Full wwPDB X-ray Structure Validation Report (i)

Jan 5, 2017 – 03:53 AM EST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

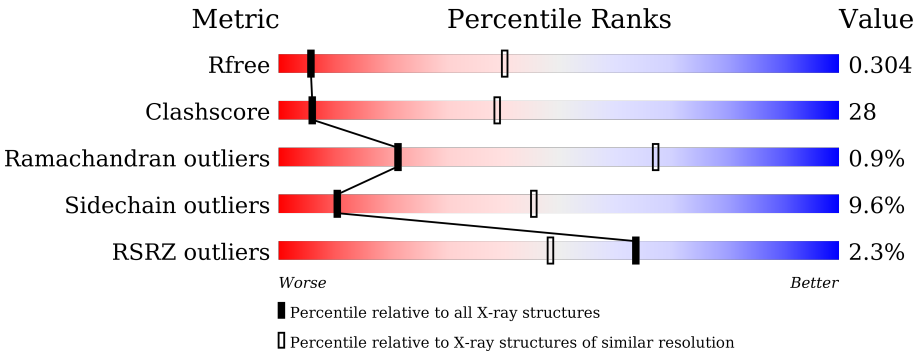
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	42% 42% 9% 6%
1	B	329	29% 33% 34%
1	G	329	29% 31% 6% 32%
1	H	329	4% 27% 35% 34%
2	C	1342	2% 44% 47% 9%
2	I	1342	4% 50% 44% 6%

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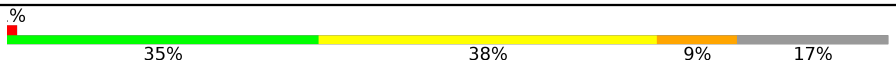
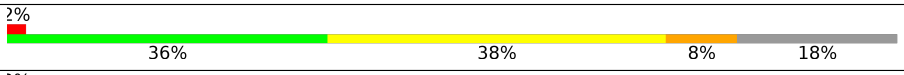
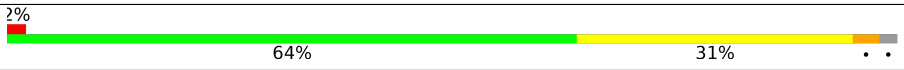
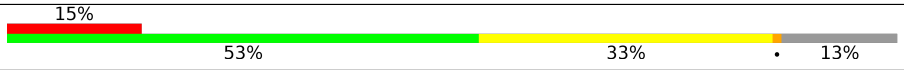
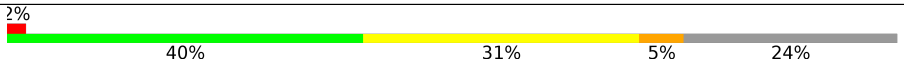
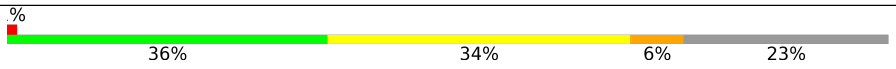
Mol	Chain	Length	Quality of chain
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

2 Entry composition

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

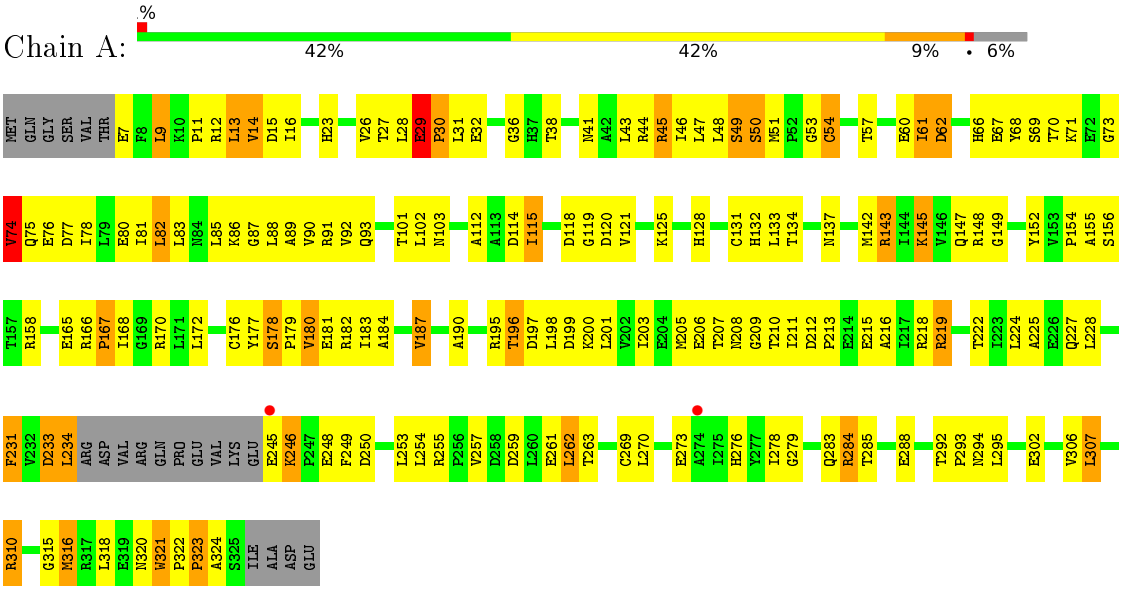
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

3 Residue-property plots (i)

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

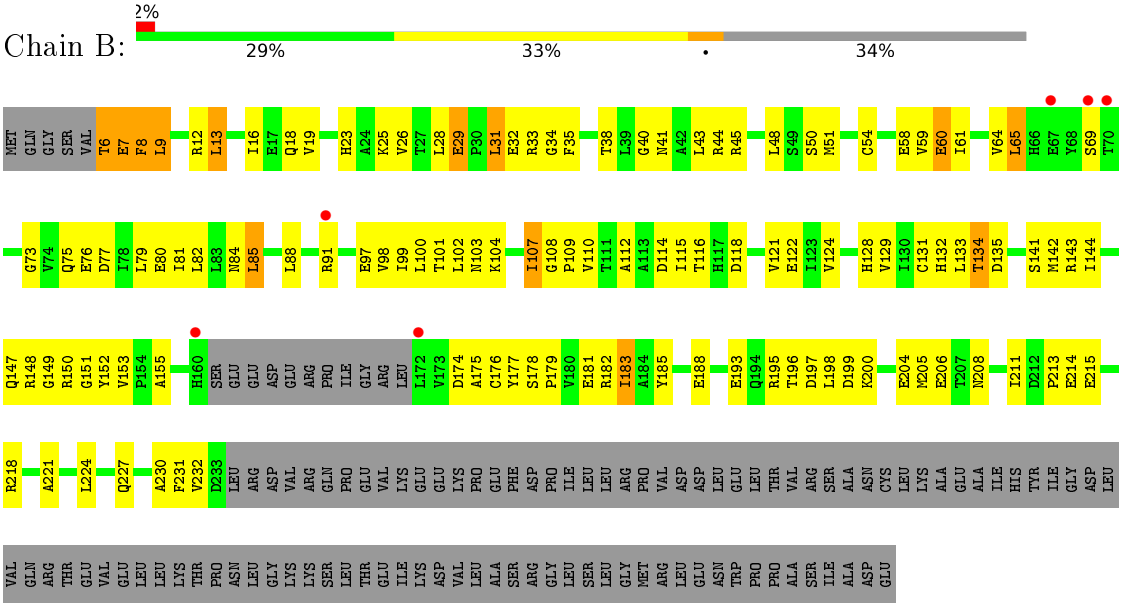
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



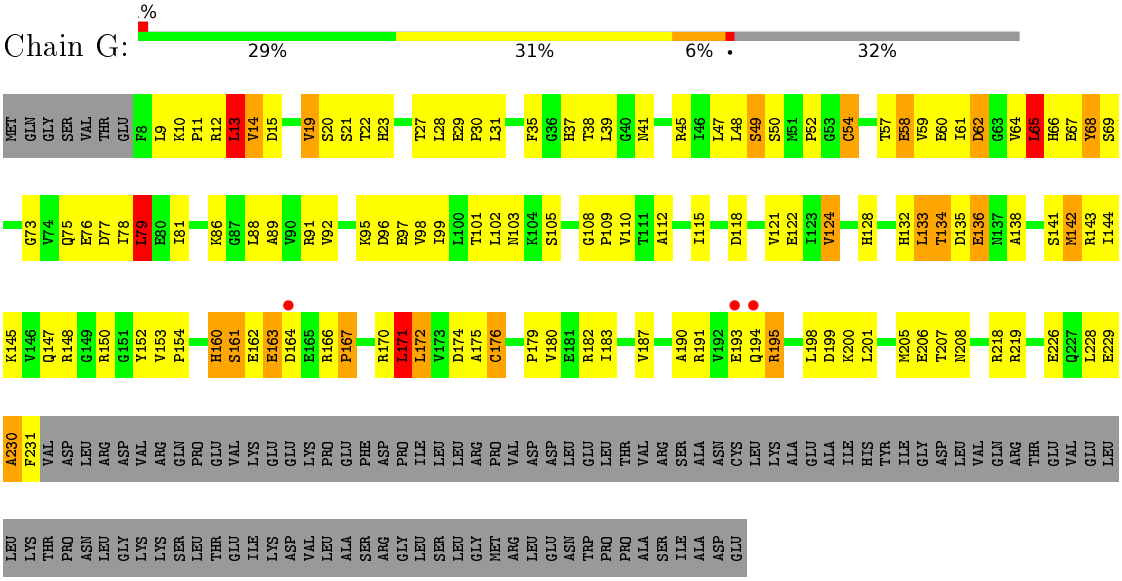
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



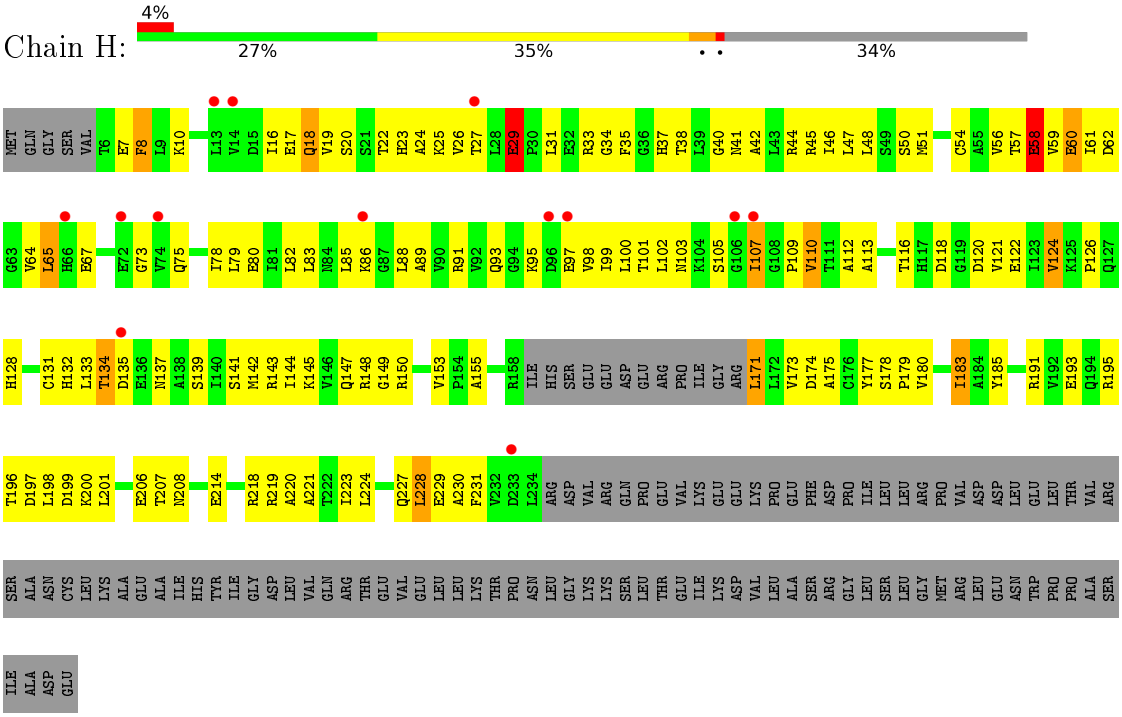
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



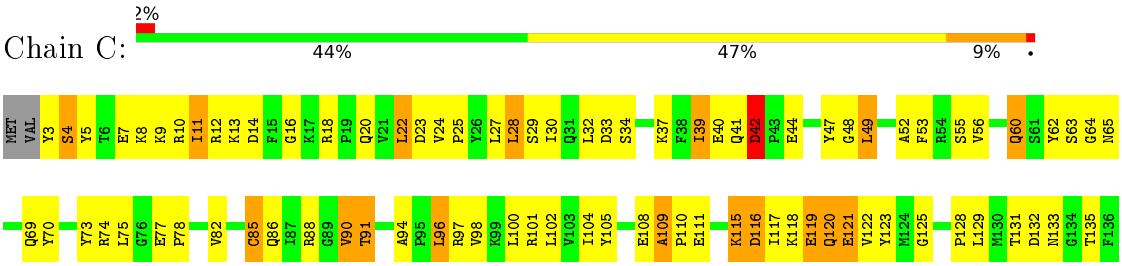
• Molecule 1: DNA-directed RNA polymerase subunit alpha

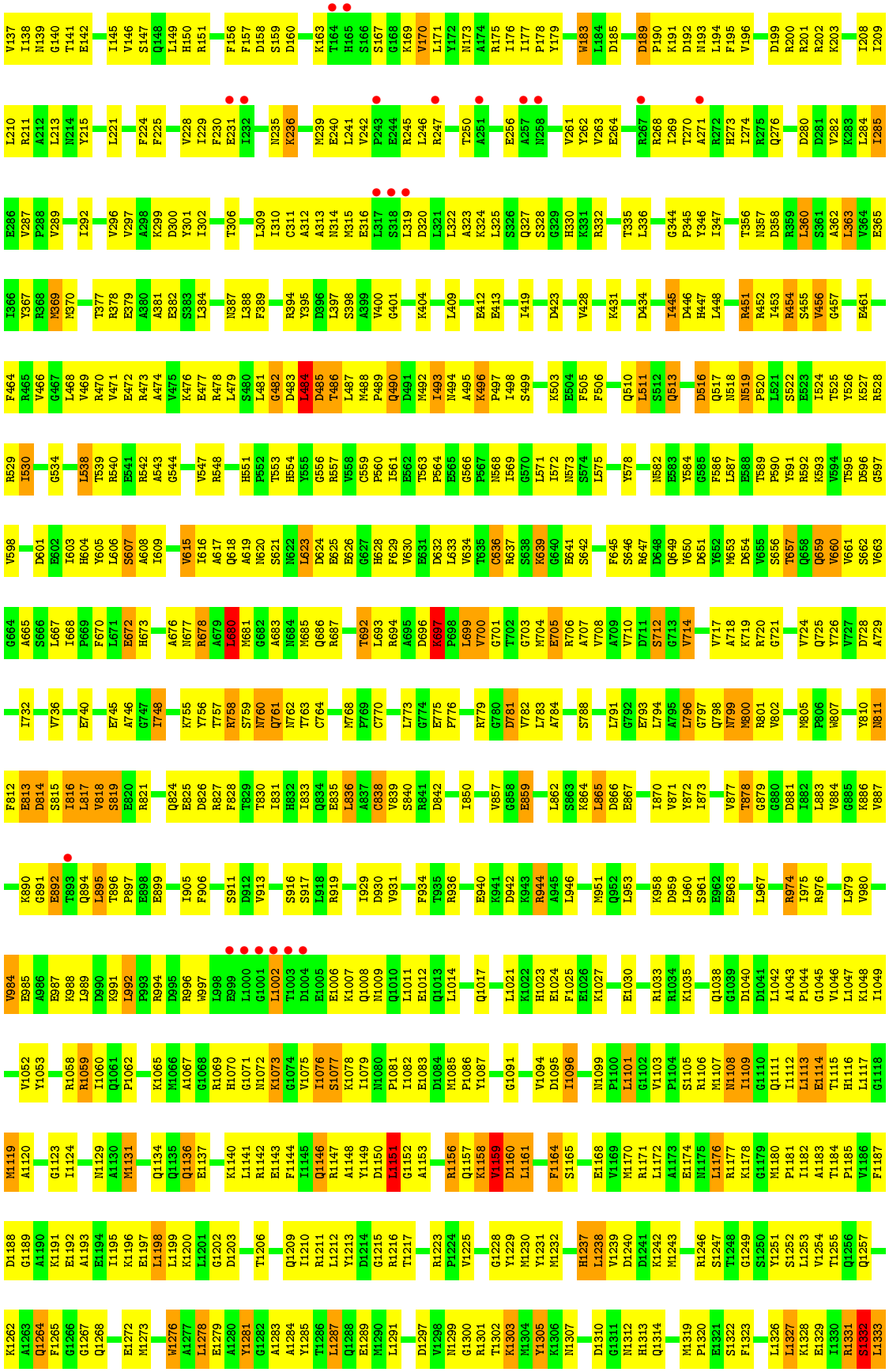
Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

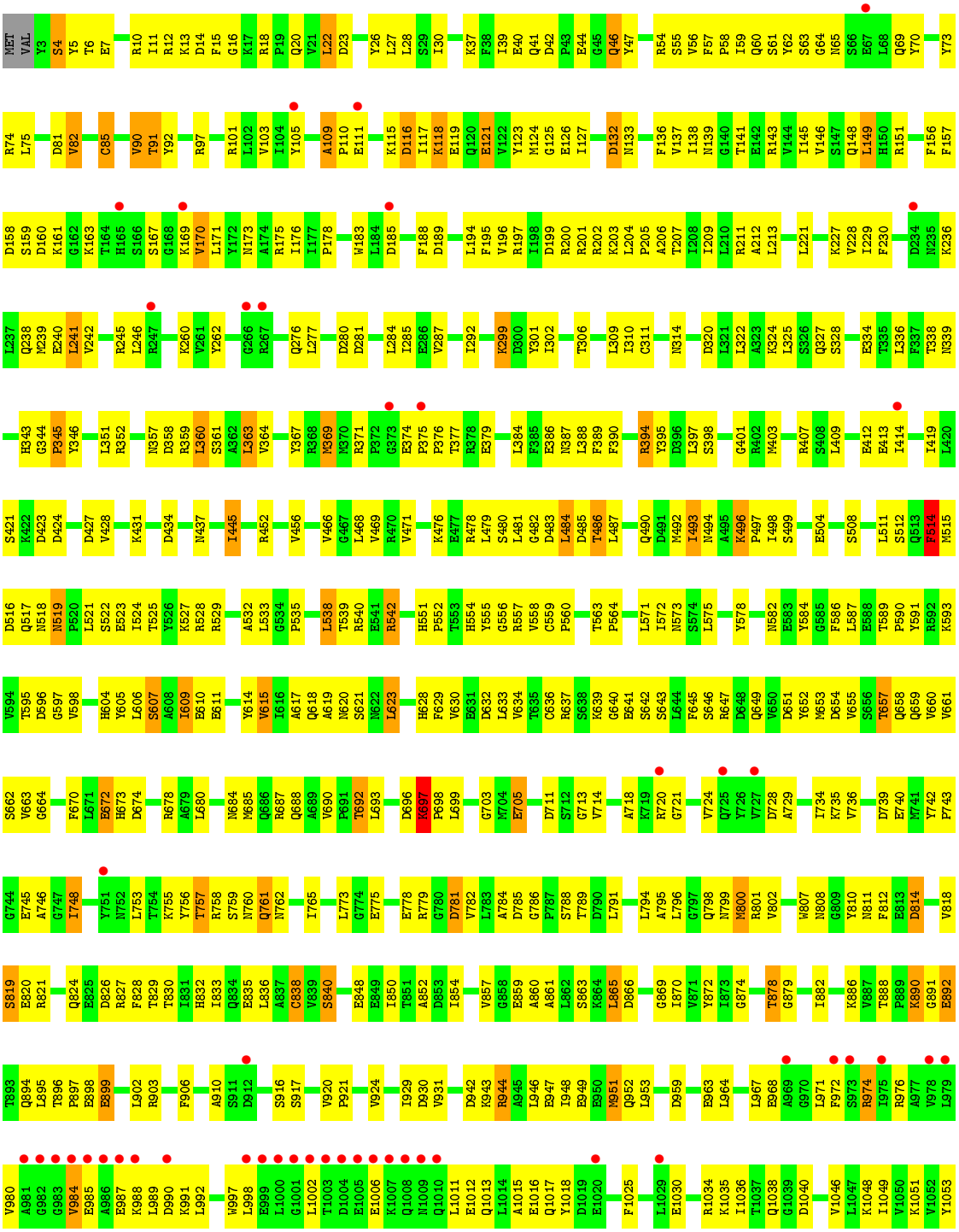
Chain C:

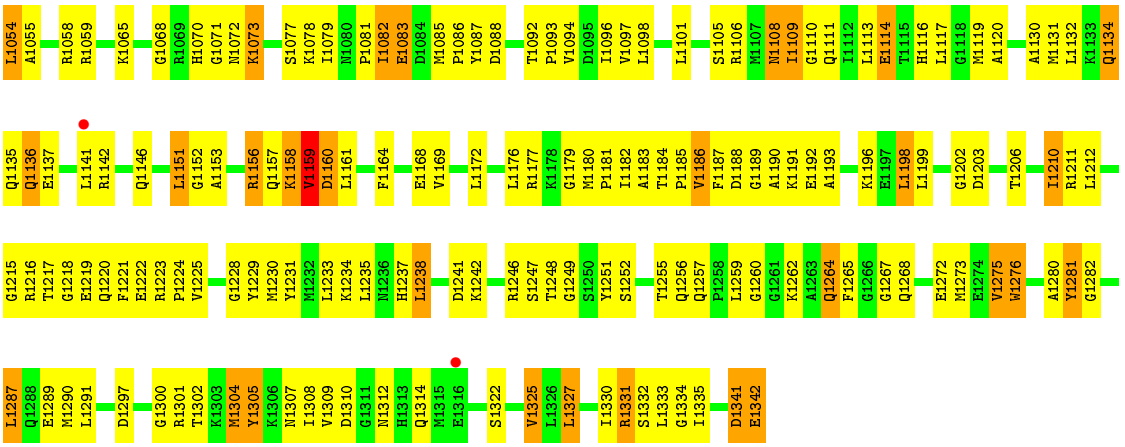




• Molecule 2: DNA-directed RNA polymerase subunit beta

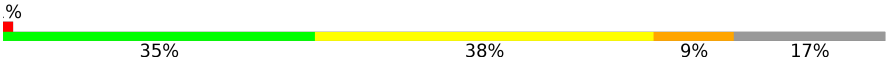
Chain I:

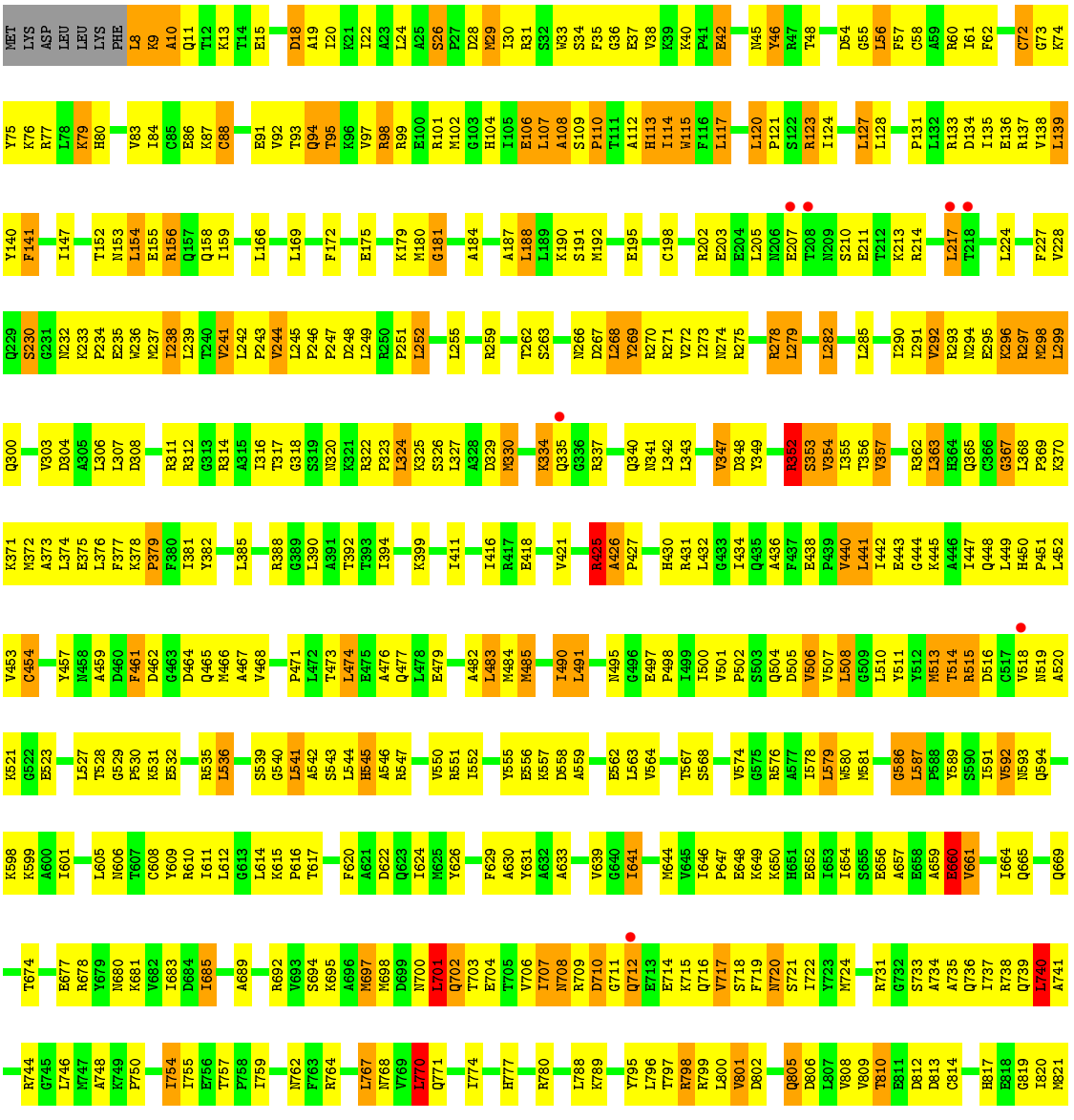


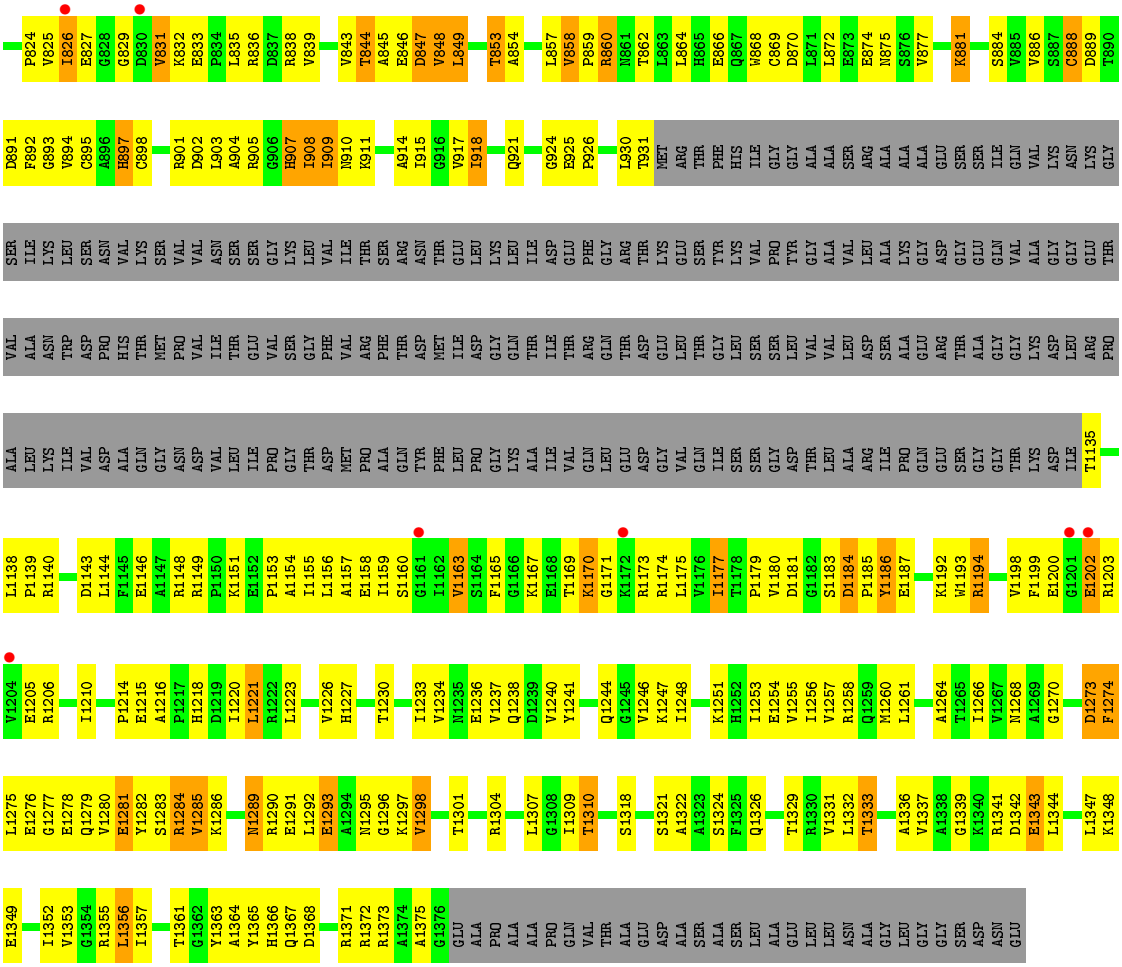


• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

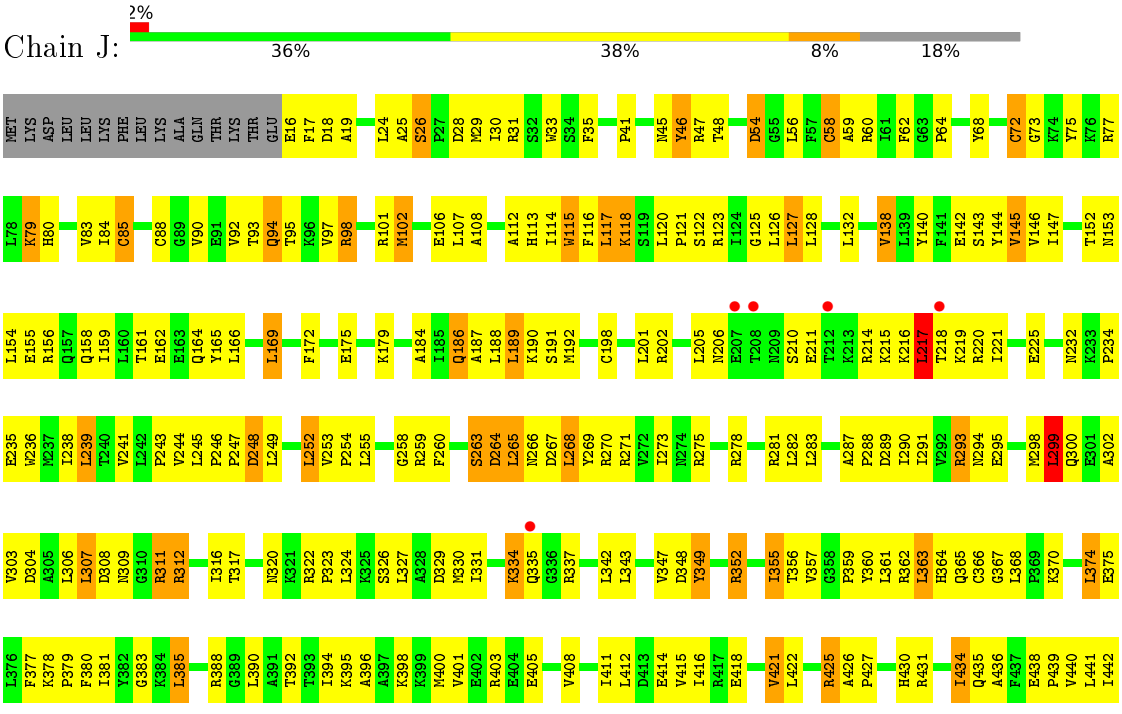


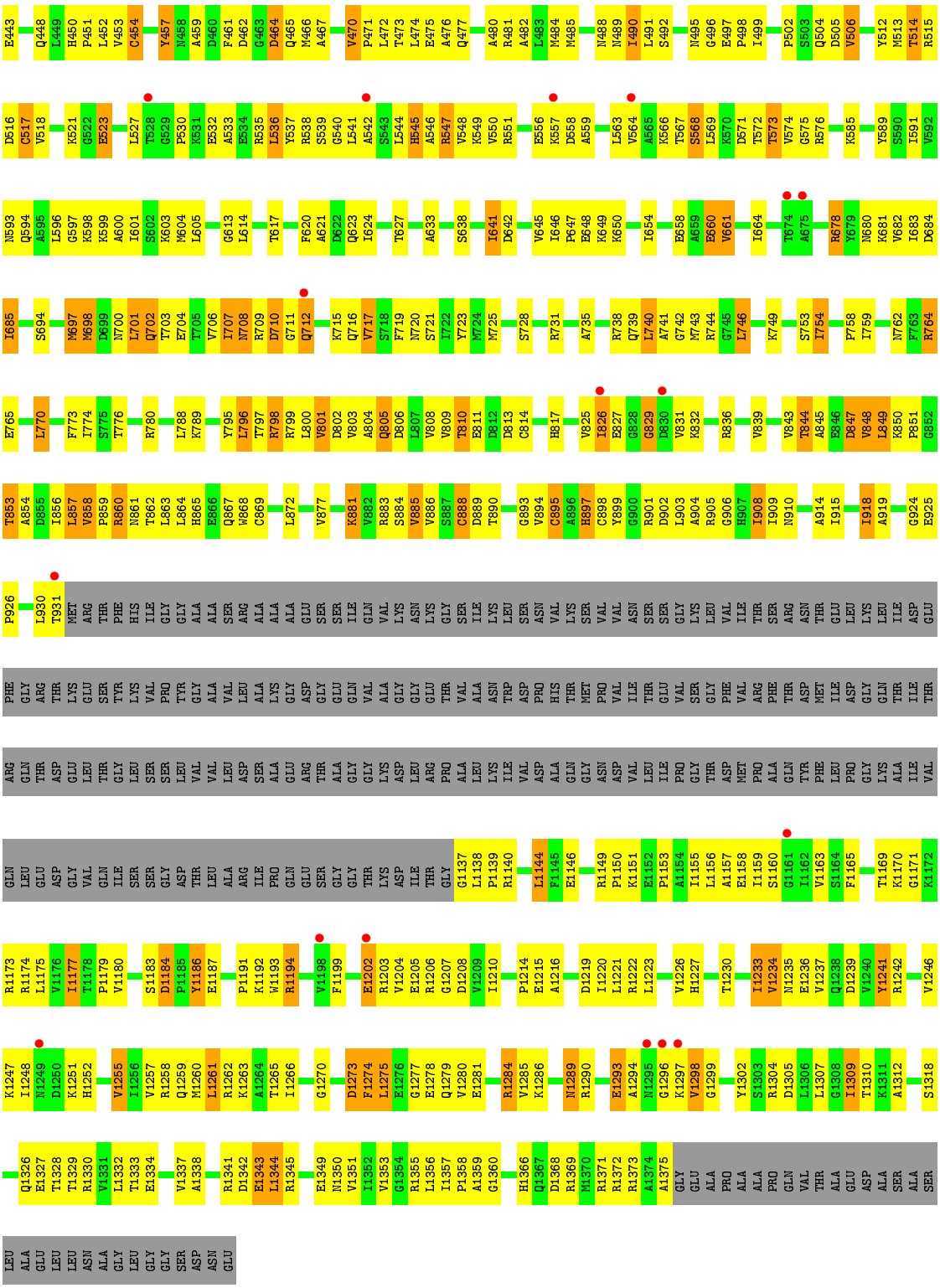




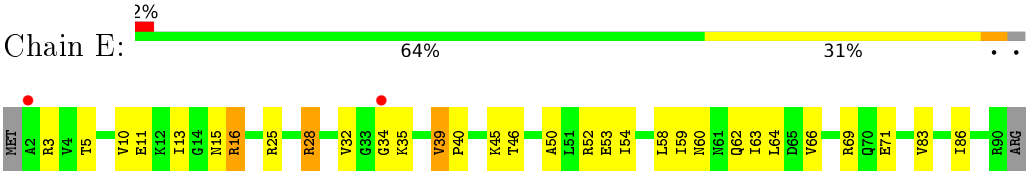
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:



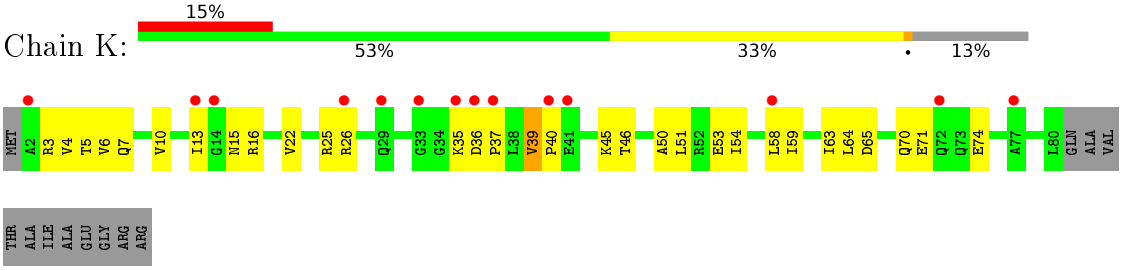


• Molecule 4: DNA-directed RNA polymerase subunit omega



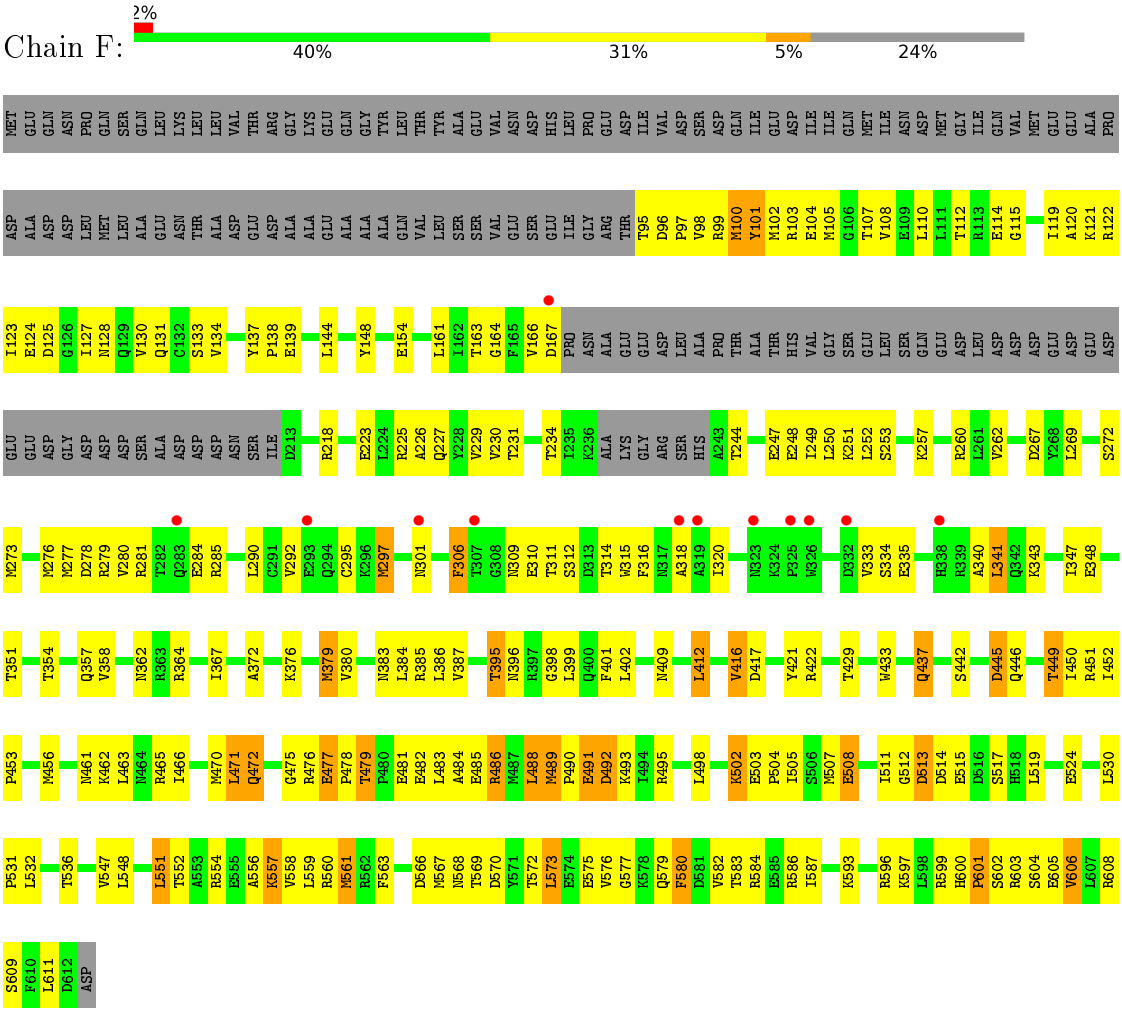
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



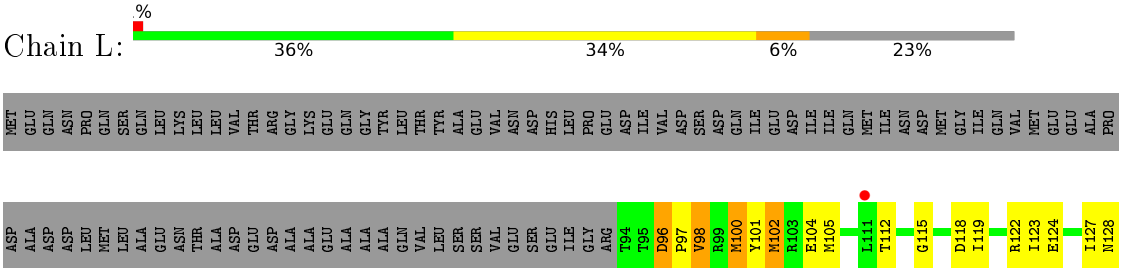
• Molecule 5: RNA polymerase sigma factor RpoD

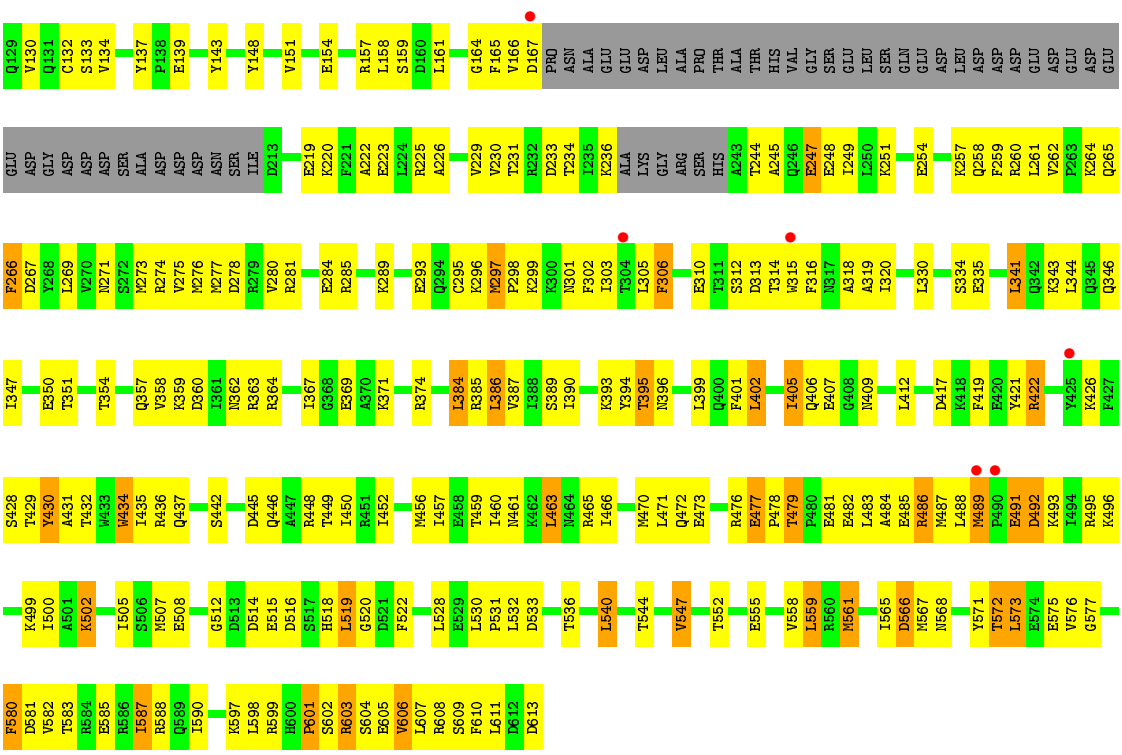
Chain F:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:




Q129 V130 Q131 C132 S133 V134 Y137 P138 E139 Y143 Y148 V151 E154 R157 L158 S159 D160 L161 G164 F165 V166 D167 PRO ASN ALA GLU GLU ASP LEU ALA PRO THR ALA THR HIS VAL GLY SER GLU LEU SER GLN GLU ASP LEU ASP ASP ASP GLU ASP GLU ASP GLU
GLU ASP GLY ASP ASP SER ALA ASP ASP ASP ASN SER ILE D213 E219 K220 F221 A222 E223 L224 R225 A226 V229 V230 T231 R232 D233 T234 T235 K236 ALA LYS GLY ARG SER HIS A243 T244 A245 Q246 E247 E248 I249 L250 K251 E254 K257 Q258 F259 R260 L261 V262 F263 K264 Q265
F266 D267 Y268 L269 V270 N271 S272 M273 R274 V275 M276 M277 D278 R279 V280 R281 E284 R285 K289 E293 Q294 C295 K296 M297 P298 K299 K300 N301 F302 I303 T304 L305 F306 E310 T311 S312 D313 T314 W315 F316 N317 A318 A319 I320 L330 S334 E335 I341 Q342 K343 L344 Q345 Q346
I347 E350 T351 T354 Q357 V358 K359 D360 I361 N362 R363 R364 I367 G368 E369 A370 K371 R374 L384 R385 L386 V387 I388 S389 I390 K393 Y394 T395 N396 L399 Q400 F401 L402 T405 Q406 E407 G408 N409 L412 D417 K418 F419 E420 Y421 R422 Y425 K426 F427
S428 T429 Y430 A431 T432 W433 W434 I435 R436 Q437 S442 D445 Q446 A447 R448 T449 I450 R451 I452 M456 I457 E458 T459 I460 N461 K462 L463 N464 R465 I466 M470 L471 Q472 E473 R476 E477 P478 T479 P480 E481 E482 L483 A484 E485 R486 M487 L488 M489 P490 E491 D492 K493 I494 R495 K496
K499 I500 A501 K502 I505 S506 M507 E508 G512 D513 D514 E515 D516 S517 H518 L519 G520 D521 F522 L528 E529 L530 P531 L532 D533 T536 L540 T544 V547 T552 E555 V558 L559 R560 M561 I565 D566 M567 N568 Y571 T572 L573 E574 E575 V576 G577
P580 D581 V582 T583 R584 E585 R586 I587 R588 Q589 I590 K597 L598 R599 H600 P601 S602 R603 S604 E605 V606 L607 R608 S609 F610 L611 D612 D613

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	185.36Å 206.28Å 308.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.60 29.90 – 3.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.90-3.60) 93.7 (29.90-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.56Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.246 , 0.305 0.245 , 0.304	Depositor DCC
R_{free} test set	1937 reflections (1.51%)	DCC
Wilson B-factor (Å^2)	142.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 91.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	55699	wwPDB-VP
Average B, all atoms (Å^2)	157.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

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

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

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

All (141) bond length outliers are listed below:

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

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

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

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

All (258) bond angle outliers are listed below:

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

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

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

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

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

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

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

There are no chirality outliers.

All (39) planarity outliers are listed below:

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

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

5.2 Too-close contacts (i)

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:HIS:HB2	1:A:205:MET:O	1.85	0.77
3:D:587:LEU:HD23	3:D:591:ILE:HG21	1.66	0.77
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.48	0.77
3:J:518:VAL:O	3:J:547:ARG:NH1	2.18	0.77
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.66	0.77
5:F:573:LEU:H	5:F:573:LEU:HD23	1.49	0.77
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.67	0.77
5:L:585:GLU:OE2	5:L:588:ARG:NH1	2.18	0.77
2:C:131:THR:HG23	2:C:133:ASN:H	1.50	0.76
3:D:418:GLU:HG3	4:E:45:LYS:H	1.50	0.76
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.68	0.76
1:A:45:ARG:NH2	2:C:1216:ARG:HA	1.99	0.76
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.65	0.76
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.51	0.76
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	1.99	0.76
3:D:109:SER:HB2	3:D:296:LYS:HE2	1.68	0.76
2:I:1072:ASN:N	2:I:1072:ASN:OD1	2.14	0.76
3:J:1263:LYS:HE2	3:J:1279:GLN:HE21	1.50	0.76
2:C:705:GLU:HB2	2:C:794:LEU:H	1.50	0.76
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.18	0.76
2:I:637:ARG:HA	2:I:642:SER:HA	1.66	0.76
2:C:1299:ASN:HD22	2:C:1303:LYS:HE2	1.49	0.76
2:C:4:SER:OG	2:C:5:TYR:N	2.16	0.76
3:J:1252:HIS:O	3:J:1255:VAL:HG13	1.85	0.76
1:B:6:THR:N	1:B:7:GLU:OE2	2.17	0.76
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.19	0.76
1:G:161:SER:O	1:G:163:GLU:N	2.18	0.76
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.68	0.75
2:I:1272:GLU:HB2	3:J:342:LEU:O	1.87	0.75
2:C:759:SER:OG	2:C:763:THR:N	2.18	0.75
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.67	0.75
3:J:1368:ASP:HA	3:J:1371:ARG:HH12	1.49	0.75
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.68	0.75
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.69	0.75
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.67	0.75
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.00	0.75
2:C:142:GLU:HB2	2:C:760:ASN:ND2	2.02	0.75
2:C:42:ASP:OD2	2:C:44:GLU:HG2	1.86	0.75
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.69	0.75
5:L:395:THR:OG1	5:L:396:ASN:N	2.16	0.75
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:ASP:OD2	2:C:44:GLU:O	2.05	0.75
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.69	0.75
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.69	0.75
2:I:1117:LEU:HD21	2:I:1182:ILE:HD12	1.68	0.75
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.69	0.75
2:C:1164:PHE:N	2:C:1168:GLU:OE1	2.18	0.75
3:J:140:TYR:OH	3:J:312:ARG:NH2	2.20	0.75
2:C:16:GLY:O	2:C:1156:ARG:HG2	1.87	0.74
2:C:149:LEU:HD12	2:C:452:ARG:O	1.86	0.74
3:J:523:GLU:OE2	3:J:547:ARG:NH1	2.18	0.74
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.20	0.74
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.69	0.74
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.68	0.74
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.68	0.74
2:C:511:LEU:HD12	2:C:511:LEU:N	2.02	0.74
2:C:759:SER:O	2:C:761:GLN:N	2.19	0.74
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.01	0.74
2:C:615:VAL:HG13	2:C:651:ASP:H	1.51	0.74
3:D:888:CYS:SG	3:D:889:ASP:N	2.61	0.74
3:J:362:ARG:H	3:J:365:GLN:HE21	1.33	0.74
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.70	0.74
2:C:1114:GLU:OE1	2:C:1230:MET:HA	1.88	0.74
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.68	0.74
1:G:9:LEU:O	1:H:227:GLN:NE2	2.21	0.74
2:C:142:GLU:CB	2:C:760:ASN:HD21	1.99	0.74
2:C:878:THR:OG1	2:C:879:GLY:N	2.19	0.74
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.23	0.74
3:D:98:ARG:HB3	3:D:248:ASP:OD2	1.88	0.74
1:A:12:ARG:H	1:A:30:PRO:HG2	1.53	0.74
3:D:45:ASN:HB3	3:D:48:THR:O	1.89	0.73
3:J:1159:ILE:HA	3:J:1206:ARG:HB3	1.70	0.73
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	1.87	0.73
5:L:343:LYS:HD2	5:L:343:LYS:H	1.52	0.73
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.23	0.73
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.69	0.73
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.69	0.73
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.88	0.73
5:L:305:LEU:HB3	5:L:315:TRP:HB3	1.70	0.73
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.69	0.73
3:D:847:ASP:HA	3:D:860:ARG:H	1.53	0.73
1:G:194:GLN:O	1:G:195:ARG:HG2	1.88	0.73

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

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

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.37	0.60
3:J:138:VAL:HG21	3:J:145:VAL:HB	1.83	0.60
5:L:476:ARG:HG3	5:L:477:GLU:N	2.15	0.60
1:B:107:ILE:HG23	1:B:135:ASP:HA	1.82	0.60
2:C:138:ILE:HG22	2:C:139:ASN:N	2.16	0.60
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.82	0.60
3:D:375:GLU:OE2	3:D:378:LYS:HD2	2.02	0.60
2:I:1247:SER:HB3	3:J:375:GLU:O	2.01	0.60
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.19	0.60
3:J:536:LEU:HD13	3:J:541:LEU:HB2	1.83	0.60
3:J:888:CYS:SG	3:J:889:ASP:N	2.75	0.60
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.37	0.60
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.66	0.60
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.66	0.60
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.02	0.60
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.67	0.60
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.83	0.60
1:A:249:PHE:HB2	1:A:253:LEU:HD12	1.82	0.60
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.83	0.60
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.37	0.60
2:C:701:GLY:O	2:C:1184:THR:N	2.25	0.60
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.32	0.60
1:A:61:ILE:HG22	1:A:62:ASP:H	1.66	0.60
1:B:151:GLY:O	1:B:177:TYR:HB2	2.02	0.60
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.20	0.60
2:C:498:ILE:H	2:C:498:ILE:HD12	1.66	0.60
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.36	0.60
3:D:363:LEU:HG	3:D:363:LEU:O	2.02	0.60
3:D:641:ILE:HD13	3:D:641:ILE:O	2.02	0.60
2:I:407:ARG:HH21	2:I:414:ILE:HG22	1.65	0.60
2:I:674:ASP:OD1	2:I:1109:ILE:N	2.34	0.60
3:J:495:ASN:ND2	3:J:497:GLU:HB2	2.17	0.60
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.17	0.59
1:G:65:LEU:CD2	1:G:65:LEU:H	2.15	0.59
1:G:228:LEU:HD22	1:H:221:ALA:HB1	1.84	0.59
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.66	0.59
3:J:521:LYS:NZ	3:J:540:GLY:O	2.24	0.59
5:L:233:ASP:O	5:L:236:LYS:HE2	2.02	0.59
5:L:245:ALA:O	5:L:249:ILE:HG13	2.01	0.59
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.31	0.59
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.67	0.59
2:C:864:LYS:HZ1	2:C:877:VAL:HG12	1.67	0.59
3:D:77:ARG:HG3	3:D:79:LYS:H	1.67	0.59
5:F:599:ARG:O	5:F:604:SER:OG	2.18	0.59
1:G:45:ARG:NH1	1:H:34:GLY:O	2.34	0.59
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.02	0.59
3:J:810:THR:HG23	3:J:811:GLU:H	1.67	0.59
5:L:127:ILE:O	5:L:130:VAL:HG22	2.02	0.59
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.17	0.59
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.83	0.59
1:G:172:LEU:HD12	1:G:172:LEU:H	1.67	0.59
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.02	0.59
2:I:1073:LYS:HE3	3:J:462:ASP:CB	2.32	0.59
2:I:1238:LEU:H	2:I:1238:LEU:HD12	1.68	0.59
2:I:4:SER:OG	2:I:5:TYR:N	2.35	0.59
1:A:9:LEU:HD13	1:A:32:GLU:OE2	2.03	0.59
1:B:34:GLY:N	1:B:199:ASP:OD2	2.29	0.59
2:C:615:VAL:HG13	2:C:651:ASP:N	2.17	0.59
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.67	0.59
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	1.85	0.59
1:H:18:GLN:HA	1:H:24:ALA:HA	1.83	0.59
2:I:159:SER:O	2:I:160:ASP:HB2	2.01	0.59
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.17	0.59
1:B:182:ARG:NH1	3:D:581:MET:SD	2.75	0.59
5:F:227:GLN:HG2	5:F:252:LEU:HA	1.84	0.59
5:F:532:LEU:O	5:F:536:THR:HG23	2.02	0.59
2:I:878:THR:OG1	2:I:879:GLY:N	2.34	0.59
3:J:527:LEU:HD21	3:J:536:LEU:HG	1.83	0.59
1:A:53:GLY:O	1:A:149:GLY:N	2.27	0.59
1:B:153:VAL:O	1:B:175:ALA:N	2.34	0.59
1:B:197:ASP:O	1:B:198:LEU:HD13	2.02	0.59
3:D:665:GLN:HG3	3:D:669:GLN:HE21	1.67	0.59
2:C:483:ASP:HB2	2:C:486:THR:HG22	1.83	0.59
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.83	0.59
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	1.84	0.59
5:F:601:PRO:CA	5:F:604:SER:HB2	2.33	0.59
1:H:113:ALA:HB2	1:H:126:PRO:HB3	1.83	0.59
2:I:778:GLU:O	2:I:781:ASP:HB2	2.03	0.59
1:A:11:PRO:CB	1:A:30:PRO:HG2	2.33	0.59
5:F:124:GLU:HA	5:F:127:ILE:HD11	1.83	0.59
1:H:58:GLU:HA	1:H:171:LEU:O	2.03	0.59

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.37	0.57
1:B:64:VAL:HG12	1:B:65:LEU:H	1.70	0.57
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.86	0.57
2:C:1268:GLN:HE22	3:D:352:ARG:NH1	2.02	0.57
3:D:356:THR:OG1	3:D:357:VAL:N	2.38	0.57
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.85	0.57
3:J:308:ASP:OD2	3:J:311:ARG:NE	2.38	0.57
3:J:425:ARG:HG2	3:J:426:ALA:H	1.68	0.57
5:L:390:ILE:O	5:L:393:LYS:HB2	2.05	0.57
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.05	0.57
5:F:461:ASN:O	5:F:465:ARG:HG2	2.04	0.57
1:G:230:ALA:HB3	1:G:231:PHE:CE2	2.39	0.57
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.87	0.57
2:I:185:ASP:HB2	2:I:197:ARG:HG3	1.87	0.57
2:I:12:ARG:NH2	2:I:698:PRO:O	2.25	0.57
2:C:936:ARG:HE	2:C:1047:LEU:HD23	1.70	0.57
2:C:468:LEU:O	2:C:471:VAL:HG12	2.04	0.57
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.33	0.57
5:F:561:MET:HA	5:F:567:MET:HE1	1.86	0.57
1:H:99:ILE:HD12	1:H:145:LYS:HB2	1.87	0.57
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.70	0.57
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.05	0.57
2:C:1238:LEU:HD12	2:C:1238:LEU:N	2.18	0.57
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.86	0.57
3:D:555:TYR:O	3:D:586:GLY:O	2.23	0.57
5:F:503:GLU:HG3	5:F:504:PRO:HD2	1.87	0.57
1:H:99:ILE:HG13	1:H:144:ILE:O	2.05	0.57
2:I:145:ILE:HB	2:I:456:VAL:HG22	1.86	0.57
1:G:75:GLN:O	2:I:729:ALA:HB2	2.04	0.57
3:J:1343:GLU:HG3	3:J:1373:ARG:NH2	2.20	0.57
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.45	0.57
2:C:596:ASP:OD2	2:C:597:GLY:N	2.36	0.57
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.68	0.57
3:D:94:GLN:O	3:D:97:VAL:HG23	2.04	0.57
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.70	0.57
2:C:980:VAL:O	2:C:984:VAL:HB	2.05	0.57
3:D:388:ARG:HB2	3:D:390:LEU:CD1	2.35	0.57
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.34	0.57
2:I:1246:ARG:NH2	2:I:1249:GLY:H	2.03	0.57
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.05	0.57
2:I:480:SER:HB3	2:I:481:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:606:LEU:HD23	2:I:611:GLU:HA	1.86	0.57
5:L:421:TYR:CE2	5:L:422:ARG:HD2	2.40	0.57
2:I:170:VAL:HG23	2:I:171:LEU:N	2.20	0.56
2:C:170:VAL:O	2:C:171:LEU:HG	2.05	0.56
2:C:886:LYS:CE	2:C:916:SER:HB3	2.35	0.56
5:F:226:ALA:O	5:F:229:VAL:HG22	2.05	0.56
5:F:379:MET:HG3	5:F:379:MET:O	2.01	0.56
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.40	0.56
2:I:239:MET:O	2:I:284:LEU:HD12	2.03	0.56
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.87	0.56
2:I:655:VAL:N	2:I:659:GLN:OE1	2.37	0.56
3:J:45:ASN:O	3:J:46:TYR:HD2	1.87	0.56
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.39	0.56
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.05	0.56
2:C:62:TYR:O	2:C:64:GLY:N	2.38	0.56
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.38	0.56
2:C:495:ALA:HB3	5:F:471:LEU:HD13	1.85	0.56
2:I:468:LEU:O	2:I:471:VAL:HG12	2.06	0.56
3:J:1203:ARG:NH1	3:J:1205:GLU:HG2	2.18	0.56
3:J:536:LEU:O	3:J:539:SER:OG	2.24	0.56
1:A:23:HIS:HB2	1:A:206:GLU:HA	1.87	0.56
3:D:224:LEU:O	3:D:228:VAL:HG23	2.04	0.56
3:D:299:LEU:O	3:D:299:LEU:HG	2.02	0.56
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.39	0.56
3:D:657:ALA:O	3:D:661:VAL:HG12	2.06	0.56
3:D:817:HIS:HE1	3:D:860:ARG:HE	1.45	0.56
5:F:343:LYS:H	5:F:343:LYS:HD2	1.70	0.56
2:I:40:GLU:O	2:I:73:TYR:OH	2.23	0.56
1:A:23:HIS:CB	1:A:206:GLU:HA	2.35	0.56
1:B:82:LEU:O	1:B:85:LEU:HB2	2.05	0.56
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.86	0.56
2:C:685:MET:HE1	2:C:1071:GLY:HA2	1.87	0.56
3:D:674:THR:HG1	3:D:677:GLU:HB2	1.71	0.56
1:G:38:THR:HG23	1:H:42:ALA:HA	1.88	0.56
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.41	0.56
2:I:615:VAL:HG13	2:I:651:ASP:H	1.69	0.56
2:I:818:VAL:HG22	2:I:1096:ILE:HG12	1.87	0.56
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.87	0.56
3:J:425:ARG:HH11	3:J:459:ALA:HA	1.69	0.56
1:G:9:LEU:HD23	1:G:10:LYS:N	2.20	0.56
1:G:73:GLY:N	2:I:728:ASP:OD2	2.35	0.56

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:466:VAL:O	2:C:470:ARG:HG2	2.05	0.56
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.15	0.56
3:D:347:VAL:HG12	3:D:348:ASP:O	2.05	0.56
1:H:44:ARG:CG	1:H:183:ILE:HD13	2.36	0.56
2:I:138:ILE:HG22	2:I:139:ASN:N	2.19	0.56
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.38	0.56
3:J:127:LEU:O	3:J:220:ARG:NH2	2.39	0.56
3:J:518:VAL:HG23	3:J:547:ARG:HH22	1.70	0.56
2:C:1299:ASN:HD22	2:C:1303:LYS:CE	2.18	0.55
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.88	0.55
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.07	0.55
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.71	0.55
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.41	0.55
3:J:709:ARG:C	3:J:711:GLY:H	2.08	0.55
3:J:849:LEU:HB3	3:J:853:THR:HG23	1.87	0.55
3:J:789:LYS:HE3	3:J:931:THR:O	2.05	0.55
1:A:49:SER:OG	1:A:50:SER:N	2.38	0.55
1:B:60:GLU:HG3	1:B:143:ARG:O	2.06	0.55
2:C:379:GLU:H	2:C:379:GLU:CD	2.08	0.55
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.41	0.55
3:D:140:TYR:HB3	5:F:100:MET:SD	2.46	0.55
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.20	0.55
1:G:191:ARG:NH1	1:G:198:LEU:H	2.04	0.55
2:I:1132:LEU:HD22	2:I:1177:ARG:NH1	2.21	0.55
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.87	0.55
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.11	0.55
3:J:156:ARG:NH2	3:J:191:SER:OG	2.37	0.55
5:L:547:VAL:HG23	5:L:603:ARG:NH1	2.21	0.55
1:A:269:CYS:O	1:A:273:GLU:HG2	2.06	0.55
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.42	0.55
1:B:99:ILE:HG13	1:B:144:ILE:O	2.05	0.55
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.37	0.55
2:C:228:VAL:HB	2:C:335:THR:OG1	2.06	0.55
2:C:607:SER:OG	2:C:608:ALA:N	2.32	0.55
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.88	0.55
1:H:60:GLU:HG2	1:H:143:ARG:HB2	1.87	0.55
2:I:1085:MET:HB2	2:I:1093:PRO:HB3	1.87	0.55
2:I:324:LYS:O	2:I:327:GLN:NE2	2.40	0.55
2:I:807:TRP:CE3	2:I:808:ASN:HB2	2.41	0.55
2:I:898:GLU:OE1	2:I:898:GLU:N	2.37	0.55
3:J:45:ASN:HB3	3:J:48:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.88	0.55
1:B:155:ALA:N	1:B:174:ASP:OD1	2.39	0.55
2:C:1076:ILE:HD11	2:C:1078:LYS:O	2.06	0.55
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.42	0.55
2:C:202:ARG:HH11	2:C:369:MET:HG2	1.71	0.55
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.89	0.55
3:J:418:GLU:HB2	4:K:45:LYS:HB2	1.88	0.55
1:A:12:ARG:N	1:A:30:PRO:HG2	2.12	0.55
2:C:55:SER:OG	2:C:56:VAL:N	2.39	0.55
2:C:637:ARG:HA	2:C:642:SER:HA	1.87	0.55
5:F:227:GLN:NE2	5:F:251:LYS:HZ1	2.03	0.55
2:I:557:ARG:HH21	2:I:607:SER:C	2.09	0.55
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.42	0.55
2:C:224:PHE:CD2	2:C:347:ILE:HG13	2.41	0.55
2:C:758:ARG:HH22	2:C:761:GLN:CG	2.08	0.55
5:F:354:THR:N	5:F:357:GLN:OE1	2.40	0.55
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.21	0.55
5:L:266:PHE:O	5:L:269:LEU:HB2	2.06	0.55
3:D:314:ARG:HH22	3:D:323:PRO:HG3	1.69	0.55
3:D:418:GLU:H	4:E:45:LYS:NZ	2.04	0.55
3:J:1159:ILE:CA	3:J:1206:ARG:HB3	2.36	0.55
3:J:1327:GLU:OE2	3:J:1329:THR:HB	2.06	0.55
3:J:490:ILE:O	3:J:499:ILE:HG22	2.06	0.55
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.88	0.55
2:C:1151:LEU:HD23	2:C:1197:GLU:OE2	2.07	0.55
3:D:152:THR:OG1	3:D:153:ASN:N	2.38	0.55
5:F:166:VAL:O	5:F:167:ASP:HB2	2.07	0.55
1:H:60:GLU:OE1	1:H:142:MET:HB2	2.06	0.55
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.41	0.55
2:I:678:ARG:NH1	2:I:1071:GLY:O	2.37	0.55
2:I:156:PHE:CE1	2:I:445:ILE:HG13	2.42	0.55
2:I:498:ILE:H	2:I:498:ILE:HD12	1.71	0.55
3:J:568:SER:OG	3:J:569:LEU:N	2.37	0.55
5:L:314:THR:O	5:L:318:ALA:HB3	2.07	0.55
3:D:1277:GLY:O	3:D:1278:GLU:HG2	2.07	0.55
3:D:425:ARG:HG2	3:D:426:ALA:H	1.71	0.55
3:D:515:ARG:O	3:D:545:HIS:HB3	2.07	0.55
1:G:150:ARG:NH1	1:H:7:GLU:O	2.32	0.55
2:I:421:SER:N	2:I:424:ASP:OD2	2.37	0.55
3:J:1174:ARG:NH2	3:J:1187:GLU:OE2	2.40	0.55
3:J:492:SER:HB2	3:J:499:ILE:HD13	1.88	0.55

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:THR:O	1:B:6:THR:OG1	2.21	0.51
2:C:894:GLN:O	2:C:894:GLN:HG3	2.11	0.51
3:D:34:SER:HB2	3:D:104:HIS:HB3	1.93	0.51
3:D:556:GLU:O	3:D:564:VAL:N	2.28	0.51
3:D:75:TYR:HD2	3:D:80:HIS:CD2	2.29	0.51
3:J:682:VAL:O	3:J:685:ILE:HG12	2.10	0.51
2:C:490:GLN:CD	5:F:472:GLN:NE2	2.64	0.50
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.11	0.50
3:D:495:ASN:OD1	3:D:495:ASN:N	2.43	0.50
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.93	0.50
4:E:50:ALA:O	4:E:54:ILE:HG12	2.11	0.50
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.11	0.50
2:I:1281:TYR:OH	3:J:434:ILE:O	2.29	0.50
1:A:57:THR:HG22	1:A:158:ARG:NH2	2.26	0.50
1:A:75:GLN:HA	2:C:729:ALA:N	2.26	0.50
2:C:1112:ILE:O	2:C:1115:THR:N	2.44	0.50
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.76	0.50
2:C:229:ILE:HG21	2:C:240:GLU:OE2	2.12	0.50
2:C:452:ARG:NH1	2:C:584:TYR:O	2.43	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE2	1.93	0.50
2:C:1267:GLY:HA3	3:D:347:VAL:O	2.12	0.50
3:D:516:ASP:OD1	3:D:516:ASP:N	2.44	0.50
3:D:664:ILE:HG21	3:D:681:LYS:HG2	1.93	0.50
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.93	0.50
2:I:921:PRO:O	2:I:924:VAL:HG22	2.11	0.50
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.27	0.50
3:J:1261:LEU:HD13	3:J:1304:ARG:HD2	1.93	0.50
1:A:207:THR:HG22	1:A:209:GLY:H	1.76	0.50
1:A:228:LEU:HA	1:A:231:PHE:HB2	1.93	0.50
2:C:397:LEU:HD12	2:C:397:LEU:N	2.26	0.50
3:D:574:VAL:O	3:D:578:ILE:HG13	2.11	0.50
1:G:65:LEU:N	1:G:65:LEU:HD22	2.26	0.50
2:I:4:SER:HB3	2:I:7:GLU:CD	2.31	0.50
2:I:623:LEU:HA	2:I:630:VAL:HG23	1.92	0.50
2:I:757:THR:O	2:I:833:ILE:HD12	2.11	0.50
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.93	0.50
2:C:323:ALA:O	2:C:327:GLN:HG3	2.12	0.50
1:A:152:TYR:OH	2:C:824:GLN:HA	2.11	0.50
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.93	0.50
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.93	0.50
2:C:618:GLN:OE1	3:D:770:LEU:HD13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:844:THR:OG1	3:D:860:ARG:O	2.20	0.50
1:G:88:LEU:HB2	1:G:128:HIS:CD2	2.46	0.50
2:I:101:ARG:HE	2:I:118:LYS:HD2	1.77	0.50
3:J:255:LEU:HB2	3:J:259:ARG:O	2.12	0.50
3:J:825:VAL:C	3:J:826:ILE:HG13	2.32	0.50
5:L:161:LEU:O	5:L:262:VAL:HG23	2.11	0.50
2:C:1268:GLN:OE1	3:D:352:ARG:HG2	2.12	0.50
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.26	0.50
3:D:188:LEU:O	3:D:191:SER:OG	2.25	0.50
3:D:839:VAL:HG12	3:D:839:VAL:O	2.12	0.50
5:F:120:ALA:HA	5:F:123:ILE:HD12	1.93	0.50
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.93	0.50
1:H:19:VAL:HB	1:H:23:HIS:CD2	2.46	0.50
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.26	0.50
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.93	0.50
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.92	0.50
3:D:1184:ASP:O	3:D:1186:TYR:N	2.45	0.50
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.47	0.50
5:F:125:ASP:N	5:F:125:ASP:OD1	2.43	0.50
5:F:292:VAL:HG13	5:F:297:MET:O	2.11	0.50
5:F:478:PRO:HB2	5:F:483:LEU:CD1	2.41	0.50
5:F:478:PRO:HB2	5:F:483:LEU:HD11	1.92	0.50
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.47	0.50
2:I:556:GLY:HA2	2:I:659:GLN:O	2.12	0.50
3:J:205:LEU:HD23	3:J:217:LEU:HG	1.94	0.50
3:J:516:ASP:OD1	3:J:516:ASP:N	2.44	0.50
1:A:114:ASP:N	1:A:114:ASP:OD1	2.44	0.50
3:D:114:ILE:HD13	3:D:304:ASP:CG	2.32	0.50
3:D:817:HIS:NE2	3:D:860:ARG:NH2	2.59	0.50
3:D:905:ARG:NH1	4:E:10:VAL:HG11	2.27	0.50
1:H:78:ILE:O	1:H:82:LEU:HG	2.12	0.50
3:J:1246:VAL:HG12	3:J:1248:ILE:HG13	1.92	0.50
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.12	0.50
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.93	0.50
3:J:77:ARG:HB3	3:J:80:HIS:CE1	2.47	0.50
1:B:16:ILE:HG12	1:B:26:VAL:CG1	2.41	0.50
2:C:1149:TYR:HE2	2:C:1180:MET:SD	2.35	0.50
2:C:1328:LYS:O	2:C:1332:SER:N	2.45	0.50
2:C:18:ARG:NH1	2:C:621:SER:O	2.45	0.50
2:C:209:ILE:O	2:C:213:LEU:HG	2.12	0.50
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.93	0.50

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.16	0.49
5:L:148:TYR:HE1	5:L:158:LEU:HD21	1.77	0.49
5:L:261:LEU:H	5:L:261:LEU:HD12	1.78	0.49
5:L:603:ARG:NH1	5:L:603:ARG:HA	2.27	0.49
1:A:321:TRP:HA	1:A:322:PRO:HA	1.64	0.49
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.94	0.49
2:C:1212:LEU:HD22	2:C:1225:VAL:CG2	2.41	0.49
2:C:959:ASP:O	2:C:963:GLU:HG2	2.12	0.49
3:D:843:VAL:HG11	3:D:897:HIS:O	2.12	0.49
1:H:64:VAL:HG12	1:H:65:LEU:H	1.77	0.49
2:I:1219:GLU:OE2	3:J:538:ARG:NH1	2.31	0.49
2:I:1220:GLN:HG2	2:I:1221:PHE:H	1.77	0.49
2:I:139:ASN:O	2:I:141:THR:HG23	2.12	0.49
2:I:158:ASP:CG	2:I:159:SER:H	2.14	0.49
2:I:674:ASP:OD1	2:I:1110:GLY:N	2.25	0.49
3:J:322:ARG:NH1	3:J:322:ARG:HB2	2.27	0.49
5:L:230:VAL:O	5:L:234:THR:HG23	2.13	0.49
1:A:262:LEU:HD21	1:A:306:VAL:HG11	1.95	0.48
2:C:1238:LEU:H	2:C:1238:LEU:CD1	2.16	0.48
2:C:1333:LEU:HD21	3:D:327:LEU:HB2	1.95	0.48
2:C:866:ASP:HA	2:C:872:TYR:CZ	2.48	0.48
2:C:90:VAL:HG12	2:C:91:THR:N	2.27	0.48
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.28	0.48
3:D:825:VAL:C	3:D:826:ILE:HG13	2.33	0.48
1:G:64:VAL:HG12	1:G:66:HIS:H	1.78	0.48
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.95	0.48
2:I:745:GLU:H	2:I:1017:GLN:HG3	1.78	0.48
2:I:367:TYR:CE2	2:I:376:PRO:HA	2.48	0.48
3:J:848:VAL:CG2	3:J:858:VAL:HG13	2.42	0.48
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.94	0.48
2:C:1079:ILE:HG23	2:C:1079:ILE:O	2.13	0.48
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.34	0.48
2:C:4:SER:HB3	2:C:7:GLU:OE2	2.14	0.48
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.29	0.48
3:D:198:CYS:O	3:D:202:ARG:HG3	2.12	0.48
3:D:318:GLY:O	3:D:320:ASN:N	2.46	0.48
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.96	0.48
1:G:67:GLU:HG3	1:G:171:LEU:HG	1.94	0.48
1:H:112:ALA:HB2	1:H:128:HIS:HB3	1.94	0.48
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.94	0.48
2:I:143:ARG:HH21	2:I:512:SER:C	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:15:PHE:CE1	2:I:1151:LEU:HD13	2.48	0.48
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.95	0.48
3:J:79:LYS:HG3	3:J:80:HIS:N	2.28	0.48
5:L:299:LYS:O	5:L:303:ILE:HG12	2.13	0.48
5:L:555:GLU:OE2	5:L:597:LYS:NZ	2.39	0.48
1:A:283:GLN:O	1:A:315:GLY:HA2	2.14	0.48
2:C:1283:ALA:HB1	3:D:479:GLU:OE2	2.13	0.48
2:C:139:ASN:O	2:C:141:THR:N	2.46	0.48
2:C:185:ASP:O	2:C:196:VAL:HA	2.14	0.48
2:C:285:ILE:HD11	2:C:287:VAL:HG12	1.95	0.48
2:C:557:ARG:NH2	2:C:608:ALA:HA	2.28	0.48
4:E:53:GLU:OE1	4:E:59:ILE:HG13	2.14	0.48
5:F:532:LEU:HD12	5:F:532:LEU:H	1.79	0.48
1:G:105:SER:HB2	1:G:138:ALA:O	2.12	0.48
1:G:91:ARG:HG3	1:G:122:GLU:HB3	1.95	0.48
1:H:179:PRO:HA	1:H:208:ASN:HD21	1.78	0.48
2:I:801:ARG:HD3	2:I:1094:VAL:HA	1.96	0.48
2:I:137:VAL:HA	2:I:141:THR:O	2.13	0.48
2:I:786:GLY:N	2:I:789:THR:OG1	2.46	0.48
3:J:395:LYS:O	3:J:398:LYS:HB3	2.14	0.48
3:J:45:ASN:O	3:J:46:TYR:CD2	2.66	0.48
3:J:613:GLY:O	3:J:617:THR:OG1	2.27	0.48
3:J:293:ARG:NH1	5:L:104:GLU:OE2	2.46	0.48
5:L:456:MET:O	5:L:459:THR:HB	2.13	0.48
1:B:152:TYR:HE1	1:B:176:CYS:HB3	1.79	0.48
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.14	0.48
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.25	0.48
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.34	0.48
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.94	0.48
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.77	0.48
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.95	0.48
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.94	0.48
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.28	0.48
1:B:211:ILE:HD11	1:B:215:GLU:OE2	2.13	0.48
2:C:20:GLN:O	2:C:20:GLN:HG3	2.14	0.48
2:C:325:LEU:O	2:C:328:SER:OG	2.31	0.48
2:I:132:ASP:N	2:I:132:ASP:OD1	2.38	0.48
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.48	0.48
2:I:629:PHE:CE2	2:I:634:VAL:HG11	2.49	0.48
2:I:658:GLN:NE2	2:I:1186:VAL:H	2.11	0.48
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.95	0.48

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:TRP:O	3:D:580:TRP:CG	2.67	0.48
5:F:489:MET:O	5:F:491:GLU:HB3	2.14	0.48
1:G:10:LYS:HE2	1:H:229:GLU:OE1	2.14	0.48
1:G:64:VAL:CG1	1:G:69:SER:HB2	2.44	0.48
2:I:195:PHE:CD1	2:I:205:PRO:HA	2.49	0.48
2:I:685:MET:HA	2:I:688:GLN:HE21	1.78	0.48
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.49	0.48
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.96	0.48
5:L:137:TYR:CE2	5:L:273:MET:HG2	2.49	0.48
1:B:108:GLY:O	1:B:133:LEU:HB2	2.13	0.48
2:C:108:GLU:OE1	2:C:108:GLU:HA	2.13	0.48
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.29	0.48
2:C:805:MET:O	2:C:805:MET:HG3	2.14	0.48
1:B:196:THR:HG23	3:D:443:GLU:CD	2.35	0.48
3:D:706:VAL:HG12	3:D:715:LYS:CB	2.44	0.48
5:F:580:PHE:C	5:F:582:VAL:H	2.17	0.48
5:F:600:HIS:CG	5:F:601:PRO:HD2	2.48	0.48
2:I:1242:LYS:HD2	3:J:465:GLN:OE1	2.14	0.48
2:I:496:LYS:HB3	2:I:497:PRO:HD3	1.96	0.48
3:J:1265:THR:HG22	3:J:1277:GLY:HA2	1.96	0.48
3:J:161:THR:HG22	3:J:164:GLN:CD	2.34	0.48
3:J:544:LEU:O	3:J:575:GLY:N	2.47	0.48
5:L:157:ARG:NH2	5:L:159:SER:OG	2.47	0.48
5:L:343:LYS:HA	5:L:346:GLN:HB3	1.95	0.48
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.48	0.47
2:C:1176:LEU:HD23	2:C:1176:LEU:HA	1.38	0.47
2:C:1341:ASP:HB3	3:D:18:ASP:OD2	2.14	0.47
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.95	0.47
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.47	0.47
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.44	0.47
5:F:453:PRO:O	5:F:456:MET:HB2	2.14	0.47
2:I:169:LYS:O	2:I:170:VAL:HG22	2.14	0.47
2:I:213:LEU:HD23	2:I:213:LEU:HA	1.56	0.47
2:I:4:SER:H	2:I:7:GLU:CD	2.17	0.47
3:J:239:LEU:HA	3:J:239:LEU:HD23	1.60	0.47
3:J:742:GLY:O	3:J:762:ASN:HB3	2.14	0.47
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.28	0.47
5:L:598:LEU:O	5:L:604:SER:OG	2.31	0.47
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.73	0.47
2:C:590:PRO:HG3	2:C:605:TYR:CE2	2.49	0.47
2:C:41:GLN:NE2	2:C:73:TYR:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:SER:HB3	2:C:7:GLU:CD	2.34	0.47
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.94	0.47
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.96	0.47
2:C:123:TYR:HB3	5:F:472:GLN:HB2	1.96	0.47
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.13	0.47
2:I:379:GLU:H	2:I:379:GLU:CD	2.15	0.47
2:I:151:ARG:HE	2:I:445:ILE:HD11	1.78	0.47
2:I:494:ASN:HD22	2:I:497:PRO:CD	2.28	0.47
2:I:658:GLN:O	2:I:660:VAL:N	2.47	0.47
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.95	0.47
3:J:598:LYS:N	3:J:728:SER:O	2.33	0.47
2:C:29:SER:O	2:C:30:ILE:C	2.52	0.47
2:C:619:ALA:HA	2:C:654:ASP:HB2	1.96	0.47
2:C:811:ASN:HA	2:C:815:SER:HB2	1.94	0.47
1:G:19:VAL:HG12	1:G:20:SER:N	2.27	0.47
2:I:1085:MET:CB	2:I:1093:PRO:HB3	2.43	0.47
2:I:367:TYR:HD1	2:I:384:LEU:HD22	1.78	0.47
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.96	0.47
3:J:1356:LEU:O	3:J:1366:HIS:CE1	2.67	0.47
5:L:515:GLU:HG2	5:L:516:ASP:N	2.29	0.47
1:B:101:THR:HG22	1:B:116:THR:HB	1.97	0.47
2:C:302:ILE:O	2:C:330:HIS:NE2	2.36	0.47
2:C:486:THR:HG23	2:C:487:LEU:H	1.79	0.47
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.96	0.47
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.73	0.47
2:I:517:GLN:CD	2:I:688:GLN:HA	2.34	0.47
2:I:785:ASP:HB3	2:I:789:THR:OG1	2.14	0.47
3:J:1226:VAL:O	3:J:1230:THR:HG22	2.14	0.47
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.49	0.47
3:J:770:LEU:O	3:J:774:ILE:HG13	2.15	0.47
2:C:129:LEU:HA	2:C:129:LEU:HD23	1.64	0.47
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.49	0.47
2:C:623:LEU:HA	2:C:630:VAL:HG23	1.96	0.47
2:C:681:MET:O	2:C:685:MET:HE2	2.15	0.47
2:C:821:ARG:HG3	2:C:825:GLU:OE1	2.15	0.47
1:G:97:GLU:HB3	1:G:147:GLN:HA	1.97	0.47
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.96	0.47
1:H:197:ASP:C	1:H:198:LEU:HD22	2.34	0.47
2:I:74:ARG:NH1	2:I:121:GLU:OE2	2.46	0.47
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.96	0.47
2:I:692:THR:OG1	2:I:693:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:720:ARG:HH21	2:I:736:VAL:HG11	1.79	0.47
3:J:299:LEU:O	3:J:300:GLN:C	2.53	0.47
3:J:658:GLU:O	3:J:661:VAL:HG13	2.14	0.47
3:J:884:SER:OG	3:J:885:VAL:N	2.48	0.47
1:A:233:ASP:O	1:A:234:LEU:HD22	2.14	0.47
1:A:307:LEU:HA	1:A:307:LEU:HD23	1.53	0.47
2:C:1142:ARG:CD	2:C:1161:LEU:HD11	2.31	0.47
2:C:1252:SER:HB3	2:C:1255:THR:O	2.14	0.47
2:C:250:THR:HA	2:C:268:ARG:HA	1.97	0.47
2:C:650:VAL:HG23	2:C:650:VAL:O	2.14	0.47
3:D:1146:GLU:HA	3:D:1146:GLU:OE2	2.15	0.47
3:D:1221:LEU:O	3:D:1221:LEU:HD22	2.15	0.47
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.62	0.47
3:D:40:LYS:HB2	3:D:54:ASP:O	2.14	0.47
3:D:744:ARG:HG3	3:D:744:ARG:O	2.15	0.47
3:D:739:GLN:OE1	3:D:744:ARG:NE	2.48	0.47
5:F:112:THR:OG1	5:F:114:GLU:HG3	2.14	0.47
2:I:13:LYS:O	2:I:1183:ALA:N	2.31	0.47
2:I:197:ARG:NH1	2:I:201:ARG:O	2.45	0.47
2:I:557:ARG:NE	2:I:587:LEU:O	2.41	0.47
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.97	0.47
3:J:1286:LYS:HD2	3:J:1290:ARG:HH21	1.78	0.47
2:I:902:LEU:HD21	5:L:611:LEU:HG	1.95	0.47
1:A:246:LYS:HB2	1:A:248:GLU:OE2	2.15	0.47
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.50	0.47
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.29	0.47
3:D:35:PHE:CE1	3:D:101:ARG:HD3	2.50	0.47
3:D:1181:ASP:CB	3:J:202:ARG:HD3	2.45	0.47
5:F:372:ALA:O	5:F:376:LYS:HG3	2.14	0.47
2:I:835:GLU:OE2	2:I:1051:LYS:HD3	2.14	0.47
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.29	0.47
5:L:390:ILE:HD11	5:L:432:THR:HG23	1.97	0.47
5:L:463:LEU:HA	5:L:463:LEU:HD23	1.68	0.47
5:L:489:MET:CE	5:L:493:LYS:HD2	2.44	0.47
5:L:603:ARG:CZ	5:L:603:ARG:HA	2.44	0.47
2:C:1120:ALA:HB1	2:C:1198:LEU:HD13	1.96	0.47
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.14	0.47
3:D:238:ILE:HG23	3:D:238:ILE:HD12	1.67	0.47
3:D:273:ILE:O	3:D:274:ASN:C	2.52	0.47
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.96	0.47
3:D:648:GLU:OE2	3:D:649:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:163:THR:O	5:F:260:ARG:NH2	2.48	0.47
5:F:276:MET:O	5:F:279:ARG:HB2	2.14	0.47
5:F:513:ASP:C	5:F:515:GLU:H	2.17	0.47
1:G:37:HIS:HB3	1:H:45:ARG:NH1	2.30	0.47
2:I:242:VAL:HG21	2:I:245:ARG:NH1	2.30	0.47
2:I:344:GLY:O	2:I:346:TYR:CG	2.68	0.47
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.29	0.47
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.97	0.47
3:J:895:CYS:O	3:J:898:CYS:N	2.43	0.47
1:A:102:LEU:HD22	1:A:103:ASN:N	2.30	0.47
1:A:27:THR:HA	1:A:201:LEU:O	2.14	0.47
1:A:284:ARG:HG3	1:A:288:GLU:OE1	2.15	0.47
2:C:1023:HIS:O	2:C:1027:LYS:HG2	2.14	0.47
5:F:379:MET:HG2	5:F:416:VAL:CG2	2.45	0.47
3:D:46:TYR:CD1	5:F:452:ILE:HG22	2.50	0.47
5:F:548:LEU:O	5:F:556:ALA:HB2	2.14	0.47
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.35	0.47
2:I:221:LEU:HD23	2:I:221:LEU:HA	1.63	0.47
2:I:854:ILE:O	2:I:857:VAL:HG22	2.15	0.47
1:G:66:HIS:HE1	2:I:874:GLY:HA2	1.76	0.47
3:J:1280:VAL:HG11	3:J:1304:ARG:CZ	2.44	0.47
3:J:128:LEU:HA	3:J:192:MET:HE1	1.96	0.47
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.95	0.47
3:J:495:ASN:O	3:J:497:GLU:N	2.48	0.47
3:J:647:PRO:HG3	3:J:697:MET:CB	2.40	0.47
1:A:28:LEU:N	1:A:28:LEU:CD1	2.72	0.47
1:B:109:PRO:HA	1:B:132:HIS:HA	1.97	0.47
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.50	0.47
3:D:279:LEU:C	3:D:279:LEU:HD23	2.35	0.47
3:D:810:THR:HG21	3:D:893:GLY:HA3	1.97	0.47
2:I:1309:VAL:HA	3:J:383:GLY:HA3	1.97	0.47
3:J:287:ALA:HB1	3:J:288:PRO:HD2	1.95	0.47
3:J:316:ILE:HA	3:J:323:PRO:HA	1.96	0.47
3:J:915:ILE:O	3:J:919:ALA:N	2.45	0.47
2:C:53:PHE:CD1	2:C:468:LEU:HD11	2.49	0.47
2:C:496:LYS:HE3	2:C:497:PRO:HD3	1.97	0.47
2:C:696:ASP:O	2:C:697:LYS:HB3	2.15	0.47
3:D:109:SER:O	3:D:110:PRO:C	2.52	0.47
3:D:238:ILE:HA	3:D:238:ILE:HD13	1.38	0.47
3:D:37:GLU:O	3:D:61:ILE:HD11	2.14	0.47
1:H:18:GLN:NE2	1:H:20:SER:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:185:ASP:HB2	2:I:197:ARG:O	2.15	0.47
2:I:62:TYR:O	2:I:64:GLY:N	2.47	0.47
2:I:753:LEU:HD21	2:I:784:ALA:CB	2.45	0.47
2:I:81:ASP:O	2:I:85:CYS:HB2	2.15	0.47
5:L:306:PHE:HE1	5:L:315:TRP:CH2	2.33	0.47
1:A:12:ARG:NH1	1:A:13:LEU:HD21	2.29	0.46
1:A:316:MET:CB	5:F:600:HIS:CE1	2.98	0.46
2:C:28:LEU:HA	2:C:28:LEU:HD23	1.40	0.46
2:C:356:THR:HG21	2:C:362:ALA:HA	1.97	0.46
3:D:1237:VAL:CG1	3:D:1253:ILE:HD13	2.46	0.46
3:D:768:ASN:OD1	3:D:771:GLN:OE1	2.33	0.46
2:I:1059:ARG:O	2:I:1234:LYS:NZ	2.43	0.46
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.97	0.46
2:I:44:GLU:HA	2:I:54:ARG:NH1	2.30	0.46
3:J:850:LYS:HB3	3:J:851:PRO:HD2	1.98	0.46
1:B:104:LYS:HG2	1:B:114:ASP:CG	2.36	0.46
1:B:188:GLU:O	1:B:200:LYS:N	2.29	0.46
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.97	0.46
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.50	0.46
2:C:169:LYS:O	2:C:170:VAL:HG22	2.15	0.46
2:C:239:MET:O	2:C:284:LEU:HD12	2.15	0.46
2:C:300:ASP:OD1	2:C:313:ALA:N	2.48	0.46
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.98	0.46
2:C:484:LEU:HD12	2:C:485:ASP:H	1.80	0.46
3:D:112:ALA:HA	3:D:238:ILE:CD1	2.46	0.46
3:D:318:GLY:C	3:D:320:ASN:H	2.18	0.46
3:D:519:ASN:OD1	3:D:709:ARG:NH1	2.48	0.46
1:H:110:VAL:HG23	1:H:131:CYS:O	2.15	0.46
1:H:155:ALA:N	1:H:174:ASP:OD1	2.43	0.46
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.57	0.46
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.96	0.46
3:J:1234:VAL:HG23	3:J:1235:ASN:N	2.30	0.46
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.80	0.46
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.16	0.46
3:J:654:ILE:O	3:J:658:GLU:HB2	2.15	0.46
3:J:804:ALA:O	3:J:806:ASP:N	2.48	0.46
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.96	0.46
1:A:14:VAL:HG22	1:A:15:ASP:N	2.26	0.46
1:A:179:PRO:HB3	1:A:211:ILE:HB	1.96	0.46
1:A:255:ARG:HB2	1:A:278:ILE:HD12	1.98	0.46
1:A:16:ILE:CG2	1:A:26:VAL:HG12	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLU:HG3	1:B:150:ARG:NE	2.26	0.46
1:A:50:SER:HB2	1:B:8:PHE:HZ	1.79	0.46
2:C:1009:ASN:O	2:C:1012:GLU:HB3	2.16	0.46
2:C:1136:GLN:NE2	2:C:1140:LYS:NZ	2.64	0.46
1:H:220:ALA:HA	1:H:223:ILE:HD12	1.97	0.46
2:I:517:GLN:O	2:I:517:GLN:HG2	2.14	0.46
2:I:617:ALA:N	2:I:652:TYR:O	2.30	0.46
2:I:657:THR:HG23	2:I:658:GLN:HG3	1.97	0.46
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.97	0.46
2:I:891:GLY:C	2:I:892:GLU:HG3	2.35	0.46
3:J:117:LEU:HA	3:J:117:LEU:HD12	1.44	0.46
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.30	0.46
3:J:521:LYS:HE3	3:J:541:LEU:O	2.15	0.46
3:J:647:PRO:CD	3:J:697:MET:HB3	2.45	0.46
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.80	0.46
1:A:77:ASP:O	1:A:80:GLU:N	2.48	0.46
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.31	0.46
2:C:128:PRO:HG2	2:C:506:PHE:CD1	2.50	0.46
2:C:705:GLU:HB2	2:C:794:LEU:N	2.27	0.46
2:C:953:LEU:HD12	2:C:953:LEU:HA	1.52	0.46
3:D:45:ASN:O	3:D:46:TYR:CB	2.63	0.46
1:G:166:ARG:N	1:G:167:PRO:HD2	2.30	0.46
1:G:98:VAL:HG22	1:G:99:ILE:H	1.79	0.46
2:I:1131:MET:CE	2:I:1141:LEU:HD12	2.46	0.46
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.14	0.46
2:I:607:SER:OG	2:I:609:ILE:HG13	2.15	0.46
2:I:653:MET:HG2	2:I:654:ASP:N	2.30	0.46
2:I:830:THR:HG22	2:I:1058:ARG:O	2.15	0.46
3:J:746:LEU:CD2	3:J:758:PRO:HG3	2.45	0.46
5:L:296:LYS:HD3	5:L:296:LYS:HA	1.71	0.46
1:B:118:ASP:HB2	1:B:121:VAL:CG2	2.46	0.46
2:C:131:THR:HG21	2:C:135:THR:OG1	2.15	0.46
2:C:247:ARG:HB2	2:C:274:ILE:CD1	2.45	0.46
2:C:262:TYR:HE1	2:C:280:ASP:OD2	1.98	0.46
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.98	0.46
3:D:721:SER:HA	3:D:724:MET:CE	2.45	0.46
5:F:253:SER:O	5:F:257:LYS:N	2.47	0.46
5:F:466:ILE:HG22	5:F:470:MET:HG3	1.97	0.46
1:H:22:THR:OG1	1:H:207:THR:O	2.33	0.46
3:J:914:ALA:O	3:J:918:ILE:HG23	2.15	0.46
5:L:316:PHE:O	5:L:320:ILE:HG13	2.16	0.46

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLN:HG3	1:A:76:GLU:OE2	2.16	0.45
2:C:864:LYS:HZ3	2:C:881:ASP:CG	2.20	0.45
2:C:896:THR:HB	2:C:897:PRO:HD2	1.96	0.45
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.98	0.45
3:D:859:PRO:HG2	3:D:862:THR:HG21	1.98	0.45
4:E:40:PRO:O	4:E:52:ARG:NH2	2.49	0.45
1:G:187:VAL:HG22	1:G:201:LEU:HD13	1.98	0.45
1:H:99:ILE:HA	1:H:144:ILE:O	2.17	0.45
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	1.98	0.45
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.97	0.45
2:I:886:LYS:O	2:I:916:SER:N	2.48	0.45
3:J:886:VAL:HA	3:J:1258:ARG:HB2	1.98	0.45
3:J:1297:LYS:NZ	3:J:1299:GLY:HA3	2.30	0.45
3:J:165:TYR:CE2	3:J:169:LEU:HD12	2.51	0.45
3:J:147:ILE:HD11	3:J:179:LYS:NZ	2.31	0.45
3:J:899:TYR:O	3:J:1251:LYS:HD3	2.16	0.45
4:K:26:ARG:NH2	4:K:36:ASP:O	2.49	0.45
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.63	0.45
5:L:532:LEU:H	5:L:532:LEU:HD12	1.81	0.45
2:C:120:GLN:CG	2:C:121:GLU:HG3	2.36	0.45
2:C:273:HIS:HA	2:C:276:GLN:OE1	2.15	0.45
2:C:448:LEU:HA	2:C:448:LEU:HD23	1.75	0.45
2:C:883:LEU:HA	2:C:883:LEU:HD23	1.73	0.45
3:D:796:LEU:HG	3:D:800:LEU:HD22	1.99	0.45
1:H:149:GLY:HA3	1:H:177:TYR:CD2	2.51	0.45
2:I:1012:GLU:HG3	2:I:1016:GLU:OE2	2.16	0.45
2:I:97:ARG:HB3	2:I:121:GLU:CB	2.46	0.45
2:I:598:VAL:HG13	2:I:628:HIS:CE1	2.51	0.45
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.50	0.45
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.98	0.45
3:J:381:ILE:HG21	3:J:401:VAL:HG11	1.97	0.45
3:J:349:TYR:CE1	3:J:472:LEU:HD11	2.51	0.45
5:L:297:MET:HG2	5:L:298:PRO:N	2.31	0.45
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.98	0.45
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.52	0.45
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.40	0.45
2:C:74:ARG:O	2:C:96:LEU:HD12	2.16	0.45
1:A:261:GLU:OE2	2:C:859:GLU:HB2	2.17	0.45
3:D:1258:ARG:NH2	3:D:1281:GLU:OE1	2.48	0.45
3:D:112:ALA:HB3	3:D:300:GLN:NE2	2.31	0.45
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:689:ALA:O	3:D:692:ARG:HB2	2.16	0.45
3:D:875:ASN:OD1	3:D:875:ASN:N	2.49	0.45
2:I:504:GLU:OE2	2:I:508:SER:HB2	2.16	0.45
2:I:538:LEU:HA	2:I:542:ARG:NE	2.31	0.45
2:I:758:ARG:HH22	2:I:761:GLN:HE21	1.63	0.45
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.97	0.45
1:B:152:TYR:CE1	1:B:176:CYS:HB3	2.52	0.45
2:C:400:VAL:H	2:C:400:VAL:HG23	1.46	0.45
2:C:720:ARG:NH2	2:C:736:VAL:HG21	2.31	0.45
3:D:1356:LEU:HA	3:D:1356:LEU:HD23	1.40	0.45
3:D:184:ALA:O	3:D:187:ALA:HB3	2.17	0.45
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.42	0.45
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.98	0.45
1:G:226:GLU:CD	1:H:10:LYS:HE2	2.37	0.45
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.58	0.45
2:I:228:VAL:HG22	2:I:245:ARG:HE	1.80	0.45
2:I:397:LEU:H	2:I:397:LEU:HD12	1.81	0.45
2:I:62:TYR:C	2:I:64:GLY:H	2.19	0.45
2:I:798:GLN:OE1	2:I:828:PHE:HD1	1.99	0.45
1:G:152:TYR:CD2	2:I:824:GLN:HG2	2.52	0.45
3:J:1262:ARG:HD2	3:J:1279:GLN:HE22	1.81	0.45
2:I:1281:TYR:OH	3:J:431:ARG:O	2.33	0.45
5:L:143:TYR:OH	5:L:265:GLN:OE1	2.12	0.45
5:L:357:GLN:HG3	5:L:357:GLN:H	1.52	0.45
5:L:470:MET:HA	5:L:473:GLU:HB3	1.98	0.45
5:L:577:GLY:O	5:L:581:ASP:N	2.50	0.45
1:A:224:LEU:C	1:A:224:LEU:HD23	2.36	0.45
1:A:233:ASP:O	1:A:234:LEU:HD13	2.17	0.45
1:B:84:ASN:ND2	1:B:129:VAL:O	2.45	0.45
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.50	0.45
2:C:1160:ASP:CG	2:C:1161:LEU:N	2.67	0.45
2:C:5:TYR:CZ	2:C:776:PRO:HB2	2.51	0.45
2:C:891:GLY:C	2:C:892:GLU:HG3	2.37	0.45
3:D:1140:ARG:NH2	3:D:1144:LEU:HD21	2.31	0.45
3:D:127:LEU:HA	3:D:127:LEU:HD12	1.46	0.45
3:D:282:LEU:HA	3:D:282:LEU:HD23	1.52	0.45
1:H:105:SER:HB3	1:H:137:ASN:O	2.17	0.45
1:H:60:GLU:OE2	1:H:143:ARG:NH1	2.50	0.45
2:I:952:GLN:OE1	2:I:1036:ILE:HG23	2.16	0.45
3:J:585:LYS:HA	3:J:585:LYS:HD3	1.68	0.45
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:419:PHE:CD1	5:L:430:TYR:CD2	3.05	0.45
5:L:533:ASP:O	5:L:536:THR:N	2.49	0.45
1:A:197:ASP:O	1:A:198:LEU:HD23	2.17	0.45
2:C:1035:LYS:O	2:C:1038:GLN:HG2	2.17	0.45
2:C:388:LEU:HA	2:C:388:LEU:HD23	1.72	0.45
2:C:5:TYR:HD1	2:C:8:LYS:HD3	1.82	0.45
3:D:107:LEU:HD22	3:D:299:LEU:HD21	1.98	0.45
3:D:285:LEU:N	3:D:285:LEU:HD12	2.32	0.45
3:D:471:PRO:HG2	3:D:471:PRO:O	2.16	0.45
3:D:528:THR:HG22	3:D:532:GLU:CD	2.37	0.45
3:D:846:GLU:HA	3:D:860:ARG:HD3	1.97	0.45
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.16	0.45
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.81	0.45
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.17	0.45
1:G:154:PRO:HB3	2:I:1059:ARG:NH2	2.32	0.45
2:I:1068:GLY:HA3	2:I:1072:ASN:HD21	1.82	0.45
2:I:1212:LEU:O	2:I:1221:PHE:N	2.46	0.45
2:I:697:LYS:HB3	2:I:697:LYS:HE2	1.79	0.45
3:J:549:LYS:HE2	3:J:571:ASP:OD2	2.17	0.45
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.98	0.45
5:L:390:ILE:HG21	5:L:390:ILE:HD13	1.74	0.45
2:C:1161:LEU:HD12	2:C:1161:LEU:HA	1.26	0.45
2:C:474:ALA:O	2:C:477:GLU:HB3	2.17	0.45
2:C:606:LEU:HD12	2:C:606:LEU:N	2.32	0.45
3:D:24:LEU:HA	3:D:24:LEU:HD13	1.74	0.45
3:D:605:LEU:HA	3:D:605:LEU:HD23	1.77	0.45
3:D:819:GLY:O	3:D:1227:HIS:HE1	1.99	0.45
5:F:433:TRP:O	5:F:437:GLN:HB3	2.17	0.45
2:I:1077:SER:OG	2:I:1078:LYS:N	2.50	0.45
2:I:511:LEU:HD12	2:I:511:LEU:N	2.32	0.45
2:I:886:LYS:H	2:I:917:SER:HB3	1.82	0.45
2:I:967:LEU:HA	2:I:967:LEU:HD12	1.84	0.45
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.46	0.45
3:J:215:LYS:O	3:J:218:THR:HG22	2.17	0.45
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.99	0.45
1:B:9:LEU:HB3	1:B:32:GLU:HG2	1.99	0.45
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.49	0.45
2:C:145:ILE:CG2	2:C:456:VAL:HG22	2.47	0.45
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.52	0.45
2:C:22:LEU:HD22	2:C:22:LEU:HA	1.82	0.45
3:D:154:LEU:HD12	3:D:154:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.98	0.45
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.50	0.45
3:D:740:LEU:HD12	3:D:740:LEU:HA	1.47	0.45
3:D:796:LEU:HA	3:D:796:LEU:HD12	1.61	0.45
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.98	0.45
5:F:364:ARG:HA	5:F:367:ILE:HD12	1.97	0.45
5:F:561:MET:HE3	5:F:561:MET:HB2	1.92	0.45
1:H:82:LEU:HD22	1:H:173:VAL:CG2	2.47	0.45
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.98	0.45
3:J:450:HIS:HE1	3:J:452:LEU:HG	1.82	0.45
3:J:701:LEU:HA	3:J:701:LEU:HD22	1.57	0.45
3:J:93:THR:HG22	3:J:94:GLN:N	2.31	0.45
5:L:96:ASP:O	5:L:98:VAL:N	2.49	0.45
2:C:1246:ARG:CZ	2:C:1249:GLY:H	2.30	0.45
2:C:159:SER:O	2:C:160:ASP:HB2	2.16	0.45
2:C:445:ILE:HG22	2:C:446:ASP:OD1	2.16	0.45
2:C:60:GLN:HG2	2:C:60:GLN:H	1.31	0.45
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.40	0.45
3:D:508:LEU:HA	3:D:508:LEU:HD12	1.62	0.45
3:D:544:LEU:HD12	3:D:544:LEU:HA	1.57	0.45
3:D:622:ASP:HB3	3:D:626:TYR:CE2	2.51	0.45
3:D:630:ALA:O	3:D:633:ALA:HB3	2.17	0.45
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.32	0.45
5:F:502:LYS:HE3	5:F:502:LYS:HB2	1.40	0.45
5:F:511:ILE:HG23	5:F:511:ILE:O	2.17	0.45
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.47	0.45
1:G:135:ASP:OD1	1:G:136:GLU:N	2.50	0.45
1:G:41:ASN:HD22	1:H:41:ASN:ND2	2.09	0.45
1:G:68:TYR:CE1	2:I:929:ILE:HG21	2.50	0.45
1:G:89:ALA:HB3	1:G:124:VAL:HG12	1.99	0.45
2:I:968:GLU:CG	2:I:1018:TYR:HE1	2.29	0.45
3:J:1337:VAL:HG23	3:J:1338:ALA:N	2.32	0.45
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.49	0.45
5:L:507:MET:HG2	5:L:520:GLY:CA	2.47	0.45
1:A:132:HIS:N	1:A:132:HIS:CD2	2.84	0.45
2:C:104:ILE:HD12	2:C:115:LYS:O	2.16	0.45
2:C:325:LEU:O	2:C:330:HIS:HB2	2.17	0.45
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.51	0.45
2:C:850:ILE:HD12	2:C:850:ILE:HG23	1.54	0.45
3:D:707:ILE:N	3:D:714:GLU:O	2.48	0.45
1:G:23:HIS:ND1	1:G:206:GLU:HG2	2.31	0.45

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:227:GLN:CG	5:F:252:LEU:HA	2.48	0.44
1:H:228:LEU:HD23	1:H:228:LEU:HA	1.59	0.44
2:I:1252:SER:HB3	2:I:1255:THR:O	2.16	0.44
2:I:361:SER:O	2:I:364:VAL:HB	2.18	0.44
2:I:494:ASN:ND2	2:I:497:PRO:HD3	2.33	0.44
2:I:796:LEU:N	2:I:796:LEU:HD12	2.33	0.44
3:J:201:LEU:HD12	3:J:221:ILE:HD13	2.00	0.44
3:J:518:VAL:HG23	3:J:547:ARG:NH2	2.33	0.44
3:J:706:VAL:HG12	3:J:715:LYS:CB	2.46	0.44
3:J:805:GLN:HB3	3:J:806:ASP:H	1.61	0.44
3:J:797:THR:CG2	3:J:924:GLY:HA3	2.36	0.44
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.99	0.44
5:L:384:LEU:HA	5:L:384:LEU:HD23	1.55	0.44
1:A:137:ASN:N	1:A:137:ASN:OD1	2.51	0.43
2:C:1195:ILE:HD13	2:C:1195:ILE:HG21	1.70	0.43
2:C:1223:ARG:HD3	2:C:1223:ARG:HH11	1.67	0.43
2:C:62:TYR:C	2:C:64:GLY:N	2.71	0.43
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.51	0.43
3:D:1257:VAL:O	3:D:1260:MET:N	2.51	0.43
3:D:1332:LEU:N	3:D:1332:LEU:HD22	2.32	0.43
3:D:1344:LEU:N	3:D:1344:LEU:HD12	2.33	0.43
3:D:381:ILE:HD13	3:D:381:ILE:HG21	1.67	0.43
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.83	0.43
2:I:672:GLU:HG2	2:I:1187:PHE:HA	2.00	0.43
5:L:161:LEU:HD12	5:L:161:LEU:HA	1.68	0.43
1:A:233:ASP:C	1:A:234:LEU:HD22	2.38	0.43
1:B:181:GLU:OE2	1:B:208:ASN:HA	2.18	0.43
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.81	0.43
2:C:479:LEU:HD23	2:C:479:LEU:HA	1.73	0.43
2:C:819:SER:HB2	2:C:1085:MET:SD	2.57	0.43
2:C:987:GLU:O	2:C:991:LYS:HG3	2.18	0.43
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	2.18	0.43
3:D:1375:ALA:HB1	3:J:853:THR:HG21	2.00	0.43
3:D:266:ASN:O	3:D:267:ASP:C	2.54	0.43
3:D:733:SER:O	3:D:736:GLN:N	2.50	0.43
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.53	0.43
1:G:66:HIS:HB2	1:G:69:SER:OG	2.18	0.43
1:H:57:THR:OG1	1:H:147:GLN:HB3	2.17	0.43
2:I:1087:TYR:OH	2:I:1218:GLY:HA2	2.17	0.43
2:I:1252:SER:HB3	2:I:1257:GLN:H	1.83	0.43
2:I:1268:GLN:HG2	3:J:467:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1301:ARG:O	2:I:1304:MET:HB3	2.18	0.43
2:I:276:GLN:O	2:I:280:ASP:N	2.43	0.43
2:I:409:LEU:HD13	2:I:427:ASP:HB3	2.00	0.43
3:J:1206:ARG:NH2	3:J:1223:LEU:HD13	2.34	0.43
3:J:265:LEU:HD23	3:J:265:LEU:HA	1.67	0.43
5:L:251:LYS:HA	5:L:254:GLU:HG2	1.99	0.43
5:L:281:ARG:HA	5:L:284:GLU:OE1	2.18	0.43
1:B:44:ARG:HG3	1:B:183:ILE:HB	2.00	0.43
2:C:1312:ASN:HD21	2:C:1314:GLN:HG3	1.83	0.43
2:C:208:ILE:O	2:C:362:ALA:HB1	2.19	0.43
2:C:571:LEU:HD23	2:C:571:LEU:HA	1.66	0.43
3:D:293:ARG:O	3:D:294:ASN:C	2.57	0.43
3:D:474:LEU:HA	3:D:474:LEU:HD12	1.60	0.43
3:D:500:ILE:O	3:D:500:ILE:HG22	2.17	0.43
1:G:133:LEU:HA	1:G:133:LEU:HD13	1.79	0.43
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.18	0.43
2:I:22:LEU:HD13	2:I:23:ASP:N	2.34	0.43
2:I:387:ASN:O	2:I:394:ARG:HB2	2.19	0.43
2:I:640:GLY:O	2:I:641:GLU:HG3	2.18	0.43
3:J:1290:ARG:HD3	3:J:1290:ARG:HA	1.78	0.43
3:J:1357:ILE:O	3:J:1359:ALA:N	2.47	0.43
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.18	0.43
1:B:100:LEU:O	1:B:143:ARG:HA	2.18	0.43
3:D:1248:ILE:HD13	3:D:1248:ILE:HG21	1.75	0.43
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.33	0.43
3:D:255:LEU:N	3:D:259:ARG:O	2.48	0.43
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.83	0.43
3:D:795:TYR:HE2	3:D:799:ARG:NE	2.15	0.43
3:D:891:ASP:CA	3:D:1281:GLU:HG3	2.47	0.43
3:D:910:ASN:ND2	4:E:15:ASN:O	2.50	0.43
5:F:552:THR:H	5:F:552:THR:HG23	1.59	0.43
2:I:1287:LEU:O	2:I:1290:MET:N	2.51	0.43
2:I:158:ASP:HB3	2:I:173:ASN:OD1	2.18	0.43
2:I:538:LEU:HA	2:I:542:ARG:NH2	2.33	0.43
2:I:811:ASN:N	2:I:811:ASN:OD1	2.46	0.43
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.81	0.43
3:J:1257:VAL:O	3:J:1260:MET:N	2.51	0.43
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.00	0.43
3:J:75:TYR:CD2	3:J:83:VAL:HG21	2.54	0.43
5:L:502:LYS:HE3	5:L:502:LYS:HB2	1.32	0.43
2:C:819:SER:HB2	2:C:1085:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.18	0.43
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.59	0.43
2:C:1196:LYS:CD	2:C:1206:THR:HG23	2.29	0.43
3:D:306:LEU:O	3:D:326:SER:HB2	2.18	0.43
3:D:541:LEU:HD23	3:D:541:LEU:HA	1.44	0.43
5:F:306:PHE:CE1	5:F:315:TRP:CD2	3.00	0.43
1:G:59:VAL:HG13	1:G:143:ARG:O	2.19	0.43
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.81	0.43
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.53	0.43
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.99	0.43
3:J:41:PRO:HB3	3:J:270:ARG:HG3	2.00	0.43
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.43	0.43
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.44	0.43
5:L:611:LEU:HD23	5:L:611:LEU:HA	1.56	0.43
2:C:1101:LEU:HA	2:C:1101:LEU:HD23	1.58	0.43
2:C:1137:GLU:HG2	2:C:1140:LYS:CG	2.49	0.43
2:C:756:TYR:CD1	2:C:756:TYR:N	2.86	0.43
3:D:1237:VAL:HG11	3:D:1253:ILE:HD13	2.00	0.43
3:D:813:ASP:HA	3:D:897:HIS:HB2	2.01	0.43
3:D:97:VAL:HG12	3:D:101:ARG:CG	2.45	0.43
5:F:103:ARG:HH11	5:F:103:ARG:HD3	1.64	0.43
1:G:47:LEU:O	1:G:180:VAL:HG11	2.19	0.43
2:I:1176:LEU:HD22	2:I:1181:PRO:HD2	2.00	0.43
3:J:118:LYS:HD2	3:J:118:LYS:HA	1.62	0.43
3:J:189:LEU:HD23	3:J:189:LEU:HA	1.77	0.43
3:J:102:MET:CE	3:J:246:PRO:HD3	2.47	0.43
2:C:1239:VAL:HG13	2:C:1240:ASP:N	2.33	0.43
2:C:409:LEU:HA	2:C:409:LEU:HD23	1.65	0.43
2:C:88:ARG:HG2	2:C:90:VAL:CG2	2.49	0.43
2:C:992:LEU:HG	2:C:997:TRP:HE1	1.84	0.43
3:D:108:ALA:CB	3:D:279:LEU:HD22	2.49	0.43
3:D:108:ALA:HB3	3:D:279:LEU:HD22	1.99	0.43
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.65	0.43
3:D:647:PRO:HG3	3:D:697:MET:CB	2.47	0.43
3:D:717:VAL:H	3:D:717:VAL:HG22	1.54	0.43
3:D:755:ILE:HG22	3:D:757:THR:H	1.83	0.43
5:F:593:LYS:O	5:F:597:LYS:N	2.50	0.43
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.99	0.43
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.53	0.43
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.18	0.43
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:705:GLU:HB2	2:I:794:LEU:H	1.83	0.43
3:J:299:LEU:O	3:J:302:ALA:N	2.51	0.43
1:A:92:VAL:HA	1:A:120:ASP:O	2.18	0.43
1:A:176:CYS:O	1:A:177:TYR:C	2.57	0.43
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.75	0.43
2:C:544:GLY:O	2:C:548:ARG:HG3	2.19	0.43
2:C:551:HIS:CE1	2:C:553:THR:HG23	2.53	0.43
2:C:830:THR:HG22	2:C:1058:ARG:O	2.19	0.43
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.48	0.43
1:G:219:ARG:HD3	1:G:219:ARG:HH11	1.67	0.43
1:H:83:LEU:HD12	1:H:86:LYS:HE2	2.01	0.43
2:I:818:VAL:O	2:I:1079:ILE:HA	2.19	0.43
2:I:159:SER:O	2:I:171:LEU:O	2.37	0.43
3:J:1140:ARG:HH21	3:J:1236:GLU:CG	2.22	0.43
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.35	0.43
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.99	0.43
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.49	0.43
5:L:576:VAL:HG12	5:L:587:ILE:CD1	2.49	0.43
1:A:102:LEU:HD23	1:A:115:ILE:HA	2.01	0.43
1:A:196:THR:OG1	1:A:197:ASP:N	2.50	0.43
1:A:320:ASN:O	1:A:323:PRO:HD3	2.18	0.43
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.64	0.43
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.18	0.43
2:C:469:VAL:O	2:C:472:GLU:HB3	2.18	0.43
2:C:760:ASN:O	2:C:761:GLN:O	2.37	0.43
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	2.00	0.43
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.52	0.43
3:D:411:ILE:HG23	3:D:411:ILE:HD12	1.69	0.43
5:F:503:GLU:CG	5:F:504:PRO:HD2	2.48	0.43
1:G:152:TYR:CE2	2:I:824:GLN:HG2	2.54	0.43
2:I:1053:TYR:N	2:I:1053:TYR:CD1	2.87	0.43
2:I:1211:ARG:HB2	2:I:1220:GLN:HE21	1.83	0.43
2:I:518:ASN:O	2:I:519:ASN:HB3	2.18	0.43
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.54	0.43
3:J:343:LEU:HA	3:J:343:LEU:HD12	1.80	0.43
5:L:295:CYS:CB	5:L:330:LEU:HD23	2.49	0.43
5:L:312:SER:OG	5:L:313:ASP:N	2.51	0.43
1:A:118:ASP:HB3	1:A:121:VAL:CG2	2.45	0.43
1:A:225:ALA:HA	1:A:228:LEU:HD12	2.00	0.43
1:A:92:VAL:HA	1:A:120:ASP:HB3	2.00	0.43
2:C:1042:LEU:HD13	2:C:1046:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:517:GLN:O	2:C:517:GLN:HG2	2.16	0.43
2:C:979:LEU:HD12	2:C:979:LEU:HA	1.72	0.43
3:D:135:ILE:HG21	3:D:135:ILE:HD13	1.65	0.43
3:D:352:ARG:HB3	3:D:467:ALA:HA	2.01	0.43
3:D:748:ALA:HA	3:D:754:ILE:HA	2.00	0.43
3:D:848:VAL:HG23	3:D:858:VAL:HG13	2.01	0.43
3:D:905:ARG:HH12	4:E:10:VAL:HG11	1.82	0.43
3:D:908:ILE:HD13	3:D:909:ILE:N	2.34	0.43
5:F:512:GLY:C	5:F:514:ASP:N	2.71	0.43
5:F:601:PRO:HA	5:F:604:SER:H	1.84	0.43
1:G:50:SER:HG	1:H:35:PHE:HZ	1.67	0.43
1:G:52:PRO:HG2	1:G:219:ARG:NE	2.29	0.43
1:H:82:LEU:HA	1:H:85:LEU:HD12	2.00	0.43
2:I:1262:LYS:HD3	2:I:1262:LYS:HA	1.83	0.43
2:I:1334:GLY:O	3:J:25:ALA:CB	2.66	0.43
2:I:1331:ARG:HA	2:I:1335:ILE:O	2.19	0.43
2:I:149:LEU:HA	2:I:149:LEU:HD12	1.62	0.43
2:I:403:MET:SD	2:I:403:MET:C	2.98	0.43
2:I:705:GLU:CD	2:I:705:GLU:H	2.20	0.43
3:D:1292:LEU:HA	3:J:1226:VAL:HG21	2.01	0.43
3:J:1257:VAL:O	3:J:1258:ARG:C	2.57	0.43
3:J:1355:ARG:HB3	3:J:1355:ARG:HE	1.52	0.43
3:J:364:HIS:CE1	3:J:365:GLN:OE1	2.72	0.43
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.82	0.42
1:A:257:VAL:HG22	1:A:276:HIS:O	2.19	0.42
2:C:1209:GLN:HA	2:C:1225:VAL:O	2.19	0.42
2:C:1268:GLN:HE22	3:D:352:ARG:HH11	1.65	0.42
2:C:493:ILE:HG22	2:C:493:ILE:H	1.49	0.42
2:C:557:ARG:HH21	2:C:608:ALA:N	2.16	0.42
2:C:632:ASP:O	2:C:647:ARG:HB2	2.19	0.42
2:C:653:MET:HG2	2:C:654:ASP:N	2.34	0.42
2:C:870:ILE:HB	2:C:944:ARG:HD3	2.01	0.42
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.48	0.42
3:D:915:ILE:HG12	3:D:915:ILE:H	1.64	0.42
3:D:93:THR:HG22	3:D:94:GLN:N	2.34	0.42
5:F:290:LEU:HB3	5:F:333:VAL:HG21	2.01	0.42
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.32	0.42
2:I:1038:GLN:HG3	2:I:1038:GLN:O	2.19	0.42
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.54	0.42
2:I:518:ASN:CG	2:I:519:ASN:N	2.72	0.42
2:I:607:SER:H	2:I:610:GLU:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	2.01	0.42
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.19	0.42
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.53	0.42
3:J:495:ASN:N	3:J:495:ASN:OD1	2.52	0.42
4:K:50:ALA:O	4:K:54:ILE:HG12	2.19	0.42
5:L:123:ILE:HG21	5:L:123:ILE:HD13	1.80	0.42
5:L:341:LEU:O	5:L:344:LEU:HB3	2.19	0.42
5:L:350:GLU:H	5:L:350:GLU:HG3	1.54	0.42
5:L:354:THR:O	5:L:358:VAL:HG23	2.19	0.42
2:C:235:ASN:OD1	2:C:236:LYS:HG2	2.19	0.42
2:C:263:VAL:HG12	2:C:264:GLU:O	2.19	0.42
2:C:490:GLN:O	2:C:492:MET:N	2.52	0.42
2:C:591:TYR:CE1	2:C:616:ILE:HG21	2.54	0.42
3:D:322:ARG:CZ	3:D:322:ARG:HB2	2.48	0.42
5:F:227:GLN:NE2	5:F:251:LYS:NZ	2.66	0.42
5:F:597:LYS:O	5:F:603:ARG:HG3	2.19	0.42
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.82	0.42
1:G:13:LEU:HG	1:G:14:VAL:N	2.34	0.42
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.84	0.42
2:I:161:LYS:H	2:I:161:LYS:HG2	1.63	0.42
2:I:194:LEU:HD12	2:I:194:LEU:HA	1.80	0.42
2:I:515:MET:CG	2:I:515:MET:O	2.67	0.42
2:I:798:GLN:NE2	2:I:827:ARG:O	2.49	0.42
2:I:894:GLN:HG3	2:I:894:GLN:O	2.18	0.42
3:J:647:PRO:HG3	3:J:697:MET:N	2.34	0.42
3:J:903:LEU:HA	3:J:903:LEU:HD12	1.93	0.42
5:L:271:ASN:O	5:L:275:VAL:HG23	2.19	0.42
5:L:572:THR:HG23	5:L:575:GLU:CB	2.43	0.42
2:C:158:ASP:CG	2:C:159:SER:N	2.71	0.42
3:D:298:MET:HE1	5:F:402:LEU:O	2.19	0.42
3:D:528:THR:HG23	3:D:529:GLY:N	2.35	0.42
3:D:544:LEU:O	3:D:574:VAL:HB	2.19	0.42
3:D:647:PRO:CG	3:D:697:MET:HB3	2.50	0.42
3:D:825:VAL:HG22	3:D:833:GLU:N	2.35	0.42
5:F:560:ARG:O	5:F:563:PHE:O	2.37	0.42
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.55	0.42
2:I:643:SER:HG	2:I:645:PHE:HE1	1.68	0.42
2:I:757:THR:OG1	2:I:758:ARG:N	2.52	0.42
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.19	0.42
3:J:127:LEU:HA	3:J:127:LEU:HD12	1.47	0.42
3:J:317:THR:HG22	3:J:322:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.53	0.42
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.86	0.42
3:J:596:LEU:HD12	3:J:601:ILE:HG13	2.01	0.42
5:L:165:PHE:HD1	5:L:259:PHE:HA	1.84	0.42
1:A:187:VAL:O	1:A:187:VAL:HG23	2.20	0.42
1:A:212:ASP:HA	1:A:213:PRO:HD3	1.93	0.42
2:C:1067:ALA:HB2	2:C:1073:LYS:HA	2.00	0.42
2:C:1322:SER:OG	2:C:1323:PHE:N	2.52	0.42
3:D:707:ILE:O	3:D:714:GLU:N	2.52	0.42
5:F:463:LEU:HA	5:F:463:LEU:HD23	1.80	0.42
5:F:470:MET:HE1	5:F:486:ARG:HH12	1.83	0.42
1:G:12:ARG:HA	1:H:231:PHE:HZ	1.81	0.42
1:H:51:MET:HB3	1:H:178:SER:CB	2.50	0.42
2:I:146:VAL:HG13	2:I:529:ARG:HB3	2.01	0.42
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.85	0.42
2:I:388:LEU:HA	2:I:388:LEU:HD23	1.76	0.42
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.42
2:I:920:VAL:HG13	2:I:1054:LEU:HD21	2.01	0.42
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.18	0.42
3:J:591:ILE:HG13	3:J:604:MET:HE2	2.00	0.42
2:I:1225:VAL:HA	3:J:638:SER:CB	2.49	0.42
3:J:810:THR:HG23	3:J:811:GLU:N	2.34	0.42
1:A:51:MET:HE1	1:A:216:ALA:HB1	2.00	0.42
1:B:31:LEU:HD13	1:B:31:LEU:HA	1.85	0.42
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	2.01	0.42
2:C:1112:ILE:O	2:C:1113:LEU:C	2.56	0.42
3:D:141:PHE:CE1	3:D:181:GLY:HA3	2.54	0.42
3:D:371:LYS:O	3:D:372:MET:C	2.54	0.42
3:D:495:ASN:O	3:D:497:GLU:N	2.53	0.42
3:D:513:MET:HE1	3:D:579:LEU:HD13	2.01	0.42
5:F:121:LYS:HD3	5:F:121:LYS:HA	1.83	0.42
5:F:357:GLN:H	5:F:357:GLN:HG3	1.58	0.42
1:G:52:PRO:CG	1:G:219:ARG:HH21	2.32	0.42
2:I:1132:LEU:HB3	2:I:1177:ARG:CZ	2.49	0.42
3:J:125:GLY:O	3:J:128:LEU:N	2.52	0.42
3:J:1356:LEU:HD23	3:J:1356:LEU:HA	1.67	0.42
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.84	0.42
3:J:83:VAL:HG13	3:J:92:VAL:HG13	2.01	0.42
3:J:844:THR:HG21	3:J:858:VAL:HG21	2.00	0.42
5:L:452:ILE:HG21	5:L:452:ILE:HD13	1.69	0.42
1:A:249:PHE:CE2	1:A:254:LEU:HG	2.55	0.42

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:CG2	1:B:177:TYR:HE2	2.32	0.42
2:C:48:GLY:N	2:C:461:GLU:OE1	2.52	0.42
2:C:499:SER:O	2:C:503:LYS:HB2	2.20	0.42
2:C:680:LEU:O	2:C:681:MET:C	2.58	0.42
2:C:865:LEU:HD23	2:C:865:LEU:HA	1.70	0.42
3:D:227:PHE:CE1	3:D:234:PRO:HG3	2.54	0.42
3:D:249:LEU:HD23	3:D:249:LEU:HA	1.71	0.42
3:D:337:ARG:HB3	3:D:1324:SER:O	2.20	0.42
3:D:357:VAL:HG22	3:D:461:PHE:CD1	2.55	0.42
3:D:411:ILE:HA	3:D:411:ILE:HD13	1.78	0.42
3:D:482:ALA:C	3:D:483:LEU:HG	2.39	0.42
3:D:609:TYR:HA	3:D:617:THR:OG1	2.20	0.42
3:D:74:LYS:HD3	3:D:75:TYR:HE1	1.85	0.42
3:D:770:LEU:HA	3:D:770:LEU:HD12	1.52	0.42
5:F:127:ILE:O	5:F:128:ASN:C	2.58	0.42
2:I:819:SER:HB2	2:I:1085:MET:CG	2.49	0.42
3:J:1150:PRO:O	3:J:1153:PRO:HG3	2.20	0.42
3:J:189:LEU:HD22	3:J:234:PRO:HB3	2.02	0.42
5:L:148:TYR:CE1	5:L:158:LEU:HD21	2.55	0.42
5:L:219:GLU:O	5:L:222:ALA:HB3	2.19	0.42
5:L:261:LEU:HD12	5:L:261:LEU:N	2.35	0.42
5:L:603:ARG:HG2	5:L:603:ARG:H	1.47	0.42
1:A:208:ASN:OD1	1:A:208:ASN:N	2.44	0.42
1:A:78:ILE:HA	1:A:78:ILE:HD13	1.79	0.42
1:B:12:ARG:O	1:B:29:GLU:O	2.37	0.42
1:B:195:ARG:HB3	1:B:198:LEU:HD21	2.02	0.42
2:C:169:LYS:HG2	2:C:169:LYS:O	2.20	0.42
2:C:269:ILE:HG23	2:C:273:HIS:CB	2.48	0.42
2:C:52:ALA:HB2	2:C:461:GLU:HG3	2.01	0.42
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.55	0.42
2:C:871:VAL:HG22	2:C:872:TYR:O	2.19	0.42
3:D:1365:TYR:O	3:D:1366:HIS:C	2.58	0.42
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.95	0.42
3:D:528:THR:HG22	3:D:532:GLU:OE1	2.20	0.42
3:D:515:ARG:CZ	3:D:719:PHE:CE2	3.02	0.42
3:D:79:LYS:HG3	3:D:80:HIS:N	2.35	0.42
5:F:551:LEU:HA	5:F:551:LEU:HD23	1.79	0.42
1:H:109:PRO:HA	1:H:132:HIS:HA	2.02	0.42
1:H:214:GLU:HG2	1:H:218:ARG:HE	1.85	0.42
2:I:836:LEU:CD1	2:I:1054:LEU:HD13	2.46	0.42
2:I:241:LEU:HA	2:I:241:LEU:HD12	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.20	0.42
2:I:718:ALA:HB3	2:I:781:ASP:H	1.85	0.42
2:I:75:LEU:HA	2:I:75:LEU:HD13	1.55	0.42
3:J:1261:LEU:HD12	3:J:1261:LEU:C	2.40	0.42
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.20	0.42
3:D:1291:GLU:CD	3:J:1302:TYR:OH	2.58	0.42
3:J:211:GLU:OE2	3:J:214:ARG:NH2	2.53	0.42
3:J:64:PRO:HG3	3:J:90:VAL:CG1	2.49	0.42
3:J:888:CYS:HB2	3:J:898:CYS:SG	2.59	0.42
5:L:599:ARG:O	5:L:604:SER:OG	2.37	0.42
1:A:101:THR:HG22	1:A:103:ASN:HD21	1.85	0.42
1:B:51:MET:HB3	1:B:178:SER:HA	2.02	0.42
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.61	0.42
2:C:100:LEU:HA	2:C:100:LEU:HD23	1.70	0.42
2:C:1144:PHE:O	2:C:1147:ARG:HB2	2.18	0.42
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.84	0.42
2:C:718:ALA:HB2	2:C:783:LEU:HD21	2.02	0.42
2:C:5:TYR:HB2	2:C:781:ASP:OD1	2.20	0.42
3:D:1177:ILE:HG13	3:D:1186:TYR:O	2.20	0.42
3:D:214:ARG:HA	3:D:217:LEU:HB2	2.02	0.42
3:D:22:ILE:HG21	3:D:22:ILE:HD13	1.79	0.42
3:D:737:ILE:O	3:D:740:LEU:N	2.49	0.42
5:F:306:PHE:HE1	5:F:315:TRP:CE2	2.37	0.42
5:F:462:LYS:HE3	5:F:488:LEU:HD11	2.01	0.42
1:H:134:THR:HG23	1:H:135:ASP:H	1.83	0.42
2:I:1233:LEU:N	2:I:1233:LEU:HD22	2.34	0.42
2:I:260:LYS:HE3	2:I:262:TYR:CE1	2.55	0.42
2:I:721:GLY:N	2:I:740:GLU:OE1	2.40	0.42
2:I:903:ARG:NH2	2:I:910:ALA:HB2	2.35	0.42
3:J:489:ASN:HA	3:J:904:ALA:HB1	2.01	0.42
5:L:363:ARG:O	5:L:367:ILE:HG13	2.20	0.42
5:L:483:LEU:CD1	5:L:483:LEU:H	2.30	0.42
2:C:179:TYR:H	2:C:397:LEU:HA	1.85	0.41
3:D:1342:ASP:OD1	3:D:1344:LEU:N	2.48	0.41
3:D:18:ASP:HB2	3:D:1373:ARG:NH1	2.35	0.41
3:D:318:GLY:C	3:D:320:ASN:N	2.73	0.41
3:D:354:VAL:HG12	3:D:355:ILE:N	2.35	0.41
3:D:490:ILE:HD13	3:D:490:ILE:HG21	1.68	0.41
3:D:8:LEU:HD23	3:D:9:LYS:H	1.84	0.41
1:G:190:ALA:O	1:G:198:LEU:HB2	2.20	0.41
1:G:231:PHE:HA	1:H:218:ARG:HH11	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:HIS:CE1	1:H:206:GLU:HG2	2.54	0.41
2:I:1136:GLN:O	2:I:1137:GLU:HB3	2.20	0.41
2:I:1161:LEU:HA	2:I:1161:LEU:HD12	1.67	0.41
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	2.02	0.41
3:J:132:LEU:O	3:J:132:LEU:HD22	2.20	0.41
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.84	0.41
3:J:482:ALA:O	3:J:488:ASN:ND2	2.54	0.41
3:J:694:SER:O	3:J:698:MET:HB2	2.20	0.41
3:J:702:GLN:HG2	3:J:703:THR:N	2.30	0.41
5:L:101:TYR:O	5:L:102:MET:C	2.57	0.41
5:L:470:MET:C	5:L:478:PRO:HD3	2.41	0.41
1:A:190:ALA:HB2	1:A:200:LYS:CB	2.41	0.41
1:A:67:GLU:HG2	1:A:67:GLU:H	1.45	0.41
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.84	0.41
2:C:1075:VAL:O	2:C:1075:VAL:HG12	2.20	0.41
2:C:700:VAL:HG21	2:C:1114:GLU:HG2	2.01	0.41
2:C:310:ILE:HG21	2:C:325:LEU:HB3	2.03	0.41
2:C:603:ILE:HG12	2:C:603:ILE:H	1.65	0.41
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.01	0.41
2:C:857:VAL:HG23	2:C:862:LEU:HD11	2.02	0.41
2:C:895:LEU:H	2:C:895:LEU:HG	1.54	0.41
2:C:96:LEU:HD12	2:C:96:LEU:HA	1.77	0.41
3:D:447:ILE:HG21	3:D:447:ILE:HD13	1.64	0.41
3:D:83:VAL:O	3:D:91:GLU:HA	2.20	0.41
5:F:227:GLN:OE1	5:F:251:LYS:NZ	2.53	0.41
5:F:230:VAL:HG13	5:F:231:THR:H	1.85	0.41
1:G:172:LEU:CD1	1:G:172:LEU:H	2.33	0.41
1:H:7:GLU:CD	1:H:8:PHE:N	2.73	0.41
2:I:1088:ASP:OD1	2:I:1092:THR:N	2.53	0.41
2:I:339:ASN:HB3	2:I:343:HIS:H	1.84	0.41
2:I:672:GLU:H	2:I:672:GLU:HG3	1.54	0.41
2:I:798:GLN:OE1	2:I:828:PHE:CD1	2.73	0.41
2:I:850:ILE:HG23	2:I:850:ILE:HD12	1.77	0.41
3:J:307:LEU:HD23	3:J:307:LEU:HA	1.19	0.41
3:J:434:ILE:HG21	3:J:434:ILE:HD13	1.46	0.41
3:J:473:THR:HG23	3:J:476:ALA:H	1.85	0.41
5:L:466:ILE:HD11	5:L:487:MET:CE	2.51	0.41
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.62	0.41
1:A:154:PRO:O	1:A:158:ARG:HG3	2.20	0.41
1:A:78:ILE:HD12	1:A:78:ILE:HG23	1.77	0.41
2:C:799:ASN:HA	2:C:1231:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1278:LEU:HD23	2:C:1278:LEU:HA	1.67	0.41
2:C:494:ASN:HD22	2:C:497:PRO:CD	2.27	0.41
2:C:676:ALA:O	2:C:677:ASN:C	2.58	0.41
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.60	0.41
2:C:1246:ARG:CZ	3:D:348:ASP:OD1	2.69	0.41
3:D:440:VAL:O	3:D:442:ILE:HG12	2.21	0.41
3:D:872:LEU:O	3:D:877:VAL:HG12	2.20	0.41
5:F:230:VAL:HG13	5:F:231:THR:N	2.36	0.41
1:G:54:CYS:HB3	1:G:148:ARG:HG2	2.01	0.41
2:I:1330:ILE:HG21	2:I:1330:ILE:HD13	1.75	0.41
2:I:363:LEU:HA	2:I:363:LEU:HD23	1.62	0.41
2:I:395:TYR:HE2	2:I:397:LEU:CD1	2.33	0.41
2:I:593:LYS:HG3	2:I:595:THR:HG23	2.02	0.41
2:I:959:ASP:O	2:I:963:GLU:HG2	2.21	0.41
3:J:1144:LEU:HD23	3:J:1144:LEU:HA	1.57	0.41
3:J:1151:LYS:O	3:J:1153:PRO:HD3	2.21	0.41
3:J:1344:LEU:HD12	3:J:1344:LEU:N	2.35	0.41
3:J:252:LEU:HD22	3:J:260:PHE:HD2	1.85	0.41
3:J:309:ASN:HB2	3:J:326:SER:HB3	2.02	0.41
3:J:331:ILE:HD13	3:J:331:ILE:HG21	1.67	0.41
3:J:352:ARG:HB3	3:J:467:ALA:HA	2.02	0.41
3:J:530:PRO:O	3:J:533:ALA:HB3	2.20	0.41
3:J:514:THR:CB	3:J:576:ARG:HG2	2.47	0.41
3:J:762:ASN:OD1	3:J:764:ARG:N	2.53	0.41
5:L:130:VAL:HA	5:L:133:SER:HB2	2.01	0.41
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.20	0.41
2:C:1120:ALA:O	2:C:1123:GLY:N	2.53	0.41
2:C:1178:LYS:HA	2:C:1178:LYS:HD3	1.55	0.41
2:C:867:GLU:HG3	2:C:867:GLU:H	1.30	0.41
3:D:10:ALA:O	3:D:11:GLN:HB2	2.21	0.41
3:D:117:LEU:HD12	3:D:117:LEU:HA	1.77	0.41
3:D:530:PRO:O	3:D:531:LYS:C	2.57	0.41
3:D:74:LYS:CD	3:D:87:LYS:HD3	2.47	0.41
1:G:226:GLU:O	1:G:229:GLU:HB2	2.20	0.41
1:G:50:SER:HB2	1:H:8:PHE:HZ	1.86	0.41
1:G:52:PRO:HG2	1:G:219:ARG:NH2	2.34	0.41
1:H:102:LEU:HA	1:H:102:LEU:HD23	1.66	0.41
2:I:1251:TYR:CD1	2:I:1301:ARG:NH2	2.89	0.41
2:I:540:ARG:H	2:I:540:ARG:HG3	1.50	0.41
2:I:819:SER:OG	2:I:820:GLU:N	2.50	0.41
3:J:1177:ILE:HG13	3:J:1186:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	2.02	0.41
3:J:270:ARG:O	3:J:273:ILE:HB	2.21	0.41
3:J:278:ARG:O	3:J:281:ARG:HB2	2.20	0.41
3:J:556:GLU:O	3:J:564:VAL:N	2.47	0.41
3:J:796:LEU:HA	3:J:796:LEU:HD12	1.61	0.41
4:K:6:VAL:HG12	4:K:51:LEU:HD13	2.02	0.41
1:B:151:GLY:O	1:B:177:TYR:CD2	2.70	0.41
2:C:9:LYS:HG2	2:C:1171:ARG:HD3	2.02	0.41
2:C:1184:THR:HG22	2:C:1185:PRO:O	2.20	0.41
2:C:149:LEU:HG	2:C:451:ARG:HH11	1.84	0.41
2:C:142:GLU:CG	2:C:760:ASN:HD21	2.31	0.41
3:D:233:LYS:HA	3:D:234:PRO:HD3	1.87	0.41
3:D:430:HIS:ND1	3:D:430:HIS:N	2.66	0.41
3:D:501:VAL:HG22	3:D:502:PRO:O	2.20	0.41
3:D:506:VAL:HG12	3:D:506:VAL:H	1.52	0.41
3:D:536:LEU:O	3:D:539:SER:OG	2.37	0.41
3:D:614:LEU:O	3:D:615:LYS:C	2.59	0.41
3:D:821:MET:HA	3:D:881:LYS:HA	2.01	0.41
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.84	0.41
3:D:95:THR:HG23	3:D:95:THR:O	2.20	0.41
5:F:161:LEU:C	5:F:262:VAL:HG23	2.41	0.41
5:F:575:GLU:O	5:F:579:GLN:HG2	2.20	0.41
2:I:1281:TYR:CE2	3:J:431:ARG:HB2	2.55	0.41
2:I:1322:SER:O	2:I:1325:VAL:N	2.53	0.41
2:I:948:ILE:O	2:I:951:MET:HB3	2.20	0.41
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.20	0.41
3:J:266:ASN:O	3:J:267:ASP:C	2.57	0.41
3:J:844:THR:HG21	3:J:858:VAL:CG2	2.50	0.41
4:K:10:VAL:HG13	4:K:16:ARG:HB2	2.02	0.41
5:L:284:GLU:OE2	5:L:359:LYS:HD2	2.20	0.41
5:L:601:PRO:HB2	5:L:605:GLU:HG2	2.01	0.41
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.64	0.41
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.35	0.41
2:C:194:LEU:HA	2:C:194:LEU:HD12	1.33	0.41
2:C:626:GLU:HB3	2:C:628:HIS:CE1	2.55	0.41
2:C:929:ILE:O	2:C:930:ASP:HB2	2.19	0.41
2:C:960:LEU:O	2:C:963:GLU:HB2	2.20	0.41
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.03	0.41
3:D:1256:ILE:HD13	3:D:1256:ILE:HA	1.74	0.41
3:D:203:GLU:O	3:D:207:GLU:HG2	2.19	0.41
3:D:334:LYS:CG	3:D:335:GLN:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.66	0.41
3:D:884:SER:OG	3:D:886:VAL:HG12	2.21	0.41
3:D:909:ILE:HA	3:D:909:ILE:HD12	1.85	0.41
1:H:17:GLU:OE1	1:H:25:LYS:HD3	2.20	0.41
1:H:195:ARG:CB	1:H:198:LEU:HD21	2.50	0.41
2:I:1132:LEU:O	2:I:1132:LEU:HD23	2.19	0.41
2:I:1301:ARG:HH11	2:I:1301:ARG:HD2	1.71	0.41
2:I:1331:ARG:HH11	2:I:1331:ARG:HD3	1.72	0.41
2:I:176:ILE:HD13	2:I:176:ILE:HG21	1.74	0.41
2:I:618:GLN:HG3	2:I:619:ALA:N	2.36	0.41
3:J:146:VAL:HG12	3:J:147:ILE:N	2.36	0.41
3:J:546:ALA:O	3:J:573:THR:HA	2.20	0.41
3:J:709:ARG:C	3:J:711:GLY:N	2.74	0.41
3:J:735:ALA:O	3:J:738:ARG:HB3	2.20	0.41
4:K:53:GLU:HB3	4:K:59:ILE:CG1	2.50	0.41
5:L:236:LYS:N	5:L:236:LYS:HD3	2.35	0.41
5:L:412:LEU:N	5:L:435:ILE:HG12	2.36	0.41
5:L:552:THR:H	5:L:552:THR:HG23	1.65	0.41
2:C:639:LYS:O	2:C:641:GLU:N	2.54	0.41
2:C:818:VAL:HG22	2:C:1096:ILE:HG12	2.03	0.41
3:D:543:SER:OG	3:D:544:LEU:N	2.52	0.41
3:D:649:LYS:HD2	3:D:652:GLU:OE1	2.21	0.41
3:D:656:GLU:O	3:D:659:ALA:N	2.54	0.41
3:D:891:ASP:O	3:D:892:PHE:HB2	2.20	0.41
4:E:32:VAL:O	4:E:34:GLY:N	2.52	0.41
5:F:223:GLU:O	5:F:226:ALA:HB3	2.21	0.41
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.63	0.41
1:H:45:ARG:HD3	1:H:45:ARG:HH11	1.69	0.41
2:I:1198:LEU:HD22	2:I:1198:LEU:HA	1.78	0.41
2:I:538:LEU:HG	2:I:538:LEU:H	1.33	0.41
2:I:696:ASP:HB3	2:I:697:LYS:H	1.62	0.41
2:I:888:THR:CG2	2:I:916:SER:OG	2.68	0.41
3:J:1175:LEU:O	3:J:1187:GLU:HA	2.21	0.41
3:J:1219:ASP:O	3:J:1220:ILE:C	2.58	0.41
3:J:72:CYS:SG	3:J:73:GLY:N	2.94	0.41
3:J:863:LEU:HD11	3:J:901:ARG:HB3	2.02	0.41
5:L:518:HIS:O	5:L:519:LEU:C	2.58	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.31	0.41
2:C:289:VAL:HG13	2:C:319:LEU:HD11	2.03	0.41
2:C:513:GLN:NE2	2:C:526:TYR:CE2	2.89	0.41
2:C:530:ILE:HD12	2:C:530:ILE:HG23	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.20	0.41
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	2.02	0.41
3:D:1158:GLU:HG3	3:D:1186:TYR:CZ	2.56	0.41
3:D:500:ILE:HG23	3:D:500:ILE:HD12	1.78	0.41
3:D:83:VAL:H	3:D:83:VAL:HG12	1.56	0.41
5:F:396:ASN:C	5:F:398:GLY:N	2.74	0.41
1:G:86:LYS:NZ	1:G:174:ASP:HB2	2.36	0.41
1:G:61:ILE:HG22	1:G:62:ASP:N	2.35	0.41
1:G:66:HIS:NE2	2:I:929:ILE:HG22	2.36	0.41
1:H:93:GLN:HB2	1:H:120:ASP:HB3	2.02	0.41
2:I:596:ASP:CG	2:I:597:GLY:H	2.23	0.41
2:I:688:GLN:HB2	2:I:1235:LEU:HD22	2.01	0.41
2:I:807:TRP:HE3	2:I:808:ASN:HB2	1.85	0.41
3:J:1160:SER:HA	3:J:1204:VAL:O	2.21	0.41
3:J:147:ILE:HD11	3:J:179:LYS:HZ3	1.85	0.41
3:J:294:ASN:HD21	5:L:402:LEU:HD23	1.85	0.41
3:J:909:ILE:HG23	3:J:909:ILE:O	2.19	0.41
1:A:112:ALA:O	1:A:115:ILE:HG13	2.20	0.41
1:A:228:LEU:HD11	1:B:224:LEU:HD23	2.03	0.41
2:C:1172:LEU:HD22	2:C:1172:LEU:O	2.21	0.41
2:C:24:VAL:HG12	2:C:25:PRO:O	2.21	0.41
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.83	0.41
2:C:548:ARG:HB3	2:C:569:ILE:O	2.21	0.41
3:D:112:ALA:O	3:D:300:GLN:NE2	2.46	0.41
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.91	0.41
3:D:390:LEU:N	3:D:390:LEU:HD12	2.36	0.41
3:D:442:ILE:HG23	3:D:442:ILE:HD12	1.72	0.41
3:D:733:SER:O	3:D:735:ALA:N	2.54	0.41
5:F:442:SER:O	5:F:445:ASP:N	2.54	0.41
1:G:118:ASP:HB3	1:G:121:VAL:HG21	2.02	0.41
1:H:44:ARG:HG3	1:H:183:ILE:HB	2.03	0.41
1:H:16:ILE:HA	1:H:26:VAL:HG13	2.03	0.41
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.86	0.41
2:I:195:PHE:CB	2:I:203:LYS:HD3	2.50	0.41
2:I:344:GLY:O	2:I:346:TYR:CD2	2.74	0.41
2:I:212:ALA:HA	2:I:359:ARG:HG3	2.03	0.41
2:I:517:GLN:O	2:I:518:ASN:C	2.60	0.41
2:I:521:LEU:HD12	2:I:521:LEU:HA	1.82	0.41
2:I:523:GLU:HG2	2:I:527:LYS:CE	2.36	0.41
2:I:617:ALA:HB3	2:I:653:MET:HB2	2.02	0.41
2:I:761:GLN:HA	2:I:762:ASN:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:794:LEU:HD21	2:I:796:LEU:HD21	2.01	0.41
2:I:829:THR:HG23	2:I:1059:ARG:HG2	2.03	0.41
3:J:425:ARG:HH11	3:J:425:ARG:HD2	1.60	0.41
5:L:124:GLU:O	5:L:128:ASN:HB2	2.19	0.41
1:A:273:GLU:OE2	1:A:293:PRO:HD2	2.21	0.41
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	2.02	0.41
2:C:138:ILE:HD11	2:C:506:PHE:HB3	2.02	0.41
2:C:719:LYS:O	2:C:779:ARG:HG3	2.21	0.41
3:D:31:ARG:CZ	3:D:106:GLU:OE2	2.69	0.41
3:D:205:LEU:C	3:D:205:LEU:HD13	2.41	0.41
4:E:62:GLN:O	4:E:66:VAL:HG23	2.21	0.41
5:F:137:TYR:HA	5:F:138:PRO:HD3	1.95	0.41
5:F:557:LYS:O	5:F:561:MET:N	2.52	0.41
1:H:191:ARG:HH12	3:J:370:LYS:HZ3	1.68	0.41
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.94	0.41
2:I:756:TYR:N	2:I:756:TYR:CD1	2.83	0.41
2:I:807:TRP:HE1	2:I:1086:PRO:HG3	1.85	0.41
3:J:1223:LEU:HA	3:J:1223:LEU:HD13	1.73	0.41
3:J:849:LEU:H	3:J:849:LEU:HD22	1.86	0.41
3:J:908:ILE:HD13	3:J:909:ILE:N	2.35	0.41
5:L:118:ASP:O	5:L:122:ARG:HG3	2.20	0.41
5:L:127:ILE:HG13	5:L:127:ILE:H	1.70	0.41
5:L:262:VAL:HG12	5:L:264:LYS:HG3	2.02	0.41
1:B:214:GLU:O	1:B:218:ARG:HG3	2.21	0.41
2:C:1049:ILE:HG21	2:C:1049:ILE:HD13	1.75	0.41
2:C:1143:GLU:OE1	2:C:1147:ARG:HD3	2.21	0.41
2:C:210:LEU:O	2:C:215:TYR:HB2	2.21	0.41
2:C:311:CYS:O	2:C:311:CYS:SG	2.79	0.41
2:C:384:LEU:O	2:C:387:ASN:N	2.54	0.41
2:C:619:ALA:HB1	2:C:657:THR:HA	2.03	0.41
2:C:667:LEU:HD23	2:C:667:LEU:HA	1.84	0.41
2:C:831:ILE:HG21	2:C:831:ILE:HD13	1.85	0.41
3:D:120:LEU:HB3	3:D:121:PRO:HD3	2.02	0.41
3:D:1291:GLU:C	3:D:1292:LEU:HD12	2.41	0.41
3:D:1364:ALA:O	3:D:1367:GLN:HB3	2.20	0.41
3:D:20:ILE:HG21	3:D:20:ILE:HD13	1.85	0.41
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.56	0.41
3:D:556:GLU:HG2	3:D:558:ASP:HB2	2.02	0.41
3:D:697:MET:O	3:D:701:LEU:HB2	2.21	0.41
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.57	0.41
2:I:1342:GLU:O	3:J:1369:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:229:ILE:HG21	2:I:240:GLU:OE2	2.20	0.41
2:I:65:ASN:O	2:I:105:TYR:HD2	2.03	0.41
2:I:865:LEU:HA	2:I:865:LEU:HD23	1.77	0.41
3:J:368:LEU:HD23	3:J:368:LEU:C	2.41	0.41
3:J:601:ILE:HG21	3:J:601:ILE:HD13	1.61	0.41
3:J:795:TYR:HE2	3:J:799:ARG:NE	2.17	0.41
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.52	0.41
1:A:12:ARG:HG2	1:A:13:LEU:H	1.85	0.40
2:C:1172:LEU:HD22	2:C:1172:LEU:C	2.42	0.40
2:C:1211:ARG:O	2:C:1211:ARG:HG3	2.21	0.40
2:C:145:ILE:HD12	2:C:145:ILE:N	2.37	0.40
2:C:328:SER:OG	2:C:330:HIS:CD2	2.73	0.40
2:C:624:ASP:OD1	2:C:625:GLU:N	2.52	0.40
2:C:929:ILE:HG21	2:C:929:ILE:HD13	1.73	0.40
3:D:1257:VAL:HA	3:D:1260:MET:HE2	2.03	0.40
3:D:1264:ALA:O	3:D:1278:GLU:N	2.34	0.40
3:D:54:ASP:OD1	3:D:54:ASP:N	2.54	0.40
3:D:770:LEU:O	3:D:774:ILE:HG13	2.21	0.40
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.80	0.40
1:G:108:GLY:HA2	1:G:109:PRO:HD3	1.90	0.40
1:G:170:ARG:O	1:G:171:LEU:HD13	2.20	0.40
1:G:75:GLN:HG2	1:G:76:GLU:OE2	2.20	0.40
1:H:19:VAL:O	1:H:23:HIS:HB3	2.21	0.40
2:I:606:LEU:HD12	2:I:606:LEU:N	2.37	0.40
2:I:663:VAL:HG23	2:I:664:GLY:N	2.36	0.40
2:I:896:THR:OG1	2:I:899:GLU:HG3	2.21	0.40
3:J:470:VAL:CG1	3:J:472:LEU:HD23	2.49	0.40
3:J:648:GLU:OE2	3:J:649:LYS:HE2	2.21	0.40
3:J:847:ASP:HA	3:J:860:ARG:H	1.86	0.40
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.48	0.40
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.86	0.40
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.56	0.40
2:C:131:THR:HG22	2:C:135:THR:N	2.11	0.40
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.03	0.40
2:C:660:VAL:HG13	2:C:661:VAL:N	2.36	0.40
2:C:725:GLN:O	2:C:725:GLN:HG2	2.21	0.40
2:C:77:GLU:HA	2:C:78:PRO:HD3	1.84	0.40
2:C:836:LEU:O	2:C:1052:VAL:N	2.44	0.40
3:D:1237:VAL:HG13	3:D:1238:GLN:N	2.36	0.40
3:D:1307:LEU:HD12	3:D:1307:LEU:N	2.36	0.40
3:D:1321:SER:HB2	3:D:1349:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:242:LEU:HD23	3:D:243:PRO:O	2.21	0.40
2:C:1243:MET:HA	3:D:353:SER:CB	2.51	0.40
5:F:269:LEU:O	5:F:272:SER:N	2.54	0.40
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.86	0.40
2:I:1332:SER:OG	3:J:327:LEU:HD13	2.21	0.40
3:J:184:ALA:O	3:J:187:ALA:HB3	2.21	0.40
1:A:182:ARG:O	1:A:183:ILE:HD12	2.21	0.40
2:C:817:LEU:HD23	2:C:1078:LYS:HB3	2.04	0.40
2:C:109:ALA:HB1	2:C:111:GLU:HA	2.02	0.40
2:C:1120:ALA:HB1	2:C:1198:LEU:CD1	2.51	0.40
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	2.03	0.40
2:C:47:TYR:HD2	2:C:47:TYR:HA	1.72	0.40
2:C:142:GLU:N	2:C:760:ASN:OD1	2.54	0.40
2:C:836:LEU:CD1	2:C:836:LEU:N	2.82	0.40
3:D:1233:ILE:O	3:D:1234:VAL:C	2.58	0.40
3:D:205:LEU:O	3:D:205:LEU:HD13	2.22	0.40
3:D:259:ARG:HD2	5:F:505:ILE:HD13	2.03	0.40
5:F:144:LEU:HA	5:F:144:LEU:HD12	1.78	0.40
5:F:379:MET:HG2	5:F:416:VAL:HG22	2.03	0.40
1:G:73:GLY:O	1:G:134:THR:HG22	2.22	0.40
1:G:20:SER:O	1:G:21:SER:C	2.59	0.40
2:I:1046:VAL:HG12	2:I:1046:VAL:H	1.59	0.40
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.73	0.40
2:I:27:LEU:HD23	2:I:27:LEU:HA	1.78	0.40
2:I:643:SER:OG	2:I:645:PHE:HE1	2.05	0.40
3:J:97:VAL:O	3:J:101:ARG:HG3	2.21	0.40
3:J:188:LEU:O	3:J:191:SER:OG	2.28	0.40
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.72	0.40
3:J:422:LEU:HA	3:J:422:LEU:HD12	1.83	0.40
3:J:847:ASP:HB3	3:J:856:ILE:CG2	2.51	0.40
3:J:836:ARG:HG3	3:J:869:CYS:HB3	2.03	0.40
5:L:587:ILE:HA	5:L:590:ILE:CD1	2.51	0.40
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.91	0.40
1:A:85:LEU:O	1:A:86:LYS:C	2.58	0.40
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.74	0.40
2:C:930:ASP:HB3	2:C:1053:TYR:HB2	2.03	0.40
2:C:1062:PRO:HA	2:C:1076:ILE:O	2.21	0.40
2:C:208:ILE:HG21	2:C:208:ILE:HD13	1.79	0.40
2:C:617:ALA:HB3	2:C:653:MET:CG	2.51	0.40
2:C:842:ASP:HB2	2:C:1045:GLY:O	2.21	0.40
3:D:1347:LEU:HG	3:D:1357:ILE:CG2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:ARG:NH2	3:D:717:VAL:HG23	2.37	0.40
3:D:592:VAL:HG22	3:D:592:VAL:H	1.69	0.40
5:F:107:THR:OG1	5:F:108:VAL:N	2.53	0.40
5:F:110:LEU:HD23	5:F:110:LEU:HA	1.73	0.40
1:A:316:MET:HB2	5:F:600:HIS:CE1	2.57	0.40
1:G:38:THR:N	1:H:45:ARG:NH1	2.70	0.40
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.61	0.40
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.70	0.40
2:I:801:ARG:HA	2:I:1228:GLY:O	2.22	0.40
2:I:1247:SER:OG	2:I:1248:THR:N	2.51	0.40
2:I:41:GLN:NE2	2:I:73:TYR:CZ	2.89	0.40
2:I:62:TYR:C	2:I:64:GLY:N	2.74	0.40
2:I:791:LEU:HD23	2:I:791:LEU:HA	1.73	0.40
2:I:861:ALA:HB1	2:I:882:ILE:HD13	2.03	0.40
2:I:976:ARG:HH12	2:I:990:ASP:HB3	1.86	0.40
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.85	0.40
3:J:872:LEU:CD2	3:J:877:VAL:HG11	2.43	0.40
5:L:112:THR:OG1	5:L:115:GLY:N	2.51	0.40
5:L:230:VAL:HG13	5:L:231:THR:N	2.36	0.40
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.86	0.40
5:L:519:LEU:C	5:L:519:LEU:HD23	2.42	0.40
5:L:565:ILE:HG22	5:L:566:ASP:OD2	2.21	0.40
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.67	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.51	0.40
1:A:76:GLU:HB3	1:A:81:ILE:HG12	2.03	0.40
1:B:112:ALA:HA	1:B:115:ILE:HD11	2.03	0.40
1:B:103:ASN:HA	1:B:141:SER:HB2	2.03	0.40
1:B:215:GLU:HA	1:B:218:ARG:CD	2.51	0.40
1:B:40:GLY:HA3	1:B:185:TYR:CD1	2.56	0.40
2:C:1251:TYR:CE1	2:C:1301:ARG:CZ	3.04	0.40
2:C:556:GLY:HA2	2:C:659:GLN:O	2.21	0.40
2:C:615:VAL:HG21	2:C:645:PHE:CD2	2.57	0.40
2:C:746:ALA:HA	2:C:974:ARG:NH2	2.34	0.40
2:C:811:ASN:N	2:C:811:ASN:OD1	2.48	0.40
2:C:1313:HIS:HD2	3:D:477:GLN:NE2	2.19	0.40
4:E:39:VAL:HG13	4:E:52:ARG:HH21	1.86	0.40
5:F:148:TYR:OH	5:F:218:ARG:HA	2.21	0.40
5:F:476:ARG:HG3	5:F:477:GLU:N	2.35	0.40
5:F:606:VAL:O	5:F:609:SER:OG	2.40	0.40
1:G:14:VAL:HG13	1:G:27:THR:HB	2.03	0.40
1:H:31:LEU:HB2	1:H:199:ASP:HB2	2.04	0.40

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

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

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

5.3 Torsion angles (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	305/329 (93%)	271 (89%)	25 (8%)	9 (3%)	5 44
1	B	213/329 (65%)	191 (90%)	20 (9%)	2 (1%)	21 67
1	G	222/329 (68%)	182 (82%)	28 (13%)	12 (5%)	2 27
1	H	213/329 (65%)	193 (91%)	20 (9%)	0	100 100
2	C	1338/1342 (100%)	1225 (92%)	103 (8%)	10 (1%)	26 72
2	I	1338/1342 (100%)	1226 (92%)	100 (8%)	12 (1%)	21 67
3	D	1162/1407 (83%)	1074 (92%)	79 (7%)	9 (1%)	24 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	J	1151/1407 (82%)	1064 (92%)	82 (7%)	5 (0%)	39 80
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100 100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100 100
5	F	461/613 (75%)	422 (92%)	37 (8%)	2 (0%)	39 80
5	L	463/613 (76%)	423 (91%)	39 (8%)	1 (0%)	52 87
All	All	7030/8222 (86%)	6424 (91%)	544 (8%)	62 (1%)	21 67

All (62) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains (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	268/286 (94%)	249 (93%)	19 (7%)	18 59
1	B	184/286 (64%)	166 (90%)	18 (10%)	10 44
1	G	191/286 (67%)	179 (94%)	12 (6%)	22 64
1	H	183/286 (64%)	165 (90%)	18 (10%)	10 44
2	C	1155/1157 (100%)	1046 (91%)	109 (9%)	11 47
2	I	1154/1157 (100%)	1046 (91%)	108 (9%)	11 47
3	D	975/1168 (84%)	875 (90%)	100 (10%)	9 42
3	J	967/1168 (83%)	869 (90%)	98 (10%)	9 43
4	E	72/75 (96%)	64 (89%)	8 (11%)	8 38
4	K	67/75 (89%)	63 (94%)	4 (6%)	24 65
5	F	416/540 (77%)	373 (90%)	43 (10%)	9 42
5	L	418/540 (77%)	372 (89%)	46 (11%)	8 39
All	All	6050/7024 (86%)	5467 (90%)	583 (10%)	10 45

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	309/329 (93%)	-0.32	2 (0%) 90 83	99, 147, 225, 245	0
1	B	217/329 (65%)	-0.02	6 (2%) 56 42	112, 194, 254, 272	0
1	G	224/329 (68%)	-0.07	3 (1%) 79 66	163, 206, 241, 270	0
1	H	217/329 (65%)	0.07	13 (5%) 25 17	146, 213, 252, 285	0
2	C	1340/1342 (99%)	-0.35	21 (1%) 74 61	74, 121, 234, 285	0
2	I	1340/1342 (99%)	-0.16	50 (3%) 45 32	86, 159, 261, 388	0
3	D	1166/1407 (82%)	-0.30	14 (1%) 81 69	72, 112, 215, 264	0
3	J	1155/1407 (82%)	-0.22	22 (1%) 70 56	86, 138, 229, 274	0
4	E	89/91 (97%)	-0.02	2 (2%) 65 50	147, 183, 216, 241	0
4	K	79/91 (86%)	0.78	14 (17%) 2 2	202, 277, 319, 350	0
5	F	467/613 (76%)	-0.23	12 (2%) 59 44	93, 165, 290, 340	0
5	L	469/613 (76%)	-0.30	7 (1%) 76 64	116, 178, 288, 353	0
All	All	7072/8222 (86%)	-0.22	166 (2%) 64 48	72, 147, 251, 388	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	8.9
3	D	335	GLN	6.3
2	I	1001	GLY	5.3
1	B	160	HIS	5.1
2	I	1000	LEU	4.9
3	J	208	THR	4.7
2	C	1002	LEU	4.4
2	I	983	GLY	4.4
2	I	998	LEU	4.4
2	I	979	LEU	4.4
2	C	251	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
5	L	489	MET	4.4
2	C	1001	GLY	4.4
2	I	981	ALA	4.4
2	I	999	GLU	4.2
2	C	231	GLU	4.2
2	C	1003	THR	4.2
5	F	319	ALA	4.2
5	F	326	TRP	4.1
2	I	1002	LEU	4.1
3	D	712	GLN	4.1
5	F	323	ASN	4.0
3	J	218	THR	4.0
2	I	414	ILE	3.8
1	H	96	ASP	3.8
2	C	319	LEU	3.8
2	C	1000	LEU	3.7
4	E	2	ALA	3.7
4	K	36	ASP	3.7
5	L	490	PRO	3.7
4	K	72	GLN	3.7
3	J	931	THR	3.6
2	I	1004	ASP	3.5
1	H	135	ASP	3.4
2	I	105	TYR	3.4
2	I	985	GLU	3.4
3	D	1202	GLU	3.4
2	I	987	GLU	3.3
4	K	33	GLY	3.3
4	K	37	PRO	3.3
1	H	106	GLY	3.2
3	J	542	ALA	3.2
2	I	1007	LYS	3.2
5	L	111	LEU	3.2
2	I	1010	GLN	3.2
5	L	425	TYR	3.2
2	I	266	GLY	3.2
1	H	97	GLU	3.1
5	F	318	ALA	3.1
2	I	1003	THR	3.1
3	J	675	ALA	3.1
1	B	172	LEU	3.1
1	H	72	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
4	K	40	PRO	3.0
5	F	325	PRO	3.0
4	K	26	ARG	3.0
5	F	338	HIS	3.0
2	I	984	VAL	3.0
2	I	727	VAL	3.0
2	I	986	ALA	3.0
1	B	69	SER	2.9
3	J	528	THR	2.9
2	C	1004	ASP	2.9
2	I	978	VAL	2.9
2	I	972	PHE	2.9
3	J	1296	GLY	2.9
1	B	70	THR	2.8
2	C	893	THR	2.8
2	C	267	ARG	2.8
3	J	830	ASP	2.8
3	J	712	GLN	2.8
2	C	258	ASN	2.8
2	I	975	ILE	2.8
5	L	315	TRP	2.8
5	F	167	ASP	2.8
4	K	2	ALA	2.8
3	D	218	THR	2.8
5	F	301	ASN	2.8
3	J	1297	LYS	2.7
2	I	1005	GLU	2.7
1	B	67	GLU	2.7
3	D	1204	VAL	2.7
2	I	751	TYR	2.7
2	I	1006	GLU	2.7
2	I	1316	GLU	2.6
2	I	973	SER	2.6
3	D	1172	LYS	2.6
3	D	1161	GLY	2.6
2	I	912	ASP	2.6
2	I	267	ARG	2.5
3	J	564	VAL	2.5
5	L	167	ASP	2.5
2	I	375	PRO	2.5
3	J	1295	ASN	2.5
1	H	66	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	830	ASP	2.5
2	C	247	ARG	2.5
3	D	207	GLU	2.5
3	J	335	GLN	2.5
2	C	317	LEU	2.5
2	I	725	GLN	2.4
2	I	165	HIS	2.4
2	I	111	GLU	2.4
3	D	826	ILE	2.4
3	D	518	VAL	2.4
3	J	826	ILE	2.4
2	I	969	ALA	2.4
4	K	35	LYS	2.4
1	G	194	GLN	2.3
5	F	283	GLN	2.3
2	I	169	LYS	2.3
1	H	14	VAL	2.3
2	I	1008	GLN	2.3
2	I	1009	ASN	2.3
3	J	1249	ASN	2.3
2	C	318	SER	2.3
5	F	332	ASP	2.3
3	D	208	THR	2.3
4	K	41	GLU	2.3
2	I	1020	GLU	2.2
1	G	164	ASP	2.2
3	D	217	LEU	2.2
2	C	257	ALA	2.2
5	F	307	THR	2.2
2	I	988	LYS	2.2
4	K	58	LEU	2.2
4	K	77	ALA	2.2
4	K	13	ILE	2.2
1	G	193	GLU	2.2
1	H	74	VAL	2.2
3	J	207	GLU	2.2
4	E	34	GLY	2.2
2	C	164	THR	2.2
2	I	247	ARG	2.2
1	H	13	LEU	2.2
1	H	27	THR	2.2
5	L	304	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	232	ILE	2.2
3	J	1202	GLU	2.2
1	H	233	ASP	2.2
1	B	91	ARG	2.1
1	A	245	GLU	2.1
1	H	107	ILE	2.1
3	J	674	THR	2.1
2	C	999	GLU	2.1
3	D	1201	GLY	2.1
5	F	293	GLU	2.1
1	A	274	ALA	2.1
2	I	234	ASP	2.1
3	J	1198	VAL	2.1
2	C	165	HIS	2.1
2	I	1141	LEU	2.1
2	I	720	ARG	2.1
3	J	1161	GLY	2.1
2	I	185	ASP	2.1
3	J	557	LYS	2.1
4	K	29	GLN	2.1
1	H	86	LYS	2.0
2	C	271	ALA	2.0
2	I	990	ASP	2.0
2	I	373	GLY	2.0
2	C	243	PRO	2.0
2	I	1029	LEU	2.0
3	J	212	THR	2.0
2	I	67	GLU	2.0
4	K	14	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	ZN	D	1502	1/1	0.81	0.13	-0.94	134,134,134,134	0
7	ZN	D	1503	1/1	0.99	0.06	-0.97	51,51,51,51	0
7	ZN	J	1503	1/1	0.95	0.09	-1.43	97,97,97,97	0
7	ZN	J	1502	1/1	0.97	0.02	-1.80	131,131,131,131	0
6	MG	D	1501	1/1	0.94	0.54	-	87,87,87,87	0
6	MG	J	1501	1/1	0.92	0.35	-	94,94,94,94	0

6.5 Other polymers

There are no such residues in this entry.