CYS:O	9:I:31:THR:N	2.49	0.43
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.51	0.43
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.43
3:A:306:ASN:OD1	3:A:313:GLN:NE2	2.51	0.43
3:A:574:GLY:O	3:A:575:LYS:C	2.61	0.43
3:A:850:VAL:O	3:A:1060:PRO:HA	2.18	0.43
3:A:1004:ASN:O	3:A:1008:GLN:HB2	2.19	0.43
3:A:1015:VAL:HG12	3:A:1015:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1094:VAL:HG12	3:A:1095:THR:N	2.32	0.43
3:A:1097:GLY:O	3:A:1098:VAL:C	2.60	0.43
4:B:204:ILE:C	4:B:205:ILE:HD12	2.43	0.43
4:B:212:LEU:HD13	4:B:409:ALA:HA	2.00	0.43
4:B:758:PHE:CZ	4:B:1044:ALA:HA	2.52	0.43
4:B:849:GLY:O	4:B:850:LEU:C	2.59	0.43
4:B:969:ARG:HG2	4:B:970:THR:N	2.33	0.43
4:B:1002:THR:HG21	4:B:1006:ILE:HB	2.00	0.43
6:E:117:THR:C	6:E:119:SER:H	2.25	0.43
6:E:145:THR:HG21	6:E:187:TYR:CE2	2.54	0.43
12:L:26:THR:C	12:L:27:LEU:HD23	2.44	0.43
3:A:7:SER:OG	4:B:1193:GLN:NE2	2.51	0.43
3:A:35:ILE:HD13	3:A:53:LEU:HD23	2.00	0.43
3:A:80:HIS:O	3:A:243:PRO:HB3	2.17	0.43
3:A:87:ALA:HB3	3:A:276:LEU:CD2	2.45	0.43
3:A:907:THR:HG22	3:A:908:LEU:H	1.82	0.43
4:B:130:VAL:CG1	4:B:131:ASP:H	2.29	0.43
4:B:288:ALA:HA	4:B:331:LEU:HD13	1.99	0.43
4:B:358:LYS:O	4:B:359:GLU:OE1	2.36	0.43
4:B:436:VAL:O	4:B:437:GLU:C	2.61	0.43
4:B:705:MET:H	4:B:710:LEU:CD1	2.32	0.43
4:B:758:PHE:CE2	4:B:1044:ALA:HA	2.53	0.43
4:B:809:MET:HE1	4:B:983:ARG:HH22	1.82	0.43
4:B:850:LEU:CD2	4:B:1009:ASP:HB3	2.48	0.43
4:B:977:GLY:CA	4:B:1099:VAL:HG21	2.30	0.43
5:C:261:ALA:O	5:C:262:LEU:C	2.61	0.43
11:K:98:LEU:HD23	11:K:98:LEU:HA	1.89	0.43
3:A:367:PRO:CB	3:A:466:SER:HA	2.47	0.43
3:A:868:TYR:C	3:A:870:GLU:N	2.76	0.43
3:A:1028:THR:O	3:A:1029:ARG:C	2.61	0.43
4:B:361:LEU:O	4:B:363:HIS:O	2.35	0.43
4:B:416:LEU:O	4:B:417:PHE:C	2.61	0.43
4:B:1152:MET:SD	4:B:1197:PRO:HD3	2.59	0.43
5:C:8:VAL:HA	5:C:21:ILE:O	2.19	0.43
5:C:135:GLN:O	5:C:136:ASP:O	2.37	0.43
6:E:69:ILE:O	6:E:73:PRO:HG3	2.19	0.43
7:F:140:ASP:OD1	7:F:141:GLY:N	2.52	0.43
10:J:9:SER:HB2	10:J:45:CYS:HB2	2.01	0.43
11:K:47:ARG:C	11:K:47:ARG:HD2	2.43	0.43
11:K:55:LYS:HD3	11:K:78:THR:OG1	2.18	0.43
12:L:27:LEU:HD13	12:L:37:LYS:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:51:CYS:C	12:L:53:HIS:N	2.75	0.43
1:D:5:DG:H1	2:R:8:C:N4	2.16	0.43
3:A:68:GLN:O	3:A:70:CYS:N	2.52	0.43
3:A:244:PRO:O	3:A:245:PRO:C	2.59	0.43
3:A:534:LEU:HD13	3:A:656:TRP:CD1	2.54	0.43
3:A:672:ASP:O	3:A:675:THR:HB	2.19	0.43
4:B:121:ASN:HA	4:B:207:GLY:CA	2.46	0.43
4:B:295:GLY:H	4:B:298:LEU:HG	1.84	0.43
4:B:329:THR:O	4:B:333:PHE:N	2.48	0.43
4:B:563:MET:HE1	4:B:580:VAL:HB	2.00	0.43
4:B:705:MET:N	4:B:710:LEU:HD12	2.34	0.43
4:B:784:ASN:HD21	4:B:788:ARG:HD2	1.84	0.43
4:B:872:GLU:CD	4:B:914:LYS:HE2	2.43	0.43
5:C:76:ASP:OD2	5:C:128:ASN:N	2.47	0.43
5:C:148:ARG:H	5:C:151:GLN:HG3	1.84	0.43
8:H:111:LEU:HD23	8:H:127:GLY:O	2.18	0.43
3:A:42:ASP:OD1	3:A:45:GLN:O	2.36	0.43
3:A:645:LEU:HD11	3:A:649:ILE:HD11	2.01	0.43
3:A:1364:ASN:HD22	3:A:1366:ARG:N	2.16	0.43
4:B:102:VAL:HG21	4:B:112:LEU:HD13	1.99	0.43
4:B:203:PHE:HE1	4:B:212:LEU:CD1	2.31	0.43
4:B:310:MET:O	4:B:313:MET:HB2	2.18	0.43
4:B:1197:PRO:O	4:B:1200:ALA:HB3	2.19	0.43
3:A:86:LEU:HB3	3:A:296:LEU:HD21	1.99	0.43
3:A:108:MET:O	3:A:109:HIS:CB	2.66	0.43
3:A:113:LEU:C	3:A:115:LEU:N	2.77	0.43
3:A:148:CYS:HB3	3:A:167:CYS:O	2.18	0.43
3:A:366:VAL:HA	3:A:367:PRO:HD2	1.81	0.43
3:A:396:PRO:HG3	3:A:416:ARG:HB3	2.00	0.43
3:A:401:GLY:H	3:A:435:HIS:HD2	1.66	0.43
3:A:852:TYR:CE2	7:F:136:ARG:NE	2.86	0.43
3:A:1046:LEU:C	3:A:1048:ASN:N	2.75	0.43
3:A:1343:ALA:O	3:A:1344:GLY:C	2.61	0.43
4:B:329:THR:O	4:B:332:ASP:HB3	2.19	0.43
4:B:601:ARG:O	4:B:605:ARG:HG3	2.19	0.43
4:B:640:VAL:HG22	4:B:651:LEU:HD23	2.01	0.43
4:B:702:LEU:HD12	4:B:702:LEU:HA	1.76	0.43
4:B:1073:TYR:N	4:B:1073:TYR:CD1	2.87	0.43
5:C:251:LEU:HG	11:K:98:LEU:HD11	2.01	0.43
6:E:121:MET:C	6:E:123:LEU:N	2.75	0.43
6:E:138:ALA:O	6:E:140:LEU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:2:A:C3'	2:R:3:C:H5'	2.43	0.43
3:A:99:ILE:O	3:A:100:LYS:C	2.61	0.43
3:A:114:LEU:HD12	3:A:142:CYS:O	2.18	0.43
3:A:337:ARG:CZ	3:A:839:ARG:CZ	2.97	0.43
3:A:412:ARG:CZ	4:B:1108:ARG:NH2	2.81	0.43
3:A:639:PRO:HG2	3:A:640:GLN:H	1.84	0.43
3:A:675:THR:HG21	3:A:736:ASN:HD21	1.77	0.43
3:A:1155:ASP:O	3:A:1190:PRO:O	2.37	0.43
3:A:1366:ARG:HG2	3:A:1366:ARG:HH11	1.84	0.43
3:A:1390:ASN:HD22	3:A:1399:ARG:CA	2.30	0.43
3:A:1441:PHE:HB2	7:F:134:ILE:HG23	2.00	0.43
4:B:702:LEU:HD22	4:B:737:THR:CG2	2.49	0.43
4:B:915:THR:HG21	4:B:934:LYS:HG2	2.00	0.43
4:B:1023:VAL:O	4:B:1024:ALA:C	2.62	0.43
4:B:1204:PHE:O	4:B:1207:LEU:HB2	2.19	0.43
8:H:47:PHE:CB	8:H:95:TYR:HD1	2.31	0.43
9:I:59:VAL:HG12	9:I:60:GLN:N	2.34	0.43
3:A:63:ARG:CA	3:A:74:MET:HE2	2.49	0.42
3:A:753:GLY:HA2	3:A:757:ASN:ND2	2.34	0.42
3:A:834:THR:HG21	3:A:1077:THR:HA	2.00	0.42
3:A:1342:GLU:HG2	6:E:212:ARG:HH11	1.83	0.42
3:A:1385:THR:HG22	3:A:1386:ARG:N	2.34	0.42
3:A:1394:THR:HG22	3:A:1395:GLY:O	2.19	0.42
3:A:1424:VAL:HG11	4:B:1139:ILE:HD13	2.00	0.42
4:B:366:GLN:O	4:B:367:LEU:O	2.36	0.42
4:B:1148:LYS:O	4:B:1152:MET:HB2	2.19	0.42
6:E:138:ALA:C	6:E:140:LEU:N	2.76	0.42
6:E:168:TYR:O	6:E:170:LEU:HD23	2.19	0.42
10:J:31:ASP:O	10:J:32:GLU:C	2.61	0.42
10:J:53:HIS:CE1	10:J:55:ASP:HA	2.54	0.42
3:A:30:ILE:O	3:A:31:SER:O	2.37	0.42
3:A:99:ILE:O	3:A:102:VAL:HB	2.19	0.42
3:A:407:ARG:HG2	3:A:430:TRP:CE2	2.54	0.42
3:A:447:GLN:HA	3:A:448:PRO:C	2.44	0.42
3:A:567:LYS:HZ2	8:H:46:LEU:CB	2.29	0.42
3:A:577:ILE:O	3:A:578:LEU:C	2.62	0.42
3:A:666:ILE:HD11	4:B:1030:LEU:CD1	2.20	0.42
3:A:673:GLY:N	3:A:674:PRO:HD2	2.33	0.42
3:A:879:GLU:CD	3:A:962:ARG:HH22	2.26	0.42
3:A:1027:ALA:O	3:A:1030:ARG:HB2	2.19	0.42
3:A:1208:THR:O	3:A:1209:MET:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:115:GLN:HG2	4:B:193:LYS:HB2	2.01	0.42
4:B:280:ILE:CG2	4:B:285:ILE:HG13	2.47	0.42
4:B:556:THR:O	4:B:557:PHE:C	2.61	0.42
4:B:757:PRO:HG2	4:B:984:HIS:CE1	2.55	0.42
4:B:834:ASN:HB2	4:B:838:SER:O	2.19	0.42
4:B:955:THR:HA	12:L:54:ARG:O	2.19	0.42
9:I:53:GLY:O	9:I:54:GLU:C	2.63	0.42
9:I:55:THR:HG21	9:I:109:ILE:CD1	2.48	0.42
3:A:55:ASP:O	3:A:56:PRO:C	2.61	0.42
3:A:113:LEU:HG	3:A:218:ASP:OD1	2.19	0.42
3:A:134:ARG:O	3:A:137:ALA:N	2.52	0.42
3:A:289:ILE:C	3:A:291:GLU:H	2.27	0.42
3:A:1148:ILE:HD12	3:A:1196:GLU:HG2	2.01	0.42
3:A:1161:THR:OG1	3:A:1170:ILE:HD11	2.20	0.42
3:A:1215:ARG:HD2	3:A:1215:ARG:HA	1.88	0.42
3:A:1368:MET:O	3:A:1369:ALA:C	2.62	0.42
4:B:113:TYR:CD2	4:B:192:LEU:HD22	2.53	0.42
4:B:806:THR:O	4:B:808:ALA:N	2.53	0.42
4:B:1177:HIS:O	4:B:1179:GLN:HG3	2.19	0.42
5:C:5:GLY:O	5:C:6:PRO:O	2.37	0.42
5:C:263:THR:C	5:C:265:MET:N	2.77	0.42
6:E:114:ASN:O	6:E:115:ASN:HB3	2.18	0.42
8:H:4:THR:O	8:H:5:LEU:HD23	2.20	0.42
9:I:46:HIS:O	9:I:47:GLU:HB2	2.18	0.42
1:D:8:DT:H2'	1:D:9:DG:C8	2.55	0.42
3:A:89:PRO:HG3	3:A:208:LEU:HD12	2.00	0.42
3:A:166:GLY:O	3:A:167:CYS:CB	2.67	0.42
3:A:367:PRO:O	3:A:368:LYS:C	2.61	0.42
3:A:565:ILE:HD13	3:A:567:LYS:HE2	2.01	0.42
3:A:751:SER:O	3:A:752:LYS:CB	2.67	0.42
3:A:1168:GLU:O	3:A:1172:LEU:HG	2.19	0.42
4:B:34:ILE:HG12	4:B:542:MET:CE	2.49	0.42
4:B:749:LEU:HD22	4:B:753:ALA:CB	2.50	0.42
4:B:1026:LEU:O	4:B:1027:ILE:C	2.63	0.42
4:B:1108:ARG:O	4:B:1108:ARG:CG	2.67	0.42
4:B:1117:GLN:HG3	4:B:1156:ASP:CG	2.43	0.42
4:B:1177:HIS:O	4:B:1179:GLN:N	2.52	0.42
6:E:16:PHE:CZ	6:E:20:LYS:HE2	2.54	0.42
7:F:116:ASP:O	7:F:117:PRO:C	2.62	0.42
8:H:143:LEU:HD12	8:H:143:LEU:N	2.34	0.42
9:I:91:ARG:HA	9:I:91:ARG:HD3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:HIS:CD2	10:J:54:VAL:N	2.88	0.42
11:K:95:ILE:O	11:K:98:LEU:HB2	2.19	0.42
1:D:10:DG:H5'	4:B:792:MET:HE3	2.01	0.42
2:R:3:C:C2'	2:R:4:C:O4'	2.67	0.42
2:R:9:A:OP1	3:A:483:ASP:OD1	2.38	0.42
3:A:151:ASP:OD1	3:A:163:SER:HA	2.19	0.42
3:A:984:LYS:O	3:A:988:LEU:HB2	2.19	0.42
3:A:1329:THR:HG22	3:A:1330:ASN:N	2.34	0.42
4:B:293:PRO:C	4:B:294:ASP:O	2.57	0.42
4:B:781:PHE:HE2	4:B:795:ILE:HD11	1.83	0.42
4:B:784:ASN:HB3	10:J:63:TYR:OH	2.18	0.42
4:B:831:SER:CB	4:B:994:TYR:OH	2.67	0.42
4:B:835:GLN:O	4:B:836:GLU:C	2.62	0.42
4:B:880:THR:O	4:B:881:ASN:HB2	2.20	0.42
5:C:242:GLN:O	5:C:246:ARG:N	2.52	0.42
8:H:57:VAL:CG1	8:H:58:THR:N	2.83	0.42
12:L:58:LYS:O	12:L:59:ALA:C	2.63	0.42
3:A:80:HIS:N	3:A:243:PRO:HB3	2.34	0.42
3:A:131:SER:OG	3:A:132:LYS:N	2.51	0.42
3:A:336:ILE:CD1	3:A:1405:THR:HG21	2.45	0.42
3:A:441:PRO:O	3:A:441:PRO:HG2	2.20	0.42
3:A:541:ILE:HD12	3:A:541:ILE:N	2.34	0.42
3:A:709:THR:O	3:A:712:GLU:N	2.52	0.42
3:A:760:GLN:CB	4:B:1021:MET:HE1	2.50	0.42
3:A:1129:GLU:O	3:A:1130:GLN:C	2.61	0.42
3:A:1150:SER:HB2	3:A:1195:LEU:CD2	2.49	0.42
3:A:1187:GLN:HA	3:A:1243:VAL:HG23	2.02	0.42
4:B:202:TYR:CD2	4:B:202:TYR:N	2.87	0.42
4:B:203:PHE:HE1	4:B:212:LEU:HD12	1.85	0.42
4:B:280:ILE:HA	4:B:281:PRO:HD2	1.85	0.42
4:B:794:ASN:O	4:B:795:ILE:HD12	2.19	0.42
4:B:841:MET:HE3	4:B:1010:LEU:HD13	2.02	0.42
5:C:214:ASN:CB	5:C:217:ASP:OD2	2.68	0.42
3:A:38:PRO:CA	3:A:270:LEU:HD23	2.49	0.42
3:A:629:LEU:CD1	3:A:645:LEU:HD21	2.48	0.42
3:A:1205:LYS:O	3:A:1206:ASP:C	2.63	0.42
4:B:307:ASP:O	4:B:308:TRP:C	2.59	0.42
4:B:797:TYR:HB3	4:B:798:TYR:CD1	2.55	0.42
4:B:1106:ARG:HH12	4:B:1118:PRO:CA	2.33	0.42
6:E:168:TYR:CB	6:E:170:LEU:HG	2.49	0.42
7:F:89:GLU:HB3	7:F:134:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:84:VAL:O	9:I:84:VAL:HG13	2.19	0.42
3:A:427:GLN:O	3:A:428:TYR:C	2.62	0.42
3:A:514:PRO:HB2	3:A:875:ALA:HB3	2.01	0.42
3:A:683:ILE:O	3:A:686:ALA:N	2.53	0.42
3:A:683:ILE:CD1	3:A:764:CYS:HB2	2.42	0.42
3:A:782:ARG:NH2	9:I:67:THR:HG22	2.34	0.42
3:A:811:GLN:O	3:A:812:GLU:C	2.61	0.42
3:A:1126:ALA:O	3:A:1128:GLN:N	2.53	0.42
4:B:269:ILE:HB	4:B:317:CYS:SG	2.60	0.42
4:B:877:PRO:O	4:B:878:GLN:HG2	2.19	0.42
4:B:879:ARG:O	4:B:880:THR:HB	2.20	0.42
4:B:995:ARG:HB2	4:B:995:ARG:HH11	1.81	0.42
4:B:1162:ILE:HG22	4:B:1163:CYS:N	2.34	0.42
5:C:39:ALA:CA	5:C:164:ALA:HB3	2.46	0.42
5:C:204:SER:O	5:C:205:LYS:C	2.63	0.42
6:E:131:THR:HG21	6:E:191:LYS:HE2	2.02	0.42
10:J:21:TYR:CA	10:J:39:LEU:HD11	2.49	0.42
3:A:339:ASN:HB3	4:B:1117:GLN:HE22	1.85	0.42
3:A:601:LYS:O	3:A:602:ASP:C	2.62	0.42
3:A:633:VAL:HG11	3:A:645:LEU:HD22	2.00	0.42
3:A:1223:ASP:C	3:A:1243:VAL:HG12	2.45	0.42
3:A:1402:PHE:O	3:A:1404:GLU:N	2.51	0.42
4:B:167:ILE:O	4:B:168:GLY:O	2.38	0.42
4:B:482:VAL:O	4:B:483:LEU:C	2.63	0.42
4:B:640:VAL:HG22	4:B:651:LEU:CD2	2.50	0.42
4:B:890:TYR:C	4:B:892:LYS:N	2.78	0.42
4:B:955:THR:CG2	12:L:54:ARG:O	2.65	0.42
4:B:1182:CYS:SG	4:B:1185:CYS:HB2	2.60	0.42
5:C:20:PHE:CD1	5:C:20:PHE:C	2.97	0.42
6:E:28:TYR:CE1	6:E:78:LEU:CD1	3.03	0.42
6:E:134:THR:C	6:E:135:PHE:HD1	2.27	0.42
8:H:31:THR:O	8:H:32:THR:OG1	2.37	0.42
9:I:87:GLN:O	9:I:88:SER:C	2.62	0.42
9:I:97:MET:HE3	9:I:97:MET:HB2	1.88	0.42
10:J:3:VAL:CG2	10:J:18:TRP:CG	3.02	0.42
10:J:27:GLU:C	10:J:29:GLU:N	2.77	0.42
1:D:5:DG:H1	2:R:8:C:H42	1.67	0.42
3:A:49:LYS:NZ	3:A:60:SER:HA	2.34	0.42
3:A:567:LYS:CD	8:H:95:TYR:CD1	3.00	0.42
3:A:598:LEU:HD22	8:H:25:ARG:CZ	2.50	0.42
3:A:637:LYS:HA	3:A:637:LYS:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1064:VAL:O	3:A:1065:GLY:C	2.63	0.42
4:B:310:MET:O	4:B:311:LEU:C	2.62	0.42
4:B:839:MET:HE1	4:B:980:PHE:CB	2.49	0.42
4:B:878:GLN:O	4:B:879:ARG:C	2.61	0.42
4:B:1197:PRO:O	4:B:1200:ALA:N	2.52	0.42
6:E:59:SER:HA	6:E:80:VAL:O	2.19	0.42
12:L:40:LEU:HD23	12:L:40:LEU:HA	1.78	0.42
3:A:59:GLY:HA2	3:A:67:CYS:SG	2.60	0.41
3:A:568:PRO:CB	5:C:221:TYR:CZ	3.03	0.41
3:A:596:THR:C	3:A:598:LEU:N	2.78	0.41
3:A:725:ALA:HA	3:A:728:LYS:HE2	2.02	0.41
4:B:105:SER:O	4:B:106:ASP:HB2	2.19	0.41
4:B:499:ASN:OD1	4:B:500:THR:N	2.53	0.41
4:B:995:ARG:HH11	4:B:995:ARG:CB	2.33	0.41
4:B:1096:ARG:O	4:B:1097:HIS:CB	2.59	0.41
4:B:1149:GLU:HG3	4:B:1153:GLU:OE1	2.20	0.41
6:E:98:ILE:O	6:E:99:HIS:C	2.62	0.41
9:I:63:GLY:O	9:I:70:ARG:NH2	2.53	0.41
3:A:225:ASN:C	3:A:227:VAL:N	2.71	0.41
3:A:265:LYS:HZ1	3:A:323:LYS:H	1.62	0.41
3:A:383:TYR:O	7:F:115:THR:HG22	2.20	0.41
3:A:675:THR:CG2	3:A:736:ASN:ND2	2.78	0.41
3:A:843:LYS:HG3	3:A:1402:PHE:CD1	2.54	0.41
3:A:1254:ALA:O	3:A:1255:GLU:HB2	2.19	0.41
4:B:55:VAL:O	4:B:59:LEU:HB3	2.19	0.41
4:B:315:LYS:O	4:B:317:CYS:N	2.53	0.41
4:B:1060:ARG:C	4:B:1062:HIS:H	2.26	0.41
4:B:1106:ARG:HH12	4:B:1118:PRO:HA	1.85	0.41
5:C:59:ALA:O	5:C:63:ILE:HG13	2.19	0.41
8:H:12:VAL:HG13	8:H:26:ILE:HG23	2.01	0.41
8:H:111:LEU:C	8:H:112:ILE:HG13	2.45	0.41
11:K:82:ASP:O	11:K:85:ASP:HB2	2.20	0.41
3:A:14:VAL:HB	3:A:1430:LEU:HD13	2.02	0.41
3:A:134:ARG:O	3:A:136:ALA:N	2.53	0.41
3:A:321:PRO:O	3:A:322:VAL:CB	2.63	0.41
3:A:384:ASN:CG	3:A:388:LEU:HD12	2.45	0.41
3:A:530:GLY:O	3:A:532:ARG:N	2.53	0.41
3:A:543:LEU:O	3:A:544:ASP:C	2.63	0.41
3:A:1158:PRO:HB3	3:A:1241:ARG:HH12	1.83	0.41
4:B:92:PHE:HD2	4:B:130:VAL:HG11	1.85	0.41
4:B:205:ILE:N	4:B:205:ILE:CD1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:546:SER:OG	4:B:631:GLY:N	2.52	0.41
4:B:579:ARG:HB2	4:B:586:TRP:HE1	1.84	0.41
4:B:941:LEU:HD21	4:B:946:ASN:HA	2.02	0.41
5:C:27:LEU:HD12	5:C:27:LEU:O	2.20	0.41
5:C:252:GLN:NE2	11:K:99:GLY:N	2.68	0.41
8:H:96:VAL:HG13	8:H:143:LEU:HG	2.02	0.41
3:A:48:ALA:C	3:A:49:LYS:HG3	2.45	0.41
3:A:401:GLY:N	3:A:435:HIS:HD2	2.18	0.41
3:A:451:HIS:HB2	3:A:454:SER:OG	2.19	0.41
3:A:463:ILE:CD1	3:A:469:ARG:HG3	2.50	0.41
3:A:474:VAL:HG13	3:A:478:TYR:HE1	1.85	0.41
3:A:515:GLN:CG	3:A:516:SER:N	2.84	0.41
3:A:531:ILE:CG2	3:A:532:ARG:N	2.84	0.41
3:A:1364:ASN:HD21	3:A:1366:ARG:NH1	2.19	0.41
4:B:53:GLN:HG2	4:B:547:VAL:HG13	2.02	0.41
4:B:276:ILE:HD11	4:B:355:ILE:CD1	2.50	0.41
4:B:368:GLU:O	4:B:371:GLU:OE1	2.37	0.41
4:B:901:PRO:O	4:B:949:VAL:O	2.38	0.41
4:B:958:GLN:C	4:B:960:GLY:N	2.79	0.41
6:E:35:VAL:C	6:E:37:LEU:N	2.78	0.41
6:E:79:TRP:HD1	6:E:96:PHE:HE1	1.67	0.41
9:I:103:CYS:SG	9:I:106:CYS:SG	2.99	0.41
11:K:65:HIS:HD2	11:K:67:PHE:CB	2.33	0.41
3:A:88:LYS:HD2	3:A:293:GLU:OE1	2.19	0.41
3:A:407:ARG:HG2	3:A:430:TRP:CZ2	2.56	0.41
3:A:518:LYS:HB2	3:A:519:PRO:HD2	2.01	0.41
3:A:1006:ILE:HG22	3:A:1007:ILE:N	2.36	0.41
3:A:1173:HIS:NE2	3:A:1227:ILE:HG23	2.35	0.41
3:A:1265:ASN:O	3:A:1266:THR:C	2.64	0.41
3:A:1378:GLN:C	3:A:1380:GLY:H	2.29	0.41
4:B:39:ARG:HG2	4:B:39:ARG:HH11	1.85	0.41
4:B:648:HIS:HB2	4:B:649:LYS:H	1.61	0.41
5:C:8:VAL:CG1	5:C:9:LYS:H	2.32	0.41
5:C:252:GLN:HG3	11:K:95:ILE:HG23	2.03	0.41
6:E:116:ILE:CG2	6:E:117:THR:N	2.84	0.41
8:H:84:ALA:HA	8:H:87:ARG:CB	2.50	0.41
8:H:117:SER:HA	8:H:122:LEU:HD23	2.02	0.41
10:J:43:ARG:H	10:J:43:ARG:HG2	1.68	0.41
11:K:35:PHE:O	11:K:70:ARG:HB2	2.21	0.41
11:K:103:THR:O	11:K:106:GLU:N	2.53	0.41
12:L:28:LYS:O	12:L:29:TYR:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:101:LYS:HG2	3:A:139:TRP:CZ2	2.55	0.41
3:A:751:SER:OG	4:B:1015:HIS:HE1	2.03	0.41
3:A:1406:VAL:CG1	3:A:1410:PHE:CE1	3.03	0.41
4:B:175:ARG:HH11	4:B:175:ARG:CG	2.34	0.41
4:B:369:GLY:C	4:B:370:PHE:CD1	2.99	0.41
4:B:377:PHE:HE2	4:B:381:MET:HE2	1.85	0.41
4:B:381:MET:HE3	4:B:381:MET:HB2	1.97	0.41
4:B:577:ALA:HB1	4:B:589:VAL:HG12	2.00	0.41
4:B:707:PRO:HG2	4:B:708:GLU:N	2.27	0.41
4:B:843:GLN:HB2	4:B:993:THR:OG1	2.20	0.41
4:B:846:ILE:CG2	4:B:974:PRO:HG2	2.51	0.41
4:B:855:PHE:HZ	4:B:857:ARG:HH12	1.64	0.41
5:C:124:LEU:O	5:C:127:ARG:CG	2.65	0.41
5:C:214:ASN:O	5:C:215:GLU:C	2.62	0.41
5:C:235:VAL:HG21	10:J:6:ARG:NH2	2.35	0.41
1:D:2:DA:H4'	3:A:1403:GLU:CD	2.46	0.41
3:A:76:GLU:O	3:A:78:PRO:CD	2.68	0.41
3:A:332:LYS:H	3:A:337:ARG:CB	2.33	0.41
3:A:542:GLU:OE1	3:A:569:LYS:HE2	2.20	0.41
3:A:992:ASP:O	3:A:993:LEU:C	2.64	0.41
3:A:1107:VAL:CG2	3:A:1383:SER:HA	2.51	0.41
4:B:120:ARG:HH22	12:L:54:ARG:HD2	1.86	0.41
4:B:188:ASP:O	4:B:192:LEU:HG	2.21	0.41
4:B:405:ARG:CZ	4:B:632:ARG:HG2	2.49	0.41
4:B:840:ILE:HB	4:B:1011:ILE:HB	2.03	0.41
4:B:911:ILE:HD11	4:B:941:LEU:CB	2.50	0.41
5:C:264:GLN:HG3	5:C:264:GLN:H	1.61	0.41
6:E:13:TRP:O	6:E:16:PHE:HB3	2.21	0.41
9:I:101:PHE:HD1	9:I:110:PHE:O	2.02	0.41
12:L:41:SER:O	12:L:44:ASP:HB2	2.21	0.41
3:A:84:ILE:HG21	3:A:239:LEU:HD23	2.01	0.41
3:A:209:ASN:O	3:A:210:ILE:C	2.64	0.41
3:A:525:GLN:HB3	4:B:835:GLN:HG2	2.01	0.41
3:A:530:GLY:O	3:A:533:LYS:N	2.53	0.41
3:A:553:VAL:HG22	3:A:652:VAL:CG2	2.51	0.41
3:A:556:TRP:CE2	3:A:558:GLY:HA2	2.56	0.41
3:A:568:PRO:HB3	5:C:221:TYR:OH	2.21	0.41
3:A:738:LYS:HZ1	5:C:194:GLU:CA	2.34	0.41
3:A:960:ILE:HD12	3:A:1021:LEU:CD2	2.50	0.41
4:B:244:LEU:HB2	4:B:249:ARG:HA	2.03	0.41
4:B:435:THR:O	4:B:435:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:616:ILE:HG12	4:B:696:GLU:HG3	2.03	0.41
4:B:1120:GLU:CG	4:B:1121:GLY:N	2.84	0.41
5:C:146:LYS:O	5:C:147:LEU:HD23	2.20	0.41
9:I:92:ARG:CG	9:I:93:LYS:N	2.84	0.41
12:L:45:ALA:C	12:L:46:VAL:HG23	2.45	0.41
3:A:19:PHE:HB3	3:A:1413:GLY:HA2	2.03	0.41
3:A:343:LYS:NZ	4:B:1156:ASP:OD2	2.49	0.41
3:A:399:HIS:NE2	3:A:462:VAL:HG21	2.36	0.41
3:A:403:LYS:O	3:A:404:TYR:O	2.39	0.41
3:A:574:GLY:O	3:A:577:ILE:HG12	2.21	0.41
3:A:622:VAL:C	3:A:623:GLY:O	2.64	0.41
3:A:942:PHE:HZ	6:E:206:GLY:HA3	1.86	0.41
3:A:1066:VAL:C	3:A:1068:ALA:N	2.79	0.41
3:A:1102:LYS:O	3:A:1103:GLU:C	2.63	0.41
3:A:1381:LEU:HD23	3:A:1381:LEU:HA	1.92	0.41
4:B:54:PHE:O	4:B:55:VAL:C	2.64	0.41
4:B:120:ARG:HH12	12:L:54:ARG:NH1	2.18	0.41
4:B:121:ASN:HD21	4:B:965:LYS:HE3	1.86	0.41
4:B:234:ILE:H	4:B:234:ILE:CD1	2.16	0.41
4:B:634:TYR:CD1	4:B:692:TYR:HB3	2.55	0.41
4:B:724:ASP:HA	4:B:725:PRO:HD2	1.95	0.41
4:B:913:GLY:HA2	4:B:938:SER:HB2	2.02	0.41
4:B:972:LYS:HD3	4:B:1098:MET:HE1	2.03	0.41
4:B:1114:LEU:O	4:B:1198:TYR:HE2	2.03	0.41
4:B:1122:ARG:C	4:B:1124:ARG:N	2.79	0.41
5:C:14:SER:HA	11:K:114:LEU:HD22	2.02	0.41
6:E:3:GLN:HG3	6:E:5:ASN:H	1.85	0.41
6:E:72:PHE:N	6:E:72:PHE:CD1	2.89	0.41
9:I:25:LEU:HD12	9:I:26:LEU:N	2.35	0.41
9:I:98:VAL:HG12	9:I:99:LEU:N	2.36	0.41
9:I:99:LEU:HB2	9:I:112:SER:OG	2.21	0.41
9:I:99:LEU:O	9:I:111:THR:HG23	2.21	0.41
10:J:12:LYS:O	10:J:13:VAL:C	2.64	0.41
11:K:47:ARG:HH11	11:K:48:ALA:N	2.19	0.41
11:K:93:SER:O	11:K:97:LYS:HG3	2.20	0.41
11:K:106:GLU:O	11:K:110:ASN:ND2	2.54	0.41
12:L:29:TYR:C	12:L:30:ILE:HG13	2.45	0.41
3:A:45:GLN:O	3:A:46:THR:C	2.63	0.41
3:A:172:PRO:HB3	3:A:185:TRP:CZ2	2.56	0.41
3:A:334:GLY:O	3:A:335:ARG:C	2.64	0.41
3:A:396:PRO:HB3	3:A:403:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:848:ILE:HG23	3:A:864:ILE:HD12	2.03	0.41
3:A:1026:LEU:HD23	3:A:1026:LEU:HA	1.90	0.41
3:A:1038:THR:O	3:A:1039:LYS:C	2.63	0.41
3:A:1102:LYS:HG2	3:A:1106:ASN:ND2	2.36	0.41
3:A:1107:VAL:HG23	3:A:1383:SER:HA	2.03	0.41
3:A:1116:LEU:H	3:A:1308:THR:CG2	2.34	0.41
4:B:380:TYR:O	4:B:384:ARG:HG2	2.21	0.41
4:B:549:THR:HG22	4:B:550:ASP:N	2.36	0.41
4:B:593:PRO:HG2	4:B:617:ARG:NH2	2.36	0.41
4:B:707:PRO:CG	4:B:708:GLU:N	2.84	0.41
4:B:737:THR:HG21	9:I:66:PRO:C	2.40	0.41
4:B:850:LEU:HD22	4:B:1009:ASP:HB3	2.02	0.41
4:B:872:GLU:CD	4:B:914:LYS:CE	2.94	0.41
4:B:992:ILE:CD1	4:B:994:TYR:CE2	3.04	0.41
4:B:1104:HIS:HB2	4:B:1122:ARG:CB	2.51	0.41
5:C:51:VAL:HG22	5:C:155:LEU:CD2	2.47	0.41
6:E:117:THR:O	6:E:120:ALA:N	2.54	0.41
6:E:136:ASN:O	6:E:137:GLU:C	2.65	0.41
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.03	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41
9:I:85:PHE:HD1	9:I:99:LEU:HD22	1.83	0.41
11:K:7:PHE:C	11:K:9:LEU:H	2.29	0.41
3:A:302:THR:O	3:A:313:GLN:NE2	2.54	0.40
3:A:332:LYS:H	3:A:337:ARG:CD	2.34	0.40
3:A:719:VAL:HG22	3:A:774:ARG:HD2	2.03	0.40
3:A:738:LYS:HA	8:H:19:ARG:NH2	2.37	0.40
3:A:871:ASP:CB	6:E:204:THR:CG2	2.98	0.40
3:A:1139:GLU:HG3	3:A:1280:GLU:O	2.20	0.40
3:A:1343:ALA:O	3:A:1346:ALA:HB3	2.20	0.40
4:B:48:LEU:O	4:B:49:ASP:C	2.64	0.40
4:B:56:ASP:CB	4:B:57:TYR:CD1	3.04	0.40
4:B:56:ASP:CB	4:B:57:TYR:HD1	2.34	0.40
4:B:283:VAL:HG13	4:B:297:ILE:HD12	2.03	0.40
4:B:284:ILE:HG12	4:B:324:ILE:HD12	2.03	0.40
4:B:293:PRO:O	4:B:294:ASP:C	2.64	0.40
4:B:313:MET:HE1	4:B:386:LEU:HD22	1.99	0.40
4:B:418:LYS:O	4:B:420:LEU:N	2.54	0.40
4:B:1177:HIS:HB2	4:B:1179:GLN:HG3	2.03	0.40
5:C:5:GLY:HA3	5:C:6:PRO:HD2	1.78	0.40
5:C:17:ASN:C	5:C:18:VAL:HG23	2.45	0.40
5:C:46:ILE:CG2	5:C:157:CYS:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:66:ARG:NH2	10:J:3:VAL:O	2.54	0.40
5:C:127:ARG:HG2	5:C:127:ARG:H	1.73	0.40
7:F:109:VAL:CG1	7:F:110:ASP:H	2.34	0.40
8:H:126:GLU:N	8:H:130:ARG:HH12	2.19	0.40
11:K:96:ASN:O	11:K:97:LYS:C	2.63	0.40
1:D:6:DC:OP2	3:A:332:LYS:NZ	2.45	0.40
2:R:2:A:H2'	2:R:3:C:C5'	2.50	0.40
3:A:14:VAL:O	3:A:15:LYS:HD3	2.20	0.40
3:A:270:LEU:O	3:A:274:ILE:HG13	2.21	0.40
3:A:474:VAL:HG13	3:A:474:VAL:O	2.20	0.40
3:A:901:LEU:CG	3:A:926:GLN:HE21	2.30	0.40
3:A:909:ASP:OD1	3:A:910:PRO:HD2	2.21	0.40
3:A:1116:LEU:CD2	3:A:1316:VAL:HG21	2.51	0.40
3:A:1224:LEU:HD11	3:A:1240:CYS:HB3	2.04	0.40
3:A:1230:GLU:C	3:A:1232:ASN:N	2.80	0.40
3:A:1345:ARG:HH11	3:A:1373:ASP:CG	2.29	0.40
4:B:530:GLY:O	4:B:531:GLN:C	2.64	0.40
4:B:818:PRO:HG3	10:J:54:VAL:HG21	2.03	0.40
6:E:137:GLU:O	6:E:140:LEU:N	2.43	0.40
6:E:182:ASP:O	6:E:186:LEU:HG	2.21	0.40
9:I:16:PRO:HA	9:I:26:LEU:O	2.21	0.40
11:K:49:GLU:C	11:K:51:LEU:N	2.79	0.40
3:A:18:GLN:O	4:B:1215:ARG:HG3	2.21	0.40
3:A:19:PHE:HA	4:B:1213:THR:O	2.22	0.40
3:A:354:SER:CA	3:A:482:PHE:CD2	3.03	0.40
3:A:379:VAL:HG22	3:A:431:LYS:HG2	2.03	0.40
3:A:432:VAL:O	3:A:434:ARG:N	2.54	0.40
3:A:913:LEU:CD1	3:A:981:LEU:O	2.69	0.40
3:A:971:PHE:O	3:A:972:HIS:C	2.64	0.40
4:B:627:PHE:O	4:B:632:ARG:NH1	2.54	0.40
4:B:952:VAL:HG13	4:B:966:VAL:HG22	2.03	0.40
4:B:1084:GLN:NE2	5:C:192:TRP:HB2	2.37	0.40
5:C:178:PHE:CD2	5:C:178:PHE:C	2.99	0.40
6:E:11:ARG:NH2	6:E:141:VAL:HG21	2.37	0.40
6:E:116:ILE:HG22	6:E:117:THR:N	2.36	0.40
3:A:30:ILE:O	3:A:31:SER:C	2.64	0.40
3:A:203:SER:O	3:A:207:ILE:HG12	2.21	0.40
3:A:205:GLU:O	3:A:208:LEU:HB2	2.22	0.40
3:A:225:ASN:ND2	3:A:228:PHE:CD1	2.90	0.40
3:A:578:LEU:O	3:A:581:ALA:N	2.51	0.40
3:A:738:LYS:C	3:A:740:LEU:N	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:738:LYS:CB	8:H:19:ARG:HH22	2.34	0.40
3:A:808:LEU:N	3:A:808:LEU:HD12	2.35	0.40
3:A:878:ILE:C	3:A:879:GLU:CG	2.94	0.40
3:A:1316:VAL:O	3:A:1322:ILE:HD13	2.21	0.40
4:B:61:ASP:OD1	4:B:61:ASP:N	2.54	0.40
4:B:171:PRO:HD2	4:B:457:LEU:HD12	2.03	0.40
4:B:281:PRO:HG2	4:B:284:ILE:CD1	2.45	0.40
4:B:288:ALA:O	4:B:331:LEU:CD1	2.70	0.40
4:B:387:LEU:HD23	4:B:393:LYS:HD2	2.03	0.40
4:B:702:LEU:CD2	4:B:735:ALA:HB1	2.51	0.40
4:B:839:MET:HE2	4:B:980:PHE:CD1	2.56	0.40
4:B:1115:THR:CG2	4:B:1199:ALA:HB2	2.50	0.40
4:B:1156:ASP:HB3	4:B:1197:PRO:CA	2.52	0.40
8:H:33:GLN:OE1	8:H:129:TYR:HE2	2.05	0.40
9:I:6:PHE:HD2	9:I:13:MET:HA	1.86	0.40
3:A:13:THR:HB	3:A:15:LYS:HE2	2.04	0.40
3:A:48:ALA:O	3:A:49:LYS:CG	2.65	0.40
3:A:508:PRO:O	3:A:511:ILE:HG13	2.21	0.40
3:A:605:MET:HE2	3:A:612:ILE:HG13	2.03	0.40
4:B:51:PHE:O	4:B:54:PHE:N	2.54	0.40
4:B:185:THR:N	4:B:188:ASP:HB2	2.36	0.40
4:B:514:LEU:HD12	4:B:514:LEU:C	2.45	0.40
4:B:803:LEU:HD13	4:B:1036:ALA:HB2	2.03	0.40
4:B:995:ARG:O	4:B:996:ARG:C	2.63	0.40
5:C:214:ASN:HB2	5:C:217:ASP:OD2	2.22	0.40
6:E:19:VAL:O	6:E:19:VAL:HG12	2.20	0.40
6:E:93:MET:HE2	6:E:120:ALA:HB1	2.04	0.40
11:K:21:ILE:HG12	11:K:33:ILE:HG12	2.03	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	
3	A	1365/1733 (79%)	1021 (75%)	253 (18%)	91 (7%)	1	7
4	B	1077/1224 (88%)	839 (78%)	169 (16%)	69 (6%)	1	8
5	C	264/318 (83%)	208 (79%)	39 (15%)	17 (6%)	1	8
6	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	2	14
7	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	2	17
8	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	2
9	I	117/122 (96%)	93 (80%)	15 (13%)	9 (8%)	1	5
10	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	8
11	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	14	43
12	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	0
All	All	3465/4173 (83%)	2654 (77%)	583 (17%)	228 (7%)	1	7

All (228) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	31	SER
3	A	48	ALA
3	A	55	ASP
3	A	56	PRO
3	A	74	MET
3	A	75	ASN
3	A	167	CYS
3	A	322	VAL
3	A	404	TYR
3	A	418	SER
3	A	543	LEU
3	A	567	LYS
3	A	597	LEU
3	A	598	LEU
3	A	628	GLY
3	A	752	LYS
3	A	846	GLU
3	A	998	LEU
3	A	1036	ARG
3	A	1127	ASP
3	A	1206	ASP
3	A	1221	LYS
3	A	1223	ASP
3	A	1392	SER

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Mol	Chain	Res	Type
3	A	1393	ASN
3	A	1403	GLU
3	A	1406	VAL
3	A	1416	ALA
4	B	65	GLU
4	B	124	TYR
4	B	174	LEU
4	B	175	ARG
4	B	200	GLY
4	B	229	ALA
4	B	364	ILE
4	B	367	LEU
4	B	531	GLN
4	B	708	GLU
4	B	709	ASP
4	B	731	VAL
4	B	751	VAL
4	B	958	GLN
4	B	959	ASP
4	B	1046	PRO
4	B	1103	ILE
4	B	1167	GLY
4	B	1176	ASN
4	B	1183	LYS
5	C	4	GLU
5	C	5	GLY
5	C	6	PRO
5	C	110	THR
5	C	142	VAL
5	C	215	GLU
7	F	73	ALA
8	H	32	THR
8	H	81	PRO
8	H	140	ALA
9	I	8	ARG
10	J	2	ILE
10	J	55	ASP
12	L	27	LEU
12	L	38	LEU
12	L	64	LEU
3	A	35	ILE
3	A	54	ASN

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Mol	Chain	Res	Type
3	A	62	ASP
3	A	87	ALA
3	A	109	HIS
3	A	135	PHE
3	A	168	GLY
3	A	332	LYS
3	A	385	ILE
3	A	419	LYS
3	A	534	LEU
3	A	568	PRO
3	A	790	ASP
3	A	986	ILE
3	A	1114	PRO
3	A	1365	TYR
3	A	1366	ARG
3	A	1379	GLY
4	B	55	VAL
4	B	168	GLY
4	B	275	TYR
4	B	346	GLU
4	B	410	GLY
4	B	480	SER
4	B	641	GLU
4	B	643	ASP
4	B	792	MET
4	B	864	LYS
4	B	866	TYR
4	B	884	ARG
4	B	891	ASP
4	B	992	ILE
4	B	1066	SER
4	B	1155	SER
5	C	136	ASP
7	F	142	SER
8	H	61	SER
8	H	77	ARG
8	H	88	SER
8	H	128	ASN
9	I	30	ARG
9	I	79	HIS
12	L	39	SER
12	L	52	GLY

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Mol	Chain	Res	Type
3	A	6	TYR
3	A	45	GLN
3	A	59	GLY
3	A	67	CYS
3	A	69	THR
3	A	335	ARG
3	A	433	GLU
3	A	596	THR
3	A	737	LEU
3	A	775	ILE
3	A	830	LYS
3	A	920	LEU
4	B	28	GLU
4	B	249	ARG
4	B	277	LYS
4	B	447	ALA
4	B	629	ASP
4	B	735	ALA
4	B	807	ARG
4	B	880	THR
4	B	1017	ILE
4	B	1099	VAL
4	B	1104	HIS
5	C	48	SER
5	C	212	PRO
5	C	227	THR
6	E	31	THR
6	E	102	GLU
6	E	103	LYS
6	E	122	LYS
6	E	139	ALA
6	E	206	GLY
7	F	128	LYS
8	H	8	ASP
8	H	17	PRO
8	H	82	PRO
8	H	135	LEU
8	H	139	ASN
9	I	9	ASP
9	I	33	SER
9	I	86	PHE
10	J	9	SER

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Mol	Chain	Res	Type
12	L	63	ARG
3	A	101	LYS
3	A	134	ARG
3	A	139	TRP
3	A	424	ILE
3	A	599	SER
3	A	1067	LEU
3	A	1097	GLY
3	A	1115	SER
3	A	1122	PRO
3	A	1405	THR
4	B	304	ASP
4	B	436	VAL
4	B	501	PRO
4	B	667	GLN
4	B	791	THR
4	B	1054	GLY
4	B	1097	HIS
4	B	1178	ASN
5	C	18	VAL
5	C	149	LYS
5	C	174	ALA
6	E	59	SER
10	J	6	ARG
12	L	50	ASP
12	L	56	LEU
3	A	58	LEU
3	A	223	GLY
3	A	400	PRO
3	A	958	VAL
3	A	972	HIS
3	A	1098	VAL
3	A	1130	GLN
3	A	1282	VAL
3	A	1351	GLU
3	A	1378	GLN
4	B	248	SER
4	B	419	THR
4	B	619	ILE
4	B	648	HIS
4	B	687	GLU
4	B	707	PRO

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Mol	Chain	Res	Type
4	B	712	PRO
4	B	764	SER
4	B	907	GLY
4	B	982	SER
4	B	1108	ARG
6	E	36	GLU
8	H	62	SER
8	H	89	LEU
9	I	47	GLU
9	I	88	SER
3	A	226	GLU
3	A	368	LYS
3	A	399	HIS
3	A	531	ILE
3	A	1014	ALA
3	A	1314	SER
3	A	1352	VAL
4	B	27	ALA
6	E	167	ARG
8	H	138	GLU
9	I	98	VAL
11	K	107	THR
12	L	59	ALA
4	B	247	GLY
3	A	336	ILE
3	A	1104	ILE
12	L	55	ILE
3	A	810	PRO
3	A	1075	PRO
3	A	1242	VAL
5	C	172	PRO
5	C	216	GLY
3	A	78	PRO
4	B	511	PRO
5	C	202	PRO
5	C	218	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1206/1520 (79%)	1123 (93%)	83 (7%)	14	41
4	B	952/1061 (90%)	874 (92%)	78 (8%)	10	35
5	C	234/274 (85%)	218 (93%)	16 (7%)	14	42
6	E	196/197 (100%)	192 (98%)	4 (2%)	48	68
7	F	74/137 (54%)	68 (92%)	6 (8%)	11	36
8	H	117/128 (91%)	113 (97%)	4 (3%)	32	59
9	I	113/116 (97%)	105 (93%)	8 (7%)	13	40
10	J	60/65 (92%)	54 (90%)	6 (10%)	7	27
11	K	99/102 (97%)	88 (89%)	11 (11%)	6	22
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	13
All	All	3091/3657 (84%)	2869 (93%)	222 (7%)	13	40

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	GLN
3	A	22	PHE
3	A	31	SER
3	A	56	PRO
3	A	70	CYS
3	A	93	VAL
3	A	247	ARG
3	A	269	ILE
3	A	302	THR
3	A	322	VAL
3	A	326	ARG
3	A	351	THR
3	A	375	THR
3	A	381	THR
3	A	385	ILE
3	A	397	ASN
3	A	434	ARG
3	A	443	LEU
3	A	445	ASN
3	A	450	LEU
3	A	451	HIS
3	A	461	LYS

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Mol	Chain	Res	Type
3	A	466	SER
3	A	474	VAL
3	A	475	THR
3	A	493	GLN
3	A	503	GLN
3	A	504	LEU
3	A	524	VAL
3	A	535	THR
3	A	590	ARG
3	A	596	THR
3	A	597	LEU
3	A	598	LEU
3	A	618	GLU
3	A	629	LEU
3	A	666	ILE
3	A	682	THR
3	A	740	LEU
3	A	741	ASN
3	A	745	GLN
3	A	756	ILE
3	A	768	GLN
3	A	821	ARG
3	A	845	LEU
3	A	849	MET
3	A	854	ASN
3	A	855	THR
3	A	858	ASN
3	A	904	THR
3	A	913	LEU
3	A	920	LEU
3	A	929	LEU
3	A	948	VAL
3	A	979	SER
3	A	1029	ARG
3	A	1035	TYR
3	A	1043	ASP
3	A	1055	ARG
3	A	1057	VAL
3	A	1077	THR
3	A	1122	PRO
3	A	1136	SER
3	A	1208	THR

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Mol	Chain	Res	Type
3	A	1212	VAL
3	A	1222	ASN
3	A	1232	ASN
3	A	1258	HIS
3	A	1264	GLU
3	A	1295	THR
3	A	1308	THR
3	A	1311	VAL
3	A	1318	THR
3	A	1332	PHE
3	A	1335	ILE
3	A	1351	GLU
3	A	1355	VAL
3	A	1359	ASP
3	A	1364	ASN
3	A	1375	MET
3	A	1376	THR
3	A	1425	SER
3	A	1442	ASP
4	B	43	LEU
4	B	57	TYR
4	B	63	ILE
4	B	98	THR
4	B	109	THR
4	B	121	ASN
4	B	175	ARG
4	B	185	THR
4	B	194	GLU
4	B	232	SER
4	B	234	ILE
4	B	254	LEU
4	B	261	ARG
4	B	268	THR
4	B	309	GLN
4	B	313	MET
4	B	317	CYS
4	B	320	ASP
4	B	331	LEU
4	B	361	LEU
4	B	387	LEU
4	B	396	ASP
4	B	408	LEU

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Mol	Chain	Res	Type
4	B	453	ILE
4	B	484	ASN
4	B	485	ARG
4	B	498	THR
4	B	513	GLN
4	B	514	LEU
4	B	538	ASN
4	B	542	MET
4	B	547	VAL
4	B	556	THR
4	B	563	MET
4	B	570	VAL
4	B	576	ASP
4	B	624	LEU
4	B	644	GLU
4	B	680	THR
4	B	723	VAL
4	B	732	SER
4	B	737	THR
4	B	762	ASN
4	B	764	SER
4	B	780	VAL
4	B	791	THR
4	B	835	GLN
4	B	839	MET
4	B	860	MET
4	B	901	PRO
4	B	915	THR
4	B	944	THR
4	B	951	GLN
4	B	953	LEU
4	B	954	VAL
4	B	976	ILE
4	B	986	GLN
4	B	987	LYS
4	B	996	ARG
4	B	997	GLU
4	B	999	MET
4	B	1002	THR
4	B	1007	VAL
4	B	1017	ILE
4	B	1021	MET

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Mol	Chain	Res	Type
4	B	1034	VAL
4	B	1049	ASP
4	B	1065	GLN
4	B	1073	TYR
4	B	1103	ILE
4	B	1111	MET
4	B	1118	PRO
4	B	1132	GLU
4	B	1133	MET
4	B	1147	LEU
4	B	1150	ARG
4	B	1151	LEU
4	B	1185	CYS
5	C	22	LEU
5	C	25	VAL
5	C	26	ASP
5	C	58	LEU
5	C	62	PHE
5	C	69	LEU
5	C	77	ILE
5	C	99	LEU
5	C	133	ILE
5	C	195	GLN
5	C	229	TYR
5	C	233	GLU
5	C	238	ILE
5	C	240	VAL
5	C	259	LEU
5	C	264	GLN
6	E	40	GLU
6	E	84	ASP
6	E	92	THR
6	E	183	PRO
7	F	79	ARG
7	F	90	ARG
7	F	103	MET
7	F	111	LEU
7	F	115	THR
7	F	133	VAL
8	H	21	ASN
8	H	27	GLU
8	H	109	LYS

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Mol	Chain	Res	Type
8	H	110	ASP
9	I	12	ASN
9	I	29	CYS
9	I	31	THR
9	I	52	ILE
9	I	75	CYS
9	I	76	PRO
9	I	87	GLN
9	I	97	MET
10	J	1	MET
10	J	2	ILE
10	J	7	CYS
10	J	22	LEU
10	J	47	ARG
10	J	48	ARG
11	K	11	LEU
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	47	ARG
11	K	50	LEU
11	K	51	LEU
11	K	63	VAL
11	K	77	THR
11	K	114	LEU
12	L	50	ASP
12	L	54	ARG
12	L	55	ILE
12	L	65	VAL
12	L	68	GLU
12	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
3	A	92	HIS
3	A	118	HIS
3	A	169	ASN
3	A	225	ASN
3	A	281	HIS

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Mol	Chain	Res	Type
3	A	339	ASN
3	A	425	GLN
3	A	435	HIS
3	A	445	ASN
3	A	493	GLN
3	A	503	GLN
3	A	517	ASN
3	A	631	HIS
3	A	698	GLN
3	A	736	ASN
3	A	741	ASN
3	A	757	ASN
3	A	760	GLN
3	A	768	GLN
3	A	786	HIS
3	A	858	ASN
3	A	877	HIS
3	A	926	GLN
3	A	953	ASN
3	A	965	GLN
3	A	968	GLN
3	A	994	GLN
3	A	1011	GLN
3	A	1033	GLN
3	A	1070	GLN
3	A	1124	HIS
3	A	1130	GLN
3	A	1188	GLN
3	A	1364	ASN
3	A	1387	HIS
3	A	1390	ASN
3	A	1393	ASN
3	A	1432	GLN
4	B	46	GLN
4	B	47	GLN
4	B	53	GLN
4	B	115	GLN
4	B	121	ASN
4	B	215	GLN
4	B	236	HIS
4	B	309	GLN
4	B	325	GLN

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Mol	Chain	Res	Type
4	B	363	HIS
4	B	415	GLN
4	B	465	ASN
4	B	484	ASN
4	B	513	GLN
4	B	515	HIS
4	B	516	ASN
4	B	518	HIS
4	B	538	ASN
4	B	744	HIS
4	B	770	GLN
4	B	822	ASN
4	B	842	ASN
4	B	862	GLN
4	B	957	ASN
4	B	975	GLN
4	B	1015	HIS
4	B	1065	GLN
4	B	1093	GLN
4	B	1117	GLN
4	B	1141	HIS
4	B	1161	HIS
4	B	1178	ASN
4	B	1179	GLN
4	B	1193	GLN
5	C	65	HIS
5	C	73	GLN
5	C	112	ASN
5	C	123	ASN
5	C	131	HIS
5	C	140	ASN
5	C	167	HIS
5	C	242	GLN
5	C	252	GLN
6	E	5	ASN
6	E	101	GLN
6	E	104	ASN
6	E	114	ASN
6	E	115	ASN
6	E	147	HIS
7	F	78	GLN
8	H	33	GLN

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Mol	Chain	Res	Type
9	I	12	ASN
10	J	53	HIS
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	3	C
2	R	9	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.