



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:04 AM UTC

PDB ID : 5UAG / pdb_00005uag
Title : Escherichia coli RNA polymerase mutant - RpoB D516V
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

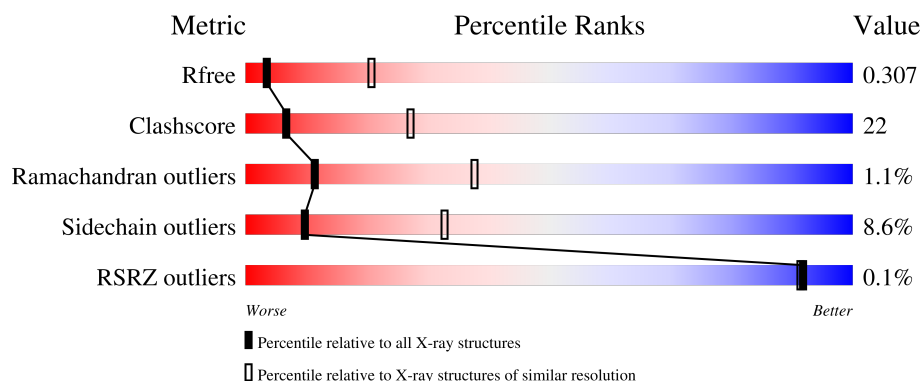
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	320	37% 31% 5% 27%
1	B	320	30% 32% • • 32%
1	G	320	36% 30% • • 29%
1	H	320	32% 33% • 32%
2	C	1342	55% 40% 5%

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Mol	Chain	Length	Quality of chain
2	I	1342	57% 39%
3	D	1407	46% 32% 5% 17%
3	J	1407	43% 33% 5% 18%
4	E	90	59% 32% 8%
4	K	90	% 54% 27% 6% 12%
5	F	613	43% 29% 24%
5	L	613	44% 28% 23%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55066 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	233	Total	C	N	O	S	0	0	0
			1812	1127	323	356	6			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	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
			10569	6632	1841	2053	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10565	6630	1840	2052	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2
I	516	VAL	ASP	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	1167	Total	C	N	O	S	0	0	0
			9065	5700	1622	1697	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	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.

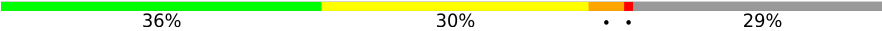
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

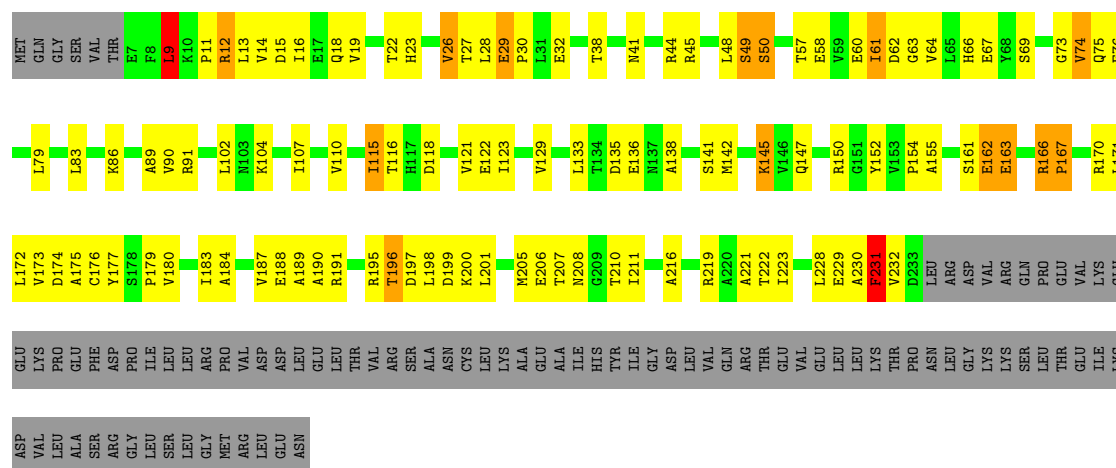
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

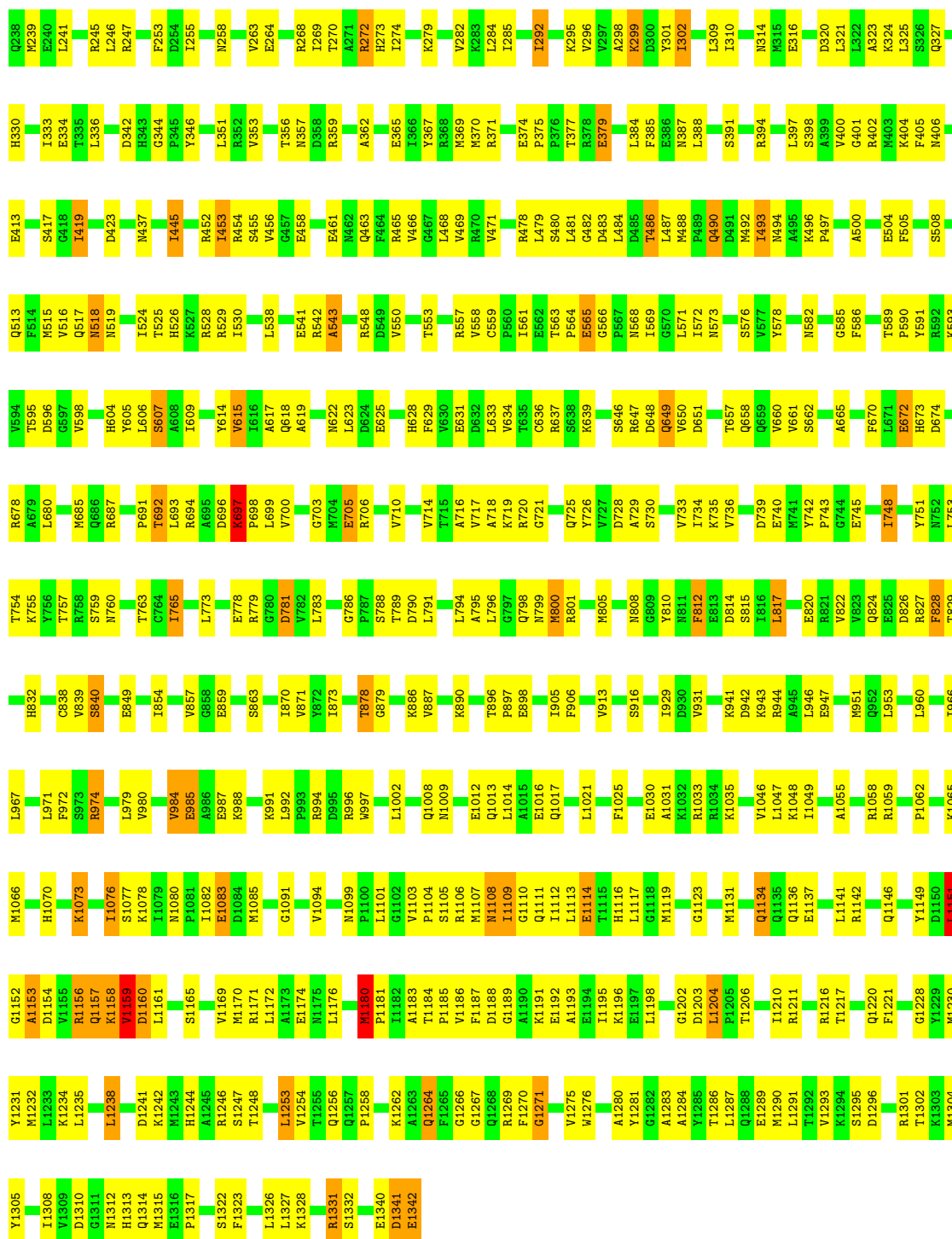
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Mg	0	0
			2	2		
6	I	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

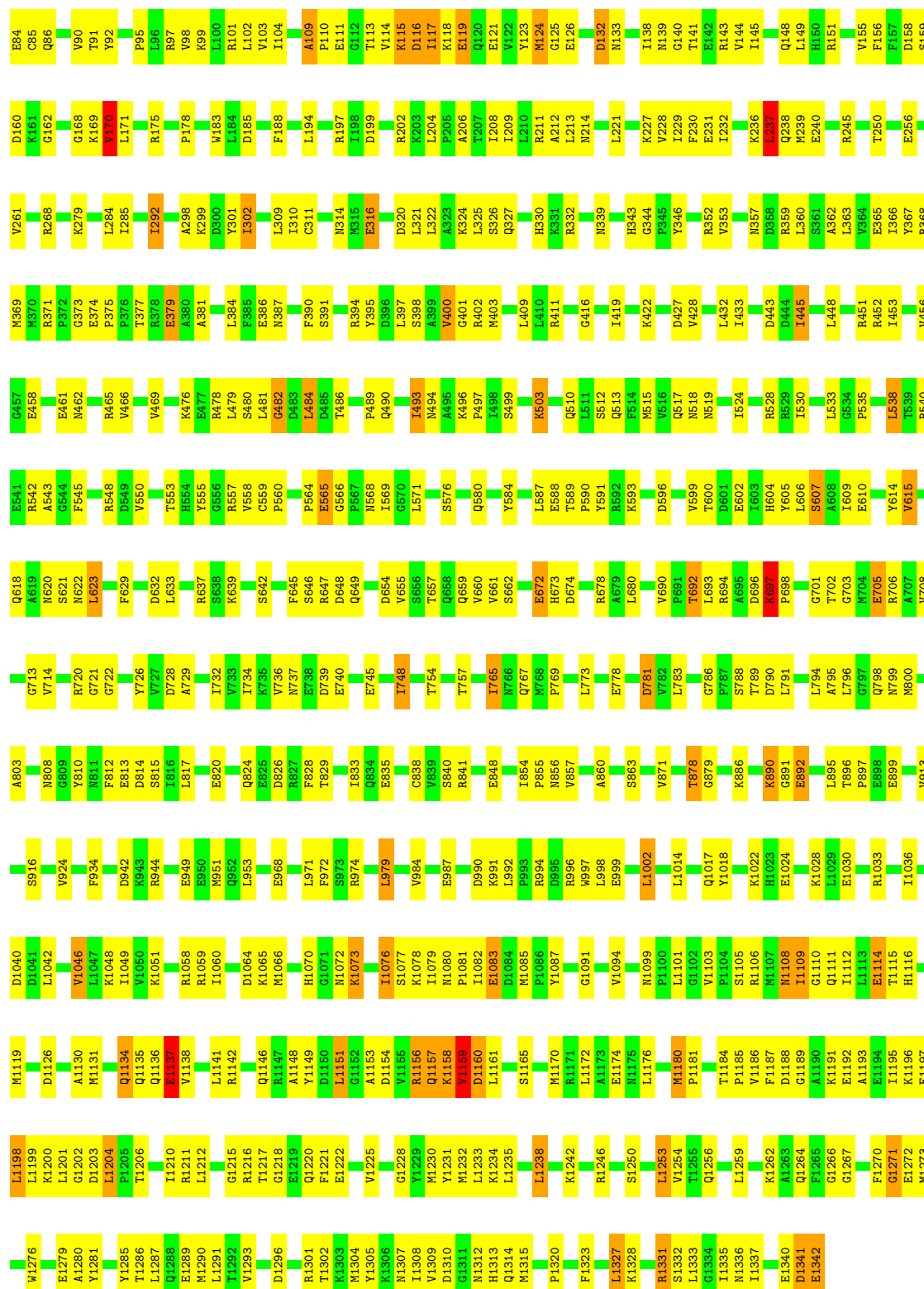
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

Chain G: 



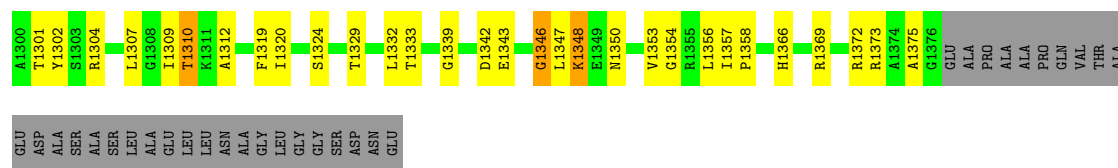




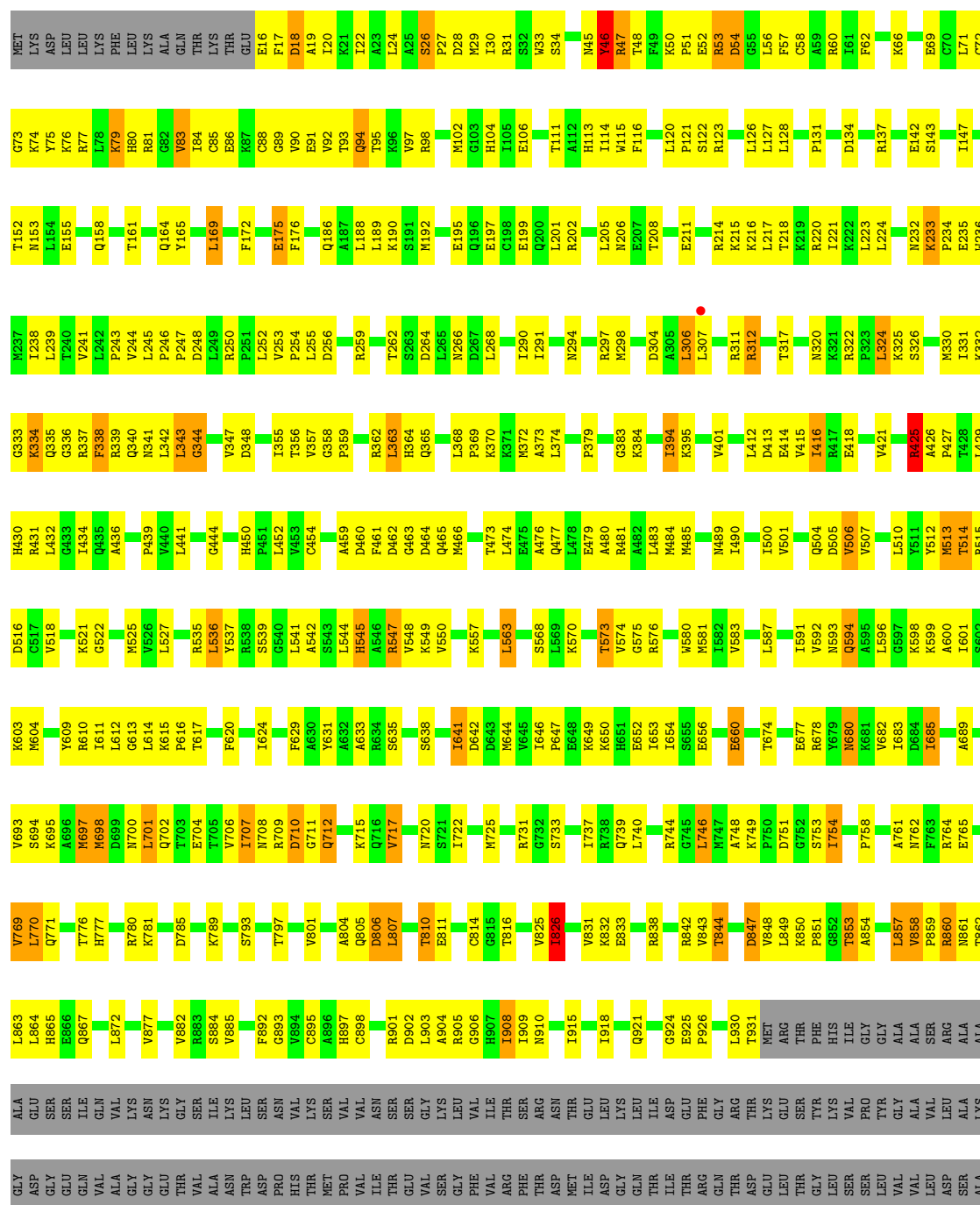
• Molecule 3: DNA-directed RNA polymerase subunit beta'

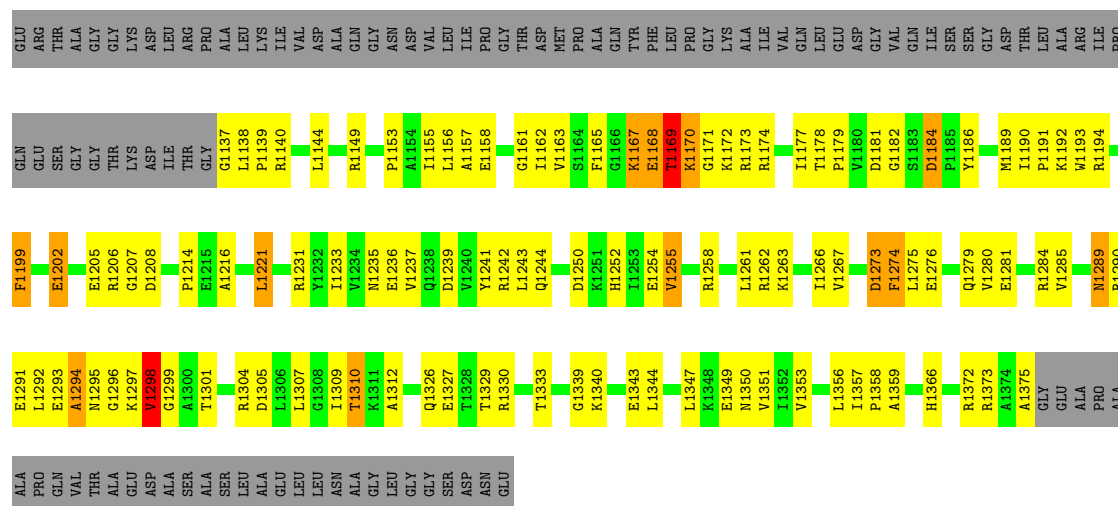
Chain D: 46% 32% 5% 17%

P1214	V1141	PRO	THR	GLY	V885	Q805	R709	B606	K521	I442	D348	F260	Q158	V83	MET
E1215	F1145	ALA	VAL	SER	D889	D806	D710	Y609	M525	I443	I355	A261	L169	I84	LYS
I1220	F1145	LEU	ALA	ILE	T890	L807	G712	G609	G526	E443	T356	T262	L189	C85	ASP
L1221	R1149	ILE	ASN	LYS	V891	V808	Q711	T609	L527	T890	V357	S263	C88	E86	LEU
G1225	P1153	VAL	THR	SER	D892	T810	K715	L612	E532	D891	G358	L265	D174	K87	LYS
V1226	A1154	ASP	PRO	ASN	G893	E811	Q716	G613	A633	E892	P359	N266	E175	C88	PHE
L1227	I1155	ALA	HIS	VAL	V894	C814	W717	L614	E534	H450	Y360	D267	K179	V92	L8
T1230	L1156	GLN	THR	LYS	C895	G815	W719	K615	E536	C454	L363	L268	M180	Q94	A10
I1233	A1157	GLY	PRO	VAL	H897	T816	R720	T617	L536	H364	Y269	Y269	Q94	T95	T12
V1234	E1158	VAL	VAL	VAL	C898	H817	S721	F629	Y537	A459	R278	R278	A184	T95	K13
V1237	I1159	ILE	ILE	ASN	R901	T820	I722	F629	R538	D460	L368	L279	L188	K96	K13
Q1238	S1160	SER	THR	SER	D902	V825	K725	A633	S539	F461	P369	K280	L189	V97	T14
L1243	I1162	GLY	GLU	GLY	L903	V825	S728	D641	L541	D462	M372	K280	K190	R93	E16
Q1244	V1163	THR	GLY	LYS	A904	L826	R731	L642	H545	G463	A373	T290	S191	R101	F17
G1245	K1167	ASP	PHE	VAL	G906	V831	G732	L646	A546	D464	M192	M102	M192	M102	D18
V1246	E1168	THR	VAL	ILE	H907	K832	G733	F647	R547	D464	G103	G103	G103	G103	A19
K1247	T1169	ARG	ARG	THR	I908	E833	S733	P647	V548	L472	L194	L194	L194	L194	I20
I1248	K1170	THR	THR	ARG	N910	L835	R737	K650	K549	T473	L201	E106	R202	E106	I22
H1252	G1171	ASN	ASN	ASN	N910	R836	Q738	H651	R551	L474	Y382	M298	L205	L107	S26
I1253	K1172	THR	THR	THR	E913	V839	L740	E652	E556	E475	L385	L306	S109	A108	P27
E1254	R1173	LEU	ILE	GLU	A914	V839	L740	L653	E557	A476	T208	T208	H113	H113	I30
V1255	R1174	PRO	ASP	LEU	I915	K842	M743	L654	D558	Q477	R311	R311	I114	I114	R31
R1258	L1175	GLY	GLY	LYS	1918	R842	R744	E656	E559	T487	T392	R312	R214	W115	W33
R1262	I1176	ALA	GLN	LEU	1918	T844	G745	A657	N560	A480	T393	G313	L217	K118	S34
K1263	I1177	ILE	THR	ILE	G924	V847	L746	E658	L563	M484	K395	R314	R220	S119	E42
I1266	P1178	VAL	THR	GLU	E925	V847	M747	L659	L563	M485	A396	R315	R220	L120	N45
V1267	V1180	GLN	ARG	PHE	P926	V848	K749	E660	S568	M486	V401	L316	L223	P121	Y46
S1272	D1181	LEU	GLN	GLY	L930	K850	P750	V661	S568	T487	L412	T317	L223	S122	R47
D1273	G1182	THR	THR	THR	T931	R851	P750	T674	S568	M488	L413	K321	E225	L126	T48
F1274	S1183	ASP	GLY	LYS	N932	V852	I754	T674	S568	M489	E414	R322	V228	L127	R53
E1275	D1184	VAL	LEU	GLU	ARG	V853	P758	E677	G575	L490	E414	R322	K233	L128	D54
G1277	P1185	THR	LEU	SER	THR	K854	I759	R678	R576	L491	V415	P323	P234	P131	G55
E1278	Y1186	GLY	THR	TYR	PHE	V858	P759	R678	R576	S492	E418	R325	P234	L132	L56
K1279	E1187	VAL	THR	LYS	HIS	R859	R764	N680	L578	S492	R417	R325	E235	R133	F57
Q1279	M1188	PRO	SER	VAL	ILE	R860	R764	N680	L578	M495	E418	R325	W236	D134	L56
V1280	M1189	GLY	SER	PRO	GLY	R861	R769	N683	N580	P498	H419	L327	V236	F57	F57
E1281	I1190	ASP	LEU	TYR	GLY	R862	V769	L683	N581	P498	P420	A328	E135	E135	R60
R1284	K1192	THR	VAL	GLY	ALA	L682	L770	L685	L591	V501	R425	R332	V241	E136	I61
V1285	W1193	LEU	VAL	ALA	ALA	L683	Q771	L685	V592	P502	A426	G333	L242	E136	R62
M1289	E1200	ARG	ASP	LEU	ARG	S694	V772	V693	V592	P502	P427	G333	V244	L139	C70
A1294	G1201	ALA	LEU	LEU	ARG	K695	H777	K695	G594	S503	T428	G336	Y140	Y140	L71
R1295	I1202	ILE	SER	GLY	ALA	L696	D785	K697	L596	S503	H430	R337	P247	F141	C72
A1296	R1203	GLY	THR	GLY	SER	N875	K789	K698	G597	L432	R431	F338	D248	E142	G73
G1296	V1204	GLY	GLY	GLN	ILE	V877	T797	L701	K598	L432	Q340	R339	P251	I147	K74
I1297	E1205	THR	GLY	GLN	ILE	V877	R798	Q702	K599	L434	R341	Q340	L252	T152	Y75
V1298	R1206	LYS	VAL	VAL	GLN	K881	W801	T705	L601	M513	L343	R345	V253	N153	K76
I1299	E1206	ASP	GLY	GLY	VAL	R882	D802	V706	S602	M514	A436	G344	L255	M154	R77
G1299	I1210	ILE	ARG	GLY	ASN	R883	D802	V706	R603	R515	F437	R345	L255	E155	L78
					LYS	S884		W708	L605	D516	P439	V347	R259	R156	K79
					LYS									Q157	H80



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





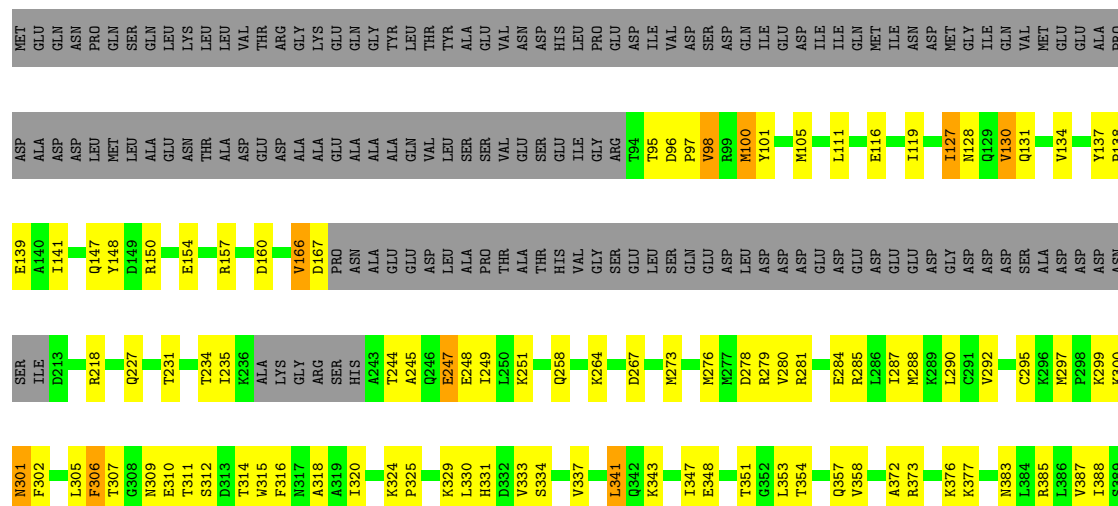
- Molecule 4: DNA-directed RNA polymerase subunit omega

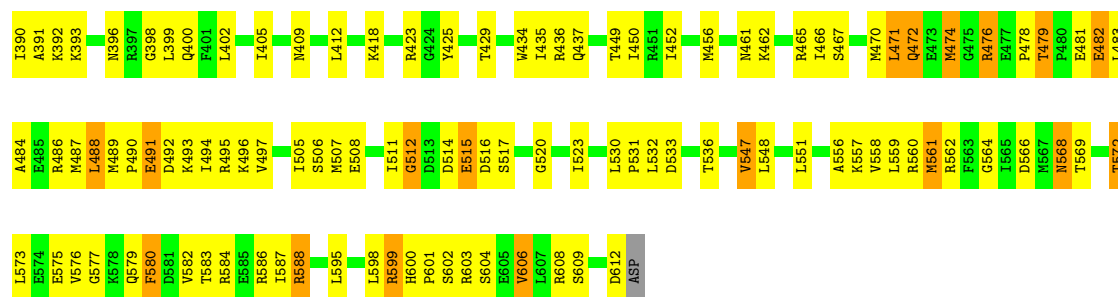


- Molecule 4: DNA-directed RNA polymerase subunit omega



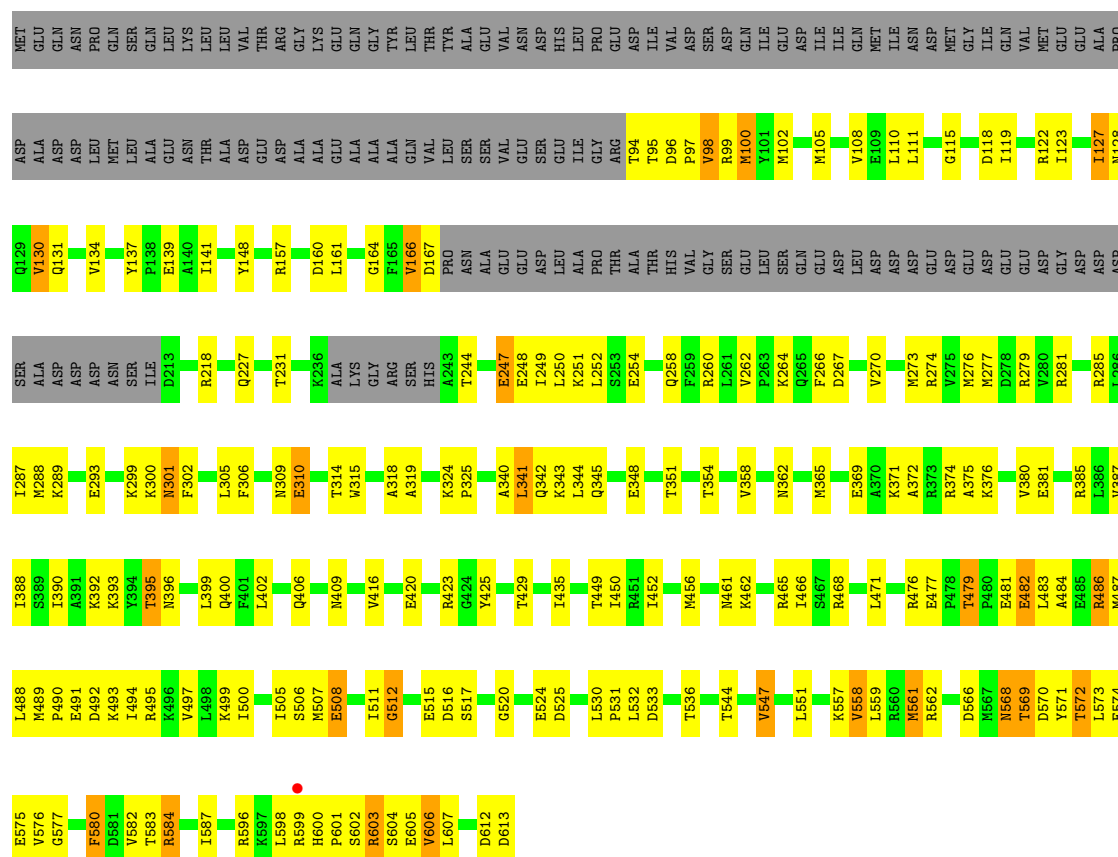
- Molecule 5: RNA polymerase sigma factor RpoD





• Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 44% 28% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.83Å 205.04Å 307.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.40 29.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.99-3.40) 88.9 (29.99-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.39Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.277 , 0.311 0.278 , 0.307	Depositor DCC
R_{free} test set	2000 reflections (1.24%)	wwPDB-VP
Wilson B-factor (Å ²)	135.9	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 101.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55066	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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	0.44	1/1834 (0.1%)	1.06	4/2485 (0.2%)
1	B	0.47	0/1697	1.33	17/2300 (0.7%)
1	G	0.49	1/1777 (0.1%)	1.06	3/2408 (0.1%)
1	H	0.44	0/1681	1.27	12/2278 (0.5%)
2	C	0.41	1/10738 (0.0%)	0.99	24/14488 (0.2%)
2	I	0.39	1/10734 (0.0%)	0.98	18/14483 (0.1%)
3	D	0.42	3/9205 (0.0%)	0.99	13/12430 (0.1%)
3	J	0.42	0/9140	1.00	19/12341 (0.2%)
4	E	0.40	0/693	0.92	0/935
4	K	0.40	0/629	0.98	2/847 (0.2%)
5	F	0.42	1/3864 (0.0%)	1.01	8/5194 (0.2%)
5	L	0.40	0/3872	1.02	3/5205 (0.1%)
All	All	0.42	8/55864 (0.0%)	1.02	123/75394 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	C	0	4
2	I	0	2
3	D	0	2
3	J	0	3
4	E	0	1
5	L	0	1
All	All	0	14

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	312	ARG	CA-C	8.91	1.56	1.52
2	I	373	GLY	C-N	8.24	1.50	1.33
1	G	29	GLU	C-N	7.77	1.52	1.33
5	F	476	ARG	CA-C	-5.83	1.48	1.52
2	C	543	ALA	CA-CB	-5.70	1.45	1.53
3	D	343	LEU	CG-CD2	-5.58	1.34	1.52
3	D	1346	GLY	CA-C	-5.43	1.45	1.52
1	A	29	GLU	C-N	5.30	1.46	1.33

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	53	ARG	N-CA-C	-10.43	93.73	110.20
3	D	53	ARG	N-CA-C	-10.02	94.36	110.20
3	J	425	ARG	NE-CZ-NH2	9.29	127.56	119.20
2	I	111	GLU	CA-C-N	8.05	131.38	120.92
2	I	111	GLU	C-N-CA	8.05	131.38	120.92
3	J	425	ARG	NE-CZ-NH1	-7.95	113.55	121.50
3	J	1199	PHE	N-CA-C	-7.89	98.12	109.96
1	B	68	TYR	CA-CB-CG	7.61	127.60	113.90
5	L	584	ARG	CB-CA-C	-7.31	106.11	116.34
2	C	111	GLU	CA-C-N	7.06	130.10	120.92
2	C	111	GLU	C-N-CA	7.06	130.10	120.92
3	D	1186	TYR	N-CA-C	7.01	120.40	109.96
3	J	54	ASP	N-CA-C	-6.95	91.55	111.00
2	I	237	LEU	N-CA-C	6.91	125.52	110.80
1	H	28	LEU	N-CA-C	6.80	120.12	108.02
2	I	316	GLU	CA-C-N	6.73	131.51	120.94
2	I	316	GLU	C-N-CA	6.73	131.51	120.94
2	C	541	GLU	CA-C-N	-6.73	111.48	120.63
2	C	541	GLU	C-N-CA	-6.73	111.48	120.63
3	D	54	ASP	N-CA-C	-6.73	92.15	111.00
3	D	1203	ARG	N-CA-C	-6.67	99.66	110.20
2	C	237	LEU	N-CA-C	6.66	125.00	110.80
2	I	813	GLU	CA-CB-CG	6.62	127.34	114.10
3	D	1199	PHE	N-CA-C	-6.62	100.03	109.96
1	G	49	SER	CA-C-N	-6.58	113.70	122.85
1	G	49	SER	C-N-CA	-6.58	113.70	122.85
1	G	12	ARG	NE-CZ-NH1	-6.53	114.97	121.50
5	L	584	ARG	N-CA-C	6.53	117.67	108.00
3	J	343	LEU	CB-CG-CD1	-6.51	91.16	110.70
5	F	476	ARG	N-CA-C	-6.49	101.67	111.34
1	B	8	PHE	N-CA-C	6.40	119.13	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	398	SER	CB-CA-C	-6.34	108.24	115.79
2	I	1271	GLY	N-CA-C	6.28	122.50	112.58
4	K	14	GLY	CA-C-N	6.28	133.53	121.54
4	K	14	GLY	C-N-CA	6.28	133.53	121.54
1	A	51	MET	N-CA-C	-6.22	100.75	110.14
1	H	200	LYS	N-CA-C	-6.17	101.07	110.14
1	B	17	GLU	N-CA-C	-6.08	97.80	108.20
5	F	588	ARG	CB-CG-CD	6.05	125.21	111.30
3	J	1298	VAL	CA-C-N	5.98	133.13	121.41
3	J	1298	VAL	C-N-CA	5.98	133.13	121.41
2	C	1264	GLN	N-CA-C	-5.93	96.72	107.75
2	I	482	GLY	CA-C-N	5.89	133.68	121.32
2	I	482	GLY	C-N-CA	5.89	133.68	121.32
3	D	913	GLU	CA-C-N	-5.87	114.61	122.42
3	D	913	GLU	C-N-CA	-5.87	114.61	122.42
2	I	543	ALA	N-CA-C	-5.86	100.11	109.96
3	J	89	GLY	N-CA-C	-5.85	99.31	113.18
1	A	28	LEU	CA-C-N	5.81	126.28	119.83
1	A	28	LEU	C-N-CA	5.81	126.28	119.83
2	I	117	ILE	N-CA-C	-5.80	100.07	108.36
1	H	31	LEU	CA-C-N	-5.78	111.23	121.29
1	H	31	LEU	C-N-CA	-5.78	111.23	121.29
3	D	343	LEU	CB-CG-CD2	-5.78	93.37	110.70
3	J	46	TYR	CA-C-N	-5.64	114.79	121.90
3	J	46	TYR	C-N-CA	-5.64	114.79	121.90
2	C	1151	LEU	CA-CB-CG	-5.63	96.60	116.30
2	I	124	MET	CA-CB-CG	-5.61	102.87	114.10
5	F	95	THR	CA-C-N	5.56	135.36	121.80
5	F	95	THR	C-N-CA	5.56	135.36	121.80
2	I	1157	GLN	N-CA-C	5.55	117.41	111.36
1	B	200	LYS	N-CA-C	-5.55	101.98	110.14
2	C	1157	GLN	CA-C-N	5.54	132.13	121.54
2	C	1157	GLN	C-N-CA	5.54	132.13	121.54
3	J	563	LEU	CB-CG-CD2	-5.54	94.09	110.70
1	B	88	LEU	N-CA-C	-5.49	100.84	109.25
2	I	162	GLY	CA-C-N	5.47	132.00	121.54
2	I	162	GLY	C-N-CA	5.47	132.00	121.54
1	B	198	LEU	N-CA-C	-5.47	101.10	109.41
2	C	162	GLY	CA-C-N	5.46	131.97	121.54
2	C	162	GLY	C-N-CA	5.46	131.97	121.54
1	H	12	ARG	N-CA-C	-5.46	100.78	109.07
5	F	436	ARG	CB-CA-C	5.45	119.83	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	THR	N-CA-C	5.43	120.05	113.38
2	I	1202	GLY	N-CA-C	-5.42	100.34	113.18
1	H	138	ALA	CA-C-N	-5.42	114.40	122.74
1	H	138	ALA	C-N-CA	-5.42	114.40	122.74
5	L	568	ASN	CB-CA-C	5.41	118.90	109.65
2	C	508	SER	N-CA-C	5.40	119.65	112.30
3	J	208	THR	N-CA-C	-5.39	100.51	109.46
2	I	1138	VAL	N-CA-C	5.38	117.78	111.05
3	D	1348	LYS	CA-CB-CG	5.38	124.86	114.10
1	B	177	TYR	N-CA-C	5.36	117.56	111.02
1	B	19	VAL	CA-C-N	5.34	131.75	121.54
1	B	19	VAL	C-N-CA	5.34	131.75	121.54
3	J	1294	ALA	CA-C-N	5.33	130.24	121.39
3	J	1294	ALA	C-N-CA	5.33	130.24	121.39
1	H	198	LEU	CA-C-N	-5.31	113.88	122.81
1	H	198	LEU	C-N-CA	-5.31	113.88	122.81
1	B	205	MET	CA-C-N	5.30	131.26	121.94
1	B	205	MET	C-N-CA	5.30	131.26	121.94
5	F	474	MET	CA-C-N	5.30	130.17	122.28
5	F	474	MET	C-N-CA	5.30	130.17	122.28
1	H	93	GLN	CB-CA-C	-5.29	99.90	110.42
3	D	1200	GLU	CB-CG-CD	-5.27	103.64	112.60
3	J	1169	THR	N-CA-CB	-5.23	101.66	110.49
1	B	29	GLU	N-CA-C	-5.22	99.76	109.06
3	D	563	LEU	CB-CG-CD2	-5.22	95.05	110.70
3	J	53	ARG	N-CA-CB	5.22	117.94	110.06
2	C	1180	MET	CG-SD-CE	-5.19	89.48	100.90
3	J	47	ARG	CG-CD-NE	5.18	123.40	112.00
2	C	649	GLN	N-CA-C	-5.15	99.83	110.80
2	C	272	ARG	CB-CA-C	-5.15	103.03	110.96
1	B	197	ASP	CA-C-N	5.14	131.45	122.82
1	B	197	ASP	C-N-CA	5.14	131.45	122.82
2	C	542	ARG	N-CA-C	5.13	116.73	111.03
1	H	17	GLU	N-CA-C	-5.13	99.42	108.20
2	I	1137	GLU	N-CA-CB	5.13	119.15	110.49
1	B	54	CYS	CA-C-N	5.11	130.82	122.81
1	B	54	CYS	C-N-CA	5.11	130.82	122.81
1	B	130	ILE	CG1-CB-CG2	-5.10	95.41	110.70
2	C	543	ALA	N-CA-C	-5.10	101.40	109.96
5	F	436	ARG	CG-CD-NE	5.08	123.17	112.00
3	J	52	GLU	N-CA-C	5.07	117.57	109.96
3	D	233	LYS	CB-CG-CD	-5.06	99.66	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	106	GLU	CA-C-N	-5.05	114.97	122.74
2	C	106	GLU	C-N-CA	-5.05	114.97	122.74
1	H	198	LEU	N-CA-C	-5.05	101.74	109.41
2	C	1271	GLY	N-CA-C	5.04	120.55	112.58
2	C	625	GLU	CA-CB-CG	5.03	124.15	114.10
3	D	208	THR	N-CA-C	-5.03	101.11	109.46
2	C	513	GLN	CA-CB-CG	5.02	124.13	114.10
2	C	812	PHE	CB-CA-C	-5.02	100.44	110.42

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
2	C	658	GLN	Sidechain
2	C	985	GLU	Mainchain
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
4	E	76	GLU	Sidechain
1	G	63	GLY	Mainchain
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1168	GLU	Mainchain
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
5	L	569	THR	Mainchain

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	1812	0	1839	113	0
1	B	1677	0	1703	130	0
1	G	1755	0	1773	107	0
1	H	1662	0	1687	116	0
2	C	10569	0	10587	460	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	10565	0	10581	453	0
3	D	9065	0	9210	449	0
3	J	9001	0	9165	479	0
4	E	691	0	695	27	0
4	K	627	0	634	26	0
5	F	3813	0	3880	163	0
5	L	3821	0	3884	157	0
6	D	2	0	0	0	0
6	I	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	55066	0	55638	2385	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (2385) 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)
2:I:1271:GLY:HA2	3:J:343:LEU:HD11	1.25	1.18
2:C:1269:ARG:HG2	3:D:343:LEU:HD12	1.24	1.11
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.35	1.08
3:J:54:ASP:OD2	3:J:60:ARG:NH1	1.89	1.03
2:I:1271:GLY:CA	3:J:343:LEU:HD11	1.87	1.03
2:C:1271:GLY:HA2	3:D:343:LEU:HD21	1.41	1.02
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.44	1.00
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.44	0.99
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.45	0.99
3:J:1167:LYS:HZ3	3:J:1170:LYS:HB2	1.27	0.98
5:F:562:ARG:HH21	5:F:573:LEU:HD23	1.28	0.98
1:B:75:GLN:HE22	1:B:132:HIS:HB2	1.29	0.95
1:A:14:VAL:HG13	1:A:15:ASP:H	1.31	0.95
5:F:595:LEU:O	5:F:599:ARG:HD3	1.66	0.95
2:C:40:GLU:O	2:C:73:TYR:OH	1.85	0.94
3:D:54:ASP:OD2	3:D:60:ARG:NH1	1.99	0.94
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.49	0.94
1:B:191:ARG:NH1	1:B:196:THR:O	2.00	0.93
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.48	0.92
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.51	0.92
2:C:1271:GLY:CA	3:D:343:LEU:HD21	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.53	0.91
2:I:674:ASP:OD1	2:I:1110:GLY:N	2.04	0.91
1:B:16:ILE:HG23	1:B:26:VAL:HG22	1.50	0.91
1:A:45:ARG:HG2	1:B:38:THR:HB	1.51	0.90
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.03	0.90
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.52	0.89
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.05	0.89
2:C:1269:ARG:HG2	3:D:343:LEU:CD1	2.02	0.89
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.05	0.88
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	1.89	0.88
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.54	0.88
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.07	0.87
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.56	0.87
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.54	0.87
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.55	0.87
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.56	0.87
2:I:18:ARG:NH1	2:I:621:SER:O	2.07	0.86
1:A:191:ARG:NH1	1:A:198:LEU:O	2.08	0.86
2:C:478:ARG:HG2	2:C:492:MET:HG2	1.57	0.86
2:I:560:PRO:O	3:J:780:ARG:NH2	2.09	0.86
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.40	0.86
3:D:392:THR:HG21	5:F:606:VAL:HA	1.58	0.86
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.58	0.85
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.59	0.85
2:I:1271:GLY:HA2	3:J:343:LEU:CD1	2.06	0.85
2:I:452:ARG:NH1	2:I:584:TYR:O	2.10	0.84
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.59	0.84
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.57	0.84
2:C:201:ARG:NH2	2:C:370:MET:O	2.09	0.84
2:C:324:LYS:O	2:C:327:GLN:NE2	2.11	0.84
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	1.92	0.83
5:L:97:PRO:HA	5:L:100:MET:HG3	1.61	0.83
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.61	0.83
2:I:721:GLY:N	2:I:740:GLU:OE1	2.12	0.83
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.61	0.82
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.61	0.82
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.11	0.82
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.15	0.81
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.26	0.81
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.61	0.81
3:D:45:ASN:HB3	3:D:48:THR:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.61	0.81
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.63	0.81
2:C:1271:GLY:HA2	3:D:343:LEU:CD2	2.11	0.81
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.09	0.81
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.63	0.81
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.44	0.80
2:C:721:GLY:N	2:C:740:GLU:OE1	2.15	0.80
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.17	0.80
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.44	0.80
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	1.97	0.80
5:L:602:SER:H	5:L:605:GLU:HG3	1.45	0.80
3:D:1263:LYS:HE2	3:D:1279:GLN:HE21	1.47	0.80
3:D:1167:LYS:HZ1	3:D:1170:LYS:HB2	1.45	0.79
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.12	0.79
1:H:158:ARG:HB3	1:H:172:LEU:HD23	1.63	0.79
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.63	0.79
1:G:83:LEU:HD23	2:I:694:ARG:HE	1.48	0.79
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.14	0.79
3:D:1263:LYS:HE2	3:D:1279:GLN:NE2	1.98	0.78
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.47	0.78
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.16	0.78
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.16	0.78
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.66	0.78
3:D:336:GLY:HA3	3:D:1324:SER:O	1.82	0.77
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.17	0.77
5:F:456:MET:HE1	5:F:497:VAL:HG13	1.65	0.77
5:L:551:LEU:HD21	5:L:598:LEU:HD21	1.65	0.77
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.65	0.77
1:B:79:LEU:HD11	3:D:526:VAL:HG21	1.65	0.77
1:B:154:PRO:HA	1:B:174:ASP:HB3	1.66	0.77
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.67	0.77
1:G:45:ARG:HG2	1:H:38:THR:HB	1.67	0.77
1:A:45:ARG:NH2	2:C:1216:ARG:HA	1.99	0.76
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.20	0.76
5:F:227:GLN:HE22	5:F:251:LYS:NZ	1.81	0.76
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.18	0.76
1:B:175:ALA:HB1	1:B:177:TYR:CE1	2.20	0.76
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.68	0.76
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.67	0.76
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.17	0.76
2:I:706:ARG:NH2	2:I:791:LEU:O	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.68	0.76
2:I:1296:ASP:HB3	2:I:1320:PRO:HB3	1.67	0.76
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.17	0.76
1:B:18:GLN:NE2	1:B:24:ALA:HB2	2.00	0.76
2:C:696:ASP:HB2	2:C:798:GLN:CG	2.15	0.76
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.68	0.76
1:B:16:ILE:HG12	1:B:26:VAL:HG13	1.68	0.75
3:D:1181:ASP:HA	3:J:202:ARG:HB3	1.68	0.75
4:K:14:GLY:O	4:K:16:ARG:N	2.20	0.75
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.67	0.75
5:F:388:ILE:O	5:F:392:LYS:HG3	1.86	0.75
2:C:1062:PRO:HA	2:C:1076:ILE:HG13	1.69	0.75
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.19	0.75
5:F:515:GLU:C	5:F:517:SER:H	1.95	0.75
1:B:153:VAL:O	1:B:175:ALA:N	2.15	0.75
4:E:13:ILE:HD12	4:E:19:LEU:HA	1.69	0.75
1:B:134:THR:HG23	1:B:135:ASP:H	1.49	0.75
3:D:418:GLU:HG3	4:E:45:LYS:H	1.51	0.75
1:H:90:VAL:HG13	1:H:123:ILE:HD12	1.69	0.75
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.69	0.74
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.20	0.74
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.67	0.74
1:G:12:ARG:H	1:G:30:PRO:HD2	1.53	0.74
1:G:231:PHE:HB3	1:H:218:ARG:HB3	1.69	0.74
3:J:127:LEU:O	3:J:220:ARG:NH2	2.20	0.74
1:A:158:ARG:NH2	1:A:173:VAL:O	2.17	0.74
1:H:27:THR:HG23	1:H:202:VAL:HG22	1.69	0.74
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.70	0.74
5:L:395:THR:OG1	5:L:396:ASN:N	2.21	0.74
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.70	0.74
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.69	0.74
5:L:601:PRO:HA	5:L:604:SER:HB3	1.69	0.74
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.70	0.73
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.69	0.73
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.70	0.73
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.69	0.73
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.69	0.73
1:H:32:GLU:HA	1:H:198:LEU:HD12	1.70	0.73
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.22	0.73
5:L:483:LEU:HD12	5:L:483:LEU:H	1.52	0.73
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.54	0.73
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.54	0.73
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.23	0.73
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.71	0.73
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.71	0.73
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.52	0.73
5:F:300:LYS:HE3	5:F:301:ASN:HD21	1.53	0.73
2:I:40:GLU:O	2:I:73:TYR:OH	2.06	0.73
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.04	0.73
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.71	0.72
3:J:709:ARG:O	3:J:711:GLY:N	2.22	0.72
3:J:1263:LYS:HE2	3:J:1279:GLN:HE21	1.54	0.72
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.37	0.72
3:D:1186:TYR:HE2	3:D:1188:GLU:HB2	1.54	0.72
3:J:114:ILE:HD11	3:J:311:ARG:HB2	1.70	0.72
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.72	0.72
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.05	0.72
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.71	0.71
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.23	0.71
2:C:40:GLU:HG2	2:C:41:GLN:N	2.05	0.71
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.72	0.71
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.73	0.71
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.56	0.71
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.73	0.71
3:D:709:ARG:O	3:D:711:GLY:N	2.24	0.71
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.71	0.71
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.24	0.71
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.25	0.71
1:A:9:LEU:O	1:B:227:GLN:NE2	2.24	0.70
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.73	0.70
1:G:14:VAL:HG13	1:G:15:ASP:H	1.56	0.70
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.72	0.70
3:D:842:ARG:NH1	3:D:1254:GLU:OE2	2.18	0.70
2:C:74:ARG:NH1	2:C:121:GLU:OE1	2.23	0.70
2:C:810:TYR:HE1	2:C:1078:LYS:HD2	1.55	0.70
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.73	0.70
1:B:18:GLN:CD	1:B:24:ALA:HB2	2.17	0.70
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.24	0.70
1:H:152:TYR:CE2	3:J:536:LEU:HD21	2.26	0.70
1:H:211:ILE:HD11	1:H:215:GLU:HG2	1.73	0.70
3:J:320:ASN:OD1	3:J:322:ARG:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:HIS:CE1	1:B:69:SER:OG	2.44	0.70
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.23	0.70
3:J:901:ARG:HD2	3:J:906:GLY:O	1.92	0.70
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	1.92	0.70
1:G:32:GLU:OE2	1:H:150:ARG:NH2	2.25	0.70
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.74	0.69
2:C:197:ARG:NH1	2:C:201:ARG:O	2.25	0.69
2:C:1315:MET:HE2	2:C:1317:PRO:HB3	1.73	0.69
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.25	0.69
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.74	0.69
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.27	0.69
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.26	0.69
2:C:705:GLU:HB2	2:C:794:LEU:H	1.57	0.69
1:G:75:GLN:HA	2:I:729:ALA:N	2.08	0.69
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	1.92	0.69
3:J:518:VAL:O	3:J:547:ARG:NH1	2.25	0.69
3:J:1169:THR:OG1	3:J:1192:LYS:HD3	1.91	0.69
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.74	0.69
2:C:41:GLN:NE2	2:C:73:TYR:O	2.26	0.69
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.73	0.69
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.72	0.69
1:G:228:LEU:O	1:G:230:ALA:N	2.23	0.69
3:J:905:ARG:NH1	3:J:910:ASN:HD21	1.90	0.69
1:H:153:VAL:HG11	1:H:158:ARG:HH11	1.57	0.69
1:H:214:GLU:HG2	1:H:218:ARG:NH2	2.06	0.69
2:I:18:ARG:NH2	2:I:622:ASN:OD1	2.25	0.69
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.58	0.69
2:C:402:ARG:NH2	2:C:419:ILE:O	2.26	0.69
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.75	0.69
3:D:1158:GLU:HG3	3:D:1186:TYR:CZ	2.28	0.69
2:I:324:LYS:O	2:I:327:GLN:NE2	2.25	0.69
2:I:452:ARG:HH21	2:I:458:GLU:CD	2.01	0.69
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.75	0.69
2:C:528:ARG:NH2	2:C:576:SER:O	2.26	0.68
2:C:565:GLU:HG2	2:C:565:GLU:O	1.92	0.68
5:F:601:PRO:HA	5:F:604:SER:HB3	1.75	0.68
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.74	0.68
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.23	0.68
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.25	0.68
5:L:244:THR:O	5:L:247:GLU:HG2	1.93	0.68
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLU:O	1:B:150:ARG:NH1	2.27	0.68
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.59	0.68
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.75	0.68
1:G:191:ARG:HH12	1:G:197:ASP:HA	1.57	0.68
3:J:680:ASN:O	3:J:683:ILE:HG22	1.93	0.68
5:L:600:HIS:CD2	5:L:601:PRO:HD2	2.28	0.68
1:G:188:GLU:O	1:G:200:LYS:N	2.23	0.68
3:D:396:ALA:HB2	5:F:609:SER:HB2	1.75	0.68
1:H:101:THR:HG22	1:H:116:THR:HG21	1.73	0.68
2:I:992:LEU:HD12	2:I:996:ARG:HB3	1.76	0.68
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.75	0.68
3:D:259:ARG:HG2	3:D:260:PHE:H	1.57	0.68
2:I:148:GLN:NE2	2:I:535:PRO:O	2.20	0.68
3:J:50:LYS:HD3	3:J:71:LEU:HD21	1.74	0.68
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.27	0.67
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.60	0.67
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.77	0.67
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.76	0.67
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.76	0.67
5:F:547:VAL:HG22	5:F:598:LEU:CD2	2.24	0.67
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.58	0.67
1:B:182:ARG:HD2	3:D:581:MET:HE1	1.76	0.67
2:C:1099:ASN:HD21	3:D:505:ASP:CG	2.03	0.67
3:D:1160:SER:HG	3:D:1203:ARG:HH12	1.41	0.67
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.28	0.67
2:C:115:LYS:HD3	2:C:116:ASP:N	2.10	0.67
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.77	0.67
5:F:166:VAL:O	5:F:167:ASP:HB2	1.94	0.67
2:I:829:THR:HA	2:I:1059:ARG:HA	1.77	0.67
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.76	0.67
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.77	0.67
3:D:310:GLY:CA	3:D:314:ARG:HD2	2.22	0.67
1:G:219:ARG:O	1:G:223:ILE:HG13	1.94	0.67
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.75	0.67
3:D:11:GLN:HG2	3:D:15:GLU:HG3	1.77	0.67
3:D:205:LEU:HD22	3:D:214:ARG:HB2	1.77	0.67
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	1.94	0.67
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.30	0.67
1:B:188:GLU:O	1:B:200:LYS:N	2.24	0.67
3:D:73:GLY:O	3:D:76:LYS:NZ	2.21	0.67
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.59	0.67
1:H:74:VAL:HG12	1:H:76:GLU:H	1.60	0.67
2:C:1304:MET:HE3	2:C:1308:ILE:HD11	1.77	0.66
3:D:885:VAL:O	3:D:1258:ARG:HD2	1.96	0.66
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.28	0.66
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.77	0.66
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.96	0.66
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.44	0.66
1:B:48:LEU:HD22	3:D:539:SER:HB3	1.77	0.66
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.76	0.66
2:C:211:ARG:NH1	2:C:357:ASN:O	2.28	0.66
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.08	0.66
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.78	0.66
3:D:54:ASP:OD2	3:D:60:ARG:HD3	1.96	0.66
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.61	0.66
3:J:514:THR:OG1	3:J:594:GLN:O	2.12	0.66
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.28	0.66
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.78	0.66
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.31	0.66
2:C:106:GLU:HB3	2:C:109:ALA:HB2	1.78	0.66
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.78	0.66
1:G:155:ALA:N	1:G:174:ASP:OD1	2.29	0.66
1:H:16:ILE:HG23	1:H:26:VAL:HG22	1.76	0.66
3:J:45:ASN:HB3	3:J:48:THR:O	1.96	0.66
1:B:182:ARG:NH1	3:D:581:MET:SD	2.69	0.66
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.31	0.66
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.78	0.66
5:F:599:ARG:NH1	5:F:599:ARG:HG2	2.10	0.66
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.76	0.66
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.14	0.66
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.77	0.66
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.14	0.66
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.78	0.66
2:C:710:VAL:HG13	2:C:717:VAL:HG21	1.77	0.65
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.78	0.65
3:J:1263:LYS:HE2	3:J:1279:GLN:NE2	2.11	0.65
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.77	0.65
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.76	0.65
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.78	0.65
3:D:1301:THR:HA	3:J:1297:LYS:HE2	1.77	0.65
2:I:1250:SER:OG	5:L:524:GLU:OE1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.78	0.65
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.79	0.65
5:F:316:PHE:HZ	5:F:334:SER:HA	1.61	0.65
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.78	0.65
1:G:155:ALA:HB2	1:G:173:VAL:C	2.21	0.65
2:I:80:PHE:HB3	2:I:84:GLU:HB2	1.79	0.65
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.25	0.65
3:J:885:VAL:O	3:J:1258:ARG:HD2	1.96	0.65
1:G:45:ARG:HH12	1:H:38:THR:H	1.45	0.65
3:J:370:LYS:HG2	3:J:441:LEU:HD12	1.77	0.65
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.32	0.65
3:J:832:LYS:HD3	3:J:1242:ARG:HH11	1.59	0.65
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.78	0.65
2:I:1242:LYS:HD2	3:J:465:GLN:OE1	1.97	0.65
3:J:473:THR:HG23	3:J:476:ALA:H	1.61	0.65
5:L:300:LYS:HE3	5:L:301:ASN:HD21	1.62	0.65
3:D:1266:ILE:HB	3:D:1274:PHE:O	1.96	0.65
3:D:515:ARG:NH2	3:D:717:VAL:O	2.30	0.65
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.77	0.65
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.78	0.65
1:G:73:GLY:N	2:I:728:ASP:OD2	2.15	0.65
2:I:211:ARG:NH1	2:I:357:ASN:O	2.29	0.65
2:I:314:ASN:O	2:I:352:ARG:NH1	2.30	0.65
2:I:580:GLN:HB2	2:I:605:TYR:HE1	1.62	0.65
1:B:74:VAL:HG12	1:B:76:GLU:H	1.60	0.64
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.30	0.64
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.08	0.64
2:C:798:GLN:OE1	2:C:827:ARG:HB2	1.97	0.64
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.63	0.64
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.79	0.64
1:G:91:ARG:HH21	1:G:122:GLU:CD	2.03	0.64
1:H:62:ASP:HB2	1:H:141:SER:O	1.98	0.64
2:I:256:GLU:HB3	2:I:261:VAL:HG22	1.79	0.64
2:C:696:ASP:CB	2:C:798:GLN:HG2	2.22	0.64
3:J:1174:ARG:HE	3:J:1189:MET:HE2	1.63	0.64
2:C:4:SER:OG	2:C:5:TYR:N	2.30	0.64
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.80	0.64
5:F:470:MET:HE2	5:F:486:ARG:HH11	1.61	0.64
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.80	0.64
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.63	0.64
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HG12	1:B:135:ASP:HA	1.79	0.64
3:D:557:LYS:HA	3:D:563:LEU:HA	1.80	0.64
1:G:150:ARG:NH1	1:H:7:GLU:O	2.30	0.64
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.13	0.64
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.79	0.64
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.31	0.64
3:D:1206:ARG:NH2	3:J:1295:ASN:OD1	2.29	0.63
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.80	0.63
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.78	0.63
1:B:53:GLY:HA3	1:B:177:TYR:O	1.99	0.63
2:C:1101:LEU:O	3:D:731:ARG:HD3	1.98	0.63
2:C:719:LYS:N	2:C:751:TYR:OH	2.26	0.63
2:C:1099:ASN:ND2	3:D:505:ASP:OD1	2.32	0.63
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.79	0.63
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.80	0.63
2:C:402:ARG:NE	2:C:417:SER:O	2.31	0.63
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.63	0.63
1:H:182:ARG:NH1	3:J:581:MET:SD	2.72	0.63
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.81	0.63
5:F:599:ARG:HG2	5:F:599:ARG:HH11	1.62	0.63
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.80	0.63
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.79	0.63
3:J:115:TRP:CZ2	3:J:1329:THR:HG23	2.34	0.63
3:J:847:ASP:OD2	3:J:860:ARG:HG2	1.98	0.63
1:G:45:ARG:NH1	1:H:38:THR:H	1.96	0.63
2:I:1042:LEU:HD22	2:I:1049:ILE:HD12	1.81	0.63
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.81	0.63
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.14	0.63
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.79	0.63
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.64	0.63
3:J:425:ARG:HH11	3:J:459:ALA:HA	1.60	0.63
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.81	0.63
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.80	0.63
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.81	0.63
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	1.80	0.63
2:I:1114:GLU:OE1	2:I:1230:MET:HA	1.98	0.63
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.81	0.62
5:F:462:LYS:O	5:F:466:ILE:HG13	1.99	0.62
3:D:156:ARG:NH2	3:D:191:SER:OG	2.33	0.62
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.26	0.62
2:C:742:TYR:O	2:C:974:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1155:ILE:HD13	3:D:1190:ILE:HD13	1.82	0.62
3:D:1183:SER:OG	3:J:206:ASN:ND2	2.32	0.62
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.81	0.62
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.39	0.62
2:I:690:VAL:HG12	2:I:1234:LYS:O	1.98	0.62
2:C:258:ASN:ND2	2:C:282:VAL:HG22	2.15	0.62
2:C:1267:GLY:HA3	3:D:347:VAL:O	1.98	0.62
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.14	0.62
2:I:30:ILE:HD12	2:I:30:ILE:H	1.64	0.62
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.64	0.62
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.64	0.62
3:D:680:ASN:O	3:D:683:ILE:HG22	1.99	0.62
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.82	0.62
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.06	0.62
2:I:979:LEU:HA	2:I:1002:LEU:HD12	1.81	0.62
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.63	0.62
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.80	0.62
1:A:92:VAL:HG23	1:A:148:ARG:NH1	2.15	0.62
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.81	0.62
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.35	0.62
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.81	0.62
3:J:1167:LYS:HZ3	3:J:1170:LYS:CB	2.07	0.62
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.82	0.62
5:F:599:ARG:HH11	5:F:599:ARG:CG	2.13	0.62
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.82	0.62
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.82	0.62
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.31	0.62
3:D:847:ASP:OD1	3:D:847:ASP:N	2.29	0.62
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.82	0.62
3:J:1153:PRO:HA	3:J:1214:PRO:O	1.99	0.62
1:H:28:LEU:HG	1:H:31:LEU:HD21	1.82	0.61
2:I:637:ARG:HA	2:I:642:SER:HA	1.82	0.61
1:A:118:ASP:H	1:A:121:VAL:HB	1.65	0.61
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.82	0.61
3:J:73:GLY:O	3:J:76:LYS:NZ	2.25	0.61
3:J:1167:LYS:HG2	3:J:1168:GLU:H	1.64	0.61
5:F:316:PHE:CZ	5:F:334:SER:HA	2.35	0.61
5:F:511:ILE:HG12	5:F:512:GLY:N	2.15	0.61
1:A:135:ASP:O	1:A:138:ALA:N	2.33	0.61
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.82	0.61
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.81	0.61
5:F:312:SER:O	5:F:315:TRP:NE1	2.34	0.61
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.64	0.61
3:J:57:PHE:HB3	3:J:98:ARG:NH2	2.15	0.61
2:C:302:ILE:O	2:C:330:HIS:NE2	2.33	0.61
3:D:872:LEU:O	3:D:877:VAL:HG12	1.99	0.61
1:G:191:ARG:NH1	1:G:197:ASP:HA	2.15	0.61
2:I:778:GLU:O	2:I:781:ASP:HB2	2.00	0.61
3:J:205:LEU:CD2	3:J:214:ARG:HB2	2.31	0.61
5:L:573:LEU:HD23	5:L:573:LEU:H	1.66	0.61
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.00	0.61
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.82	0.61
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.82	0.61
1:H:154:PRO:HB3	3:J:525:MET:HE1	1.83	0.61
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	2.01	0.61
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.64	0.61
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.16	0.61
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.81	0.61
2:C:115:LYS:HD3	2:C:116:ASP:H	1.66	0.61
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.36	0.61
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.82	0.61
3:J:205:LEU:HD22	3:J:214:ARG:HB2	1.83	0.61
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.82	0.61
1:A:218:ARG:HG3	1:B:231:PHE:O	2.01	0.61
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.16	0.61
5:F:306:PHE:HE1	5:F:315:TRP:CG	2.19	0.61
2:I:371:ARG:HB3	2:I:374:GLU:OE2	2.01	0.61
2:I:565:GLU:HG2	2:I:565:GLU:O	2.00	0.61
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.31	0.60
1:G:45:ARG:NH1	1:H:34:GLY:O	2.32	0.60
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.83	0.60
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.83	0.60
2:C:615:VAL:HG13	2:C:651:ASP:H	1.65	0.60
3:D:598:LYS:N	3:D:728:SER:O	2.26	0.60
3:D:697:MET:O	3:D:701:LEU:HB2	2.01	0.60
3:J:436:ALA:HB3	3:J:485:MET:HA	1.84	0.60
5:L:461:ASN:HB3	5:L:465:ARG:HH21	1.66	0.60
2:C:1248:THR:HG21	5:F:531:PRO:HG3	1.81	0.60
2:I:737:ASN:HB3	2:I:739:ASP:OD1	2.01	0.60
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.36	0.60
3:J:901:ARG:HA	3:J:908:ILE:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ILE:HG23	1:B:142:MET:HE1	1.82	0.60
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.16	0.60
2:C:406:ASN:ND2	2:C:413:GLU:O	2.34	0.60
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.84	0.60
3:D:844:THR:HG21	3:D:858:VAL:HG21	1.83	0.60
3:J:26:SER:HB2	3:J:236:TRP:CE2	2.37	0.60
3:J:343:LEU:HD12	3:J:344:GLY:HA3	1.83	0.60
3:J:462:ASP:OD2	3:J:464:ASP:OD2	2.17	0.60
5:L:507:MET:HG2	5:L:520:GLY:CA	2.32	0.60
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.82	0.60
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.84	0.60
5:F:479:THR:HG23	5:F:481:GLU:H	1.65	0.60
3:J:418:GLU:HG3	4:K:45:LYS:H	1.66	0.60
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.32	0.60
5:L:314:THR:O	5:L:318:ALA:HB3	2.01	0.60
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.36	0.60
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.82	0.60
5:L:461:ASN:O	5:L:465:ARG:HG2	2.02	0.60
2:C:517:GLN:HE21	2:C:760:ASN:H	1.50	0.60
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.83	0.60
1:G:9:LEU:O	1:H:227:GLN:NE2	2.35	0.60
3:J:807:LEU:HD23	3:J:915:ILE:HG13	1.82	0.60
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.37	0.60
3:J:1289:ASN:O	3:J:1290:ARG:NH1	2.35	0.60
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.66	0.60
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.84	0.60
2:I:810:TYR:HD2	3:J:359:PRO:HG2	1.66	0.59
3:J:152:THR:HG21	3:J:176:PHE:HB2	1.85	0.59
3:J:892:PHE:CD1	3:J:1281:GLU:HG2	2.37	0.59
5:L:511:ILE:HG13	5:L:512:GLY:N	2.17	0.59
1:A:12:ARG:H	1:A:30:PRO:HD2	1.66	0.59
1:A:75:GLN:HA	2:C:729:ALA:N	2.17	0.59
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.85	0.59
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.82	0.59
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.35	0.59
3:J:298:MET:SD	5:L:402:LEU:HB3	2.42	0.59
1:B:41:ASN:O	1:B:45:ARG:HG3	2.02	0.59
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.37	0.59
5:F:244:THR:O	5:F:247:GLU:HG2	2.01	0.59
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.66	0.59
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:960:LEU:HB3	2:C:1025:PHE:HE2	1.67	0.59
3:D:473:THR:HG23	3:D:476:ALA:H	1.67	0.59
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.67	0.59
2:C:517:GLN:NE2	2:C:760:ASN:H	2.01	0.59
3:D:179:LYS:HB2	3:D:184:ALA:HB2	1.83	0.59
2:I:1286:THR:N	3:J:479:GLU:OE2	2.31	0.59
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.43	0.59
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.67	0.59
3:D:259:ARG:HG2	3:D:260:PHE:N	2.17	0.59
2:C:905:ILE:O	5:F:599:ARG:HD2	2.02	0.59
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.85	0.59
2:I:124:MET:HG3	2:I:124:MET:O	2.02	0.59
2:I:896:THR:HB	2:I:897:PRO:HD2	1.85	0.59
1:B:219:ARG:O	1:B:223:ILE:HG13	2.02	0.59
3:D:642:ASP:HA	3:D:764:ARG:HH21	1.67	0.59
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.85	0.59
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.03	0.59
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.37	0.59
5:L:166:VAL:O	5:L:167:ASP:HB2	2.02	0.59
5:F:483:LEU:H	5:F:483:LEU:HD12	1.67	0.59
2:I:841:ARG:NE	3:J:256:ASP:HB3	2.18	0.59
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.50	0.59
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.33	0.59
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.02	0.58
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.67	0.58
3:D:34:SER:OG	3:D:104:HIS:ND1	2.36	0.58
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.38	0.58
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.85	0.58
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.33	0.58
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.38	0.58
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.67	0.58
5:L:108:VAL:HG11	5:L:381:GLU:C	2.27	0.58
5:L:532:LEU:H	5:L:532:LEU:HD12	1.67	0.58
2:C:98:VAL:C	2:C:121:GLU:HA	2.28	0.58
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.86	0.58
2:C:204:LEU:HD11	2:C:369:MET:HG3	1.85	0.58
2:C:801:ARG:HD3	2:C:1094:VAL:HA	1.85	0.58
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.68	0.58
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.85	0.58
3:J:722:ILE:HA	3:J:725:MET:HE3	1.85	0.58
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.18	0.58
1:G:135:ASP:HB3	1:G:138:ALA:HB2	1.83	0.58
5:L:511:ILE:HG13	5:L:512:GLY:H	1.67	0.58
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.01	0.58
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.10	0.58
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.85	0.58
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.38	0.58
3:D:11:GLN:NE2	3:D:15:GLU:OE1	2.36	0.58
3:D:817:HIS:CE1	3:D:860:ARG:HH21	2.20	0.58
2:I:12:ARG:NH2	2:I:698:PRO:O	2.22	0.58
1:A:23:HIS:HE1	1:A:204:GLU:CG	2.17	0.58
1:B:64:VAL:HG11	1:B:69:SER:CB	2.34	0.58
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.85	0.58
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.86	0.58
3:D:1181:ASP:HB3	3:J:202:ARG:HH11	1.68	0.58
3:D:1263:LYS:CE	3:D:1279:GLN:HE21	2.16	0.58
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.03	0.58
5:F:572:THR:HG23	5:F:575:GLU:HG3	1.86	0.58
1:H:48:LEU:HD21	3:J:535:ARG:O	2.02	0.58
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.86	0.58
3:D:722:ILE:HA	3:D:725:MET:HE3	1.85	0.58
2:I:515:MET:HE3	2:I:517:GLN:HB2	1.85	0.58
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.86	0.58
3:J:195:GLU:O	3:J:199:GLU:HG3	2.02	0.58
3:J:221:ILE:HA	3:J:224:LEU:HD12	1.86	0.58
3:J:1326:GLN:OE1	3:J:1330:ARG:NH2	2.37	0.58
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.84	0.58
3:D:298:MET:SD	5:F:402:LEU:HB3	2.44	0.58
3:D:414:GLU:O	4:E:45:LYS:NZ	2.25	0.58
5:F:423:ARG:HD2	5:F:425:TYR:CE2	2.39	0.58
2:I:159:SER:O	2:I:160:ASP:HB2	2.04	0.58
2:I:871:VAL:O	2:I:944:ARG:NH1	2.36	0.58
2:C:298:ALA:N	2:C:334:GLU:O	2.30	0.58
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.85	0.58
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.31	0.58
1:H:153:VAL:HG11	1:H:158:ARG:NH1	2.18	0.58
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.84	0.58
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.86	0.58
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.04	0.58
5:F:280:VAL:HG21	5:F:358:VAL:HG11	1.84	0.58
5:F:461:ASN:O	5:F:465:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:ALA:O	1:H:46:ILE:HG13	2.03	0.58
2:I:228:VAL:HG22	2:I:245:ARG:HE	1.69	0.58
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.86	0.57
3:J:770:LEU:H	3:J:770:LEU:HD22	1.69	0.57
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.86	0.57
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.39	0.57
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.16	0.57
5:F:276:MET:O	5:F:279:ARG:HB2	2.04	0.57
4:K:26:ARG:NH1	4:K:29:GLN:OE1	2.37	0.57
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.40	0.57
2:I:185:ASP:HB2	2:I:197:ARG:HG3	1.86	0.57
3:J:27:PRO:HB3	3:J:241:VAL:HG23	1.85	0.57
1:A:14:VAL:CG1	1:A:15:ASP:H	2.13	0.57
2:C:40:GLU:HG2	2:C:41:GLN:H	1.69	0.57
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.86	0.57
2:C:557:ARG:HH21	2:C:607:SER:C	2.12	0.57
2:C:815:SER:HB2	2:C:1077:SER:HB3	1.85	0.57
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.87	0.57
3:D:1171:GLY:O	3:D:1172:LYS:HG3	2.05	0.57
2:I:1197:GLU:O	2:I:1200:LYS:HB2	2.04	0.57
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.86	0.57
2:C:179:TYR:H	2:C:397:LEU:HA	1.69	0.57
3:D:843:VAL:HG11	3:D:897:HIS:O	2.04	0.57
2:I:156:PHE:CE1	2:I:443:ASP:HB2	2.38	0.57
2:I:250:THR:HA	2:I:268:ARG:HA	1.86	0.57
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.68	0.57
5:F:601:PRO:O	5:F:602:SER:OG	2.18	0.57
1:A:23:HIS:ND1	1:A:205:MET:O	2.37	0.57
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.85	0.57
1:H:79:LEU:O	1:H:82:LEU:HB2	2.05	0.57
3:J:394:ILE:HG23	5:L:536:THR:HG22	1.86	0.57
1:G:49:SER:OG	1:G:50:SER:N	2.34	0.57
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.87	0.57
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.86	0.57
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.70	0.57
1:A:45:ARG:HG2	1:B:38:THR:CB	2.31	0.57
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.86	0.57
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.38	0.57
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.87	0.57
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.31	0.57
3:D:205:LEU:CD2	3:D:214:ARG:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:316:ILE:HA	3:D:323:PRO:HA	1.86	0.57
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.87	0.57
3:D:814:CYS:HB2	3:D:889:ASP:HB3	1.87	0.57
1:H:51:MET:O	1:H:150:ARG:HA	2.04	0.57
2:C:105:TYR:CE1	2:C:111:GLU:HB3	2.40	0.56
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.86	0.56
5:F:97:PRO:HA	5:F:100:MET:HG3	1.87	0.56
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.71	0.56
2:I:994:ARG:HD2	2:I:997:TRP:CZ2	2.40	0.56
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.39	0.56
2:C:214:ASN:HB2	2:C:359:ARG:HD2	1.86	0.56
2:C:582:ASN:N	2:C:586:PHE:O	2.26	0.56
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.87	0.56
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.06	0.56
3:D:317:THR:HB	3:D:324:LEU:HB3	1.87	0.56
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.87	0.56
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.87	0.56
5:F:511:ILE:HG12	5:F:512:GLY:H	1.69	0.56
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.86	0.56
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.86	0.56
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.87	0.56
3:J:325:LYS:HE2	3:J:330:MET:HG2	1.86	0.56
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.05	0.56
2:C:832:HIS:ND1	2:C:1058:ARG:HD2	2.20	0.56
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.05	0.56
1:G:172:LEU:HD12	1:G:172:LEU:H	1.70	0.56
1:H:41:ASN:ND2	2:I:1217:THR:O	2.39	0.56
2:I:739:ASP:OD1	2:I:739:ASP:N	2.37	0.56
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.86	0.56
2:I:812:PHE:N	2:I:815:SER:OG	2.38	0.56
2:I:1099:ASN:HD21	3:J:505:ASP:CG	2.13	0.56
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.03	0.56
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.87	0.56
4:K:13:ILE:HD12	4:K:19:LEU:HA	1.86	0.56
1:B:140:ILE:HD11	1:B:142:MET:HE3	1.87	0.56
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.69	0.56
3:D:26:SER:HB2	3:D:236:TRP:CZ2	2.40	0.56
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.88	0.56
2:I:607:SER:N	2:I:610:GLU:HB2	2.20	0.56
5:L:164:GLY:O	5:L:260:ARG:HB2	2.05	0.56
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.46	0.56
3:D:56:LEU:H	3:D:56:LEU:HD12	1.70	0.56
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.06	0.56
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.87	0.56
2:I:934:PHE:HA	2:I:1040:ASP:OD2	2.06	0.56
5:L:612:ASP:N	5:L:612:ASP:OD1	2.37	0.56
2:C:30:ILE:H	2:C:30:ILE:HD12	1.71	0.56
2:C:356:THR:HG21	2:C:362:ALA:HA	1.87	0.56
2:C:829:THR:HA	2:C:1059:ARG:HA	1.87	0.56
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.87	0.56
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.06	0.56
1:H:7:GLU:HG2	1:H:8:PHE:H	1.71	0.56
2:I:1259:LEU:HD23	5:L:524:GLU:HB3	1.88	0.56
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.21	0.56
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.86	0.56
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	1.88	0.56
2:C:490:GLN:HG3	5:F:472:GLN:NE2	2.20	0.56
2:C:1114:GLU:OE1	2:C:1230:MET:HA	2.05	0.56
2:C:1326:LEU:HD21	3:D:337:ARG:NE	2.20	0.56
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.88	0.56
2:I:1272:GLU:N	3:J:343:LEU:HD11	2.21	0.56
1:B:102:LEU:HD23	1:B:115:ILE:HA	1.87	0.56
2:C:628:HIS:HB3	2:C:647:ARG:HH21	1.71	0.56
3:D:259:ARG:CD	5:F:505:ILE:HD13	2.36	0.56
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.70	0.56
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.06	0.56
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.70	0.56
1:B:154:PRO:HA	1:B:174:ASP:CB	2.35	0.56
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.88	0.56
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.87	0.56
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.87	0.56
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.87	0.56
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.88	0.56
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.45	0.56
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.86	0.56
3:D:770:LEU:H	3:D:770:LEU:HD22	1.70	0.56
3:D:1162:ILE:O	3:D:1178:THR:N	2.36	0.56
3:D:53:ARG:HB2	3:D:54:ASP:OD1	2.05	0.55
5:F:515:GLU:C	5:F:517:SER:N	2.60	0.55
5:F:612:ASP:OD1	5:F:612:ASP:N	2.40	0.55
1:G:14:VAL:HG13	1:G:15:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:VAL:HG12	1:H:76:GLU:HB2	1.87	0.55
1:H:108:GLY:O	1:H:133:LEU:HB2	2.06	0.55
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.88	0.55
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.35	0.55
3:J:843:VAL:HG11	3:J:897:HIS:O	2.06	0.55
1:B:35:PHE:HA	1:B:38:THR:HG22	1.89	0.55
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.88	0.55
1:H:81:ILE:HG23	1:H:131:CYS:HB3	1.87	0.55
1:H:211:ILE:HD11	1:H:215:GLU:CG	2.36	0.55
2:I:20:GLN:O	2:I:20:GLN:HG3	2.06	0.55
2:I:895:LEU:HB2	2:I:899:GLU:HB2	1.88	0.55
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.36	0.55
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.88	0.55
1:H:55:ALA:HB3	1:H:177:TYR:CD1	2.41	0.55
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.89	0.55
5:L:343:LYS:H	5:L:343:LYS:HD2	1.71	0.55
1:B:102:LEU:O	1:B:141:SER:HA	2.06	0.55
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.88	0.55
2:C:1247:SER:HB3	3:D:375:GLU:O	2.07	0.55
3:D:30:ILE:HD13	3:D:243:PRO:HD3	1.88	0.55
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.88	0.55
4:E:86:ILE:C	4:E:88:GLU:N	2.62	0.55
2:I:143:ARG:NH2	2:I:512:SER:O	2.40	0.55
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.89	0.55
2:I:655:VAL:N	2:I:659:GLN:OE1	2.39	0.55
3:J:514:THR:HB	3:J:576:ARG:HG2	1.88	0.55
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.68	0.55
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.88	0.55
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.86	0.55
3:D:317:THR:HG22	3:D:322:ARG:O	2.07	0.55
3:D:1273:ASP:HB2	3:D:1276:GLU:HB2	1.89	0.55
3:D:1302:TYR:CE1	3:J:1297:LYS:HD3	2.41	0.55
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.71	0.55
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.88	0.55
2:I:1136:GLN:O	2:I:1137:GLU:HG2	2.07	0.55
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.88	0.55
1:A:92:VAL:HA	1:A:120:ASP:O	2.07	0.55
2:C:387:ASN:HA	2:C:391:SER:HB2	1.88	0.55
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.88	0.55
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.88	0.55
3:D:1284:ARG:HH22	3:J:1292:LEU:HD11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.87	0.55
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.87	0.55
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.88	0.55
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.36	0.55
1:H:225:ALA:HA	1:H:228:LEU:HB2	1.89	0.55
2:I:115:LYS:HD3	2:I:116:ASP:H	1.72	0.55
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.46	0.55
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.72	0.55
4:K:32:VAL:O	4:K:34:GLY:N	2.38	0.55
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.06	0.55
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.38	0.55
3:D:901:ARG:HD2	3:D:906:GLY:O	2.06	0.55
4:E:8:ASP:HB2	4:E:55:GLU:HG2	1.88	0.55
5:F:227:GLN:HE22	5:F:251:LYS:HZ2	1.53	0.55
2:I:125:GLY:CA	2:I:499:SER:HB2	2.36	0.55
3:J:128:LEU:HA	3:J:192:MET:HE1	1.89	0.55
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.42	0.54
3:D:511:TYR:CG	3:D:728:SER:HB3	2.42	0.54
2:I:448:LEU:HG	2:I:553:THR:OG1	2.07	0.54
5:L:276:MET:O	5:L:279:ARG:HB2	2.07	0.54
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.89	0.54
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.89	0.54
2:C:778:GLU:O	2:C:781:ASP:HB2	2.08	0.54
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.90	0.54
3:D:45:ASN:O	3:D:46:TYR:HD2	1.89	0.54
1:H:172:LEU:H	1:H:172:LEU:HD12	1.72	0.54
2:I:324:LYS:HA	2:I:327:GLN:HE21	1.72	0.54
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.89	0.54
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.42	0.54
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.41	0.54
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.89	0.54
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.71	0.54
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.42	0.54
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.08	0.54
2:I:754:THR:N	2:I:767:GLN:OE1	2.36	0.54
3:J:211:GLU:OE2	3:J:214:ARG:NH1	2.34	0.54
5:L:287:ILE:HD11	5:L:344:LEU:HD22	1.90	0.54
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.42	0.54
3:D:895:CYS:SG	3:D:898:CYS:HB2	2.47	0.54
5:F:111:LEU:HD13	5:F:116:GLU:HA	1.88	0.54
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:872:LEU:O	3:J:877:VAL:HG12	2.08	0.54
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.88	0.54
2:C:538:LEU:HD23	2:C:543:ALA:CB	2.37	0.54
3:J:642:ASP:HA	3:J:764:ARG:HH21	1.71	0.54
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.36	0.54
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.38	0.54
3:J:56:LEU:HD12	3:J:56:LEU:H	1.72	0.54
3:J:77:ARG:HG3	3:J:79:LYS:H	1.72	0.54
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.88	0.54
2:C:452:ARG:HH21	2:C:458:GLU:CD	2.15	0.54
3:D:214:ARG:HA	3:D:217:LEU:HB3	1.89	0.54
3:D:396:ALA:HB2	5:F:609:SER:CB	2.37	0.54
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.73	0.54
3:D:850:LYS:HD3	3:D:875:ASN:ND2	2.23	0.54
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.24	0.54
1:G:9:LEU:HD13	1:G:32:GLU:HG2	1.90	0.54
1:G:23:HIS:HB2	1:G:205:MET:O	2.08	0.54
1:G:211:ILE:HG21	1:G:216:ALA:HB2	1.90	0.54
2:I:599:VAL:HG21	2:I:623:LEU:HD22	1.89	0.54
3:J:525:MET:O	3:J:548:VAL:HG13	2.08	0.54
5:L:94:THR:OG1	5:L:95:THR:N	2.34	0.54
5:L:134:VAL:HG22	5:L:273:MET:HE1	1.90	0.54
5:L:289:LYS:HA	5:L:293:GLU:OE1	2.07	0.54
2:C:1211:ARG:HE	2:C:1220:GLN:NE2	2.06	0.54
5:F:577:GLY:C	5:F:583:THR:HG23	2.32	0.54
1:G:107:ILE:HG13	1:G:136:GLU:HA	1.90	0.54
1:H:48:LEU:CD2	3:J:535:ARG:HG3	2.38	0.54
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.23	0.54
1:A:172:LEU:H	1:A:172:LEU:HD12	1.73	0.54
3:D:748:ALA:O	3:D:777:HIS:HD2	1.91	0.54
5:F:547:VAL:CG2	5:F:598:LEU:CD2	2.86	0.54
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.73	0.54
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.73	0.54
3:J:785:ASP:O	3:J:789:LYS:HG3	2.08	0.54
1:B:29:GLU:CB	1:B:200:LYS:HG3	2.32	0.53
2:C:992:LEU:HD23	2:C:992:LEU:H	1.73	0.53
3:D:694:SER:OG	3:D:738:ARG:NE	2.40	0.53
5:F:315:TRP:HZ2	5:F:341:LEU:HD11	1.73	0.53
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.89	0.53
2:C:829:THR:HG23	2:C:1059:ARG:HA	1.89	0.53
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ARG:HG2	1:H:38:THR:CB	2.37	0.53
1:G:91:ARG:NH2	1:G:122:GLU:OE2	2.39	0.53
1:G:228:LEU:HD23	1:H:225:ALA:HB2	1.90	0.53
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.89	0.53
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.23	0.53
5:L:507:MET:HG2	5:L:520:GLY:HA3	1.91	0.53
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.08	0.53
2:I:892:GLU:OE1	3:J:66:LYS:NZ	2.40	0.53
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.41	0.53
3:D:11:GLN:HG2	3:D:15:GLU:CG	2.38	0.53
1:G:187:VAL:HG12	1:G:201:LEU:HD13	1.91	0.53
1:H:201:LEU:HG	1:H:203:ILE:CD1	2.38	0.53
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.90	0.53
3:J:102:MET:HE3	3:J:246:PRO:HD3	1.91	0.53
2:C:239:MET:O	2:C:284:LEU:HD12	2.09	0.53
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.90	0.53
3:D:34:SER:HG	3:D:104:HIS:HD1	1.52	0.53
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.89	0.53
4:E:58:LEU:HD12	4:E:58:LEU:H	1.74	0.53
5:F:315:TRP:CZ2	5:F:341:LEU:HD11	2.44	0.53
3:J:111:THR:O	3:J:239:LEU:N	2.35	0.53
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.91	0.53
2:I:1197:GLU:HA	2:I:1200:LYS:HD2	1.90	0.53
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.23	0.53
3:J:233:LYS:HD3	3:J:235:GLU:OE1	2.09	0.53
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.90	0.53
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.42	0.53
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.90	0.53
1:G:195:ARG:HG3	1:G:196:THR:N	2.23	0.53
2:I:132:ASP:OD1	2:I:132:ASP:N	2.38	0.53
3:J:46:TYR:CD1	5:L:452:ILE:HG22	2.43	0.53
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.44	0.53
3:J:761:ALA:H	3:J:771:GLN:HE22	1.56	0.53
3:J:931:THR:OG1	3:J:1244:GLN:NE2	2.42	0.53
5:L:372:ALA:O	5:L:376:LYS:HG3	2.09	0.53
2:C:739:ASP:N	2:C:739:ASP:OD1	2.40	0.53
2:C:817:LEU:HD23	2:C:1078:LYS:HB3	1.91	0.53
3:D:201:LEU:HD11	3:D:220:ARG:HH11	1.72	0.53
3:D:892:PHE:CD1	3:D:1281:GLU:HG2	2.43	0.53
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.89	0.53
2:C:65:ASN:HB3	2:C:105:TYR:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.22	0.53
5:F:295:CYS:O	5:F:329:LYS:HD3	2.09	0.53
3:J:46:TYR:CD1	5:L:500:ILE:HG21	2.44	0.53
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.23	0.53
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.44	0.53
3:J:259:ARG:HD2	5:L:505:ILE:CD1	2.39	0.53
5:L:569:THR:OG1	5:L:570:ASP:N	2.42	0.53
1:B:27:THR:HG23	1:B:202:VAL:HG22	1.90	0.52
2:C:65:ASN:HB3	2:C:105:TYR:CD2	2.44	0.52
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.91	0.52
3:D:369:PRO:HB3	3:D:444:GLY:O	2.09	0.52
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.90	0.52
3:D:1167:LYS:HZ3	3:D:1170:LYS:HB2	1.73	0.52
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.24	0.52
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.39	0.52
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.91	0.52
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.91	0.52
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.91	0.52
3:J:264:ASP:OD2	5:L:506:SER:OG	2.24	0.52
1:B:54:CYS:SG	1:B:148:ARG:HG3	2.49	0.52
2:C:1103:VAL:HG11	2:C:1112:ILE:HD11	1.91	0.52
3:D:16:GLU:O	3:D:1369:ARG:NH2	2.43	0.52
3:D:1225:GLY:HA3	3:J:1294:ALA:O	2.10	0.52
4:E:32:VAL:O	4:E:34:GLY:N	2.43	0.52
1:H:40:GLY:HA3	1:H:185:TYR:CD1	2.45	0.52
2:I:168:GLY:C	2:I:170:VAL:H	2.16	0.52
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.24	0.52
5:L:572:THR:HG23	5:L:575:GLU:CB	2.39	0.52
1:B:75:GLN:NE2	1:B:132:HIS:HB2	2.11	0.52
3:D:114:ILE:O	3:D:118:LYS:N	2.27	0.52
3:D:115:TRP:CZ2	3:D:1329:THR:HG23	2.44	0.52
1:G:161:SER:O	1:G:163:GLU:N	2.42	0.52
2:I:40:GLU:HG2	2:I:41:GLN:N	2.24	0.52
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.37	0.52
3:J:34:SER:OG	3:J:104:HIS:ND1	2.42	0.52
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	1.92	0.52
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.92	0.52
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.74	0.52
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.75	0.52
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.73	0.52
1:H:8:PHE:HB2	1:H:10:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:259:ARG:HD3	5:F:505:ILE:HD13	1.92	0.52
1:G:155:ALA:H	1:G:174:ASP:CG	2.16	0.52
3:J:609:TYR:HD1	3:J:610:ARG:HH11	1.57	0.52
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.44	0.52
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.42	0.52
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.75	0.52
2:I:672:GLU:HB3	2:I:1187:PHE:HD2	1.75	0.52
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	1.91	0.52
3:J:460:ASP:HB2	3:J:462:ASP:OD1	2.10	0.52
2:C:272:ARG:HD3	2:C:273:HIS:CD2	2.44	0.52
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.92	0.52
3:D:809:VAL:HG23	3:D:915:ILE:HD13	1.91	0.52
5:F:487:MET:HA	5:F:487:MET:HE2	1.91	0.52
5:F:511:ILE:CG1	5:F:512:GLY:H	2.23	0.52
1:G:166:ARG:O	1:G:167:PRO:C	2.52	0.52
1:H:187:VAL:HG13	1:H:199:ASP:HB3	1.91	0.52
2:I:1077:SER:HA	3:J:356:THR:OG1	2.09	0.52
3:J:600:ALA:O	3:J:603:LYS:HG2	2.09	0.52
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.91	0.52
3:J:797:THR:O	3:J:801:VAL:HG12	2.09	0.52
3:J:1261:LEU:HD13	3:J:1304:ARG:HD2	1.92	0.52
5:L:166:VAL:N	5:L:258:GLN:O	2.28	0.52
1:B:11:PRO:O	1:B:12:ARG:HG3	2.09	0.52
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.92	0.52
3:D:491:LEU:HD11	3:D:609:TYR:CE1	2.45	0.52
1:G:38:THR:HG1	1:H:45:ARG:NH1	2.07	0.52
1:G:45:ARG:CG	1:H:38:THR:HB	2.39	0.52
2:I:227:LYS:NZ	2:I:298:ALA:HB1	2.24	0.52
1:A:32:GLU:HA	1:A:198:LEU:HD22	1.91	0.52
2:C:538:LEU:HD23	2:C:543:ALA:HB2	1.92	0.52
3:D:850:LYS:HD3	3:D:875:ASN:HD21	1.75	0.52
3:J:201:LEU:HD22	3:J:217:LEU:CD1	2.40	0.52
3:J:644:MET:HB2	3:J:764:ARG:HG3	1.90	0.52
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.91	0.52
3:J:902:ASP:OD1	3:J:903:LEU:N	2.42	0.52
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.92	0.52
2:C:208:ILE:O	2:C:362:ALA:HB1	2.10	0.52
3:D:521:LYS:NZ	3:D:540:GLY:O	2.32	0.52
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.91	0.52
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.10	0.52
3:D:1301:THR:HG23	3:J:1301:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:15:PHE:CZ	2:I:1151:LEU:HD12	2.45	0.52
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.90	0.52
3:J:142:GLU:OE2	5:L:100:MET:HE2	2.10	0.52
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.91	0.51
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.45	0.51
3:D:1375:ALA:HB1	3:J:853:THR:HG21	1.92	0.51
5:F:548:LEU:HD23	5:F:551:LEU:HD12	1.92	0.51
2:I:722:GLY:HA2	2:I:737:ASN:OD1	2.09	0.51
3:J:75:TYR:CD2	3:J:83:VAL:HG21	2.45	0.51
1:A:189:ALA:HB1	1:A:191:ARG:NH1	2.25	0.51
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.74	0.51
3:D:525:MET:O	3:D:548:VAL:HG13	2.10	0.51
2:I:402:ARG:HG2	2:I:416:GLY:N	2.25	0.51
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.91	0.51
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.25	0.51
3:J:695:LYS:HA	3:J:698:MET:HB2	1.91	0.51
3:D:1302:TYR:OH	3:J:1291:GLU:HG2	2.10	0.51
2:I:564:PRO:HG2	2:I:568:ASN:O	2.11	0.51
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.92	0.51
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.25	0.51
3:D:1302:TYR:H	3:J:1297:LYS:HE2	1.73	0.51
2:I:62:TYR:C	2:I:64:GLY:H	2.19	0.51
3:J:91:GLU:HG3	3:J:91:GLU:O	2.11	0.51
3:J:1170:LYS:C	3:J:1172:LYS:H	2.18	0.51
1:A:228:LEU:HA	1:A:231:PHE:HB2	1.92	0.51
3:D:513:MET:HE1	3:D:579:LEU:HD22	1.92	0.51
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.92	0.51
3:D:789:LYS:HE3	3:D:931:THR:C	2.35	0.51
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.41	0.51
1:H:9:LEU:HD12	1:H:195:ARG:HH21	1.73	0.51
2:I:104:ILE:O	2:I:114:VAL:HG23	2.10	0.51
2:I:632:ASP:HA	2:I:647:ARG:HD2	1.92	0.51
3:J:847:ASP:HA	3:J:860:ARG:H	1.75	0.51
5:L:572:THR:O	5:L:576:VAL:HG23	2.10	0.51
2:C:5:TYR:HB2	2:C:781:ASP:OD1	2.10	0.51
2:C:759:SER:OG	2:C:763:THR:N	2.40	0.51
5:F:147:GLN:HE22	5:F:150:ARG:HH11	1.59	0.51
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.10	0.51
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.93	0.51
3:J:137:ARG:O	3:J:142:GLU:HB2	2.11	0.51
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.71	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.10	0.51
1:A:201:LEU:HG	1:A:203:ILE:HG13	1.93	0.51
2:C:253:PHE:O	2:C:255:ILE:HG13	2.11	0.51
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.26	0.51
3:D:574:VAL:O	3:D:578:ILE:HG13	2.11	0.51
1:H:190:ALA:N	1:H:198:LEU:O	2.27	0.51
3:J:418:GLU:H	4:K:45:LYS:NZ	2.08	0.51
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.91	0.51
5:F:582:VAL:CG1	5:F:586:ARG:HG2	2.41	0.51
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.93	0.51
5:L:348:GLU:HG2	5:L:354:THR:HA	1.91	0.51
1:B:61:ILE:HG23	1:B:142:MET:CE	2.40	0.51
1:B:219:ARG:HA	1:B:222:THR:HB	1.92	0.51
2:C:518:ASN:O	2:C:691:PRO:HD3	2.10	0.51
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.92	0.51
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.10	0.51
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.91	0.51
1:G:221:ALA:HB1	1:H:228:LEU:HD22	1.93	0.51
2:I:238:GLN:OE1	2:I:284:LEU:HD21	2.10	0.51
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.45	0.51
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	1.92	0.51
3:J:1158:GLU:HG3	3:J:1186:TYR:CZ	2.46	0.51
5:L:479:THR:HG23	5:L:481:GLU:H	1.76	0.51
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.92	0.51
1:A:218:ARG:NH1	1:B:231:PHE:O	2.44	0.51
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.93	0.51
2:C:808:ASN:H	3:D:633:ALA:HB2	1.76	0.51
5:F:235:ILE:HA	5:F:245:ALA:HB2	1.93	0.51
1:G:175:ALA:HB1	1:G:177:TYR:CZ	2.46	0.51
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.92	0.51
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.93	0.51
3:J:513:MET:O	3:J:575:GLY:HA3	2.11	0.51
3:J:700:ASN:O	3:J:704:GLU:HB2	2.10	0.51
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.10	0.51
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.46	0.50
1:G:74:VAL:HG22	1:G:76:GLU:H	1.75	0.50
3:J:462:ASP:CG	3:J:464:ASP:OD2	2.54	0.50
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.94	0.50
5:F:288:MET:SD	5:F:299:LYS:HE2	2.50	0.50
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.92	0.50
1:G:29:GLU:OE1	1:G:200:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:GLU:OE2	1:H:143:ARG:HB2	2.12	0.50
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.26	0.50
1:H:182:ARG:HD2	3:J:581:MET:HE1	1.93	0.50
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.08	0.50
3:J:615:LYS:NZ	4:K:7:GLN:HG2	2.27	0.50
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.44	0.50
1:B:46:ILE:HD11	1:B:224:LEU:HD13	1.93	0.50
1:B:67:GLU:N	1:B:67:GLU:OE1	2.44	0.50
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.93	0.50
2:C:1085:MET:HA	2:C:1085:MET:HE2	1.92	0.50
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.92	0.50
3:J:22:ILE:HG22	3:J:1340:LYS:O	2.12	0.50
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.92	0.50
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.42	0.50
3:D:902:ASP:OD1	3:D:903:LEU:N	2.44	0.50
2:I:133:ASN:ND2	2:I:713:GLY:HA3	2.26	0.50
3:J:259:ARG:HD2	5:L:505:ILE:HD13	1.92	0.50
1:B:211:ILE:HD11	1:B:215:GLU:HG2	1.94	0.50
2:C:548:ARG:HB3	2:C:569:ILE:O	2.12	0.50
2:C:745:GLU:HG3	2:C:1017:GLN:CB	2.34	0.50
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.44	0.50
2:C:1246:ARG:HH11	2:C:1266:GLY:HA2	1.76	0.50
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.93	0.50
3:D:842:ARG:HH12	3:D:1254:GLU:CD	2.15	0.50
1:H:59:VAL:O	1:H:171:LEU:HB2	2.11	0.50
3:J:850:LYS:HG2	3:J:857:LEU:HD23	1.94	0.50
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.94	0.50
1:B:56:VAL:HG22	1:B:146:VAL:HG22	1.94	0.50
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.94	0.50
3:D:108:ALA:HB2	3:D:280:LYS:HG2	1.93	0.50
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.19	0.50
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.30	0.50
3:D:1273:ASP:O	3:D:1275:LEU:N	2.45	0.50
1:G:189:ALA:HA	1:G:199:ASP:HA	1.94	0.50
1:H:84:ASN:ND2	1:H:129:VAL:O	2.44	0.50
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	1.94	0.50
3:J:18:ASP:HB2	3:J:1373:ARG:NH2	2.26	0.50
1:A:91:ARG:HH21	1:A:122:GLU:CD	2.20	0.50
3:D:1225:GLY:CA	3:J:1294:ALA:O	2.60	0.50
1:G:61:ILE:HG22	1:G:62:ASP:H	1.77	0.50
1:H:211:ILE:HD11	1:H:215:GLU:CD	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:488:LEU:H	5:L:488:LEU:HD12	1.77	0.50
2:C:980:VAL:HA	2:C:984:VAL:HA	1.94	0.50
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	1.94	0.50
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.26	0.50
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.44	0.50
4:E:69:ARG:HA	4:E:72:GLN:OE1	2.11	0.50
2:I:607:SER:H	2:I:610:GLU:HB2	1.75	0.50
3:J:609:TYR:OH	3:J:905:ARG:HA	2.11	0.50
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.26	0.50
5:L:250:LEU:O	5:L:254:GLU:HG2	2.12	0.50
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.93	0.50
1:A:190:ALA:H	1:A:199:ASP:HA	1.76	0.50
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.93	0.50
2:I:346:TYR:CE2	2:I:433:ILE:HG23	2.47	0.50
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.94	0.50
3:J:1171:GLY:O	3:J:1172:LYS:HG3	2.12	0.50
1:A:38:THR:HA	1:B:45:ARG:HD3	1.94	0.49
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.94	0.49
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.94	0.49
1:G:90:VAL:HG22	1:G:91:ARG:H	1.77	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.49
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.47	0.49
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.93	0.49
3:J:848:VAL:HG12	3:J:857:LEU:HD11	1.93	0.49
5:L:247:GLU:O	5:L:251:LYS:HG3	2.12	0.49
1:B:190:ALA:N	1:B:198:LEU:O	2.42	0.49
1:H:191:ARG:NH1	3:J:413:ASP:OD2	2.46	0.49
5:L:251:LYS:HA	5:L:254:GLU:HG2	1.94	0.49
2:C:566:GLY:O	2:C:569:ILE:HG13	2.11	0.49
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.94	0.49
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.40	0.49
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.94	0.49
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.94	0.49
4:E:80:LEU:O	4:E:84:THR:OG1	2.19	0.49
5:F:292:VAL:HG13	5:F:297:MET:O	2.12	0.49
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.93	0.49
2:I:480:SER:HB3	2:I:481:LEU:HD22	1.94	0.49
2:I:1272:GLU:H	3:J:343:LEU:HD11	1.77	0.49
2:I:1276:TRP:HD1	2:I:1279:GLU:OE1	1.96	0.49
1:A:49:SER:OG	1:A:50:SER:N	2.45	0.49
1:A:91:ARG:NH2	1:A:122:GLU:OE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.52	0.49
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.47	0.49
2:C:561:ILE:HD11	2:C:665:ALA:HB1	1.94	0.49
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.94	0.49
3:D:128:LEU:HA	3:D:192:MET:HE1	1.95	0.49
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.47	0.49
3:D:647:PRO:CG	3:D:697:MET:HB3	2.39	0.49
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.94	0.49
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.47	0.49
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.78	0.49
3:J:317:THR:HG22	3:J:322:ARG:O	2.12	0.49
3:J:1156:LEU:HA	3:J:1208:ASP:O	2.12	0.49
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.47	0.49
2:C:854:ILE:HB	2:C:857:VAL:HG21	1.95	0.49
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.95	0.49
2:C:1328:LYS:O	2:C:1332:SER:N	2.44	0.49
3:D:514:THR:OG1	3:D:594:GLN:O	2.30	0.49
3:D:931:THR:HG22	3:D:932:MET:H	1.78	0.49
1:H:153:VAL:HB	1:H:175:ALA:HB3	1.95	0.49
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.94	0.49
2:I:365:GLU:OE2	2:I:368:ARG:NH2	2.44	0.49
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	1.94	0.49
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.13	0.49
2:I:1271:GLY:C	3:J:343:LEU:HD11	2.36	0.49
2:I:1281:TYR:OH	3:J:434:ILE:O	2.30	0.49
2:C:247:ARG:NH2	2:C:274:ILE:HD12	2.28	0.49
5:F:515:GLU:O	5:F:517:SER:N	2.45	0.49
5:F:573:LEU:HD13	5:F:588:ARG:NE	2.27	0.49
5:F:580:PHE:C	5:F:582:VAL:H	2.21	0.49
2:I:229:ILE:HG21	2:I:240:GLU:OE2	2.12	0.49
2:I:705:GLU:HB2	2:I:794:LEU:H	1.78	0.49
2:I:812:PHE:O	2:I:1099:ASN:ND2	2.45	0.49
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.13	0.49
5:L:148:TYR:OH	5:L:218:ARG:HA	2.12	0.49
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.95	0.49
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.27	0.49
1:B:173:VAL:HG12	1:B:174:ASP:H	1.78	0.49
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.95	0.49
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.95	0.49
3:D:360:TYR:OH	3:D:442:ILE:HD11	2.13	0.49
3:D:491:LEU:HA	3:D:498:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:492:SER:HB3	3:D:495:ASN:O	2.13	0.49
3:D:702:GLN:O	3:D:718:SER:N	2.37	0.49
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.38	0.49
5:F:148:TYR:OH	5:F:218:ARG:HA	2.12	0.49
1:G:45:ARG:CD	2:I:1083:GLU:HB3	2.42	0.49
2:I:103:VAL:HB	2:I:113:THR:HG22	1.95	0.49
2:I:620:ASN:O	2:I:620:ASN:ND2	2.45	0.49
2:I:891:GLY:O	2:I:892:GLU:HG3	2.13	0.49
3:J:697:MET:O	3:J:701:LEU:HB2	2.13	0.49
1:A:29:GLU:OE1	1:A:200:LYS:HG3	2.12	0.49
1:A:152:TYR:CZ	2:C:824:GLN:HA	2.48	0.49
2:C:564:PRO:HG2	2:C:568:ASN:O	2.13	0.49
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.77	0.49
3:D:654:ILE:O	3:D:658:GLU:HB2	2.12	0.49
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.94	0.49
1:G:175:ALA:HB1	1:G:177:TYR:CE1	2.47	0.49
2:I:194:LEU:HD11	2:I:432:LEU:CD2	2.43	0.49
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.12	0.49
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.47	0.49
2:I:860:ALA:O	2:I:863:SER:OG	2.25	0.49
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.47	0.49
5:L:533:ASP:O	5:L:536:THR:N	2.46	0.49
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.95	0.49
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.53	0.49
2:I:1099:ASN:ND2	3:J:505:ASP:OD1	2.46	0.49
3:J:264:ASP:HB3	3:J:324:LEU:HB2	1.95	0.49
5:L:315:TRP:O	5:L:319:ALA:HB3	2.12	0.49
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.94	0.48
1:B:53:GLY:O	1:B:177:TYR:HB3	2.13	0.48
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.42	0.48
2:C:180:ARG:NH2	2:C:465:ARG:HH12	2.11	0.48
2:C:559:CYS:CB	2:C:662:SER:HB3	2.42	0.48
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.13	0.48
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.46	0.48
5:L:119:ILE:O	5:L:123:ILE:HG13	2.13	0.48
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.28	0.48
1:A:14:VAL:HG13	1:A:15:ASP:N	2.11	0.48
1:B:16:ILE:CG2	1:B:26:VAL:HG22	2.34	0.48
3:D:306:LEU:O	3:D:326:SER:HB2	2.13	0.48
3:D:436:ALA:HB3	3:D:485:MET:HA	1.94	0.48
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:511:ILE:CG1	5:F:512:GLY:N	2.76	0.48
2:I:545:PHE:CZ	3:J:781:LYS:HG3	2.48	0.48
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.28	0.48
3:J:797:THR:CG2	3:J:924:GLY:HA3	2.41	0.48
3:J:1184:ASP:O	3:J:1186:TYR:N	2.46	0.48
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.94	0.48
1:H:54:CYS:SG	1:H:148:ARG:HG3	2.53	0.48
2:I:98:VAL:O	2:I:121:GLU:HA	2.14	0.48
2:I:1309:VAL:HA	3:J:383:GLY:HA3	1.95	0.48
2:I:1328:LYS:O	2:I:1332:SER:N	2.45	0.48
3:J:425:ARG:NH1	3:J:464:ASP:CG	2.71	0.48
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.78	0.48
5:L:340:ALA:HA	5:L:343:LYS:NZ	2.27	0.48
1:A:23:HIS:HE1	1:A:204:GLU:HG3	1.78	0.48
1:B:48:LEU:CD2	3:D:535:ARG:HG3	2.42	0.48
1:B:108:GLY:O	1:B:133:LEU:HB2	2.12	0.48
3:D:514:THR:HG23	3:D:596:LEU:HB2	1.94	0.48
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.42	0.48
2:I:208:ILE:O	2:I:362:ALA:HB1	2.14	0.48
5:L:137:TYR:HE1	5:L:351:THR:HB	1.78	0.48
1:B:9:LEU:HB2	1:B:32:GLU:OE1	2.14	0.48
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.29	0.48
2:C:298:ALA:HB3	2:C:334:GLU:HB2	1.95	0.48
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.29	0.48
2:C:1009:ASN:O	2:C:1012:GLU:HB3	2.12	0.48
5:F:343:LYS:H	5:F:343:LYS:HD2	1.78	0.48
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.44	0.48
1:G:83:LEU:HD23	2:I:694:ARG:NE	2.23	0.48
3:J:22:ILE:O	3:J:1339:GLY:HA2	2.13	0.48
1:A:176:CYS:O	1:A:177:TYR:C	2.55	0.48
2:C:62:TYR:C	2:C:64:GLY:H	2.21	0.48
2:C:263:VAL:HG21	2:C:273:HIS:CG	2.49	0.48
2:C:820:GLU:N	2:C:1080:ASN:O	2.46	0.48
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.77	0.48
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.48
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.77	0.48
2:I:596:ASP:C	2:I:648:ASP:OD1	2.57	0.48
2:I:606:LEU:HD21	2:I:614:TYR:CD1	2.48	0.48
2:I:1304:MET:HE3	2:I:1308:ILE:HD11	1.94	0.48
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.14	0.48
3:J:152:THR:OG1	3:J:153:ASN:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:490:ILE:HA	3:J:500:ILE:HG13	1.94	0.48
3:J:844:THR:HG23	3:J:864:LEU:HD11	1.96	0.48
5:L:134:VAL:HA	5:L:273:MET:HE1	1.95	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.14	0.48
5:L:456:MET:HE1	5:L:497:VAL:HG13	1.95	0.48
5:L:573:LEU:HG	5:L:574:GLU:OE1	2.13	0.48
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.43	0.48
3:D:527:LEU:HD22	3:D:533:ALA:HA	1.96	0.48
3:D:1234:VAL:O	3:D:1238:GLN:HB2	2.14	0.48
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.95	0.48
1:H:100:LEU:HD11	1:H:121:VAL:CG2	2.42	0.48
2:I:344:GLY:HA3	2:I:346:TYR:CE1	2.48	0.48
2:I:548:ARG:HB3	2:I:569:ILE:O	2.14	0.48
2:C:728:ASP:OD1	2:C:729:ALA:N	2.47	0.48
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.43	0.48
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.95	0.48
3:D:1266:ILE:HD13	3:D:1272:SER:HB3	1.96	0.48
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.94	0.48
5:F:281:ARG:O	5:F:285:ARG:HG3	2.14	0.48
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.96	0.48
2:I:15:PHE:HZ	2:I:1151:LEU:HD12	1.78	0.48
2:I:810:TYR:HE1	2:I:1078:LYS:HD2	1.74	0.48
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.60	0.48
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	1.95	0.48
2:I:1059:ARG:O	2:I:1234:LYS:NZ	2.46	0.48
2:I:1246:ARG:HH11	2:I:1266:GLY:HA2	1.78	0.48
2:I:1253:LEU:HD11	3:J:253:VAL:HG11	1.96	0.48
3:J:88:CYS:O	3:J:90:VAL:N	2.47	0.48
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.13	0.48
5:L:227:GLN:HG2	5:L:252:LEU:HA	1.95	0.48
2:C:149:LEU:HD12	2:C:452:ARG:O	2.14	0.48
5:F:484:ALA:HB1	5:F:491:GLU:HG3	1.96	0.48
2:I:728:ASP:OD1	2:I:729:ALA:N	2.47	0.48
2:I:1085:MET:HE2	2:I:1085:MET:HA	1.96	0.48
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.96	0.48
3:J:306:LEU:O	3:J:326:SER:HB2	2.13	0.48
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.96	0.48
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.14	0.48
2:C:854:ILE:O	2:C:857:VAL:HG22	2.13	0.48
2:C:1315:MET:CE	2:C:1317:PRO:HB3	2.42	0.48
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:109:ALA:HB1	2:I:110:PRO:O	2.14	0.48
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.96	0.48
2:I:878:THR:OG1	2:I:879:GLY:N	2.45	0.48
5:L:423:ARG:HD2	5:L:425:TYR:CE2	2.49	0.48
2:C:488:MET:C	2:C:490:GLN:H	2.21	0.47
3:D:600:ALA:O	3:D:603:LYS:HG2	2.14	0.47
1:H:51:MET:C	1:H:150:ARG:HG2	2.39	0.47
2:I:138:ILE:HG22	2:I:139:ASN:N	2.29	0.47
2:I:155:VAL:HA	2:I:175:ARG:O	2.14	0.47
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.48	0.47
2:I:206:ALA:O	2:I:209:ILE:HG22	2.13	0.47
3:J:16:GLU:HG3	3:J:17:PHE:H	1.78	0.47
3:J:362:ARG:H	3:J:365:GLN:HE21	1.62	0.47
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.22	0.47
3:J:557:LYS:HA	3:J:563:LEU:HA	1.96	0.47
3:J:576:ARG:NH1	3:J:593:ASN:O	2.46	0.47
5:L:515:GLU:C	5:L:517:SER:N	2.72	0.47
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.49	0.47
2:C:1238:LEU:O	2:C:1241:ASP:HB2	2.14	0.47
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.49	0.47
3:D:785:ASP:O	3:D:789:LYS:N	2.39	0.47
5:F:314:THR:O	5:F:318:ALA:HB3	2.14	0.47
3:J:192:MET:HE2	3:J:197:GLU:OE2	2.13	0.47
3:J:516:ASP:N	3:J:516:ASP:OD1	2.47	0.47
3:J:596:LEU:HD12	3:J:601:ILE:HG13	1.96	0.47
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.14	0.47
5:L:515:GLU:HG2	5:L:516:ASP:N	2.29	0.47
1:B:66:HIS:CE1	1:B:68:TYR:CD1	3.02	0.47
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.78	0.47
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.48	0.47
3:D:141:PHE:HA	3:D:180:MET:HE2	1.95	0.47
3:D:515:ARG:O	3:D:545:HIS:HB3	2.14	0.47
4:E:21:LEU:HD12	4:E:21:LEU:HA	1.74	0.47
5:F:532:LEU:O	5:F:536:THR:HG23	2.14	0.47
2:I:996:ARG:HD2	2:I:999:GLU:OE1	2.13	0.47
3:J:334:LYS:HA	3:J:335:GLN:HA	1.58	0.47
3:J:369:PRO:HB3	3:J:444:GLY:O	2.15	0.47
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.96	0.47
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.96	0.47
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.50	0.47
2:C:169:LYS:O	2:C:170:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.68	0.47
2:I:808:ASN:H	3:J:633:ALA:HB2	1.79	0.47
3:J:317:THR:CG2	3:J:320:ASN:HB3	2.44	0.47
1:B:53:GLY:HA3	1:B:177:TYR:C	2.39	0.47
1:B:79:LEU:HD11	3:D:526:VAL:HG11	1.96	0.47
4:E:3:ARG:HB2	4:E:48:VAL:HG13	1.96	0.47
1:G:228:LEU:HG	1:H:221:ALA:HB1	1.97	0.47
2:I:1148:ALA:HA	2:I:1201:LEU:CD2	2.43	0.47
3:J:810:THR:HG23	3:J:811:GLU:H	1.80	0.47
1:A:166:ARG:O	1:A:167:PRO:C	2.58	0.47
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.96	0.47
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.96	0.47
4:E:82:ALA:O	4:E:85:ALA:HB3	2.13	0.47
4:E:86:ILE:C	4:E:88:GLU:H	2.20	0.47
1:H:55:ALA:HB3	1:H:177:TYR:HD1	1.78	0.47
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.95	0.47
1:B:211:ILE:HD11	1:B:215:GLU:CD	2.39	0.47
2:C:229:ILE:HD13	2:C:334:GLU:HG2	1.97	0.47
2:C:859:GLU:O	2:C:863:SER:N	2.47	0.47
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.14	0.47
3:D:652:GLU:O	3:D:656:GLU:HG3	2.14	0.47
3:D:810:THR:HG23	3:D:811:GLU:H	1.79	0.47
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.97	0.47
5:F:396:ASN:C	5:F:398:GLY:H	2.22	0.47
1:G:62:ASP:OD1	1:G:141:SER:OG	2.32	0.47
2:I:60:GLN:O	2:I:476:LYS:HE2	2.15	0.47
2:I:1312:ASN:ND2	2:I:1314:GLN:HE21	2.08	0.47
3:J:343:LEU:HD12	3:J:344:GLY:CA	2.45	0.47
3:J:372:MET:HE2	3:J:372:MET:HB3	1.66	0.47
3:J:591:ILE:HG13	3:J:604:MET:HE2	1.97	0.47
5:L:606:VAL:HG13	5:L:607:LEU:HD12	1.96	0.47
1:A:230:ALA:O	1:A:233:ASP:O	2.33	0.47
2:C:138:ILE:HG22	2:C:139:ASN:N	2.30	0.47
2:C:180:ARG:CZ	2:C:465:ARG:HH12	2.28	0.47
2:C:494:ASN:HB3	2:C:497:PRO:HD2	1.95	0.47
2:C:812:PHE:HZ	3:D:503:SER:HB2	1.79	0.47
3:D:244:VAL:HA	3:D:269:TYR:OH	2.14	0.47
2:I:47:TYR:OH	2:I:398:SER:HB2	2.14	0.47
3:J:58:CYS:SG	3:J:60:ARG:HB3	2.55	0.47
3:J:594:GLN:HG3	3:J:596:LEU:HD22	1.97	0.47
3:J:650:LYS:HZ1	3:J:762:ASN:HD22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:748:ALA:O	3:J:777:HIS:HD2	1.98	0.47
3:J:793:SER:O	3:J:797:THR:HG23	2.14	0.47
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.72	0.47
1:B:201:LEU:HG	1:B:203:ILE:CD1	2.45	0.47
2:C:183:TRP:HB2	2:C:199:ASP:HA	1.97	0.47
2:C:371:ARG:HD3	2:C:374:GLU:OE2	2.15	0.47
2:C:698:PRO:HG3	2:C:1231:TYR:CE2	2.49	0.47
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.15	0.47
3:D:290:ILE:H	3:D:290:ILE:HD12	1.80	0.47
3:D:801:VAL:O	3:D:805:GLN:HB2	2.15	0.47
3:D:914:ALA:O	3:D:918:ILE:HG23	2.14	0.47
5:F:134:VAL:HA	5:F:273:MET:HE1	1.96	0.47
5:F:139:GLU:HG2	5:F:351:THR:HA	1.97	0.47
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.96	0.47
1:H:192:VAL:HB	1:H:195:ARG:HB2	1.96	0.47
2:I:9:LYS:O	2:I:1172:LEU:HA	2.15	0.47
3:J:514:THR:CB	3:J:576:ARG:HG2	2.45	0.47
3:J:598:LYS:O	3:J:601:ILE:HG22	2.15	0.47
4:K:59:ILE:HD12	4:K:64:LEU:HD21	1.97	0.47
2:C:67:GLU:HB3	2:C:103:VAL:CG2	2.44	0.47
2:C:615:VAL:HG13	2:C:651:ASP:N	2.30	0.47
2:C:1326:LEU:HD21	3:D:337:ARG:CZ	2.45	0.47
3:D:1176:VAL:HA	3:D:1186:TYR:O	2.15	0.47
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.50	0.47
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.96	0.47
1:H:191:ARG:O	1:H:191:ARG:HG2	2.10	0.47
2:I:149:LEU:HD12	2:I:452:ARG:O	2.15	0.47
2:I:519:ASN:ND2	2:I:796:LEU:HD23	2.30	0.47
2:I:979:LEU:HA	2:I:1002:LEU:CD1	2.44	0.47
2:I:1272:GLU:HG2	2:I:1276:TRP:CZ2	2.50	0.47
3:J:649:LYS:O	3:J:653:ILE:HG13	2.15	0.47
1:B:22:THR:OG1	1:B:207:THR:O	2.32	0.46
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.96	0.46
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.97	0.46
1:G:45:ARG:HH12	1:H:38:THR:N	2.11	0.46
2:I:208:ILE:HG12	2:I:362:ALA:HB1	1.97	0.46
2:I:379:GLU:CD	2:I:379:GLU:H	2.22	0.46
2:I:891:GLY:C	2:I:892:GLU:HG3	2.39	0.46
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.95	0.46
5:L:388:ILE:O	5:L:392:LYS:HG3	2.16	0.46
2:C:98:VAL:O	2:C:121:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:GLU:HG3	2:C:107:ARG:N	2.30	0.46
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.45	0.46
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.15	0.46
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.59	0.46
3:J:142:GLU:O	3:J:143:SER:OG	2.30	0.46
3:J:516:ASP:HA	3:J:545:HIS:HB2	1.97	0.46
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.96	0.46
3:J:544:LEU:O	3:J:574:VAL:HB	2.15	0.46
3:J:615:LYS:HZ3	4:K:7:GLN:HG2	1.80	0.46
1:B:158:ARG:HG2	1:B:172:LEU:HD23	1.97	0.46
2:C:299:LYS:HG2	2:C:334:GLU:OE1	2.15	0.46
1:G:79:LEU:HD11	2:I:693:LEU:HD21	1.96	0.46
1:H:34:GLY:N	1:H:199:ASP:OD2	2.49	0.46
1:H:173:VAL:HG12	1:H:174:ASP:H	1.80	0.46
2:I:214:ASN:HB2	2:I:359:ARG:HD2	1.97	0.46
2:I:496:LYS:HB3	2:I:496:LYS:HE3	1.58	0.46
2:I:499:SER:O	2:I:503:LYS:HB2	2.16	0.46
2:I:720:ARG:NE	2:I:736:VAL:HG11	2.30	0.46
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.16	0.46
3:J:364:HIS:CD2	4:K:4:VAL:HG23	2.50	0.46
5:L:342:GLN:OE1	5:L:345:GLN:NE2	2.48	0.46
5:L:583:THR:HG22	5:L:584:ARG:H	1.79	0.46
1:A:234:LEU:H	1:B:218:ARG:HH12	1.63	0.46
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.96	0.46
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.50	0.46
5:F:147:GLN:HE22	5:F:150:ARG:NH1	2.13	0.46
1:G:58:GLU:CD	1:G:145:LYS:HE3	2.40	0.46
1:G:197:ASP:O	1:G:198:LEU:HD23	2.14	0.46
1:H:53:GLY:HA3	1:H:177:TYR:C	2.40	0.46
2:I:232:ILE:HD13	2:I:326:SER:OG	2.15	0.46
3:J:74:LYS:NZ	3:J:86:GLU:OE1	2.43	0.46
3:J:297:ARG:HB3	5:L:97:PRO:HB3	1.97	0.46
3:J:504:GLN:OE1	3:J:731:ARG:NH1	2.49	0.46
3:J:518:VAL:HG12	3:J:707:ILE:HD13	1.98	0.46
3:J:930:LEU:HD23	3:J:1244:GLN:HG3	1.98	0.46
3:J:1297:LYS:HG3	3:J:1299:GLY:H	1.80	0.46
5:L:487:MET:HE2	5:L:487:MET:HA	1.97	0.46
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.51	0.46
2:C:606:LEU:HD21	2:C:614:TYR:HD1	1.81	0.46
2:C:906:PHE:CE2	5:F:608:ARG:HD3	2.50	0.46
3:D:253:VAL:HG21	5:F:523:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:278:ARG:HH11	3:D:295:GLU:CD	2.22	0.46
3:D:733:SER:O	3:D:737:ILE:HG12	2.14	0.46
5:F:418:LYS:HD2	5:F:434:TRP:CZ2	2.50	0.46
1:G:152:TYR:CZ	2:I:824:GLN:HA	2.51	0.46
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.98	0.46
2:I:703:GLY:N	2:I:705:GLU:OE2	2.47	0.46
2:I:1327:LEU:HG	2:I:1337:ILE:HG23	1.96	0.46
3:J:34:SER:HG	3:J:104:HIS:HD1	1.58	0.46
3:J:583:VAL:HG21	3:J:592:VAL:HG11	1.97	0.46
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.98	0.46
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.58	0.46
2:C:169:LYS:O	2:C:169:LYS:HG2	2.15	0.46
2:C:301:TYR:CE2	2:C:333:ILE:HA	2.50	0.46
2:C:1059:ARG:O	2:C:1234:LYS:NZ	2.43	0.46
3:J:30:ILE:HD13	3:J:243:PRO:HD3	1.97	0.46
3:J:53:ARG:HB2	3:J:54:ASP:OD1	2.16	0.46
3:J:290:ILE:H	3:J:290:ILE:HD12	1.80	0.46
1:A:61:ILE:HG22	1:A:62:ASP:H	1.80	0.46
3:D:45:ASN:O	3:D:46:TYR:HB3	2.15	0.46
3:D:77:ARG:HH21	5:F:568:ASN:HA	1.80	0.46
3:D:140:TYR:O	3:D:297:ARG:NH1	2.48	0.46
3:D:513:MET:HE2	3:D:513:MET:HB3	1.58	0.46
3:D:1301:THR:HG23	3:J:1301:THR:CG2	2.45	0.46
5:F:96:ASP:O	5:F:98:VAL:N	2.48	0.46
1:G:45:ARG:NH1	1:H:38:THR:N	2.63	0.46
2:I:786:GLY:N	2:I:789:THR:OG1	2.48	0.46
3:J:848:VAL:O	3:J:857:LEU:HD12	2.15	0.46
5:L:108:VAL:HG11	5:L:381:GLU:O	2.16	0.46
5:L:580:PHE:C	5:L:582:VAL:H	2.23	0.46
2:C:1191:LYS:O	2:C:1195:ILE:HG13	2.16	0.46
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.16	0.46
3:D:93:THR:HG22	3:D:94:GLN:H	1.80	0.46
3:D:416:ILE:HD13	3:D:416:ILE:HA	1.75	0.46
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.30	0.46
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.57	0.46
1:G:176:CYS:O	1:G:177:TYR:C	2.59	0.46
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.81	0.46
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.77	0.46
2:I:1101:LEU:HB3	3:J:731:ARG:HD3	1.97	0.46
3:J:85:CYS:HB3	3:J:88:CYS:O	2.16	0.46
5:L:248:GLU:O	5:L:252:LEU:N	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:248:GLU:HA	5:L:251:LYS:HZ1	1.81	0.46
2:C:57:PHE:HD1	2:C:58:PRO:HA	1.81	0.46
2:C:323:ALA:O	2:C:327:GLN:HG3	2.16	0.46
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.50	0.46
2:C:734:ILE:O	2:C:748:ILE:HB	2.15	0.46
2:C:1291:LEU:HD11	3:D:1354:GLY:HA2	1.97	0.46
2:C:1312:ASN:OD1	2:C:1314:GLN:HG3	2.15	0.46
3:D:75:TYR:OH	3:D:86:GLU:OE1	2.34	0.46
3:D:744:ARG:O	3:D:759:ILE:HB	2.16	0.46
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.97	0.46
1:H:74:VAL:HG22	1:H:133:LEU:HD12	1.96	0.46
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.98	0.46
3:J:1168:GLU:OE1	3:J:1173:ARG:HG3	2.15	0.46
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.98	0.46
5:L:557:LYS:O	5:L:561:MET:HB2	2.16	0.46
1:B:110:VAL:O	1:B:130:ILE:HB	2.15	0.46
2:C:211:ARG:HB2	2:C:362:ALA:HB2	1.96	0.46
2:C:617:ALA:HA	2:C:636:CYS:SG	2.56	0.46
3:D:609:TYR:OH	3:D:905:ARG:HA	2.16	0.46
3:D:877:VAL:O	3:D:877:VAL:HG13	2.16	0.46
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.30	0.46
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.98	0.46
5:F:507:MET:HG2	5:F:520:GLY:CA	2.45	0.46
1:H:67:GLU:OE1	1:H:67:GLU:N	2.49	0.46
2:I:57:PHE:HD1	2:I:58:PRO:HA	1.81	0.46
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.97	0.46
2:I:886:LYS:CE	2:I:916:SER:HB3	2.45	0.46
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.98	0.46
3:J:591:ILE:HG23	3:J:604:MET:HE2	1.98	0.46
3:J:631:TYR:O	3:J:635:SER:N	2.49	0.46
3:J:694:SER:O	3:J:698:MET:HB2	2.16	0.46
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.98	0.46
3:J:1205:GLU:N	3:J:1208:ASP:OD2	2.49	0.46
1:B:74:VAL:HG12	1:B:76:GLU:HB2	1.98	0.45
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.74	0.45
2:C:263:VAL:HG21	2:C:273:HIS:CD2	2.51	0.45
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.16	0.45
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.98	0.45
2:C:871:VAL:O	2:C:944:ARG:NH1	2.48	0.45
2:C:1248:THR:HG21	5:F:531:PRO:CG	2.45	0.45
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:507:MET:HG2	5:F:520:GLY:HA3	1.98	0.45
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.15	0.45
2:I:672:GLU:HB3	2:I:1187:PHE:CD2	2.51	0.45
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.98	0.45
2:I:1331:ARG:HA	2:I:1335:ILE:O	2.15	0.45
3:J:515:ARG:NH2	3:J:717:VAL:O	2.49	0.45
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.51	0.45
2:C:725:GLN:HE22	2:C:966:ILE:HG23	1.81	0.45
2:C:730:SER:O	2:C:753:LEU:HB2	2.16	0.45
2:C:896:THR:HB	2:C:897:PRO:HD2	1.98	0.45
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.52	0.45
3:D:152:THR:OG1	3:D:153:ASN:N	2.42	0.45
3:D:814:CYS:SG	3:D:816:THR:HG22	2.56	0.45
3:D:1141:VAL:HG13	3:D:1237:VAL:HG23	1.98	0.45
5:F:512:GLY:C	5:F:514:ASP:H	2.24	0.45
5:F:562:ARG:HD2	5:F:562:ARG:HA	1.77	0.45
2:I:115:LYS:HD3	2:I:116:ASP:N	2.30	0.45
2:I:494:ASN:HB3	2:I:497:PRO:CD	2.46	0.45
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.98	0.45
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.16	0.45
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.51	0.45
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.98	0.45
3:J:746:LEU:CD2	3:J:758:PRO:HG3	2.46	0.45
3:J:860:ARG:HB3	3:J:861:ASN:H	1.68	0.45
5:L:601:PRO:O	5:L:602:SER:OG	2.21	0.45
2:C:615:VAL:HG22	2:C:650:VAL:HA	1.99	0.45
2:C:685:MET:HE3	2:C:685:MET:HB2	1.69	0.45
3:D:42:GLU:OE1	3:D:42:GLU:N	2.47	0.45
3:D:820:ILE:HG22	3:D:1227:HIS:HD1	1.80	0.45
5:F:227:GLN:HE22	5:F:251:LYS:HZ1	1.60	0.45
5:F:372:ALA:O	5:F:376:LYS:HG3	2.17	0.45
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.99	0.45
1:G:232:VAL:C	1:H:218:ARG:HH12	2.24	0.45
2:I:91:THR:HB	2:I:138:ILE:O	2.16	0.45
2:I:734:ILE:O	2:I:748:ILE:HB	2.17	0.45
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.82	0.45
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	1.97	0.45
3:J:1327:GLU:OE2	3:J:1329:THR:HB	2.17	0.45
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.52	0.45
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.63	0.45
5:L:481:GLU:O	5:L:484:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.97	0.45
1:A:179:PRO:HA	1:A:208:ASN:ND2	2.31	0.45
1:A:223:ILE:HD13	1:B:8:PHE:HE1	1.81	0.45
2:C:18:ARG:NH1	2:C:622:ASN:OD1	2.40	0.45
2:C:298:ALA:HB3	2:C:334:GLU:CB	2.47	0.45
2:C:516:VAL:HG23	2:C:526:HIS:HD2	1.82	0.45
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.65	0.45
3:D:1171:GLY:HA2	3:D:1193:TRP:CH2	2.51	0.45
5:F:306:PHE:CE1	5:F:315:TRP:CG	3.02	0.45
5:F:320:ILE:HG21	5:F:331:HIS:NE2	2.30	0.45
5:F:354:THR:O	5:F:358:VAL:HG23	2.16	0.45
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.65	0.45
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.40	0.45
2:I:1285:TYR:CE2	3:J:1356:LEU:HD11	2.52	0.45
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.80	0.45
3:J:749:LYS:HG3	3:J:751:ASP:HB3	1.97	0.45
3:J:884:SER:OG	3:J:1254:GLU:OE1	2.15	0.45
1:A:6:THR:OG1	1:A:7:GLU:N	2.45	0.45
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.17	0.45
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.31	0.45
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.99	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.45
2:C:1313:HIS:N	4:E:31:GLN:OE1	2.40	0.45
3:D:109:SER:HB2	3:D:296:LYS:HE2	1.99	0.45
3:D:347:VAL:HG12	3:D:348:ASP:O	2.16	0.45
3:J:689:ALA:O	3:J:693:VAL:HG23	2.16	0.45
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.32	0.45
5:L:557:LYS:NZ	5:L:561:MET:HE1	2.32	0.45
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.98	0.45
2:C:733:VAL:CG1	2:C:748:ILE:HG13	2.47	0.45
2:C:1290:MET:HE2	2:C:1290:MET:HB2	1.85	0.45
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.51	0.45
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.66	0.45
3:D:320:ASN:OD1	3:D:322:ARG:HB3	2.16	0.45
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.60	0.45
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.63	0.45
1:H:74:VAL:CG1	1:H:76:GLU:HB2	2.47	0.45
1:H:214:GLU:O	1:H:218:ARG:HG3	2.16	0.45
2:I:854:ILE:O	2:I:857:VAL:HG22	2.16	0.45
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.99	0.45
3:J:214:ARG:HA	3:J:217:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:650:LYS:O	3:J:654:ILE:HG13	2.17	0.45
5:L:596:ARG:HG3	5:L:599:ARG:HH21	1.82	0.45
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.47	0.45
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.15	0.45
3:D:849:LEU:H	3:D:849:LEU:HD22	1.82	0.45
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.97	0.45
1:G:211:ILE:CG2	1:G:216:ALA:HB2	2.45	0.45
1:H:177:TYR:O	1:H:178:SER:C	2.59	0.45
2:I:465:ARG:O	2:I:469:VAL:HG13	2.17	0.45
2:I:524:ILE:HD13	2:I:708:VAL:HG13	1.97	0.45
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.52	0.45
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.98	0.45
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.81	0.45
5:L:128:ASN:HA	5:L:131:GLN:NE2	2.21	0.45
5:L:354:THR:O	5:L:358:VAL:HG23	2.17	0.45
5:L:465:ARG:HG2	5:L:465:ARG:H	1.37	0.45
1:B:25:LYS:HE2	1:B:202:VAL:HG11	1.99	0.45
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.83	0.45
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.97	0.45
3:D:432:LEU:HD21	3:D:489:ASN:CB	2.47	0.45
3:D:1297:LYS:N	3:D:1298:VAL:HA	2.30	0.45
2:I:80:PHE:HB3	2:I:84:GLU:CB	2.44	0.45
3:J:749:LYS:HG2	3:J:753:SER:O	2.17	0.45
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.99	0.45
5:L:603:ARG:HH11	5:L:603:ARG:HA	1.82	0.45
1:A:117:HIS:CE1	1:A:118:ASP:O	2.69	0.45
1:A:177:TYR:O	1:A:178:SER:HB2	2.17	0.45
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.65	0.45
2:C:480:SER:HB3	2:C:481:LEU:HD22	1.99	0.45
3:D:114:ILE:HD11	3:D:311:ARG:CB	2.37	0.45
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.82	0.45
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.99	0.45
3:D:504:GLN:OE1	3:D:731:ARG:NH1	2.50	0.45
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.98	0.45
5:F:306:PHE:HE1	5:F:315:TRP:CD2	2.35	0.45
1:G:74:VAL:CG2	1:G:76:GLU:HB2	2.47	0.45
2:I:4:SER:HB2	2:I:7:GLU:HG3	1.99	0.45
2:I:74:ARG:HG2	2:I:75:LEU:N	2.31	0.45
2:I:208:ILE:HG12	2:I:362:ALA:CB	2.47	0.45
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.17	0.45
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:245:LEU:O	3:J:250:ARG:NH2	2.50	0.45
3:J:363:LEU:O	3:J:363:LEU:HG	2.16	0.45
3:J:1266:ILE:HG13	3:J:1276:GLU:O	2.17	0.45
1:B:112:ALA:O	1:B:115:ILE:HG13	2.17	0.45
3:D:62:PHE:O	3:D:101:ARG:HD2	2.17	0.45
3:D:432:LEU:HD21	3:D:489:ASN:HB2	1.98	0.45
5:F:101:TYR:HE2	5:F:388:ILE:HD11	1.82	0.45
1:H:31:LEU:HD13	1:H:31:LEU:HA	1.75	0.45
2:I:402:ARG:HG2	2:I:416:GLY:H	1.82	0.45
2:I:411:ARG:NH2	2:I:427:ASP:OD2	2.43	0.45
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.99	0.45
3:J:733:SER:O	3:J:737:ILE:HG12	2.17	0.45
3:J:825:VAL:C	3:J:826:ILE:HG13	2.41	0.45
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.71	0.45
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.99	0.44
2:C:53:PHE:O	2:C:57:PHE:HB2	2.17	0.44
2:C:1281:TYR:OH	3:D:434:ILE:O	2.35	0.44
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.32	0.44
1:G:13:LEU:HD22	1:H:231:PHE:CD1	2.52	0.44
1:G:154:PRO:HB2	2:I:1059:ARG:HH21	1.83	0.44
2:I:810:TYR:HE2	3:J:359:PRO:HD2	1.82	0.44
2:I:1262:LYS:HA	2:I:1262:LYS:HD3	1.68	0.44
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.18	0.44
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.78	0.44
3:J:838:ARG:NH1	3:J:1250:ASP:OD1	2.50	0.44
3:J:1236:GLU:O	3:J:1239:ASP:HB2	2.17	0.44
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.32	0.44
5:L:483:LEU:HA	5:L:486:ARG:NH1	2.32	0.44
2:C:517:GLN:HE21	2:C:759:SER:HB2	1.83	0.44
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.52	0.44
3:D:1170:LYS:C	3:D:1172:LYS:H	2.25	0.44
2:I:1198:LEU:HD22	2:I:1198:LEU:HA	1.74	0.44
2:I:1312:ASN:HD21	2:I:1314:GLN:NE2	2.09	0.44
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.58	0.44
3:J:122:SER:O	3:J:126:LEU:HG	2.17	0.44
3:J:613:GLY:O	3:J:617:THR:OG1	2.30	0.44
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.17	0.44
3:J:1290:ARG:HD3	3:J:1294:ALA:CB	2.48	0.44
2:C:159:SER:O	2:C:160:ASP:HB2	2.16	0.44
2:C:1161:LEU:HD21	2:C:1165:SER:HB3	1.99	0.44
3:D:901:ARG:HA	3:D:908:ILE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1273:ASP:OD1	3:D:1273:ASP:N	2.47	0.44
4:E:83:VAL:HA	4:E:86:ILE:HG12	1.98	0.44
5:F:157:ARG:HB3	5:F:160:ASP:OD2	2.17	0.44
5:F:166:VAL:O	5:F:258:GLN:NE2	2.45	0.44
1:H:40:GLY:HA3	1:H:185:TYR:CG	2.53	0.44
1:H:41:ASN:CG	2:I:1217:THR:HA	2.43	0.44
1:H:224:LEU:HD12	1:H:224:LEU:HA	1.63	0.44
2:I:156:PHE:CD1	2:I:443:ASP:HB2	2.52	0.44
3:J:850:LYS:HB3	3:J:851:PRO:HD2	1.99	0.44
1:A:45:ARG:NH1	1:B:38:THR:H	2.14	0.44
1:A:115:ILE:HG22	1:A:116:THR:H	1.81	0.44
1:B:57:THR:O	1:B:173:VAL:N	2.46	0.44
2:C:210:LEU:O	2:C:215:TYR:HB2	2.18	0.44
2:C:692:THR:OG1	2:C:693:LEU:N	2.50	0.44
2:C:703:GLY:N	2:C:705:GLU:OE2	2.37	0.44
2:C:828:PHE:HD1	2:C:828:PHE:HA	1.60	0.44
2:C:1142:ARG:CD	2:C:1161:LEU:HD22	2.46	0.44
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.98	0.44
3:D:825:VAL:C	3:D:826:ILE:HG13	2.43	0.44
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.75	0.44
1:H:211:ILE:CD1	1:H:215:GLU:HG2	2.46	0.44
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.72	0.44
2:I:588:GLU:HG3	2:I:605:TYR:HD1	1.82	0.44
3:J:29:MET:O	3:J:29:MET:HG3	2.18	0.44
3:J:739:GLN:HA	3:J:744:ARG:HB3	1.99	0.44
1:A:175:ALA:HB1	1:A:177:TYR:CE1	2.53	0.44
2:C:685:MET:SD	2:C:1073:LYS:HG3	2.57	0.44
3:D:26:SER:HB2	3:D:236:TRP:CE2	2.52	0.44
3:D:342:LEU:HA	3:D:343:LEU:HA	1.82	0.44
3:D:748:ALA:O	3:D:777:HIS:CD2	2.70	0.44
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.99	0.44
1:H:197:ASP:OD1	1:H:197:ASP:N	2.50	0.44
2:I:462:ASN:O	2:I:466:VAL:HG23	2.17	0.44
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.32	0.44
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.83	0.44
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.98	0.44
3:J:218:THR:HG21	3:J:1275:LEU:HD21	1.99	0.44
3:J:430:HIS:HA	3:J:921:GLN:HB3	2.00	0.44
5:L:462:LYS:O	5:L:466:ILE:HG13	2.17	0.44
1:A:23:HIS:CE1	1:A:204:GLU:HG3	2.53	0.44
2:C:805:MET:HE3	2:C:805:MET:HB2	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:THR:C	1:G:28:LEU:HD12	2.43	0.44
1:H:41:ASN:HA	1:H:44:ARG:NH1	2.33	0.44
2:I:74:ARG:NH2	2:I:97:ARG:HG3	2.32	0.44
2:I:145:ILE:HB	2:I:456:VAL:HG22	1.99	0.44
3:J:268:LEU:HG	3:J:324:LEU:HD22	1.99	0.44
3:J:908:ILE:HD13	3:J:909:ILE:O	2.17	0.44
5:L:139:GLU:HG2	5:L:351:THR:HA	2.00	0.44
1:A:13:LEU:H	1:A:13:LEU:HD23	1.83	0.44
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.52	0.44
3:D:1145:PHE:O	3:D:1309:ILE:HG12	2.17	0.44
2:I:566:GLY:O	2:I:569:ILE:HG13	2.18	0.44
3:J:1263:LYS:CE	3:J:1279:GLN:HE21	2.26	0.44
5:L:96:ASP:O	5:L:98:VAL:N	2.51	0.44
5:L:161:LEU:C	5:L:262:VAL:HG23	2.43	0.44
1:A:51:MET:HE2	1:A:220:ALA:HB2	2.00	0.44
2:C:10:ARG:HA	2:C:1172:LEU:HD23	2.00	0.44
2:C:46:GLN:OE1	2:C:47:TYR:N	2.49	0.44
2:C:263:VAL:HG12	2:C:264:GLU:O	2.18	0.44
2:C:596:ASP:C	2:C:648:ASP:OD1	2.61	0.44
2:C:1158:LYS:C	2:C:1159:VAL:HG22	2.43	0.44
2:C:1295:SER:OG	3:D:346:ARG:O	2.35	0.44
3:D:1172:LYS:HB3	3:D:1189:MET:HB3	2.00	0.44
3:D:1302:TYR:CD1	3:J:1297:LYS:HD3	2.52	0.44
5:F:138:PRO:HD2	5:F:353:LEU:HD11	2.00	0.44
2:I:11:ILE:HD13	2:I:11:ILE:HA	1.89	0.44
2:I:62:TYR:O	2:I:64:GLY:N	2.50	0.44
5:L:515:GLU:HG2	5:L:516:ASP:H	1.83	0.44
1:A:27:THR:C	1:A:28:LEU:HD12	2.43	0.44
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.53	0.44
2:C:226:GLU:HB3	2:C:245:ARG:HH22	1.82	0.44
2:C:500:ALA:O	2:C:504:GLU:HB2	2.16	0.44
3:D:126:LEU:HD13	3:D:223:LEU:HD21	2.00	0.44
3:D:1284:ARG:NH2	3:J:1292:LEU:HD11	2.33	0.44
5:F:548:LEU:HD22	5:F:556:ALA:HA	1.98	0.44
5:F:557:LYS:O	5:F:561:MET:HB2	2.18	0.44
2:I:75:LEU:HD13	2:I:75:LEU:HA	1.59	0.44
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.48	0.44
3:J:75:TYR:N	3:J:75:TYR:CD1	2.85	0.44
3:J:1243:LEU:HA	3:J:1243:LEU:HD12	1.70	0.44
5:L:105:MET:HE2	5:L:105:MET:HB2	1.89	0.44
5:L:115:GLY:HA2	5:L:118:ASP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:157:ARG:HB3	5:L:160:ASP:OD2	2.18	0.44
1:B:84:ASN:CG	3:D:551:ARG:HH22	2.26	0.43
2:C:486:THR:HG23	2:C:487:LEU:H	1.81	0.43
3:D:45:ASN:O	3:D:46:TYR:CD2	2.70	0.43
3:D:598:LYS:O	3:D:601:ILE:HG22	2.18	0.43
3:D:613:GLY:O	3:D:617:THR:OG1	2.25	0.43
3:D:825:VAL:O	3:D:826:ILE:C	2.60	0.43
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.99	0.43
2:I:13:LYS:NZ	2:I:1148:ALA:O	2.51	0.43
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	1.99	0.43
5:L:390:ILE:O	5:L:393:LYS:HB2	2.17	0.43
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	2.00	0.43
1:A:50:SER:HB2	1:B:8:PHE:CZ	2.53	0.43
1:A:162:GLU:HB3	1:A:163:GLU:H	1.58	0.43
2:C:124:MET:HE2	2:C:493:ILE:CD1	2.49	0.43
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.99	0.43
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.52	0.43
3:D:356:THR:OG1	3:D:357:VAL:N	2.48	0.43
3:D:516:ASP:HA	3:D:545:HIS:CB	2.48	0.43
3:D:646:ILE:HG22	3:D:647:PRO:HD2	1.99	0.43
3:D:843:VAL:CG1	3:D:897:HIS:O	2.66	0.43
3:D:891:ASP:OD2	3:D:1285:VAL:HG12	2.19	0.43
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.53	0.43
2:I:102:LEU:O	2:I:116:ASP:HA	2.18	0.43
2:I:169:LYS:O	2:I:170:VAL:HG22	2.18	0.43
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.53	0.43
2:I:212:ALA:HA	2:I:359:ARG:HG3	1.99	0.43
2:I:593:LYS:HB3	2:I:602:GLU:HG3	1.99	0.43
3:J:215:LYS:HD2	3:J:216:LYS:HG3	1.99	0.43
5:L:266:PHE:O	5:L:270:VAL:HG23	2.18	0.43
2:C:214:ASN:CB	2:C:359:ARG:HD2	2.48	0.43
3:D:94:GLN:O	3:D:97:VAL:HG22	2.18	0.43
3:D:142:GLU:OE2	5:F:100:MET:HE2	2.18	0.43
3:D:189:LEU:HB3	3:D:234:PRO:HB2	2.01	0.43
3:D:606:ASN:OD1	3:D:610:ARG:NE	2.51	0.43
5:F:343:LYS:O	5:F:347:ILE:HG13	2.17	0.43
5:F:533:ASP:O	5:F:536:THR:N	2.51	0.43
1:G:219:ARG:HA	1:G:222:THR:HB	2.00	0.43
1:H:175:ALA:HB1	1:H:177:TYR:CE1	2.52	0.43
2:I:828:PHE:HZ	2:I:1232:MET:O	2.01	0.43
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.32	0.43
3:J:294:ASN:HD22	5:L:406:GLN:HE21	1.66	0.43
3:J:425:ARG:HH11	3:J:425:ARG:HD2	1.47	0.43
3:J:842:ARG:HB3	3:J:882:VAL:HG11	2.00	0.43
3:J:1162:ILE:O	3:J:1178:THR:N	2.51	0.43
5:L:137:TYR:O	5:L:141:ILE:HG12	2.18	0.43
5:L:309:ASN:HB3	5:L:310:GLU:H	1.69	0.43
1:A:132:HIS:O	1:A:133:LEU:HD22	2.18	0.43
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.01	0.43
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.81	0.43
3:D:264:ASP:OD2	5:F:506:SER:OG	2.31	0.43
5:F:515:GLU:O	5:F:515:GLU:HG2	2.18	0.43
1:H:115:ILE:HG22	1:H:116:THR:H	1.82	0.43
2:I:119:GLU:HG3	2:I:489:PRO:CD	2.47	0.43
2:I:557:ARG:HH21	2:I:607:SER:C	2.26	0.43
2:I:803:ALA:HB2	2:I:1094:VAL:HG21	2.00	0.43
3:J:804:ALA:O	3:J:806:ASP:N	2.52	0.43
3:J:1168:GLU:OE1	3:J:1173:ARG:NH1	2.51	0.43
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	2.00	0.43
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.65	0.43
1:A:207:THR:HG22	1:A:209:GLY:H	1.84	0.43
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.99	0.43
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.63	0.43
2:C:878:THR:OG1	2:C:879:GLY:N	2.50	0.43
3:D:248:ASP:O	3:D:251:PRO:HG3	2.19	0.43
1:H:183:ILE:CD1	1:H:205:MET:HG3	2.48	0.43
2:I:339:ASN:HB3	2:I:343:HIS:H	1.82	0.43
2:I:890:LYS:HE2	2:I:891:GLY:H	1.84	0.43
2:I:1192:GLU:CD	3:J:641:ILE:HD12	2.43	0.43
1:B:31:LEU:HD13	1:B:31:LEU:HA	1.92	0.43
2:C:20:GLN:HG3	2:C:20:GLN:O	2.19	0.43
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.53	0.43
2:C:1008:GLN:O	2:C:1012:GLU:HB2	2.17	0.43
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.90	0.43
3:D:179:LYS:HB2	3:D:184:ALA:CB	2.46	0.43
5:F:127:ILE:O	5:F:130:VAL:HG22	2.18	0.43
5:F:561:MET:HG2	5:F:576:VAL:CG2	2.47	0.43
1:H:134:THR:HG23	1:H:135:ASP:N	2.33	0.43
2:I:560:PRO:HB3	3:J:776:THR:HG21	1.99	0.43
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.65	0.43
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:127:ILE:O	5:L:130:VAL:HG22	2.18	0.43
1:B:153:VAL:N	1:B:175:ALA:O	2.49	0.43
2:C:996:ARG:HA	2:C:996:ARG:HD3	1.46	0.43
1:G:44:ARG:HA	1:G:183:ILE:HG21	2.00	0.43
2:I:71:VAL:HB	2:I:99:LYS:HB2	2.00	0.43
2:I:239:MET:O	2:I:284:LEU:HD12	2.18	0.43
2:I:1126:ASP:O	2:I:1130:ALA:N	2.48	0.43
2:I:1272:GLU:H	3:J:343:LEU:CD1	2.31	0.43
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.53	0.43
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.53	0.43
3:J:322:ARG:HB2	3:J:322:ARG:NH1	2.34	0.43
3:J:342:LEU:HA	3:J:343:LEU:HD12	1.99	0.43
3:J:436:ALA:N	3:J:484:MET:O	2.31	0.43
3:J:642:ASP:HA	3:J:764:ARG:NH2	2.34	0.43
3:J:1356:LEU:HD23	3:J:1356:LEU:HA	1.84	0.43
1:B:23:HIS:HD1	1:B:206:GLU:HG2	1.83	0.43
2:C:124:MET:HG3	2:C:124:MET:O	2.18	0.43
2:C:148:GLN:O	2:C:453:ILE:HA	2.18	0.43
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.34	0.43
2:C:718:ALA:HB2	2:C:783:LEU:HD23	2.01	0.43
2:C:941:LYS:HB2	2:C:946:LEU:HG	2.00	0.43
3:D:328:ALA:O	3:D:332:LYS:HB2	2.19	0.43
3:D:343:LEU:HD13	3:D:344:GLY:CA	2.48	0.43
5:F:470:MET:HE2	5:F:486:ARG:NH1	2.32	0.43
2:I:86:GLN:HA	2:I:140:GLY:HA2	2.00	0.43
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.99	0.43
2:I:808:ASN:HA	3:J:629:PHE:HB3	2.00	0.43
2:I:820:GLU:N	2:I:1080:ASN:O	2.52	0.43
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.65	0.43
3:J:599:LYS:HD3	3:J:599:LYS:HA	1.57	0.43
3:J:683:ILE:HG21	3:J:683:ILE:HD13	1.83	0.43
1:A:231:PHE:HE2	1:B:39:LEU:HD13	1.82	0.43
1:A:238:ARG:HA	1:B:13:LEU:HA	1.99	0.43
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.18	0.43
2:C:221:LEU:HD11	2:C:314:ASN:HB2	2.00	0.43
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.01	0.43
2:C:1220:GLN:HG2	2:C:1221:PHE:H	1.84	0.43
3:D:18:ASP:HB2	3:D:1373:ARG:NH2	2.34	0.43
3:D:605:LEU:HD23	3:D:605:LEU:HA	1.72	0.43
5:F:166:VAL:HG23	5:F:258:GLN:O	2.18	0.43
2:I:139:ASN:C	2:I:141:THR:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:968:GLU:OE2	2:I:1022:LYS:NZ	2.39	0.43
2:I:1212:LEU:O	2:I:1221:PHE:N	2.52	0.43
3:J:527:LEU:HD21	3:J:536:LEU:HG	2.01	0.43
3:J:761:ALA:H	3:J:771:GLN:NE2	2.16	0.43
1:B:18:GLN:HG3	1:B:20:SER:O	2.17	0.43
2:C:209:ILE:O	2:C:213:LEU:N	2.52	0.43
2:C:211:ARG:HD3	2:C:357:ASN:C	2.44	0.43
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.31	0.43
3:D:807:LEU:HD23	3:D:915:ILE:HG13	2.01	0.43
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.49	0.43
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.18	0.43
3:D:1278:GLU:HG3	3:D:1279:GLN:N	2.33	0.43
1:G:23:HIS:HB2	1:G:206:GLU:HA	2.01	0.43
1:G:32:GLU:HA	1:G:198:LEU:CD2	2.48	0.43
1:G:166:ARG:N	1:G:167:PRO:HD2	2.34	0.43
1:G:223:ILE:HD13	1:H:8:PHE:CZ	2.54	0.43
2:I:213:LEU:HA	2:I:213:LEU:HD23	1.76	0.43
2:I:232:ILE:HD12	2:I:330:HIS:O	2.19	0.43
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.01	0.43
2:I:1313:HIS:O	4:K:28:ARG:NH1	2.52	0.43
3:J:356:THR:OG1	3:J:357:VAL:N	2.48	0.43
3:J:358:GLY:N	3:J:359:PRO:HD3	2.34	0.43
3:J:683:ILE:HD11	3:J:754:ILE:HG23	2.01	0.43
3:J:810:THR:HG21	3:J:893:GLY:HA3	2.00	0.43
5:L:100:MET:HE2	5:L:100:MET:HB3	1.93	0.43
1:A:45:ARG:NH1	1:B:38:THR:N	2.67	0.42
2:C:109:ALA:HB1	2:C:110:PRO:O	2.19	0.42
2:C:943:LYS:O	2:C:947:GLU:HG3	2.19	0.42
2:C:1270:PHE:N	3:D:343:LEU:HD11	2.34	0.42
3:D:1307:LEU:HB3	3:D:1312:ALA:HB2	2.01	0.42
5:F:137:TYR:O	5:F:141:ILE:HG12	2.19	0.42
5:F:474:MET:HE2	5:F:482:GLU:OE1	2.18	0.42
2:I:1149:TYR:N	2:I:1149:TYR:CD2	2.87	0.42
2:I:1191:LYS:O	2:I:1195:ILE:HG13	2.19	0.42
2:I:1315:MET:HE3	2:I:1315:MET:HB2	1.88	0.42
3:J:342:LEU:HA	3:J:343:LEU:HA	1.33	0.42
5:L:465:ARG:HB3	5:L:468:ARG:HH22	1.84	0.42
5:L:483:LEU:HD12	5:L:483:LEU:N	2.29	0.42
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.54	0.42
2:C:55:SER:OG	2:C:56:VAL:N	2.51	0.42
2:C:211:ARG:O	2:C:359:ARG:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1151:LEU:HD12	2:C:1151:LEU:HA	1.70	0.42
3:D:609:TYR:HD1	3:D:610:ARG:HH11	1.67	0.42
3:D:1267:VAL:O	3:D:1274:PHE:CE1	2.72	0.42
1:H:102:LEU:O	1:H:141:SER:HA	2.19	0.42
1:H:118:ASP:HB2	1:H:121:VAL:CG2	2.49	0.42
2:I:194:LEU:HD11	2:I:432:LEU:HD23	2.02	0.42
2:I:629:PHE:O	2:I:647:ARG:NH2	2.52	0.42
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.19	0.42
3:J:331:ILE:O	3:J:337:ARG:HA	2.19	0.42
3:J:522:GLY:O	3:J:525:MET:HG2	2.19	0.42
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.84	0.42
5:L:166:VAL:HG23	5:L:258:GLN:O	2.19	0.42
5:L:544:THR:O	5:L:547:VAL:HG12	2.19	0.42
1:A:90:VAL:HG22	1:A:91:ARG:H	1.84	0.42
1:B:48:LEU:HD11	3:D:538:ARG:HB2	1.99	0.42
1:B:64:VAL:HG11	1:B:69:SER:HB2	2.00	0.42
1:B:175:ALA:HB1	1:B:177:TYR:CZ	2.53	0.42
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.19	0.42
2:C:292:ILE:HG23	2:C:295:LYS:HB2	2.00	0.42
2:C:619:ALA:HB1	2:C:657:THR:HA	2.00	0.42
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.54	0.42
3:D:746:LEU:CD2	3:D:758:PRO:HG3	2.49	0.42
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	2.01	0.42
3:D:1298:VAL:CB	3:D:1299:GLY:HA3	2.49	0.42
5:F:320:ILE:HG12	5:F:330:LEU:HB2	2.02	0.42
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.00	0.42
5:F:547:VAL:CG2	5:F:598:LEU:HD22	2.50	0.42
1:G:22:THR:O	1:G:207:THR:HB	2.19	0.42
2:I:362:ALA:O	2:I:366:ILE:HG13	2.19	0.42
2:I:397:LEU:HB3	2:I:401:GLY:HA3	2.00	0.42
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.52	0.42
3:J:51:PRO:HB2	3:J:57:PHE:O	2.19	0.42
3:J:54:ASP:OD1	3:J:54:ASP:N	2.51	0.42
3:J:483:LEU:HD22	4:K:17:PHE:HE1	1.85	0.42
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.85	0.42
4:K:60:ASN:OD1	4:K:62:GLN:HB3	2.18	0.42
1:A:166:ARG:N	1:A:167:PRO:HD2	2.34	0.42
2:C:705:GLU:CD	2:C:705:GLU:H	2.27	0.42
2:C:800:MET:HE1	2:C:822:VAL:HG13	2.00	0.42
3:D:268:LEU:HG	3:D:324:LEU:HD22	2.01	0.42
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.19	0.42
4:E:51:LEU:HD23	4:E:51:LEU:HA	1.88	0.42
5:F:306:PHE:O	5:F:307:THR:C	2.60	0.42
2:I:14:ASP:OD2	2:I:1156:ARG:NE	2.50	0.42
2:I:279:LYS:HB3	2:I:279:LYS:HE3	1.74	0.42
2:I:702:THR:HA	2:I:1184:THR:O	2.20	0.42
2:I:1158:LYS:HG3	2:I:1159:VAL:N	2.34	0.42
3:J:18:ASP:HB2	3:J:1373:ARG:HH21	1.84	0.42
3:J:161:THR:HG22	3:J:164:GLN:CD	2.44	0.42
3:J:518:VAL:HA	3:J:547:ARG:CZ	2.49	0.42
3:J:682:VAL:HA	3:J:685:ILE:HD13	2.01	0.42
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.79	0.42
2:C:553:THR:O	2:C:557:ARG:HD2	2.19	0.42
2:C:887:VAL:HB	2:C:913:VAL:HG22	2.01	0.42
3:D:252:LEU:HD23	3:D:262:THR:HB	2.01	0.42
3:D:516:ASP:OD1	3:D:516:ASP:N	2.50	0.42
3:D:797:THR:O	3:D:801:VAL:HG12	2.18	0.42
5:F:556:ALA:O	5:F:560:ARG:HG3	2.20	0.42
1:G:11:PRO:HD3	1:H:227:GLN:CD	2.45	0.42
1:G:41:ASN:CG	2:I:1218:GLY:HA3	2.45	0.42
1:H:136:GLU:CG	1:H:137:ASN:H	2.31	0.42
2:I:316:GLU:H	2:I:316:GLU:CD	2.27	0.42
2:I:538:LEU:H	2:I:538:LEU:HG	1.44	0.42
2:I:757:THR:C	2:I:833:ILE:HD12	2.44	0.42
2:I:795:ALA:HB1	2:I:1231:TYR:OH	2.19	0.42
3:J:480:ALA:O	3:J:485:MET:N	2.52	0.42
1:B:64:VAL:HG11	1:B:69:SER:HB3	2.02	0.42
1:B:96:ASP:O	1:B:97:GLU:HG2	2.20	0.42
2:C:48:GLY:N	2:C:461:GLU:OE1	2.53	0.42
2:C:136:PHE:O	2:C:142:GLU:HA	2.19	0.42
2:C:494:ASN:HD22	2:C:497:PRO:HD3	1.84	0.42
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.85	0.42
2:C:1232:MET:HE2	2:C:1232:MET:HB3	1.87	0.42
3:D:546:ALA:O	3:D:573:THR:HA	2.19	0.42
3:D:749:LYS:HB2	3:D:750:PRO:HD2	2.01	0.42
1:G:11:PRO:HA	1:G:30:PRO:HB2	2.02	0.42
1:G:23:HIS:CB	1:G:206:GLU:HA	2.49	0.42
1:H:59:VAL:HG12	1:H:61:ILE:HD13	2.01	0.42
2:I:139:ASN:O	2:I:141:THR:HG23	2.20	0.42
2:I:301:TYR:HB2	2:I:311:CYS:SG	2.60	0.42
2:I:387:ASN:HA	2:I:391:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:890:LYS:HE2	2:I:891:GLY:N	2.34	0.42
2:I:1065:LYS:CD	2:I:1235:LEU:HD12	2.50	0.42
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.54	0.42
3:J:930:LEU:HD11	3:J:1241:TYR:CZ	2.55	0.42
1:B:177:TYR:O	1:B:178:SER:C	2.62	0.42
1:B:201:LEU:HG	1:B:203:ILE:HD13	2.01	0.42
2:C:7:GLU:HG2	2:C:706:ARG:NH1	2.35	0.42
2:C:367:TYR:CD1	2:C:384:LEU:HD22	2.55	0.42
2:C:1332:SER:HA	3:D:102:MET:HE1	2.00	0.42
3:D:70:CYS:SG	3:D:85:CYS:HB2	2.60	0.42
3:D:839:VAL:HG13	3:D:882:VAL:HG21	2.02	0.42
3:D:850:LYS:HB3	3:D:851:PRO:HD2	2.01	0.42
3:D:1158:GLU:HG3	3:D:1186:TYR:OH	2.19	0.42
3:D:1372:ARG:HG3	3:J:854:ALA:HB2	2.02	0.42
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.86	0.42
2:I:52:ALA:HB2	2:I:461:GLU:HG3	2.01	0.42
2:I:367:TYR:HD1	2:I:384:LEU:HD22	1.83	0.42
2:I:673:HIS:O	2:I:1109:ILE:HG22	2.19	0.42
2:I:1064:ASP:O	2:I:1076:ILE:HG22	2.19	0.42
3:J:102:MET:HE2	3:J:102:MET:HB3	1.95	0.42
3:J:232:ASN:HA	3:J:236:TRP:CZ3	2.54	0.42
5:L:161:LEU:HD12	5:L:161:LEU:HA	1.69	0.42
2:C:92:TYR:O	2:C:128:PRO:HA	2.20	0.42
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.86	0.42
2:C:716:ALA:O	2:C:783:LEU:HB2	2.20	0.42
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.84	0.42
2:C:840:SER:O	2:C:1047:LEU:N	2.43	0.42
3:D:220:ARG:NH1	3:D:224:LEU:HD11	2.35	0.42
3:D:343:LEU:HD22	3:D:343:LEU:HA	1.35	0.42
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.81	0.42
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.82	0.42
4:E:15:ASN:O	4:E:16:ARG:HB3	2.19	0.42
5:F:390:ILE:O	5:F:393:LYS:HB2	2.19	0.42
5:F:488:LEU:H	5:F:488:LEU:HG	1.47	0.42
1:G:102:LEU:HB3	1:G:142:MET:HG2	2.01	0.42
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.55	0.42
2:I:204:LEU:HD23	2:I:204:LEU:HA	1.84	0.42
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.45	0.42
3:J:425:ARG:HD2	3:J:459:ALA:HA	2.02	0.42
1:A:67:GLU:HB3	1:A:82:LEU:HD11	2.01	0.42
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:LEU:HD21	2:C:524:ILE:HD12	2.02	0.42
2:C:468:LEU:O	2:C:471:VAL:HG12	2.20	0.42
2:C:849:GLU:HB2	2:C:887:VAL:HG23	2.01	0.42
2:C:1192:GLU:O	2:C:1196:LYS:N	2.31	0.42
3:D:291:ILE:HD13	5:F:409:ASN:HB3	2.02	0.42
3:D:560:ASN:O	3:D:560:ASN:ND2	2.53	0.42
3:D:683:ILE:HD11	3:D:754:ILE:CG2	2.50	0.42
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	2.02	0.42
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.79	0.42
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.34	0.42
1:H:71:LYS:HD2	1:H:71:LYS:HA	1.85	0.42
1:H:89:ALA:HB3	1:H:124:VAL:HG12	2.02	0.42
2:I:81:ASP:HA	2:I:92:TYR:HE1	1.85	0.42
2:I:403:MET:HE3	2:I:403:MET:HB3	1.95	0.42
2:I:528:ARG:NH1	2:I:576:SER:O	2.52	0.42
2:I:734:ILE:HD11	2:I:783:LEU:HD11	2.01	0.42
3:J:325:LYS:HE2	3:J:330:MET:HA	2.02	0.42
3:J:1158:GLU:O	3:J:1206:ARG:NH1	2.52	0.42
1:A:40:GLY:HA3	1:A:185:TYR:CD2	2.55	0.42
1:A:236:ASP:HA	1:B:14:VAL:HG13	2.02	0.42
2:C:117:ILE:HD12	2:C:488:MET:HG2	2.01	0.42
2:C:1283:ALA:HA	3:D:479:GLU:CD	2.45	0.42
3:D:420:PRO:O	3:D:471:PRO:HD2	2.20	0.42
3:D:833:GLU:HA	3:D:834:PRO:HD3	1.85	0.42
3:D:1243:LEU:HD12	3:D:1243:LEU:HA	1.81	0.42
3:D:1375:ALA:CB	3:J:853:THR:HG21	2.50	0.42
2:I:237:LEU:HD13	2:I:237:LEU:HA	1.64	0.42
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.02	0.42
2:I:1158:LYS:C	2:I:1159:VAL:HG22	2.45	0.42
2:I:1170:MET:HE3	2:I:1170:MET:HB3	1.78	0.42
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.84	0.42
2:I:1336:ASN:ND2	3:J:29:MET:HE3	2.34	0.42
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.50	0.42
3:J:1231:ARG:HG3	3:J:1235:ASN:OD1	2.20	0.42
4:K:66:VAL:HG22	4:K:69:ARG:NH2	2.29	0.42
5:L:110:LEU:HD23	5:L:110:LEU:HA	1.83	0.42
5:L:288:MET:SD	5:L:299:LYS:HE2	2.60	0.42
5:L:489:MET:HE2	5:L:493:LYS:HB2	2.01	0.42
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.85	0.41
1:A:236:ASP:HA	1:B:14:VAL:O	2.20	0.41
1:B:7:GLU:O	1:B:8:PHE:CD2	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	2.02	0.41
5:F:383:ASN:HB2	5:F:412:LEU:HD21	2.03	0.41
2:I:1106:ARG:NE	3:J:731:ARG:HH21	2.17	0.41
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.20	0.41
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.52	0.41
3:J:165:TYR:O	3:J:169:LEU:HB2	2.20	0.41
3:J:506:VAL:H	3:J:506:VAL:HG12	1.59	0.41
3:J:510:LEU:HG	3:J:513:MET:HE2	2.01	0.41
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	2.02	0.41
5:L:374:ARG:HH11	5:L:374:ARG:HD2	1.69	0.41
1:A:93:GLN:H	1:A:120:ASP:HB3	1.84	0.41
2:C:147:SER:OG	2:C:455:SER:HB3	2.20	0.41
2:C:316:GLU:H	2:C:316:GLU:CD	2.28	0.41
2:C:325:LEU:O	2:C:330:HIS:HB2	2.20	0.41
2:C:810:TYR:CD1	2:C:1078:LYS:HD2	2.52	0.41
2:C:1253:LEU:CD1	3:D:253:VAL:HG11	2.50	0.41
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	2.01	0.41
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.56	0.41
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.50	0.41
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.35	0.41
4:E:86:ILE:O	4:E:88:GLU:N	2.53	0.41
5:F:348:GLU:HG2	5:F:354:THR:HA	2.01	0.41
5:F:580:PHE:HD1	5:F:580:PHE:HA	1.51	0.41
1:G:115:ILE:HG22	1:G:116:THR:H	1.85	0.41
1:H:175:ALA:HB1	1:H:177:TYR:CZ	2.55	0.41
2:I:606:LEU:HD21	2:I:614:TYR:HD1	1.85	0.41
2:I:796:LEU:O	2:I:1233:LEU:HD12	2.19	0.41
2:I:1060:ILE:HD11	2:I:1066:MET:SD	2.60	0.41
2:I:1276:TRP:CZ2	3:J:801:VAL:HG11	2.55	0.41
3:J:172:PHE:HB3	3:J:175:GLU:OE2	2.20	0.41
3:J:355:ILE:HG21	3:J:466:MET:HG3	2.01	0.41
3:J:1261:LEU:HA	3:J:1305:ASP:O	2.20	0.41
5:L:315:TRP:CZ2	5:L:341:LEU:HD11	2.55	0.41
5:L:483:LEU:H	5:L:483:LEU:CD1	2.28	0.41
1:B:100:LEU:O	1:B:144:ILE:HG22	2.19	0.41
2:C:786:GLY:N	2:C:789:THR:OG1	2.51	0.41
3:D:647:PRO:HG3	3:D:697:MET:CB	2.43	0.41
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.51	0.41
4:E:77:ALA:O	4:E:80:LEU:HB2	2.19	0.41
5:F:396:ASN:C	5:F:398:GLY:N	2.78	0.41
1:G:67:GLU:H	1:G:67:GLU:HG2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:158:ASP:CG	2:I:159:SER:H	2.28	0.41
2:I:409:LEU:HD13	2:I:427:ASP:HB3	2.01	0.41
3:J:79:LYS:O	3:J:81:ARG:HG2	2.20	0.41
3:J:201:LEU:HD22	3:J:217:LEU:HD11	2.02	0.41
3:J:218:THR:HG21	3:J:1275:LEU:HD11	2.02	0.41
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.20	0.41
3:J:797:THR:HG22	3:J:924:GLY:CA	2.46	0.41
1:A:50:SER:CB	1:B:8:PHE:CZ	3.03	0.41
1:B:14:VAL:HG23	1:B:27:THR:O	2.19	0.41
2:C:139:ASN:O	2:C:141:THR:HG23	2.20	0.41
2:C:799:ASN:HA	2:C:1231:TYR:HA	2.02	0.41
2:C:1246:ARG:HG2	2:C:1247:SER:N	2.35	0.41
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.45	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.86	0.41
3:D:490:ILE:H	3:D:490:ILE:HD13	1.86	0.41
1:H:60:GLU:HG3	1:H:143:ARG:O	2.20	0.41
2:I:803:ALA:CB	2:I:1094:VAL:HG21	2.50	0.41
2:I:1313:HIS:HB2	3:J:474:LEU:HD13	2.02	0.41
3:J:34:SER:HB2	3:J:104:HIS:HB3	2.01	0.41
3:J:186:GLN:HB2	3:J:238:ILE:HG21	2.01	0.41
1:B:155:ALA:N	1:B:174:ASP:OD1	2.45	0.41
1:B:173:VAL:HG12	1:B:174:ASP:N	2.35	0.41
1:B:190:ALA:O	1:B:198:LEU:HB2	2.19	0.41
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.20	0.41
2:C:1107:MET:HG2	3:D:740:LEU:HD11	2.02	0.41
3:D:322:ARG:HB2	3:D:322:ARG:CZ	2.50	0.41
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.02	0.41
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.35	0.41
5:F:105:MET:HE2	5:F:105:MET:HB2	1.90	0.41
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.84	0.41
1:G:89:ALA:HB1	1:G:210:THR:CG2	2.51	0.41
3:J:481:ARG:O	3:J:485:MET:HB2	2.20	0.41
3:J:1262:ARG:HD2	3:J:1279:GLN:HE22	1.86	0.41
1:A:224:LEU:HA	1:A:224:LEU:HD12	1.54	0.41
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.85	0.41
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.53	0.41
2:C:230:PHE:CE1	2:C:239:MET:HB2	2.55	0.41
2:C:342:ASP:O	2:C:437:ASN:CG	2.63	0.41
2:C:478:ARG:CG	2:C:492:MET:HG2	2.40	0.41
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	2.02	0.41
2:C:1241:ASP:O	2:C:1244:HIS:CE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:281:ARG:HH11	3:D:281:ARG:HD3	1.68	0.41
3:D:1332:LEU:HD13	3:D:1332:LEU:HA	1.85	0.41
2:I:213:LEU:HB3	2:I:422:LYS:HD2	2.02	0.41
2:I:1070:HIS:CD2	2:I:1111:GLN:HA	2.55	0.41
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.86	0.41
3:J:746:LEU:HG	3:J:758:PRO:HB3	2.02	0.41
3:J:1165:PHE:HD2	3:J:1173:ARG:NE	2.18	0.41
1:A:8:PHE:O	1:A:9:LEU:HD23	2.19	0.41
1:A:187:VAL:HG23	1:A:187:VAL:O	2.20	0.41
1:A:207:THR:HG22	1:A:208:ASN:N	2.34	0.41
1:B:142:MET:HB3	1:B:142:MET:HE2	1.73	0.41
1:B:211:ILE:HA	1:B:211:ILE:HD12	1.67	0.41
2:C:75:LEU:HA	2:C:75:LEU:HD13	1.79	0.41
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.66	0.41
2:C:1152:GLY:O	2:C:1153:ALA:CB	2.68	0.41
3:D:903:LEU:HD12	3:D:903:LEU:HA	1.86	0.41
5:F:373:ARG:HH12	5:F:377:LYS:HZ1	1.68	0.41
5:F:467:SER:O	5:F:471:LEU:HB2	2.20	0.41
1:G:76:GLU:OE2	1:G:76:GLU:N	2.54	0.41
1:G:179:PRO:HA	1:G:208:ASN:ND2	2.36	0.41
2:I:696:ASP:HB2	2:I:798:GLN:CG	2.40	0.41
2:I:696:ASP:HB3	2:I:697:LYS:H	1.62	0.41
2:I:701:GLY:O	2:I:1184:THR:N	2.37	0.41
3:J:416:ILE:HG12	3:J:441:LEU:CD2	2.49	0.41
3:J:804:ALA:O	3:J:805:GLN:C	2.62	0.41
5:L:476:ARG:HG3	5:L:477:GLU:HG2	2.01	0.41
1:B:178:SER:HB2	1:B:180:VAL:HG22	2.01	0.41
1:B:211:ILE:HD11	1:B:215:GLU:CG	2.51	0.41
2:C:13:LYS:O	2:C:1183:ALA:N	2.43	0.41
2:C:62:TYR:O	2:C:64:GLY:N	2.53	0.41
2:C:146:VAL:HG13	2:C:529:ARG:HB3	2.02	0.41
2:C:516:VAL:H	2:C:526:HIS:HD2	1.69	0.41
2:C:618:GLN:CG	3:D:770:LEU:HD21	2.50	0.41
2:C:1066:MET:HG2	2:C:1234:LYS:HA	2.03	0.41
2:C:1283:ALA:HB1	2:C:1286:THR:HB	2.02	0.41
2:C:1301:ARG:HG3	2:C:1302:THR:H	1.85	0.41
3:D:85:CYS:HB3	3:D:88:CYS:O	2.20	0.41
3:D:169:LEU:HD23	3:D:173:GLY:HA2	2.01	0.41
3:D:683:ILE:HG21	3:D:683:ILE:HD13	1.84	0.41
3:D:1347:LEU:HG	3:D:1357:ILE:HG23	2.02	0.41
5:F:402:LEU:HA	5:F:405:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:VAL:HG12	1:H:91:ARG:H	1.86	0.41
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.62	0.41
2:I:231:GLU:HG2	2:I:332:ARG:NH2	2.36	0.41
2:I:799:ASN:HA	2:I:1231:TYR:HA	2.03	0.41
2:I:1109:ILE:HD12	2:I:1109:ILE:HA	1.89	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.03	0.41
3:J:93:THR:HG22	3:J:94:GLN:H	1.86	0.41
3:J:580:TRP:HH2	3:J:587:LEU:O	2.03	0.41
3:J:591:ILE:HG23	3:J:592:VAL:HG13	2.02	0.41
3:J:814:CYS:SG	3:J:816:THR:HG22	2.61	0.41
1:A:187:VAL:CG1	1:A:201:LEU:HD13	2.51	0.41
1:A:189:ALA:HB1	1:A:191:ARG:HH12	1.84	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.21	0.41
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.88	0.41
1:B:140:ILE:HD11	1:B:142:MET:CE	2.51	0.41
2:C:136:PHE:O	2:C:143:ARG:N	2.43	0.41
2:C:379:GLU:CD	2:C:379:GLU:H	2.28	0.41
2:C:674:ASP:O	3:D:772:TYR:OH	2.28	0.41
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.50	0.41
2:C:972:PHE:HB2	2:C:994:ARG:HH21	1.86	0.41
2:C:1170:MET:HE3	2:C:1170:MET:HB3	1.87	0.41
3:D:121:PRO:O	3:D:122:SER:C	2.63	0.41
3:D:429:LEU:HD13	3:D:429:LEU:HA	1.85	0.41
3:D:705:THR:OG1	3:D:718:SER:HA	2.21	0.41
3:D:860:ARG:HB3	3:D:861:ASN:H	1.67	0.41
3:D:1154:ALA:N	3:D:1214:PRO:O	2.46	0.41
5:F:281:ARG:HA	5:F:284:GLU:OE1	2.21	0.41
5:F:391:ALA:HB3	5:F:405:ILE:HG22	2.03	0.41
5:F:575:GLU:O	5:F:579:GLN:HG2	2.21	0.41
1:G:13:LEU:HD23	1:G:13:LEU:H	1.85	0.41
1:H:67:GLU:HA	1:H:78:ILE:HG21	2.03	0.41
1:H:116:THR:O	1:H:116:THR:HG23	2.21	0.41
2:I:62:TYR:C	2:I:64:GLY:N	2.79	0.41
2:I:149:LEU:HD11	2:I:451:ARG:HB3	2.03	0.41
2:I:211:ARG:HD3	2:I:357:ASN:O	2.20	0.41
2:I:409:LEU:HD11	2:I:428:VAL:HG23	2.03	0.41
2:I:540:ARG:H	2:I:540:ARG:HG3	1.64	0.41
2:I:620:ASN:OD1	3:J:769:VAL:HG23	2.21	0.41
2:I:726:TYR:CE2	2:I:728:ASP:HB2	2.56	0.41
2:I:924:VAL:HG12	2:I:1058:ARG:NH2	2.35	0.41
2:I:1046:VAL:HG21	2:I:1049:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1149:TYR:N	2:I:1149:TYR:HD2	2.19	0.41
2:I:1157:GLN:HG3	2:I:1158:LYS:O	2.20	0.41
2:I:1270:PHE:CE1	2:I:1290:MET:HG2	2.56	0.41
3:J:215:LYS:O	3:J:218:THR:HG22	2.21	0.41
3:J:291:ILE:HD13	5:L:409:ASN:HB3	2.03	0.41
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.86	0.41
3:J:521:LYS:HD2	3:J:541:LEU:O	2.21	0.41
3:J:549:LYS:HA	3:J:570:LYS:O	2.21	0.41
3:J:620:PHE:CE1	3:J:624:ILE:HD11	2.55	0.41
3:J:1192:LYS:HE3	3:J:1192:LYS:HB2	1.99	0.41
5:L:324:LYS:HB3	5:L:325:PRO:HD2	2.03	0.41
1:A:118:ASP:HB3	1:A:121:VAL:CG2	2.50	0.41
1:A:228:LEU:HA	1:A:228:LEU:HD23	1.95	0.41
1:B:6:THR:OG1	1:B:7:GLU:N	2.48	0.41
1:B:113:ALA:HB2	1:B:126:PRO:HB3	2.02	0.41
2:C:91:THR:HA	2:C:138:ILE:O	2.21	0.41
2:C:279:LYS:HB3	2:C:279:LYS:HE3	1.88	0.41
3:D:805:GLN:OE1	3:D:1348:LYS:HD3	2.21	0.41
5:F:584:ARG:HA	5:F:584:ARG:NH1	2.36	0.41
1:G:11:PRO:HD2	1:H:227:GLN:HA	2.03	0.41
1:G:195:ARG:HG2	1:G:198:LEU:HG	2.02	0.41
1:H:39:LEU:HD23	1:H:39:LEU:HA	1.95	0.41
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	2.04	0.41
2:I:1151:LEU:HD22	2:I:1197:GLU:OE2	2.20	0.41
2:I:1281:TYR:OH	3:J:431:ARG:O	2.36	0.41
3:J:484:MET:HE2	3:J:484:MET:HB3	1.85	0.41
3:J:620:PHE:O	3:J:624:ILE:HG13	2.21	0.41
3:J:833:GLU:OE1	3:J:1242:ARG:HD3	2.20	0.41
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.36	0.41
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.90	0.41
1:A:60:GLU:HB2	1:A:170:ARG:HD3	2.03	0.40
1:A:166:ARG:NH1	1:A:168:ILE:HG12	2.36	0.40
1:B:82:LEU:HD22	1:B:173:VAL:HG22	2.03	0.40
2:C:578:TYR:HB3	2:C:590:PRO:HG2	2.02	0.40
2:C:719:LYS:O	2:C:779:ARG:HG3	2.21	0.40
2:C:898:GLU:OE1	2:C:898:GLU:N	2.50	0.40
3:D:46:TYR:CD1	5:F:452:ILE:HG22	2.56	0.40
3:D:594:GLN:HG3	3:D:596:LEU:HD22	2.04	0.40
4:E:50:ALA:O	4:E:54:ILE:HG12	2.21	0.40
5:F:601:PRO:CA	5:F:604:SER:HB3	2.49	0.40
1:H:205:MET:HG2	1:H:206:GLU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:18:ARG:HH12	2:I:622:ASN:HA	1.85	0.40
2:I:230:PHE:CE1	2:I:239:MET:HB2	2.56	0.40
3:J:473:THR:HG23	3:J:476:ALA:N	2.33	0.40
3:J:1144:LEU:HD23	3:J:1144:LEU:HA	1.89	0.40
4:K:7:GLN:NE2	4:K:7:GLN:O	2.54	0.40
5:L:111:LEU:HD23	5:L:111:LEU:HA	1.77	0.40
2:C:720:ARG:NH2	2:C:736:VAL:HG21	2.36	0.40
2:C:1341:ASP:HB3	3:D:18:ASP:OD2	2.21	0.40
3:D:372:MET:HE2	3:D:372:MET:HB3	1.73	0.40
5:F:357:GLN:H	5:F:357:GLN:HG3	1.71	0.40
2:I:10:ARG:HA	2:I:1172:LEU:CD2	2.37	0.40
2:I:953:LEU:HD12	2:I:953:LEU:HA	1.94	0.40
2:I:1225:VAL:HA	3:J:638:SER:CB	2.51	0.40
5:L:161:LEU:O	5:L:262:VAL:HG23	2.21	0.40
1:A:54:CYS:HB3	1:A:148:ARG:HG3	2.04	0.40
1:A:83:LEU:CD2	2:C:694:ARG:HE	2.23	0.40
2:C:213:LEU:HD23	2:C:385:PHE:HE2	1.87	0.40
2:C:401:GLY:O	2:C:405:PHE:HB2	2.21	0.40
2:C:516:VAL:HG23	2:C:526:HIS:CD2	2.56	0.40
2:C:754:THR:O	2:C:755:LYS:HD2	2.21	0.40
2:C:897:PRO:HB3	5:F:564:GLY:C	2.47	0.40
2:C:1104:PRO:HG2	3:D:725:MET:SD	2.62	0.40
3:D:521:LYS:HB3	3:D:541:LEU:O	2.20	0.40
5:F:111:LEU:HD23	5:F:111:LEU:HA	1.83	0.40
5:F:276:MET:HE2	5:F:276:MET:HB2	1.79	0.40
3:J:338:PHE:O	3:J:340:GLN:N	2.54	0.40
3:J:481:ARG:NH1	4:K:3:ARG:O	2.54	0.40
3:J:650:LYS:NZ	3:J:762:ASN:HD22	2.19	0.40
3:J:1168:GLU:O	3:J:1169:THR:C	2.64	0.40
3:J:1357:ILE:C	3:J:1359:ALA:H	2.29	0.40
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.89	0.40
2:C:1013:GLN:NE2	2:C:1016:GLU:OE2	2.55	0.40
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.21	0.40
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.53	0.40
3:D:461:PHE:HD2	3:D:461:PHE:HA	1.70	0.40
3:D:591:ILE:HG23	3:D:592:VAL:HG13	2.03	0.40
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.54	0.40
1:G:207:THR:HG22	1:G:208:ASN:N	2.36	0.40
2:I:23:ASP:OD1	2:I:23:ASP:N	2.51	0.40
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	2.04	0.40
3:J:557:LYS:HB2	3:J:557:LYS:HE3	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1173:ARG:N	3:J:1190:ILE:O	2.51	0.40
4:K:26:ARG:O	4:K:29:GLN:HB2	2.22	0.40
5:L:481:GLU:OE1	5:L:495:ARG:NH2	2.53	0.40
1:A:45:ARG:HH21	2:C:1216:ARG:HA	1.83	0.40
1:A:57:THR:O	1:A:173:VAL:HG22	2.21	0.40
1:A:181:GLU:HB3	1:A:206:GLU:HG3	2.03	0.40
1:A:234:LEU:H	1:B:218:ARG:NH1	2.19	0.40
2:C:61:SER:HB3	2:C:479:LEU:HB3	2.04	0.40
2:C:164:THR:C	2:C:166:SER:H	2.30	0.40
2:C:388:LEU:HA	2:C:388:LEU:HD23	1.84	0.40
2:C:631:GLU:OE1	2:C:631:GLU:N	2.53	0.40
2:C:674:ASP:OD1	2:C:1110:GLY:N	2.45	0.40
2:C:1276:TRP:CH2	3:D:801:VAL:HG11	2.56	0.40
3:D:480:ALA:O	3:D:485:MET:N	2.55	0.40
3:D:697:MET:HG3	3:D:698:MET:N	2.36	0.40
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	2.02	0.40
4:E:78:ALA:C	4:E:80:LEU:H	2.29	0.40
5:F:465:ARG:HG2	5:F:465:ARG:H	1.42	0.40
1:H:8:PHE:HB2	1:H:10:LYS:HZ2	1.85	0.40
2:I:227:LYS:HZ3	2:I:298:ALA:HB1	1.84	0.40
2:I:757:THR:O	2:I:833:ILE:HD12	2.21	0.40
2:I:835:GLU:OE2	2:I:1051:LYS:HD3	2.21	0.40
2:I:1301:ARG:HG3	2:I:1302:THR:H	1.86	0.40
3:J:581:MET:HE2	3:J:581:MET:HB3	1.83	0.40
3:J:647:PRO:HG3	3:J:697:MET:HB3	2.04	0.40
3:J:652:GLU:O	3:J:656:GLU:HG3	2.21	0.40
5:L:380:VAL:HG22	5:L:416:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/320 (72%)	201 (87%)	25 (11%)	5 (2%)	5	24
1	B	213/320 (67%)	186 (87%)	24 (11%)	3 (1%)	9	31
1	G	225/320 (70%)	193 (86%)	26 (12%)	6 (3%)	4	20
1	H	212/320 (66%)	189 (89%)	19 (9%)	4 (2%)	6	26
2	C	1338/1342 (100%)	1229 (92%)	99 (7%)	10 (1%)	18	47
2	I	1338/1342 (100%)	1227 (92%)	100 (8%)	11 (1%)	16	44
3	D	1163/1407 (83%)	1067 (92%)	86 (7%)	10 (1%)	14	42
3	J	1151/1407 (82%)	1054 (92%)	81 (7%)	16 (1%)	9	31
4	E	87/90 (97%)	82 (94%)	5 (6%)	0	100	100
4	K	77/90 (86%)	72 (94%)	3 (4%)	2 (3%)	4	21
5	F	462/613 (75%)	421 (91%)	36 (8%)	5 (1%)	11	38
5	L	463/613 (76%)	422 (91%)	39 (8%)	2 (0%)	30	59
All	All	6960/8184 (85%)	6343 (91%)	543 (8%)	74 (1%)	11	38

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	GLU
1	A	232	VAL
2	C	170	VAL
2	C	484	LEU
2	C	1137	GLU
2	C	1153	ALA
2	C	1159	VAL
3	D	10	ALA
3	D	1274	PHE
3	D	1294	ALA
5	F	512	GLY
5	F	569	THR
1	G	162	GLU
1	G	167	PRO
1	G	229	GLU
1	G	231	PHE
2	I	170	VAL
2	I	484	LEU
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP

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Mol	Chain	Res	Type
3	J	332	LYS
3	J	1169	THR
4	K	15	ASN
5	L	512	GLY
1	A	167	PRO
2	C	697	LYS
2	C	1158	LYS
3	D	19	ALA
3	D	332	LYS
3	D	712	GLN
3	D	1169	THR
1	H	178	SER
2	I	697	LYS
2	I	1154	ASP
3	J	19	ALA
3	J	334	LYS
3	J	339	ARG
3	J	341	ASN
3	J	712	GLN
5	F	515	GLU
1	G	9	LEU
1	H	193	GLU
2	I	1158	LYS
3	J	333	GLY
3	J	1167	LYS
1	A	14	VAL
1	A	162	GLU
1	B	13	LEU
1	B	138	ALA
1	H	177	TYR
3	J	338	PHE
2	C	63	SER
2	C	573	ASN
3	D	806	ASP
1	G	196	THR
2	I	63	SER
3	J	710	ASP
5	L	166	VAL
5	F	516	ASP
1	H	138	ALA
3	J	806	ASP
3	J	344	GLY

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Mol	Chain	Res	Type
3	J	826	ILE
3	J	831	VAL
4	K	14	GLY
3	D	826	ILE
3	D	831	VAL
1	B	178	SER
3	J	336	GLY
2	C	1186	VAL
5	F	166	VAL
2	I	1186	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/279 (72%)	190 (94%)	11 (6%)	19	46
1	B	186/279 (67%)	172 (92%)	14 (8%)	12	38
1	G	193/279 (69%)	177 (92%)	16 (8%)	10	35
1	H	183/279 (66%)	174 (95%)	9 (5%)	22	49
2	C	1155/1157 (100%)	1057 (92%)	98 (8%)	10	33
2	I	1154/1157 (100%)	1052 (91%)	102 (9%)	9	31
3	D	962/1168 (82%)	876 (91%)	86 (9%)	9	31
3	J	960/1168 (82%)	871 (91%)	89 (9%)	8	29
4	E	72/74 (97%)	64 (89%)	8 (11%)	6	21
4	K	67/74 (90%)	62 (92%)	5 (8%)	12	38
5	F	417/540 (77%)	378 (91%)	39 (9%)	8	29
5	L	418/540 (77%)	383 (92%)	35 (8%)	10	34
All	All	5968/6994 (85%)	5456 (91%)	512 (9%)	10	33

All (512) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	19	VAL
1	A	26	VAL
1	A	50	SER
1	A	61	ILE
1	A	74	VAL
1	A	115	ILE
1	A	129	VAL
1	A	133	LEU
1	A	227	GLN
1	A	231	PHE
1	B	7	GLU
1	B	8	PHE
1	B	9	LEU
1	B	50	SER
1	B	61	ILE
1	B	64	VAL
1	B	68	TYR
1	B	103	ASN
1	B	115	ILE
1	B	123	ILE
1	B	133	LEU
1	B	176	CYS
1	B	198	LEU
1	B	211	ILE
2	C	11	ILE
2	C	39	ILE
2	C	60	GLN
2	C	82	VAL
2	C	90	VAL
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	132	ASP
2	C	170	VAL
2	C	237	LEU
2	C	285	ILE
2	C	292	ILE
2	C	299	LYS
2	C	302	ILE

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Mol	Chain	Res	Type
2	C	320	ASP
2	C	321	LEU
2	C	353	VAL
2	C	377	THR
2	C	379	GLU
2	C	394	ARG
2	C	400	VAL
2	C	419	ILE
2	C	423	ASP
2	C	445	ILE
2	C	453	ILE
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	518	ASN
2	C	550	VAL
2	C	558	VAL
2	C	565	GLU
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	791	LEU
2	C	800	MET
2	C	817	LEU
2	C	826	ASP
2	C	828	PHE

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Mol	Chain	Res	Type
2	C	840	SER
2	C	878	THR
2	C	890	LYS
2	C	951	MET
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	1002	LEU
2	C	1046	VAL
2	C	1073	LYS
2	C	1076	ILE
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	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1160	ASP
2	C	1174	GLU
2	C	1180	MET
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1238	LEU
2	C	1253	LEU
2	C	1254	VAL
2	C	1264	GLN
2	C	1293	VAL
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1340	GLU
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	12	THR
3	D	13	LYS

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Mol	Chain	Res	Type
3	D	18	ASP
3	D	20	ILE
3	D	26	SER
3	D	46	TYR
3	D	79	LYS
3	D	83	VAL
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	97	VAL
3	D	169	LEU
3	D	175	GLU
3	D	244	VAL
3	D	252	LEU
3	D	255	LEU
3	D	306	LEU
3	D	312	ARG
3	D	324	LEU
3	D	343	LEU
3	D	374	LEU
3	D	394	ILE
3	D	401	VAL
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	454	CYS
3	D	490	ILE
3	D	501	VAL
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	568	SER
3	D	573	THR
3	D	594	GLN
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU

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Mol	Chain	Res	Type
3	D	678	ARG
3	D	680	ASN
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	746	LEU
3	D	754	ILE
3	D	769	VAL
3	D	770	LEU
3	D	807	LEU
3	D	810	THR
3	D	826	ILE
3	D	844	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	908	ILE
3	D	918	ILE
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1194	ARG
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL
3	D	1310	THR
3	D	1333	THR
3	D	1343	GLU
4	E	3	ARG
4	E	5	THR

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Mol	Chain	Res	Type
4	E	13	ILE
4	E	16	ARG
4	E	21	LEU
4	E	28	ARG
4	E	39	VAL
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	127	ILE
5	F	130	VAL
5	F	154	GLU
5	F	247	GLU
5	F	264	LYS
5	F	267	ASP
5	F	301	ASN
5	F	305	LEU
5	F	306	PHE
5	F	310	GLU
5	F	341	LEU
5	F	400	GLN
5	F	429	THR
5	F	437	GLN
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	476	ARG
5	F	479	THR
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	494	ILE
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	580	PHE
5	F	587	ILE
5	F	599	ARG

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Mol	Chain	Res	Type
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
1	G	9	LEU
1	G	18	GLN
1	G	19	VAL
1	G	26	VAL
1	G	50	SER
1	G	61	ILE
1	G	64	VAL
1	G	74	VAL
1	G	115	ILE
1	G	129	VAL
1	G	133	LEU
1	G	145	LYS
1	G	162	GLU
1	G	163	GLU
1	G	166	ARG
1	G	231	PHE
1	H	50	SER
1	H	61	ILE
1	H	64	VAL
1	H	103	ASN
1	H	115	ILE
1	H	130	ILE
1	H	133	LEU
1	H	176	CYS
1	H	198	LEU
2	I	11	ILE
2	I	39	ILE
2	I	60	GLN
2	I	82	VAL
2	I	90	VAL
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	132	ASP
2	I	170	VAL
2	I	237	LEU
2	I	285	ILE

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Mol	Chain	Res	Type
2	I	292	ILE
2	I	299	LYS
2	I	302	ILE
2	I	320	ASP
2	I	321	LEU
2	I	353	VAL
2	I	360	LEU
2	I	377	THR
2	I	379	GLU
2	I	394	ARG
2	I	400	VAL
2	I	419	ILE
2	I	445	ILE
2	I	453	ILE
2	I	484	LEU
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	503	LYS
2	I	510	GLN
2	I	518	ASN
2	I	538	LEU
2	I	542	ARG
2	I	550	VAL
2	I	558	VAL
2	I	565	GLU
2	I	589	THR
2	I	600	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE
2	I	615	VAL
2	I	623	LEU
2	I	633	LEU
2	I	639	LYS
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE

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Mol	Chain	Res	Type
2	I	765	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	800	MET
2	I	817	LEU
2	I	826	ASP
2	I	840	SER
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	951	MET
2	I	974	ARG
2	I	979	LEU
2	I	984	VAL
2	I	1002	LEU
2	I	1046	VAL
2	I	1073	LYS
2	I	1076	ILE
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	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1160	ASP
2	I	1174	GLU
2	I	1180	MET
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1238	LEU
2	I	1253	LEU
2	I	1254	VAL
2	I	1264	GLN
2	I	1293	VAL
2	I	1310	ASP
2	I	1327	LEU

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Mol	Chain	Res	Type
2	I	1331	ARG
2	I	1340	GLU
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	26	SER
3	J	46	TYR
3	J	79	LYS
3	J	83	VAL
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	97	VAL
3	J	169	LEU
3	J	175	GLU
3	J	233	LYS
3	J	244	VAL
3	J	252	LEU
3	J	255	LEU
3	J	306	LEU
3	J	312	ARG
3	J	324	LEU
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	401	VAL
3	J	416	ILE
3	J	425	ARG
3	J	429	LEU
3	J	454	CYS
3	J	501	VAL
3	J	506	VAL
3	J	507	VAL
3	J	513	MET
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	568	SER
3	J	573	THR

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Mol	Chain	Res	Type
3	J	594	GLN
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	678	ARG
3	J	680	ASN
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
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	769	VAL
3	J	770	LEU
3	J	807	LEU
3	J	810	THR
3	J	826	ILE
3	J	844	THR
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
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	1194	ARG
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL

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Mol	Chain	Res	Type
3	J	1273	ASP
3	J	1274	PHE
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1298	VAL
3	J	1310	THR
3	J	1333	THR
3	J	1343	GLU
4	K	3	ARG
4	K	13	ILE
4	K	21	LEU
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	127	ILE
5	L	130	VAL
5	L	247	GLU
5	L	264	LYS
5	L	267	ASP
5	L	301	ASN
5	L	305	LEU
5	L	306	PHE
5	L	310	GLU
5	L	341	LEU
5	L	395	THR
5	L	400	GLN
5	L	429	THR
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	479	THR
5	L	482	GLU
5	L	486	ARG
5	L	494	ILE
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET

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Mol	Chain	Res	Type
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	580	PHE
5	L	587	ILE
5	L	603	ARG
5	L	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	HIS
1	B	186	ASN
1	B	194	GLN
2	C	31	GLN
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	165	HIS
2	C	273	HIS
2	C	494	ASN
2	C	517	GLN
2	C	526	HIS
2	C	618	GLN
2	C	620	ASN
2	C	659	GLN
2	C	799	ASN
2	C	1013	GLN
2	C	1023	HIS
2	C	1116	HIS
2	C	1146	GLN
2	C	1220	GLN
2	C	1288	GLN
2	C	1299	ASN
2	C	1313	HIS
2	C	1314	GLN
2	C	1336	ASN
3	D	94	GLN
3	D	196	GLN
3	D	200	GLN
3	D	294	ASN
3	D	419	HIS

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Mol	Chain	Res	Type
3	D	450	HIS
3	D	594	GLN
3	D	702	GLN
3	D	777	HIS
3	D	792	ASN
3	D	867	GLN
3	D	910	ASN
3	D	1218	HIS
3	D	1326	GLN
4	E	7	GLN
4	E	15	ASN
5	F	129	GLN
5	F	131	GLN
5	F	147	GLN
5	F	227	GLN
5	F	301	ASN
5	F	309	ASN
5	F	362	ASN
5	F	446	GLN
5	F	455	HIS
5	F	469	GLN
5	F	600	HIS
1	G	23	HIS
1	G	84	ASN
1	G	194	GLN
1	H	128	HIS
2	I	69	GLN
2	I	139	ASN
2	I	165	HIS
2	I	327	GLN
2	I	343	HIS
2	I	494	ASN
2	I	513	GLN
2	I	618	GLN
2	I	673	HIS
2	I	677	ASN
2	I	688	GLN
2	I	725	GLN
2	I	799	ASN
2	I	952	GLN
2	I	1017	GLN
2	I	1108	ASN

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Mol	Chain	Res	Type
2	I	1111	GLN
2	I	1116	HIS
2	I	1209	GLN
2	I	1220	GLN
2	I	1299	ASN
2	I	1313	HIS
2	I	1314	GLN
2	I	1324	ASN
2	I	1336	ASN
3	J	94	GLN
3	J	196	GLN
3	J	200	GLN
3	J	206	ASN
3	J	364	HIS
3	J	365	GLN
3	J	419	HIS
3	J	465	GLN
3	J	489	ASN
3	J	594	GLN
3	J	702	GLN
3	J	716	GLN
3	J	777	HIS
3	J	867	GLN
3	J	910	ASN
3	J	929	GLN
3	J	1227	HIS
3	J	1244	GLN
3	J	1279	GLN
4	K	7	GLN
4	K	61	ASN
4	K	72	GLN
5	L	128	ASN
5	L	131	GLN
5	L	301	ASN
5	L	345	GLN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN
5	L	455	HIS
5	L	464	ASN
5	L	568	ASN
5	L	600	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	233/320 (72%)	-0.53	0 100 100	105, 144, 198, 236	0
1	B	217/320 (67%)	-0.39	1 (0%) 87 78	121, 192, 243, 265	0
1	G	227/320 (70%)	-0.41	0 100 100	162, 195, 234, 271	0
1	H	216/320 (67%)	-0.26	1 (0%) 87 78	175, 215, 240, 264	0
2	C	1340/1342 (99%)	-0.50	1 (0%) 92 91	78, 133, 242, 297	0
2	I	1340/1342 (99%)	-0.44	0 100 100	104, 171, 269, 334	0
3	D	1167/1407 (82%)	-0.52	1 (0%) 92 91	83, 120, 204, 261	0
3	J	1155/1407 (82%)	-0.47	1 (0%) 92 91	99, 146, 228, 277	0
4	E	89/90 (98%)	-0.64	0 100 100	118, 156, 179, 198	0
4	K	79/90 (87%)	-0.47	1 (1%) 75 61	211, 251, 298, 305	0
5	F	468/613 (76%)	-0.48	0 100 100	115, 167, 295, 326	0
5	L	469/613 (76%)	-0.51	1 (0%) 91 87	130, 181, 301, 320	0
All	All	7000/8184 (85%)	-0.47	7 (0%) 92 91	78, 156, 252, 334	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	45	GLY	2.6
1	B	85	LEU	2.3
3	J	307	LEU	2.2
4	K	16	ARG	2.2
1	H	220	ALA	2.1
5	L	599	ARG	2.1
3	D	340	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
6	MG	D	2002	1/1	0.25	0.21	189,189,189,189	0
6	MG	I	1401	1/1	0.30	0.09	189,189,189,189	0
6	MG	J	2001	1/1	0.50	0.10	189,189,189,189	0
6	MG	D	2001	1/1	0.59	0.12	189,189,189,189	0
7	ZN	D	2003	1/1	0.91	0.11	189,189,189,189	0
7	ZN	D	2004	1/1	0.92	0.13	189,189,189,189	0
7	ZN	J	2003	1/1	0.95	0.07	189,189,189,189	0
7	ZN	J	2002	1/1	0.97	0.06	310,310,310,310	0

6.5 Other polymers [i](#)

There are no such residues in this entry.