



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 09:06 PM EDT

PDB ID : 5UAQ
Title : Escherichia coli RNA polymerase RpoB H526Y mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.60 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:

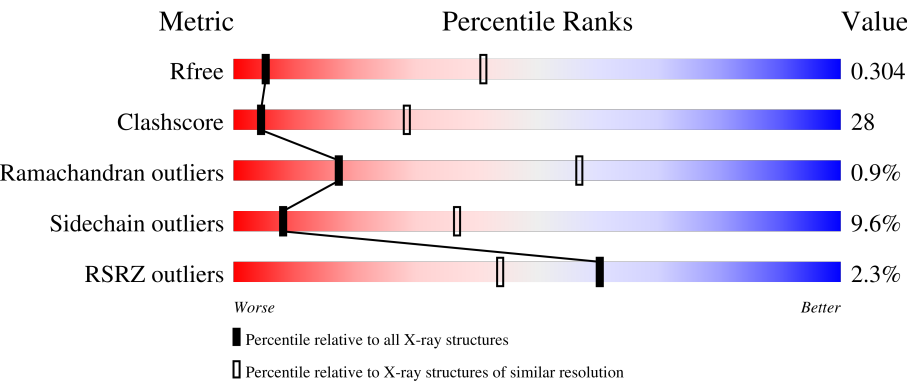
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	<div><div></div><div>4%</div><div>50%</div><div>44%</div><div>6%</div></div>
3	D	1407	<div><div></div><div>%</div><div>35%</div><div>38%</div><div>9%</div><div>17%</div></div>
3	J	1407	<div><div></div><div>2%</div><div>36%</div><div>38%</div><div>8%</div><div>18%</div></div>
4	E	91	<div><div></div><div>2%</div><div>64%</div><div>31%</div><div>• •</div></div>
4	K	91	<div><div></div><div>15%</div><div>53%</div><div>33%</div><div>•</div><div>13%</div></div>
5	F	613	<div><div></div><div>2%</div><div>40%</div><div>31%</div><div>5%</div><div>24%</div></div>
5	L	613	<div><div></div><div>%</div><div>36%</div><div>34%</div><div>6%</div><div>23%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55699 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2403	1505	421	469	8			
1	B	217	Total	C	N	O	S	0	0	0
			1672	1044	295	327	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10572	6634	1839	2056	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10568	6632	1838	2055	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	526	TYR	HIS	engineered mutation	UNP P0A8V2
I	526	TYR	HIS	engineered mutation	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9029	5676	1620	1687	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	467	Total	C	N	O	S	0	0	0
			3806	2385	677	721	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

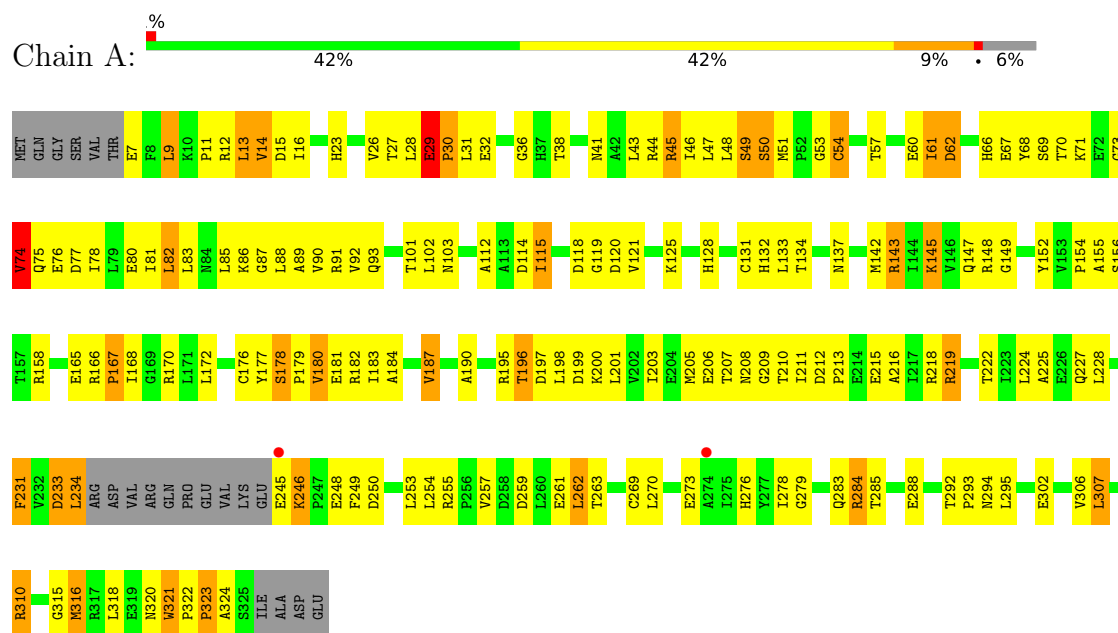
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	J	2	Total	Zn	0	0
			2	2		

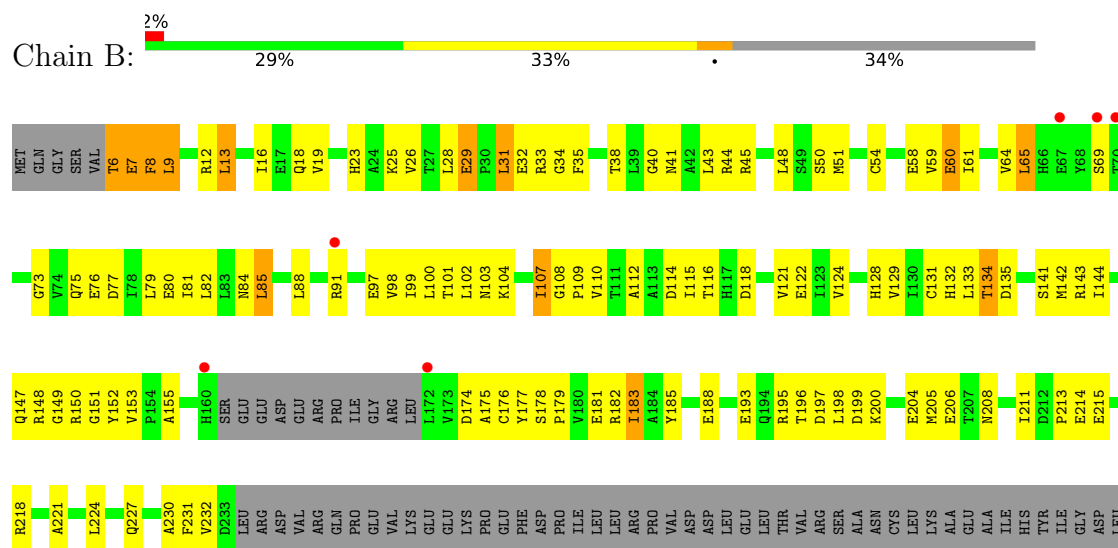
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

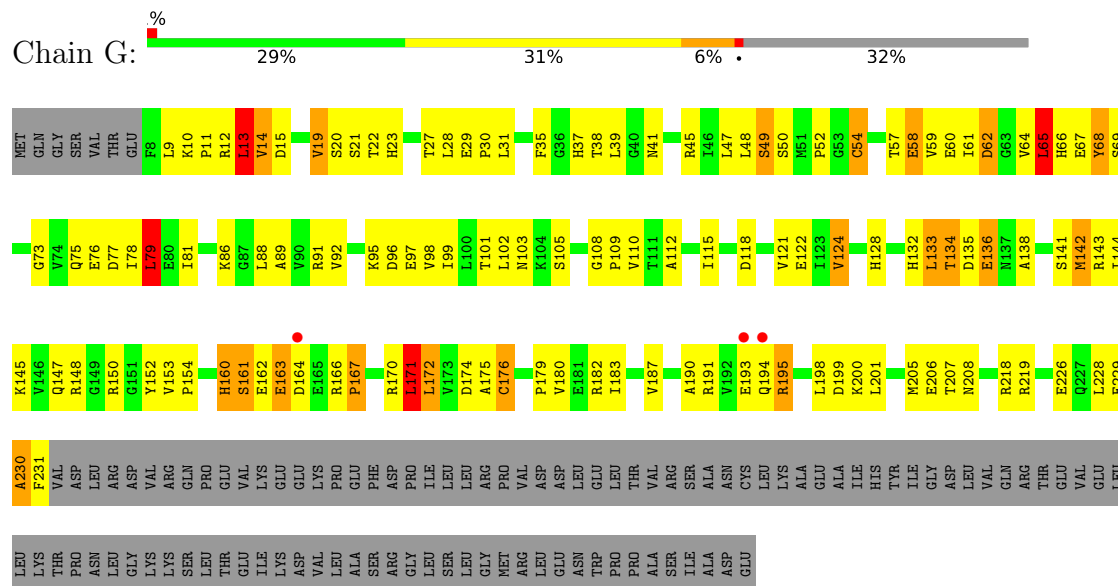


• Molecule 1: DNA-directed RNA polymerase subunit alpha

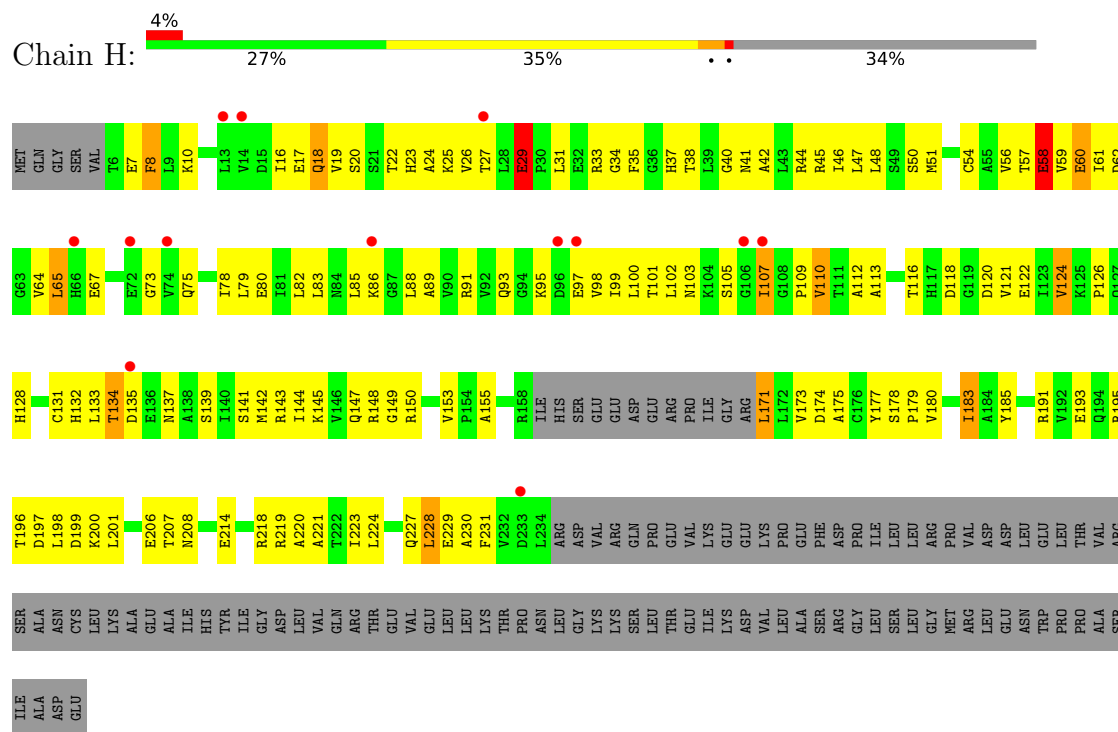


VAL GLN ARG THR GLU VAL LEU LEU LYS THR PRO ASN LEU GLY LYS SER LEU THR VAL LEU LEU ALA SER ARG LEU LEU MET ARG LEU LEU GLU ASN TRP PRO PRO ALA ILE SER ASP GLU

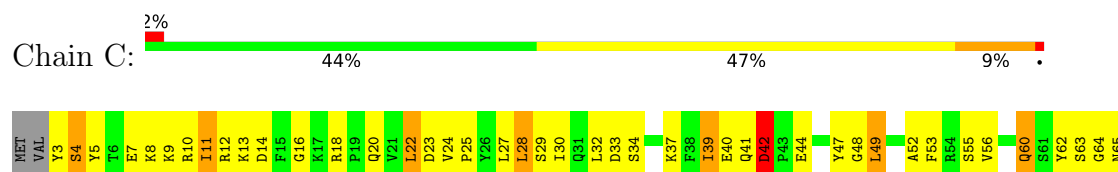
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

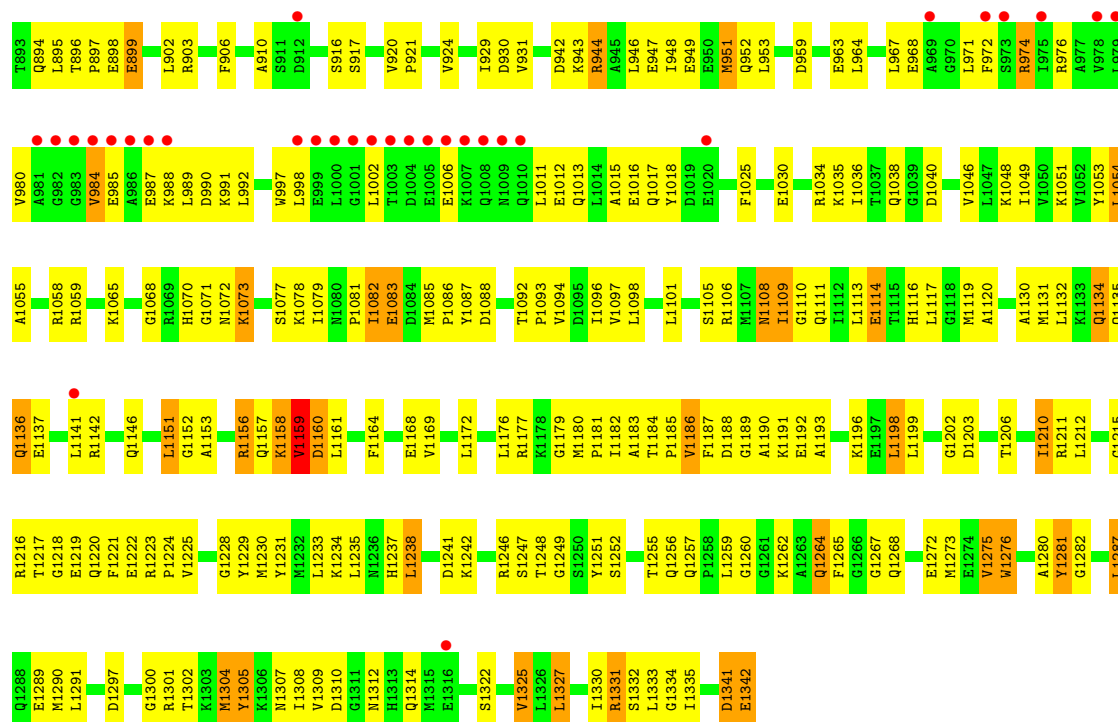


• Molecule 2: DNA-directed RNA polymerase subunit beta

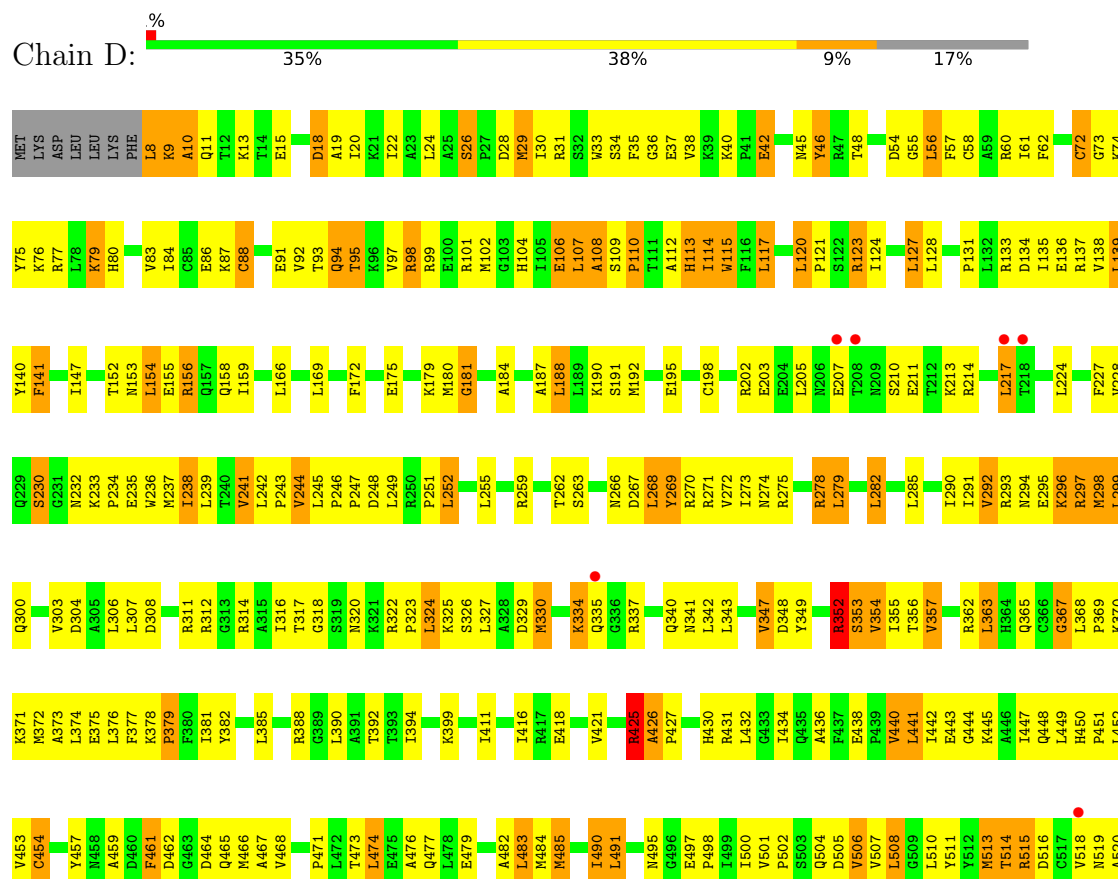


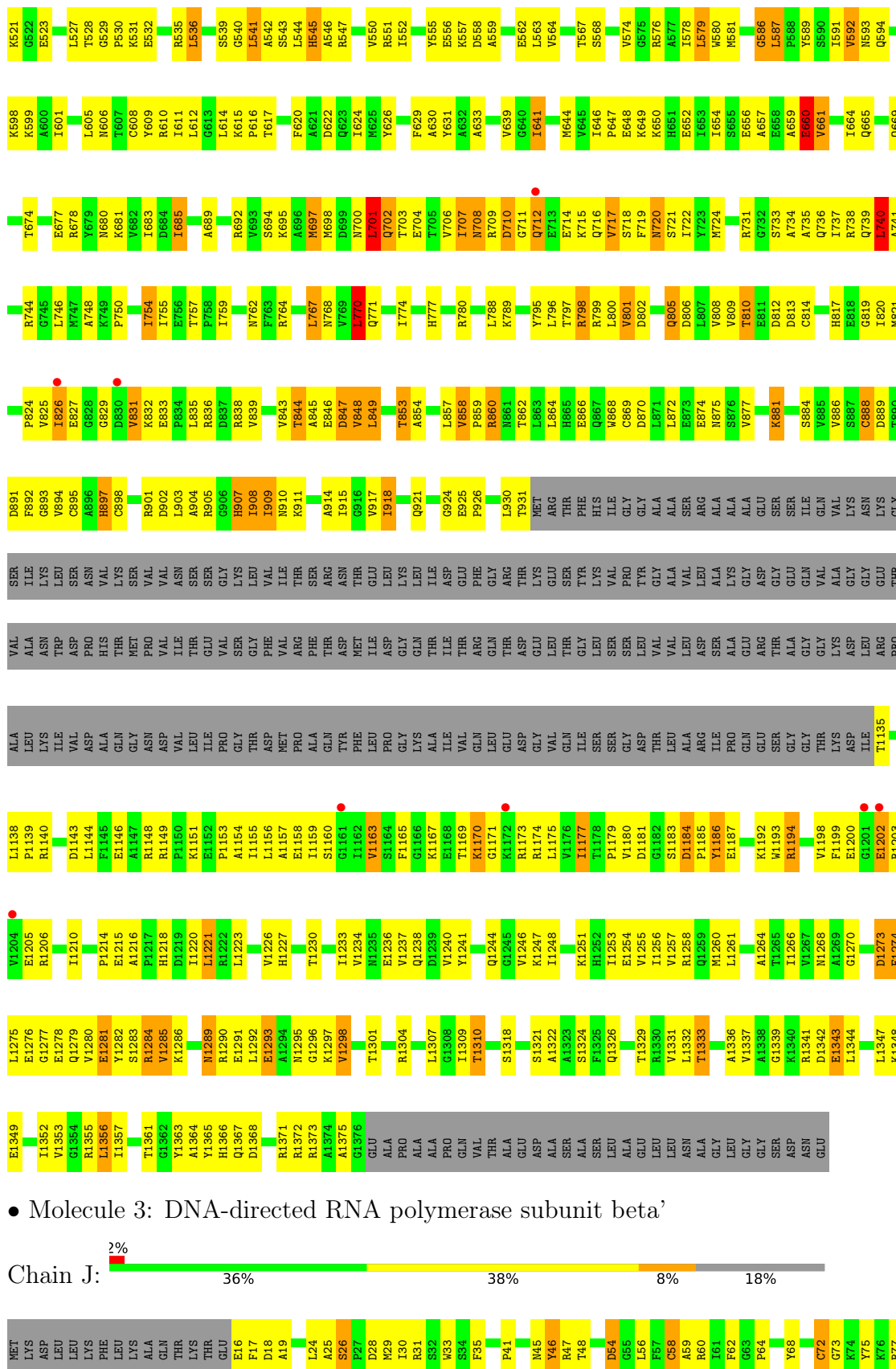
M119	V1052	V984	F812	G664	V598	R529	F464	L366	E286	L210	V137	Q89
A1120	Y1053	E985	E813	A665	D601	I530	R465	Y367	V287	R211	I138	Y70
G1123	E986	E987	D814	S666	E601	G534	G466	R368	P289	A212	M139	
I1124	E988	S815	S815	E602	G534		G467	M369	F289	L213	G140	
	R1058	R893	L816	I603	I603	L538	L468	M370	L292	N214	T141	
M1129	R1059	R894	R817	P669	H604	T539	V469	T377	L292	N215	R74	
A1130	L1060	L895	V818	F670	G605	R540	R470	R378	V296	L221	L75	
M1131	Q1061	R896	S819	L671	L606	E541	V471	R379	V297	L221	G76	
	P1062	T897	E820	E672	S607	R542	E472	E379	V297	F224	E77	
	E988	G747	H673	H673	A608	A543	R473	A381	K299	F225	P78	
	R994	I748			I609	G544	A474	A382	D300	F225		
Q1134	K1065		A676	A676			V475	S382	D300		V82	
Q1135	Q1135		R677	R677	V615		E476	S383	Y301	V228	L149	
Q1136	A1067		R678	R678	I616	V547	E477	L384	I302	V228	H150	
E1137	G1068		A679	A679	E478	R548	E477			F230	R151	
	R1069		Q618	Q618	R478			N387	T306	E231	F156	
K1140	H1070		R758	R758	L479	H551	S480	F389	L309	L232	F157	
L1141	G1071		S759	S759	L479		S480		L310	L232	R88	
R1142	N1072		N620	N620	A619	H552	L481		C311	L241	D158	
E1143	K1073		G682	G682	N620	T553	G482		A312	L241	G89	
F1144	G1074		H684	H684	S621	H554	D482		L322	L241	V90	
	I1145		L623	L623	H622		L483		A323	L241	T91	
Q1146	T1075		L623	L623	L623		L483		K322	L241	A94	
Q1147	T1076		L623	L623	L623		L483		A323	L241	P95	
R1147	T1077		L623	L623	L623		L483		A323	L241	R96	
A1148	S1077		L623	L623	L623		L483		A323	L241	R97	
A1149	K1078		L623	L623	L623		L483		A323	L241	V98	
Y1149	I1079		L623	L623	L623		L483		A323	L241	R99	
D1150	H1080		L623	L623	L623		L483		A323	L241	D100	
	I1081		L623	L623	L623		L483		A323	L241	R101	
E1151	T1082		L623	L623	L623		L483		A323	L241	L102	
A1152	K1083		L623	L623	L623		L483		A323	L241	L103	
	E1083		L623	L623	L623		L483		A323	L241	W103	
	D1084		L623	L623	L623		L483		A323	L241	Y104	
	T1085		L623	L623	L623		L483		A323	L241	Y105	
R1156	P1086		L623	L623	L623		L483		A323	L241	E108	
Q1157	Y1087		L623	L623	L623		L483		A323	L241	A109	
			L623	L623	L623		L483		A323	L241	P110	
L1158			L623	L623	L623		L483		A323	L241	E111	
V1159			L623	L623	L623		L483		A323	L241	K115	
L1161			L623	L623	L623		L483		A323	L241	D116	
			L623	L623	L623		L483		A323	L241	I117	
F1164			L623	L623	L623		L483		A323	L241	K118	
S1165			L623	L623	L623		L483		A323	L241	E119	
			L623	L623	L623		L483		A323	L241	Q120	
E1168			L623	L623	L623		L483		A323	L241	E121	
V1169			L623	L623	L623		L483		A323	L241	V122	
M1170			L623	L623	L623		L483		A323	L241	Y123	
R1171			L623	L623	L623		L483		A323	L241	M124	
L1172			L623	L623	L623		L483		A323	L241	G125	
A1173			L623	L623	L623		L483		A323	L241		
E1174			L623	L623	L623		L483		A323	L241	P128	
N1175			L623	L623	L623		L483		A323	L241	L129	
L1176			L623	L623	L623		L483		A323	L241	M130	
R1177			L623	L623	L623		L483		A323	L241	T131	
K1178			L623	L623	L623		L483		A323	L241	R201	
			L623	L623	L623		L483		A323	L241	R202	
G1179			L623	L623	L623		L483		A323	L241	K203	
G1180			L623	L623	L623		L483		A323	L241	G134	
M1180			L623	L623	L623		L483		A323	L241	T208	
P1181			L623	L623	L623		L483		A323	L241	L209	
L1182			L623	L623	L623		L483		A323	L241		
A1183			L623	L623	L623		L483		A323	L241		
E1184			L623	L623	L623		L483		A323	L241		
T1184			L623	L623	L623		L483		A323	L241		
			L623	L623	L623		L483		A323	L241		
P1185			L623	L623	L623		L483		A323	L241		
L1186			L623	L623	L623		L483		A323	L241		
F1187			L623	L623	L623		L483		A323	L241		



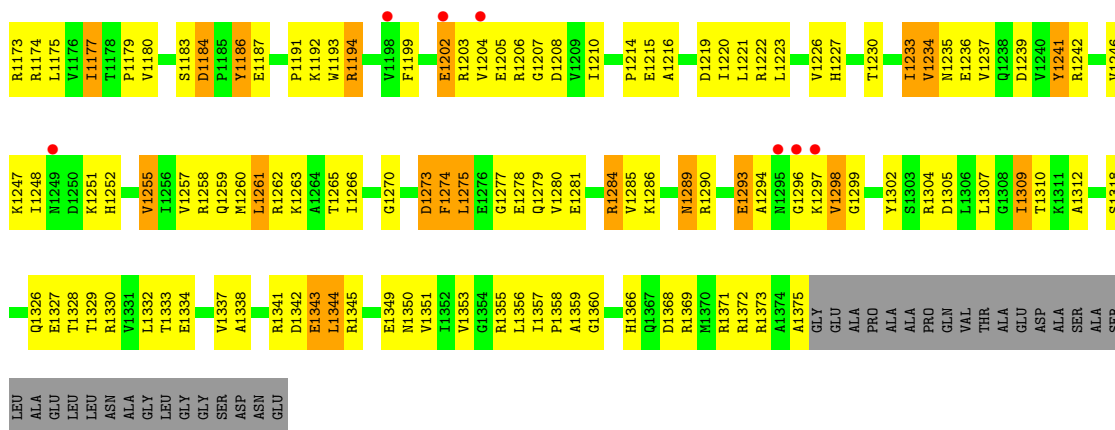


- Molecule 3: DNA-directed RNA polymerase subunit beta'

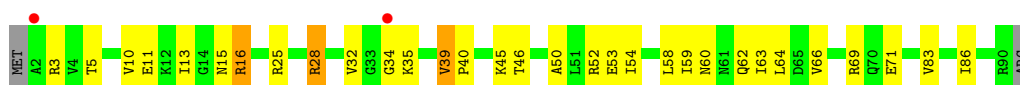




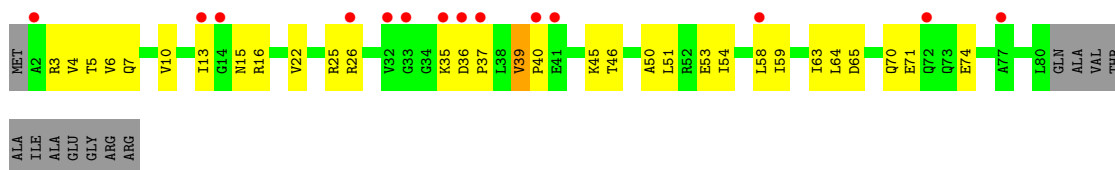
WORLDWIDE
PDB
PROTEIN DATA BANK



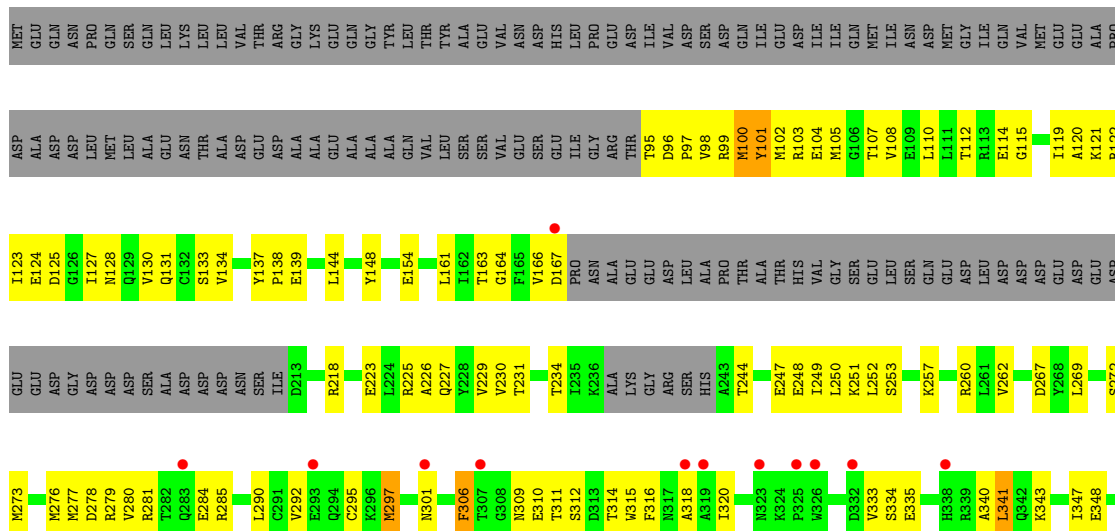
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.36Å 206.28Å 308.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.60 29.90 – 3.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.90-3.60) 93.7 (29.90-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.56Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.246 , 0.305 0.246 , 0.304	Depositor DCC
R_{free} test set	1932 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	142.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 91.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55699	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	4/2435 (0.2%)	1.07	12/3300 (0.4%)
1	B	0.75	1/1692 (0.1%)	1.01	5/2293 (0.2%)
1	G	0.58	0/1751	1.05	9/2373 (0.4%)
1	H	0.59	0/1686	0.91	4/2285 (0.2%)
2	C	1.17	37/10741 (0.3%)	1.21	65/14492 (0.4%)
2	I	0.80	7/10737 (0.1%)	0.97	15/14487 (0.1%)
3	D	1.21	60/9246 (0.6%)	1.24	74/12478 (0.6%)
3	J	1.02	27/9168 (0.3%)	1.13	52/12374 (0.4%)
4	E	0.65	0/693	0.83	0/935
4	K	0.38	0/629	0.61	0/847
5	F	0.82	2/3857 (0.1%)	1.05	10/5184 (0.2%)
5	L	0.77	3/3872 (0.1%)	0.99	12/5205 (0.2%)
All	All	0.98	141/56507 (0.2%)	1.10	258/76253 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	G	0	1
2	C	0	11
2	I	0	2
3	D	0	12
3	J	0	9
5	F	0	1
5	L	0	1
All	All	0	39

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	811	ASN	CB-CG	-9.14	1.30	1.51
1	A	131	CYS	CB-SG	-8.93	1.67	1.82
3	J	145	VAL	CB-CG2	-8.81	1.34	1.52
2	C	636	CYS	CB-SG	-8.52	1.67	1.82
3	J	72	CYS	CB-SG	-7.87	1.68	1.82
3	D	814	CYS	CB-SG	-7.77	1.69	1.82
2	C	183	TRP	CB-CG	-7.71	1.36	1.50
3	J	115	TRP	CB-CG	-7.67	1.36	1.50
3	D	244	VAL	CB-CG1	-7.63	1.36	1.52
3	D	457	TYR	CE2-CZ	-7.57	1.28	1.38
1	B	131	CYS	CB-SG	-7.47	1.69	1.82
3	D	292	VAL	CB-CG1	-7.43	1.37	1.52
2	C	1285	TYR	CB-CG	-7.33	1.40	1.51
3	D	303	VAL	CB-CG2	-7.26	1.37	1.52
2	C	764	CYS	CB-SG	-7.18	1.70	1.82
3	D	349	TYR	CE2-CZ	-7.18	1.29	1.38
3	D	426	ALA	C-N	-7.16	1.20	1.34
3	J	1353	VAL	CB-CG1	-7.15	1.37	1.52
2	C	1076	ILE	CB-CG2	-7.15	1.30	1.52
3	D	349	TYR	CG-CD1	-7.14	1.29	1.39
3	D	868	TRP	CB-CG	-7.04	1.37	1.50
3	D	511	TYR	CD2-CE2	-7.02	1.28	1.39
3	D	72	CYS	CB-SG	-6.99	1.70	1.82
2	C	1276	TRP	CB-CG	-6.92	1.37	1.50
3	J	198	CYS	CB-SG	-6.90	1.70	1.82
2	C	807	TRP	CB-CG	-6.89	1.37	1.50
3	D	457	TYR	CD2-CE2	-6.89	1.29	1.39
2	C	838	CYS	CB-SG	-6.83	1.70	1.82
3	J	145	VAL	CB-CG1	-6.81	1.38	1.52
2	I	1275	VAL	CB-CG2	-6.77	1.38	1.52
3	D	1337	VAL	CB-CG1	-6.71	1.38	1.52
2	I	1281	TYR	CE1-CZ	-6.60	1.29	1.38
3	D	894	VAL	CB-CG1	-6.59	1.39	1.52
2	I	1276	TRP	CE3-CZ3	-6.53	1.27	1.38
3	J	349	TYR	CE1-CZ	-6.51	1.30	1.38
3	D	917	VAL	CB-CG2	-6.46	1.39	1.52
3	D	895	CYS	CB-SG	-6.43	1.71	1.82
3	D	347	VAL	CB-CG2	-6.42	1.39	1.52
5	L	96	ASP	C-N	-6.42	1.22	1.34
3	J	85	CYS	CB-SG	-6.38	1.71	1.82
3	D	453	VAL	CB-CG1	-6.37	1.39	1.52
3	J	885	VAL	CB-CG1	-6.37	1.39	1.52
2	I	1325	VAL	CB-CG2	-6.34	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	236	TRP	CB-CG	-6.34	1.38	1.50
3	J	303	VAL	CB-CG1	-6.32	1.39	1.52
2	C	137	VAL	CB-CG2	-6.31	1.39	1.52
3	D	236	TRP	CG-CD1	-6.28	1.27	1.36
3	J	801	VAL	CB-CG2	-6.24	1.39	1.52
3	D	898	CYS	CB-SG	-6.23	1.71	1.82
3	D	115	TRP	CB-CG	-6.22	1.39	1.50
5	F	101	TYR	CD2-CE2	-6.21	1.30	1.39
2	I	1305	TYR	CD1-CE1	-6.19	1.30	1.39
2	C	663	VAL	CB-CG2	-6.13	1.40	1.52
2	C	660	VAL	CB-CG1	-6.02	1.40	1.52
2	C	1096	ILE	CB-CG2	-6.01	1.34	1.52
3	J	303	VAL	CB-CG2	-6.01	1.40	1.52
2	C	85	CYS	CB-SG	-6.01	1.72	1.82
2	C	934	PHE	CD2-CE2	-6.01	1.27	1.39
2	C	1329	GLU	CG-CD	-5.99	1.43	1.51
3	D	421	VAL	CB-CG1	-5.99	1.40	1.52
3	D	639	VAL	CB-CG1	-5.98	1.40	1.52
3	D	457	TYR	CG-CD1	-5.97	1.31	1.39
2	C	592	ARG	CB-CG	-5.97	1.36	1.52
3	J	307	LEU	CG-CD2	-5.97	1.29	1.51
3	J	421	VAL	CB-CG1	-5.96	1.40	1.52
5	L	434	TRP	CB-CG	-5.95	1.39	1.50
3	D	115	TRP	CE3-CZ3	-5.93	1.28	1.38
3	D	354	VAL	CB-CG2	-5.92	1.40	1.52
3	D	1363	TYR	CD2-CE2	-5.91	1.30	1.39
3	J	894	VAL	CB-CG1	-5.89	1.40	1.52
3	D	511	TYR	CB-CG	-5.82	1.43	1.51
2	C	505	PHE	CB-CG	-5.76	1.41	1.51
3	D	631	TYR	CE2-CZ	-5.76	1.31	1.38
3	D	454	CYS	CB-SG	-5.73	1.72	1.81
3	D	511	TYR	CD1-CE1	-5.72	1.30	1.39
3	D	608	CYS	CB-SG	-5.72	1.72	1.81
2	C	1069	ARG	CG-CD	-5.71	1.37	1.51
2	C	663	VAL	CB-CG1	-5.68	1.41	1.52
3	J	868	TRP	CB-CG	-5.66	1.40	1.50
3	J	144	TYR	CE2-CZ	-5.66	1.31	1.38
2	C	1281	TYR	CE2-CZ	-5.63	1.31	1.38
2	C	464	PHE	CB-CG	-5.63	1.41	1.51
3	D	468	VAL	CB-CG1	-5.62	1.41	1.52
3	D	347	VAL	CB-CG1	-5.62	1.41	1.52
3	D	801	VAL	CB-CG1	-5.60	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	895	CYS	CB-SG	-5.60	1.72	1.81
3	D	438	GLU	CG-CD	5.59	1.60	1.51
3	D	421	VAL	CB-CG2	-5.55	1.41	1.52
2	C	810	TYR	CG-CD1	-5.53	1.31	1.39
3	J	512	TYR	CD2-CE2	-5.51	1.31	1.39
3	J	723	TYR	CE1-CZ	-5.51	1.31	1.38
3	J	457	TYR	CD2-CE2	-5.45	1.31	1.39
3	D	592	VAL	CB-CG1	-5.45	1.41	1.52
2	C	810	TYR	CB-CG	-5.44	1.43	1.51
3	J	512	TYR	CD1-CE1	-5.43	1.31	1.39
3	D	660	GLU	CB-CG	-5.43	1.41	1.52
3	D	141	PHE	CB-CG	-5.40	1.42	1.51
2	C	659	GLN	CB-CG	-5.39	1.38	1.52
2	I	899	GLU	CG-CD	-5.39	1.43	1.51
3	D	138	VAL	CB-CG2	-5.37	1.41	1.52
3	D	269	TYR	CD1-CE1	-5.37	1.31	1.39
3	D	292	VAL	CB-CG2	-5.36	1.41	1.52
3	D	1331	VAL	CB-CG2	-5.35	1.41	1.52
2	C	770	CYS	CB-SG	-5.35	1.73	1.81
3	D	357	VAL	CB-CG2	-5.34	1.41	1.52
2	C	1305	TYR	CG-CD2	-5.34	1.32	1.39
3	D	120	LEU	C-N	-5.32	1.24	1.34
3	J	241	VAL	CB-CG1	-5.32	1.41	1.52
3	D	349	TYR	CE1-CZ	-5.30	1.31	1.38
2	I	1305	TYR	CB-CG	-5.30	1.43	1.51
1	A	68	TYR	CD1-CE1	-5.30	1.31	1.39
2	C	389	PHE	CB-CG	-5.30	1.42	1.51
3	D	57	PHE	CB-CG	-5.29	1.42	1.51
3	D	801	VAL	CB-CG2	-5.29	1.41	1.52
3	J	1241	TYR	CE1-CZ	-5.28	1.31	1.38
3	D	1363	TYR	CD1-CE1	-5.28	1.31	1.39
3	D	123	ARG	CB-CG	-5.26	1.38	1.52
2	C	505	PHE	CD1-CE1	-5.26	1.28	1.39
1	A	180	VAL	CB-CG1	-5.25	1.41	1.52
2	C	782	VAL	CB-CG1	-5.23	1.41	1.52
3	J	295	GLU	CB-CG	-5.23	1.42	1.52
3	D	440	VAL	CB-CG1	-5.21	1.42	1.52
5	L	522	PHE	CB-CG	-5.19	1.42	1.51
2	C	708	VAL	CB-CG1	-5.17	1.42	1.52
2	C	816	ILE	CB-CG2	-5.14	1.36	1.52
2	C	530	ILE	CB-CG2	-5.11	1.37	1.52
2	C	700	VAL	CB-CG1	-5.09	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	517	CYS	CB-SG	-5.09	1.73	1.81
1	A	187	VAL	CB-CG1	-5.09	1.42	1.52
2	C	456	VAL	CB-CG1	-5.09	1.42	1.52
3	D	269	TYR	CD2-CE2	-5.09	1.31	1.39
2	C	884	VAL	CB-CG1	-5.07	1.42	1.52
3	D	272	VAL	CB-CG2	-5.07	1.42	1.52
3	D	349	TYR	CB-CG	-5.07	1.44	1.51
5	F	508	GLU	CB-CG	-5.07	1.42	1.52
3	D	1353	VAL	CB-CG2	-5.03	1.42	1.52
3	D	461	PHE	CG-CD2	-5.02	1.31	1.38
3	D	353	SER	CB-OG	-5.01	1.35	1.42
3	D	1337	VAL	CB-CG2	-5.01	1.42	1.52
2	C	934	PHE	CD1-CE1	-5.01	1.29	1.39
3	J	116	PHE	CE2-CZ	-5.01	1.27	1.37

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1287	LEU	CB-CG-CD2	-14.16	86.92	111.00
3	D	376	LEU	CB-CG-CD2	-10.83	92.59	111.00
3	D	114	ILE	CG1-CB-CG2	-10.71	87.84	111.40
2	C	796	LEU	CB-CG-CD2	-9.94	94.10	111.00
3	D	188	LEU	CB-CG-CD2	-9.88	94.20	111.00
3	J	117	LEU	CB-CG-CD1	-9.86	94.25	111.00
3	D	888	CYS	CA-CB-SG	-9.74	96.47	114.00
3	J	1261	LEU	CB-CG-CD2	-9.68	94.54	111.00
3	D	245	LEU	CB-CG-CD2	-8.95	95.79	111.00
3	D	299	LEU	CB-CG-CD1	-8.92	95.84	111.00
3	D	541	LEU	CA-CB-CG	-8.91	94.81	115.30
3	J	307	LEU	CB-CG-CD2	-8.91	95.86	111.00
3	J	189	LEU	CA-CB-CG	-8.89	94.86	115.30
2	I	1327	LEU	CA-CB-CG	-8.81	95.04	115.30
2	C	680	LEU	CB-CG-CD1	-8.73	96.16	111.00
2	C	758	ARG	NE-CZ-NH2	-8.72	115.94	120.30
2	C	42	ASP	C-N-CD	-8.71	101.43	120.60
2	C	49	LEU	CA-CB-CG	-8.58	95.57	115.30
1	B	9	LEU	C-N-CA	8.54	143.04	121.70
3	D	117	LEU	CB-CG-CD1	-8.52	96.52	111.00
2	C	32	LEU	CB-CG-CD2	-8.47	96.61	111.00
3	J	198	CYS	CA-CB-SG	-8.42	98.85	114.00
1	G	54	CYS	CA-CB-SG	-8.37	98.94	114.00
3	D	1261	LEU	CB-CG-CD2	-8.28	96.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	865	LEU	CB-CG-CD2	-8.20	97.06	111.00
5	L	519	LEU	CB-CG-CD2	-8.19	97.08	111.00
3	J	239	LEU	CB-CG-CD2	-8.17	97.11	111.00
3	D	271	ARG	NE-CZ-NH1	-8.16	116.22	120.30
5	L	384	LEU	CB-CG-CD2	-8.15	97.14	111.00
1	A	29	GLU	C-N-CD	-8.09	102.81	120.60
2	C	575	LEU	CB-CG-CD1	-8.09	97.25	111.00
5	F	412	LEU	CB-CG-CD1	-7.93	97.52	111.00
3	D	123	ARG	CG-CD-NE	-7.87	95.27	111.80
2	C	1161	LEU	CA-CB-CG	-7.80	97.35	115.30
1	G	68	TYR	CB-CG-CD2	-7.80	116.32	121.00
2	C	1278	LEU	CB-CG-CD1	-7.73	97.85	111.00
1	G	48	LEU	CA-CB-CG	-7.73	97.53	115.30
2	C	540	ARG	NE-CZ-NH1	-7.72	116.44	120.30
3	J	245	LEU	CB-CG-CD1	-7.71	97.89	111.00
3	J	888	CYS	CA-CB-SG	-7.71	100.13	114.00
2	C	836	LEU	CB-CG-CD2	-7.69	97.92	111.00
2	C	1291	LEU	CB-CG-CD2	-7.65	98.00	111.00
3	J	434	ILE	CG1-CB-CG2	-7.50	94.90	111.40
5	F	379	MET	CA-CB-CG	-7.46	100.62	113.30
3	J	1344	LEU	CA-CB-CG	-7.40	98.27	115.30
1	H	228	LEU	CA-CB-CG	-7.38	98.33	115.30
1	G	68	TYR	CB-CG-CD1	7.36	125.42	121.00
2	C	680	LEU	CA-CB-CG	7.33	132.16	115.30
2	C	800	MET	CG-SD-CE	7.31	111.90	100.20
3	D	282	LEU	CB-CG-CD2	-7.31	98.57	111.00
3	D	441	LEU	CB-CG-CD1	-7.31	98.57	111.00
2	C	699	LEU	CA-CB-CG	-7.29	98.52	115.30
3	J	166	LEU	CB-CG-CD2	-7.22	98.72	111.00
3	J	470	VAL	C-N-CD	-7.22	104.72	120.60
3	J	127	LEU	CB-CG-CD2	-7.15	98.84	111.00
5	F	519	LEU	CA-CB-CG	-7.12	98.91	115.30
3	J	217	LEU	CA-CB-CG	7.11	131.66	115.30
3	D	918	ILE	CG1-CB-CG2	-7.08	95.81	111.40
5	F	602	SER	N-CA-C	-7.08	91.87	111.00
1	A	54	CYS	CA-CB-SG	-7.07	101.28	114.00
2	I	1287	LEU	CB-CG-CD2	-7.03	99.04	111.00
2	C	96	LEU	CA-CB-CG	-7.03	99.13	115.30
2	I	363	LEU	CA-CB-CG	-7.03	99.14	115.30
3	J	1233	ILE	CG1-CB-CG2	-7.02	95.96	111.40
2	I	241	LEU	CA-CB-CG	-6.92	99.38	115.30
3	J	307	LEU	CA-CB-CG	-6.89	99.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	540	LEU	CB-CG-CD2	-6.86	99.34	111.00
1	B	85	LEU	CA-CB-CG	-6.82	99.61	115.30
2	C	762	ASN	C-N-CA	-6.80	104.69	121.70
2	C	1101	LEU	CB-CG-CD2	-6.80	99.45	111.00
2	C	75	LEU	CB-CG-CD1	-6.78	99.48	111.00
3	D	416	ILE	CG1-CB-CG2	-6.77	96.50	111.40
2	C	1151	LEU	CA-CB-CG	-6.76	99.74	115.30
2	C	1327	LEU	CB-CG-CD2	-6.76	99.50	111.00
3	D	1361	THR	CA-CB-CG2	-6.75	102.96	112.40
2	C	818	VAL	CA-CB-CG2	-6.74	100.80	110.90
3	J	118	LYS	CD-CE-NZ	6.72	127.16	111.70
5	F	498	LEU	CB-CG-CD1	-6.69	99.62	111.00
2	C	1333	LEU	CB-CG-CD2	-6.68	99.64	111.00
3	J	1144	LEU	CA-CB-CG	-6.67	99.96	115.30
3	D	1355	ARG	NE-CZ-NH1	-6.67	116.97	120.30
2	C	28	LEU	CA-CB-CG	-6.64	100.03	115.30
2	I	838	CYS	CA-CB-SG	-6.62	102.09	114.00
2	C	1326	LEU	CB-CG-CD1	-6.61	99.76	111.00
1	B	28	LEU	CA-CB-CG	-6.61	100.11	115.30
3	J	162	GLU	CA-CB-CG	6.53	127.76	113.40
2	C	668	ILE	CG1-CB-CG2	-6.49	97.12	111.40
3	D	166	LEU	CB-CG-CD1	-6.47	100.00	111.00
3	D	508	LEU	CB-CG-CD1	-6.46	100.03	111.00
2	I	149	LEU	CB-CG-CD1	-6.45	100.03	111.00
3	D	299	LEU	CA-CB-CG	-6.45	100.48	115.30
3	J	1261	LEU	CB-CG-CD1	-6.43	100.07	111.00
3	J	289	ASP	CB-CG-OD1	-6.43	112.52	118.30
3	D	279	LEU	CB-CG-CD2	-6.41	100.10	111.00
3	J	374	LEU	CA-CB-CG	6.41	130.03	115.30
5	L	405	ILE	CG1-CB-CG2	-6.39	97.35	111.40
2	C	454	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	C	1303	LYS	CA-CB-CG	6.38	127.43	113.40
2	C	454	ARG	CG-CD-NE	-6.37	98.42	111.80
2	C	1176	LEU	CB-CG-CD2	-6.37	100.17	111.00
2	C	367	TYR	CB-CG-CD1	-6.36	117.18	121.00
3	J	126	LEU	CA-CB-CG	6.35	129.91	115.30
1	G	142	MET	CA-CB-CG	-6.34	102.52	113.30
3	D	297	ARG	NE-CZ-NH1	-6.32	117.14	120.30
5	L	559	LEU	CA-CB-CG	-6.32	100.76	115.30
2	C	1113	LEU	CB-CG-CD2	-6.31	100.27	111.00
2	C	367	TYR	CB-CG-CD2	6.29	124.77	121.00
5	L	386	LEU	CB-CG-CD2	-6.27	100.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	MET	CB-CG-SD	-6.25	93.64	112.40
1	A	316	MET	CA-CB-CG	-6.25	102.67	113.30
1	G	79	LEU	CB-CG-CD2	-6.22	100.43	111.00
5	F	519	LEU	CB-CG-CD1	-6.21	100.45	111.00
3	D	180	MET	CG-SD-CE	6.15	110.04	100.20
3	D	324	LEU	CB-CG-CD2	-6.15	100.55	111.00
3	J	566	LYS	N-CA-CB	6.13	121.64	110.60
1	G	195	ARG	N-CA-CB	6.12	121.62	110.60
3	D	449	LEU	CB-CG-CD2	-6.12	100.59	111.00
3	J	138	VAL	CG1-CB-CG2	-6.11	101.13	110.90
3	D	275	ARG	NE-CZ-NH1	-6.09	117.25	120.30
3	D	88	CYS	CA-CB-SG	-6.09	103.04	114.00
2	C	481	LEU	CA-CB-CG	6.07	129.26	115.30
5	L	402	LEU	CB-CG-CD2	-6.06	100.69	111.00
2	C	1281	TYR	C-N-CA	-6.04	109.62	122.30
3	D	740	LEU	CB-CG-CD1	-6.03	100.75	111.00
3	D	491	LEU	CB-CG-CD2	-6.00	100.81	111.00
2	C	513	GLN	CB-CA-C	-5.97	98.46	110.40
3	D	139	LEU	CB-CG-CD2	-5.95	100.88	111.00
3	J	723	TYR	CB-CG-CD2	5.95	124.57	121.00
1	B	131	CYS	CA-CB-SG	-5.94	103.30	114.00
3	J	464	ASP	CB-CG-OD1	5.93	123.64	118.30
3	J	58	CYS	CA-CB-SG	-5.89	103.40	114.00
3	J	268	LEU	CB-CG-CD2	-5.88	101.01	111.00
3	J	264	ASP	CB-CG-OD2	-5.86	113.03	118.30
3	D	770	LEU	CB-CG-CD1	-5.84	101.08	111.00
2	I	699	LEU	CA-CB-CG	5.83	128.71	115.30
3	D	608	CYS	CA-CB-SG	-5.82	103.53	114.00
3	J	249	LEU	CA-CB-CG	-5.79	101.99	115.30
3	D	107	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	G	65	LEU	CA-CB-CG	5.76	128.56	115.30
3	D	515	ARG	N-CA-C	-5.75	95.47	111.00
3	D	701	LEU	CA-CB-CG	5.75	128.52	115.30
3	J	355	ILE	CG1-CB-CG2	-5.74	98.77	111.40
3	J	311	ARG	NE-CZ-NH2	-5.74	117.43	120.30
3	D	137	ARG	CG-CD-NE	-5.73	99.77	111.80
3	D	780	ARG	NE-CZ-NH2	5.72	123.16	120.30
3	D	56	LEU	CB-CG-CD1	-5.72	101.28	111.00
3	J	453	VAL	CG1-CB-CG2	-5.72	101.75	110.90
2	C	838	CYS	CA-CB-SG	-5.71	103.71	114.00
3	D	102	MET	CG-SD-CE	-5.71	91.06	100.20
3	J	263	SER	CB-CA-C	-5.71	99.25	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	293	ARG	NE-CZ-NH1	-5.71	117.45	120.30
3	D	579	LEU	CB-CG-CD1	-5.69	101.32	111.00
2	I	1304	MET	CB-CG-SD	-5.69	95.32	112.40
3	J	723	TYR	CB-CG-CD1	-5.69	117.58	121.00
3	D	449	LEU	CB-CG-CD1	-5.68	101.35	111.00
3	J	1247	LYS	CB-CG-CD	-5.67	96.85	111.60
3	D	432	LEU	CA-CB-CG	-5.65	102.31	115.30
2	C	484	LEU	CA-CB-CG	5.65	128.29	115.30
3	D	644	MET	CG-SD-CE	5.64	109.23	100.20
2	C	1232	MET	CG-SD-CE	5.63	109.21	100.20
2	I	336	LEU	CB-CG-CD2	-5.61	101.46	111.00
2	C	200	ARG	CG-CD-NE	-5.60	100.04	111.80
5	L	528	LEU	CB-CG-CD1	-5.60	101.48	111.00
3	J	1309	ILE	CG1-CB-CG2	-5.60	99.09	111.40
3	D	252	LEU	CB-CG-CD1	-5.59	101.49	111.00
3	D	296	LYS	CD-CE-NZ	5.59	124.56	111.70
3	D	511	TYR	CB-CG-CD2	-5.59	117.64	121.00
2	I	533	LEU	CB-CG-CD2	-5.59	101.49	111.00
2	I	865	LEU	CB-CG-CD2	-5.59	101.50	111.00
3	D	474	LEU	CB-CG-CD1	-5.58	101.51	111.00
2	C	363	LEU	CB-CG-CD2	-5.58	101.51	111.00
3	D	154	LEU	CB-CG-CD1	-5.58	101.52	111.00
3	D	268	LEU	CA-CB-CG	-5.54	102.55	115.30
2	C	678	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	D	127	LEU	CA-CB-CG	-5.54	102.57	115.30
2	C	1160	ASP	C-N-CA	5.53	135.54	121.70
2	C	712	SER	C-N-CA	-5.53	110.69	122.30
2	C	818	VAL	CG1-CB-CG2	-5.53	102.06	110.90
1	H	29	GLU	C-N-CD	-5.52	108.45	120.60
5	L	463	LEU	CA-CB-CG	-5.52	102.61	115.30
1	G	142	MET	CB-CG-SD	5.51	128.92	112.40
3	D	38	VAL	CA-CB-CG2	-5.50	102.64	110.90
3	D	275	ARG	NE-CZ-NH2	5.50	123.05	120.30
3	D	107	LEU	CB-CG-CD1	-5.50	101.65	111.00
2	C	511	LEU	CA-CB-CG	-5.50	102.65	115.30
2	C	1287	LEU	CA-CB-CG	-5.48	102.70	115.30
3	D	239	LEU	CB-CG-CD2	-5.48	101.69	111.00
3	J	107	LEU	CA-CB-CG	5.47	127.87	115.30
3	D	238	ILE	CA-CB-CG1	-5.46	100.62	111.00
3	D	298	MET	CA-CB-CG	-5.46	104.01	113.30
5	F	557	LYS	CD-CE-NZ	5.45	124.24	111.70
2	C	791	LEU	CB-CG-CD1	-5.45	101.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1160	ASP	CB-CG-OD1	5.45	123.21	118.30
5	L	602	SER	N-CA-C	-5.45	96.28	111.00
2	C	1264	GLN	N-CA-C	-5.42	96.38	111.00
3	J	329	ASP	CB-CG-OD1	5.41	123.17	118.30
3	D	241	VAL	CB-CA-C	-5.40	101.14	111.40
1	A	262	LEU	CA-CB-CG	-5.38	102.92	115.30
3	J	1234	VAL	CG1-CB-CG2	-5.38	102.29	110.90
2	C	96	LEU	CB-CG-CD2	-5.37	101.87	111.00
3	J	299	LEU	CB-CG-CD1	-5.37	101.88	111.00
2	I	1259	LEU	CA-CB-CG	-5.36	102.97	115.30
1	A	143	ARG	CG-CD-NE	5.36	123.05	111.80
3	D	252	LEU	CB-CG-CD2	5.36	120.11	111.00
3	J	605	LEU	CB-CG-CD2	-5.35	101.91	111.00
2	C	1131	MET	CG-SD-CE	5.34	108.74	100.20
2	C	1119	MET	CB-CG-SD	-5.33	96.41	112.40
3	D	838	ARG	CB-CG-CD	5.30	125.39	111.60
3	D	352	ARG	CG-CD-NE	-5.30	100.67	111.80
3	D	485	MET	CG-SD-CE	5.28	108.65	100.20
1	H	58	GLU	CB-CA-C	-5.28	99.85	110.40
3	J	385	LEU	CA-CB-CG	-5.27	103.18	115.30
2	I	1241	ASP	N-CA-C	-5.27	96.78	111.00
1	A	307	LEU	CA-CB-CG	-5.26	103.20	115.30
3	D	370	LYS	CA-CB-CG	5.26	124.96	113.40
3	D	1337	VAL	CA-CB-CG2	-5.26	103.01	110.90
5	F	416	VAL	CA-CB-CG2	-5.25	103.03	110.90
3	D	311	ARG	NE-CZ-NH2	-5.24	117.68	120.30
3	J	127	LEU	CA-CB-CG	-5.24	103.25	115.30
3	D	42	GLU	CA-CB-CG	5.24	124.92	113.40
1	H	95	LYS	CA-CB-CG	5.24	124.92	113.40
2	C	1059	ARG	N-CA-CB	5.22	120.00	110.60
2	C	1170	MET	CA-CB-CG	-5.22	104.43	113.30
1	A	323	PRO	C-N-CA	5.22	134.74	121.70
2	I	1160	ASP	C-N-CA	5.22	134.74	121.70
1	A	74	VAL	CG1-CB-CG2	-5.21	102.56	110.90
2	C	865	LEU	CA-CB-CG	-5.21	103.31	115.30
3	J	1328	THR	CA-CB-CG2	-5.21	105.11	112.40
2	C	1273	MET	CG-SD-CE	-5.20	91.88	100.20
3	J	796	LEU	CA-CB-CG	-5.20	103.35	115.30
2	C	482	GLY	N-CA-C	5.19	126.08	113.10
3	J	829	GLY	N-CA-C	-5.19	100.12	113.10
3	J	154	LEU	CB-CG-CD1	-5.17	102.21	111.00
2	I	1054	LEU	CB-CG-CD1	-5.16	102.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	907	HIS	N-CA-CB	-5.16	101.31	110.60
5	F	551	LEU	CA-CB-CG	-5.15	103.46	115.30
3	J	265	LEU	CB-CG-CD2	-5.14	102.26	111.00
3	D	343	LEU	CA-CB-CG	-5.12	103.52	115.30
3	D	767	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	82	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	131	CYS	CA-CB-SG	-5.10	104.82	114.00
3	D	1356	LEU	CA-CB-CG	-5.09	103.58	115.30
3	D	425	ARG	NE-CZ-NH1	-5.07	117.76	120.30
2	C	1332	SER	CB-CA-C	-5.07	100.47	110.10
3	J	271	ARG	CB-CG-CD	-5.07	98.43	111.60
3	D	156	ARG	NE-CZ-NH2	-5.07	117.77	120.30
5	L	430	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	A	45	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	C	813	GLU	CA-CB-CG	-5.06	102.28	113.40
5	L	430	TYR	CB-CG-CD1	5.06	124.03	121.00
2	C	451	ARG	CG-CD-NE	-5.05	101.19	111.80
2	C	177	ILE	CG1-CB-CG2	-5.03	100.34	111.40
1	A	48	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	B	31	LEU	CB-CG-CD1	-5.02	102.46	111.00
3	D	278	ARG	NE-CZ-NH1	-5.02	117.79	120.30
5	F	386	LEU	CA-CB-CG	5.02	126.84	115.30
3	D	1246	VAL	CA-CB-CG2	-5.01	103.39	110.90
3	D	909	ILE	CG1-CB-CG2	-5.00	100.39	111.40

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	TRP	Peptide
1	A	49	SER	Mainchain
2	C	1077	SER	Mainchain
2	C	109	ALA	Peptide
2	C	1107	MET	Mainchain
2	C	1164	PHE	Mainchain
2	C	1332	SER	Mainchain
2	C	236	LYS	Peptide
2	C	473	ARG	Mainchain
2	C	560	PRO	Mainchain
2	C	573	ASN	Mainchain
2	C	683	ALA	Mainchain
2	C	686	GLN	Mainchain

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Mol	Chain	Res	Type	Group
3	D	113	HIS	Mainchain
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
3	D	1310	THR	Mainchain
3	D	181	GLY	Mainchain
3	D	308	ASP	Mainchain
3	D	367	GLY	Mainchain
3	D	379	PRO	Mainchain
3	D	425	ARG	Mainchain
3	D	483	LEU	Mainchain
3	D	914	ALA	Mainchain
3	D	921	GLN	Mainchain
5	F	601	PRO	Peptide
1	G	171	LEU	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	102	MET	Mainchain
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
3	J	1305	ASP	Mainchain
3	J	143	SER	Mainchain
3	J	186	GLN	Mainchain
3	J	248	ASP	Mainchain
3	J	299	LEU	Mainchain
3	J	475	GLU	Mainchain
5	L	601	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2403	0	2453	197	0
1	B	1672	0	1693	112	0
1	G	1730	0	1756	145	0
1	H	1667	0	1689	123	1
2	C	10572	0	10584	657	3
2	I	10568	0	10578	602	0
3	D	9107	0	9308	612	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	9029	0	9225	587	0
4	E	691	0	695	22	0
4	K	627	0	634	26	0
5	F	3806	0	3873	199	2
5	L	3821	0	3884	190	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	55699	0	56372	3190	3

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 28.

All (3190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:O	1:A:28:LEU:HD12	1.10	1.23
2:I:27:LEU:O	2:I:528:ARG:NH1	1.78	1.17
1:A:27:THR:O	1:A:28:LEU:CD1	1.93	1.17
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.36	1.08
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.16	1.08
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.36	1.07
1:A:12:ARG:H	1:A:30:PRO:CG	1.67	1.06
2:C:758:ARG:HH22	2:C:761:GLN:HG3	1.22	1.04
1:A:45:ARG:HG2	1:B:38:THR:HB	1.40	1.04
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.40	1.04
2:C:324:LYS:O	2:C:327:GLN:NE2	1.89	1.03
1:A:27:THR:C	1:A:28:LEU:HD12	1.78	1.02
2:C:1142:ARG:HD3	2:C:1161:LEU:HD11	1.43	1.01
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.42	1.00
1:A:12:ARG:H	1:A:30:PRO:HG3	1.22	1.00
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.23	0.99
2:I:560:PRO:O	3:J:780:ARG:NH2	1.96	0.99
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.00	0.98
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.46	0.97
2:I:821:ARG:HH21	2:I:1082:ILE:HG21	1.27	0.96
2:C:131:THR:HG22	2:C:135:THR:H	1.27	0.96
3:J:418:GLU:HG3	4:K:45:LYS:H	1.30	0.95
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.28	0.95
3:D:56:LEU:H	3:D:56:LEU:HD12	1.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:GLU:HB2	2:C:760:ASN:HD21	1.30	0.94
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.46	0.94
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.30	0.93
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.49	0.93
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.51	0.92
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.52	0.92
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.52	0.92
1:A:27:THR:C	1:A:28:LEU:CD1	2.36	0.92
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.53	0.91
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.49	0.91
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.51	0.91
2:I:890:LYS:NZ	2:I:891:GLY:O	2.02	0.91
1:A:11:PRO:HA	1:A:30:PRO:CG	2.01	0.90
1:A:12:ARG:N	1:A:30:PRO:HG3	1.86	0.90
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.04	0.90
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.51	0.90
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.51	0.90
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.54	0.90
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.04	0.90
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.53	0.89
1:A:11:PRO:HA	1:A:30:PRO:HB2	1.54	0.89
1:A:11:PRO:CA	1:A:30:PRO:HG2	2.03	0.89
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.54	0.89
3:D:42:GLU:OE2	5:F:451:ARG:NH2	2.05	0.89
2:I:18:ARG:NH1	2:I:621:SER:O	2.05	0.89
2:I:523:GLU:HG2	2:I:527:LYS:HE3	1.55	0.88
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.54	0.88
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.37	0.88
3:D:1291:GLU:OE1	3:J:1302:TYR:OH	1.91	0.88
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.55	0.87
2:C:930:ASP:OD2	2:C:931:VAL:N	2.08	0.86
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.57	0.86
2:C:758:ARG:NH2	2:C:761:GLN:HG3	1.91	0.86
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.08	0.86
1:G:231:PHE:HD1	1:H:218:ARG:HG2	1.40	0.86
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.40	0.85
5:L:132:CYS:SG	5:L:257:LYS:NZ	2.48	0.85
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.41	0.85
1:H:101:THR:HG22	1:H:116:THR:HB	1.58	0.85
3:D:817:HIS:CE1	3:D:860:ARG:HE	1.93	0.85
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.10	0.85
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.59	0.85
5:L:244:THR:O	5:L:247:GLU:HG2	1.77	0.85
2:I:1307:ASN:HB3	2:I:1312:ASN:O	1.75	0.85
1:A:11:PRO:HA	1:A:30:PRO:CB	2.07	0.84
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.09	0.84
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.58	0.84
1:B:16:ILE:HG23	1:B:26:VAL:HG22	1.57	0.84
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.59	0.83
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.26	0.83
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.61	0.83
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.58	0.83
3:D:11:GLN:HG2	3:D:15:GLU:HG3	1.60	0.83
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.40	0.83
2:I:344:GLY:O	2:I:346:TYR:N	2.10	0.83
1:A:12:ARG:N	1:A:30:PRO:CG	2.40	0.83
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.61	0.83
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.43	0.83
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.60	0.82
2:I:452:ARG:NH1	2:I:584:TYR:O	2.12	0.82
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.42	0.82
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.44	0.82
3:D:75:TYR:OH	3:D:86:GLU:OE1	1.95	0.82
1:A:7:GLU:O	1:B:150:ARG:NH2	2.12	0.82
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.10	0.82
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.60	0.82
5:F:121:LYS:NZ	5:F:421:TYR:OH	2.10	0.82
2:I:930:ASP:OD2	2:I:931:VAL:N	2.12	0.82
1:A:29:GLU:O	1:A:31:LEU:N	2.13	0.81
3:D:557:LYS:HA	3:D:563:LEU:HA	1.62	0.81
5:F:470:MET:SD	5:F:486:ARG:NH1	2.53	0.81
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.45	0.81
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.63	0.81
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	1.95	0.81
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.62	0.81
3:D:930:LEU:HD22	3:D:1244:GLN:HG3	1.63	0.81
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.63	0.81
3:D:128:LEU:HA	3:D:192:MET:HE1	1.61	0.80
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.62	0.80
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.44	0.80
3:J:514:THR:OG1	3:J:594:GLN:O	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.15	0.80
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.62	0.80
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.15	0.80
2:I:1312:ASN:HD21	2:I:1314:GLN:NE2	1.79	0.80
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.64	0.80
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.64	0.80
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.59	0.79
1:A:89:ALA:H	1:A:125:LYS:HD3	1.47	0.79
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.64	0.79
3:D:327:LEU:HA	3:D:330:MET:HG3	1.62	0.79
2:I:761:GLN:HG2	2:I:762:ASN:OD1	1.82	0.79
2:I:860:ALA:O	2:I:863:SER:OG	2.01	0.79
1:G:12:ARG:HD2	1:H:230:ALA:HB1	1.62	0.79
2:C:721:GLY:N	2:C:740:GLU:OE1	2.13	0.79
3:D:515:ARG:NH2	3:D:717:VAL:O	2.16	0.79
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.15	0.79
1:B:16:ILE:HG12	1:B:26:VAL:HG13	1.65	0.79
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.65	0.79
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.16	0.79
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.15	0.79
3:J:810:THR:HG21	3:J:893:GLY:HA3	1.65	0.79
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	1.65	0.78
1:G:41:ASN:HD22	1:H:41:ASN:HD22	1.32	0.78
1:H:23:HIS:ND1	1:H:206:GLU:HG2	1.97	0.78
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.65	0.78
2:I:1114:GLU:OE1	2:I:1230:MET:HA	1.82	0.78
5:F:483:LEU:H	5:F:483:LEU:HD12	1.46	0.78
2:I:30:ILE:HD12	2:I:30:ILE:H	1.48	0.78
1:A:7:GLU:HG3	1:B:150:ARG:HE	1.49	0.78
1:A:14:VAL:HG22	1:A:15:ASP:H	1.48	0.78
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.64	0.78
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.18	0.78
3:J:518:VAL:HG11	3:J:707:ILE:HD13	1.64	0.78
1:B:76:GLU:OE2	1:B:132:HIS:N	2.13	0.78
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.66	0.78
1:A:60:GLU:CD	1:A:143:ARG:HH21	1.88	0.78
2:C:133:ASN:O	2:C:527:LYS:NZ	2.17	0.78
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.64	0.78
3:D:1140:ARG:NH2	3:D:1236:GLU:HG2	1.99	0.77
1:H:59:VAL:O	1:H:171:LEU:N	2.16	0.77
2:I:703:GLY:N	2:I:705:GLU:OE2	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:HIS:HB2	1:A:205:MET:O	1.85	0.77
3:D:587:LEU:HD23	3:D:591:ILE:HG21	1.66	0.77
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.48	0.77
3:J:518:VAL:O	3:J:547:ARG:NH1	2.18	0.77
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.66	0.77
5:F:573:LEU:HD23	5:F:573:LEU:H	1.49	0.77
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.67	0.77
5:L:585:GLU:OE2	5:L:588:ARG:NH1	2.18	0.77
2:C:131:THR:HG23	2:C:133:ASN:H	1.50	0.76
3:D:418:GLU:HG3	4:E:45:LYS:H	1.50	0.76
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.68	0.76
1:A:45:ARG:NH2	2:C:1216:ARG:HA	1.99	0.76
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.65	0.76
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.51	0.76
3:D:109:SER:HB2	3:D:296:LYS:HE2	1.68	0.76
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	1.99	0.76
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.14	0.76
3:J:1263:LYS:HE2	3:J:1279:GLN:HE21	1.50	0.76
2:C:705:GLU:HB2	2:C:794:LEU:H	1.50	0.76
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.18	0.76
2:I:637:ARG:HA	2:I:642:SER:HA	1.66	0.76
2:C:4:SER:OG	2:C:5:TYR:N	2.16	0.76
2:C:1299:ASN:HD22	2:C:1303:LYS:HE2	1.49	0.76
3:J:1252:HIS:O	3:J:1255:VAL:HG13	1.85	0.76
1:B:6:THR:N	1:B:7:GLU:OE2	2.17	0.76
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.19	0.76
1:G:161:SER:O	1:G:163:GLU:N	2.18	0.76
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.68	0.75
2:I:1272:GLU:HB2	3:J:342:LEU:O	1.87	0.75
2:C:759:SER:OG	2:C:763:THR:N	2.18	0.75
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.67	0.75
3:J:1368:ASP:HA	3:J:1371:ARG:HH12	1.49	0.75
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.68	0.75
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.69	0.75
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.67	0.75
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.00	0.75
2:C:142:GLU:HB2	2:C:760:ASN:ND2	2.02	0.75
2:C:42:ASP:OD2	2:C:44:GLU:HG2	1.86	0.75
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.69	0.75
5:L:395:THR:OG1	5:L:396:ASN:N	2.16	0.75
2:C:42:ASP:OD2	2:C:44:GLU:O	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.69	0.75
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.69	0.75
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.69	0.75
2:I:1117:LEU:HD21	2:I:1182:ILE:HD12	1.68	0.75
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.69	0.75
2:C:1164:PHE:N	2:C:1168:GLU:OE1	2.18	0.75
3:J:140:TYR:OH	3:J:312:ARG:NH2	2.20	0.75
2:C:16:GLY:O	2:C:1156:ARG:HG2	1.87	0.74
2:C:149:LEU:HD12	2:C:452:ARG:O	1.86	0.74
3:J:523:GLU:OE2	3:J:547:ARG:NH1	2.18	0.74
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.20	0.74
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.68	0.74
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.69	0.74
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.68	0.74
2:C:511:LEU:HD12	2:C:511:LEU:N	2.02	0.74
2:C:759:SER:O	2:C:761:GLN:N	2.19	0.74
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.01	0.74
2:C:615:VAL:HG13	2:C:651:ASP:H	1.51	0.74
3:D:888:CYS:SG	3:D:889:ASP:N	2.61	0.74
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.70	0.74
3:J:362:ARG:H	3:J:365:GLN:HE21	1.33	0.74
2:C:1114:GLU:OE1	2:C:1230:MET:HA	1.88	0.74
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.68	0.74
1:G:9:LEU:O	1:H:227:GLN:NE2	2.21	0.74
2:C:142:GLU:CB	2:C:760:ASN:HD21	1.99	0.74
2:C:878:THR:OG1	2:C:879:GLY:N	2.19	0.74
3:D:98:ARG:HB3	3:D:248:ASP:OD2	1.88	0.74
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.23	0.74
1:A:12:ARG:H	1:A:30:PRO:HG2	1.53	0.74
3:D:45:ASN:HB3	3:D:48:THR:O	1.89	0.73
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	1.87	0.73
3:J:1159:ILE:HA	3:J:1206:ARG:HB3	1.70	0.73
5:L:343:LYS:H	5:L:343:LYS:HD2	1.52	0.73
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.23	0.73
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.69	0.73
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.69	0.73
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.88	0.73
5:L:305:LEU:HB3	5:L:315:TRP:HB3	1.70	0.73
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.69	0.73
3:D:847:ASP:HA	3:D:860:ARG:H	1.53	0.73
1:G:194:GLN:O	1:G:195:ARG:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:148:GLN:NE2	2:I:535:PRO:O	2.18	0.73
1:H:50:SER:HA	1:H:150:ARG:O	1.88	0.73
1:A:166:ARG:O	1:A:168:ILE:N	2.22	0.73
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.70	0.73
2:I:207:THR:HG21	2:I:351:LEU:HG	1.70	0.73
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.71	0.73
2:I:758:ARG:HH22	2:I:761:GLN:HG3	1.54	0.73
1:A:87:GLY:O	1:A:125:LYS:NZ	2.21	0.73
2:C:131:THR:CG2	2:C:135:THR:H	2.02	0.73
3:D:1183:SER:OG	3:J:206:ASN:ND2	2.22	0.72
3:J:152:THR:OG1	3:J:153:ASN:N	2.22	0.72
3:J:403:ARG:HB3	3:J:405:GLU:HG3	1.71	0.72
5:L:97:PRO:HA	5:L:100:MET:HG3	1.70	0.72
1:A:32:GLU:HA	1:A:198:LEU:HD22	1.71	0.72
3:D:314:ARG:NH2	3:D:323:PRO:HG3	2.04	0.72
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.24	0.72
2:I:819:SER:HB2	2:I:1085:MET:SD	2.29	0.72
3:J:435:GLN:HB2	3:J:457:TYR:OH	1.89	0.72
3:D:399:LYS:NZ	5:F:611:LEU:O	2.23	0.72
2:C:30:ILE:H	2:C:30:ILE:HD12	1.53	0.72
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.70	0.72
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.71	0.72
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.23	0.72
1:B:82:LEU:HA	1:B:85:LEU:HD12	1.71	0.72
3:D:73:GLY:O	3:D:76:LYS:NZ	2.17	0.72
2:I:1312:ASN:ND2	2:I:1314:GLN:HE21	1.82	0.72
1:A:36:GLY:HA3	1:A:187:VAL:HG11	1.71	0.72
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.29	0.72
5:F:395:THR:OG1	5:F:396:ASN:N	2.23	0.72
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.72	0.72
3:J:576:ARG:NH1	3:J:593:ASN:O	2.21	0.72
1:A:261:GLU:CD	2:C:859:GLU:H	1.93	0.72
3:D:598:LYS:O	3:D:601:ILE:HG22	1.89	0.72
3:J:905:ARG:NH1	3:J:910:ASN:HD21	1.88	0.72
5:L:512:GLY:O	5:L:514:ASP:N	2.23	0.72
1:G:79:LEU:HD21	2:I:756:TYR:OH	1.89	0.72
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.70	0.72
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.71	0.72
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.20	0.71
5:L:386:LEU:O	5:L:389:SER:OG	2.05	0.71
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:617:ALA:HA	2:C:636:CYS:SG	2.29	0.71
2:C:1131:MET:HE1	2:C:1141:LEU:HA	1.72	0.71
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.72	0.71
2:I:836:LEU:HD13	2:I:1054:LEU:HD13	1.70	0.71
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.05	0.71
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.23	0.71
2:C:1202:GLY:O	2:C:1203:ASP:HB2	1.90	0.71
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.24	0.71
2:C:90:VAL:HG12	2:C:91:THR:H	1.55	0.71
2:C:696:ASP:HB2	2:C:798:GLN:CG	2.19	0.71
2:I:1268:GLN:HE22	3:J:352:ARG:NH1	1.88	0.71
3:J:56:LEU:HD12	3:J:56:LEU:H	1.56	0.71
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.73	0.71
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.71	0.71
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.70	0.71
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.71	0.71
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.72	0.71
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.54	0.71
2:C:703:GLY:N	2:C:705:GLU:OE2	2.23	0.71
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.73	0.71
2:C:980:VAL:HA	2:C:984:VAL:HA	1.72	0.71
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.71	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.73	0.71
3:D:35:PHE:HD1	3:D:101:ARG:HB3	1.55	0.71
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.72	0.71
1:G:49:SER:OG	1:G:50:SER:N	2.23	0.71
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.71	0.71
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.71	0.70
5:L:601:PRO:HA	5:L:604:SER:HB2	1.74	0.70
1:A:13:LEU:H	1:A:13:LEU:HD23	1.56	0.70
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.72	0.70
1:H:102:LEU:HB2	1:H:142:MET:H	1.56	0.70
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.31	0.70
2:I:1333:LEU:HD22	3:J:307:LEU:HD22	1.73	0.70
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.23	0.70
5:L:561:MET:HA	5:L:567:MET:HE1	1.73	0.70
1:A:310:ARG:O	5:F:608:ARG:NH1	2.24	0.70
1:B:12:ARG:O	1:B:13:LEU:HG	1.91	0.70
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.73	0.70
1:G:66:HIS:CE1	2:I:874:GLY:HA2	2.26	0.70
1:A:29:GLU:HB3	1:A:30:PRO:CD	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.27	0.70
2:I:1223:ARG:NH1	3:J:721:SER:OG	2.24	0.70
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.74	0.70
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.22	0.70
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.74	0.70
5:F:601:PRO:HA	5:F:604:SER:HB2	1.72	0.70
3:J:1177:ILE:HD12	3:J:1186:TYR:HB3	1.74	0.70
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.25	0.70
1:A:172:LEU:H	1:A:172:LEU:HD12	1.55	0.70
3:J:557:LYS:HA	3:J:563:LEU:HA	1.73	0.70
5:L:412:LEU:HB2	5:L:435:ILE:HD11	1.73	0.70
3:D:902:ASP:OD1	3:D:903:LEU:N	2.25	0.70
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.07	0.70
5:L:483:LEU:HD12	5:L:483:LEU:H	1.57	0.70
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.73	0.69
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.74	0.69
5:F:97:PRO:HA	5:F:100:MET:HG3	1.73	0.69
5:F:600:HIS:CD2	5:F:601:PRO:HD2	2.26	0.69
2:I:521:LEU:HA	2:I:524:ILE:HG22	1.75	0.69
2:I:109:ALA:HB1	2:I:110:PRO:C	2.13	0.69
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.57	0.69
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.23	0.69
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.24	0.69
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.72	0.69
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.07	0.69
3:J:210:SER:O	3:J:214:ARG:HG2	1.92	0.69
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.28	0.69
2:C:8:LYS:HE3	2:C:1171:ARG:CZ	2.23	0.69
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	1.72	0.69
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.73	0.69
1:H:60:GLU:HG3	1:H:143:ARG:O	1.92	0.69
3:J:360:TYR:OH	3:J:448:GLN:OE1	2.05	0.69
3:D:248:ASP:O	3:D:251:PRO:HG3	1.92	0.69
3:D:708:ASN:HB3	3:D:712:GLN:O	1.92	0.69
3:J:202:ARG:NH2	3:J:225:GLU:OE1	2.25	0.69
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.74	0.69
3:J:1341:ARG:NH1	3:J:1343:GLU:OE2	2.26	0.69
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.73	0.69
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.22	0.69
2:C:582:ASN:HB3	2:C:586:PHE:H	1.57	0.69
1:G:218:ARG:HG3	1:H:231:PHE:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.73	0.68
1:G:92:VAL:O	1:G:148:ARG:NH2	2.25	0.68
1:G:134:THR:HG23	1:G:135:ASP:H	1.56	0.68
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.28	0.68
1:A:31:LEU:HB2	1:A:199:ASP:O	1.94	0.68
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.74	0.68
3:D:293:ARG:NH1	5:F:104:GLU:OE2	2.27	0.68
3:D:674:THR:OG1	3:D:677:GLU:HB2	1.94	0.68
5:F:247:GLU:HA	5:F:250:LEU:HD12	1.74	0.68
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.76	0.68
2:C:618:GLN:HG3	2:C:619:ALA:N	2.05	0.68
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.08	0.68
5:L:101:TYR:O	5:L:104:GLU:N	2.26	0.68
5:L:281:ARG:O	5:L:285:ARG:HG3	1.93	0.68
2:C:656:SER:OG	2:C:657:THR:N	2.22	0.68
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.75	0.68
3:D:74:LYS:HD2	3:D:87:LYS:HD3	1.75	0.68
3:D:817:HIS:CE1	3:D:860:ARG:NE	2.61	0.68
3:J:1137:GLY:O	3:J:1140:ARG:HB3	1.93	0.68
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.73	0.68
3:D:1266:ILE:HD12	3:D:1273:ASP:O	1.94	0.68
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.24	0.68
2:C:563:THR:OG1	2:C:564:PRO:HD2	1.93	0.68
1:H:61:ILE:HB	1:H:64:VAL:O	1.94	0.68
3:J:98:ARG:HB3	3:J:248:ASP:OD2	1.94	0.68
3:J:102:MET:HE2	3:J:246:PRO:HD3	1.76	0.68
3:J:362:ARG:H	3:J:365:GLN:NE2	1.91	0.68
2:C:74:ARG:HH12	2:C:121:GLU:CD	1.96	0.68
1:A:227:GLN:NE2	1:B:9:LEU:O	2.27	0.68
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.75	0.68
3:D:709:ARG:O	3:D:711:GLY:N	2.27	0.68
5:F:306:PHE:HE1	5:F:315:TRP:CD2	2.11	0.68
1:G:79:LEU:HD23	1:G:79:LEU:H	1.59	0.68
2:I:890:LYS:HE2	2:I:891:GLY:H	1.58	0.68
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.74	0.68
2:C:27:LEU:O	2:C:528:ARG:NH1	2.27	0.68
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.74	0.68
2:C:1211:ARG:HD3	2:C:1213:TYR:OH	1.94	0.68
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.74	0.68
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.12	0.68
4:K:70:GLN:NE2	4:K:74:GLU:OE2	2.16	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:724:VAL:HG23	2:I:775:GLU:O	1.94	0.67
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.77	0.67
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.75	0.67
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.76	0.67
3:J:847:ASP:OD1	3:J:847:ASP:N	2.23	0.67
1:A:7:GLU:OE1	1:B:150:ARG:NH2	2.28	0.67
1:A:73:GLY:O	1:A:134:THR:HG22	1.95	0.67
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.76	0.67
3:D:262:THR:OG1	3:D:263:SER:N	2.24	0.67
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.59	0.67
2:I:517:GLN:NE2	2:I:687:ARG:O	2.26	0.67
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.75	0.67
1:A:45:ARG:HG2	1:B:38:THR:CB	2.21	0.67
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.28	0.67
3:J:773:PHE:O	3:J:776:THR:HB	1.95	0.67
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.60	0.67
3:D:210:SER:O	3:D:214:ARG:HG2	1.95	0.67
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.10	0.67
2:I:607:SER:N	2:I:610:GLU:OE1	2.27	0.67
1:G:75:GLN:HA	2:I:729:ALA:N	2.09	0.67
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.94	0.67
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.77	0.67
2:C:494:ASN:HD22	2:C:497:PRO:HD3	1.58	0.67
5:F:479:THR:HG23	5:F:481:GLU:H	1.58	0.67
2:C:520:PRO:HG3	2:C:714:VAL:HG21	1.77	0.67
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	1.94	0.67
2:I:629:PHE:O	2:I:647:ARG:NH2	2.28	0.67
3:J:700:ASN:O	3:J:704:GLU:HB2	1.95	0.67
3:J:1263:LYS:CE	3:J:1279:GLN:HE21	2.08	0.67
1:G:22:THR:O	1:G:207:THR:N	2.27	0.67
1:H:67:GLU:O	1:H:78:ILE:HB	1.95	0.67
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.60	0.66
3:D:694:SER:OG	3:D:738:ARG:NE	2.28	0.66
2:I:818:VAL:O	2:I:1079:ILE:HD12	1.95	0.66
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.75	0.66
5:F:461:ASN:HB3	5:F:465:ARG:NH2	2.11	0.66
1:B:214:GLU:OE2	1:B:218:ARG:NH2	2.26	0.66
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.10	0.66
2:I:55:SER:OG	2:I:56:VAL:N	2.28	0.66
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.35	0.66
1:G:231:PHE:HA	1:H:218:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.77	0.66
3:J:1215:GLU:N	3:J:1215:GLU:OE2	2.28	0.66
5:F:227:GLN:HE22	5:F:251:LYS:HZ1	1.42	0.66
1:G:52:PRO:HG2	1:G:219:ARG:HE	1.60	0.66
1:G:231:PHE:CD1	1:H:218:ARG:HG2	2.29	0.66
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.78	0.66
3:J:743:MET:HB2	3:J:759:ILE:O	1.96	0.66
3:J:902:ASP:OD1	3:J:903:LEU:N	2.29	0.66
3:D:56:LEU:HD12	3:D:56:LEU:N	2.04	0.66
3:D:1160:SER:HG	3:D:1203:ARG:HH12	1.44	0.66
5:F:139:GLU:HG2	5:F:351:THR:HA	1.77	0.66
2:C:1131:MET:HE1	2:C:1141:LEU:HD12	1.78	0.66
3:D:77:ARG:HB3	3:D:80:HIS:CE1	2.31	0.66
3:D:362:ARG:H	3:D:365:GLN:HE21	1.43	0.66
1:G:76:GLU:OE1	1:G:132:HIS:N	2.21	0.66
2:I:886:LYS:CE	2:I:916:SER:HB3	2.26	0.66
3:D:77:ARG:HB3	3:D:80:HIS:ND1	2.10	0.66
3:D:392:THR:HG21	5:F:606:VAL:HA	1.78	0.66
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.36	0.66
5:L:139:GLU:HG2	5:L:351:THR:HA	1.77	0.66
5:L:461:ASN:O	5:L:465:ARG:HG2	1.95	0.66
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.78	0.66
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.14	0.66
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.61	0.66
2:C:3:TYR:CE1	2:C:11:ILE:HD11	2.32	0.65
2:C:1131:MET:CE	2:C:1141:LEU:HD12	2.26	0.65
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.95	0.65
3:D:708:ASN:OD1	3:D:708:ASN:N	2.25	0.65
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.12	0.65
2:C:566:GLY:O	2:C:569:ILE:HG13	1.96	0.65
2:C:816:ILE:O	2:C:1076:ILE:HD12	1.96	0.65
3:J:218:THR:HG21	3:J:1275:LEU:HD11	1.78	0.65
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.31	0.65
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	1.96	0.65
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.30	0.65
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.31	0.65
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.26	0.65
2:C:125:GLY:HA2	2:C:499:SER:HB2	1.78	0.65
1:G:12:ARG:HG2	1:G:13:LEU:HD23	1.76	0.65
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.28	0.65
2:I:176:ILE:HD11	2:I:428:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.29	0.65
1:G:12:ARG:HA	1:H:231:PHE:CZ	2.32	0.65
3:J:491:LEU:HD23	3:J:498:PRO:HA	1.77	0.65
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.79	0.65
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.78	0.65
3:D:1372:ARG:O	3:D:1375:ALA:HB3	1.96	0.65
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	1.77	0.65
1:A:29:GLU:N	1:A:30:PRO:HD2	2.12	0.65
3:D:109:SER:CB	3:D:296:LYS:HE2	2.26	0.65
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.79	0.65
3:J:416:ILE:HG12	3:J:441:LEU:CD2	2.26	0.65
3:J:514:THR:HB	3:J:576:ARG:HG2	1.78	0.65
1:A:156:SER:HB2	2:C:1059:ARG:HH22	1.61	0.65
3:D:721:SER:HA	3:D:724:MET:HE2	1.78	0.65
3:D:827:GLU:HB3	3:D:832:LYS:HD2	1.78	0.65
1:G:102:LEU:HD22	1:G:103:ASN:H	1.60	0.65
3:J:436:ALA:HB3	3:J:485:MET:HA	1.79	0.65
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.27	0.65
3:J:1140:ARG:NE	3:J:1144:LEU:HD11	2.11	0.65
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.26	0.65
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.11	0.65
3:D:298:MET:SD	5:F:402:LEU:HB3	2.37	0.65
2:I:755:LYS:O	2:I:757:THR:HG22	1.97	0.65
2:I:758:ARG:NH2	2:I:761:GLN:HG3	2.10	0.65
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.30	0.65
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.31	0.65
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.79	0.64
2:C:891:GLY:O	2:C:892:GLU:HG3	1.97	0.64
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.79	0.64
2:I:866:ASP:HA	2:I:872:TYR:OH	1.97	0.64
2:C:42:ASP:OD2	2:C:44:GLU:N	2.30	0.64
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.79	0.64
3:J:290:ILE:H	3:J:290:ILE:HD12	1.62	0.64
3:J:901:ARG:HD2	3:J:906:GLY:O	1.97	0.64
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.12	0.64
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.79	0.64
2:I:57:PHE:HD1	2:I:58:PRO:HA	1.63	0.64
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.79	0.64
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.79	0.64
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.77	0.64
3:J:1159:ILE:HD12	3:J:1206:ARG:HD2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:512:GLY:C	5:L:514:ASP:H	2.00	0.64
3:D:709:ARG:C	3:D:711:GLY:H	2.01	0.64
3:D:768:ASN:N	3:D:771:GLN:OE1	2.26	0.64
5:F:512:GLY:O	5:F:514:ASP:N	2.30	0.64
3:J:1140:ARG:HE	3:J:1144:LEU:HD11	1.61	0.64
1:B:81:ILE:O	1:B:85:LEU:HG	1.97	0.64
2:C:522:SER:O	2:C:525:THR:HG22	1.97	0.64
1:G:45:ARG:HG2	1:H:38:THR:HB	1.78	0.64
2:I:890:LYS:HE2	2:I:891:GLY:N	2.13	0.64
2:I:1065:LYS:HE2	3:J:462:ASP:O	1.98	0.64
3:J:544:LEU:O	3:J:574:VAL:HB	1.97	0.64
3:J:1140:ARG:NH2	3:J:1236:GLU:HG2	2.12	0.64
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.78	0.64
5:L:573:LEU:HD23	5:L:573:LEU:H	1.63	0.64
1:A:263:THR:N	1:A:302:GLU:OE2	2.26	0.64
2:C:12:ARG:HH21	2:C:793:GLU:CD	2.01	0.64
2:C:1101:LEU:O	3:D:731:ARG:HD3	1.97	0.64
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.79	0.64
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.79	0.64
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.78	0.64
1:A:71:LYS:HB3	1:A:74:VAL:CG1	2.27	0.64
1:A:261:GLU:OE1	2:C:859:GLU:N	2.28	0.64
1:G:95:LYS:NZ	1:G:118:ASP:OD2	2.30	0.64
3:J:709:ARG:O	3:J:711:GLY:N	2.31	0.64
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.80	0.64
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.80	0.64
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.79	0.64
5:L:457:ILE:HA	5:L:460:ILE:HD12	1.80	0.64
1:A:71:LYS:HB3	1:A:74:VAL:HG11	1.80	0.63
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.80	0.63
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.33	0.63
3:D:317:THR:HG22	3:D:322:ARG:O	1.98	0.63
5:F:244:THR:O	5:F:247:GLU:HG2	1.99	0.63
2:I:1268:GLN:OE1	3:J:352:ARG:HG2	1.98	0.63
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.79	0.63
3:J:598:LYS:O	3:J:601:ILE:HG22	1.98	0.63
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.38	0.63
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.34	0.63
2:I:759:SER:O	2:I:761:GLN:N	2.26	0.63
3:J:216:LYS:HA	3:J:219:LYS:HE3	1.80	0.63
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:PRO:HA	1:G:208:ASN:ND2	2.13	0.63
1:A:27:THR:C	1:A:28:LEU:HD13	2.18	0.63
5:F:582:VAL:CG1	5:F:586:ARG:HG2	2.27	0.63
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.34	0.63
2:I:1217:THR:OG1	2:I:1219:GLU:HG2	1.98	0.63
3:J:115:TRP:CZ2	3:J:1329:THR:HG23	2.34	0.63
2:C:582:ASN:HB3	2:C:586:PHE:N	2.12	0.63
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.62	0.63
3:D:901:ARG:HA	3:D:908:ILE:HA	1.79	0.63
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.32	0.63
2:C:557:ARG:HH21	2:C:607:SER:C	2.01	0.63
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.79	0.63
3:J:470:VAL:HG12	3:J:472:LEU:HD23	1.80	0.63
3:J:1326:GLN:OE1	3:J:1330:ARG:NH2	2.31	0.63
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.79	0.63
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.63	0.63
2:I:161:LYS:HA	2:I:170:VAL:HA	1.81	0.63
1:B:50:SER:HA	1:B:150:ARG:O	1.99	0.63
2:C:158:ASP:OD1	2:C:159:SER:N	2.32	0.63
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.81	0.63
5:L:164:GLY:O	5:L:260:ARG:HB2	1.99	0.63
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.33	0.62
2:C:1319:MET:HG3	2:C:1320:PRO:HD2	1.81	0.62
1:G:11:PRO:HB3	1:G:30:PRO:O	1.98	0.62
1:G:14:VAL:HG13	1:G:15:ASP:H	1.64	0.62
2:I:518:ASN:O	2:I:522:SER:HB3	1.99	0.62
1:G:118:ASP:HB3	1:G:121:VAL:CG2	2.29	0.62
2:C:4:SER:H	2:C:7:GLU:CD	2.01	0.62
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.33	0.62
3:D:156:ARG:NH2	3:D:191:SER:OG	2.32	0.62
3:D:1282:TYR:O	3:D:1285:VAL:HG12	1.99	0.62
5:F:134:VAL:HG22	5:F:273:MET:HE3	1.80	0.62
2:I:821:ARG:NH2	2:I:1082:ILE:HG21	2.08	0.62
1:A:118:ASP:H	1:A:121:VAL:HB	1.64	0.62
1:A:152:TYR:CZ	2:C:824:GLN:HA	2.34	0.62
3:D:1177:ILE:HD12	3:D:1186:TYR:HB3	1.81	0.62
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.32	0.62
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.81	0.62
5:L:540:LEU:HD12	5:L:610:PHE:CD1	2.34	0.62
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.80	0.62
3:D:388:ARG:HB2	3:D:390:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:ASP:HB2	1:H:121:VAL:CG2	2.29	0.62
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.63	0.62
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.81	0.62
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.82	0.62
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.28	0.62
2:C:1024:GLU:HA	2:C:1027:LYS:HD3	1.81	0.62
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.82	0.62
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.35	0.62
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.82	0.62
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.82	0.62
2:C:109:ALA:HB1	2:C:110:PRO:C	2.19	0.62
2:C:131:THR:HG23	2:C:133:ASN:N	2.15	0.62
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.21	0.62
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.11	0.62
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.82	0.62
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	1.81	0.62
2:C:23:ASP:OD1	2:C:23:ASP:N	2.32	0.62
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.64	0.62
5:F:354:THR:O	5:F:358:VAL:HG23	1.98	0.62
3:J:620:PHE:CE1	3:J:624:ILE:HD11	2.35	0.62
3:J:1270:GLY:HA3	3:J:1298:VAL:HG22	1.81	0.62
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.82	0.61
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.82	0.61
2:C:878:THR:N	2:C:881:ASP:OD2	2.24	0.61
5:F:461:ASN:HB3	5:F:465:ARG:HH21	1.64	0.61
2:I:227:LYS:O	2:I:245:ARG:NH2	2.33	0.61
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.32	0.61
2:C:836:LEU:HD12	2:C:836:LEU:N	2.15	0.61
3:D:697:MET:SD	3:D:741:ALA:HB3	2.40	0.61
2:C:710:VAL:HG13	2:C:717:VAL:HG21	1.82	0.61
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.81	0.61
1:G:60:GLU:O	1:G:142:MET:HB2	2.00	0.61
2:I:658:GLN:O	2:I:661:VAL:HG22	2.01	0.61
2:I:1273:MET:HG2	2:I:1276:TRP:CZ3	2.35	0.61
3:J:356:THR:OG1	3:J:357:VAL:N	2.34	0.61
5:F:316:PHE:HZ	5:F:334:SER:HA	1.64	0.61
2:I:896:THR:HB	2:I:897:PRO:HD2	1.81	0.61
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.66	0.61
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.81	0.61
3:D:891:ASP:HA	3:D:1281:GLU:HG3	1.82	0.61
3:J:418:GLU:H	4:K:45:LYS:NZ	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:CYS:HA	1:A:148:ARG:HA	1.83	0.61
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.16	0.61
1:G:66:HIS:NE2	2:I:929:ILE:HA	2.14	0.61
2:I:1246:ARG:HG2	2:I:1247:SER:N	2.15	0.61
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.82	0.61
3:J:502:PRO:HB3	3:J:506:VAL:HG21	1.83	0.61
3:D:316:ILE:HA	3:D:323:PRO:HA	1.82	0.61
1:A:218:ARG:HG3	1:B:231:PHE:O	2.01	0.61
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.83	0.61
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.36	0.61
2:C:601:ASP:OD1	2:C:601:ASP:N	2.32	0.61
3:J:647:PRO:CG	3:J:697:MET:HB3	2.30	0.61
1:A:190:ALA:H	1:A:199:ASP:HA	1.66	0.61
2:C:488:MET:O	2:C:490:GLN:N	2.32	0.61
1:G:152:TYR:HD1	1:G:176:CYS:HB3	1.65	0.61
2:I:466:VAL:O	2:I:469:VAL:HG22	2.01	0.61
5:L:426:LYS:HE2	5:L:428:SER:OG	2.01	0.61
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.81	0.61
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.82	0.60
2:C:316:GLU:H	2:C:316:GLU:CD	2.04	0.60
2:C:667:LEU:HD21	2:C:704:MET:HB2	1.82	0.60
3:D:762:ASN:OD1	3:D:764:ARG:N	2.33	0.60
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.82	0.60
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	1.84	0.60
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.34	0.60
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.35	0.60
2:I:346:TYR:OH	2:I:437:ASN:OD1	2.02	0.60
2:I:697:LYS:HA	2:I:795:ALA:HB2	1.83	0.60
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.25	0.60
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.47	0.60
2:C:156:PHE:CZ	2:C:158:ASP:HB2	2.37	0.60
2:C:510:GLN:OE1	2:C:534:GLY:HA2	2.00	0.60
2:C:1246:ARG:NH2	3:D:348:ASP:OD1	2.34	0.60
3:D:147:ILE:HG13	3:D:147:ILE:O	2.01	0.60
3:D:514:THR:O	3:D:514:THR:OG1	2.19	0.60
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.14	0.60
3:D:1280:VAL:CG1	3:D:1304:ARG:HH21	2.04	0.60
3:J:697:MET:SD	3:J:741:ALA:HB3	2.41	0.60
5:L:226:ALA:O	5:L:229:VAL:HG22	2.01	0.60
2:C:256:GLU:HB3	2:C:261:VAL:HG13	1.82	0.60
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.37	0.60
3:J:138:VAL:HG21	3:J:145:VAL:HB	1.83	0.60
5:L:476:ARG:HG3	5:L:477:GLU:N	2.15	0.60
1:B:107:ILE:HG23	1:B:135:ASP:HA	1.82	0.60
2:C:138:ILE:HG22	2:C:139:ASN:N	2.16	0.60
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.82	0.60
3:D:375:GLU:OE2	3:D:378:LYS:HD2	2.02	0.60
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.19	0.60
2:I:1247:SER:HB3	3:J:375:GLU:O	2.01	0.60
3:J:536:LEU:HD13	3:J:541:LEU:HB2	1.83	0.60
3:J:888:CYS:SG	3:J:889:ASP:N	2.75	0.60
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.37	0.60
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.02	0.60
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.67	0.60
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.66	0.60
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.66	0.60
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.83	0.60
1:A:249:PHE:HB2	1:A:253:LEU:HD12	1.82	0.60
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.83	0.60
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.37	0.60
2:C:701:GLY:O	2:C:1184:THR:N	2.25	0.60
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.32	0.60
1:A:61:ILE:HG22	1:A:62:ASP:H	1.66	0.60
1:B:151:GLY:O	1:B:177:TYR:HB2	2.02	0.60
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.20	0.60
2:C:498:ILE:H	2:C:498:ILE:HD12	1.66	0.60
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.36	0.60
3:D:363:LEU:HG	3:D:363:LEU:O	2.02	0.60
3:D:641:ILE:O	3:D:641:ILE:HD13	2.02	0.60
2:I:407:ARG:HH21	2:I:414:ILE:HG22	1.65	0.60
2:I:674:ASP:OD1	2:I:1109:ILE:N	2.34	0.60
3:J:495:ASN:ND2	3:J:497:GLU:HB2	2.17	0.60
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.17	0.59
1:G:65:LEU:H	1:G:65:LEU:CD2	2.15	0.59
1:G:228:LEU:HD22	1:H:221:ALA:HB1	1.84	0.59
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.66	0.59
3:J:521:LYS:NZ	3:J:540:GLY:O	2.24	0.59
5:L:233:ASP:O	5:L:236:LYS:HE2	2.02	0.59
5:L:245:ALA:O	5:L:249:ILE:HG13	2.01	0.59
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.31	0.59
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.32	0.59
2:C:864:LYS:HZ1	2:C:877:VAL:HG12	1.67	0.59
3:D:77:ARG:HG3	3:D:79:LYS:H	1.67	0.59
5:F:599:ARG:O	5:F:604:SER:OG	2.18	0.59
1:G:45:ARG:NH1	1:H:34:GLY:O	2.34	0.59
3:J:810:THR:HG23	3:J:811:GLU:H	1.67	0.59
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.02	0.59
5:L:127:ILE:O	5:L:130:VAL:HG22	2.02	0.59
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.17	0.59
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.83	0.59
1:G:172:LEU:HD12	1:G:172:LEU:H	1.67	0.59
2:I:4:SER:OG	2:I:5:TYR:N	2.35	0.59
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.02	0.59
2:I:1073:LYS:HE3	3:J:462:ASP:CB	2.32	0.59
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.68	0.59
1:A:9:LEU:HD13	1:A:32:GLU:OE2	2.03	0.59
1:B:34:GLY:N	1:B:199:ASP:OD2	2.29	0.59
2:C:615:VAL:HG13	2:C:651:ASP:N	2.17	0.59
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.67	0.59
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	1.85	0.59
1:H:18:GLN:HA	1:H:24:ALA:HA	1.83	0.59
2:I:159:SER:O	2:I:160:ASP:HB2	2.01	0.59
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.17	0.59
1:B:182:ARG:NH1	3:D:581:MET:SD	2.75	0.59
5:F:227:GLN:HG2	5:F:252:LEU:HA	1.84	0.59
5:F:532:LEU:O	5:F:536:THR:HG23	2.02	0.59
2:I:878:THR:OG1	2:I:879:GLY:N	2.34	0.59
3:J:527:LEU:HD21	3:J:536:LEU:HG	1.83	0.59
1:A:53:GLY:O	1:A:149:GLY:N	2.27	0.59
1:B:153:VAL:O	1:B:175:ALA:N	2.34	0.59
1:B:197:ASP:O	1:B:198:LEU:HD13	2.02	0.59
3:D:665:GLN:HG3	3:D:669:GLN:HE21	1.67	0.59
2:C:483:ASP:HB2	2:C:486:THR:HG22	1.83	0.59
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.83	0.59
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	1.84	0.59
5:F:601:PRO:CA	5:F:604:SER:HB2	2.33	0.59
1:H:113:ALA:HB2	1:H:126:PRO:HB3	1.83	0.59
2:I:778:GLU:O	2:I:781:ASP:HB2	2.03	0.59
1:A:11:PRO:CB	1:A:30:PRO:HG2	2.33	0.59
5:F:124:GLU:HA	5:F:127:ILE:HD11	1.83	0.59
1:H:58:GLU:HA	1:H:171:LEU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.37	0.59
2:I:692:THR:OG1	2:I:827:ARG:O	2.20	0.59
5:L:479:THR:HG23	5:L:481:GLU:H	1.68	0.59
3:D:242:LEU:HD23	3:D:242:LEU:C	2.24	0.59
1:G:65:LEU:H	1:G:65:LEU:HD22	1.68	0.59
1:H:197:ASP:O	1:H:198:LEU:HD13	2.03	0.59
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.85	0.58
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.85	0.58
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.83	0.58
3:J:516:ASP:HA	3:J:545:HIS:HB2	1.83	0.58
3:J:551:ARG:HA	3:J:568:SER:O	2.03	0.58
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	1.85	0.58
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.33	0.58
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.31	0.58
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.06	0.58
2:I:632:ASP:O	2:I:647:ARG:HB2	2.02	0.58
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.32	0.58
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.38	0.58
1:A:201:LEU:HG	1:A:203:ILE:HG13	1.85	0.58
3:J:335:GLN:HG2	3:J:343:LEU:HD13	1.85	0.58
5:L:544:THR:HG22	5:L:607:LEU:HD21	1.85	0.58
3:D:97:VAL:HG11	3:D:101:ARG:CZ	2.34	0.58
5:F:105:MET:HE3	5:F:385:ARG:HG2	1.86	0.58
2:I:143:ARG:NH2	2:I:512:SER:O	2.37	0.58
2:I:314:ASN:O	2:I:352:ARG:NH1	2.29	0.58
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.38	0.58
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.86	0.58
3:J:155:GLU:N	3:J:158:GLN:OE1	2.33	0.58
3:J:843:VAL:HG11	3:J:897:HIS:O	2.03	0.58
5:L:225:ARG:O	5:L:229:VAL:HG13	2.04	0.58
4:E:83:VAL:HA	4:E:86:ILE:HG12	1.86	0.58
2:I:696:ASP:HB2	2:I:798:GLN:CG	2.32	0.58
3:J:1219:ASP:O	3:J:1222:ARG:N	2.36	0.58
3:J:1368:ASP:HA	3:J:1371:ARG:NH1	2.19	0.58
2:C:732:ILE:HD13	2:C:783:LEU:HD12	1.84	0.58
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.68	0.58
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.36	0.58
3:D:612:LEU:N	3:D:612:LEU:HD12	2.18	0.58
5:F:281:ARG:HG2	5:F:285:ARG:HD2	1.85	0.58
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.85	0.58
1:G:22:THR:HB	1:G:207:THR:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:CB	1:A:30:PRO:CD	2.79	0.58
2:C:1246:ARG:HG2	2:C:1247:SER:N	2.18	0.58
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.85	0.58
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.85	0.58
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.85	0.58
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.19	0.58
2:I:1030:GLU:OE2	2:I:1034:ARG:NH2	2.37	0.58
2:I:1120:ALA:HB1	2:I:1198:LEU:HD12	1.85	0.58
3:J:259:ARG:CZ	5:L:505:ILE:HD11	2.34	0.58
3:J:403:ARG:NE	3:J:405:GLU:OE2	2.24	0.58
2:C:49:LEU:HB2	2:C:73:TYR:CZ	2.39	0.58
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.33	0.58
2:C:169:LYS:HE2	2:C:190:PRO:O	2.03	0.58
5:F:137:TYR:CE2	5:F:273:MET:HG2	2.38	0.58
1:G:69:SER:O	1:G:78:ILE:HG12	2.03	0.58
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.39	0.58
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.86	0.58
3:D:418:GLU:H	4:E:45:LYS:HZ2	1.51	0.58
3:D:839:VAL:CG1	3:D:864:LEU:HD12	2.34	0.58
2:I:810:TYR:CZ	3:J:359:PRO:HD2	2.39	0.58
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.84	0.58
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.86	0.57
3:D:622:ASP:HB3	3:D:626:TYR:HE2	1.69	0.57
2:I:523:GLU:OE2	2:I:527:LYS:NZ	2.27	0.57
3:J:94:GLN:O	3:J:97:VAL:HG23	2.04	0.57
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.87	0.57
2:C:312:ALA:HB3	2:C:315:MET:HE3	1.85	0.57
1:G:52:PRO:HG2	1:G:219:ARG:HH21	1.67	0.57
2:I:206:ALA:O	2:I:209:ILE:HG22	2.04	0.57
2:I:836:LEU:N	2:I:836:LEU:HD12	2.19	0.57
3:J:1156:LEU:HD22	3:J:1156:LEU:N	2.19	0.57
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.18	0.57
1:A:11:PRO:CA	1:A:30:PRO:CG	2.70	0.57
2:C:1253:LEU:O	2:C:1253:LEU:HD22	2.04	0.57
2:I:1260:GLY:HA2	2:I:1264:GLN:O	2.04	0.57
1:B:151:GLY:O	1:B:177:TYR:HD2	1.88	0.57
3:D:274:ASN:OD1	5:F:446:GLN:NE2	2.38	0.57
5:F:137:TYR:CD2	5:F:273:MET:HG2	2.39	0.57
2:I:371:ARG:HB3	2:I:374:GLU:OE2	2.04	0.57
3:J:298:MET:SD	5:L:402:LEU:HB3	2.44	0.57
3:J:600:ALA:O	3:J:603:LYS:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.37	0.57
1:B:64:VAL:HG12	1:B:65:LEU:H	1.70	0.57
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.86	0.57
2:C:1268:GLN:HE22	3:D:352:ARG:NH1	2.02	0.57
3:D:356:THR:OG1	3:D:357:VAL:N	2.38	0.57
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.85	0.57
3:J:308:ASP:OD2	3:J:311:ARG:NE	2.38	0.57
3:J:425:ARG:HG2	3:J:426:ALA:H	1.68	0.57
5:L:390:ILE:O	5:L:393:LYS:HB2	2.05	0.57
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.05	0.57
5:F:461:ASN:O	5:F:465:ARG:HG2	2.04	0.57
1:G:230:ALA:HB3	1:G:231:PHE:CE2	2.39	0.57
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.87	0.57
2:I:12:ARG:NH2	2:I:698:PRO:O	2.25	0.57
2:I:185:ASP:HB2	2:I:197:ARG:HG3	1.87	0.57
2:C:468:LEU:O	2:C:471:VAL:HG12	2.04	0.57
2:C:936:ARG:HE	2:C:1047:LEU:HD23	1.70	0.57
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.33	0.57
5:F:561:MET:HA	5:F:567:MET:HE1	1.86	0.57
1:H:99:ILE:HD12	1:H:145:LYS:HB2	1.87	0.57
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.05	0.57
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.70	0.57
2:C:1238:LEU:HD12	2:C:1238:LEU:N	2.18	0.57
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.86	0.57
3:D:555:TYR:O	3:D:586:GLY:O	2.23	0.57
5:F:503:GLU:HG3	5:F:504:PRO:HD2	1.87	0.57
1:G:75:GLN:O	2:I:729:ALA:HB2	2.04	0.57
1:H:99:ILE:HG13	1:H:144:ILE:O	2.05	0.57
2:I:145:ILE:HB	2:I:456:VAL:HG22	1.86	0.57
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.45	0.57
3:J:1343:GLU:HG3	3:J:1373:ARG:NH2	2.20	0.57
2:C:596:ASP:OD2	2:C:597:GLY:N	2.36	0.57
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.68	0.57
3:D:94:GLN:O	3:D:97:VAL:HG23	2.04	0.57
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.70	0.57
2:C:980:VAL:O	2:C:984:VAL:HB	2.05	0.57
3:D:388:ARG:HB2	3:D:390:LEU:CD1	2.35	0.57
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.34	0.57
2:I:480:SER:HB3	2:I:481:LEU:HD22	1.86	0.57
2:I:606:LEU:HD23	2:I:611:GLU:HA	1.86	0.57
2:I:1246:ARG:NH2	2:I:1249:GLY:H	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.05	0.57
5:L:421:TYR:CE2	5:L:422:ARG:HD2	2.40	0.57
2:I:170:VAL:HG23	2:I:171:LEU:N	2.20	0.56
2:C:170:VAL:O	2:C:171:LEU:HG	2.05	0.56
2:C:886:LYS:CE	2:C:916:SER:HB3	2.35	0.56
5:F:226:ALA:O	5:F:229:VAL:HG22	2.05	0.56
5:F:379:MET:O	5:F:379:MET:HG3	2.01	0.56
2:I:239:MET:O	2:I:284:LEU:HD12	2.03	0.56
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.87	0.56
2:I:655:VAL:N	2:I:659:GLN:OE1	2.37	0.56
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.39	0.56
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.40	0.56
3:J:45:ASN:O	3:J:46:TYR:HD2	1.87	0.56
1:A:23:HIS:HB2	1:A:206:GLU:HA	1.87	0.56
2:C:62:TYR:O	2:C:64:GLY:N	2.38	0.56
2:C:495:ALA:HB3	5:F:471:LEU:HD13	1.85	0.56
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.05	0.56
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.38	0.56
3:D:224:LEU:O	3:D:228:VAL:HG23	2.04	0.56
3:D:299:LEU:O	3:D:299:LEU:HG	2.02	0.56
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.39	0.56
3:D:657:ALA:O	3:D:661:VAL:HG12	2.06	0.56
3:D:817:HIS:HE1	3:D:860:ARG:HE	1.45	0.56
5:F:343:LYS:H	5:F:343:LYS:HD2	1.70	0.56
2:I:40:GLU:O	2:I:73:TYR:OH	2.23	0.56
2:I:468:LEU:O	2:I:471:VAL:HG12	2.06	0.56
3:J:536:LEU:O	3:J:539:SER:OG	2.24	0.56
3:J:1203:ARG:NH1	3:J:1205:GLU:HG2	2.18	0.56
1:A:23:HIS:CB	1:A:206:GLU:HA	2.35	0.56
1:B:82:LEU:O	1:B:85:LEU:HB2	2.05	0.56
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.86	0.56
2:C:685:MET:HE1	2:C:1071:GLY:HA2	1.87	0.56
3:D:674:THR:HG1	3:D:677:GLU:HB2	1.71	0.56
1:G:38:THR:HG23	1:H:42:ALA:HA	1.88	0.56
2:I:615:VAL:HG13	2:I:651:ASP:H	1.69	0.56
2:I:818:VAL:HG22	2:I:1096:ILE:HG12	1.87	0.56
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.41	0.56
3:J:425:ARG:HH11	3:J:459:ALA:HA	1.69	0.56
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.87	0.56
1:G:9:LEU:HD23	1:G:10:LYS:N	2.20	0.56
1:G:73:GLY:N	2:I:728:ASP:OD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:101:ARG:HH21	2:I:118:LYS:HE3	1.71	0.56
2:I:870:ILE:HB	2:I:944:ARG:HD3	1.86	0.56
2:I:1252:SER:O	2:I:1256:GLN:HA	2.06	0.56
3:J:735:ALA:O	3:J:739:GLN:HG3	2.06	0.56
3:J:741:ALA:O	3:J:762:ASN:ND2	2.39	0.56
3:J:1230:THR:O	3:J:1234:VAL:HG22	2.05	0.56
1:B:112:ALA:HB2	1:B:128:HIS:HB3	1.86	0.56
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.46	0.56
2:C:887:VAL:HB	2:C:913:VAL:HG21	1.87	0.56
2:C:905:ILE:O	5:F:599:ARG:NH1	2.27	0.56
1:G:102:LEU:O	1:G:141:SER:HB2	2.06	0.56
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.87	0.56
1:H:191:ARG:HH12	3:J:370:LYS:NZ	2.03	0.56
2:I:888:THR:HG23	2:I:916:SER:OG	2.06	0.56
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.05	0.56
2:C:561:ILE:O	2:C:680:LEU:HD12	2.05	0.56
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	2.20	0.56
5:F:225:ARG:O	5:F:229:VAL:HG13	2.05	0.56
2:I:158:ASP:OD1	2:I:159:SER:N	2.37	0.56
3:J:620:PHE:O	3:J:624:ILE:HG13	2.06	0.56
3:J:930:LEU:HD11	3:J:1241:TYR:CZ	2.41	0.56
2:C:22:LEU:HD13	2:C:23:ASP:N	2.21	0.56
2:C:211:ARG:HD3	2:C:357:ASN:O	2.06	0.56
2:C:768:MET:O	2:C:784:ALA:HB1	2.06	0.56
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.21	0.56
2:I:720:ARG:HA	2:I:779:ARG:HG3	1.86	0.56
2:I:1282:GLY:O	3:J:1360:GLY:HA3	2.06	0.56
1:A:36:GLY:CA	1:A:187:VAL:HG11	2.36	0.56
2:C:170:VAL:HG23	2:C:171:LEU:N	2.21	0.56
2:C:828:PHE:HB3	2:C:1060:ILE:HD12	1.88	0.56
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.87	0.56
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.87	0.56
3:D:700:ASN:O	3:D:704:GLU:HB2	2.06	0.56
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.87	0.56
2:I:136:PHE:O	2:I:143:ARG:N	2.33	0.56
2:I:538:LEU:HA	2:I:542:ARG:CZ	2.35	0.56
2:I:673:HIS:HB3	2:I:1109:ILE:CG2	2.32	0.56
2:I:891:GLY:O	2:I:892:GLU:HG3	2.06	0.56
3:J:621:ALA:HA	3:J:624:ILE:HD12	1.87	0.56
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.88	0.56
2:C:397:LEU:H	2:C:397:LEU:HD12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:466:VAL:O	2:C:470:ARG:HG2	2.05	0.56
3:D:347:VAL:HG12	3:D:348:ASP:O	2.05	0.56
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.15	0.56
1:H:44:ARG:CG	1:H:183:ILE:HD13	2.36	0.56
2:I:138:ILE:HG22	2:I:139:ASN:N	2.19	0.56
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.38	0.56
3:J:127:LEU:O	3:J:220:ARG:NH2	2.39	0.56
3:J:518:VAL:HG23	3:J:547:ARG:HH22	1.70	0.56
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.88	0.55
2:C:1299:ASN:HD22	2:C:1303:LYS:CE	2.18	0.55
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.71	0.55
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.07	0.55
3:J:709:ARG:C	3:J:711:GLY:H	2.08	0.55
3:J:789:LYS:HE3	3:J:931:THR:O	2.05	0.55
3:J:849:LEU:HB3	3:J:853:THR:HG23	1.87	0.55
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.41	0.55
1:A:49:SER:OG	1:A:50:SER:N	2.38	0.55
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.41	0.55
1:B:60:GLU:HG3	1:B:143:ARG:O	2.06	0.55
2:C:379:GLU:CD	2:C:379:GLU:H	2.08	0.55
3:D:140:TYR:HB3	5:F:100:MET:SD	2.46	0.55
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.20	0.55
1:G:191:ARG:NH1	1:G:198:LEU:H	2.04	0.55
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.87	0.55
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.11	0.55
2:I:1132:LEU:HD22	2:I:1177:ARG:NH1	2.21	0.55
3:J:156:ARG:NH2	3:J:191:SER:OG	2.37	0.55
5:L:547:VAL:HG23	5:L:603:ARG:NH1	2.21	0.55
1:A:269:CYS:O	1:A:273:GLU:HG2	2.06	0.55
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.42	0.55
1:B:99:ILE:HG13	1:B:144:ILE:O	2.05	0.55
2:C:228:VAL:HB	2:C:335:THR:OG1	2.06	0.55
2:C:607:SER:OG	2:C:608:ALA:N	2.32	0.55
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.37	0.55
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.88	0.55
1:H:60:GLU:HG2	1:H:143:ARG:HB2	1.87	0.55
2:I:324:LYS:O	2:I:327:GLN:NE2	2.40	0.55
2:I:807:TRP:CE3	2:I:808:ASN:HB2	2.41	0.55
2:I:898:GLU:OE1	2:I:898:GLU:N	2.37	0.55
2:I:1085:MET:HB2	2:I:1093:PRO:HB3	1.87	0.55
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:45:ASN:HB3	3:J:48:THR:O	2.06	0.55
1:B:155:ALA:N	1:B:174:ASP:OD1	2.39	0.55
2:C:202:ARG:HH11	2:C:369:MET:HG2	1.71	0.55
2:C:1076:ILE:HD11	2:C:1078:LYS:O	2.06	0.55
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.42	0.55
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.89	0.55
3:J:418:GLU:HB2	4:K:45:LYS:HB2	1.88	0.55
1:A:12:ARG:N	1:A:30:PRO:HG2	2.12	0.55
2:C:55:SER:OG	2:C:56:VAL:N	2.39	0.55
2:C:637:ARG:HA	2:C:642:SER:HA	1.87	0.55
5:F:227:GLN:NE2	5:F:251:LYS:HZ1	2.03	0.55
2:I:557:ARG:HH21	2:I:607:SER:C	2.09	0.55
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.42	0.55
2:C:224:PHE:CD2	2:C:347:ILE:HG13	2.41	0.55
2:C:758:ARG:HH22	2:C:761:GLN:CG	2.08	0.55
5:F:354:THR:N	5:F:357:GLN:OE1	2.40	0.55
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.21	0.55
5:L:266:PHE:O	5:L:269:LEU:HB2	2.06	0.55
3:D:314:ARG:HH22	3:D:323:PRO:HG3	1.69	0.55
3:D:418:GLU:H	4:E:45:LYS:NZ	2.04	0.55
3:J:490:ILE:O	3:J:499:ILE:HG22	2.06	0.55
3:J:1159:ILE:CA	3:J:1206:ARG:HB3	2.36	0.55
3:J:1327:GLU:OE2	3:J:1329:THR:HB	2.06	0.55
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.88	0.55
2:C:1151:LEU:HD23	2:C:1197:GLU:OE2	2.07	0.55
3:D:152:THR:OG1	3:D:153:ASN:N	2.38	0.55
5:F:166:VAL:O	5:F:167:ASP:HB2	2.07	0.55
1:H:60:GLU:OE1	1:H:142:MET:HB2	2.06	0.55
2:I:156:PHE:CE1	2:I:445:ILE:HG13	2.42	0.55
2:I:498:ILE:H	2:I:498:ILE:HD12	1.71	0.55
2:I:678:ARG:NH1	2:I:1071:GLY:O	2.37	0.55
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.41	0.55
3:J:568:SER:OG	3:J:569:LEU:N	2.37	0.55
5:L:314:THR:O	5:L:318:ALA:HB3	2.07	0.55
3:D:425:ARG:HG2	3:D:426:ALA:H	1.71	0.55
3:D:515:ARG:O	3:D:545:HIS:HB3	2.07	0.55
3:D:1277:GLY:O	3:D:1278:GLU:HG2	2.07	0.55
1:G:150:ARG:NH1	1:H:7:GLU:O	2.32	0.55
2:I:421:SER:N	2:I:424:ASP:OD2	2.37	0.55
3:J:492:SER:HB2	3:J:499:ILE:HD13	1.88	0.55
3:J:1174:ARG:NH2	3:J:1187:GLU:OE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:297:VAL:HG12	2:C:315:MET:O	2.06	0.55
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.89	0.55
3:D:58:CYS:SG	3:D:60:ARG:N	2.80	0.55
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.55
2:I:1077:SER:HA	3:J:356:THR:OG1	2.06	0.55
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.88	0.55
2:I:1184:THR:HG23	2:I:1189:GLY:CA	2.36	0.55
2:I:1333:LEU:HD22	3:J:307:LEU:CD2	2.37	0.55
3:J:411:ILE:O	3:J:414:GLU:HB2	2.06	0.55
3:J:845:ALA:CB	3:J:881:LYS:HD2	2.37	0.55
1:B:35:PHE:HA	1:B:38:THR:HG22	1.89	0.54
1:B:43:LEU:HD21	1:B:221:ALA:HB2	1.89	0.54
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.89	0.54
3:D:121:PRO:HD2	3:D:123:ARG:NH2	2.22	0.54
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.89	0.54
5:F:484:ALA:HB1	5:F:491:GLU:HG3	1.88	0.54
1:H:82:LEU:HD23	1:H:85:LEU:HD12	1.89	0.54
2:I:133:ASN:OD1	2:I:713:GLY:HA3	2.07	0.54
2:I:397:LEU:O	2:I:398:SER:OG	2.25	0.54
3:J:1356:LEU:O	3:J:1366:HIS:HE1	1.89	0.54
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.88	0.54
1:A:234:LEU:HB2	1:B:218:ARG:NH2	2.22	0.54
2:C:1124:ILE:HG21	2:C:1180:MET:HG3	1.89	0.54
3:D:518:VAL:HG11	3:D:707:ILE:HD13	1.89	0.54
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.88	0.54
2:I:514:PHE:HE2	2:I:760:ASN:HB3	1.72	0.54
2:I:557:ARG:NH2	2:I:607:SER:O	2.40	0.54
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.42	0.54
2:I:1132:LEU:HD22	2:I:1177:ARG:HH12	1.71	0.54
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.89	0.54
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	2.09	0.54
4:K:15:ASN:O	4:K:16:ARG:HB3	2.08	0.54
1:A:158:ARG:HH21	1:A:172:LEU:HB3	1.73	0.54
2:C:189:ASP:OD1	2:C:193:ASN:N	2.22	0.54
2:C:518:ASN:OD1	2:C:519:ASN:N	2.40	0.54
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.41	0.54
2:C:1281:TYR:CE2	3:D:431:ARG:HG3	2.43	0.54
3:D:1165:PHE:HE1	3:D:1200:GLU:HB3	1.72	0.54
5:F:316:PHE:O	5:F:320:ILE:HG13	2.07	0.54
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.89	0.54
1:H:40:GLY:HA3	1:H:185:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:97:VAL:HG11	3:J:101:ARG:NH2	2.22	0.54
3:J:418:GLU:HG3	4:K:45:LYS:N	2.11	0.54
1:A:83:LEU:CD2	2:C:694:ARG:HE	2.21	0.54
2:C:175:ARG:NH1	2:C:183:TRP:HZ3	2.06	0.54
3:D:244:VAL:HA	3:D:269:TYR:OH	2.07	0.54
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.89	0.54
3:D:1295:ASN:CG	3:D:1298:VAL:HB	2.27	0.54
1:G:152:TYR:CD1	1:G:176:CYS:HB3	2.41	0.54
1:G:153:VAL:O	1:G:175:ALA:N	2.38	0.54
1:H:7:GLU:CD	1:H:8:PHE:H	2.10	0.54
1:H:61:ILE:HG22	1:H:64:VAL:H	1.72	0.54
3:J:1194:ARG:N	3:J:1194:ARG:HD2	2.22	0.54
1:A:90:VAL:HG22	1:A:91:ARG:H	1.73	0.54
2:C:247:ARG:HH12	2:C:271:ALA:HB2	1.72	0.54
2:C:801:ARG:HB2	2:C:1229:TYR:CZ	2.43	0.54
5:F:316:PHE:CZ	5:F:334:SER:HA	2.42	0.54
5:F:569:THR:OG1	5:F:570:ASP:N	2.30	0.54
2:I:617:ALA:HA	2:I:636:CYS:SG	2.47	0.54
2:I:1275:VAL:HG22	2:I:1287:LEU:HD11	1.89	0.54
3:J:97:VAL:HG11	3:J:101:ARG:CZ	2.37	0.54
3:J:481:ARG:NH1	4:K:3:ARG:O	2.40	0.54
4:K:35:LYS:NZ	4:K:71:GLU:OE2	2.38	0.54
5:L:316:PHE:HZ	5:L:334:SER:HA	1.72	0.54
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.90	0.54
2:C:149:LEU:HD13	2:C:453:ILE:HG12	1.89	0.54
2:C:262:TYR:CZ	2:C:282:VAL:HG21	2.43	0.54
2:C:519:ASN:C	2:C:519:ASN:OD1	2.45	0.54
2:C:866:ASP:HA	2:C:872:TYR:OH	2.07	0.54
3:D:19:ALA:O	3:D:20:ILE:HG13	2.07	0.54
3:D:24:LEU:HB2	3:D:232:ASN:OD1	2.08	0.54
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.22	0.54
3:D:369:PRO:HB3	3:D:444:GLY:O	2.07	0.54
3:D:702:GLN:O	3:D:718:SER:N	2.22	0.54
1:G:102:LEU:HD13	1:G:103:ASN:N	2.23	0.54
2:I:4:SER:HB3	2:I:7:GLU:OE2	2.08	0.54
1:B:19:VAL:HB	1:B:23:HIS:HD2	1.70	0.54
1:B:134:THR:HG23	1:B:135:ASP:N	2.22	0.54
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.36	0.54
3:D:520:ALA:HB3	3:D:546:ALA:HB2	1.88	0.54
2:I:146:VAL:O	2:I:511:LEU:HD23	2.08	0.54
3:J:474:LEU:O	3:J:477:GLN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.90	0.54
1:A:316:MET:SD	5:F:600:HIS:ND1	2.81	0.54
2:C:97:ARG:HH22	5:F:475:GLY:HA3	1.73	0.54
1:G:77:ASP:OD2	2:I:755:LYS:NZ	2.36	0.54
1:H:219:ARG:O	1:H:223:ILE:HG13	2.07	0.54
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.08	0.54
3:J:58:CYS:SG	3:J:59:ALA:N	2.80	0.54
4:K:53:GLU:HB3	4:K:59:ILE:HG13	1.88	0.54
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.89	0.54
2:C:886:LYS:H	2:C:917:SER:HB3	1.73	0.54
2:C:1281:TYR:OH	3:D:431:ARG:O	2.24	0.54
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.22	0.54
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.89	0.54
3:J:620:PHE:CD1	3:J:624:ILE:HD11	2.43	0.54
5:L:460:ILE:O	5:L:463:LEU:HB2	2.08	0.54
3:D:362:ARG:H	3:D:365:GLN:NE2	2.06	0.54
5:F:343:LYS:O	5:F:347:ILE:HG13	2.08	0.54
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.90	0.54
2:I:673:HIS:CB	2:I:1109:ILE:HG22	2.36	0.54
3:J:905:ARG:CZ	3:J:910:ASN:HD21	2.20	0.54
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.43	0.53
3:D:40:LYS:O	3:D:55:GLY:HA2	2.08	0.53
3:D:1158:GLU:HB3	3:D:1186:TYR:CE1	2.43	0.53
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.73	0.53
5:F:470:MET:CE	5:F:486:ARG:HH12	2.21	0.53
2:I:412:GLU:HB3	2:I:413:GLU:OE1	2.08	0.53
3:J:1371:ARG:HB3	3:J:1371:ARG:CZ	2.39	0.53
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.23	0.53
1:A:207:THR:HG22	1:A:208:ASN:N	2.23	0.53
3:D:293:ARG:O	3:D:296:LYS:N	2.41	0.53
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.44	0.53
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.91	0.53
1:G:67:GLU:O	1:G:78:ILE:HB	2.08	0.53
2:I:808:ASN:H	3:J:633:ALA:HB2	1.72	0.53
2:I:1116:HIS:HE1	3:J:641:ILE:N	2.01	0.53
3:J:442:ILE:HG22	3:J:443:GLU:O	2.08	0.53
3:J:623:GLN:O	3:J:627:THR:HG22	2.08	0.53
4:K:59:ILE:HD13	4:K:63:ILE:HG21	1.91	0.53
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.91	0.53
1:A:47:LEU:HD13	1:A:183:ILE:HG12	1.90	0.53
1:A:88:LEU:HD12	1:A:125:LYS:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:HB2	5:F:601:PRO:HB3	1.90	0.53
1:B:25:LYS:HG3	1:B:204:GLU:HB2	1.90	0.53
2:C:412:GLU:HB3	2:C:413:GLU:OE1	2.09	0.53
2:C:985:GLU:HG2	2:C:988:LYS:HD2	1.89	0.53
3:D:30:ILE:CG2	3:D:243:PRO:HG3	2.38	0.53
3:D:744:ARG:O	3:D:759:ILE:HB	2.08	0.53
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.37	0.53
1:H:103:ASN:HA	1:H:141:SER:HB2	1.88	0.53
2:I:301:TYR:HB2	2:I:311:CYS:SG	2.48	0.53
2:I:1142:ARG:HD3	2:I:1161:LEU:HD11	1.91	0.53
3:J:1169:THR:CG2	3:J:1192:LYS:HD3	2.37	0.53
1:B:175:ALA:HB1	1:B:177:TYR:CZ	2.44	0.53
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.91	0.53
3:D:808:VAL:HG12	3:D:809:VAL:N	2.23	0.53
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.91	0.53
2:I:632:ASP:HA	2:I:647:ARG:HD2	1.90	0.53
2:I:963:GLU:O	2:I:967:LEU:HB2	2.08	0.53
3:J:58:CYS:SG	3:J:60:ARG:N	2.79	0.53
3:J:647:PRO:HD3	3:J:697:MET:HB3	1.91	0.53
3:J:808:VAL:HG12	3:J:809:VAL:N	2.23	0.53
2:C:529:ARG:O	2:C:530:ILE:HD13	2.08	0.53
2:C:667:LEU:CD2	2:C:704:MET:HB2	2.38	0.53
2:C:755:LYS:O	2:C:757:THR:HG23	2.09	0.53
2:C:1136:GLN:HE21	2:C:1140:LYS:HZ3	1.56	0.53
2:C:1257:GLN:HE22	3:D:340:GLN:HE21	1.56	0.53
2:C:1281:TYR:HE2	3:D:431:ARG:HG3	1.73	0.53
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.43	0.53
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.08	0.53
3:D:124:ILE:HG12	3:D:237:MET:SD	2.48	0.53
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.74	0.53
5:F:230:VAL:O	5:F:234:THR:HG23	2.08	0.53
5:F:512:GLY:C	5:F:514:ASP:H	2.12	0.53
1:G:13:LEU:HA	1:G:28:LEU:HA	1.89	0.53
1:G:31:LEU:HB2	1:G:199:ASP:HB2	1.90	0.53
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.73	0.53
3:J:1157:ALA:O	3:J:1207:GLY:N	2.39	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.44	0.53
2:C:759:SER:HG	2:C:763:THR:N	2.05	0.53
3:D:262:THR:O	5:F:507:MET:HB2	2.09	0.53
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.43	0.53
5:F:124:GLU:O	5:F:127:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:133:SER:OG	5:F:364:ARG:HD2	2.08	0.53
1:G:77:ASP:OD2	2:I:729:ALA:HB1	2.09	0.53
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.90	0.53
2:I:195:PHE:HE1	2:I:205:PRO:HG3	1.73	0.53
3:J:263:SER:OG	3:J:264:ASP:N	2.41	0.53
3:J:440:VAL:O	3:J:442:ILE:HG12	2.08	0.53
3:J:795:TYR:CE2	3:J:799:ARG:NE	2.77	0.53
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.72	0.53
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	1.91	0.53
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.43	0.53
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.73	0.53
2:I:57:PHE:CD1	2:I:58:PRO:HA	2.42	0.53
2:I:202:ARG:HH11	2:I:369:MET:CG	2.21	0.53
2:I:478:ARG:NH2	2:I:487:LEU:HD13	2.24	0.53
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.09	0.53
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.73	0.53
3:J:123:ARG:HD2	3:J:1337:VAL:HG11	1.91	0.53
3:J:572:THR:HG21	3:J:589:TYR:OH	2.08	0.53
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.08	0.53
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.91	0.53
5:F:281:ARG:O	5:F:285:ARG:HG3	2.09	0.53
1:G:182:ARG:NH2	1:G:206:GLU:OE2	2.42	0.53
3:J:363:LEU:HG	3:J:363:LEU:O	2.08	0.53
2:C:724:VAL:HG23	2:C:775:GLU:O	2.09	0.53
2:C:799:ASN:C	2:C:799:ASN:HD22	2.12	0.53
2:C:835:GLU:C	2:C:836:LEU:HD12	2.29	0.53
2:C:1305:TYR:HE1	3:D:379:PRO:HG3	1.73	0.53
3:D:62:PHE:O	3:D:101:ARG:HD2	2.09	0.53
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.41	0.53
3:J:93:THR:HG22	3:J:94:GLN:H	1.74	0.53
3:J:1140:ARG:NH2	3:J:1144:LEU:HD21	2.24	0.53
2:C:720:ARG:NE	2:C:736:VAL:HG11	2.24	0.53
2:C:1124:ILE:HB	2:C:1180:MET:HB2	1.91	0.53
2:C:1247:SER:HB3	3:D:375:GLU:O	2.09	0.53
3:D:26:SER:OG	3:D:28:ASP:N	2.42	0.53
3:D:35:PHE:CD1	3:D:101:ARG:HB3	2.41	0.53
3:D:56:LEU:H	3:D:56:LEU:CD1	2.14	0.53
3:D:552:ILE:HG21	3:D:589:TYR:CE1	2.44	0.53
3:D:1349:GLU:OE2	3:D:1349:GLU:N	2.36	0.53
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.44	0.53
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.74	0.52
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.91	0.52
3:D:521:LYS:NZ	3:D:540:GLY:O	2.20	0.52
3:D:1226:VAL:O	3:D:1230:THR:HG22	2.09	0.52
5:F:445:ASP:OD2	5:F:451:ARG:HD2	2.09	0.52
1:G:60:GLU:HB2	1:G:170:ARG:NH1	2.23	0.52
2:I:582:ASN:HB3	2:I:586:PHE:N	2.24	0.52
2:I:698:PRO:HG3	2:I:1231:TYR:CE2	2.44	0.52
2:I:739:ASP:OD1	2:I:739:ASP:N	2.42	0.52
3:J:514:THR:HG23	3:J:596:LEU:HB2	1.89	0.52
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.90	0.52
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.74	0.52
3:D:140:TYR:O	3:D:297:ARG:NH1	2.42	0.52
3:D:1156:LEU:HD22	3:D:1156:LEU:N	2.24	0.52
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.90	0.52
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.09	0.52
5:F:315:TRP:CH2	5:F:341:LEU:HD11	2.44	0.52
1:G:68:TYR:HE1	2:I:929:ILE:HG21	1.72	0.52
3:J:421:VAL:HG22	3:J:439:PRO:HG3	1.91	0.52
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.91	0.52
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.91	0.52
5:L:601:PRO:CA	5:L:604:SER:HB2	2.39	0.52
2:C:69:GLN:HG3	2:C:101:ARG:HB3	1.91	0.52
2:C:378:ARG:NH1	2:C:382:GLU:OE2	2.41	0.52
2:C:1272:GLU:HB2	3:D:342:LEU:O	2.09	0.52
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.42	0.52
3:D:195:GLU:O	3:D:198:CYS:HB2	2.09	0.52
3:D:1309:ILE:HG13	3:D:1310:THR:H	1.74	0.52
5:F:114:GLU:HG3	5:F:115:GLY:N	2.24	0.52
5:F:486:ARG:HB2	5:F:486:ARG:CZ	2.38	0.52
3:J:708:ASN:HB3	3:J:712:GLN:O	2.09	0.52
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.40	0.52
1:B:197:ASP:C	1:B:198:LEU:HD22	2.30	0.52
2:C:98:VAL:C	2:C:121:GLU:HA	2.30	0.52
2:C:158:ASP:CG	2:C:159:SER:H	2.12	0.52
2:C:490:GLN:NE2	5:F:472:GLN:HE22	2.08	0.52
2:C:797:GLY:N	2:C:1231:TYR:OH	2.40	0.52
2:C:1193:ALA:O	2:C:1197:GLU:N	2.32	0.52
3:D:77:ARG:HG3	3:D:79:LYS:HB3	1.90	0.52
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.10	0.52
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.24	0.52
1:B:61:ILE:HB	1:B:64:VAL:O	2.10	0.52
2:C:3:TYR:HE1	2:C:11:ILE:HD11	1.74	0.52
2:C:799:ASN:ND2	2:C:799:ASN:O	2.41	0.52
2:C:992:LEU:HD23	2:C:992:LEU:H	1.75	0.52
3:D:1179:PRO:CD	3:D:1184:ASP:HA	2.40	0.52
5:F:376:LYS:O	5:F:380:VAL:HG23	2.10	0.52
2:I:514:PHE:CE2	2:I:760:ASN:HB3	2.45	0.52
3:J:201:LEU:HD13	3:J:221:ILE:HB	1.92	0.52
1:A:125:LYS:HE2	1:A:128:HIS:CG	2.44	0.52
1:A:249:PHE:C	5:F:605:GLU:OE2	2.48	0.52
2:C:62:TYR:CZ	2:C:476:LYS:HB3	2.44	0.52
2:C:62:TYR:C	2:C:64:GLY:H	2.13	0.52
2:C:906:PHE:CE2	5:F:608:ARG:HG3	2.45	0.52
3:D:179:LYS:HB2	3:D:184:ALA:HB2	1.91	0.52
3:D:442:ILE:HG22	3:D:443:GLU:O	2.09	0.52
4:E:15:ASN:O	4:E:16:ARG:HB3	2.09	0.52
1:G:182:ARG:O	1:G:183:ILE:HD12	2.10	0.52
2:I:127:ILE:HG13	2:I:127:ILE:O	2.09	0.52
2:I:515:MET:HG2	2:I:515:MET:O	2.09	0.52
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.91	0.52
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.90	0.52
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.43	0.52
1:B:215:GLU:HA	1:B:218:ARG:HD2	1.91	0.52
2:C:300:ASP:OD1	2:C:312:ALA:HA	2.09	0.52
3:D:436:ALA:HB3	3:D:485:MET:HA	1.92	0.52
1:H:195:ARG:HB3	1:H:198:LEU:HD21	1.92	0.52
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.92	0.52
2:I:670:PHE:HA	2:I:672:GLU:OE2	2.09	0.52
2:I:972:PHE:CZ	2:I:998:LEU:HD11	2.45	0.52
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.92	0.52
3:D:45:ASN:O	3:D:46:TYR:HB3	2.09	0.52
3:D:473:THR:HG23	3:D:476:ALA:H	1.75	0.52
3:D:528:THR:O	3:D:551:ARG:HB3	2.09	0.52
3:D:674:THR:N	3:D:677:GLU:OE1	2.37	0.52
2:I:598:VAL:HG13	2:I:628:HIS:HE1	1.75	0.52
2:I:1035:LYS:O	2:I:1038:GLN:HG2	2.10	0.52
1:B:77:ASP:O	1:B:81:ILE:HG13	2.10	0.52
2:C:397:LEU:O	2:C:398:SER:OG	2.24	0.52
2:C:692:THR:OG1	2:C:693:LEU:N	2.42	0.52
3:D:31:ARG:NE	3:D:106:GLU:OE2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.91	0.52
5:F:479:THR:HG23	5:F:481:GLU:N	2.25	0.52
2:I:325:LEU:O	2:I:328:SER:OG	2.28	0.52
3:J:142:GLU:OE2	5:L:100:MET:HE2	2.10	0.52
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.91	0.52
1:A:187:VAL:CG1	1:A:201:LEU:HD13	2.39	0.52
1:A:261:GLU:CD	2:C:859:GLU:HB2	2.31	0.52
2:C:189:ASP:OD1	2:C:192:ASP:N	2.43	0.52
3:D:789:LYS:NZ	3:D:931:THR:O	2.42	0.52
3:D:847:ASP:CA	3:D:860:ARG:H	2.20	0.52
2:I:582:ASN:HB3	2:I:586:PHE:H	1.75	0.52
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.92	0.51
3:D:270:ARG:NH2	5:F:449:THR:HG23	2.25	0.51
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	1.91	0.51
2:I:299:LYS:HG2	2:I:334:GLU:OE1	2.11	0.51
2:I:551:HIS:CG	2:I:552:PRO:HD2	2.45	0.51
2:I:564:PRO:HD2	2:I:572:ILE:HB	1.92	0.51
2:I:1210:ILE:O	2:I:1224:PRO:HA	2.09	0.51
3:J:518:VAL:HA	3:J:547:ARG:CZ	2.40	0.51
3:J:850:LYS:HG2	3:J:857:LEU:HD23	1.92	0.51
5:L:448:ARG:NH2	5:L:500:ILE:O	2.43	0.51
1:B:60:GLU:OE1	1:B:142:MET:HB2	2.10	0.51
2:C:268:ARG:HH21	2:C:270:THR:CG2	2.23	0.51
2:C:553:THR:O	2:C:557:ARG:HD2	2.11	0.51
3:D:290:ILE:H	3:D:290:ILE:HD12	1.75	0.51
1:H:134:THR:HG23	1:H:135:ASP:N	2.24	0.51
3:J:471:PRO:HB3	3:J:476:ALA:HB1	1.92	0.51
3:J:817:HIS:CD2	3:J:860:ARG:HH21	2.28	0.51
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.73	0.51
5:L:431:ALA:O	5:L:434:TRP:N	2.43	0.51
1:A:250:ASP:HB2	5:F:601:PRO:CB	2.40	0.51
2:C:201:ARG:NH2	2:C:370:MET:O	2.37	0.51
2:C:543:ALA:O	2:C:548:ARG:NH1	2.43	0.51
2:C:1246:ARG:NH2	2:C:1249:GLY:H	2.08	0.51
3:D:805:GLN:OE1	3:D:1348:LYS:HD3	2.10	0.51
1:G:112:ALA:HB2	1:G:128:HIS:HB3	1.92	0.51
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.93	0.51
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.93	0.51
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.91	0.51
5:L:580:PHE:C	5:L:582:VAL:H	2.14	0.51
1:A:155:ALA:CA	1:A:158:ARG:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.24	0.51
2:C:358:ASP:OD1	2:C:360:LEU:N	2.44	0.51
2:C:1137:GLU:HG2	2:C:1140:LYS:HG2	1.92	0.51
2:C:1279:GLU:HG2	3:D:1357:ILE:HD13	1.92	0.51
5:F:227:GLN:HE22	5:F:251:LYS:NZ	2.06	0.51
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.74	0.51
1:H:62:ASP:OD1	1:H:142:MET:HB3	2.11	0.51
3:J:77:ARG:HG3	3:J:79:LYS:H	1.76	0.51
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.09	0.51
5:F:164:GLY:O	5:F:260:ARG:HB2	2.11	0.51
1:H:60:GLU:CD	1:H:143:ARG:H	2.12	0.51
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.92	0.51
2:I:397:LEU:HD12	2:I:397:LEU:N	2.26	0.51
2:I:812:PHE:CE2	3:J:451:PRO:HB3	2.46	0.51
1:A:91:ARG:HD3	1:A:210:THR:O	2.10	0.51
5:F:101:TYR:O	5:F:104:GLU:N	2.42	0.51
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.46	0.51
2:I:197:ARG:NH2	2:I:203:LYS:HB2	2.26	0.51
2:I:1046:VAL:HG21	2:I:1049:ILE:HD11	1.92	0.51
3:J:54:ASP:OD1	3:J:54:ASP:N	2.42	0.51
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	1.91	0.51
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.11	0.51
1:G:9:LEU:HD12	1:G:195:ARG:NH2	2.25	0.51
1:H:153:VAL:O	1:H:175:ALA:N	2.43	0.51
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.93	0.51
3:J:56:LEU:HD12	3:J:56:LEU:N	2.24	0.51
3:J:114:ILE:HB	3:J:304:ASP:OD1	2.11	0.51
3:J:405:GLU:O	3:J:408:VAL:HG22	2.10	0.51
3:J:470:VAL:HG12	3:J:472:LEU:CD2	2.41	0.51
2:C:14:ASP:OD2	2:C:1156:ARG:NE	2.42	0.51
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.11	0.51
2:I:943:LYS:O	2:I:947:GLU:HG3	2.11	0.51
2:I:1131:MET:HE2	2:I:1141:LEU:HA	1.91	0.51
2:C:195:PHE:CD1	2:C:203:LYS:HG2	2.46	0.51
2:C:231:GLU:HG2	2:C:332:ARG:NH2	2.26	0.51
3:D:45:ASN:O	3:D:46:TYR:HD2	1.93	0.51
3:D:849:LEU:HD13	3:D:849:LEU:H	1.76	0.51
3:D:1165:PHE:CE1	3:D:1200:GLU:HB3	2.46	0.51
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.19	0.51
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.11	0.51
3:J:1158:GLU:HB3	3:J:1186:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:THR:O	1:B:6:THR:OG1	2.21	0.51
2:C:894:GLN:O	2:C:894:GLN:HG3	2.11	0.51
3:D:34:SER:HB2	3:D:104:HIS:HB3	1.93	0.51
3:D:75:TYR:HD2	3:D:80:HIS:CD2	2.29	0.51
3:D:556:GLU:O	3:D:564:VAL:N	2.28	0.51
3:J:682:VAL:O	3:J:685:ILE:HG12	2.10	0.51
2:C:490:GLN:CD	5:F:472:GLN:NE2	2.64	0.50
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.11	0.50
3:D:495:ASN:N	3:D:495:ASN:OD1	2.43	0.50
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.93	0.50
4:E:50:ALA:O	4:E:54:ILE:HG12	2.11	0.50
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.11	0.50
2:I:1281:TYR:OH	3:J:434:ILE:O	2.29	0.50
1:A:57:THR:HG22	1:A:158:ARG:NH2	2.26	0.50
1:A:75:GLN:HA	2:C:729:ALA:N	2.26	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE2	1.93	0.50
2:C:229:ILE:HG21	2:C:240:GLU:OE2	2.12	0.50
2:C:452:ARG:NH1	2:C:584:TYR:O	2.43	0.50
2:C:1112:ILE:O	2:C:1115:THR:N	2.44	0.50
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.76	0.50
2:C:1267:GLY:HA3	3:D:347:VAL:O	2.12	0.50
3:D:516:ASP:OD1	3:D:516:ASP:N	2.44	0.50
3:D:664:ILE:HG21	3:D:681:LYS:HG2	1.93	0.50
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.93	0.50
2:I:921:PRO:O	2:I:924:VAL:HG22	2.11	0.50
3:J:1261:LEU:HD13	3:J:1304:ARG:HD2	1.93	0.50
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.27	0.50
1:A:207:THR:HG22	1:A:209:GLY:H	1.76	0.50
1:A:228:LEU:HA	1:A:231:PHE:HB2	1.93	0.50
2:C:397:LEU:HD12	2:C:397:LEU:N	2.26	0.50
3:D:574:VAL:O	3:D:578:ILE:HG13	2.11	0.50
1:G:65:LEU:HD22	1:G:65:LEU:N	2.26	0.50
2:I:4:SER:HB3	2:I:7:GLU:CD	2.31	0.50
2:I:623:LEU:HA	2:I:630:VAL:HG23	1.92	0.50
2:I:757:THR:O	2:I:833:ILE:HD12	2.11	0.50
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.93	0.50
1:A:152:TYR:OH	2:C:824:GLN:HA	2.11	0.50
2:C:323:ALA:O	2:C:327:GLN:HG3	2.12	0.50
2:C:618:GLN:OE1	3:D:770:LEU:HD13	2.12	0.50
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.93	0.50
3:D:844:THR:OG1	3:D:860:ARG:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.93	0.50
1:G:88:LEU:HB2	1:G:128:HIS:CD2	2.46	0.50
2:I:101:ARG:HE	2:I:118:LYS:HD2	1.77	0.50
3:J:255:LEU:HB2	3:J:259:ARG:O	2.12	0.50
3:J:825:VAL:C	3:J:826:ILE:HG13	2.32	0.50
5:L:161:LEU:O	5:L:262:VAL:HG23	2.11	0.50
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.26	0.50
2:C:1268:GLN:OE1	3:D:352:ARG:HG2	2.12	0.50
3:D:188:LEU:O	3:D:191:SER:OG	2.25	0.50
3:D:839:VAL:HG12	3:D:839:VAL:O	2.12	0.50
5:F:120:ALA:HA	5:F:123:ILE:HD12	1.93	0.50
1:H:19:VAL:HB	1:H:23:HIS:CD2	2.46	0.50
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.93	0.50
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.26	0.50
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.93	0.50
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.92	0.50
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.47	0.50
3:D:1184:ASP:O	3:D:1186:TYR:N	2.45	0.50
5:F:125:ASP:OD1	5:F:125:ASP:N	2.43	0.50
5:F:292:VAL:HG13	5:F:297:MET:O	2.11	0.50
5:F:478:PRO:HB2	5:F:483:LEU:CD1	2.41	0.50
5:F:478:PRO:HB2	5:F:483:LEU:HD11	1.92	0.50
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.47	0.50
2:I:556:GLY:HA2	2:I:659:GLN:O	2.12	0.50
3:J:205:LEU:HD23	3:J:217:LEU:HG	1.94	0.50
3:J:516:ASP:N	3:J:516:ASP:OD1	2.44	0.50
1:A:114:ASP:N	1:A:114:ASP:OD1	2.44	0.50
3:D:114:ILE:HD13	3:D:304:ASP:CG	2.32	0.50
3:D:817:HIS:NE2	3:D:860:ARG:NH2	2.59	0.50
3:D:905:ARG:NH1	4:E:10:VAL:HG11	2.27	0.50
1:H:78:ILE:O	1:H:82:LEU:HG	2.12	0.50
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.93	0.50
3:J:77:ARG:HB3	3:J:80:HIS:CE1	2.47	0.50
3:J:1246:VAL:HG12	3:J:1248:ILE:HG13	1.92	0.50
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.12	0.50
1:B:16:ILE:HG12	1:B:26:VAL:CG1	2.41	0.50
2:C:18:ARG:NH1	2:C:621:SER:O	2.45	0.50
2:C:209:ILE:O	2:C:213:LEU:HG	2.12	0.50
2:C:1149:TYR:HE2	2:C:1180:MET:SD	2.35	0.50
2:C:1328:LYS:O	2:C:1332:SER:N	2.45	0.50
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1371:ARG:CZ	3:D:1371:ARG:HB3	2.42	0.50
5:L:166:VAL:O	5:L:167:ASP:HB2	2.12	0.50
5:L:289:LYS:HE3	5:L:293:GLU:HG2	1.93	0.50
1:A:76:GLU:N	1:A:76:GLU:OE2	2.45	0.50
1:A:177:TYR:O	1:A:178:SER:HB2	2.11	0.50
2:C:566:GLY:H	2:C:569:ILE:CG1	2.23	0.50
2:C:705:GLU:H	2:C:705:GLU:CD	2.14	0.50
3:D:847:ASP:OD1	3:D:847:ASP:N	2.33	0.50
3:D:1183:SER:OG	3:D:1185:PRO:HD3	2.12	0.50
3:D:1347:LEU:O	3:D:1348:LYS:C	2.50	0.50
3:D:1347:LEU:HG	3:D:1357:ILE:HG23	1.93	0.50
1:G:99:ILE:HA	1:G:144:ILE:O	2.12	0.50
3:J:349:TYR:CD1	3:J:472:LEU:HD11	2.47	0.50
3:J:481:ARG:O	3:J:485:MET:HB2	2.12	0.50
3:J:800:LEU:O	3:J:803:VAL:HG12	2.12	0.50
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.38	0.50
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.93	0.49
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.94	0.49
2:C:1103:VAL:HG22	2:C:1111:GLN:NE2	2.27	0.49
5:F:281:ARG:HA	5:F:284:GLU:OE1	2.11	0.49
2:I:521:LEU:O	2:I:525:THR:N	2.40	0.49
2:I:866:ASP:HA	2:I:872:TYR:CZ	2.46	0.49
3:J:244:VAL:HA	3:J:269:TYR:OH	2.11	0.49
5:L:265:GLN:O	5:L:269:LEU:HG	2.12	0.49
1:A:318:LEU:HD11	5:F:600:HIS:NE2	2.28	0.49
2:C:496:LYS:HD2	2:C:496:LYS:C	2.32	0.49
2:C:1151:LEU:CD1	2:C:1198:LEU:HD23	2.41	0.49
2:C:1197:GLU:O	2:C:1200:LYS:HB2	2.11	0.49
2:C:1253:LEU:HD13	2:C:1253:LEU:C	2.32	0.49
3:D:93:THR:HG22	3:D:94:GLN:H	1.77	0.49
3:D:712:GLN:H	3:D:712:GLN:CD	2.15	0.49
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.43	0.49
2:I:23:ASP:OD1	2:I:23:ASP:N	2.44	0.49
2:I:358:ASP:OD1	2:I:360:LEU:HB3	2.12	0.49
2:I:1199:LEU:HD13	2:I:1206:THR:HA	1.94	0.49
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.94	0.49
3:J:491:LEU:HD22	3:J:496:GLY:O	2.12	0.49
5:L:407:GLU:HG3	5:L:442:SER:OG	2.12	0.49
5:L:572:THR:O	5:L:576:VAL:HG23	2.12	0.49
1:A:102:LEU:HB2	1:A:115:ILE:HG23	1.94	0.49
1:B:149:GLY:HA3	1:B:177:TYR:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:490:GLN:HG3	5:F:472:GLN:OE1	2.11	0.49
3:D:870:ASP:O	3:D:874:GLU:HG2	2.12	0.49
3:D:1159:ILE:CA	3:D:1206:ARG:HB3	2.41	0.49
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.42	0.49
2:I:794:LEU:CD2	2:I:796:LEU:HD11	2.43	0.49
3:J:804:ALA:O	3:J:805:GLN:C	2.51	0.49
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.13	0.49
1:A:29:GLU:CB	1:A:30:PRO:HD3	2.38	0.49
1:A:75:GLN:C	2:C:729:ALA:HB2	2.33	0.49
2:C:799:ASN:C	2:C:799:ASN:ND2	2.65	0.49
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.76	0.49
3:D:514:THR:OG1	3:D:594:GLN:O	2.30	0.49
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.12	0.49
3:D:1333:THR:O	3:D:1336:ALA:N	2.46	0.49
5:F:276:MET:O	5:F:280:VAL:HG23	2.12	0.49
2:I:1070:HIS:CD2	2:I:1111:GLN:HA	2.47	0.49
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	2.13	0.49
3:J:642:ASP:HA	3:J:764:ARG:HH21	1.75	0.49
3:J:903:LEU:HD23	3:J:905:ARG:HD3	1.93	0.49
5:L:248:GLU:HA	5:L:251:LYS:HE3	1.95	0.49
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.94	0.49
5:L:606:VAL:HG22	5:L:607:LEU:HD12	1.95	0.49
2:C:446:ASP:OD1	2:C:547:VAL:HG12	2.11	0.49
2:C:615:VAL:HG22	2:C:650:VAL:HA	1.94	0.49
3:D:19:ALA:CB	3:D:1373:ARG:HH22	2.26	0.49
3:D:291:ILE:O	3:D:292:VAL:C	2.47	0.49
3:D:1154:ALA:N	3:D:1214:PRO:O	2.34	0.49
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.47	0.49
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.95	0.49
1:H:73:GLY:HA2	1:H:134:THR:CG2	2.40	0.49
3:J:597:GLY:O	3:J:601:ILE:HB	2.12	0.49
3:J:844:THR:HB	3:J:860:ARG:O	2.12	0.49
2:C:516:ASP:OD1	2:C:517:GLN:N	2.44	0.49
2:C:801:ARG:O	2:C:1095:ASP:HB2	2.12	0.49
2:C:896:THR:OG1	2:C:899:GLU:HG3	2.11	0.49
3:D:367:GLY:N	3:D:448:GLN:O	2.42	0.49
5:F:314:THR:O	5:F:318:ALA:HB3	2.12	0.49
1:G:166:ARG:O	1:G:167:PRO:C	2.51	0.49
1:H:47:LEU:HD13	1:H:183:ILE:HG21	1.93	0.49
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.94	0.49
2:I:1132:LEU:HB3	2:I:1177:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:545:HIS:NE2	3:J:719:PHE:HE1	2.11	0.49
2:C:98:VAL:O	2:C:121:GLU:HA	2.13	0.49
2:C:518:ASN:O	2:C:519:ASN:HB2	2.12	0.49
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.12	0.49
2:C:1136:GLN:O	2:C:1137:GLU:HB3	2.11	0.49
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.95	0.49
1:G:23:HIS:ND1	1:G:205:MET:O	2.45	0.49
1:G:228:LEU:HD21	1:H:224:LEU:HD23	1.94	0.49
1:G:228:LEU:O	1:G:231:PHE:HD2	1.95	0.49
2:I:658:GLN:NE2	2:I:1186:VAL:HG23	2.27	0.49
2:I:807:TRP:HB2	2:I:1097:VAL:HG11	1.95	0.49
5:L:161:LEU:C	5:L:262:VAL:HG23	2.33	0.49
5:L:601:PRO:HB3	5:L:608:ARG:NH2	2.28	0.49
1:A:46:ILE:HD11	1:B:38:THR:HG21	1.95	0.49
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.95	0.49
3:D:227:PHE:O	3:D:230:SER:HB3	2.12	0.49
5:F:340:ALA:HA	5:F:343:LYS:NZ	2.28	0.49
1:H:19:VAL:HB	1:H:23:HIS:HD2	1.77	0.49
1:H:133:LEU:HD12	1:H:133:LEU:HA	1.64	0.49
2:I:1130:ALA:O	2:I:1134:GLN:N	2.46	0.49
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.13	0.49
3:J:85:CYS:HB3	3:J:88:CYS:O	2.11	0.49
3:J:454:CYS:SG	3:J:461:PHE:CZ	3.06	0.49
3:J:1165:PHE:HD2	3:J:1173:ARG:CD	2.26	0.49
3:J:1184:ASP:O	3:J:1186:TYR:N	2.46	0.49
4:K:59:ILE:HD12	4:K:64:LEU:HD21	1.95	0.49
5:L:289:LYS:HA	5:L:293:GLU:OE1	2.13	0.49
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.95	0.49
2:C:191:LYS:O	2:C:192:ASP:HB2	2.13	0.49
2:C:478:ARG:HG2	2:C:492:MET:HG2	1.95	0.49
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.43	0.49
2:C:1284:ALA:CB	3:D:1356:LEU:HD22	2.41	0.49
3:D:1283:SER:O	3:D:1286:LYS:N	2.45	0.49
1:G:75:GLN:HA	2:I:729:ALA:H	1.78	0.49
1:G:160:HIS:CG	1:G:161:SER:N	2.80	0.49
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.95	0.49
1:H:60:GLU:CG	1:H:143:ARG:HB2	2.42	0.49
2:I:20:GLN:HG2	2:I:1156:ARG:NH2	2.27	0.49
2:I:90:VAL:HG12	2:I:91:THR:H	1.77	0.49
2:I:175:ARG:NH1	2:I:200:ARG:HH12	2.11	0.49
3:J:334:LYS:HB3	5:L:516:ASP:OD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.16	0.49
5:L:148:TYR:HE1	5:L:158:LEU:HD21	1.77	0.49
5:L:261:LEU:H	5:L:261:LEU:HD12	1.78	0.49
5:L:603:ARG:NH1	5:L:603:ARG:HA	2.27	0.49
1:A:321:TRP:HA	1:A:322:PRO:HA	1.64	0.49
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.94	0.49
2:C:959:ASP:O	2:C:963:GLU:HG2	2.12	0.49
2:C:1212:LEU:HD22	2:C:1225:VAL:CG2	2.41	0.49
3:D:843:VAL:HG11	3:D:897:HIS:O	2.12	0.49
1:H:64:VAL:HG12	1:H:65:LEU:H	1.77	0.49
2:I:139:ASN:O	2:I:141:THR:HG23	2.12	0.49
2:I:158:ASP:CG	2:I:159:SER:H	2.14	0.49
2:I:674:ASP:OD1	2:I:1110:GLY:N	2.25	0.49
2:I:1219:GLU:OE2	3:J:538:ARG:NH1	2.31	0.49
2:I:1220:GLN:HG2	2:I:1221:PHE:H	1.77	0.49
3:J:322:ARG:HB2	3:J:322:ARG:NH1	2.27	0.49
5:L:230:VAL:O	5:L:234:THR:HG23	2.13	0.49
1:A:262:LEU:HD21	1:A:306:VAL:HG11	1.95	0.48
2:C:90:VAL:HG12	2:C:91:THR:N	2.27	0.48
2:C:866:ASP:HA	2:C:872:TYR:CZ	2.48	0.48
2:C:1238:LEU:H	2:C:1238:LEU:CD1	2.16	0.48
2:C:1333:LEU:HD21	3:D:327:LEU:HB2	1.95	0.48
3:D:825:VAL:C	3:D:826:ILE:HG13	2.33	0.48
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.28	0.48
1:G:64:VAL:HG12	1:G:66:HIS:H	1.78	0.48
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.95	0.48
2:I:367:TYR:CE2	2:I:376:PRO:HA	2.48	0.48
2:I:745:GLU:H	2:I:1017:GLN:HG3	1.78	0.48
3:J:848:VAL:CG2	3:J:858:VAL:HG13	2.42	0.48
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.94	0.48
2:C:4:SER:HB3	2:C:7:GLU:OE2	2.14	0.48
2:C:1079:ILE:O	2:C:1079:ILE:HG23	2.13	0.48
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.34	0.48
3:D:198:CYS:O	3:D:202:ARG:HG3	2.12	0.48
3:D:318:GLY:O	3:D:320:ASN:N	2.46	0.48
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.96	0.48
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.29	0.48
1:G:67:GLU:HG3	1:G:171:LEU:HG	1.94	0.48
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.94	0.48
1:H:112:ALA:HB2	1:H:128:HIS:HB3	1.94	0.48
2:I:15:PHE:CE1	2:I:1151:LEU:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:143:ARG:HH21	2:I:512:SER:C	2.15	0.48
3:J:79:LYS:HG3	3:J:80:HIS:N	2.28	0.48
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.95	0.48
5:L:299:LYS:O	5:L:303:ILE:HG12	2.13	0.48
5:L:555:GLU:OE2	5:L:597:LYS:NZ	2.39	0.48
1:A:283:GLN:O	1:A:315:GLY:HA2	2.14	0.48
2:C:139:ASN:O	2:C:141:THR:N	2.46	0.48
2:C:185:ASP:O	2:C:196:VAL:HA	2.14	0.48
2:C:285:ILE:HD11	2:C:287:VAL:HG12	1.95	0.48
2:C:557:ARG:NH2	2:C:608:ALA:HA	2.28	0.48
2:C:1283:ALA:HB1	3:D:479:GLU:OE2	2.13	0.48
4:E:53:GLU:OE1	4:E:59:ILE:HG13	2.14	0.48
5:F:532:LEU:H	5:F:532:LEU:HD12	1.79	0.48
1:G:91:ARG:HG3	1:G:122:GLU:HB3	1.95	0.48
1:G:105:SER:HB2	1:G:138:ALA:O	2.12	0.48
1:H:179:PRO:HA	1:H:208:ASN:HD21	1.78	0.48
2:I:137:VAL:HA	2:I:141:THR:O	2.13	0.48
2:I:786:GLY:N	2:I:789:THR:OG1	2.46	0.48
2:I:801:ARG:HD3	2:I:1094:VAL:HA	1.96	0.48
3:J:45:ASN:O	3:J:46:TYR:CD2	2.66	0.48
3:J:293:ARG:NH1	5:L:104:GLU:OE2	2.46	0.48
3:J:395:LYS:O	3:J:398:LYS:HB3	2.14	0.48
3:J:613:GLY:O	3:J:617:THR:OG1	2.27	0.48
5:L:456:MET:O	5:L:459:THR:HB	2.13	0.48
1:B:152:TYR:HE1	1:B:176:CYS:HB3	1.79	0.48
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.14	0.48
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.25	0.48
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.34	0.48
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.77	0.48
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.94	0.48
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.95	0.48
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.94	0.48
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.28	0.48
1:B:211:ILE:HD11	1:B:215:GLU:OE2	2.13	0.48
2:C:20:GLN:HG3	2:C:20:GLN:O	2.14	0.48
2:C:325:LEU:O	2:C:328:SER:OG	2.31	0.48
2:I:132:ASP:OD1	2:I:132:ASP:N	2.38	0.48
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.48	0.48
2:I:629:PHE:CE2	2:I:634:VAL:HG11	2.49	0.48
2:I:658:GLN:NE2	2:I:1186:VAL:H	2.11	0.48
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:512:GLY:C	5:L:514:ASP:N	2.63	0.48
1:B:206:GLU:OE2	3:D:531:LYS:HE2	2.14	0.48
2:C:40:GLU:O	2:C:73:TYR:OH	2.32	0.48
2:C:42:ASP:OD2	2:C:44:GLU:C	2.51	0.48
2:C:685:MET:SD	2:C:1073:LYS:HG3	2.54	0.48
3:D:9:LYS:HE2	3:D:9:LYS:HB3	1.66	0.48
3:D:36:GLY:HA3	3:D:61:ILE:HG23	1.95	0.48
5:F:483:LEU:HD12	5:F:483:LEU:N	2.22	0.48
5:F:583:THR:HG22	5:F:584:ARG:HG2	1.95	0.48
1:G:153:VAL:N	1:G:175:ALA:O	2.33	0.48
2:I:800:MET:O	2:I:1229:TYR:HA	2.13	0.48
3:J:337:ARG:HH11	3:J:1327:GLU:HA	1.79	0.48
3:J:681:LYS:O	3:J:684:ASP:HB2	2.14	0.48
5:L:276:MET:O	5:L:280:VAL:HG23	2.14	0.48
2:C:524:ILE:HD12	2:C:712:SER:HB2	1.94	0.48
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.14	0.48
3:D:34:SER:HG	3:D:104:HIS:CG	2.29	0.48
3:D:278:ARG:NH1	3:D:295:GLU:OE1	2.39	0.48
3:D:490:ILE:HG12	3:D:491:LEU:HG	1.95	0.48
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.13	0.48
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.14	0.48
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.95	0.48
1:G:190:ALA:HB2	1:G:200:LYS:CB	2.32	0.48
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.78	0.48
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.13	0.48
3:J:515:ARG:HH21	3:J:717:VAL:HG23	1.79	0.48
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.96	0.48
3:J:708:ASN:OD1	3:J:708:ASN:N	2.46	0.48
3:J:797:THR:O	3:J:801:VAL:HG13	2.12	0.48
2:C:10:ARG:CZ	2:C:697:LYS:HD3	2.44	0.48
2:C:886:LYS:O	2:C:916:SER:N	2.47	0.48
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.96	0.48
3:D:244:VAL:HG23	3:D:244:VAL:O	2.14	0.48
3:D:709:ARG:C	3:D:711:GLY:N	2.67	0.48
5:F:114:GLU:HG3	5:F:115:GLY:H	1.78	0.48
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.96	0.48
5:L:394:TYR:OH	5:L:436:ARG:HD2	2.12	0.48
1:A:61:ILE:HG23	1:A:142:MET:CB	2.39	0.48
1:A:166:ARG:O	1:A:166:ARG:HD2	2.14	0.48
2:C:42:ASP:CG	2:C:44:GLU:HG2	2.33	0.48
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:TRP:O	3:D:580:TRP:CG	2.67	0.48
5:F:489:MET:O	5:F:491:GLU:HB3	2.14	0.48
1:G:10:LYS:HE2	1:H:229:GLU:OE1	2.14	0.48
1:G:64:VAL:CG1	1:G:69:SER:HB2	2.44	0.48
2:I:195:PHE:CD1	2:I:205:PRO:HA	2.49	0.48
2:I:685:MET:HA	2:I:688:GLN:HE21	1.78	0.48
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.49	0.48
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.96	0.48
5:L:137:TYR:CE2	5:L:273:MET:HG2	2.49	0.48
1:B:108:GLY:O	1:B:133:LEU:HB2	2.13	0.48
1:B:196:THR:HG23	3:D:443:GLU:CD	2.35	0.48
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.29	0.48
2:C:108:GLU:OE1	2:C:108:GLU:HA	2.13	0.48
2:C:805:MET:O	2:C:805:MET:HG3	2.14	0.48
3:D:706:VAL:HG12	3:D:715:LYS:CB	2.44	0.48
5:F:580:PHE:C	5:F:582:VAL:H	2.17	0.48
5:F:600:HIS:CG	5:F:601:PRO:HD2	2.48	0.48
2:I:496:LYS:HB3	2:I:497:PRO:HD3	1.96	0.48
2:I:1242:LYS:HD2	3:J:465:GLN:OE1	2.14	0.48
3:J:161:THR:HG22	3:J:164:GLN:CD	2.34	0.48
3:J:544:LEU:O	3:J:575:GLY:N	2.47	0.48
3:J:1265:THR:HG22	3:J:1277:GLY:HA2	1.96	0.48
5:L:157:ARG:NH2	5:L:159:SER:OG	2.47	0.48
5:L:343:LYS:HA	5:L:346:GLN:HB3	1.95	0.48
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.48	0.47
2:C:1176:LEU:HD23	2:C:1176:LEU:HA	1.38	0.47
2:C:1341:ASP:HB3	3:D:18:ASP:OD2	2.14	0.47
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.44	0.47
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.95	0.47
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.47	0.47
5:F:453:PRO:O	5:F:456:MET:HB2	2.14	0.47
2:I:4:SER:H	2:I:7:GLU:CD	2.17	0.47
2:I:169:LYS:O	2:I:170:VAL:HG22	2.14	0.47
2:I:213:LEU:HA	2:I:213:LEU:HD23	1.56	0.47
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.28	0.47
3:J:239:LEU:HA	3:J:239:LEU:HD23	1.60	0.47
3:J:742:GLY:O	3:J:762:ASN:HB3	2.14	0.47
5:L:598:LEU:O	5:L:604:SER:OG	2.31	0.47
2:C:4:SER:HB3	2:C:7:GLU:CD	2.34	0.47
2:C:41:GLN:NE2	2:C:73:TYR:O	2.46	0.47
2:C:123:TYR:HB3	5:F:472:GLN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.73	0.47
2:C:590:PRO:HG3	2:C:605:TYR:CE2	2.49	0.47
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.94	0.47
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.96	0.47
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.13	0.47
2:I:151:ARG:HE	2:I:445:ILE:HD11	1.78	0.47
2:I:379:GLU:CD	2:I:379:GLU:H	2.15	0.47
2:I:494:ASN:HD22	2:I:497:PRO:CD	2.28	0.47
2:I:658:GLN:O	2:I:660:VAL:N	2.47	0.47
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.95	0.47
3:J:598:LYS:N	3:J:728:SER:O	2.33	0.47
2:C:29:SER:O	2:C:30:ILE:C	2.52	0.47
2:C:619:ALA:HA	2:C:654:ASP:HB2	1.96	0.47
2:C:811:ASN:HA	2:C:815:SER:HB2	1.94	0.47
1:G:19:VAL:HG12	1:G:20:SER:N	2.27	0.47
2:I:367:TYR:HD1	2:I:384:LEU:HD22	1.78	0.47
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.96	0.47
2:I:1085:MET:CB	2:I:1093:PRO:HB3	2.43	0.47
3:J:1356:LEU:O	3:J:1366:HIS:CE1	2.67	0.47
5:L:515:GLU:HG2	5:L:516:ASP:N	2.29	0.47
1:B:101:THR:HG22	1:B:116:THR:HB	1.97	0.47
2:C:302:ILE:O	2:C:330:HIS:NE2	2.36	0.47
2:C:486:THR:HG23	2:C:487:LEU:H	1.79	0.47
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.96	0.47
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.73	0.47
2:I:517:GLN:CD	2:I:688:GLN:HA	2.34	0.47
2:I:785:ASP:HB3	2:I:789:THR:OG1	2.14	0.47
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.49	0.47
3:J:770:LEU:O	3:J:774:ILE:HG13	2.15	0.47
3:J:1226:VAL:O	3:J:1230:THR:HG22	2.14	0.47
2:C:129:LEU:HD23	2:C:129:LEU:HA	1.64	0.47
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.49	0.47
2:C:623:LEU:HA	2:C:630:VAL:HG23	1.96	0.47
2:C:681:MET:O	2:C:685:MET:HE2	2.15	0.47
2:C:821:ARG:HG3	2:C:825:GLU:OE1	2.15	0.47
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.96	0.47
1:G:97:GLU:HB3	1:G:147:GLN:HA	1.97	0.47
1:H:197:ASP:C	1:H:198:LEU:HD22	2.34	0.47
2:I:74:ARG:NH1	2:I:121:GLU:OE2	2.46	0.47
2:I:692:THR:OG1	2:I:693:LEU:N	2.47	0.47
2:I:720:ARG:HH21	2:I:736:VAL:HG11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.96	0.47
3:J:299:LEU:O	3:J:300:GLN:C	2.53	0.47
3:J:658:GLU:O	3:J:661:VAL:HG13	2.14	0.47
3:J:884:SER:OG	3:J:885:VAL:N	2.48	0.47
1:A:233:ASP:O	1:A:234:LEU:HD22	2.14	0.47
1:A:307:LEU:HA	1:A:307:LEU:HD23	1.53	0.47
2:C:250:THR:HA	2:C:268:ARG:HA	1.97	0.47
2:C:650:VAL:HG23	2:C:650:VAL:O	2.14	0.47
2:C:1142:ARG:CD	2:C:1161:LEU:HD11	2.31	0.47
2:C:1252:SER:HB3	2:C:1255:THR:O	2.14	0.47
3:D:40:LYS:HB2	3:D:54:ASP:O	2.14	0.47
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.62	0.47
3:D:739:GLN:OE1	3:D:744:ARG:NE	2.48	0.47
3:D:744:ARG:O	3:D:744:ARG:HG3	2.15	0.47
3:D:1146:GLU:HA	3:D:1146:GLU:OE2	2.15	0.47
3:D:1221:LEU:O	3:D:1221:LEU:HD22	2.15	0.47
5:F:112:THR:OG1	5:F:114:GLU:HG3	2.14	0.47
2:I:13:LYS:O	2:I:1183:ALA:N	2.31	0.47
2:I:197:ARG:NH1	2:I:201:ARG:O	2.45	0.47
2:I:557:ARG:NE	2:I:587:LEU:O	2.41	0.47
2:I:902:LEU:HD21	5:L:611:LEU:HG	1.95	0.47
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.97	0.47
3:J:1286:LYS:HD2	3:J:1290:ARG:HH21	1.78	0.47
1:A:246:LYS:HB2	1:A:248:GLU:OE2	2.15	0.47
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.50	0.47
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.29	0.47
2:C:1120:ALA:HB1	2:C:1198:LEU:HD13	1.96	0.47
3:D:35:PHE:CE1	3:D:101:ARG:HD3	2.50	0.47
3:D:238:ILE:HG23	3:D:238:ILE:HD12	1.67	0.47
3:D:273:ILE:O	3:D:274:ASN:C	2.52	0.47
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.96	0.47
3:D:648:GLU:OE2	3:D:649:LYS:HE2	2.14	0.47
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.14	0.47
3:D:1181:ASP:CB	3:J:202:ARG:HD3	2.45	0.47
5:F:163:THR:O	5:F:260:ARG:NH2	2.48	0.47
5:F:276:MET:O	5:F:279:ARG:HB2	2.14	0.47
5:F:372:ALA:O	5:F:376:LYS:HG3	2.14	0.47
5:F:513:ASP:C	5:F:515:GLU:H	2.17	0.47
1:G:37:HIS:HB3	1:H:45:ARG:NH1	2.30	0.47
2:I:242:VAL:HG21	2:I:245:ARG:NH1	2.30	0.47
2:I:344:GLY:O	2:I:346:TYR:CG	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.29	0.47
2:I:835:GLU:OE2	2:I:1051:LYS:HD3	2.14	0.47
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.29	0.47
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.97	0.47
3:J:895:CYS:O	3:J:898:CYS:N	2.43	0.47
5:L:390:ILE:HD11	5:L:432:THR:HG23	1.97	0.47
5:L:463:LEU:HD23	5:L:463:LEU:HA	1.68	0.47
5:L:489:MET:CE	5:L:493:LYS:HD2	2.44	0.47
5:L:603:ARG:HA	5:L:603:ARG:CZ	2.44	0.47
1:A:27:THR:HA	1:A:201:LEU:O	2.14	0.47
1:A:102:LEU:HD22	1:A:103:ASN:N	2.30	0.47
1:A:284:ARG:HG3	1:A:288:GLU:OE1	2.15	0.47
2:C:1023:HIS:O	2:C:1027:LYS:HG2	2.14	0.47
3:D:46:TYR:CD1	5:F:452:ILE:HG22	2.50	0.47
5:F:379:MET:HG2	5:F:416:VAL:CG2	2.45	0.47
5:F:548:LEU:O	5:F:556:ALA:HB2	2.14	0.47
1:G:66:HIS:HE1	2:I:874:GLY:HA2	1.76	0.47
2:I:221:LEU:HD23	2:I:221:LEU:HA	1.63	0.47
2:I:854:ILE:O	2:I:857:VAL:HG22	2.15	0.47
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.35	0.47
3:J:128:LEU:HA	3:J:192:MET:HE1	1.96	0.47
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.95	0.47
3:J:495:ASN:O	3:J:497:GLU:N	2.48	0.47
3:J:647:PRO:HG3	3:J:697:MET:CB	2.40	0.47
3:J:1280:VAL:HG11	3:J:1304:ARG:CZ	2.44	0.47
1:A:28:LEU:CD1	1:A:28:LEU:N	2.72	0.47
1:B:109:PRO:HA	1:B:132:HIS:HA	1.97	0.47
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.50	0.47
3:D:279:LEU:HD23	3:D:279:LEU:C	2.35	0.47
3:D:810:THR:HG21	3:D:893:GLY:HA3	1.97	0.47
2:I:1309:VAL:HA	3:J:383:GLY:HA3	1.97	0.47
3:J:287:ALA:HB1	3:J:288:PRO:HD2	1.95	0.47
3:J:316:ILE:HA	3:J:323:PRO:HA	1.96	0.47
3:J:915:ILE:O	3:J:919:ALA:N	2.45	0.47
2:C:53:PHE:CD1	2:C:468:LEU:HD11	2.49	0.47
2:C:496:LYS:HE3	2:C:497:PRO:HD3	1.97	0.47
2:C:696:ASP:O	2:C:697:LYS:HB3	2.15	0.47
3:D:37:GLU:O	3:D:61:ILE:HD11	2.14	0.47
3:D:109:SER:O	3:D:110:PRO:C	2.52	0.47
3:D:238:ILE:HA	3:D:238:ILE:HD13	1.38	0.47
1:H:18:GLN:NE2	1:H:20:SER:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:62:TYR:O	2:I:64:GLY:N	2.47	0.47
2:I:81:ASP:O	2:I:85:CYS:HB2	2.15	0.47
2:I:185:ASP:HB2	2:I:197:ARG:O	2.15	0.47
2:I:753:LEU:HD21	2:I:784:ALA:CB	2.45	0.47
5:L:306:PHE:HE1	5:L:315:TRP:CH2	2.33	0.47
1:A:12:ARG:NH1	1:A:13:LEU:HD21	2.29	0.46
1:A:316:MET:CB	5:F:600:HIS:CE1	2.98	0.46
2:C:28:LEU:HA	2:C:28:LEU:HD23	1.40	0.46
2:C:356:THR:HG21	2:C:362:ALA:HA	1.97	0.46
3:D:768:ASN:OD1	3:D:771:GLN:OE1	2.33	0.46
3:D:1237:VAL:CG1	3:D:1253:ILE:HD13	2.46	0.46
2:I:44:GLU:HA	2:I:54:ARG:NH1	2.30	0.46
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.97	0.46
2:I:1059:ARG:O	2:I:1234:LYS:NZ	2.43	0.46
3:J:850:LYS:HB3	3:J:851:PRO:HD2	1.98	0.46
1:B:104:LYS:HG2	1:B:114:ASP:CG	2.36	0.46
1:B:188:GLU:O	1:B:200:LYS:N	2.29	0.46
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.50	0.46
2:C:169:LYS:O	2:C:170:VAL:HG22	2.15	0.46
2:C:239:MET:O	2:C:284:LEU:HD12	2.15	0.46
2:C:300:ASP:OD1	2:C:313:ALA:N	2.48	0.46
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.98	0.46
2:C:484:LEU:HD12	2:C:485:ASP:H	1.80	0.46
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.97	0.46
3:D:112:ALA:HA	3:D:238:ILE:CD1	2.46	0.46
3:D:318:GLY:C	3:D:320:ASN:H	2.18	0.46
3:D:519:ASN:OD1	3:D:709:ARG:NH1	2.48	0.46
1:H:110:VAL:HG23	1:H:131:CYS:O	2.15	0.46
1:H:155:ALA:N	1:H:174:ASP:OD1	2.43	0.46
2:I:409:LEU:HA	2:I:409:LEU:HD23	1.57	0.46
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.96	0.46
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.16	0.46
3:J:654:ILE:O	3:J:658:GLU:HB2	2.15	0.46
3:J:804:ALA:O	3:J:806:ASP:N	2.48	0.46
3:J:1234:VAL:HG23	3:J:1235:ASN:N	2.30	0.46
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.80	0.46
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.96	0.46
1:A:7:GLU:HG3	1:B:150:ARG:NE	2.26	0.46
1:A:14:VAL:HG22	1:A:15:ASP:N	2.26	0.46
1:A:16:ILE:CG2	1:A:26:VAL:HG12	2.37	0.46
1:A:50:SER:HB2	1:B:8:PHE:HZ	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:HB3	1:A:211:ILE:HB	1.96	0.46
1:A:255:ARG:HB2	1:A:278:ILE:HD12	1.98	0.46
2:C:1009:ASN:O	2:C:1012:GLU:HB3	2.16	0.46
2:C:1136:GLN:NE2	2:C:1140:LYS:NZ	2.64	0.46
1:H:220:ALA:HA	1:H:223:ILE:HD12	1.97	0.46
2:I:517:GLN:O	2:I:517:GLN:HG2	2.14	0.46
2:I:617:ALA:N	2:I:652:TYR:O	2.30	0.46
2:I:657:THR:HG23	2:I:658:GLN:HG3	1.97	0.46
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.97	0.46
2:I:891:GLY:C	2:I:892:GLU:HG3	2.35	0.46
3:J:117:LEU:HD12	3:J:117:LEU:HA	1.44	0.46
3:J:521:LYS:HE3	3:J:541:LEU:O	2.15	0.46
3:J:647:PRO:CD	3:J:697:MET:HB3	2.45	0.46
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.30	0.46
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.80	0.46
1:A:77:ASP:O	1:A:80:GLU:N	2.48	0.46
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.31	0.46
2:C:128:PRO:HG2	2:C:506:PHE:CD1	2.50	0.46
2:C:705:GLU:HB2	2:C:794:LEU:N	2.27	0.46
2:C:953:LEU:HA	2:C:953:LEU:HD12	1.52	0.46
3:D:45:ASN:O	3:D:46:TYR:CB	2.63	0.46
1:G:98:VAL:HG22	1:G:99:ILE:H	1.79	0.46
1:G:166:ARG:N	1:G:167:PRO:HD2	2.30	0.46
2:I:607:SER:OG	2:I:609:ILE:HG13	2.15	0.46
2:I:653:MET:HG2	2:I:654:ASP:N	2.30	0.46
2:I:830:THR:HG22	2:I:1058:ARG:O	2.15	0.46
2:I:1131:MET:CE	2:I:1141:LEU:HD12	2.46	0.46
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.14	0.46
3:J:746:LEU:CD2	3:J:758:PRO:HG3	2.45	0.46
5:L:296:LYS:HD3	5:L:296:LYS:HA	1.71	0.46
1:B:118:ASP:HB2	1:B:121:VAL:CG2	2.46	0.46
2:C:131:THR:HG21	2:C:135:THR:OG1	2.15	0.46
2:C:247:ARG:HB2	2:C:274:ILE:CD1	2.45	0.46
2:C:262:TYR:HE1	2:C:280:ASP:OD2	1.98	0.46
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.98	0.46
3:D:721:SER:HA	3:D:724:MET:CE	2.45	0.46
5:F:253:SER:O	5:F:257:LYS:N	2.47	0.46
5:F:466:ILE:HG22	5:F:470:MET:HG3	1.97	0.46
1:H:22:THR:OG1	1:H:207:THR:O	2.33	0.46
3:J:914:ALA:O	3:J:918:ILE:HG23	2.15	0.46
5:L:316:PHE:O	5:L:320:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:O	1:A:180:VAL:HG21	2.15	0.46
1:A:166:ARG:N	1:A:167:PRO:HD2	2.30	0.46
2:C:4:SER:O	2:C:7:GLU:HB2	2.16	0.46
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.98	0.46
2:C:704:MET:O	2:C:707:ALA:N	2.48	0.46
2:C:911:SER:OG	2:C:913:VAL:HG12	2.16	0.46
2:C:1164:PHE:O	2:C:1168:GLU:HB2	2.14	0.46
3:D:377:PHE:O	3:D:378:LYS:C	2.54	0.46
5:F:396:ASN:C	5:F:398:GLY:H	2.19	0.46
1:H:44:ARG:HG2	1:H:183:ILE:HD13	1.97	0.46
2:I:27:LEU:HG	2:I:711:ASP:OD2	2.16	0.46
2:I:183:TRP:HB2	2:I:199:ASP:CA	2.39	0.46
2:I:571:LEU:HA	2:I:571:LEU:HD23	1.56	0.46
2:I:796:LEU:H	2:I:796:LEU:HD12	1.81	0.46
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.50	0.46
3:J:16:GLU:HB3	3:J:17:PHE:HD2	1.79	0.46
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.31	0.46
3:J:282:LEU:HD23	3:J:282:LEU:HA	1.71	0.46
3:J:905:ARG:NH1	3:J:910:ASN:ND2	2.59	0.46
5:L:315:TRP:O	5:L:319:ALA:HB3	2.16	0.46
1:A:152:TYR:CE1	2:C:824:GLN:HG2	2.51	0.46
2:C:171:LEU:HD23	2:C:171:LEU:HA	1.68	0.46
2:C:564:PRO:HD2	2:C:572:ILE:HB	1.98	0.46
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.50	0.46
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.48	0.46
3:D:614:LEU:O	3:D:617:THR:N	2.49	0.46
3:D:620:PHE:O	3:D:624:ILE:HG13	2.16	0.46
3:D:812:ASP:HB2	3:D:911:LYS:NZ	2.30	0.46
3:D:1167:LYS:HZ3	3:D:1170:LYS:HB2	1.79	0.46
3:D:1181:ASP:HB2	3:J:202:ARG:HD3	1.97	0.46
3:D:1251:LYS:O	3:D:1254:GLU:N	2.49	0.46
1:G:58:GLU:OE1	1:G:145:LYS:HD2	2.16	0.46
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.98	0.46
2:I:468:LEU:HD23	2:I:468:LEU:HA	1.40	0.46
2:I:593:LYS:HA	2:I:652:TYR:CD2	2.51	0.46
2:I:796:LEU:O	2:I:1233:LEU:HD12	2.16	0.46
2:I:1238:LEU:HD12	2:I:1238:LEU:N	2.28	0.46
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.96	0.46
3:J:377:PHE:O	3:J:378:LYS:C	2.54	0.46
3:J:544:LEU:HD12	3:J:544:LEU:HA	1.69	0.46
3:J:885:VAL:O	3:J:1258:ARG:HD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.97	0.46
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.85	0.46
2:C:1332:SER:OG	3:D:327:LEU:HD13	2.15	0.46
3:D:37:GLU:HA	3:D:104:HIS:CE1	2.50	0.46
3:D:722:ILE:HG21	3:D:722:ILE:HD13	1.46	0.46
3:D:846:GLU:HA	3:D:860:ARG:CD	2.45	0.46
2:I:395:TYR:HE2	2:I:397:LEU:HD11	1.81	0.46
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.51	0.46
2:I:1101:LEU:HD23	2:I:1101:LEU:HA	1.65	0.46
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.16	0.46
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.98	0.46
5:L:515:GLU:HG2	5:L:516:ASP:H	1.81	0.46
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.58	0.46
1:A:90:VAL:HG22	1:A:91:ARG:N	2.30	0.46
1:A:322:PRO:HA	1:A:323:PRO:HD3	1.77	0.46
2:C:34:SER:OG	2:C:457:GLY:N	2.44	0.46
2:C:958:LYS:O	2:C:961:SER:OG	2.30	0.46
3:D:1240:VAL:O	3:D:1244:GLN:HG2	2.16	0.46
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.81	0.46
5:F:384:LEU:HD22	5:F:409:ASN:ND2	2.31	0.46
5:F:524:GLU:O	5:F:524:GLU:HG3	2.16	0.46
1:G:29:GLU:O	1:G:199:ASP:O	2.34	0.46
1:H:88:LEU:HA	1:H:88:LEU:HD12	1.72	0.46
2:I:367:TYR:CE1	2:I:371:ARG:HD2	2.51	0.46
2:I:756:TYR:HD1	2:I:756:TYR:H	1.61	0.46
2:I:810:TYR:CE2	3:J:359:PRO:HG2	2.50	0.46
3:J:112:ALA:HA	3:J:238:ILE:CD1	2.46	0.46
3:J:474:LEU:HA	3:J:477:GLN:HG3	1.97	0.46
3:J:740:LEU:HD12	3:J:740:LEU:HA	1.54	0.46
3:J:827:GLU:O	3:J:829:GLY:N	2.34	0.46
5:L:139:GLU:CG	5:L:351:THR:HA	2.44	0.46
1:A:60:GLU:OE1	1:A:143:ARG:NE	2.38	0.46
1:A:181:GLU:HB3	1:A:206:GLU:HG3	1.98	0.46
2:C:525:THR:HG21	2:C:687:ARG:CD	2.42	0.46
3:D:211:GLU:OE2	3:D:214:ARG:NH1	2.48	0.46
3:D:362:ARG:HA	3:D:626:TYR:OH	2.15	0.46
3:D:441:LEU:HA	3:D:441:LEU:HD13	1.63	0.46
2:I:421:SER:O	2:I:424:ASP:N	2.47	0.46
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.81	0.46
3:J:865:HIS:ND1	3:J:867:GLN:HB2	2.31	0.46
5:L:119:ILE:O	5:L:122:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLN:HG3	1:A:76:GLU:OE2	2.16	0.45
2:C:864:LYS:HZ3	2:C:881:ASP:CG	2.20	0.45
2:C:896:THR:HB	2:C:897:PRO:HD2	1.96	0.45
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.98	0.45
3:D:859:PRO:HG2	3:D:862:THR:HG21	1.98	0.45
4:E:40:PRO:O	4:E:52:ARG:NH2	2.49	0.45
1:G:187:VAL:HG22	1:G:201:LEU:HD13	1.98	0.45
1:H:99:ILE:HA	1:H:144:ILE:O	2.17	0.45
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.97	0.45
2:I:886:LYS:O	2:I:916:SER:N	2.48	0.45
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	1.98	0.45
3:J:147:ILE:HD11	3:J:179:LYS:NZ	2.31	0.45
3:J:165:TYR:CE2	3:J:169:LEU:HD12	2.51	0.45
3:J:886:VAL:HA	3:J:1258:ARG:HB2	1.98	0.45
3:J:899:TYR:O	3:J:1251:LYS:HD3	2.16	0.45
3:J:1297:LYS:NZ	3:J:1299:GLY:HA3	2.30	0.45
4:K:26:ARG:NH2	4:K:36:ASP:O	2.49	0.45
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.63	0.45
5:L:532:LEU:H	5:L:532:LEU:HD12	1.81	0.45
2:C:120:GLN:CG	2:C:121:GLU:HG3	2.36	0.45
2:C:273:HIS:HA	2:C:276:GLN:OE1	2.15	0.45
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.75	0.45
2:C:883:LEU:HA	2:C:883:LEU:HD23	1.73	0.45
3:D:796:LEU:HG	3:D:800:LEU:HD22	1.99	0.45
1:H:149:GLY:HA3	1:H:177:TYR:CD2	2.51	0.45
2:I:97:ARG:HB3	2:I:121:GLU:CB	2.46	0.45
2:I:598:VAL:HG13	2:I:628:HIS:CE1	2.51	0.45
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.50	0.45
2:I:1012:GLU:HG3	2:I:1016:GLU:OE2	2.16	0.45
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.98	0.45
3:J:349:TYR:CE1	3:J:472:LEU:HD11	2.51	0.45
3:J:381:ILE:HG21	3:J:401:VAL:HG11	1.97	0.45
5:L:297:MET:HG2	5:L:298:PRO:N	2.31	0.45
1:A:261:GLU:OE2	2:C:859:GLU:HB2	2.17	0.45
2:C:74:ARG:O	2:C:96:LEU:HD12	2.16	0.45
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.52	0.45
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.40	0.45
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.98	0.45
3:D:112:ALA:HB3	3:D:300:GLN:NE2	2.31	0.45
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.97	0.45
3:D:689:ALA:O	3:D:692:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:875:ASN:OD1	3:D:875:ASN:N	2.49	0.45
3:D:1258:ARG:NH2	3:D:1281:GLU:OE1	2.48	0.45
2:I:504:GLU:OE2	2:I:508:SER:HB2	2.16	0.45
2:I:538:LEU:HA	2:I:542:ARG:NE	2.31	0.45
2:I:758:ARG:HH22	2:I:761:GLN:HE21	1.63	0.45
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.97	0.45
1:B:152:TYR:CE1	1:B:176:CYS:HB3	2.52	0.45
2:C:400:VAL:H	2:C:400:VAL:HG23	1.46	0.45
2:C:720:ARG:NH2	2:C:736:VAL:HG21	2.31	0.45
3:D:184:ALA:O	3:D:187:ALA:HB3	2.17	0.45
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.42	0.45
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.98	0.45
3:D:1356:LEU:HA	3:D:1356:LEU:HD23	1.40	0.45
1:G:152:TYR:CD2	2:I:824:GLN:HG2	2.52	0.45
1:G:226:GLU:CD	1:H:10:LYS:HE2	2.37	0.45
2:I:62:TYR:C	2:I:64:GLY:H	2.19	0.45
2:I:228:VAL:HG22	2:I:245:ARG:HE	1.80	0.45
2:I:397:LEU:HD12	2:I:397:LEU:H	1.81	0.45
2:I:798:GLN:OE1	2:I:828:PHE:HD1	1.99	0.45
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.58	0.45
2:I:1281:TYR:OH	3:J:431:ARG:O	2.33	0.45
3:J:1262:ARG:HD2	3:J:1279:GLN:HE22	1.81	0.45
5:L:143:TYR:OH	5:L:265:GLN:OE1	2.12	0.45
5:L:357:GLN:H	5:L:357:GLN:HG3	1.52	0.45
5:L:470:MET:HA	5:L:473:GLU:HB3	1.98	0.45
5:L:577:GLY:O	5:L:581:ASP:N	2.50	0.45
1:A:224:LEU:HD23	1:A:224:LEU:C	2.36	0.45
1:A:233:ASP:O	1:A:234:LEU:HD13	2.17	0.45
1:B:84:ASN:ND2	1:B:129:VAL:O	2.45	0.45
2:C:5:TYR:CZ	2:C:776:PRO:HB2	2.51	0.45
2:C:891:GLY:C	2:C:892:GLU:HG3	2.37	0.45
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.50	0.45
2:C:1160:ASP:CG	2:C:1161:LEU:N	2.67	0.45
3:D:127:LEU:HD12	3:D:127:LEU:HA	1.46	0.45
3:D:282:LEU:HA	3:D:282:LEU:HD23	1.52	0.45
3:D:1140:ARG:NH2	3:D:1144:LEU:HD21	2.31	0.45
1:H:60:GLU:OE2	1:H:143:ARG:NH1	2.50	0.45
1:H:105:SER:HB3	1:H:137:ASN:O	2.17	0.45
2:I:952:GLN:OE1	2:I:1036:ILE:HG23	2.16	0.45
3:J:585:LYS:HD3	3:J:585:LYS:HA	1.68	0.45
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:419:PHE:CD1	5:L:430:TYR:CD2	3.05	0.45
5:L:533:ASP:O	5:L:536:THR:N	2.49	0.45
1:A:197:ASP:O	1:A:198:LEU:HD23	2.17	0.45
2:C:5:TYR:HD1	2:C:8:LYS:HD3	1.82	0.45
2:C:388:LEU:HD23	2:C:388:LEU:HA	1.72	0.45
2:C:1035:LYS:O	2:C:1038:GLN:HG2	2.17	0.45
3:D:107:LEU:HD22	3:D:299:LEU:HD21	1.98	0.45
3:D:285:LEU:HD12	3:D:285:LEU:N	2.32	0.45
3:D:471:PRO:HG2	3:D:471:PRO:O	2.16	0.45
3:D:528:THR:HG22	3:D:532:GLU:CD	2.37	0.45
3:D:846:GLU:HA	3:D:860:ARG:HD3	1.97	0.45
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.16	0.45
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.81	0.45
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.17	0.45
1:G:154:PRO:HB3	2:I:1059:ARG:NH2	2.32	0.45
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.79	0.45
2:I:1068:GLY:HA3	2:I:1072:ASN:HD21	1.82	0.45
2:I:1212:LEU:O	2:I:1221:PHE:N	2.46	0.45
3:J:549:LYS:HE2	3:J:571:ASP:OD2	2.17	0.45
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.98	0.45
5:L:390:ILE:HG21	5:L:390:ILE:HD13	1.74	0.45
2:C:474:ALA:O	2:C:477:GLU:HB3	2.17	0.45
2:C:606:LEU:HD12	2:C:606:LEU:N	2.32	0.45
2:C:1161:LEU:HD12	2:C:1161:LEU:HA	1.26	0.45
3:D:24:LEU:HA	3:D:24:LEU:HD13	1.74	0.45
3:D:605:LEU:HA	3:D:605:LEU:HD23	1.77	0.45
3:D:819:GLY:O	3:D:1227:HIS:HE1	1.99	0.45
5:F:433:TRP:O	5:F:437:GLN:HB3	2.17	0.45
2:I:511:LEU:N	2:I:511:LEU:HD12	2.32	0.45
2:I:886:LYS:H	2:I:917:SER:HB3	1.82	0.45
2:I:967:LEU:HD12	2:I:967:LEU:HA	1.84	0.45
2:I:1077:SER:OG	2:I:1078:LYS:N	2.50	0.45
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.46	0.45
3:J:215:LYS:O	3:J:218:THR:HG22	2.17	0.45
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.99	0.45
1:B:9:LEU:HB3	1:B:32:GLU:HG2	1.99	0.45
2:C:22:LEU:HD22	2:C:22:LEU:HA	1.82	0.45
2:C:145:ILE:CG2	2:C:456:VAL:HG22	2.47	0.45
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.52	0.45
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.49	0.45
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:154:LEU:N	3:D:154:LEU:HD12	2.31	0.45
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.98	0.45
3:D:740:LEU:HD12	3:D:740:LEU:HA	1.47	0.45
3:D:796:LEU:HD12	3:D:796:LEU:HA	1.61	0.45
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.98	0.45
5:F:364:ARG:HA	5:F:367:ILE:HD12	1.97	0.45
5:F:561:MET:HE3	5:F:561:MET:HB2	1.92	0.45
1:H:82:LEU:HD22	1:H:173:VAL:CG2	2.47	0.45
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.98	0.45
3:J:93:THR:HG22	3:J:94:GLN:N	2.31	0.45
3:J:450:HIS:HE1	3:J:452:LEU:HG	1.82	0.45
3:J:701:LEU:HD22	3:J:701:LEU:HA	1.57	0.45
5:L:96:ASP:O	5:L:98:VAL:N	2.49	0.45
2:C:60:GLN:H	2:C:60:GLN:HG2	1.31	0.45
2:C:159:SER:O	2:C:160:ASP:HB2	2.16	0.45
2:C:445:ILE:HG22	2:C:446:ASP:OD1	2.16	0.45
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.40	0.45
2:C:1246:ARG:CZ	2:C:1249:GLY:H	2.30	0.45
3:D:508:LEU:HD12	3:D:508:LEU:HA	1.62	0.45
3:D:544:LEU:HA	3:D:544:LEU:HD12	1.57	0.45
3:D:622:ASP:HB3	3:D:626:TYR:CE2	2.51	0.45
3:D:630:ALA:O	3:D:633:ALA:HB3	2.17	0.45
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.32	0.45
5:F:502:LYS:HE3	5:F:502:LYS:HB2	1.40	0.45
5:F:511:ILE:O	5:F:511:ILE:HG23	2.17	0.45
1:G:41:ASN:HD22	1:H:41:ASN:ND2	2.09	0.45
1:G:68:TYR:CE1	2:I:929:ILE:HG21	2.50	0.45
1:G:89:ALA:HB3	1:G:124:VAL:HG12	1.99	0.45
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.47	0.45
1:G:135:ASP:OD1	1:G:136:GLU:N	2.50	0.45
2:I:968:GLU:CG	2:I:1018:TYR:HE1	2.29	0.45
3:J:1337:VAL:HG23	3:J:1338:ALA:N	2.32	0.45
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.49	0.45
5:L:507:MET:HG2	5:L:520:GLY:CA	2.47	0.45
1:A:132:HIS:CD2	1:A:132:HIS:N	2.84	0.45
2:C:104:ILE:HD12	2:C:115:LYS:O	2.16	0.45
2:C:325:LEU:O	2:C:330:HIS:HB2	2.17	0.45
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.51	0.45
2:C:850:ILE:HG23	2:C:850:ILE:HD12	1.54	0.45
3:D:707:ILE:N	3:D:714:GLU:O	2.48	0.45
1:G:23:HIS:ND1	1:G:206:GLU:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:HIS:HB3	1:H:45:ARG:NH2	2.31	0.45
1:G:57:THR:HG22	1:G:58:GLU:HG2	1.99	0.45
2:I:1164:PHE:N	2:I:1168:GLU:OE1	2.49	0.45
3:J:438:GLU:OE2	3:J:481:ARG:NH2	2.34	0.45
1:A:89:ALA:HB3	1:A:125:LYS:HD2	1.99	0.44
1:B:100:LEU:HG	1:B:118:ASP:OD2	2.18	0.44
1:B:196:THR:HG23	3:D:443:GLU:CG	2.47	0.44
2:C:102:LEU:O	2:C:116:ASP:HA	2.17	0.44
2:C:230:PHE:O	2:C:332:ARG:HA	2.17	0.44
3:D:45:ASN:O	3:D:46:TYR:CD2	2.70	0.44
3:D:385:LEU:HA	3:D:385:LEU:HD23	1.78	0.44
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.99	0.44
3:D:704:GLU:O	3:D:706:VAL:HG22	2.16	0.44
3:D:854:ALA:HB2	3:J:1372:ARG:HE	1.81	0.44
3:D:907:HIS:CE1	4:E:11:GLU:OE2	2.70	0.44
3:D:1165:PHE:HD2	3:D:1173:ARG:CD	2.30	0.44
3:D:1278:GLU:OE1	3:D:1278:GLU:HA	2.16	0.44
1:H:65:LEU:O	1:H:171:LEU:HD11	2.18	0.44
3:J:121:PRO:O	3:J:122:SER:C	2.52	0.44
3:J:645:VAL:HB	3:J:701:LEU:HD23	1.99	0.44
3:J:749:LYS:HD3	3:J:753:SER:HB2	1.98	0.44
3:J:814:CYS:HB3	3:J:890:THR:OG1	2.17	0.44
3:J:839:VAL:O	3:J:839:VAL:HG12	2.16	0.44
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.98	0.44
3:J:1266:ILE:H	3:J:1266:ILE:HG13	1.42	0.44
3:J:1280:VAL:CG1	3:J:1304:ARG:HE	2.30	0.44
5:L:405:ILE:HD13	5:L:405:ILE:HG21	1.43	0.44
5:L:446:GLN:HE21	5:L:446:GLN:HB3	1.56	0.44
1:A:28:LEU:O	1:A:31:LEU:CD1	2.66	0.44
1:A:233:ASP:OD2	1:A:233:ASP:N	2.30	0.44
1:A:250:ASP:OD2	5:F:605:GLU:HA	2.17	0.44
1:B:147:GLN:HG3	1:B:148:ARG:H	1.81	0.44
2:C:150:HIS:CG	2:C:454:ARG:HH21	2.35	0.44
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.99	0.44
2:C:484:LEU:CD1	2:C:485:ASP:H	2.30	0.44
2:C:490:GLN:CD	5:F:472:GLN:HE22	2.21	0.44
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.64	0.44
3:D:665:GLN:HG3	3:D:669:GLN:NE2	2.32	0.44
3:D:845:ALA:CB	3:D:881:LYS:HD2	2.47	0.44
3:D:903:LEU:HD13	3:D:909:ILE:HD13	1.99	0.44
1:G:77:ASP:O	1:G:81:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:LEU:HA	1:H:31:LEU:HD13	1.67	0.44
2:I:389:PHE:CD2	2:I:389:PHE:N	2.85	0.44
2:I:478:ARG:HG2	2:I:492:MET:HG2	2.00	0.44
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.48	0.44
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	2.00	0.44
3:J:269:TYR:O	3:J:273:ILE:HG13	2.16	0.44
3:J:283:LEU:HD23	3:J:283:LEU:HA	1.67	0.44
3:J:388:ARG:HB2	3:J:390:LEU:HD13	2.00	0.44
3:J:744:ARG:O	3:J:759:ILE:HB	2.17	0.44
2:C:39:ILE:HG23	2:C:39:ILE:O	2.18	0.44
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.48	0.44
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.81	0.44
2:C:1237:HIS:O	2:C:1238:LEU:C	2.56	0.44
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.52	0.44
3:D:241:VAL:HG12	3:D:242:LEU:N	2.32	0.44
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.00	0.44
3:D:664:ILE:HG23	3:D:664:ILE:HD12	1.74	0.44
3:D:733:SER:O	3:D:734:ALA:C	2.56	0.44
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.18	0.44
3:D:1216:ALA:HB1	3:D:1218:HIS:HD2	1.81	0.44
3:D:1279:GLN:H	3:D:1279:GLN:HG2	1.60	0.44
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.32	0.44
5:F:269:LEU:HA	5:F:269:LEU:HD23	1.60	0.44
1:G:101:THR:O	1:G:103:ASN:ND2	2.50	0.44
1:G:136:GLU:C	1:G:138:ALA:H	2.20	0.44
2:I:44:GLU:HA	2:I:54:ARG:HH12	1.81	0.44
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.99	0.44
3:J:264:ASP:N	3:J:264:ASP:OD2	2.51	0.44
3:J:349:TYR:CE2	3:J:379:PRO:HG2	2.48	0.44
3:J:480:ALA:O	3:J:485:MET:N	2.50	0.44
3:J:749:LYS:HG2	3:J:753:SER:O	2.18	0.44
3:J:1165:PHE:HD2	3:J:1173:ARG:NE	2.14	0.44
5:L:157:ARG:CZ	5:L:159:SER:OG	2.65	0.44
1:A:285:THR:HG23	1:A:288:GLU:H	1.83	0.44
1:A:292:THR:OG1	1:A:295:LEU:HD12	2.17	0.44
2:C:518:ASN:O	2:C:519:ASN:CB	2.64	0.44
2:C:1136:GLN:NE2	2:C:1140:LYS:HZ3	2.13	0.44
2:C:1158:LYS:C	2:C:1159:VAL:HG22	2.37	0.44
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.52	0.44
3:D:184:ALA:O	3:D:188:LEU:N	2.42	0.44
3:D:1270:GLY:O	3:D:1298:VAL:HG11	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:HIS:HB3	1:H:45:ARG:CZ	2.47	0.44
1:G:65:LEU:CD2	1:G:65:LEU:N	2.80	0.44
2:I:15:PHE:CD2	2:I:1190:ALA:HB2	2.51	0.44
2:I:22:LEU:HD22	2:I:22:LEU:HA	1.74	0.44
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.81	0.44
2:I:496:LYS:HB3	2:I:496:LYS:HE3	1.81	0.44
2:I:746:ALA:HA	2:I:974:ARG:HH21	1.82	0.44
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.15	0.44
3:J:396:ALA:O	3:J:400:MET:HG3	2.18	0.44
1:B:33:ARG:NH1	2:C:1081:PRO:HG3	2.32	0.44
2:C:694:ARG:HB2	2:C:798:GLN:NE2	2.33	0.44
2:C:759:SER:C	2:C:761:GLN:N	2.70	0.44
2:C:815:SER:HB3	2:C:1077:SER:HB3	2.00	0.44
3:D:606:ASN:OD1	3:D:610:ARG:NE	2.51	0.44
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.98	0.44
3:D:1268:ASN:HB2	3:D:1301:THR:OG1	2.17	0.44
5:F:557:LYS:O	5:F:561:MET:HB2	2.18	0.44
2:I:42:ASP:OD2	2:I:44:GLU:HG2	2.18	0.44
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.82	0.44
2:I:82:VAL:HG22	2:I:92:TYR:CZ	2.51	0.44
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.53	0.44
2:I:211:ARG:HD3	2:I:357:ASN:O	2.17	0.44
2:I:558:VAL:HG13	2:I:573:ASN:HB3	1.98	0.44
3:J:24:LEU:HA	3:J:24:LEU:HD13	1.51	0.44
5:L:151:VAL:HG11	5:L:158:LEU:CD2	2.47	0.44
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.18	0.44
1:A:118:ASP:OD2	1:A:119:GLY:N	2.50	0.44
2:C:616:ILE:O	2:C:636:CYS:HB3	2.17	0.44
2:C:833:ILE:HD13	2:C:929:ILE:HD11	2.00	0.44
3:D:355:ILE:O	3:D:355:ILE:HG13	2.18	0.44
3:D:434:ILE:HG21	3:D:434:ILE:HD13	1.71	0.44
3:D:767:LEU:HD12	3:D:767:LEU:N	2.32	0.44
5:F:383:ASN:HB2	5:F:412:LEU:HD21	2.00	0.44
1:G:61:ILE:CG1	1:G:171:LEU:HD23	2.48	0.44
2:I:209:ILE:O	2:I:212:ALA:N	2.51	0.44
2:I:607:SER:N	2:I:610:GLU:HB2	2.33	0.44
2:I:670:PHE:CE2	2:I:1113:LEU:HB3	2.52	0.44
2:I:1011:LEU:O	2:I:1015:ALA:N	2.43	0.44
3:J:395:LYS:HE2	5:L:536:THR:HG21	2.00	0.44
3:J:1289:ASN:OD1	3:J:1290:ARG:CZ	2.66	0.44
2:C:1117:LEU:HD21	2:C:1182:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1240:ASP:HB3	3:D:445:LYS:CD	2.43	0.44
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.42	0.44
3:D:515:ARG:HH21	3:D:717:VAL:HG23	1.83	0.44
3:D:1290:ARG:HA	3:D:1290:ARG:HD3	1.81	0.44
5:F:295:CYS:SG	5:F:333:VAL:HB	2.58	0.44
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.19	0.44
2:I:1220:GLN:HG2	2:I:1221:PHE:N	2.33	0.44
3:J:19:ALA:HA	3:J:1344:LEU:HD12	1.98	0.44
3:J:75:TYR:N	3:J:75:TYR:CD1	2.86	0.44
3:J:452:LEU:HA	3:J:452:LEU:HD23	1.73	0.44
3:J:490:ILE:HG21	3:J:490:ILE:HD13	1.69	0.44
3:J:682:VAL:HA	3:J:685:ILE:HD13	1.99	0.44
3:J:770:LEU:HA	3:J:770:LEU:HD12	1.66	0.44
1:A:179:PRO:O	1:A:207:THR:HG23	2.17	0.44
1:B:60:GLU:CD	1:B:142:MET:HB2	2.38	0.44
2:C:49:LEU:HB2	2:C:73:TYR:OH	2.17	0.44
2:C:247:ARG:HH21	2:C:274:ILE:HG21	1.83	0.44
2:C:1253:LEU:HD13	2:C:1254:VAL:N	2.33	0.44
5:F:127:ILE:O	5:F:130:VAL:N	2.51	0.44
5:F:412:LEU:HA	5:F:412:LEU:HD12	1.73	0.44
5:F:517:SER:O	5:F:517:SER:OG	2.35	0.44
1:G:96:ASP:O	1:G:148:ARG:HG3	2.18	0.44
1:H:103:ASN:HA	1:H:141:SER:CB	2.47	0.44
2:I:277:LEU:O	2:I:281:ASP:N	2.51	0.44
2:I:367:TYR:CD2	2:I:376:PRO:HA	2.52	0.44
2:I:532:ALA:HB1	2:I:538:LEU:HD11	2.00	0.44
2:I:614:TYR:CD1	2:I:652:TYR:CE1	3.05	0.44
2:I:953:LEU:HD12	2:I:953:LEU:HA	1.56	0.44
2:I:971:LEU:CD2	2:I:1018:TYR:HB2	2.48	0.44
2:I:980:VAL:O	2:I:984:VAL:HB	2.17	0.44
3:J:860:ARG:HB3	3:J:861:ASN:H	1.68	0.44
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.48	0.44
3:J:1332:LEU:HD13	3:J:1332:LEU:HA	1.77	0.44
5:L:166:VAL:HG23	5:L:258:GLN:O	2.18	0.44
5:L:220:LYS:O	5:L:223:GLU:HB3	2.18	0.44
5:L:484:ALA:HB1	5:L:491:GLU:CG	2.48	0.44
1:B:183:ILE:O	1:B:183:ILE:HD12	2.18	0.44
2:C:605:TYR:C	2:C:606:LEU:HD12	2.38	0.44
3:D:26:SER:HB3	3:D:29:MET:HB2	2.00	0.44
3:D:703:THR:HA	3:D:717:VAL:HA	2.00	0.44
3:D:827:GLU:C	3:D:829:GLY:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:227:GLN:CG	5:F:252:LEU:HA	2.48	0.44
1:H:228:LEU:HA	1:H:228:LEU:HD23	1.59	0.44
2:I:361:SER:O	2:I:364:VAL:HB	2.18	0.44
2:I:494:ASN:ND2	2:I:497:PRO:HD3	2.33	0.44
2:I:796:LEU:HD12	2:I:796:LEU:N	2.33	0.44
2:I:1252:SER:HB3	2:I:1255:THR:O	2.16	0.44
3:J:201:LEU:HD12	3:J:221:ILE:HD13	2.00	0.44
3:J:518:VAL:HG23	3:J:547:ARG:NH2	2.33	0.44
3:J:706:VAL:HG12	3:J:715:LYS:CB	2.46	0.44
3:J:797:THR:CG2	3:J:924:GLY:HA3	2.36	0.44
3:J:805:GLN:HB3	3:J:806:ASP:H	1.61	0.44
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.99	0.44
5:L:384:LEU:HD23	5:L:384:LEU:HA	1.55	0.44
1:A:137:ASN:OD1	1:A:137:ASN:N	2.51	0.43
2:C:62:TYR:C	2:C:64:GLY:N	2.71	0.43
2:C:1195:ILE:HG21	2:C:1195:ILE:HD13	1.70	0.43
2:C:1223:ARG:HH11	2:C:1223:ARG:HD3	1.67	0.43
3:D:381:ILE:HD13	3:D:381:ILE:HG21	1.67	0.43
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.51	0.43
3:D:1257:VAL:O	3:D:1260:MET:N	2.51	0.43
3:D:1332:LEU:N	3:D:1332:LEU:HD22	2.32	0.43
3:D:1344:LEU:HD12	3:D:1344:LEU:N	2.33	0.43
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.83	0.43
2:I:672:GLU:HG2	2:I:1187:PHE:HA	2.00	0.43
5:L:161:LEU:HA	5:L:161:LEU:HD12	1.68	0.43
1:A:233:ASP:C	1:A:234:LEU:HD22	2.38	0.43
1:B:181:GLU:OE2	1:B:208:ASN:HA	2.18	0.43
2:C:479:LEU:HA	2:C:479:LEU:HD23	1.73	0.43
2:C:819:SER:HB2	2:C:1085:MET:SD	2.57	0.43
2:C:987:GLU:O	2:C:991:LYS:HG3	2.18	0.43
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.81	0.43
3:D:266:ASN:O	3:D:267:ASP:C	2.54	0.43
3:D:733:SER:O	3:D:736:GLN:N	2.50	0.43
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	2.18	0.43
3:D:1375:ALA:HB1	3:J:853:THR:HG21	2.00	0.43
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.53	0.43
1:G:66:HIS:HB2	1:G:69:SER:OG	2.18	0.43
1:H:57:THR:OG1	1:H:147:GLN:HB3	2.17	0.43
2:I:276:GLN:O	2:I:280:ASP:N	2.43	0.43
2:I:409:LEU:HD13	2:I:427:ASP:HB3	2.00	0.43
2:I:1087:TYR:OH	2:I:1218:GLY:HA2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1252:SER:HB3	2:I:1257:GLN:H	1.83	0.43
2:I:1268:GLN:HG2	3:J:467:ALA:HB1	2.00	0.43
2:I:1301:ARG:O	2:I:1304:MET:HB3	2.18	0.43
3:J:265:LEU:HA	3:J:265:LEU:HD23	1.67	0.43
3:J:1206:ARG:NH2	3:J:1223:LEU:HD13	2.34	0.43
5:L:251:LYS:HA	5:L:254:GLU:HG2	1.99	0.43
5:L:281:ARG:HA	5:L:284:GLU:OE1	2.18	0.43
1:B:44:ARG:HG3	1:B:183:ILE:HB	2.00	0.43
2:C:208:ILE:O	2:C:362:ALA:HB1	2.19	0.43
2:C:571:LEU:HA	2:C:571:LEU:HD23	1.66	0.43
2:C:1312:ASN:HD21	2:C:1314:GLN:HG3	1.83	0.43
3:D:293:ARG:O	3:D:294:ASN:C	2.57	0.43
3:D:474:LEU:HA	3:D:474:LEU:HD12	1.60	0.43
3:D:500:ILE:HG22	3:D:500:ILE:O	2.17	0.43
1:G:133:LEU:HA	1:G:133:LEU:HD13	1.79	0.43
2:I:22:LEU:HD13	2:I:23:ASP:N	2.34	0.43
2:I:387:ASN:O	2:I:394:ARG:HB2	2.19	0.43
2:I:640:GLY:O	2:I:641:GLU:HG3	2.18	0.43
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.18	0.43
3:J:1290:ARG:HA	3:J:1290:ARG:HD3	1.78	0.43
3:J:1357:ILE:O	3:J:1359:ALA:N	2.47	0.43
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.18	0.43
1:B:100:LEU:O	1:B:143:ARG:HA	2.18	0.43
3:D:255:LEU:N	3:D:259:ARG:O	2.48	0.43
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.83	0.43
3:D:795:TYR:HE2	3:D:799:ARG:NE	2.15	0.43
3:D:891:ASP:CA	3:D:1281:GLU:HG3	2.47	0.43
3:D:910:ASN:ND2	4:E:15:ASN:O	2.50	0.43
3:D:1248:ILE:HG21	3:D:1248:ILE:HD13	1.75	0.43
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.33	0.43
5:F:552:THR:H	5:F:552:THR:HG23	1.59	0.43
2:I:158:ASP:HB3	2:I:173:ASN:OD1	2.18	0.43
2:I:538:LEU:HA	2:I:542:ARG:NH2	2.33	0.43
2:I:811:ASN:N	2:I:811:ASN:OD1	2.46	0.43
2:I:1287:LEU:O	2:I:1290:MET:N	2.51	0.43
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.81	0.43
3:J:75:TYR:CD2	3:J:83:VAL:HG21	2.54	0.43
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.00	0.43
3:J:1257:VAL:O	3:J:1260:MET:N	2.51	0.43
5:L:502:LYS:HE3	5:L:502:LYS:HB2	1.32	0.43
2:C:819:SER:HB2	2:C:1085:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.18	0.43
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.59	0.43
2:C:1196:LYS:CD	2:C:1206:THR:HG23	2.29	0.43
3:D:306:LEU:O	3:D:326:SER:HB2	2.18	0.43
3:D:541:LEU:HA	3:D:541:LEU:HD23	1.44	0.43
5:F:306:PHE:CE1	5:F:315:TRP:CD2	3.00	0.43
1:G:59:VAL:HG13	1:G:143:ARG:O	2.19	0.43
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.99	0.43
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.53	0.43
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.81	0.43
3:J:41:PRO:HB3	3:J:270:ARG:HG3	2.00	0.43
3:J:385:LEU:HA	3:J:385:LEU:HD23	1.43	0.43
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.44	0.43
5:L:611:LEU:HD23	5:L:611:LEU:HA	1.56	0.43
2:C:756:TYR:CD1	2:C:756:TYR:N	2.86	0.43
2:C:1101:LEU:HD23	2:C:1101:LEU:HA	1.58	0.43
2:C:1137:GLU:HG2	2:C:1140:LYS:CG	2.49	0.43
3:D:97:VAL:HG12	3:D:101:ARG:CG	2.45	0.43
3:D:813:ASP:HA	3:D:897:HIS:HB2	2.01	0.43
3:D:1237:VAL:HG11	3:D:1253:ILE:HD13	2.00	0.43
5:F:103:ARG:HH11	5:F:103:ARG:HD3	1.64	0.43
1:G:47:LEU:O	1:G:180:VAL:HG11	2.19	0.43
2:I:1176:LEU:HD22	2:I:1181:PRO:HD2	2.00	0.43
3:J:102:MET:CE	3:J:246:PRO:HD3	2.47	0.43
3:J:118:LYS:HA	3:J:118:LYS:HD2	1.62	0.43
3:J:189:LEU:HD23	3:J:189:LEU:HA	1.77	0.43
2:C:88:ARG:HG2	2:C:90:VAL:CG2	2.49	0.43
2:C:409:LEU:HD23	2:C:409:LEU:HA	1.65	0.43
2:C:992:LEU:HG	2:C:997:TRP:HE1	1.84	0.43
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.65	0.43
2:C:1239:VAL:HG13	2:C:1240:ASP:N	2.33	0.43
3:D:108:ALA:CB	3:D:279:LEU:HD22	2.49	0.43
3:D:108:ALA:HB3	3:D:279:LEU:HD22	1.99	0.43
3:D:647:PRO:HG3	3:D:697:MET:CB	2.47	0.43
3:D:717:VAL:H	3:D:717:VAL:HG22	1.54	0.43
3:D:755:ILE:HG22	3:D:757:THR:H	1.83	0.43
5:F:593:LYS:O	5:F:597:LYS:N	2.50	0.43
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.99	0.43
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.54	0.43
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.18	0.43
2:I:705:GLU:HB2	2:I:794:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.53	0.43
3:J:299:LEU:O	3:J:302:ALA:N	2.51	0.43
1:A:92:VAL:HA	1:A:120:ASP:O	2.18	0.43
1:A:176:CYS:O	1:A:177:TYR:C	2.57	0.43
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.75	0.43
2:C:544:GLY:O	2:C:548:ARG:HG3	2.19	0.43
2:C:551:HIS:CE1	2:C:553:THR:HG23	2.53	0.43
2:C:830:THR:HG22	2:C:1058:ARG:O	2.19	0.43
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.48	0.43
1:G:219:ARG:HH11	1:G:219:ARG:HD3	1.67	0.43
1:H:83:LEU:HD12	1:H:86:LYS:HE2	2.01	0.43
2:I:159:SER:O	2:I:171:LEU:O	2.37	0.43
2:I:818:VAL:O	2:I:1079:ILE:HA	2.19	0.43
3:J:1140:ARG:HH21	3:J:1236:GLU:CG	2.22	0.43
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.35	0.43
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.99	0.43
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.49	0.43
5:L:576:VAL:HG12	5:L:587:ILE:CD1	2.49	0.43
1:A:102:LEU:HD23	1:A:115:ILE:HA	2.01	0.43
1:A:196:THR:OG1	1:A:197:ASP:N	2.50	0.43
1:A:320:ASN:O	1:A:323:PRO:HD3	2.18	0.43
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.64	0.43
2:C:469:VAL:O	2:C:472:GLU:HB3	2.18	0.43
2:C:760:ASN:O	2:C:761:GLN:O	2.37	0.43
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.52	0.43
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.18	0.43
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	2.00	0.43
3:D:411:ILE:HD12	3:D:411:ILE:HG23	1.69	0.43
5:F:503:GLU:CG	5:F:504:PRO:HD2	2.48	0.43
1:G:152:TYR:CE2	2:I:824:GLN:HG2	2.54	0.43
2:I:518:ASN:O	2:I:519:ASN:HB3	2.18	0.43
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.54	0.43
2:I:1053:TYR:CD1	2:I:1053:TYR:N	2.87	0.43
2:I:1211:ARG:HB2	2:I:1220:GLN:HE21	1.83	0.43
3:J:343:LEU:HD12	3:J:343:LEU:HA	1.80	0.43
5:L:295:CYS:CB	5:L:330:LEU:HD23	2.49	0.43
5:L:312:SER:OG	5:L:313:ASP:N	2.51	0.43
1:A:92:VAL:HA	1:A:120:ASP:HB3	2.00	0.43
1:A:118:ASP:HB3	1:A:121:VAL:CG2	2.45	0.43
1:A:225:ALA:HA	1:A:228:LEU:HD12	2.00	0.43
2:C:517:GLN:O	2:C:517:GLN:HG2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:979:LEU:HD12	2:C:979:LEU:HA	1.72	0.43
2:C:1042:LEU:HD13	2:C:1046:VAL:HG22	2.01	0.43
3:D:135:ILE:HG21	3:D:135:ILE:HD13	1.65	0.43
3:D:352:ARG:HB3	3:D:467:ALA:HA	2.01	0.43
3:D:748:ALA:HA	3:D:754:ILE:HA	2.00	0.43
3:D:848:VAL:HG23	3:D:858:VAL:HG13	2.01	0.43
3:D:905:ARG:HH12	4:E:10:VAL:HG11	1.82	0.43
3:D:908:ILE:HD13	3:D:909:ILE:N	2.34	0.43
3:D:1292:LEU:HA	3:J:1226:VAL:HG21	2.01	0.43
5:F:512:GLY:C	5:F:514:ASP:N	2.71	0.43
5:F:601:PRO:HA	5:F:604:SER:H	1.84	0.43
1:G:50:SER:HG	1:H:35:PHE:HZ	1.67	0.43
1:G:52:PRO:HG2	1:G:219:ARG:NE	2.29	0.43
1:H:82:LEU:HA	1:H:85:LEU:HD12	2.00	0.43
2:I:149:LEU:HA	2:I:149:LEU:HD12	1.62	0.43
2:I:403:MET:SD	2:I:403:MET:C	2.98	0.43
2:I:705:GLU:CD	2:I:705:GLU:H	2.20	0.43
2:I:1262:LYS:HA	2:I:1262:LYS:HD3	1.83	0.43
2:I:1331:ARG:HA	2:I:1335:ILE:O	2.19	0.43
2:I:1334:GLY:O	3:J:25:ALA:CB	2.66	0.43
3:J:364:HIS:CE1	3:J:365:GLN:OE1	2.72	0.43
3:J:1257:VAL:O	3:J:1258:ARG:C	2.57	0.43
3:J:1355:ARG:HE	3:J:1355:ARG:HB3	1.52	0.43
1:A:257:VAL:HG22	1:A:276:HIS:O	2.19	0.42
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.82	0.42
2:C:493:ILE:H	2:C:493:ILE:HG22	1.49	0.42
2:C:557:ARG:HH21	2:C:608:ALA:N	2.16	0.42
2:C:632:ASP:O	2:C:647:ARG:HB2	2.19	0.42
2:C:653:MET:HG2	2:C:654:ASP:N	2.34	0.42
2:C:870:ILE:HB	2:C:944:ARG:HD3	2.01	0.42
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.48	0.42
2:C:1209:GLN:HA	2:C:1225:VAL:O	2.19	0.42
2:C:1268:GLN:HE22	3:D:352:ARG:HH11	1.65	0.42
3:D:93:THR:HG22	3:D:94:GLN:N	2.34	0.42
3:D:915:ILE:H	3:D:915:ILE:HG12	1.64	0.42
5:F:290:LEU:HB3	5:F:333:VAL:HG21	2.01	0.42
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.32	0.42
2:I:518:ASN:CG	2:I:519:ASN:N	2.72	0.42
2:I:607:SER:H	2:I:610:GLU:HB2	1.83	0.42
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	2.01	0.42
2:I:1038:GLN:O	2:I:1038:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.54	0.42
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.53	0.42
3:J:495:ASN:N	3:J:495:ASN:OD1	2.52	0.42
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.19	0.42
4:K:50:ALA:O	4:K:54:ILE:HG12	2.19	0.42
5:L:123:ILE:HD13	5:L:123:ILE:HG21	1.80	0.42
5:L:341:LEU:O	5:L:344:LEU:HB3	2.19	0.42
5:L:350:GLU:H	5:L:350:GLU:HG3	1.54	0.42
5:L:354:THR:O	5:L:358:VAL:HG23	2.19	0.42
2:C:235:ASN:OD1	2:C:236:LYS:HG2	2.19	0.42
2:C:263:VAL:HG12	2:C:264:GLU:O	2.19	0.42
2:C:490:GLN:O	2:C:492:MET:N	2.52	0.42
2:C:591:TYR:CE1	2:C:616:ILE:HG21	2.54	0.42
3:D:322:ARG:HB2	3:D:322:ARG:CZ	2.48	0.42
5:F:227:GLN:NE2	5:F:251:LYS:NZ	2.66	0.42
5:F:597:LYS:O	5:F:603:ARG:HG3	2.19	0.42
5:F:611:LEU:HA	5:F:611:LEU:HD23	1.82	0.42
1:G:13:LEU:HG	1:G:14:VAL:N	2.34	0.42
2:I:161:LYS:H	2:I:161:LYS:HG2	1.63	0.42
2:I:194:LEU:HD12	2:I:194:LEU:HA	1.80	0.42
2:I:515:MET:O	2:I:515:MET:CG	2.67	0.42
2:I:798:GLN:NE2	2:I:827:ARG:O	2.49	0.42
2:I:894:GLN:HG3	2:I:894:GLN:O	2.18	0.42
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.84	0.42
3:J:647:PRO:HG3	3:J:697:MET:N	2.34	0.42
3:J:903:LEU:HD12	3:J:903:LEU:HA	1.93	0.42
5:L:271:ASN:O	5:L:275:VAL:HG23	2.19	0.42
5:L:572:THR:HG23	5:L:575:GLU:CB	2.43	0.42
2:C:158:ASP:CG	2:C:159:SER:N	2.71	0.42
3:D:298:MET:HE1	5:F:402:LEU:O	2.19	0.42
3:D:528:THR:HG23	3:D:529:GLY:N	2.35	0.42
3:D:544:LEU:O	3:D:574:VAL:HB	2.19	0.42
3:D:647:PRO:CG	3:D:697:MET:HB3	2.50	0.42
3:D:825:VAL:HG22	3:D:833:GLU:N	2.35	0.42
5:F:560:ARG:O	5:F:563:PHE:O	2.37	0.42
2:I:643:SER:HG	2:I:645:PHE:HE1	1.68	0.42
2:I:757:THR:OG1	2:I:758:ARG:N	2.52	0.42
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.55	0.42
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.53	0.42
3:J:127:LEU:HD12	3:J:127:LEU:HA	1.47	0.42
3:J:317:THR:HG22	3:J:322:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.86	0.42
3:J:596:LEU:HD12	3:J:601:ILE:HG13	2.01	0.42
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.19	0.42
5:L:165:PHE:HD1	5:L:259:PHE:HA	1.84	0.42
1:A:187:VAL:HG23	1:A:187:VAL:O	2.20	0.42
1:A:212:ASP:HA	1:A:213:PRO:HD3	1.93	0.42
2:C:1067:ALA:HB2	2:C:1073:LYS:HA	2.00	0.42
2:C:1322:SER:OG	2:C:1323:PHE:N	2.52	0.42
3:D:707:ILE:O	3:D:714:GLU:N	2.52	0.42
5:F:463:LEU:HD23	5:F:463:LEU:HA	1.80	0.42
5:F:470:MET:HE1	5:F:486:ARG:HH12	1.83	0.42
1:G:12:ARG:HA	1:H:231:PHE:HZ	1.81	0.42
1:H:51:MET:HB3	1:H:178:SER:CB	2.50	0.42
2:I:146:VAL:HG13	2:I:529:ARG:HB3	2.01	0.42
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.85	0.42
2:I:388:LEU:HD23	2:I:388:LEU:HA	1.76	0.42
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.42
2:I:920:VAL:HG13	2:I:1054:LEU:HD21	2.01	0.42
2:I:1225:VAL:HA	3:J:638:SER:CB	2.49	0.42
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.18	0.42
3:J:591:ILE:HG13	3:J:604:MET:HE2	2.00	0.42
3:J:810:THR:HG23	3:J:811:GLU:N	2.34	0.42
1:A:51:MET:HE1	1:A:216:ALA:HB1	2.00	0.42
1:B:31:LEU:HD13	1:B:31:LEU:HA	1.85	0.42
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	2.01	0.42
2:C:1112:ILE:O	2:C:1113:LEU:C	2.56	0.42
3:D:141:PHE:CE1	3:D:181:GLY:HA3	2.54	0.42
3:D:371:LYS:O	3:D:372:MET:C	2.54	0.42
3:D:495:ASN:O	3:D:497:GLU:N	2.53	0.42
3:D:513:MET:HE1	3:D:579:LEU:HD13	2.01	0.42
5:F:121:LYS:HA	5:F:121:LYS:HD3	1.83	0.42
5:F:357:GLN:H	5:F:357:GLN:HG3	1.58	0.42
1:G:52:PRO:CG	1:G:219:ARG:HH21	2.32	0.42
2:I:1132:LEU:HB3	2:I:1177:ARG:CZ	2.49	0.42
3:J:83:VAL:HG13	3:J:92:VAL:HG13	2.01	0.42
3:J:125:GLY:O	3:J:128:LEU:N	2.52	0.42
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.84	0.42
3:J:844:THR:HG21	3:J:858:VAL:HG21	2.00	0.42
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.67	0.42
5:L:452:ILE:HG21	5:L:452:ILE:HD13	1.69	0.42
1:A:249:PHE:CE2	1:A:254:LEU:HG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:SER:OG	2:C:455:SER:HB3	2.19	0.42
2:C:468:LEU:HA	2:C:468:LEU:HD23	1.77	0.42
2:C:1099:ASN:HD21	3:D:505:ASP:CG	2.22	0.42
3:D:88:CYS:SG	3:D:88:CYS:O	2.77	0.42
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.48	0.42
3:D:461:PHE:HD2	3:D:461:PHE:HA	1.64	0.42
3:D:491:LEU:HD23	3:D:491:LEU:HA	1.71	0.42
5:F:95:THR:OG1	5:F:96:ASP:N	2.52	0.42
5:F:396:ASN:O	5:F:398:GLY:N	2.53	0.42
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.70	0.42
2:I:196:VAL:HG12	2:I:204:LEU:O	2.19	0.42
2:I:229:ILE:HB	2:I:240:GLU:HB2	2.01	0.42
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.81	0.42
2:I:1105:SER:HB2	3:J:731:ARG:HG2	2.01	0.42
2:I:1164:PHE:O	2:I:1168:GLU:HB2	2.19	0.42
3:J:599:LYS:HD3	3:J:599:LYS:HA	1.36	0.42
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.34	0.42
1:B:109:PRO:HG3	1:B:132:HIS:CD2	2.55	0.42
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.85	0.42
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.50	0.42
2:C:700:VAL:HG11	2:C:1114:GLU:HG2	2.00	0.42
2:C:745:GLU:N	2:C:1017:GLN:HG3	2.34	0.42
2:C:794:LEU:HD21	2:C:796:LEU:HD11	2.02	0.42
2:C:797:GLY:O	2:C:1231:TYR:OH	2.37	0.42
3:D:188:LEU:HA	3:D:188:LEU:HD23	1.87	0.42
3:D:262:THR:O	3:D:262:THR:HG23	2.18	0.42
3:D:559:ALA:HB3	3:D:562:GLU:O	2.20	0.42
3:D:576:ARG:NH1	3:D:593:ASN:O	2.52	0.42
3:D:831:VAL:O	3:D:831:VAL:HG13	2.20	0.42
3:D:1342:ASP:OD1	3:D:1343:GLU:N	2.53	0.42
2:I:46:GLN:OE1	2:I:47:TYR:N	2.52	0.42
2:I:338:THR:CG2	2:I:345:PRO:HB3	2.50	0.42
3:J:113:HIS:O	3:J:114:ILE:C	2.57	0.42
3:J:146:VAL:HG23	3:J:158:GLN:O	2.19	0.42
3:J:557:LYS:O	3:J:559:ALA:N	2.52	0.42
3:J:660:GLU:O	3:J:664:ILE:HG12	2.20	0.42
3:J:698:MET:O	3:J:702:GLN:HB3	2.20	0.42
3:J:797:THR:HG22	3:J:924:GLY:CA	2.35	0.42
3:J:1179:PRO:HG2	3:J:1183:SER:O	2.19	0.42
5:L:482:GLU:O	5:L:486:ARG:NH2	2.53	0.42
1:A:219:ARG:O	1:A:222:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:CG2	1:B:177:TYR:HE2	2.32	0.42
2:C:48:GLY:N	2:C:461:GLU:OE1	2.52	0.42
2:C:499:SER:O	2:C:503:LYS:HB2	2.20	0.42
2:C:680:LEU:O	2:C:681:MET:C	2.58	0.42
2:C:865:LEU:HD23	2:C:865:LEU:HA	1.70	0.42
3:D:74:LYS:HD3	3:D:75:TYR:HE1	1.85	0.42
3:D:227:PHE:CE1	3:D:234:PRO:HG3	2.54	0.42
3:D:249:LEU:HD23	3:D:249:LEU:HA	1.71	0.42
3:D:337:ARG:HB3	3:D:1324:SER:O	2.20	0.42
3:D:357:VAL:HG22	3:D:461:PHE:CD1	2.55	0.42
3:D:411:ILE:HA	3:D:411:ILE:HD13	1.78	0.42
3:D:482:ALA:C	3:D:483:LEU:HG	2.39	0.42
3:D:609:TYR:HA	3:D:617:THR:OG1	2.20	0.42
3:D:770:LEU:HD12	3:D:770:LEU:HA	1.52	0.42
5:F:127:ILE:O	5:F:128:ASN:C	2.58	0.42
2:I:819:SER:HB2	2:I:1085:MET:CG	2.49	0.42
3:J:189:LEU:HD22	3:J:234:PRO:HB3	2.02	0.42
3:J:1150:PRO:O	3:J:1153:PRO:HG3	2.20	0.42
5:L:148:TYR:CE1	5:L:158:LEU:HD21	2.55	0.42
5:L:219:GLU:O	5:L:222:ALA:HB3	2.19	0.42
5:L:261:LEU:HD12	5:L:261:LEU:N	2.35	0.42
5:L:603:ARG:H	5:L:603:ARG:HG2	1.47	0.42
1:A:78:ILE:HA	1:A:78:ILE:HD13	1.79	0.42
1:A:208:ASN:N	1:A:208:ASN:OD1	2.44	0.42
1:B:12:ARG:O	1:B:29:GLU:O	2.37	0.42
1:B:195:ARG:HB3	1:B:198:LEU:HD21	2.02	0.42
2:C:52:ALA:HB2	2:C:461:GLU:HG3	2.01	0.42
2:C:169:LYS:O	2:C:169:LYS:HG2	2.20	0.42
2:C:269:ILE:HG23	2:C:273:HIS:CB	2.48	0.42
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.55	0.42
2:C:871:VAL:HG22	2:C:872:TYR:O	2.19	0.42
3:D:79:LYS:HG3	3:D:80:HIS:N	2.35	0.42
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.95	0.42
3:D:515:ARG:CZ	3:D:719:PHE:CE2	3.02	0.42
3:D:528:THR:HG22	3:D:532:GLU:OE1	2.20	0.42
3:D:1291:GLU:CD	3:J:1302:TYR:OH	2.58	0.42
3:D:1365:TYR:O	3:D:1366:HIS:C	2.58	0.42
5:F:551:LEU:HA	5:F:551:LEU:HD23	1.79	0.42
1:H:109:PRO:HA	1:H:132:HIS:HA	2.02	0.42
1:H:214:GLU:HG2	1:H:218:ARG:HE	1.85	0.42
2:I:75:LEU:HD13	2:I:75:LEU:HA	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:241:LEU:HD12	2:I:241:LEU:HA	1.71	0.42
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.20	0.42
2:I:718:ALA:HB3	2:I:781:ASP:H	1.85	0.42
2:I:836:LEU:CD1	2:I:1054:LEU:HD13	2.46	0.42
3:J:64:PRO:HG3	3:J:90:VAL:CG1	2.49	0.42
3:J:211:GLU:OE2	3:J:214:ARG:NH2	2.53	0.42
3:J:888:CYS:HB2	3:J:898:CYS:SG	2.59	0.42
3:J:1261:LEU:HD12	3:J:1261:LEU:C	2.40	0.42
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.20	0.42
5:L:599:ARG:O	5:L:604:SER:OG	2.37	0.42
1:A:101:THR:HG22	1:A:103:ASN:HD21	1.85	0.42
1:B:51:MET:HB3	1:B:178:SER:HA	2.02	0.42
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.61	0.42
2:C:5:TYR:HB2	2:C:781:ASP:OD1	2.20	0.42
2:C:100:LEU:HA	2:C:100:LEU:HD23	1.70	0.42
2:C:718:ALA:HB2	2:C:783:LEU:HD21	2.02	0.42
2:C:1144:PHE:O	2:C:1147:ARG:HB2	2.18	0.42
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.84	0.42
3:D:22:ILE:HD13	3:D:22:ILE:HG21	1.79	0.42
3:D:214:ARG:HA	3:D:217:LEU:HB2	2.02	0.42
3:D:737:ILE:O	3:D:740:LEU:N	2.49	0.42
3:D:1177:ILE:HG13	3:D:1186:TYR:O	2.20	0.42
5:F:306:PHE:HE1	5:F:315:TRP:CE2	2.37	0.42
5:F:462:LYS:HE3	5:F:488:LEU:HD11	2.01	0.42
1:H:134:THR:HG23	1:H:135:ASP:H	1.83	0.42
2:I:260:LYS:HE3	2:I:262:TYR:CE1	2.55	0.42
2:I:721:GLY:N	2:I:740:GLU:OE1	2.40	0.42
2:I:903:ARG:NH2	2:I:910:ALA:HB2	2.35	0.42
2:I:1233:LEU:HD22	2:I:1233:LEU:N	2.34	0.42
3:J:489:ASN:HA	3:J:904:ALA:HB1	2.01	0.42
5:L:363:ARG:O	5:L:367:ILE:HG13	2.20	0.42
5:L:483:LEU:H	5:L:483:LEU:CD1	2.30	0.42
2:C:179:TYR:H	2:C:397:LEU:HA	1.85	0.41
3:D:8:LEU:HD23	3:D:9:LYS:H	1.84	0.41
3:D:18:ASP:HB2	3:D:1373:ARG:NH1	2.35	0.41
3:D:318:GLY:C	3:D:320:ASN:N	2.73	0.41
3:D:354:VAL:HG12	3:D:355:ILE:N	2.35	0.41
3:D:490:ILE:HG21	3:D:490:ILE:HD13	1.68	0.41
3:D:1342:ASP:OD1	3:D:1344:LEU:N	2.48	0.41
1:G:190:ALA:O	1:G:198:LEU:HB2	2.20	0.41
1:G:231:PHE:HA	1:H:218:ARG:HH11	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:HIS:CE1	1:H:206:GLU:HG2	2.54	0.41
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	2.02	0.41
2:I:1136:GLN:O	2:I:1137:GLU:HB3	2.20	0.41
2:I:1161:LEU:HD12	2:I:1161:LEU:HA	1.67	0.41
3:J:132:LEU:O	3:J:132:LEU:HD22	2.20	0.41
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.84	0.41
3:J:482:ALA:O	3:J:488:ASN:ND2	2.54	0.41
3:J:694:SER:O	3:J:698:MET:HB2	2.20	0.41
3:J:702:GLN:HG2	3:J:703:THR:N	2.30	0.41
5:L:101:TYR:O	5:L:102:MET:C	2.57	0.41
5:L:470:MET:C	5:L:478:PRO:HD3	2.41	0.41
1:A:67:GLU:H	1:A:67:GLU:HG2	1.45	0.41
1:A:190:ALA:HB2	1:A:200:LYS:CB	2.41	0.41
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.84	0.41
2:C:96:LEU:HD12	2:C:96:LEU:HA	1.77	0.41
2:C:310:ILE:HG21	2:C:325:LEU:HB3	2.03	0.41
2:C:603:ILE:H	2:C:603:ILE:HG12	1.65	0.41
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.01	0.41
2:C:700:VAL:HG21	2:C:1114:GLU:HG2	2.01	0.41
2:C:857:VAL:HG23	2:C:862:LEU:HD11	2.02	0.41
2:C:895:LEU:H	2:C:895:LEU:HG	1.54	0.41
2:C:1075:VAL:O	2:C:1075:VAL:HG12	2.20	0.41
3:D:83:VAL:O	3:D:91:GLU:HA	2.20	0.41
3:D:447:ILE:HD13	3:D:447:ILE:HG21	1.64	0.41
5:F:227:GLN:OE1	5:F:251:LYS:NZ	2.53	0.41
5:F:230:VAL:HG13	5:F:231:THR:H	1.85	0.41
1:G:172:LEU:H	1:G:172:LEU:CD1	2.33	0.41
1:H:7:GLU:CD	1:H:8:PHE:N	2.73	0.41
2:I:339:ASN:HB3	2:I:343:HIS:H	1.84	0.41
2:I:672:GLU:H	2:I:672:GLU:HG3	1.54	0.41
2:I:798:GLN:OE1	2:I:828:PHE:CD1	2.73	0.41
2:I:850:ILE:HD12	2:I:850:ILE:HG23	1.77	0.41
2:I:1088:ASP:OD1	2:I:1092:THR:N	2.53	0.41
3:J:307:LEU:HA	3:J:307:LEU:HD23	1.19	0.41
3:J:434:ILE:HG21	3:J:434:ILE:HD13	1.46	0.41
3:J:473:THR:HG23	3:J:476:ALA:H	1.85	0.41
5:L:466:ILE:HD11	5:L:487:MET:CE	2.51	0.41
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.62	0.41
1:A:78:ILE:HD12	1:A:78:ILE:HG23	1.77	0.41
1:A:154:PRO:O	1:A:158:ARG:HG3	2.20	0.41
2:C:494:ASN:HD22	2:C:497:PRO:CD	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:676:ALA:O	2:C:677:ASN:C	2.58	0.41
2:C:799:ASN:HA	2:C:1231:TYR:HA	2.02	0.41
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.60	0.41
2:C:1246:ARG:CZ	3:D:348:ASP:OD1	2.69	0.41
2:C:1278:LEU:HA	2:C:1278:LEU:HD23	1.67	0.41
3:D:440:VAL:O	3:D:442:ILE:HG12	2.21	0.41
3:D:872:LEU:O	3:D:877:VAL:HG12	2.20	0.41
5:F:230:VAL:HG13	5:F:231:THR:N	2.36	0.41
1:G:54:CYS:HB3	1:G:148:ARG:HG2	2.01	0.41
2:I:363:LEU:HA	2:I:363:LEU:HD23	1.62	0.41
2:I:395:TYR:HE2	2:I:397:LEU:CD1	2.33	0.41
2:I:593:LYS:HG3	2:I:595:THR:HG23	2.02	0.41
2:I:959:ASP:O	2:I:963:GLU:HG2	2.21	0.41
2:I:1330:ILE:HD13	2:I:1330:ILE:HG21	1.75	0.41
3:J:252:LEU:HD22	3:J:260:PHE:HD2	1.85	0.41
3:J:309:ASN:HB2	3:J:326:SER:HB3	2.02	0.41
3:J:331:ILE:HD13	3:J:331:ILE:HG21	1.67	0.41
3:J:352:ARG:HB3	3:J:467:ALA:HA	2.02	0.41
3:J:514:THR:CB	3:J:576:ARG:HG2	2.47	0.41
3:J:530:PRO:O	3:J:533:ALA:HB3	2.20	0.41
3:J:762:ASN:OD1	3:J:764:ARG:N	2.53	0.41
3:J:1144:LEU:HA	3:J:1144:LEU:HD23	1.57	0.41
3:J:1151:LYS:O	3:J:1153:PRO:HD3	2.21	0.41
3:J:1344:LEU:HD12	3:J:1344:LEU:N	2.35	0.41
5:L:130:VAL:HA	5:L:133:SER:HB2	2.01	0.41
2:C:867:GLU:H	2:C:867:GLU:HG3	1.30	0.41
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.20	0.41
2:C:1120:ALA:O	2:C:1123:GLY:N	2.53	0.41
2:C:1178:LYS:HD3	2:C:1178:LYS:HA	1.55	0.41
3:D:10:ALA:O	3:D:11:GLN:HB2	2.21	0.41
3:D:74:LYS:CD	3:D:87:LYS:HD3	2.47	0.41
3:D:117:LEU:HA	3:D:117:LEU:HD12	1.77	0.41
3:D:530:PRO:O	3:D:531:LYS:C	2.57	0.41
1:G:50:SER:HB2	1:H:8:PHE:HZ	1.86	0.41
1:G:52:PRO:HG2	1:G:219:ARG:NH2	2.34	0.41
1:G:226:GLU:O	1:G:229:GLU:HB2	2.20	0.41
1:H:102:LEU:HA	1:H:102:LEU:HD23	1.66	0.41
2:I:540:ARG:H	2:I:540:ARG:HG3	1.50	0.41
2:I:819:SER:OG	2:I:820:GLU:N	2.50	0.41
2:I:1251:TYR:CD1	2:I:1301:ARG:NH2	2.89	0.41
3:J:270:ARG:O	3:J:273:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:278:ARG:O	3:J:281:ARG:HB2	2.20	0.41
3:J:556:GLU:O	3:J:564:VAL:N	2.47	0.41
3:J:796:LEU:HD12	3:J:796:LEU:HA	1.61	0.41
3:J:1177:ILE:HG13	3:J:1186:TYR:O	2.21	0.41
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	2.02	0.41
4:K:6:VAL:HG12	4:K:51:LEU:HD13	2.02	0.41
1:B:151:GLY:O	1:B:177:TYR:CD2	2.70	0.41
2:C:9:LYS:HG2	2:C:1171:ARG:HD3	2.02	0.41
2:C:142:GLU:CG	2:C:760:ASN:HD21	2.31	0.41
2:C:149:LEU:HG	2:C:451:ARG:HH11	1.84	0.41
2:C:1184:THR:HG22	2:C:1185:PRO:O	2.20	0.41
3:D:95:THR:O	3:D:95:THR:HG23	2.20	0.41
3:D:233:LYS:HA	3:D:234:PRO:HD3	1.87	0.41
3:D:430:HIS:ND1	3:D:430:HIS:N	2.66	0.41
3:D:501:VAL:HG22	3:D:502:PRO:O	2.20	0.41
3:D:506:VAL:H	3:D:506:VAL:HG12	1.52	0.41
3:D:536:LEU:O	3:D:539:SER:OG	2.37	0.41
3:D:614:LEU:O	3:D:615:LYS:C	2.59	0.41
3:D:821:MET:HA	3:D:881:LYS:HA	2.01	0.41
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.84	0.41
5:F:161:LEU:C	5:F:262:VAL:HG23	2.41	0.41
5:F:575:GLU:O	5:F:579:GLN:HG2	2.20	0.41
2:I:948:ILE:O	2:I:951:MET:HB3	2.20	0.41
2:I:1281:TYR:CE2	3:J:431:ARG:HB2	2.55	0.41
2:I:1322:SER:O	2:I:1325:VAL:N	2.53	0.41
3:J:266:ASN:O	3:J:267:ASP:C	2.57	0.41
3:J:844:THR:HG21	3:J:858:VAL:CG2	2.50	0.41
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.20	0.41
4:K:10:VAL:HG13	4:K:16:ARG:HB2	2.02	0.41
5:L:284:GLU:OE2	5:L:359:LYS:HD2	2.20	0.41
5:L:601:PRO:HB2	5:L:605:GLU:HG2	2.01	0.41
1:A:43:LEU:HA	1:A:43:LEU:HD23	1.64	0.41
2:C:194:LEU:HA	2:C:194:LEU:HD12	1.33	0.41
2:C:626:GLU:HB3	2:C:628:HIS:CE1	2.55	0.41
2:C:929:ILE:O	2:C:930:ASP:HB2	2.19	0.41
2:C:960:LEU:O	2:C:963:GLU:HB2	2.20	0.41
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.35	0.41
3:D:203:GLU:O	3:D:207:GLU:HG2	2.19	0.41
3:D:334:LYS:CG	3:D:335:GLN:H	2.32	0.41
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.66	0.41
3:D:884:SER:OG	3:D:886:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:909:ILE:HD12	3:D:909:ILE:HA	1.85	0.41
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.03	0.41
3:D:1256:ILE:HA	3:D:1256:ILE:HD13	1.74	0.41
1:H:17:GLU:OE1	1:H:25:LYS:HD3	2.20	0.41
1:H:195:ARG:CB	1:H:198:LEU:HD21	2.50	0.41
2:I:176:ILE:HD13	2:I:176:ILE:HG21	1.74	0.41
2:I:618:GLN:HG3	2:I:619:ALA:N	2.36	0.41
2:I:1132:LEU:O	2:I:1132:LEU:HD23	2.19	0.41
2:I:1301:ARG:HH11	2:I:1301:ARG:HD2	1.71	0.41
2:I:1331:ARG:HH11	2:I:1331:ARG:HD3	1.72	0.41
3:J:146:VAL:HG12	3:J:147:ILE:N	2.36	0.41
3:J:546:ALA:O	3:J:573:THR:HA	2.20	0.41
3:J:709:ARG:C	3:J:711:GLY:N	2.74	0.41
3:J:735:ALA:O	3:J:738:ARG:HB3	2.20	0.41
4:K:53:GLU:HB3	4:K:59:ILE:CG1	2.50	0.41
5:L:236:LYS:HD3	5:L:236:LYS:N	2.35	0.41
5:L:412:LEU:N	5:L:435:ILE:HG12	2.36	0.41
5:L:552:THR:H	5:L:552:THR:HG23	1.65	0.41
2:C:639:LYS:O	2:C:641:GLU:N	2.54	0.41
2:C:818:VAL:HG22	2:C:1096:ILE:HG12	2.03	0.41
3:D:543:SER:OG	3:D:544:LEU:N	2.52	0.41
3:D:649:LYS:HD2	3:D:652:GLU:OE1	2.21	0.41
3:D:656:GLU:O	3:D:659:ALA:N	2.54	0.41
3:D:891:ASP:O	3:D:892:PHE:HB2	2.20	0.41
4:E:32:VAL:O	4:E:34:GLY:N	2.52	0.41
5:F:223:GLU:O	5:F:226:ALA:HB3	2.21	0.41
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.63	0.41
1:H:45:ARG:HH11	1:H:45:ARG:HD3	1.69	0.41
2:I:538:LEU:H	2:I:538:LEU:HG	1.33	0.41
2:I:696:ASP:HB3	2:I:697:LYS:H	1.62	0.41
2:I:888:THR:CG2	2:I:916:SER:OG	2.68	0.41
2:I:1198:LEU:HD22	2:I:1198:LEU:HA	1.78	0.41
3:J:72:CYS:SG	3:J:73:GLY:N	2.94	0.41
3:J:863:LEU:HD11	3:J:901:ARG:HB3	2.02	0.41
3:J:1175:LEU:O	3:J:1187:GLU:HA	2.21	0.41
3:J:1219:ASP:O	3:J:1220:ILE:C	2.58	0.41
5:L:518:HIS:O	5:L:519:LEU:C	2.58	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.31	0.41
2:C:289:VAL:HG13	2:C:319:LEU:HD11	2.03	0.41
2:C:513:GLN:NE2	2:C:526:TYR:CE2	2.89	0.41
2:C:530:ILE:HG23	2:C:530:ILE:HD12	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.20	0.41
3:D:83:VAL:H	3:D:83:VAL:HG12	1.56	0.41
3:D:500:ILE:HD12	3:D:500:ILE:HG23	1.78	0.41
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	2.02	0.41
3:D:1158:GLU:HG3	3:D:1186:TYR:CZ	2.56	0.41
5:F:396:ASN:C	5:F:398:GLY:N	2.74	0.41
1:G:61:ILE:HG22	1:G:62:ASP:N	2.35	0.41
1:G:66:HIS:NE2	2:I:929:ILE:HG22	2.36	0.41
1:G:86:LYS:NZ	1:G:174:ASP:HB2	2.36	0.41
1:H:93:GLN:HB2	1:H:120:ASP:HB3	2.02	0.41
2:I:596:ASP:CG	2:I:597:GLY:H	2.23	0.41
2:I:688:GLN:HB2	2:I:1235:LEU:HD22	2.01	0.41
2:I:807:TRP:HE3	2:I:808:ASN:HB2	1.85	0.41
3:J:147:ILE:HD11	3:J:179:LYS:HZ3	1.85	0.41
3:J:294:ASN:HD21	5:L:402:LEU:HD23	1.85	0.41
3:J:909:ILE:O	3:J:909:ILE:HG23	2.19	0.41
3:J:1160:SER:HA	3:J:1204:VAL:O	2.21	0.41
1:A:112:ALA:O	1:A:115:ILE:HG13	2.20	0.41
1:A:228:LEU:HD11	1:B:224:LEU:HD23	2.03	0.41
1:A:273:GLU:OE2	1:A:293:PRO:HD2	2.21	0.41
2:C:24:VAL:HG12	2:C:25:PRO:O	2.21	0.41
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.83	0.41
2:C:138:ILE:HD11	2:C:506:PHE:HB3	2.02	0.41
2:C:548:ARG:HB3	2:C:569:ILE:O	2.21	0.41
2:C:719:LYS:O	2:C:779:ARG:HG3	2.21	0.41
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	2.02	0.41
2:C:1172:LEU:HD22	2:C:1172:LEU:O	2.21	0.41
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.91	0.41
3:D:31:ARG:CZ	3:D:106:GLU:OE2	2.69	0.41
3:D:112:ALA:O	3:D:300:GLN:NE2	2.46	0.41
3:D:205:LEU:C	3:D:205:LEU:HD13	2.41	0.41
3:D:390:LEU:N	3:D:390:LEU:HD12	2.36	0.41
3:D:442:ILE:HD12	3:D:442:ILE:HG23	1.72	0.41
3:D:733:SER:O	3:D:735:ALA:N	2.54	0.41
4:E:62:GLN:O	4:E:66:VAL:HG23	2.21	0.41
5:F:137:TYR:HA	5:F:138:PRO:HD3	1.95	0.41
5:F:442:SER:O	5:F:445:ASP:N	2.54	0.41
5:F:557:LYS:O	5:F:561:MET:N	2.52	0.41
1:G:118:ASP:HB3	1:G:121:VAL:HG21	2.02	0.41
1:H:16:ILE:HA	1:H:26:VAL:HG13	2.03	0.41
1:H:44:ARG:HG3	1:H:183:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:ARG:HH12	3:J:370:LYS:HZ3	1.68	0.41
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.94	0.41
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.86	0.41
2:I:195:PHE:CB	2:I:203:LYS:HD3	2.50	0.41
2:I:212:ALA:HA	2:I:359:ARG:HG3	2.03	0.41
2:I:344:GLY:O	2:I:346:TYR:CD2	2.74	0.41
2:I:517:GLN:O	2:I:518:ASN:C	2.60	0.41
2:I:521:LEU:HA	2:I:521:LEU:HD12	1.82	0.41
2:I:523:GLU:HG2	2:I:527:LYS:CE	2.36	0.41
2:I:617:ALA:HB3	2:I:653:MET:HB2	2.02	0.41
2:I:756:TYR:CD1	2:I:756:TYR:N	2.83	0.41
2:I:761:GLN:HA	2:I:762:ASN:HA	1.84	0.41
2:I:794:LEU:HD21	2:I:796:LEU:HD21	2.01	0.41
2:I:807:TRP:HE1	2:I:1086:PRO:HG3	1.85	0.41
2:I:829:THR:HG23	2:I:1059:ARG:HG2	2.03	0.41
3:J:425:ARG:HH11	3:J:425:ARG:HD2	1.60	0.41
3:J:849:LEU:HD22	3:J:849:LEU:H	1.86	0.41
3:J:908:ILE:HD13	3:J:909:ILE:N	2.35	0.41
3:J:1223:LEU:HD13	3:J:1223:LEU:HA	1.73	0.41
5:L:118:ASP:O	5:L:122:ARG:HG3	2.20	0.41
5:L:124:GLU:O	5:L:128:ASN:HB2	2.19	0.41
5:L:127:ILE:H	5:L:127:ILE:HG13	1.70	0.41
5:L:262:VAL:HG12	5:L:264:LYS:HG3	2.02	0.41
1:B:214:GLU:O	1:B:218:ARG:HG3	2.21	0.41
2:C:210:LEU:O	2:C:215:TYR:HB2	2.21	0.41
2:C:311:CYS:SG	2:C:311:CYS:O	2.79	0.41
2:C:384:LEU:O	2:C:387:ASN:N	2.54	0.41
2:C:619:ALA:HB1	2:C:657:THR:HA	2.03	0.41
2:C:667:LEU:HD23	2:C:667:LEU:HA	1.84	0.41
2:C:831:ILE:HG21	2:C:831:ILE:HD13	1.85	0.41
2:C:1049:ILE:HD13	2:C:1049:ILE:HG21	1.75	0.41
2:C:1143:GLU:OE1	2:C:1147:ARG:HD3	2.21	0.41
3:D:20:ILE:HG21	3:D:20:ILE:HD13	1.85	0.41
3:D:120:LEU:HB3	3:D:121:PRO:HD3	2.02	0.41
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.56	0.41
3:D:556:GLU:HG2	3:D:558:ASP:HB2	2.02	0.41
3:D:697:MET:O	3:D:701:LEU:HB2	2.21	0.41
3:D:1291:GLU:C	3:D:1292:LEU:HD12	2.41	0.41
3:D:1364:ALA:O	3:D:1367:GLN:HB3	2.20	0.41
2:I:65:ASN:O	2:I:105:TYR:HD2	2.03	0.41
2:I:229:ILE:HG21	2:I:240:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:865:LEU:HD23	2:I:865:LEU:HA	1.77	0.41
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.57	0.41
2:I:1342:GLU:O	3:J:1369:ARG:NH2	2.54	0.41
3:J:368:LEU:HD23	3:J:368:LEU:C	2.41	0.41
3:J:601:ILE:HG21	3:J:601:ILE:HD13	1.61	0.41
3:J:795:TYR:HE2	3:J:799:ARG:NE	2.17	0.41
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.52	0.41
1:A:12:ARG:HG2	1:A:13:LEU:H	1.85	0.40
2:C:145:ILE:N	2:C:145:ILE:HD12	2.37	0.40
2:C:328:SER:OG	2:C:330:HIS:CD2	2.73	0.40
2:C:624:ASP:OD1	2:C:625:GLU:N	2.52	0.40
2:C:929:ILE:HD13	2:C:929:ILE:HG21	1.73	0.40
2:C:1172:LEU:HD22	2:C:1172:LEU:C	2.42	0.40
2:C:1211:ARG:O	2:C:1211:ARG:HG3	2.21	0.40
3:D:54:ASP:N	3:D:54:ASP:OD1	2.54	0.40
3:D:770:LEU:O	3:D:774:ILE:HG13	2.21	0.40
3:D:1257:VAL:HA	3:D:1260:MET:HE2	2.03	0.40
3:D:1264:ALA:O	3:D:1278:GLU:N	2.34	0.40
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.80	0.40
1:G:75:GLN:HG2	1:G:76:GLU:OE2	2.20	0.40
1:G:108:GLY:HA2	1:G:109:PRO:HD3	1.90	0.40
1:G:170:ARG:O	1:G:171:LEU:HD13	2.20	0.40
1:H:19:VAL:O	1:H:23:HIS:HB3	2.21	0.40
2:I:606:LEU:HD12	2:I:606:LEU:N	2.37	0.40
2:I:663:VAL:HG23	2:I:664:GLY:N	2.36	0.40
2:I:896:THR:OG1	2:I:899:GLU:HG3	2.21	0.40
3:J:470:VAL:CG1	3:J:472:LEU:HD23	2.49	0.40
3:J:648:GLU:OE2	3:J:649:LYS:HE2	2.21	0.40
3:J:847:ASP:HA	3:J:860:ARG:H	1.86	0.40
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.48	0.40
2:C:77:GLU:HA	2:C:78:PRO:HD3	1.84	0.40
2:C:131:THR:HG22	2:C:135:THR:N	2.11	0.40
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.03	0.40
2:C:660:VAL:HG13	2:C:661:VAL:N	2.36	0.40
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.56	0.40
2:C:725:GLN:O	2:C:725:GLN:HG2	2.21	0.40
2:C:836:LEU:O	2:C:1052:VAL:N	2.44	0.40
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.86	0.40
2:C:1243:MET:HA	3:D:353:SER:CB	2.51	0.40
3:D:242:LEU:HD23	3:D:243:PRO:O	2.21	0.40
3:D:1237:VAL:HG13	3:D:1238:GLN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1307:LEU:N	3:D:1307:LEU:HD12	2.36	0.40
3:D:1321:SER:HB2	3:D:1349:GLU:OE2	2.21	0.40
5:F:269:LEU:O	5:F:272:SER:N	2.54	0.40
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.86	0.40
2:I:1332:SER:OG	3:J:327:LEU:HD13	2.21	0.40
3:J:184:ALA:O	3:J:187:ALA:HB3	2.21	0.40
1:A:182:ARG:O	1:A:183:ILE:HD12	2.21	0.40
2:C:47:TYR:HD2	2:C:47:TYR:HA	1.72	0.40
2:C:109:ALA:HB1	2:C:111:GLU:HA	2.02	0.40
2:C:142:GLU:N	2:C:760:ASN:OD1	2.54	0.40
2:C:817:LEU:HD23	2:C:1078:LYS:HB3	2.04	0.40
2:C:836:LEU:N	2:C:836:LEU:CD1	2.82	0.40
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	2.03	0.40
2:C:1120:ALA:HB1	2:C:1198:LEU:CD1	2.51	0.40
3:D:205:LEU:HD13	3:D:205:LEU:O	2.22	0.40
3:D:259:ARG:HD2	5:F:505:ILE:HD13	2.03	0.40
3:D:1233:ILE:O	3:D:1234:VAL:C	2.58	0.40
5:F:144:LEU:HA	5:F:144:LEU:HD12	1.78	0.40
5:F:379:MET:HG2	5:F:416:VAL:HG22	2.03	0.40
1:G:20:SER:O	1:G:21:SER:C	2.59	0.40
1:G:73:GLY:O	1:G:134:THR:HG22	2.22	0.40
2:I:27:LEU:HD23	2:I:27:LEU:HA	1.78	0.40
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.73	0.40
2:I:643:SER:OG	2:I:645:PHE:HE1	2.05	0.40
2:I:1046:VAL:H	2:I:1046:VAL:HG12	1.59	0.40
3:J:97:VAL:O	3:J:101:ARG:HG3	2.21	0.40
3:J:188:LEU:O	3:J:191:SER:OG	2.28	0.40
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.72	0.40
3:J:422:LEU:HA	3:J:422:LEU:HD12	1.83	0.40
3:J:836:ARG:HG3	3:J:869:CYS:HB3	2.03	0.40
3:J:847:ASP:HB3	3:J:856:ILE:CG2	2.51	0.40
5:L:587:ILE:HA	5:L:590:ILE:CD1	2.51	0.40
1:A:85:LEU:O	1:A:86:LYS:C	2.58	0.40
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.91	0.40
1:A:316:MET:HB2	5:F:600:HIS:CE1	2.57	0.40
1:B:88:LEU:HA	1:B:88:LEU:HD12	1.74	0.40
2:C:208:ILE:HD13	2:C:208:ILE:HG21	1.79	0.40
2:C:617:ALA:HB3	2:C:653:MET:CG	2.51	0.40
2:C:842:ASP:HB2	2:C:1045:GLY:O	2.21	0.40
2:C:930:ASP:HB3	2:C:1053:TYR:HB2	2.03	0.40
2:C:1062:PRO:HA	2:C:1076:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:ARG:NH2	3:D:717:VAL:HG23	2.37	0.40
3:D:592:VAL:H	3:D:592:VAL:HG22	1.69	0.40
3:D:1347:LEU:HG	3:D:1357:ILE:CG2	2.50	0.40
5:F:107:THR:OG1	5:F:108:VAL:N	2.53	0.40
5:F:110:LEU:HD23	5:F:110:LEU:HA	1.73	0.40
1:G:38:THR:N	1:H:45:ARG:NH1	2.70	0.40
2:I:41:GLN:NE2	2:I:73:TYR:CZ	2.89	0.40
2:I:62:TYR:C	2:I:64:GLY:N	2.74	0.40
2:I:791:LEU:HA	2:I:791:LEU:HD23	1.73	0.40
2:I:801:ARG:HA	2:I:1228:GLY:O	2.22	0.40
2:I:861:ALA:HB1	2:I:882:ILE:HD13	2.03	0.40
2:I:976:ARG:HH12	2:I:990:ASP:HB3	1.86	0.40
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.61	0.40
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.70	0.40
2:I:1247:SER:OG	2:I:1248:THR:N	2.51	0.40
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.85	0.40
3:J:872:LEU:CD2	3:J:877:VAL:HG11	2.43	0.40
5:L:112:THR:OG1	5:L:115:GLY:N	2.51	0.40
5:L:230:VAL:HG13	5:L:231:THR:N	2.36	0.40
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.86	0.40
5:L:519:LEU:C	5:L:519:LEU:HD23	2.42	0.40
5:L:565:ILE:HG22	5:L:566:ASP:OD2	2.21	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.51	0.40
1:A:76:GLU:HB3	1:A:81:ILE:HG12	2.03	0.40
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.67	0.40
1:B:40:GLY:HA3	1:B:185:TYR:CD1	2.56	0.40
1:B:103:ASN:HA	1:B:141:SER:HB2	2.03	0.40
1:B:112:ALA:HA	1:B:115:ILE:HD11	2.03	0.40
1:B:215:GLU:HA	1:B:218:ARG:CD	2.51	0.40
2:C:556:GLY:HA2	2:C:659:GLN:O	2.21	0.40
2:C:615:VAL:HG21	2:C:645:PHE:CD2	2.57	0.40
2:C:746:ALA:HA	2:C:974:ARG:NH2	2.34	0.40
2:C:811:ASN:OD1	2:C:811:ASN:N	2.48	0.40
2:C:1251:TYR:CE1	2:C:1301:ARG:CZ	3.04	0.40
2:C:1313:HIS:HD2	3:D:477:GLN:NE2	2.19	0.40
4:E:39:VAL:HG13	4:E:52:ARG:HH21	1.86	0.40
5:F:148:TYR:OH	5:F:218:ARG:HA	2.21	0.40
5:F:476:ARG:HG3	5:F:477:GLU:N	2.35	0.40
5:F:606:VAL:O	5:F:609:SER:OG	2.40	0.40
1:G:14:VAL:HG13	1:G:27:THR:HB	2.03	0.40
1:H:31:LEU:HB2	1:H:199:ASP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:VAL:HG22	1:H:99:ILE:H	1.87	0.40
2:I:109:ALA:HB1	2:I:111:GLU:HA	2.03	0.40
2:I:239:MET:HG2	2:I:240:GLU:O	2.21	0.40
2:I:729:ALA:O	2:I:755:LYS:HD3	2.22	0.40
3:J:201:LEU:HD22	3:J:217:LEU:HD13	2.02	0.40
3:J:215:LYS:HD2	3:J:216:LYS:N	2.36	0.40
3:J:268:LEU:HD13	3:J:306:LEU:HD23	2.04	0.40
3:J:392:THR:HG21	5:L:609:SER:HB3	2.04	0.40
5:L:343:LYS:O	5:L:347:ILE:HG13	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:ASP:OD1	5:F:554:ARG:NH2[4_455]	1.99	0.21
2:C:44:GLU:OE1	5:F:596:ARG:NH1[4_455]	2.05	0.15
2:C:940:GLU:OE1	1:H:139:SER:OG[4_455]	2.05	0.15

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/329 (93%)	271 (89%)	25 (8%)	9 (3%)	4	33
1	B	213/329 (65%)	191 (90%)	20 (9%)	2 (1%)	17	57
1	G	222/329 (68%)	182 (82%)	28 (13%)	12 (5%)	2	19
1	H	213/329 (65%)	193 (91%)	20 (9%)	0	100	100
2	C	1338/1342 (100%)	1225 (92%)	103 (8%)	10 (1%)	22	61
2	I	1338/1342 (100%)	1226 (92%)	100 (8%)	12 (1%)	17	57
3	D	1162/1407 (83%)	1074 (92%)	79 (7%)	9 (1%)	19	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	1151/1407 (82%)	1064 (92%)	82 (7%)	5 (0%)	34	71
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	461/613 (75%)	422 (92%)	37 (8%)	2 (0%)	34	71
5	L	463/613 (76%)	423 (91%)	39 (8%)	1 (0%)	47	79
All	All	7030/8222 (86%)	6424 (91%)	544 (8%)	62 (1%)	17	57

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	30	PRO
1	A	324	ALA
1	B	232	VAL
2	C	345	PRO
2	C	516	ASP
2	C	519	ASN
2	C	1159	VAL
3	D	10	ALA
1	G	13	LEU
1	G	14	VAL
1	G	62	ASP
1	G	162	GLU
2	I	516	ASP
2	I	1159	VAL
1	B	13	LEU
2	C	170	VAL
1	G	172	LEU
2	I	170	VAL
2	I	519	ASN
2	I	761	GLN
3	J	108	ALA
1	A	294	ASN
2	C	697	LYS
2	C	761	GLN
3	D	110	PRO
3	D	586	GLY
1	G	19	VAL
2	I	345	PRO
1	A	14	VAL

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Mol	Chain	Res	Type
1	A	167	PRO
2	C	1158	LYS
3	D	806	ASP
1	G	136	GLU
1	G	164	ASP
2	I	697	LYS
3	J	710	ASP
1	A	62	ASP
2	C	63	SER
2	C	760	ASN
3	D	710	ASP
5	F	477	GLU
1	G	49	SER
1	G	167	PRO
1	G	230	ALA
2	I	63	SER
2	I	484	LEU
2	I	514	PHE
2	I	1158	LYS
1	A	196	THR
3	D	108	ALA
5	F	513	ASP
1	G	134	THR
3	J	831	VAL
3	D	826	ILE
3	D	831	VAL
3	J	1180	VAL
5	L	477	GLU
2	I	1186	VAL
3	J	826	ILE
3	D	1180	VAL
1	A	178	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/286 (94%)	249 (93%)	19 (7%)	14	48
1	B	184/286 (64%)	166 (90%)	18 (10%)	8	36
1	G	191/286 (67%)	179 (94%)	12 (6%)	18	53
1	H	183/286 (64%)	165 (90%)	18 (10%)	8	36
2	C	1155/1157 (100%)	1046 (91%)	109 (9%)	8	38
2	I	1154/1157 (100%)	1046 (91%)	108 (9%)	8	38
3	D	975/1168 (84%)	875 (90%)	100 (10%)	7	34
3	J	967/1168 (83%)	869 (90%)	98 (10%)	7	34
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	31
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	54
5	F	416/540 (77%)	373 (90%)	43 (10%)	7	34
5	L	418/540 (77%)	372 (89%)	46 (11%)	6	31
All	All	6050/7024 (86%)	5467 (90%)	583 (10%)	8	37

All (583) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	29	GLU
1	A	50	SER
1	A	61	ILE
1	A	74	VAL
1	A	115	ILE
1	A	133	LEU
1	A	145	LYS
1	A	165	GLU
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	A	233	ASP
1	A	234	LEU
1	A	245	GLU
1	A	246	LYS
1	A	284	ARG
1	A	310	ARG
1	B	6	THR
1	B	7	GLU
1	B	8	PHE

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Mol	Chain	Res	Type
1	B	18	GLN
1	B	29	GLU
1	B	58	GLU
1	B	60	GLU
1	B	65	LEU
1	B	75	GLN
1	B	79	LEU
1	B	80	GLU
1	B	97	GLU
1	B	107	ILE
1	B	110	VAL
1	B	124	VAL
1	B	134	THR
1	B	183	ILE
1	B	193	GLU
2	C	4	SER
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE
2	C	42	ASP
2	C	60	GLN
2	C	70	TYR
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	132	ASP
2	C	167	SER
2	C	189	ASP
2	C	285	ILE
2	C	299	LYS
2	C	306	THR
2	C	320	ASP
2	C	360	LEU
2	C	369	MET

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Mol	Chain	Res	Type
2	C	377	THR
2	C	394	ARG
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	496	LYS
2	C	538	LEU
2	C	539	THR
2	C	542	ARG
2	C	554	HIS
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	706	ARG
2	C	714	VAL
2	C	748	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	799	ASN
2	C	800	MET
2	C	814	ASP
2	C	817	LEU
2	C	819	SER

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Mol	Chain	Res	Type
2	C	826	ASP
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	919	ARG
2	C	944	ARG
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1006	GLU
2	C	1040	ASP
2	C	1073	LYS
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1198	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1238	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	9	LYS

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Mol	Chain	Res	Type
3	D	18	ASP
3	D	26	SER
3	D	29	MET
3	D	46	TYR
3	D	79	LYS
3	D	84	ILE
3	D	94	GLN
3	D	95	THR
3	D	98	ARG
3	D	106	GLU
3	D	159	ILE
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	217	LEU
3	D	230	SER
3	D	252	LEU
3	D	312	ARG
3	D	324	LEU
3	D	330	MET
3	D	334	LYS
3	D	352	ARG
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	425	ARG
3	D	454	CYS
3	D	490	ILE
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	514	THR
3	D	523	GLU
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
3	D	587	LEU
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU

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Mol	Chain	Res	Type
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	805	GLN
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	1135	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG

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Mol	Chain	Res	Type
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1333	THR
3	D	1343	GLU
4	E	3	ARG
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	28	ARG
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	154	GLU
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	306	PHE
5	F	310	GLU
5	F	335	GLU
5	F	341	LEU
5	F	395	THR
5	F	401	PHE
5	F	417	ASP
5	F	422	ARG
5	F	429	THR
5	F	437	GLN
5	F	445	ASP
5	F	449	THR
5	F	450	ILE

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Mol	Chain	Res	Type
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	482	GLU
5	F	485	GLU
5	F	486	ARG
5	F	488	LEU
5	F	489	MET
5	F	491	GLU
5	F	492	ASP
5	F	502	LYS
5	F	508	GLU
5	F	530	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	587	ILE
5	F	606	VAL
1	G	13	LEU
1	G	58	GLU
1	G	65	LEU
1	G	79	LEU
1	G	124	VAL
1	G	133	LEU
1	G	160	HIS
1	G	161	SER
1	G	163	GLU
1	G	171	LEU
1	G	176	CYS
1	G	193	GLU
1	H	8	PHE
1	H	18	GLN
1	H	27	THR
1	H	29	GLU
1	H	58	GLU
1	H	60	GLU
1	H	65	LEU

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Mol	Chain	Res	Type
1	H	75	GLN
1	H	79	LEU
1	H	80	GLU
1	H	97	GLU
1	H	107	ILE
1	H	110	VAL
1	H	124	VAL
1	H	134	THR
1	H	171	LEU
1	H	183	ILE
1	H	193	GLU
2	I	4	SER
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	46	GLN
2	I	60	GLN
2	I	70	TYR
2	I	82	VAL
2	I	85	CYS
2	I	90	VAL
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	132	ASP
2	I	167	SER
2	I	189	ASP
2	I	285	ILE
2	I	299	LYS
2	I	306	THR
2	I	320	ASP
2	I	360	LEU
2	I	369	MET
2	I	377	THR
2	I	394	ARG
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP

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Mol	Chain	Res	Type
2	I	445	ILE
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	496	LYS
2	I	514	PHE
2	I	538	LEU
2	I	539	THR
2	I	542	ARG
2	I	554	HIS
2	I	589	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	639	LYS
2	I	657	THR
2	I	672	GLU
2	I	680	LEU
2	I	684	ASN
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	757	THR
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	819	SER
2	I	826	ASP
2	I	840	SER
2	I	859	GLU
2	I	878	THR

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Mol	Chain	Res	Type
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	944	ARG
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	984	VAL
2	I	992	LEU
2	I	1002	LEU
2	I	1006	GLU
2	I	1040	ASP
2	I	1073	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1198	LEU
2	I	1210	ILE
2	I	1237	HIS
2	I	1238	LEU
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	26	SER
3	J	29	MET
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	84	ILE

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Mol	Chain	Res	Type
3	J	94	GLN
3	J	95	THR
3	J	98	ARG
3	J	159	ILE
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	217	LEU
3	J	252	LEU
3	J	312	ARG
3	J	324	LEU
3	J	330	MET
3	J	334	LYS
3	J	352	ARG
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	425	ARG
3	J	430	HIS
3	J	454	CYS
3	J	490	ILE
3	J	506	VAL
3	J	513	MET
3	J	514	THR
3	J	523	GLU
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	568	SER
3	J	573	THR
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU

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Mol	Chain	Res	Type
3	J	702	GLN
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	764	ARG
3	J	770	LEU
3	J	788	LEU
3	J	798	ARG
3	J	805	GLN
3	J	810	THR
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	881	LYS
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL
3	J	1273	ASP
3	J	1274	PHE
3	J	1275	LEU
3	J	1278	GLU
3	J	1281	GLU

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Mol	Chain	Res	Type
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	154	GLU
5	L	247	GLU
5	L	266	PHE
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	306	PHE
5	L	310	GLU
5	L	335	GLU
5	L	341	LEU
5	L	395	THR
5	L	401	PHE
5	L	417	ASP
5	L	422	ARG
5	L	429	THR
5	L	437	GLN
5	L	445	ASP
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	492	ASP

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Mol	Chain	Res	Type
5	L	502	LYS
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	587	ILE
5	L	603	ARG
5	L	606	VAL
5	L	613	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	343	HIS
2	C	494	ASN
2	C	628	HIS
2	C	761	GLN
2	C	799	ASN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1136	GLN
2	C	1146	GLN
2	C	1237	HIS
2	C	1288	GLN
2	C	1299	ASN
2	C	1307	ASN
2	C	1313	HIS
2	C	1314	GLN
3	D	94	GLN
3	D	200	GLN
3	D	340	GLN
3	D	365	GLN

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Mol	Chain	Res	Type
3	D	450	HIS
3	D	594	GLN
3	D	669	GLN
3	D	702	GLN
3	D	716	GLN
3	D	907	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1218	HIS
3	D	1227	HIS
5	F	131	GLN
5	F	362	ASN
5	F	396	ASN
5	F	406	GLN
5	F	446	GLN
5	F	472	GLN
5	F	518	HIS
1	G	41	ASN
1	H	132	HIS
2	I	139	ASN
2	I	343	HIS
2	I	494	ASN
2	I	628	HIS
2	I	658	GLN
2	I	688	GLN
2	I	760	ASN
2	I	761	GLN
2	I	1116	HIS
2	I	1146	GLN
2	I	1220	GLN
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	206	ASN
3	J	294	ASN
3	J	364	HIS
3	J	365	GLN
3	J	419	HIS
3	J	560	ASN
3	J	702	GLN
3	J	716	GLN
3	J	817	HIS

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Mol	Chain	Res	Type
3	J	910	ASN
3	J	929	GLN
3	J	1259	GLN
3	J	1268	ASN
3	J	1279	GLN
3	J	1366	HIS
4	K	7	GLN
5	L	129	GLN
5	L	227	GLN
5	L	446	GLN
5	L	455	HIS
5	L	472	GLN
5	L	600	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	309/329 (93%)	-0.31	2 (0%) 89 81	99, 147, 225, 245	0
1	B	217/329 (65%)	-0.01	6 (2%) 53 37	112, 194, 254, 272	0
1	G	224/329 (68%)	-0.07	3 (1%) 77 63	163, 206, 241, 270	0
1	H	217/329 (65%)	0.07	13 (5%) 21 12	146, 213, 252, 285	0
2	C	1340/1342 (99%)	-0.35	21 (1%) 72 57	74, 121, 234, 285	0
2	I	1340/1342 (99%)	-0.16	48 (3%) 42 28	86, 159, 261, 388	0
3	D	1166/1407 (82%)	-0.30	14 (1%) 79 66	72, 112, 215, 264	0
3	J	1155/1407 (82%)	-0.22	24 (2%) 63 48	86, 138, 229, 274	0
4	E	89/91 (97%)	-0.02	2 (2%) 62 45	147, 183, 216, 241	0
4	K	79/91 (86%)	0.79	14 (17%) 1 1	202, 277, 319, 350	0
5	F	467/613 (76%)	-0.23	12 (2%) 56 40	93, 165, 290, 340	0
5	L	469/613 (76%)	-0.29	7 (1%) 73 60	116, 178, 288, 353	0
All	All	7072/8222 (86%)	-0.22	166 (2%) 60 44	72, 147, 251, 388	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.1
3	D	335	GLN	6.4
2	I	1001	GLY	5.5
1	B	160	HIS	5.0
2	I	1000	LEU	5.0
3	J	208	THR	4.7
2	C	1002	LEU	4.6
2	I	983	GLY	4.5
2	I	981	ALA	4.5
2	C	251	ALA	4.4
5	L	489	MET	4.4

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Mol	Chain	Res	Type	RSRZ
2	C	1003	THR	4.4
2	I	998	LEU	4.4
2	C	231	GLU	4.4
2	C	1001	GLY	4.3
2	I	979	LEU	4.3
5	F	319	ALA	4.2
2	I	999	GLU	4.2
2	I	1002	LEU	4.2
3	D	712	GLN	4.1
5	F	326	TRP	4.1
5	F	323	ASN	4.0
2	I	414	ILE	4.0
3	J	218	THR	3.9
1	H	96	ASP	3.8
4	E	2	ALA	3.8
2	C	319	LEU	3.8
4	K	36	ASP	3.7
4	K	72	GLN	3.7
2	C	1000	LEU	3.7
5	L	490	PRO	3.6
4	K	33	GLY	3.6
2	I	1004	ASP	3.6
3	J	931	THR	3.5
3	D	1202	GLU	3.5
1	H	135	ASP	3.5
2	I	105	TYR	3.4
4	K	37	PRO	3.4
2	I	987	GLU	3.3
5	L	111	LEU	3.3
1	H	106	GLY	3.3
2	I	985	GLU	3.2
3	J	542	ALA	3.2
2	I	266	GLY	3.2
2	I	1007	LYS	3.2
5	L	425	TYR	3.2
2	I	1010	GLN	3.2
2	I	984	VAL	3.1
2	I	1003	THR	3.1
5	F	318	ALA	3.1
1	H	72	GLU	3.1
1	H	97	GLU	3.1
3	J	675	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
4	K	40	PRO	3.1
1	B	172	LEU	3.0
5	F	338	HIS	3.0
4	K	26	ARG	3.0
2	I	986	ALA	3.0
2	I	727	VAL	3.0
3	J	528	THR	2.9
2	C	1004	ASP	2.9
3	J	1296	GLY	2.9
5	L	315	TRP	2.9
5	F	325	PRO	2.9
2	I	975	ILE	2.9
2	I	972	PHE	2.9
3	J	712	GLN	2.9
3	J	830	ASP	2.9
2	C	893	THR	2.8
4	K	2	ALA	2.9
2	C	258	ASN	2.8
1	B	69	SER	2.8
2	C	267	ARG	2.8
2	I	978	VAL	2.8
1	B	70	THR	2.8
3	D	1204	VAL	2.8
3	D	218	THR	2.7
3	J	1297	LYS	2.7
5	F	167	ASP	2.7
2	I	1005	GLU	2.7
5	F	301	ASN	2.7
2	I	973	SER	2.7
2	I	751	TYR	2.7
1	B	67	GLU	2.7
2	I	1006	GLU	2.6
2	I	1316	GLU	2.6
3	D	1161	GLY	2.6
3	J	1295	ASN	2.6
2	I	375	PRO	2.5
2	I	912	ASP	2.5
2	I	267	ARG	2.5
2	C	317	LEU	2.5
3	D	1172	LYS	2.5
3	J	335	GLN	2.5
5	L	167	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	247	ARG	2.5
3	D	830	ASP	2.5
3	D	207	GLU	2.5
3	D	518	VAL	2.5
3	J	564	VAL	2.5
1	H	66	HIS	2.5
4	K	35	LYS	2.4
2	I	111	GLU	2.4
3	D	826	ILE	2.4
3	J	826	ILE	2.4
2	I	165	HIS	2.4
2	I	725	GLN	2.4
2	I	169	LYS	2.4
3	J	1249	ASN	2.4
2	I	969	ALA	2.4
2	I	1009	ASN	2.3
1	G	194	GLN	2.3
5	F	283	GLN	2.3
2	C	318	SER	2.3
2	I	1020	GLU	2.3
5	F	332	ASP	2.3
1	G	164	ASP	2.3
3	D	208	THR	2.3
2	C	232	ILE	2.3
2	I	1008	GLN	2.3
3	D	217	LEU	2.3
4	K	41	GLU	2.2
1	H	14	VAL	2.2
1	H	27	THR	2.2
4	K	13	ILE	2.2
2	I	988	LYS	2.2
1	H	74	VAL	2.2
2	C	257	ALA	2.2
4	E	34	GLY	2.2
1	B	91	ARG	2.2
4	K	77	ALA	2.2
4	K	14	GLY	2.2
1	A	245	GLU	2.2
2	I	247	ARG	2.2
3	J	1202	GLU	2.2
4	K	58	LEU	2.2
1	H	13	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	193	GLU	2.2
2	C	164	THR	2.2
3	J	207	GLU	2.2
5	F	307	THR	2.1
5	L	304	THR	2.1
1	H	107	ILE	2.1
3	D	1201	GLY	2.1
2	C	271	ALA	2.1
5	F	293	GLU	2.1
2	I	234	ASP	2.1
1	A	274	ALA	2.1
2	I	720	ARG	2.1
3	J	1161	GLY	2.1
2	C	999	GLU	2.1
3	J	557	LYS	2.1
3	J	674	THR	2.1
3	J	732	GLY	2.1
2	I	185	ASP	2.1
2	I	67	GLU	2.1
2	I	373	GLY	2.1
3	J	1198	VAL	2.0
4	K	32	VAL	2.0
1	H	86	LYS	2.0
2	I	1141	LEU	2.0
2	C	165	HIS	2.0
2	C	243	PRO	2.0
3	J	1204	VAL	2.0
1	H	233	ASP	2.0
3	J	708	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	ZN	D	1502	1/1	0.81	0.13	134,134,134,134	0
6	MG	J	1501	1/1	0.92	0.35	94,94,94,94	0
6	MG	D	1501	1/1	0.94	0.54	87,87,87,87	0
7	ZN	J	1503	1/1	0.95	0.09	97,97,97,97	0
7	ZN	J	1502	1/1	0.97	0.02	131,131,131,131	0
7	ZN	D	1503	1/1	0.99	0.06	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.