



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:32 am BST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

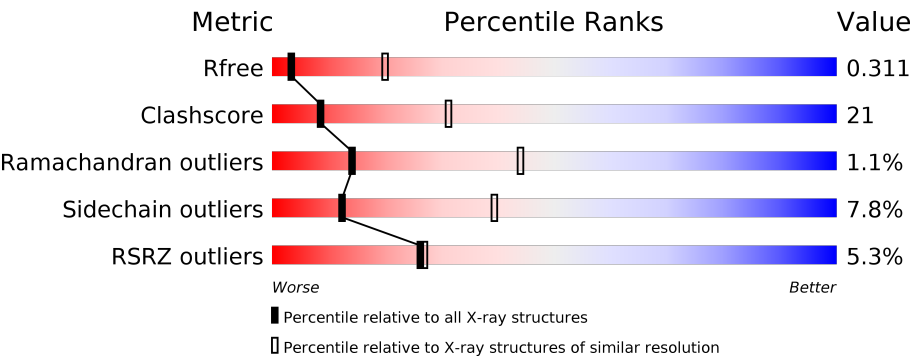
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	320	<div><div></div><div><div></div><div>39%</div><div>30%</div><div></div><div>27%</div></div></div>
1	B	320	<div><div>7%</div><div><div></div><div>32%</div><div>32%</div><div></div><div>32%</div></div></div>
1	G	320	<div><div>3%</div><div><div></div><div>36%</div><div>30%</div><div></div><div>29%</div></div></div>
1	H	320	<div><div>7%</div><div><div></div><div>33%</div><div>32%</div><div></div><div>33%</div></div></div>
2	C	1342	<div><div>4%</div><div><div></div><div>57%</div><div>39%</div><div></div></div></div>
2	I	1342	<div><div>7%</div><div><div></div><div>58%</div><div>38%</div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div></div><div>2%47%31%17%</div><div></div></div>
3	J	1407	<div><div></div><div>4%45%33%18%</div><div></div></div>
4	E	90	<div><div></div><div>3%60%30%9%</div><div></div></div>
4	K	90	<div><div></div><div>22%54%27%7%12%</div><div></div></div>
5	F	613	<div><div></div><div>4%45%28%24%</div><div></div></div>
5	L	613	<div><div></div><div>4%45%28%23%</div><div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55066 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1812	1127	323	356	6			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10569	6632	1841	2053	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10565	6630	1840	2052	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2
I	516	VAL	ASP	engineered mutation	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1167	Total	C	N	O	S	0	0	0
			9065	5700	1622	1697	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

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

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

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

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

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

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

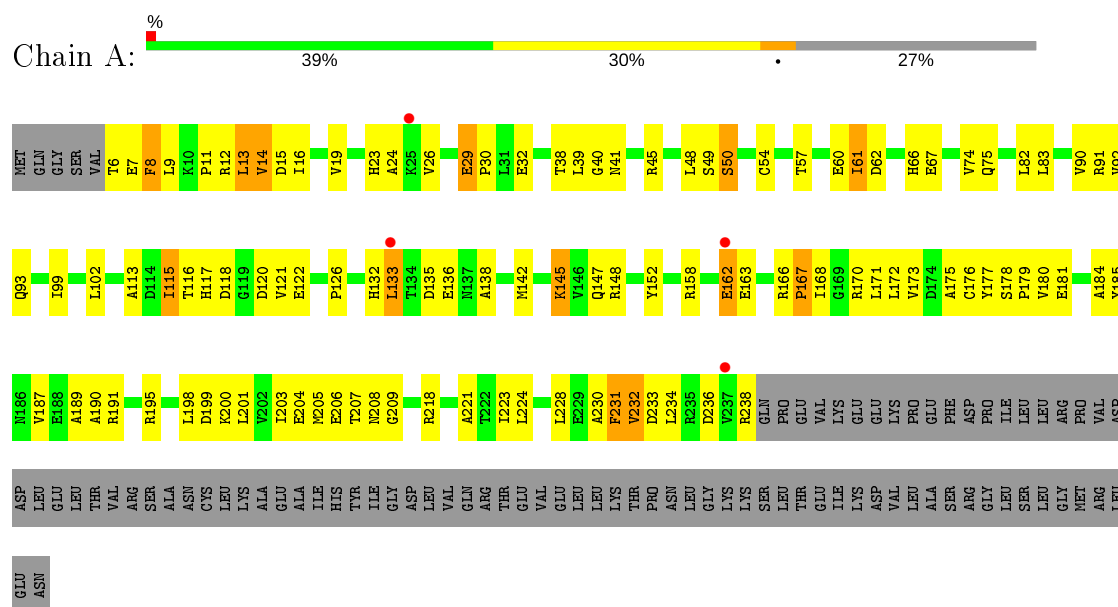
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

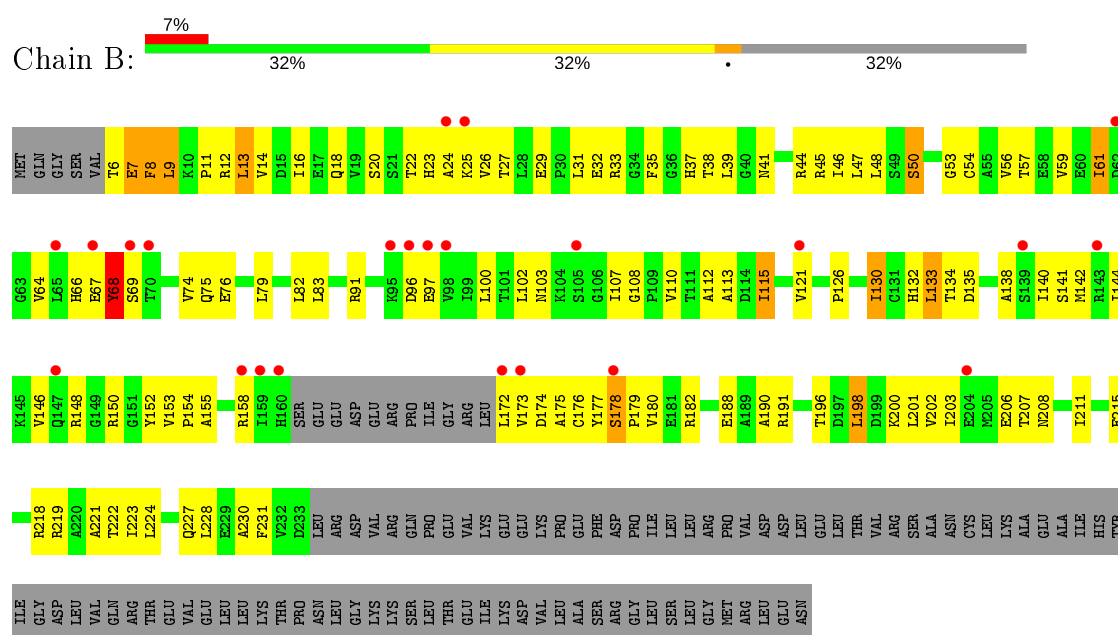
### 3 Residue-property plots [i](#)

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

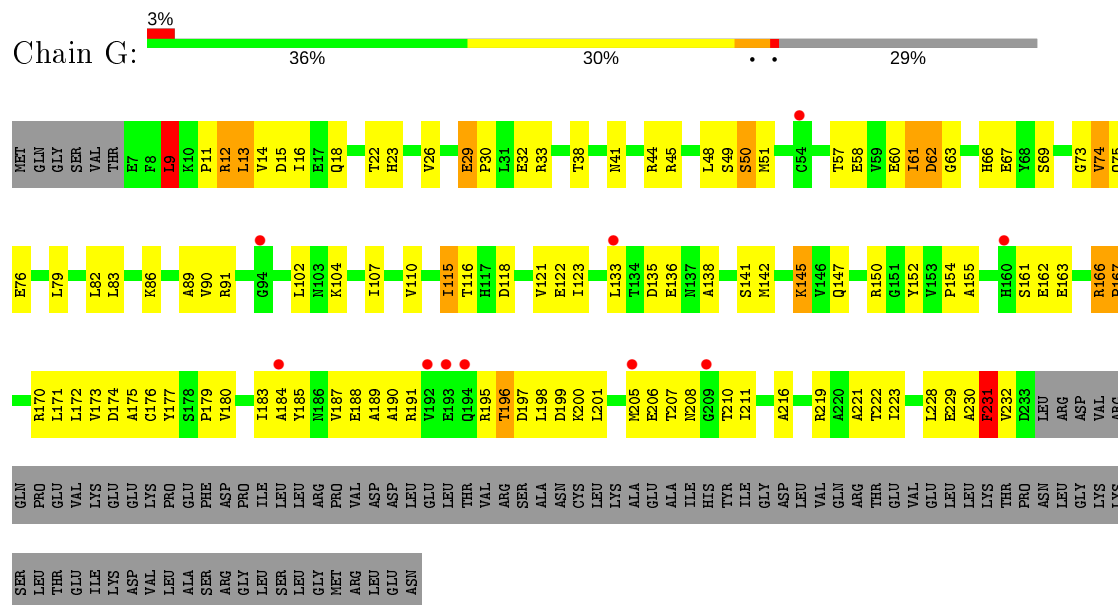
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



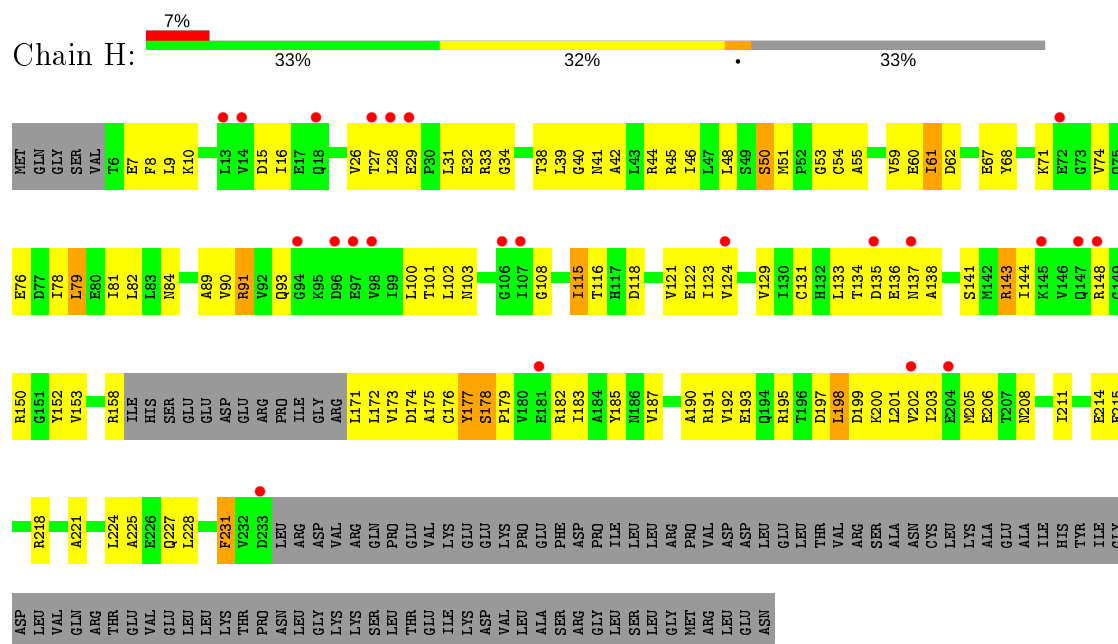
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



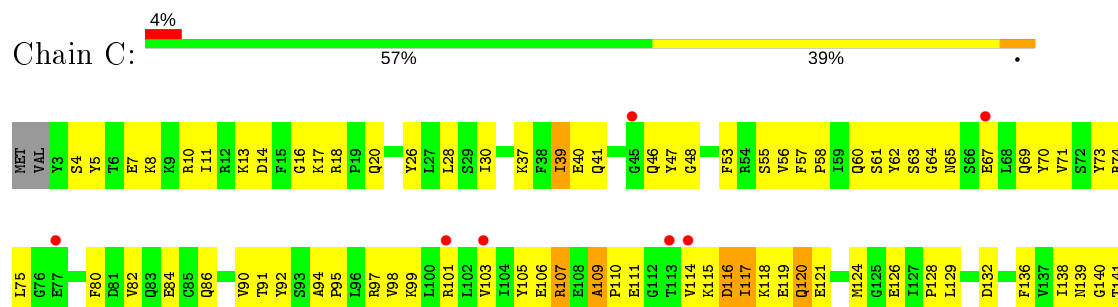
- Molecule 1: DNA-directed RNA polymerase subunit alpha

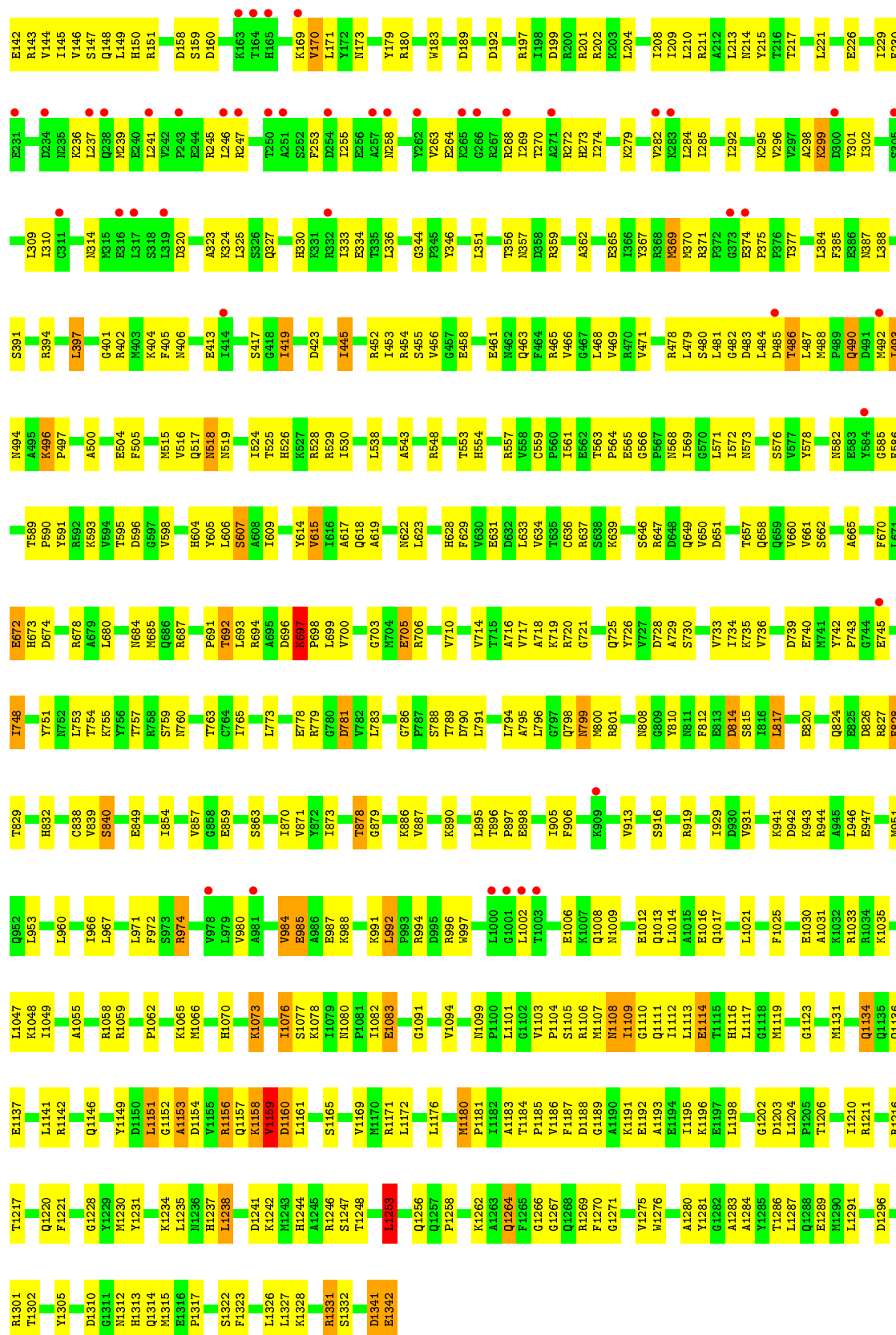


- Molecule 1: DNA-directed RNA polymerase subunit alpha



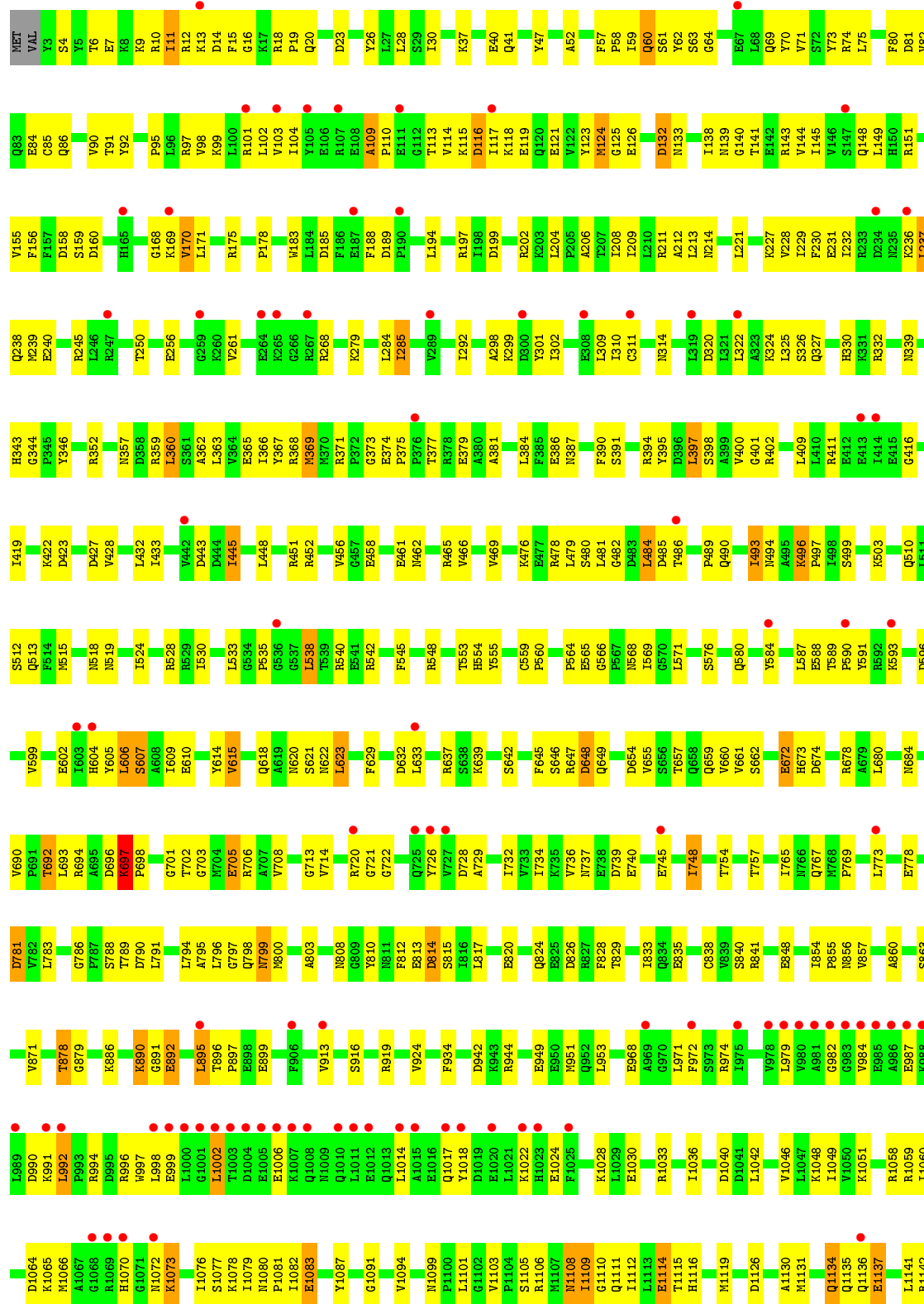
- Molecule 2: DNA-directed RNA polymerase subunit beta

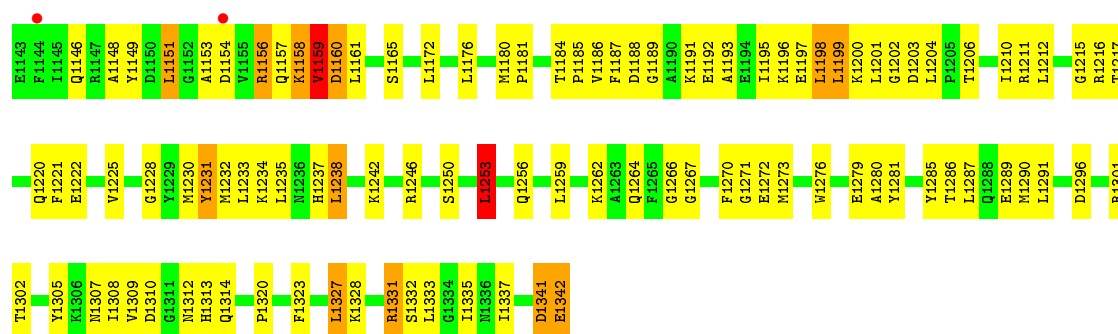




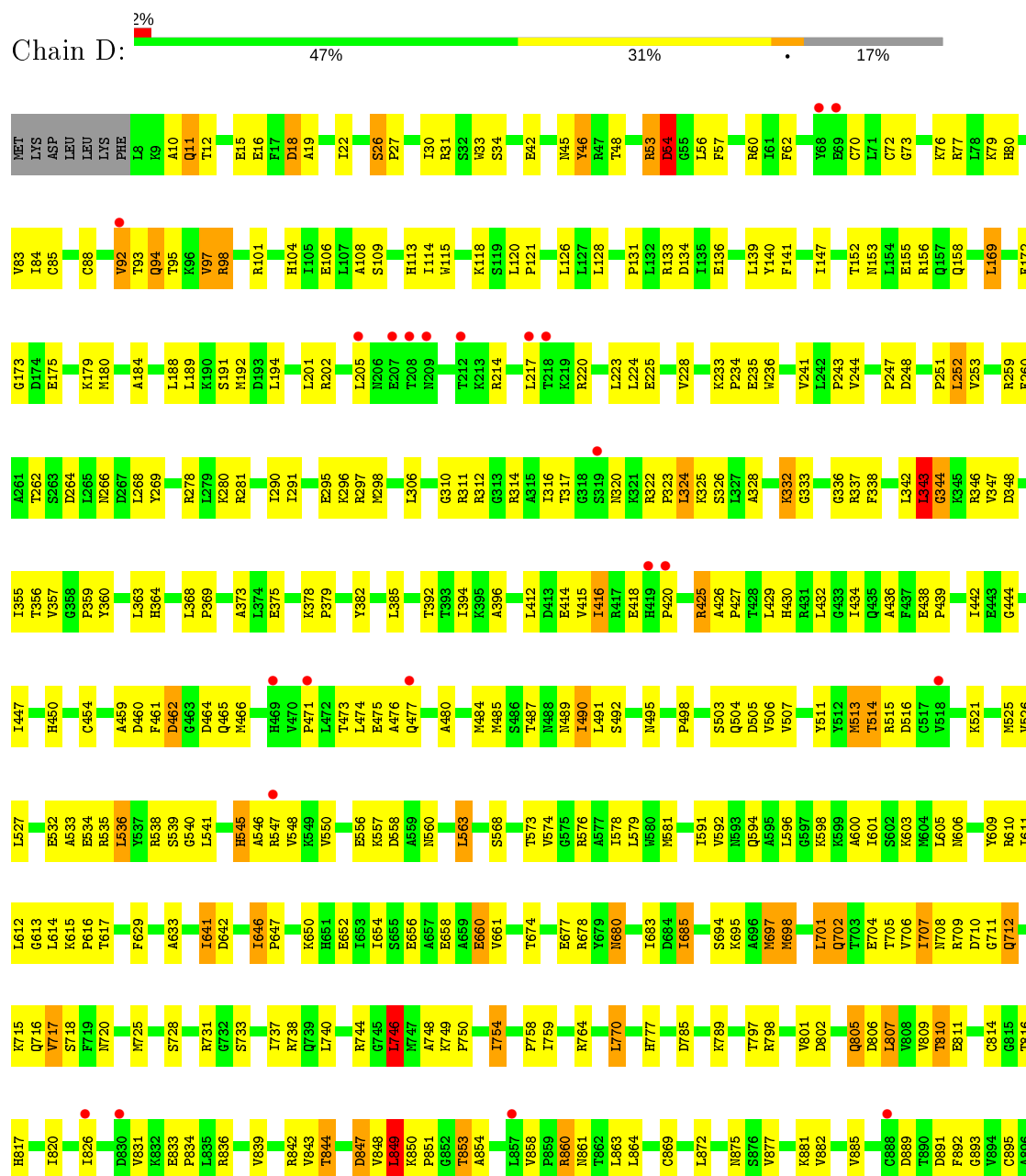
● Molecule 2: DNA-directed RNA polymerase subunit beta

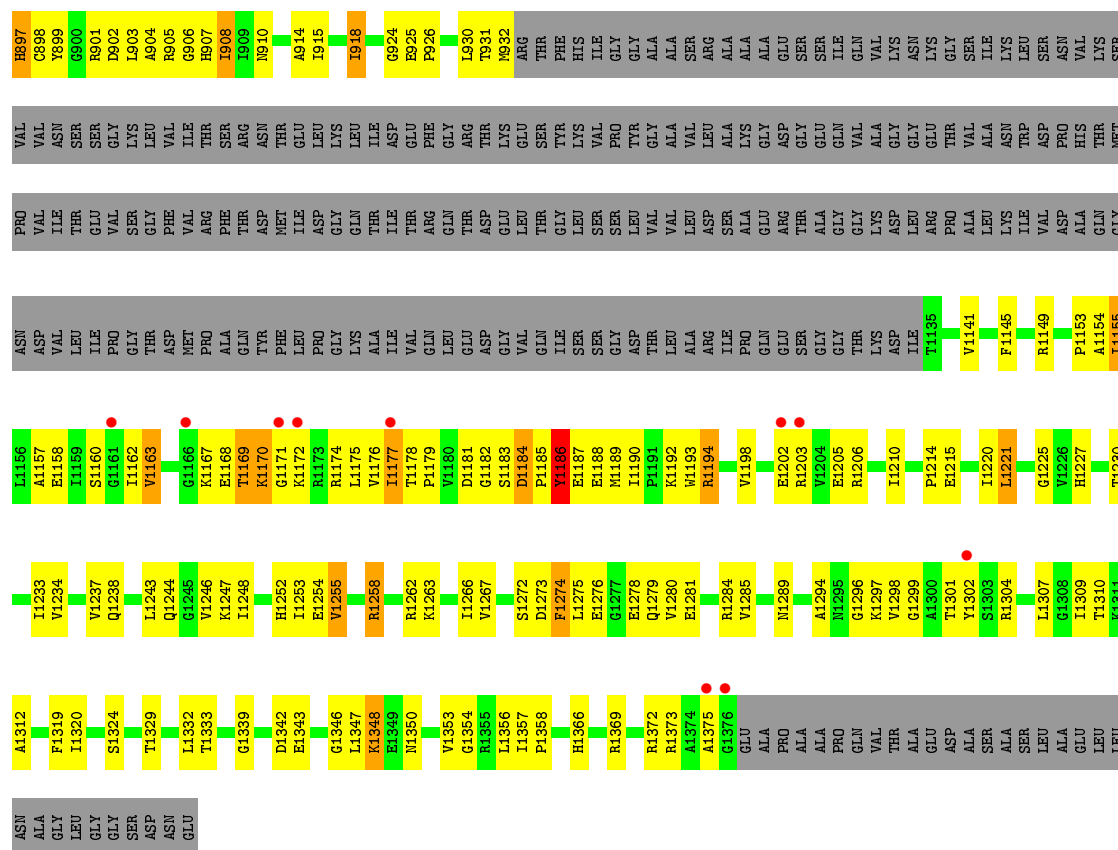




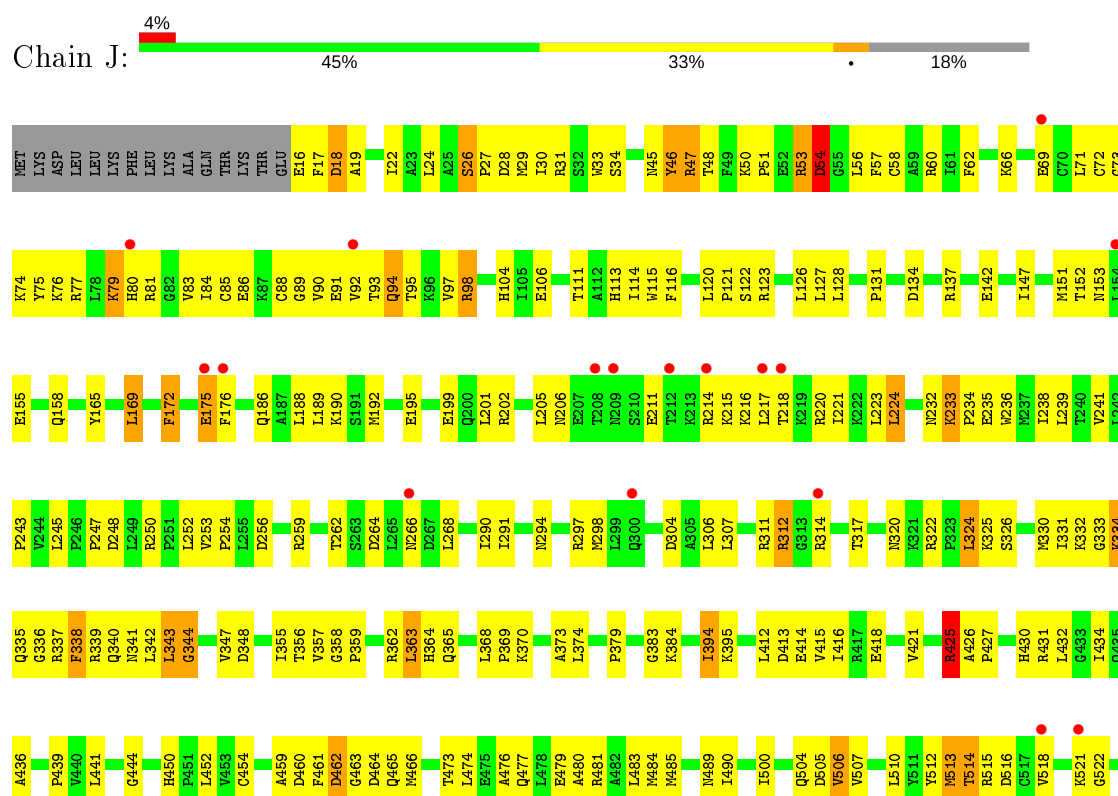


• Molecule 3: DNA-directed RNA polymerase subunit beta'

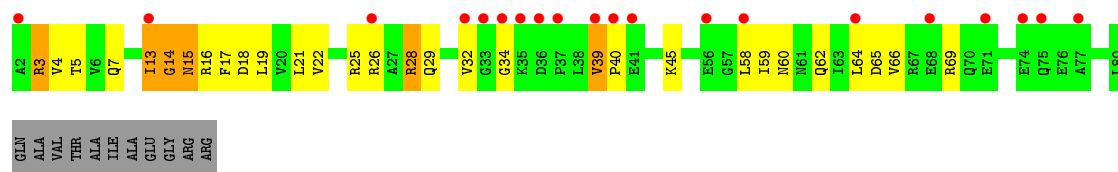




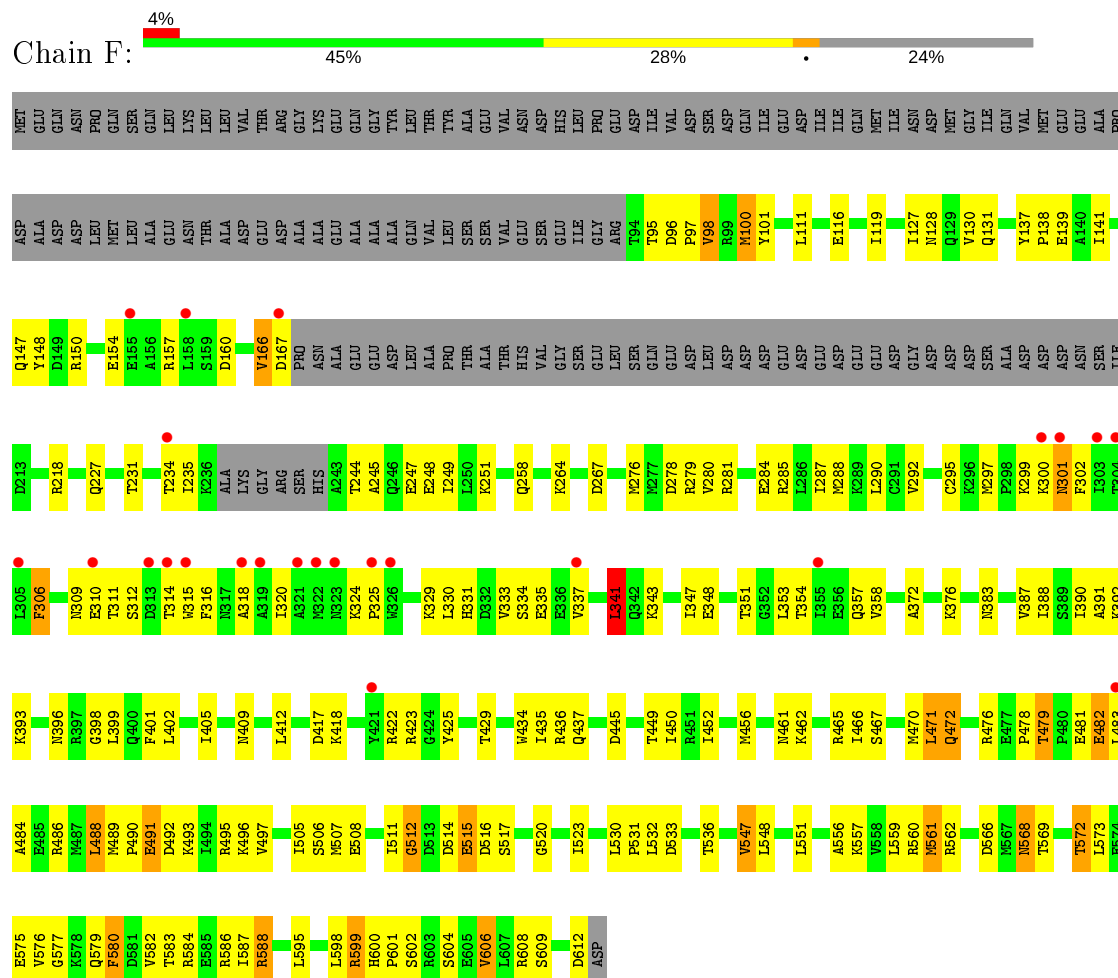
• Molecule 3: DNA-directed RNA polymerase subunit beta'



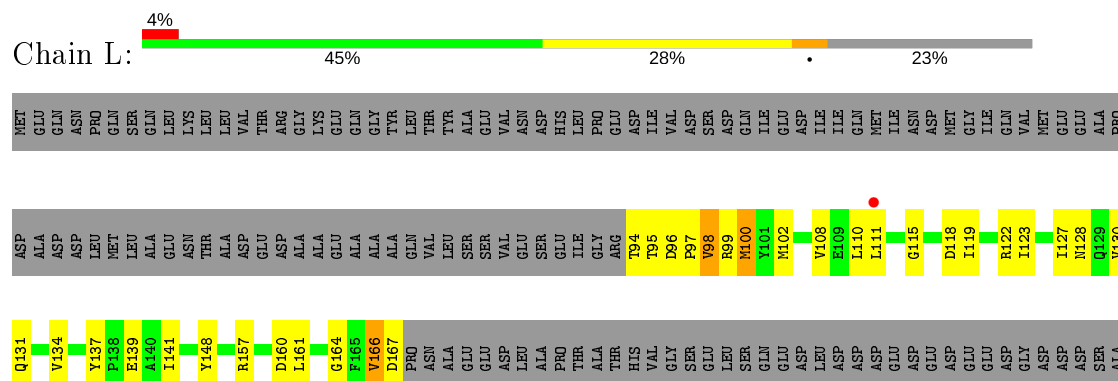




• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD



M567	M568	T569	D570	Y571	T572	L573	E574	E575	V576	G577	F580	D581	V582	T583	R584	I587	R596	K597	L598	R599	H600	P601	S602	R603	S604	E605	V606	L607	D612	D613																					
E478	T479	P480	E481	E482	L483	A484	E485	R486	M487	L488	M489	P490	E491	D492	R495	K499	I500	I505	S506	N507	E508	I511	G512	D513	D514	E515	D516	S517	G520	E524	D525	L530	P531	L532	D533	T536	T544	V547	L551	K557	V558	L559	R560	M561	R562	D566					
A375	K376	V380	E381	V387	I388	S389	I390	A391	K392	K393	T394	T395	R396	I399	Q400	F401	L402	Q406	N409	V416	D417	F420	R421	R422	R423	Q424	Y425	T429	I435	D445	T449	I450	R451	I452	N461	K462	R465	I466	S467	R468	Q469	N470	L471	R476	E477						
K289	L290	E293	K299	K300	N301	F302	F306	N309	E310	T311	S312	D313	T314	W315	F316	N317	A318	A319	I320	A321	N322	N323	K324	P325	E328	E335	E336	V337	R338	R339	A340	I341	K342	K343	L344	Q345	E348	T351	T354	V358	N362	E369	A370	K371	A372	R373	R374				
ASP	ASP	ASP	ASN	SER	ILE	D213	R218	Q227	T231	K236	ALA	LYS	GLY	ARG	SER	HIS	A243	T244	E247	E248	I249	L249	L250	K251	L252	S253	E254	Q258	F259	R260	L261	V262	P263	K264	Q265	F266	D267	V270	M273	R274	V275	M276	M277	D278	R279	V280	R281	R285	L286	I287	M288

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.83Å 205.04Å 307.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.40 29.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.99-3.40) 89.0 (29.99-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.39Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.277 , 0.311 0.277 , 0.311	Depositor DCC
$R_{free}$ test set	1977 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	135.9	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 85.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	55066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.46	1/1834 (0.1%)	0.85	0/2485
1	B	0.45	0/1697	1.00	3/2300 (0.1%)
1	G	0.52	1/1777 (0.1%)	0.93	5/2408 (0.2%)
1	H	0.44	0/1681	0.98	3/2278 (0.1%)
2	C	0.44	0/10738	0.83	7/14488 (0.0%)
2	I	0.42	1/10734 (0.0%)	0.81	12/14483 (0.1%)
3	D	0.45	0/9205	0.84	12/12430 (0.1%)
3	J	0.45	0/9140	0.88	22/12341 (0.2%)
4	E	0.43	0/693	0.76	1/935 (0.1%)
4	K	0.43	0/629	0.81	2/847 (0.2%)
5	F	0.42	0/3864	0.83	5/5194 (0.1%)
5	L	0.43	0/3872	0.83	3/5205 (0.1%)
All	All	0.44	3/55864 (0.0%)	0.85	75/75394 (0.1%)

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

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

All (3) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	29	GLU	C-N	9.36	1.52	1.34
2	I	373	GLY	C-N	7.20	1.50	1.34
1	A	29	GLU	C-N	6.31	1.46	1.34

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	425	ARG	NE-CZ-NH2	14.52	127.56	120.30
3	J	425	ARG	NE-CZ-NH1	-13.50	113.55	120.30
3	J	343	LEU	CB-CG-CD1	-11.67	91.16	111.00
1	G	12	ARG	NE-CZ-NH1	-10.66	114.97	120.30
3	D	343	LEU	CB-CG-CD2	-10.37	93.37	111.00
1	G	62	ASP	CB-CG-OD2	10.00	127.30	118.30
3	J	563	LEU	CB-CG-CD2	-9.95	94.09	111.00
3	D	563	LEU	CB-CG-CD2	-9.38	95.05	111.00
2	C	1151	LEU	CA-CB-CG	-8.13	96.60	115.30
2	C	397	LEU	CA-CB-CG	7.70	133.01	115.30
3	J	314	ARG	NE-CZ-NH2	-7.66	116.47	120.30
3	J	899	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	B	68	TYR	CA-CB-CG	7.47	127.60	113.40
1	G	33	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	130	ILE	CG1-CB-CG2	-7.27	95.41	111.40
3	J	54	ASP	N-CA-C	-7.20	91.55	111.00
3	J	314	ARG	NE-CZ-NH1	7.20	123.90	120.30
5	F	341	LEU	CB-CG-CD2	-7.12	98.89	111.00
4	K	28	ARG	NE-CZ-NH2	-7.12	116.74	120.30
3	J	857	LEU	CA-CB-CG	7.03	131.47	115.30
3	D	54	ASP	N-CA-C	-6.98	92.15	111.00
3	J	1274	PHE	CB-CG-CD2	-6.96	115.93	120.80
2	C	1180	MET	CG-SD-CE	-6.70	89.48	100.20
3	J	746	LEU	CA-CB-CG	6.64	130.56	115.30
2	C	107	ARG	NE-CZ-NH2	6.62	123.61	120.30
5	L	449	THR	CA-CB-CG2	-6.49	103.32	112.40
3	J	53	ARG	N-CA-C	-6.40	93.73	111.00
2	I	813	GLU	CA-CB-CG	6.33	127.34	113.40
1	G	62	ASP	CB-CG-OD1	-6.29	112.64	118.30
3	J	1274	PHE	CB-CG-CD1	6.21	125.15	120.80
3	D	53	ARG	N-CA-C	-6.16	94.36	111.00
2	I	124	MET	CA-CB-CG	-6.13	102.87	113.30
3	D	460	ASP	CB-CA-C	5.98	122.37	110.40
1	H	79	LEU	CA-CB-CG	5.98	129.05	115.30
2	I	1253	LEU	CA-CB-CG	5.80	128.64	115.30
3	J	849	LEU	CA-CB-CG	5.77	128.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	28	ARG	NE-CZ-NH1	5.76	123.18	120.30
3	J	224	LEU	CA-CB-CG	5.64	128.28	115.30
3	J	1243	LEU	CB-CG-CD1	-5.63	101.43	111.00
2	I	648	ASP	CB-CG-OD1	-5.62	113.24	118.30
2	I	397	LEU	CA-CB-CG	5.56	128.10	115.30
3	J	47	ARG	CG-CD-NE	5.52	123.40	111.80
2	C	1253	LEU	CA-CB-CG	5.52	127.99	115.30
3	J	89	GLY	N-CA-C	-5.52	99.31	113.10
5	L	571	TYR	CB-CG-CD1	-5.52	117.69	121.00
2	I	1199	LEU	CA-CB-CG	5.51	127.98	115.30
5	F	95	THR	C-N-CA	5.46	135.36	121.70
3	J	151	MET	CA-CB-CG	5.45	122.56	113.30
1	H	50	SER	C-N-CA	-5.43	108.12	121.70
5	F	436	ARG	CG-CD-NE	5.42	123.17	111.80
3	D	1258	ARG	NE-CZ-NH1	-5.41	117.60	120.30
2	I	285	ILE	CG1-CB-CG2	-5.41	99.51	111.40
2	I	237	LEU	N-CA-C	5.38	125.52	111.00
3	J	563	LEU	CA-CB-CG	5.35	127.61	115.30
5	L	470	MET	CA-CB-CG	-5.34	104.23	113.30
3	D	746	LEU	CA-CB-CG	5.30	127.50	115.30
2	C	1264	GLN	N-CA-C	-5.29	96.72	111.00
1	H	93	GLN	CB-CA-C	-5.25	99.90	110.40
1	B	50	SER	C-N-CA	-5.25	108.58	121.70
3	J	899	TYR	CB-CG-CD1	5.24	124.15	121.00
5	F	588	ARG	CB-CG-CD	5.24	125.21	111.60
3	D	1186	TYR	CB-CG-CD2	-5.21	117.88	121.00
3	D	1348	LYS	CA-CB-CG	5.21	124.86	113.40
2	C	237	LEU	N-CA-C	5.18	125.00	111.00
3	J	1298	VAL	C-N-CA	5.16	133.13	122.30
2	I	360	LEU	CA-CB-CG	5.12	127.08	115.30
2	I	1202	GLY	N-CA-C	-5.11	100.34	113.10
2	I	606	LEU	CB-CG-CD2	-5.09	102.34	111.00
3	D	899	TYR	CB-CG-CD2	-5.09	117.95	121.00
2	I	982	GLY	C-N-CA	-5.08	111.62	122.30
3	D	344	GLY	N-CA-C	-5.08	100.40	113.10
3	D	849	LEU	CA-CB-CG	5.08	126.97	115.30
1	G	82	LEU	CA-CB-CG	5.05	126.92	115.30
5	F	341	LEU	CB-CA-C	-5.04	100.63	110.20
4	E	76	GLU	OE1-CD-OE2	-5.01	117.29	123.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

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

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1812	0	1839	111	0
1	B	1677	0	1703	127	0
1	G	1755	0	1773	105	0
1	H	1662	0	1687	111	0
2	C	10569	0	10587	439	0
2	I	10565	0	10581	437	0
3	D	9065	0	9210	430	0
3	J	9001	0	9165	461	0
4	E	691	0	695	26	0
4	K	627	0	634	26	0
5	F	3813	0	3880	150	0
5	L	3821	0	3884	149	0
6	D	2	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	55066	0	55638	2292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 21.

All (2292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1271:GLY:HA2	3:J:343:LEU:HD11	1.25	1.18
2:C:1269:ARG:HG2	3:D:343:LEU:HD12	1.24	1.11
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.35	1.08
3:D:1167:LYS:HZ3	3:D:1170:LYS:HB2	1.18	1.06
3:J:54:ASP:OD2	3:J:60:ARG:NH1	1.89	1.03
2:I:1271:GLY:CA	3:J:343:LEU:HD11	1.87	1.03
2:C:1271:GLY:HA2	3:D:343:LEU:HD21	1.41	1.02
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.44	1.00
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.44	0.99
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.45	0.99
3:J:1167:LYS:HZ3	3:J:1170:LYS:HB2	1.27	0.98
5:F:562:ARG:HH21	5:F:573:LEU:HD23	1.28	0.98
1:B:75:GLN:HE22	1:B:132:HIS:HB2	1.29	0.95
1:A:14:VAL:HG13	1:A:15:ASP:H	1.31	0.95
5:F:595:LEU:O	5:F:599:ARG:HD3	1.66	0.95
2:C:40:GLU:O	2:C:73:TYR:OH	1.85	0.94
3:D:54:ASP:OD2	3:D:60:ARG:NH1	1.99	0.94
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.49	0.94
1:B:191:ARG:NH1	1:B:196:THR:O	2.00	0.93
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.48	0.92
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.51	0.92
2:C:1271:GLY:CA	3:D:343:LEU:HD21	1.99	0.91
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.53	0.91
2:I:674:ASP:OD1	2:I:1110:GLY:N	2.04	0.91
1:B:16:ILE:HG23	1:B:26:VAL:HG22	1.50	0.91
1:A:45:ARG:HG2	1:B:38:THR:HB	1.51	0.90
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.03	0.90
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.52	0.89
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.05	0.89
2:C:1269:ARG:HG2	3:D:343:LEU:CD1	2.02	0.89
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.05	0.88
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	1.89	0.88
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.54	0.88
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.07	0.87
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.56	0.87
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.54	0.87
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.55	0.87
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:18:ARG:NH1	2:I:621:SER:O	2.07	0.86
1:A:191:ARG:NH1	1:A:198:LEU:O	2.08	0.86
2:C:478:ARG:HG2	2:C:492:MET:HG2	1.57	0.86
2:I:560:PRO:O	3:J:780:ARG:NH2	2.09	0.86
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.40	0.86
3:D:392:THR:HG21	5:F:606:VAL:HA	1.58	0.86
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.58	0.85
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.59	0.85
2:I:1271:GLY:HA2	3:J:343:LEU:CD1	2.06	0.85
2:I:452:ARG:NH1	2:I:584:TYR:O	2.10	0.84
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.59	0.84
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.57	0.84
2:C:201:ARG:NH2	2:C:370:MET:O	2.09	0.84
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.57	0.84
2:C:324:LYS:O	2:C:327:GLN:NE2	2.11	0.84
5:L:97:PRO:HA	5:L:100:MET:HG3	1.61	0.83
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.61	0.83
2:I:721:GLY:N	2:I:740:GLU:OE1	2.12	0.83
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	1.92	0.83
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.61	0.82
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.61	0.82
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.11	0.82
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.15	0.81
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.61	0.81
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.26	0.81
3:D:45:ASN:HB3	3:D:48:THR:O	1.80	0.81
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.61	0.81
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.63	0.81
2:C:1271:GLY:HA2	3:D:343:LEU:CD2	2.11	0.81
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.09	0.81
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.63	0.81
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.44	0.80
2:C:721:GLY:N	2:C:740:GLU:OE1	2.15	0.80
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.17	0.80
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.44	0.80
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	1.97	0.80
5:L:602:SER:H	5:L:605:GLU:HG3	1.45	0.80
3:D:1263:LYS:HE2	3:D:1279:GLN:HE21	1.47	0.80
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.12	0.79
1:H:158:ARG:HB3	1:H:172:LEU:HD23	1.63	0.79
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:LEU:HD23	2:I:694:ARG:HE	1.48	0.79
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.14	0.79
3:D:1263:LYS:HE2	3:D:1279:GLN:NE2	1.98	0.78
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.47	0.78
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.16	0.78
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.16	0.78
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.66	0.78
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.17	0.77
3:D:336:GLY:HA3	3:D:1324:SER:O	1.82	0.77
5:L:551:LEU:HD21	5:L:598:LEU:HD21	1.65	0.77
1:B:79:LEU:HD11	3:D:526:VAL:HG21	1.65	0.77
1:B:154:PRO:HA	1:B:174:ASP:HB3	1.66	0.77
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.67	0.77
1:G:45:ARG:HG2	1:H:38:THR:HB	1.67	0.77
1:A:45:ARG:NH2	2:C:1216:ARG:HA	1.99	0.76
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.20	0.76
5:F:227:GLN:HE22	5:F:251:LYS:NZ	1.81	0.76
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.18	0.76
1:B:175:ALA:HB1	1:B:177:TYR:CE1	2.20	0.76
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.68	0.76
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.67	0.76
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.17	0.76
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.68	0.76
2:I:706:ARG:NH2	2:I:791:LEU:O	2.18	0.76
2:I:1296:ASP:HB3	2:I:1320:PRO:HB3	1.67	0.76
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.17	0.76
1:B:18:GLN:NE2	1:B:24:ALA:HB2	2.00	0.76
2:C:696:ASP:HB2	2:C:798:GLN:CG	2.15	0.76
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.68	0.76
1:B:16:ILE:HG12	1:B:26:VAL:HG13	1.68	0.75
3:D:1181:ASP:HA	3:J:202:ARG:HB3	1.68	0.75
4:K:14:GLY:O	4:K:16:ARG:N	2.20	0.75
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.67	0.75
5:F:388:ILE:O	5:F:392:LYS:HG3	1.86	0.75
2:C:1062:PRO:HA	2:C:1076:ILE:HG13	1.69	0.75
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.19	0.75
1:B:153:VAL:O	1:B:175:ALA:N	2.15	0.75
4:E:13:ILE:HD12	4:E:19:LEU:HA	1.69	0.75
1:B:134:THR:HG23	1:B:135:ASP:H	1.49	0.75
3:D:418:GLU:HG3	4:E:45:LYS:H	1.51	0.75
1:H:90:VAL:HG13	1:H:123:ILE:HD12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.69	0.74
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.20	0.74
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.67	0.74
1:G:12:ARG:H	1:G:30:PRO:HD2	1.53	0.74
1:G:231:PHE:HB3	1:H:218:ARG:HB3	1.69	0.74
3:J:127:LEU:O	3:J:220:ARG:NH2	2.20	0.74
1:A:158:ARG:NH2	1:A:173:VAL:O	2.17	0.74
1:H:27:THR:HG23	1:H:202:VAL:HG22	1.69	0.74
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.70	0.74
5:L:395:THR:OG1	5:L:396:ASN:N	2.21	0.74
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.70	0.74
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.69	0.74
5:L:601:PRO:HA	5:L:604:SER:HB3	1.69	0.74
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.70	0.73
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.70	0.73
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.69	0.73
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.69	0.73
1:H:32:GLU:HA	1:H:198:LEU:HD12	1.70	0.73
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.22	0.73
5:L:483:LEU:H	5:L:483:LEU:HD12	1.52	0.73
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	1.89	0.73
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.54	0.73
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.54	0.73
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.23	0.73
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.71	0.73
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.71	0.73
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.52	0.73
5:F:300:LYS:HE3	5:F:301:ASN:HD21	1.53	0.73
2:I:40:GLU:O	2:I:73:TYR:OH	2.06	0.73
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.04	0.73
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.71	0.72
3:J:709:ARG:O	3:J:711:GLY:N	2.22	0.72
3:J:1263:LYS:HE2	3:J:1279:GLN:HE21	1.54	0.72
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.37	0.72
3:D:1186:TYR:HE2	3:D:1188:GLU:HB2	1.54	0.72
3:J:114:ILE:HD11	3:J:311:ARG:HB2	1.70	0.72
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.72	0.72
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.05	0.72
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.71	0.71
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.23	0.71
2:C:40:GLU:HG2	2:C:41:GLN:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.72	0.71
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.73	0.71
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.56	0.71
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.73	0.71
3:D:709:ARG:O	3:D:711:GLY:N	2.24	0.71
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.71	0.71
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.24	0.71
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.25	0.71
1:A:9:LEU:O	1:B:227:GLN:NE2	2.24	0.70
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.73	0.70
1:G:14:VAL:HG13	1:G:15:ASP:H	1.56	0.70
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.72	0.70
3:D:842:ARG:NH1	3:D:1254:GLU:OE2	2.18	0.70
2:C:74:ARG:NH1	2:C:121:GLU:OE1	2.23	0.70
2:C:810:TYR:HE1	2:C:1078:LYS:HD2	1.55	0.70
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.73	0.70
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.24	0.70
5:F:515:GLU:C	5:F:517:SER:H	1.95	0.70
1:H:152:TYR:CE2	3:J:536:LEU:HD21	2.26	0.70
1:H:211:ILE:HD11	1:H:215:GLU:HG2	1.73	0.70
3:J:320:ASN:OD1	3:J:322:ARG:HB3	1.91	0.70
1:B:66:HIS:CE1	1:B:69:SER:OG	2.44	0.70
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.23	0.70
3:J:901:ARG:HD2	3:J:906:GLY:O	1.92	0.70
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	1.92	0.70
1:G:32:GLU:OE2	1:H:150:ARG:NH2	2.25	0.70
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.74	0.69
2:C:197:ARG:NH1	2:C:201:ARG:O	2.25	0.69
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.25	0.69
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.74	0.69
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.27	0.69
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.26	0.69
2:C:705:GLU:HB2	2:C:794:LEU:H	1.57	0.69
1:G:75:GLN:HA	2:I:729:ALA:N	2.08	0.69
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	1.92	0.69
3:J:1169:THR:OG1	3:J:1192:LYS:HD3	1.91	0.69
3:J:518:VAL:O	3:J:547:ARG:NH1	2.25	0.69
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.74	0.69
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.73	0.69
2:C:41:GLN:NE2	2:C:73:TYR:O	2.26	0.69
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:LEU:O	1:G:230:ALA:N	2.23	0.69
3:J:905:ARG:NH1	3:J:910:ASN:HD21	1.90	0.69
1:H:153:VAL:HG11	1:H:158:ARG:HH11	1.57	0.69
1:H:214:GLU:HG2	1:H:218:ARG:NH2	2.06	0.69
2:I:18:ARG:NH2	2:I:622:ASN:OD1	2.25	0.69
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.58	0.69
3:D:1158:GLU:HG3	3:D:1186:TYR:CZ	2.28	0.69
2:I:324:LYS:O	2:I:327:GLN:NE2	2.25	0.69
2:C:402:ARG:NH2	2:C:419:ILE:O	2.26	0.69
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.75	0.69
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.75	0.69
2:C:528:ARG:NH2	2:C:576:SER:O	2.26	0.68
2:C:565:GLU:HG2	2:C:565:GLU:O	1.92	0.68
5:F:601:PRO:HA	5:F:604:SER:HB3	1.75	0.68
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.74	0.68
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.25	0.68
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.23	0.68
5:L:244:THR:O	5:L:247:GLU:HG2	1.93	0.68
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.74	0.68
1:A:7:GLU:O	1:B:150:ARG:NH1	2.27	0.68
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.59	0.68
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.75	0.68
1:G:191:ARG:HH12	1:G:197:ASP:HA	1.57	0.68
3:J:680:ASN:O	3:J:683:ILE:HG22	1.93	0.68
5:L:600:HIS:CD2	5:L:601:PRO:HD2	2.28	0.68
1:G:188:GLU:O	1:G:200:LYS:N	2.23	0.68
3:D:396:ALA:HB2	5:F:609:SER:HB2	1.75	0.68
1:H:101:THR:HG22	1:H:116:THR:HG21	1.73	0.68
2:I:992:LEU:HD12	2:I:996:ARG:HB3	1.76	0.68
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.75	0.68
3:D:259:ARG:HG2	3:D:260:PHE:H	1.57	0.68
2:I:148:GLN:NE2	2:I:535:PRO:O	2.20	0.68
3:J:50:LYS:HD3	3:J:71:LEU:HD21	1.74	0.68
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.27	0.67
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.60	0.67
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.77	0.67
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.76	0.67
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.76	0.67
5:F:547:VAL:HG22	5:F:598:LEU:CD2	2.24	0.67
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.58	0.67
3:D:1160:SER:HG	3:D:1203:ARG:HH12	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.28	0.67
2:C:115:LYS:HD3	2:C:116:ASP:N	2.10	0.67
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.77	0.67
5:F:166:VAL:O	5:F:167:ASP:HB2	1.94	0.67
2:I:829:THR:HA	2:I:1059:ARG:HA	1.77	0.67
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.76	0.67
3:D:310:GLY:CA	3:D:314:ARG:HD2	2.22	0.67
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.77	0.67
1:G:219:ARG:O	1:G:223:ILE:HG13	1.94	0.67
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.75	0.67
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	1.94	0.67
3:D:11:GLN:HG2	3:D:15:GLU:HG3	1.77	0.67
3:D:205:LEU:HD22	3:D:214:ARG:HB2	1.77	0.67
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.30	0.67
1:B:188:GLU:O	1:B:200:LYS:N	2.24	0.67
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.27	0.67
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.59	0.67
3:D:73:GLY:O	3:D:76:LYS:NZ	2.21	0.67
1:H:74:VAL:HG12	1:H:76:GLU:H	1.60	0.67
3:D:885:VAL:O	3:D:1258:ARG:HD2	1.96	0.66
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.28	0.66
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.96	0.66
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.77	0.66
1:B:48:LEU:HD22	3:D:539:SER:HB3	1.77	0.66
2:C:211:ARG:NH1	2:C:357:ASN:O	2.28	0.66
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.76	0.66
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.08	0.66
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.78	0.66
3:D:54:ASP:OD2	3:D:60:ARG:HD3	1.96	0.66
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.61	0.66
3:J:514:THR:OG1	3:J:594:GLN:O	2.12	0.66
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.28	0.66
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.78	0.66
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.31	0.66
2:C:106:GLU:HB3	2:C:109:ALA:HB2	1.78	0.66
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.78	0.66
1:G:155:ALA:N	1:G:174:ASP:OD1	2.29	0.66
1:H:16:ILE:HG23	1:H:26:VAL:HG22	1.76	0.66
3:J:45:ASN:HB3	3:J:48:THR:O	1.96	0.66
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.31	0.66
1:B:182:ARG:NH1	3:D:581:MET:SD	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.78	0.66
5:F:599:ARG:HG2	5:F:599:ARG:NH1	2.10	0.66
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.76	0.66
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.77	0.66
1:B:18:GLN:CD	1:B:24:ALA:HB2	2.17	0.66
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.14	0.66
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.78	0.66
2:C:710:VAL:HG13	2:C:717:VAL:HG21	1.77	0.65
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.78	0.65
3:J:1263:LYS:HE2	3:J:1279:GLN:NE2	2.11	0.65
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.77	0.65
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.76	0.65
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.78	0.65
2:I:1250:SER:OG	5:L:524:GLU:OE1	2.14	0.65
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.78	0.65
3:D:1301:THR:HA	3:J:1297:LYS:HE2	1.77	0.65
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.79	0.65
5:F:316:PHE:HZ	5:F:334:SER:HA	1.61	0.65
2:I:80:PHE:HB3	2:I:84:GLU:HB2	1.79	0.65
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.25	0.65
3:J:885:VAL:O	3:J:1258:ARG:HD2	1.96	0.65
1:G:45:ARG:HH12	1:H:38:THR:H	1.45	0.65
3:J:832:LYS:HD3	3:J:1242:ARG:HH11	1.59	0.65
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.32	0.65
3:J:370:LYS:HG2	3:J:441:LEU:HD12	1.77	0.65
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.78	0.65
2:I:1242:LYS:HD2	3:J:465:GLN:OE1	1.97	0.65
3:J:473:THR:HG23	3:J:476:ALA:H	1.61	0.65
5:L:300:LYS:HE3	5:L:301:ASN:HD21	1.62	0.65
3:D:1266:ILE:HB	3:D:1274:PHE:O	1.96	0.65
3:D:515:ARG:NH2	3:D:717:VAL:O	2.30	0.65
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.77	0.65
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.78	0.65
2:I:314:ASN:O	2:I:352:ARG:NH1	2.30	0.65
2:I:211:ARG:NH1	2:I:357:ASN:O	2.29	0.65
2:I:580:GLN:HB2	2:I:605:TYR:HE1	1.62	0.65
1:G:73:GLY:N	2:I:728:ASP:OD2	2.15	0.65
1:B:74:VAL:HG12	1:B:76:GLU:H	1.60	0.64
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.30	0.64
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.08	0.64
2:C:798:GLN:OE1	2:C:827:ARG:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.63	0.64
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.79	0.64
1:H:62:ASP:HB2	1:H:141:SER:O	1.98	0.64
2:I:256:GLU:HB3	2:I:261:VAL:HG22	1.79	0.64
2:C:696:ASP:CB	2:C:798:GLN:HG2	2.22	0.64
2:I:452:ARG:HH21	2:I:458:GLU:CD	2.01	0.64
2:C:4:SER:OG	2:C:5:TYR:N	2.30	0.64
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.80	0.64
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.80	0.64
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.63	0.64
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.79	0.64
1:B:107:ILE:HG12	1:B:135:ASP:HA	1.79	0.64
3:D:557:LYS:HA	3:D:563:LEU:HA	1.80	0.64
1:G:150:ARG:NH1	1:H:7:GLU:O	2.30	0.64
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.13	0.64
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.79	0.64
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.31	0.64
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.80	0.63
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.78	0.63
3:D:1206:ARG:NH2	3:J:1295:ASN:OD1	2.29	0.63
1:B:53:GLY:HA3	1:B:177:TYR:O	1.99	0.63
2:C:1101:LEU:O	3:D:731:ARG:HD3	1.98	0.63
2:C:1099:ASN:ND2	3:D:505:ASP:OD1	2.32	0.63
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.79	0.63
2:C:719:LYS:N	2:C:751:TYR:OH	2.26	0.63
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.80	0.63
2:C:402:ARG:NE	2:C:417:SER:O	2.31	0.63
1:H:182:ARG:NH1	3:J:581:MET:SD	2.72	0.63
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.63	0.63
5:F:599:ARG:HG2	5:F:599:ARG:HH11	1.62	0.63
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.80	0.63
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.79	0.63
3:J:115:TRP:CZ2	3:J:1329:THR:HG23	2.34	0.63
3:J:847:ASP:OD2	3:J:860:ARG:HG2	1.98	0.63
1:G:45:ARG:NH1	1:H:38:THR:H	1.96	0.63
2:I:1042:LEU:HD22	2:I:1049:ILE:HD12	1.81	0.63
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.14	0.63
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.79	0.63
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.64	0.63
3:J:425:ARG:HH11	3:J:459:ALA:HA	1.60	0.63
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.80	0.63
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	1.80	0.63
2:I:1114:GLU:OE1	2:I:1230:MET:HA	1.98	0.63
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.81	0.62
5:F:462:LYS:O	5:F:466:ILE:HG13	1.99	0.62
3:D:156:ARG:NH2	3:D:191:SER:OG	2.33	0.62
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.26	0.62
2:C:742:TYR:O	2:C:974:ARG:NH2	2.32	0.62
3:D:1155:ILE:HD13	3:D:1190:ILE:HD13	1.82	0.62
3:D:1183:SER:OG	3:J:206:ASN:ND2	2.32	0.62
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.81	0.62
2:I:690:VAL:HG12	2:I:1234:LYS:O	1.98	0.62
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.39	0.62
2:C:1267:GLY:HA3	3:D:347:VAL:O	1.98	0.62
2:C:258:ASN:ND2	2:C:282:VAL:HG22	2.15	0.62
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.14	0.62
2:C:1099:ASN:HD21	3:D:505:ASP:CG	2.03	0.62
2:I:30:ILE:HD12	2:I:30:ILE:H	1.64	0.62
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.64	0.62
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.64	0.62
3:D:680:ASN:O	3:D:683:ILE:HG22	1.99	0.62
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.82	0.62
2:I:979:LEU:HA	2:I:1002:LEU:HD12	1.81	0.62
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.80	0.62
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.63	0.62
1:A:92:VAL:HG23	1:A:148:ARG:NH1	2.15	0.62
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.81	0.62
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.35	0.62
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.81	0.62
3:J:1167:LYS:HZ3	3:J:1170:LYS:CB	2.07	0.62
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.82	0.62
5:F:599:ARG:CG	5:F:599:ARG:HH11	2.13	0.62
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.82	0.62
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.82	0.62
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.31	0.62
3:D:847:ASP:OD1	3:D:847:ASP:N	2.29	0.62
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.82	0.62
3:J:1153:PRO:HA	3:J:1214:PRO:O	1.99	0.62
1:H:28:LEU:HG	1:H:31:LEU:HD21	1.82	0.61
2:I:637:ARG:HA	2:I:642:SER:HA	1.82	0.61
1:A:118:ASP:H	1:A:121:VAL:HB	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.82	0.61
3:J:1167:LYS:HG2	3:J:1168:GLU:H	1.64	0.61
3:J:73:GLY:O	3:J:76:LYS:NZ	2.25	0.61
5:F:316:PHE:CZ	5:F:334:SER:HA	2.35	0.61
5:F:511:ILE:HG12	5:F:512:GLY:N	2.15	0.61
1:A:135:ASP:O	1:A:138:ALA:N	2.33	0.61
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.82	0.61
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.65	0.61
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.81	0.61
5:F:312:SER:O	5:F:315:TRP:NE1	2.34	0.61
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.64	0.61
3:J:57:PHE:HB3	3:J:98:ARG:NH2	2.15	0.61
2:C:302:ILE:O	2:C:330:HIS:NE2	2.33	0.61
3:D:872:LEU:O	3:D:877:VAL:HG12	1.99	0.61
1:G:191:ARG:NH1	1:G:197:ASP:HA	2.15	0.61
2:I:778:GLU:O	2:I:781:ASP:HB2	2.00	0.61
3:J:205:LEU:CD2	3:J:214:ARG:HB2	2.31	0.61
5:L:573:LEU:H	5:L:573:LEU:HD23	1.66	0.61
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.00	0.61
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.82	0.61
1:G:155:ALA:HB2	1:G:173:VAL:C	2.21	0.61
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.82	0.61
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	2.01	0.61
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.64	0.61
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.16	0.61
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.81	0.61
2:C:115:LYS:HD3	2:C:116:ASP:H	1.66	0.61
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.36	0.61
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.82	0.61
3:J:205:LEU:HD22	3:J:214:ARG:HB2	1.83	0.61
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.82	0.61
1:A:218:ARG:HG3	1:B:231:PHE:O	2.01	0.61
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.16	0.61
5:F:306:PHE:HE1	5:F:315:TRP:CG	2.19	0.61
2:I:371:ARG:HB3	2:I:374:GLU:OE2	2.01	0.61
2:I:565:GLU:O	2:I:565:GLU:HG2	2.00	0.61
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.31	0.60
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.83	0.60
1:G:45:ARG:NH1	1:H:34:GLY:O	2.32	0.60
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.83	0.60
2:C:615:VAL:HG13	2:C:651:ASP:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:697:MET:O	3:D:701:LEU:HB2	2.01	0.60
3:D:598:LYS:N	3:D:728:SER:O	2.26	0.60
1:G:49:SER:OG	1:G:50:SER:N	2.34	0.60
3:J:436:ALA:HB3	3:J:485:MET:HA	1.84	0.60
5:L:461:ASN:HB3	5:L:465:ARG:HH21	1.66	0.60
2:C:1248:THR:HG21	5:F:531:PRO:HG3	1.81	0.60
2:I:737:ASN:HB3	2:I:739:ASP:OD1	2.01	0.60
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.36	0.60
3:J:901:ARG:HA	3:J:908:ILE:HA	1.84	0.60
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.16	0.60
2:C:406:ASN:ND2	2:C:413:GLU:O	2.34	0.60
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.84	0.60
3:D:844:THR:HG21	3:D:858:VAL:HG21	1.83	0.60
3:J:26:SER:HB2	3:J:236:TRP:CE2	2.37	0.60
3:J:343:LEU:HD12	3:J:344:GLY:HA3	1.83	0.60
3:J:462:ASP:OD2	3:J:464:ASP:OD2	2.17	0.60
5:L:507:MET:HG2	5:L:520:GLY:CA	2.32	0.60
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.82	0.60
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.84	0.60
5:F:479:THR:HG23	5:F:481:GLU:H	1.65	0.60
3:J:418:GLU:HG3	4:K:45:LYS:H	1.66	0.60
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.32	0.60
5:L:314:THR:O	5:L:318:ALA:HB3	2.01	0.60
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.36	0.60
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.82	0.60
5:L:461:ASN:O	5:L:465:ARG:HG2	2.02	0.60
2:C:517:GLN:HE21	2:C:760:ASN:H	1.50	0.60
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.83	0.60
1:G:9:LEU:O	1:H:227:GLN:NE2	2.35	0.60
3:J:1289:ASN:O	3:J:1290:ARG:NH1	2.35	0.60
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.37	0.60
3:J:807:LEU:HD23	3:J:915:ILE:HG13	1.82	0.60
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.66	0.60
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.84	0.60
2:I:810:TYR:HD2	3:J:359:PRO:HG2	1.66	0.59
3:J:892:PHE:CD1	3:J:1281:GLU:HG2	2.37	0.59
3:J:152:THR:HG21	3:J:176:PHE:HB2	1.85	0.59
5:L:511:ILE:HG13	5:L:512:GLY:N	2.17	0.59
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.85	0.59
1:A:12:ARG:H	1:A:30:PRO:HD2	1.66	0.59
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLN:HA	2:C:729:ALA:N	2.17	0.59
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.35	0.59
1:G:91:ARG:HH21	1:G:122:GLU:CD	2.03	0.59
3:J:298:MET:SD	5:L:402:LEU:HB3	2.42	0.59
1:B:41:ASN:O	1:B:45:ARG:HG3	2.02	0.59
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.37	0.59
5:F:244:THR:O	5:F:247:GLU:HG2	2.01	0.59
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.66	0.59
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.67	0.59
2:C:960:LEU:HB3	2:C:1025:PHE:HE2	1.67	0.59
3:D:473:THR:HG23	3:D:476:ALA:H	1.67	0.59
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.67	0.59
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.35	0.59
2:C:517:GLN:NE2	2:C:760:ASN:H	2.01	0.59
3:D:179:LYS:HB2	3:D:184:ALA:HB2	1.83	0.59
2:I:1286:THR:N	3:J:479:GLU:OE2	2.31	0.59
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.43	0.59
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.67	0.59
3:D:259:ARG:HG2	3:D:260:PHE:N	2.17	0.59
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.85	0.59
2:C:905:ILE:O	5:F:599:ARG:HD2	2.02	0.59
2:I:124:MET:HG3	2:I:124:MET:O	2.02	0.59
2:I:896:THR:HB	2:I:897:PRO:HD2	1.85	0.59
1:B:219:ARG:O	1:B:223:ILE:HG13	2.02	0.59
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.85	0.59
3:D:642:ASP:HA	3:D:764:ARG:HH21	1.67	0.59
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.03	0.59
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.37	0.59
5:L:166:VAL:O	5:L:167:ASP:HB2	2.02	0.59
5:F:483:LEU:H	5:F:483:LEU:HD12	1.67	0.59
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.50	0.59
2:I:841:ARG:NE	3:J:256:ASP:HB3	2.18	0.59
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.33	0.59
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.67	0.58
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.02	0.58
3:D:34:SER:OG	3:D:104:HIS:ND1	2.36	0.58
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.33	0.58
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.85	0.58
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.67	0.58
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.38	0.58
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:532:LEU:HD12	5:L:532:LEU:H	1.67	0.58
2:C:801:ARG:HD3	2:C:1094:VAL:HA	1.85	0.58
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.68	0.58
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.86	0.58
2:C:204:LEU:HD11	2:C:369:MET:HG3	1.85	0.58
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.85	0.58
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.85	0.58
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.18	0.58
1:G:135:ASP:HB3	1:G:138:ALA:HB2	1.83	0.58
5:L:511:ILE:HG13	5:L:512:GLY:H	1.67	0.58
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.01	0.58
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.38	0.58
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.85	0.58
3:D:11:GLN:NE2	3:D:15:GLU:OE1	2.36	0.58
3:D:817:HIS:CE1	3:D:860:ARG:HH21	2.20	0.58
2:I:12:ARG:NH2	2:I:698:PRO:O	2.22	0.58
1:A:23:HIS:HE1	1:A:204:GLU:CG	2.17	0.58
1:B:64:VAL:HG11	1:B:69:SER:CB	2.34	0.58
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.85	0.58
3:D:1181:ASP:HB3	3:J:202:ARG:HH11	1.68	0.58
3:D:1263:LYS:CE	3:D:1279:GLN:HE21	2.16	0.58
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.86	0.58
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.03	0.58
5:F:572:THR:HG23	5:F:575:GLU:HG3	1.86	0.58
1:H:48:LEU:HD21	3:J:535:ARG:O	2.02	0.58
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.86	0.58
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.86	0.58
3:J:1326:GLN:OE1	3:J:1330:ARG:NH2	2.37	0.58
3:J:195:GLU:O	3:J:199:GLU:HG3	2.02	0.58
3:J:221:ILE:HA	3:J:224:LEU:HD12	1.86	0.58
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.84	0.58
3:D:414:GLU:O	4:E:45:LYS:NZ	2.25	0.58
3:D:298:MET:SD	5:F:402:LEU:HB3	2.44	0.58
5:F:423:ARG:HD2	5:F:425:TYR:CE2	2.39	0.58
2:I:159:SER:O	2:I:160:ASP:HB2	2.04	0.58
2:I:871:VAL:O	2:I:944:ARG:NH1	2.36	0.58
2:C:298:ALA:N	2:C:334:GLU:O	2.30	0.58
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.85	0.58
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.31	0.58
1:H:153:VAL:HG11	1:H:158:ARG:NH1	2.18	0.58
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.86	0.58
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.04	0.58
5:F:280:VAL:HG21	5:F:358:VAL:HG11	1.84	0.58
5:F:461:ASN:O	5:F:465:ARG:HG2	2.03	0.58
1:H:42:ALA:O	1:H:46:ILE:HG13	2.03	0.58
2:I:228:VAL:HG22	2:I:245:ARG:HE	1.69	0.58
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.86	0.57
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.86	0.57
3:J:770:LEU:HD22	3:J:770:LEU:H	1.69	0.57
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.39	0.57
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.16	0.57
5:F:276:MET:O	5:F:279:ARG:HB2	2.04	0.57
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.06	0.57
4:K:26:ARG:NH1	4:K:29:GLN:OE1	2.37	0.57
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.40	0.57
2:I:185:ASP:HB2	2:I:197:ARG:HG3	1.86	0.57
3:J:27:PRO:HB3	3:J:241:VAL:HG23	1.85	0.57
1:A:14:VAL:CG1	1:A:15:ASP:H	2.13	0.57
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.86	0.57
2:C:40:GLU:HG2	2:C:41:GLN:H	1.69	0.57
2:C:815:SER:HB2	2:C:1077:SER:HB3	1.85	0.57
3:D:1171:GLY:O	3:D:1172:LYS:HG3	2.05	0.57
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.87	0.57
2:I:1197:GLU:O	2:I:1200:LYS:HB2	2.04	0.57
1:A:14:VAL:HG13	1:A:15:ASP:N	2.11	0.57
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.86	0.57
2:C:179:TYR:H	2:C:397:LEU:HA	1.69	0.57
3:D:843:VAL:HG11	3:D:897:HIS:O	2.04	0.57
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.68	0.57
2:I:250:THR:HA	2:I:268:ARG:HA	1.86	0.57
2:I:156:PHE:CE1	2:I:443:ASP:HB2	2.38	0.57
5:F:601:PRO:O	5:F:602:SER:OG	2.18	0.57
1:A:23:HIS:ND1	1:A:205:MET:O	2.37	0.57
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.85	0.57
1:H:79:LEU:O	1:H:82:LEU:HB2	2.05	0.57
3:J:394:ILE:HG23	5:L:536:THR:HG22	1.86	0.57
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.87	0.57
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.86	0.57
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.70	0.57
1:A:45:ARG:HG2	1:B:38:THR:CB	2.31	0.57
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.86	0.57
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.87	0.57
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.31	0.57
3:D:205:LEU:CD2	3:D:214:ARG:HB2	2.35	0.57
3:D:316:ILE:HA	3:D:323:PRO:HA	1.86	0.57
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.87	0.57
3:D:814:CYS:HB2	3:D:889:ASP:HB3	1.87	0.57
1:H:51:MET:O	1:H:150:ARG:HA	2.04	0.57
2:C:105:TYR:CE1	2:C:111:GLU:HB3	2.40	0.56
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.86	0.56
5:F:97:PRO:HA	5:F:100:MET:HG3	1.87	0.56
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.71	0.56
2:I:994:ARG:HD2	2:I:997:TRP:CZ2	2.40	0.56
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.39	0.56
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.06	0.56
2:C:214:ASN:HB2	2:C:359:ARG:HD2	1.86	0.56
2:C:582:ASN:N	2:C:586:PHE:O	2.26	0.56
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.87	0.56
3:D:317:THR:HB	3:D:324:LEU:HB3	1.87	0.56
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.87	0.56
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.87	0.56
5:F:511:ILE:HG12	5:F:512:GLY:H	1.69	0.56
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.87	0.56
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.86	0.56
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.05	0.56
3:J:325:LYS:HE2	3:J:330:MET:HG2	1.86	0.56
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.86	0.56
1:H:41:ASN:ND2	2:I:1217:THR:O	2.39	0.56
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.86	0.56
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.03	0.56
2:I:739:ASP:N	2:I:739:ASP:OD1	2.37	0.56
2:I:812:PHE:N	2:I:815:SER:OG	2.38	0.56
4:K:13:ILE:HD12	4:K:19:LEU:HA	1.86	0.56
2:C:832:HIS:ND1	2:C:1058:ARG:HD2	2.20	0.56
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.05	0.56
1:G:172:LEU:HD12	1:G:172:LEU:H	1.70	0.56
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.87	0.56
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.69	0.56
3:D:26:SER:HB2	3:D:236:TRP:CZ2	2.40	0.56
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.88	0.56
2:I:607:SER:N	2:I:610:GLU:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:164:GLY:O	5:L:260:ARG:HB2	2.05	0.56
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.87	0.56
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.88	0.56
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.46	0.56
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.06	0.56
3:D:56:LEU:HD12	3:D:56:LEU:H	1.70	0.56
2:I:934:PHE:HA	2:I:1040:ASP:OD2	2.06	0.56
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.87	0.56
5:L:612:ASP:OD1	5:L:612:ASP:N	2.37	0.56
2:C:829:THR:HA	2:C:1059:ARG:HA	1.87	0.56
2:C:30:ILE:H	2:C:30:ILE:HD12	1.71	0.56
2:C:356:THR:HG21	2:C:362:ALA:HA	1.87	0.56
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.87	0.56
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.06	0.56
1:H:7:GLU:HG2	1:H:8:PHE:H	1.71	0.56
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	1.88	0.56
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.21	0.56
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.86	0.56
2:I:1259:LEU:HD23	5:L:524:GLU:HB3	1.88	0.56
2:C:1114:GLU:OE1	2:C:1230:MET:HA	2.05	0.56
2:C:490:GLN:HG3	5:F:472:GLN:NE2	2.20	0.56
2:C:1326:LEU:HD21	3:D:337:ARG:NE	2.20	0.56
2:I:1272:GLU:N	3:J:343:LEU:HD11	2.21	0.56
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.88	0.56
1:B:102:LEU:HD23	1:B:115:ILE:HA	1.87	0.56
2:C:628:HIS:HB3	2:C:647:ARG:HH21	1.71	0.56
3:D:259:ARG:CD	5:F:505:ILE:HD13	2.36	0.56
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.70	0.56
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.70	0.56
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.06	0.56
1:B:154:PRO:HA	1:B:174:ASP:CB	2.35	0.56
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.88	0.56
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.87	0.56
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.87	0.56
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.88	0.56
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.45	0.56
3:D:1162:ILE:O	3:D:1178:THR:N	2.36	0.56
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.86	0.56
3:D:770:LEU:H	3:D:770:LEU:HD22	1.70	0.56
3:D:53:ARG:HB2	3:D:54:ASP:OD1	2.05	0.55
5:F:612:ASP:OD1	5:F:612:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:VAL:HG13	1:G:15:ASP:N	2.21	0.55
1:H:108:GLY:O	1:H:133:LEU:HB2	2.06	0.55
1:H:74:VAL:HG12	1:H:76:GLU:HB2	1.87	0.55
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.88	0.55
3:J:843:VAL:HG11	3:J:897:HIS:O	2.06	0.55
1:B:35:PHE:HA	1:B:38:THR:HG22	1.89	0.55
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.88	0.55
1:H:211:ILE:HD11	1:H:215:GLU:CG	2.36	0.55
1:H:81:ILE:HG23	1:H:131:CYS:HB3	1.87	0.55
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.36	0.55
2:I:20:GLN:HG3	2:I:20:GLN:O	2.06	0.55
2:I:895:LEU:HB2	2:I:899:GLU:HB2	1.88	0.55
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.88	0.55
1:H:55:ALA:HB3	1:H:177:TYR:CD1	2.41	0.55
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.89	0.55
5:L:343:LYS:H	5:L:343:LYS:HD2	1.71	0.55
1:B:102:LEU:O	1:B:141:SER:HA	2.06	0.55
2:C:1247:SER:HB3	3:D:375:GLU:O	2.07	0.55
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.88	0.55
3:D:30:ILE:HD13	3:D:243:PRO:HD3	1.88	0.55
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.88	0.55
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.89	0.55
2:I:143:ARG:NH2	2:I:512:SER:O	2.40	0.55
2:I:655:VAL:N	2:I:659:GLN:OE1	2.39	0.55
3:J:514:THR:HB	3:J:576:ARG:HG2	1.88	0.55
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.68	0.55
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.88	0.55
3:D:1273:ASP:HB2	3:D:1276:GLU:HB2	1.89	0.55
3:D:317:THR:HG22	3:D:322:ARG:O	2.07	0.55
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.86	0.55
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.71	0.55
3:D:1302:TYR:CE1	3:J:1297:LYS:HD3	2.41	0.55
5:L:94:THR:OG1	5:L:95:THR:N	2.34	0.55
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.88	0.55
2:I:1136:GLN:O	2:I:1137:GLU:HG2	2.07	0.55
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.88	0.55
1:A:92:VAL:HA	1:A:120:ASP:O	2.07	0.55
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.88	0.55
2:C:387:ASN:HA	2:C:391:SER:HB2	1.88	0.55
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.88	0.55
3:D:513:MET:HE1	3:D:579:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.87	0.55
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.87	0.55
3:D:1284:ARG:HH22	3:J:1292:LEU:HD11	1.72	0.55
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.88	0.55
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.36	0.55
1:H:225:ALA:HA	1:H:228:LEU:HB2	1.89	0.55
2:I:115:LYS:HD3	2:I:116:ASP:H	1.72	0.55
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.46	0.55
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.72	0.55
4:K:32:VAL:O	4:K:34:GLY:N	2.38	0.55
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.06	0.55
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.38	0.55
3:D:901:ARG:HD2	3:D:906:GLY:O	2.06	0.55
4:E:8:ASP:HB2	4:E:55:GLU:HG2	1.88	0.55
5:F:227:GLN:HE22	5:F:251:LYS:HZ3	1.53	0.55
2:I:125:GLY:CA	2:I:499:SER:HB2	2.36	0.55
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.42	0.54
3:D:511:TYR:CG	3:D:728:SER:HB3	2.42	0.54
2:I:448:LEU:HG	2:I:553:THR:OG1	2.07	0.54
5:L:276:MET:O	5:L:279:ARG:HB2	2.07	0.54
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.90	0.54
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.89	0.54
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.89	0.54
2:C:778:GLU:O	2:C:781:ASP:HB2	2.08	0.54
3:D:45:ASN:O	3:D:46:TYR:HD2	1.89	0.54
1:H:172:LEU:H	1:H:172:LEU:HD12	1.72	0.54
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.42	0.54
2:I:324:LYS:HA	2:I:327:GLN:HE21	1.72	0.54
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.89	0.54
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.41	0.54
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.89	0.54
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.71	0.54
2:C:1315:MET:HE2	2:C:1317:PRO:HB3	1.90	0.54
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.42	0.54
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.08	0.54
2:I:754:THR:N	2:I:767:GLN:OE1	2.36	0.54
3:J:211:GLU:OE2	3:J:214:ARG:NH1	2.34	0.54
5:L:287:ILE:HD11	5:L:344:LEU:HD22	1.90	0.54
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.42	0.54
3:D:895:CYS:SG	3:D:898:CYS:HB2	2.47	0.54
5:F:111:LEU:HD13	5:F:116:GLU:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.43	0.54
3:J:872:LEU:O	3:J:877:VAL:HG12	2.08	0.54
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.88	0.54
2:C:538:LEU:HD23	2:C:543:ALA:CB	2.37	0.54
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.36	0.54
3:J:642:ASP:HA	3:J:764:ARG:HH21	1.71	0.54
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.38	0.54
3:J:56:LEU:H	3:J:56:LEU:HD12	1.72	0.54
3:J:77:ARG:HG3	3:J:79:LYS:H	1.72	0.54
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.88	0.54
5:L:108:VAL:HG11	5:L:381:GLU:C	2.27	0.54
2:C:98:VAL:C	2:C:121:GLU:HA	2.28	0.54
3:D:214:ARG:HA	3:D:217:LEU:HB3	1.89	0.54
3:D:396:ALA:HB2	5:F:609:SER:CB	2.37	0.54
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.73	0.54
3:D:850:LYS:HD3	3:D:875:ASN:ND2	2.23	0.54
1:G:211:ILE:HG21	1:G:216:ALA:HB2	1.90	0.54
1:G:23:HIS:HB2	1:G:205:MET:O	2.08	0.54
1:G:9:LEU:HD13	1:G:32:GLU:HG2	1.90	0.54
2:I:599:VAL:HG21	2:I:623:LEU:HD22	1.89	0.54
3:J:525:MET:O	3:J:548:VAL:HG13	2.08	0.54
5:L:289:LYS:HA	5:L:293:GLU:OE1	2.07	0.54
2:C:1211:ARG:HE	2:C:1220:GLN:NE2	2.06	0.54
1:G:107:ILE:HG13	1:G:136:GLU:HA	1.90	0.54
1:H:48:LEU:CD2	3:J:535:ARG:HG3	2.38	0.54
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.23	0.54
1:A:172:LEU:H	1:A:172:LEU:HD12	1.73	0.54
3:D:748:ALA:O	3:D:777:HIS:HD2	1.91	0.54
5:F:547:VAL:CG2	5:F:598:LEU:CD2	2.86	0.54
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.73	0.54
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.10	0.54
3:J:785:ASP:O	3:J:789:LYS:HG3	2.08	0.54
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.73	0.54
1:B:29:GLU:CB	1:B:200:LYS:HG3	2.32	0.53
2:C:992:LEU:H	2:C:992:LEU:HD23	1.73	0.53
3:D:694:SER:OG	3:D:738:ARG:NE	2.40	0.53
5:F:315:TRP:HZ2	5:F:341:LEU:HD11	1.73	0.53
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.89	0.53
2:C:829:THR:HG23	2:C:1059:ARG:HA	1.89	0.53
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.90	0.53
1:G:91:ARG:NH2	1:G:122:GLU:OE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:LEU:HD23	1:H:225:ALA:HB2	1.90	0.53
1:G:45:ARG:HG2	1:H:38:THR:CB	2.37	0.53
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.23	0.53
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.89	0.53
5:L:507:MET:HG2	5:L:520:GLY:HA3	1.91	0.53
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.08	0.53
2:I:892:GLU:OE1	3:J:66:LYS:NZ	2.40	0.53
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.41	0.53
3:D:11:GLN:HG2	3:D:15:GLU:CG	2.38	0.53
1:G:187:VAL:HG12	1:G:201:LEU:HD13	1.91	0.53
1:H:201:LEU:HG	1:H:203:ILE:CD1	2.38	0.53
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.90	0.53
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.90	0.53
2:C:239:MET:O	2:C:284:LEU:HD12	2.09	0.53
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.89	0.53
3:D:34:SER:HG	3:D:104:HIS:HD1	1.52	0.53
4:E:58:LEU:H	4:E:58:LEU:HD12	1.74	0.53
5:F:315:TRP:CZ2	5:F:341:LEU:HD11	2.44	0.53
3:J:111:THR:O	3:J:239:LEU:N	2.35	0.53
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.91	0.53
2:I:1197:GLU:HA	2:I:1200:LYS:HD2	1.90	0.53
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.23	0.53
3:J:233:LYS:HD3	3:J:235:GLU:OE1	2.09	0.53
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.90	0.53
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.90	0.53
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.42	0.53
4:E:86:ILE:C	4:E:88:GLU:N	2.62	0.53
1:G:195:ARG:HG3	1:G:196:THR:N	2.23	0.53
2:I:132:ASP:N	2:I:132:ASP:OD1	2.38	0.53
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.44	0.53
3:J:46:TYR:CD1	5:L:452:ILE:HG22	2.43	0.53
3:J:761:ALA:H	3:J:771:GLN:HE22	1.56	0.53
3:J:931:THR:OG1	3:J:1244:GLN:NE2	2.42	0.53
5:L:372:ALA:O	5:L:376:LYS:HG3	2.09	0.53
1:B:140:ILE:HD11	1:B:142:MET:HE3	1.91	0.53
2:C:739:ASP:OD1	2:C:739:ASP:N	2.40	0.53
2:C:817:LEU:HD23	2:C:1078:LYS:HB3	1.91	0.53
3:D:892:PHE:CD1	3:D:1281:GLU:HG2	2.43	0.53
3:D:201:LEU:HD11	3:D:220:ARG:HH11	1.72	0.53
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.89	0.53
2:C:65:ASN:HB3	2:C:105:TYR:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.22	0.53
5:F:295:CYS:O	5:F:329:LYS:HD3	2.09	0.53
3:J:46:TYR:CD1	5:L:500:ILE:HG21	2.44	0.53
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.23	0.53
2:C:557:ARG:HH21	2:C:607:SER:C	2.12	0.53
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.44	0.53
3:J:259:ARG:HD2	5:L:505:ILE:CD1	2.39	0.53
5:L:569:THR:OG1	5:L:570:ASP:N	2.42	0.53
1:B:27:THR:HG23	1:B:202:VAL:HG22	1.90	0.52
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.91	0.52
2:C:65:ASN:HB3	2:C:105:TYR:CD2	2.44	0.52
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.24	0.52
3:D:369:PRO:HB3	3:D:444:GLY:O	2.09	0.52
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.90	0.52
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.39	0.52
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.91	0.52
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.91	0.52
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.91	0.52
1:B:54:CYS:SG	1:B:148:ARG:HG3	2.49	0.52
2:C:1103:VAL:HG11	2:C:1112:ILE:HD11	1.91	0.52
3:D:1225:GLY:HA3	3:J:1294:ALA:O	2.10	0.52
3:D:16:GLU:O	3:D:1369:ARG:NH2	2.43	0.52
4:E:32:VAL:O	4:E:34:GLY:N	2.43	0.52
1:H:40:GLY:HA3	1:H:185:TYR:CD1	2.45	0.52
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.24	0.52
5:L:572:THR:HG23	5:L:575:GLU:CB	2.39	0.52
1:B:75:GLN:NE2	1:B:132:HIS:HB2	2.11	0.52
3:D:114:ILE:O	3:D:118:LYS:N	2.27	0.52
3:D:115:TRP:CZ2	3:D:1329:THR:HG23	2.44	0.52
5:F:515:GLU:C	5:F:517:SER:N	2.60	0.52
1:G:161:SER:O	1:G:163:GLU:N	2.42	0.52
2:I:40:GLU:HG2	2:I:41:GLN:N	2.24	0.52
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.37	0.52
3:J:34:SER:OG	3:J:104:HIS:ND1	2.42	0.52
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	1.92	0.52
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.92	0.52
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.74	0.52
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.75	0.52
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.73	0.52
1:H:8:PHE:HB2	1:H:10:LYS:NZ	2.25	0.52
1:H:191:ARG:HG2	1:H:191:ARG:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:259:ARG:HD3	5:F:505:ILE:HD13	1.92	0.52
3:J:609:TYR:HD1	3:J:610:ARG:HH11	1.57	0.52
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.44	0.52
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.42	0.52
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	1.91	0.52
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.75	0.52
2:I:672:GLU:HB3	2:I:1187:PHE:HD2	1.75	0.52
3:J:460:ASP:HB2	3:J:462:ASP:OD1	2.10	0.52
2:C:272:ARG:HD3	2:C:273:HIS:CD2	2.44	0.52
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.92	0.52
3:D:809:VAL:HG23	3:D:915:ILE:HD13	1.91	0.52
5:F:511:ILE:CG1	5:F:512:GLY:H	2.23	0.52
1:H:187:VAL:HG13	1:H:199:ASP:HB3	1.91	0.52
2:I:1077:SER:HA	3:J:356:THR:OG1	2.09	0.52
3:J:1261:LEU:HD13	3:J:1304:ARG:HD2	1.92	0.52
3:J:600:ALA:O	3:J:603:LYS:HG2	2.09	0.52
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.91	0.52
3:J:797:THR:O	3:J:801:VAL:HG12	2.09	0.52
5:L:166:VAL:N	5:L:258:GLN:O	2.28	0.52
1:B:11:PRO:O	1:B:12:ARG:HG3	2.09	0.52
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.92	0.52
3:D:491:LEU:HD11	3:D:609:TYR:CE1	2.45	0.52
1:G:45:ARG:CG	1:H:38:THR:HB	2.39	0.52
2:I:227:LYS:NZ	2:I:298:ALA:HB1	2.24	0.52
1:A:32:GLU:HA	1:A:198:LEU:HD22	1.91	0.52
2:C:538:LEU:HD23	2:C:543:ALA:HB2	1.92	0.52
3:D:152:THR:OG1	3:D:153:ASN:N	2.42	0.52
3:D:850:LYS:HD3	3:D:875:ASN:HD21	1.75	0.52
2:I:1099:ASN:HD21	3:J:505:ASP:CG	2.13	0.52
3:J:201:LEU:HD22	3:J:217:LEU:CD1	2.40	0.52
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.91	0.52
3:J:644:MET:HB2	3:J:764:ARG:HG3	1.90	0.52
3:J:902:ASP:OD1	3:J:903:LEU:N	2.42	0.52
2:C:208:ILE:O	2:C:362:ALA:HB1	2.10	0.52
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.10	0.52
3:D:521:LYS:NZ	3:D:540:GLY:O	2.32	0.52
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.91	0.52
2:I:15:PHE:CZ	2:I:1151:LEU:HD12	2.45	0.52
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.90	0.52
3:D:1301:THR:HG23	3:J:1301:THR:HG22	1.92	0.52
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.45	0.51
3:D:1375:ALA:HB1	3:J:853:THR:HG21	1.92	0.51
5:F:548:LEU:HD23	5:F:551:LEU:HD12	1.92	0.51
2:I:722:GLY:HA2	2:I:737:ASN:OD1	2.09	0.51
3:J:75:TYR:CD2	3:J:83:VAL:HG21	2.45	0.51
1:A:189:ALA:HB1	1:A:191:ARG:NH1	2.25	0.51
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.74	0.51
3:D:525:MET:O	3:D:548:VAL:HG13	2.10	0.51
2:I:402:ARG:HG2	2:I:416:GLY:N	2.25	0.51
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.91	0.51
3:J:695:LYS:HA	3:J:698:MET:HB2	1.91	0.51
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.25	0.51
2:I:564:PRO:HG2	2:I:568:ASN:O	2.11	0.51
3:D:1302:TYR:OH	3:J:1291:GLU:HG2	2.10	0.51
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.92	0.51
3:D:1302:TYR:H	3:J:1297:LYS:HE2	1.73	0.51
3:D:322:ARG:HB2	3:D:322:ARG:NH1	2.25	0.51
3:J:91:GLU:O	3:J:91:GLU:HG3	2.11	0.51
1:A:228:LEU:HA	1:A:231:PHE:HB2	1.92	0.51
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.41	0.51
1:H:9:LEU:HD12	1:H:195:ARG:HH21	1.73	0.51
2:I:104:ILE:O	2:I:114:VAL:HG23	2.10	0.51
2:I:632:ASP:HA	2:I:647:ARG:HD2	1.92	0.51
3:J:847:ASP:HA	3:J:860:ARG:H	1.75	0.51
5:L:572:THR:O	5:L:576:VAL:HG23	2.10	0.51
2:C:5:TYR:HB2	2:C:781:ASP:OD1	2.10	0.51
2:C:759:SER:OG	2:C:763:THR:N	2.40	0.51
5:F:147:GLN:HE22	5:F:150:ARG:HH11	1.59	0.51
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.10	0.51
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.93	0.51
3:J:137:ARG:O	3:J:142:GLU:HB2	2.11	0.51
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.71	0.51
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.10	0.51
1:A:201:LEU:HG	1:A:203:ILE:HG13	1.93	0.51
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.26	0.51
2:C:253:PHE:O	2:C:255:ILE:HG13	2.11	0.51
3:D:574:VAL:O	3:D:578:ILE:HG13	2.11	0.51
1:H:190:ALA:N	1:H:198:LEU:O	2.27	0.51
3:J:418:GLU:H	4:K:45:LYS:NZ	2.08	0.51
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.91	0.51
5:F:582:VAL:CG1	5:F:586:ARG:HG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.93	0.51
5:L:348:GLU:HG2	5:L:354:THR:HA	1.91	0.51
1:B:61:ILE:HG23	1:B:142:MET:CE	2.40	0.51
1:B:219:ARG:HA	1:B:222:THR:HB	1.92	0.51
2:C:518:ASN:O	2:C:691:PRO:HD3	2.10	0.51
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.92	0.51
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.10	0.51
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.91	0.51
1:G:221:ALA:HB1	1:H:228:LEU:HD22	1.93	0.51
2:I:238:GLN:OE1	2:I:284:LEU:HD21	2.10	0.51
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.45	0.51
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	1.92	0.51
3:J:1158:GLU:HG3	3:J:1186:TYR:CZ	2.46	0.51
5:L:479:THR:HG23	5:L:481:GLU:H	1.76	0.51
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.92	0.51
1:A:218:ARG:NH1	1:B:231:PHE:O	2.44	0.51
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.93	0.51
2:C:808:ASN:H	3:D:633:ALA:HB2	1.76	0.51
5:F:235:ILE:HA	5:F:245:ALA:HB2	1.93	0.51
1:G:175:ALA:HB1	1:G:177:TYR:CZ	2.46	0.51
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.92	0.51
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.10	0.51
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.93	0.51
3:J:513:MET:O	3:J:575:GLY:HA3	2.11	0.51
3:J:591:ILE:HG13	3:J:604:MET:HE2	1.93	0.51
3:J:700:ASN:O	3:J:704:GLU:HB2	2.10	0.51
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.46	0.50
1:G:74:VAL:HG22	1:G:76:GLU:H	1.75	0.50
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.94	0.50
5:F:288:MET:SD	5:F:299:LYS:HE2	2.50	0.50
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.92	0.50
1:G:29:GLU:OE1	1:G:200:LYS:HG3	2.11	0.50
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.26	0.50
1:H:60:GLU:OE2	1:H:143:ARG:HB2	2.12	0.50
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.08	0.50
3:J:615:LYS:NZ	4:K:7:GLN:HG2	2.27	0.50
1:B:46:ILE:HD11	1:B:224:LEU:HD13	1.93	0.50
1:B:67:GLU:OE1	1:B:67:GLU:N	2.44	0.50
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.93	0.50
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.44	0.50
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:22:ILE:HG22	3:J:1340:LYS:O	2.12	0.50
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.92	0.50
2:C:1315:MET:CE	2:C:1317:PRO:HB3	2.42	0.50
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.42	0.50
3:D:902:ASP:OD1	3:D:903:LEU:N	2.44	0.50
2:I:133:ASN:ND2	2:I:713:GLY:HA3	2.26	0.50
3:J:259:ARG:HD2	5:L:505:ILE:HD13	1.92	0.50
1:B:211:ILE:HD11	1:B:215:GLU:HG2	1.94	0.50
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.44	0.50
2:C:1246:ARG:HH11	2:C:1266:GLY:HA2	1.76	0.50
2:C:548:ARG:HB3	2:C:569:ILE:O	2.12	0.50
2:C:745:GLU:HG3	2:C:1017:GLN:CB	2.34	0.50
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.93	0.50
1:H:59:VAL:O	1:H:171:LEU:HB2	2.11	0.50
3:J:850:LYS:HG2	3:J:857:LEU:HD23	1.94	0.50
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.94	0.50
1:B:56:VAL:HG22	1:B:146:VAL:HG22	1.94	0.50
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.94	0.50
3:D:108:ALA:HB2	3:D:280:LYS:HG2	1.93	0.50
3:D:1273:ASP:O	3:D:1275:LEU:N	2.45	0.50
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.30	0.50
1:G:189:ALA:HA	1:G:199:ASP:HA	1.94	0.50
1:H:84:ASN:ND2	1:H:129:VAL:O	2.44	0.50
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	1.94	0.50
3:J:18:ASP:HB2	3:J:1373:ARG:NH2	2.26	0.50
1:G:61:ILE:HG22	1:G:62:ASP:H	1.77	0.50
3:D:1225:GLY:CA	3:J:1294:ALA:O	2.60	0.50
5:L:488:LEU:H	5:L:488:LEU:HD12	1.77	0.50
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	1.94	0.50
2:C:980:VAL:HA	2:C:984:VAL:HA	1.94	0.50
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.26	0.50
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.44	0.50
4:E:69:ARG:HA	4:E:72:GLN:OE1	2.11	0.50
2:I:607:SER:H	2:I:610:GLU:HB2	1.75	0.50
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.26	0.50
3:J:609:TYR:OH	3:J:905:ARG:HA	2.11	0.50
5:L:250:LEU:O	5:L:254:GLU:HG2	2.12	0.50
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.93	0.50
1:A:190:ALA:H	1:A:199:ASP:HA	1.76	0.50
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.93	0.50
2:I:346:TYR:CE2	2:I:433:ILE:HG23	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1171:GLY:O	3:J:1172:LYS:HG3	2.12	0.50
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.94	0.50
1:A:38:THR:HA	1:B:45:ARG:HD3	1.94	0.49
1:B:61:ILE:HG23	1:B:142:MET:HE2	1.94	0.49
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.94	0.49
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.94	0.49
1:G:90:VAL:HG22	1:G:91:ARG:H	1.77	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.49
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.47	0.49
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.93	0.49
3:J:848:VAL:HG12	3:J:857:LEU:HD11	1.93	0.49
5:L:247:GLU:O	5:L:251:LYS:HG3	2.12	0.49
1:B:190:ALA:N	1:B:198:LEU:O	2.42	0.49
3:D:513:MET:HE1	3:D:579:LEU:HB2	1.94	0.49
1:H:191:ARG:NH1	3:J:413:ASP:OD2	2.46	0.49
5:L:251:LYS:HA	5:L:254:GLU:HG2	1.94	0.49
2:C:566:GLY:O	2:C:569:ILE:HG13	2.11	0.49
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.94	0.49
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.40	0.49
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.94	0.49
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.94	0.49
4:E:80:LEU:O	4:E:84:THR:OG1	2.19	0.49
5:F:292:VAL:HG13	5:F:297:MET:O	2.12	0.49
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.93	0.49
2:I:1276:TRP:HD1	2:I:1279:GLU:OE1	1.96	0.49
2:I:480:SER:HB3	2:I:481:LEU:HD22	1.94	0.49
2:I:1272:GLU:H	3:J:343:LEU:HD11	1.77	0.49
1:A:91:ARG:NH2	1:A:122:GLU:OE2	2.44	0.49
1:A:49:SER:OG	1:A:50:SER:N	2.45	0.49
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.52	0.49
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.47	0.49
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.94	0.49
2:C:561:ILE:HD11	2:C:665:ALA:HB1	1.94	0.49
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.47	0.49
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.47	0.49
3:D:647:PRO:CG	3:D:697:MET:HB3	2.39	0.49
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.94	0.49
3:J:1156:LEU:HA	3:J:1208:ASP:O	2.12	0.49
3:J:317:THR:HG22	3:J:322:ARG:O	2.12	0.49
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.78	0.49
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1328:LYS:O	2:C:1332:SER:N	2.44	0.49
2:C:452:ARG:HH21	2:C:458:GLU:CD	2.15	0.49
2:C:854:ILE:HB	2:C:857:VAL:HG21	1.95	0.49
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.95	0.49
3:D:514:THR:OG1	3:D:594:GLN:O	2.30	0.49
3:D:931:THR:HG22	3:D:932:MET:H	1.78	0.49
1:H:153:VAL:HB	1:H:175:ALA:HB3	1.95	0.49
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	1.94	0.49
2:I:1281:TYR:OH	3:J:434:ILE:O	2.30	0.49
2:I:365:GLU:OE2	2:I:368:ARG:NH2	2.44	0.49
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.94	0.49
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.13	0.49
2:C:247:ARG:NH2	2:C:274:ILE:HD12	2.28	0.49
5:F:515:GLU:O	5:F:517:SER:N	2.45	0.49
5:F:577:GLY:C	5:F:583:THR:HG23	2.32	0.49
5:F:573:LEU:HD13	5:F:588:ARG:NE	2.27	0.49
2:I:229:ILE:HG21	2:I:240:GLU:OE2	2.12	0.49
2:I:705:GLU:HB2	2:I:794:LEU:H	1.78	0.49
2:I:812:PHE:O	2:I:1099:ASN:ND2	2.45	0.49
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.13	0.49
5:L:148:TYR:OH	5:L:218:ARG:HA	2.12	0.49
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.95	0.49
1:B:173:VAL:HG12	1:B:174:ASP:H	1.78	0.49
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.27	0.49
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.95	0.49
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.95	0.49
3:D:360:TYR:OH	3:D:442:ILE:HD11	2.13	0.49
3:D:491:LEU:HA	3:D:498:PRO:HA	1.95	0.49
3:D:492:SER:HB3	3:D:495:ASN:O	2.13	0.49
3:D:702:GLN:O	3:D:718:SER:N	2.37	0.49
5:F:148:TYR:OH	5:F:218:ARG:HA	2.12	0.49
2:I:103:VAL:HB	2:I:113:THR:HG22	1.95	0.49
1:G:45:ARG:CD	2:I:1083:GLU:HB3	2.42	0.49
2:I:620:ASN:O	2:I:620:ASN:ND2	2.45	0.49
2:I:891:GLY:O	2:I:892:GLU:HG3	2.13	0.49
3:J:697:MET:O	3:J:701:LEU:HB2	2.13	0.49
1:A:152:TYR:CZ	2:C:824:GLN:HA	2.48	0.49
1:A:29:GLU:OE1	1:A:200:LYS:HG3	2.12	0.49
2:C:564:PRO:HG2	2:C:568:ASN:O	2.13	0.49
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.77	0.49
3:D:654:ILE:O	3:D:658:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.94	0.49
1:G:175:ALA:HB1	1:G:177:TYR:CE1	2.47	0.49
2:I:194:LEU:HD11	2:I:432:LEU:CD2	2.43	0.49
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.12	0.49
2:I:860:ALA:O	2:I:863:SER:OG	2.25	0.49
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.47	0.49
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.47	0.49
5:L:533:ASP:O	5:L:536:THR:N	2.46	0.49
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.95	0.49
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.53	0.49
2:I:1099:ASN:ND2	3:J:505:ASP:OD1	2.46	0.49
3:J:264:ASP:HB3	3:J:324:LEU:HB2	1.95	0.49
5:L:315:TRP:O	5:L:319:ALA:HB3	2.12	0.49
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.94	0.48
1:B:53:GLY:O	1:B:177:TYR:HB3	2.13	0.48
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.13	0.48
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.42	0.48
2:C:180:ARG:NH2	2:C:465:ARG:HH12	2.11	0.48
2:C:559:CYS:CB	2:C:662:SER:HB3	2.42	0.48
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.46	0.48
5:L:119:ILE:O	5:L:123:ILE:HG13	2.13	0.48
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.28	0.48
1:B:16:ILE:CG2	1:B:26:VAL:HG22	2.34	0.48
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.14	0.48
3:D:306:LEU:O	3:D:326:SER:HB2	2.13	0.48
3:D:436:ALA:HB3	3:D:485:MET:HA	1.94	0.48
5:F:511:ILE:CG1	5:F:512:GLY:N	2.76	0.48
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.28	0.48
2:I:545:PHE:CZ	3:J:781:LYS:HG3	2.48	0.48
3:J:1184:ASP:O	3:J:1186:TYR:N	2.46	0.48
3:J:797:THR:CG2	3:J:924:GLY:HA3	2.41	0.48
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.94	0.48
1:H:54:CYS:SG	1:H:148:ARG:HG3	2.53	0.48
2:I:98:VAL:O	2:I:121:GLU:HA	2.14	0.48
2:I:1328:LYS:O	2:I:1332:SER:N	2.45	0.48
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.78	0.48
2:I:1309:VAL:HA	3:J:383:GLY:HA3	1.95	0.48
5:L:340:ALA:HA	5:L:343:LYS:NZ	2.27	0.48
1:A:23:HIS:HE1	1:A:204:GLU:HG3	1.78	0.48
1:B:108:GLY:O	1:B:133:LEU:HB2	2.12	0.48
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:CD2	3:D:535:ARG:HG3	2.42	0.48
3:D:514:THR:HG23	3:D:596:LEU:HB2	1.94	0.48
2:I:208:ILE:O	2:I:362:ALA:HB1	2.14	0.48
5:L:137:TYR:HE1	5:L:351:THR:HB	1.78	0.48
1:B:9:LEU:HB2	1:B:32:GLU:OE1	2.14	0.48
2:C:1009:ASN:O	2:C:1012:GLU:HB3	2.12	0.48
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.29	0.48
2:C:298:ALA:HB3	2:C:334:GLU:HB2	1.95	0.48
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.29	0.48
5:F:343:LYS:H	5:F:343:LYS:HD2	1.78	0.48
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.44	0.48
1:G:83:LEU:HD23	2:I:694:ARG:NE	2.23	0.48
3:J:22:ILE:O	3:J:1339:GLY:HA2	2.13	0.48
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.48
2:C:263:VAL:HG21	2:C:273:HIS:CG	2.49	0.48
2:C:820:GLU:N	2:C:1080:ASN:O	2.46	0.48
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.77	0.48
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.77	0.48
2:I:606:LEU:HD21	2:I:614:TYR:CD1	2.48	0.48
3:J:152:THR:OG1	3:J:153:ASN:N	2.45	0.48
3:J:490:ILE:HA	3:J:500:ILE:HG13	1.94	0.48
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.14	0.48
3:J:844:THR:HG23	3:J:864:LEU:HD11	1.96	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.14	0.48
5:L:573:LEU:HG	5:L:574:GLU:OE1	2.13	0.48
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.43	0.48
3:D:1234:VAL:O	3:D:1238:GLN:HB2	2.14	0.48
3:D:527:LEU:HD22	3:D:533:ALA:HA	1.96	0.48
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.95	0.48
1:H:100:LEU:HD11	1:H:121:VAL:CG2	2.42	0.48
2:I:344:GLY:HA3	2:I:346:TYR:CE1	2.48	0.48
2:I:548:ARG:HB3	2:I:569:ILE:O	2.14	0.48
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.43	0.48
2:C:728:ASP:OD1	2:C:729:ALA:N	2.47	0.48
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.95	0.48
3:D:1266:ILE:HD13	3:D:1272:SER:HB3	1.96	0.48
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.94	0.48
5:F:281:ARG:O	5:F:285:ARG:HG3	2.14	0.48
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.96	0.48
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	1.95	0.48
2:I:810:TYR:HE1	2:I:1078:LYS:HD2	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1246:ARG:HH11	2:I:1266:GLY:HA2	1.78	0.48
2:I:15:PHE:HZ	2:I:1151:LEU:HD12	1.78	0.48
2:I:168:GLY:C	2:I:170:VAL:H	2.16	0.48
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.60	0.48
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.13	0.48
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.28	0.48
2:I:1253:LEU:HD11	3:J:253:VAL:HG11	1.96	0.48
3:J:88:CYS:O	3:J:90:VAL:N	2.47	0.48
5:L:227:GLN:HG2	5:L:252:LEU:HA	1.95	0.48
2:C:149:LEU:HD12	2:C:452:ARG:O	2.14	0.48
5:F:484:ALA:HB1	5:F:491:GLU:HG3	1.96	0.48
2:I:728:ASP:OD1	2:I:729:ALA:N	2.47	0.48
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.96	0.48
3:J:306:LEU:O	3:J:326:SER:HB2	2.13	0.48
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.14	0.48
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.96	0.48
2:C:854:ILE:O	2:C:857:VAL:HG22	2.13	0.48
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.13	0.48
2:I:1059:ARG:O	2:I:1234:LYS:NZ	2.46	0.48
2:I:109:ALA:HB1	2:I:110:PRO:O	2.14	0.48
2:I:797:GLY:O	2:I:1231:TYR:OH	2.28	0.48
2:I:878:THR:OG1	2:I:879:GLY:N	2.45	0.48
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.96	0.48
5:L:423:ARG:HD2	5:L:425:TYR:CE2	2.49	0.48
3:D:600:ALA:O	3:D:603:LYS:HG2	2.14	0.47
2:I:138:ILE:HG22	2:I:139:ASN:N	2.29	0.47
2:I:155:VAL:HA	2:I:175:ARG:O	2.14	0.47
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.48	0.47
2:I:206:ALA:O	2:I:209:ILE:HG22	2.13	0.47
3:J:16:GLU:HG3	3:J:17:PHE:H	1.78	0.47
3:J:362:ARG:H	3:J:365:GLN:HE21	1.62	0.47
3:J:557:LYS:HA	3:J:563:LEU:HA	1.96	0.47
3:J:576:ARG:NH1	3:J:593:ASN:O	2.46	0.47
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.49	0.47
1:A:6:THR:OG1	1:A:7:GLU:N	2.45	0.47
2:C:1238:LEU:O	2:C:1241:ASP:HB2	2.14	0.47
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.49	0.47
3:D:785:ASP:O	3:D:789:LYS:N	2.39	0.47
5:F:314:THR:O	5:F:318:ALA:HB3	2.14	0.47
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.14	0.47
3:J:516:ASP:N	3:J:516:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:596:LEU:HD12	3:J:601:ILE:HG13	1.96	0.47
5:L:515:GLU:HG2	5:L:516:ASP:N	2.29	0.47
1:B:66:HIS:CE1	1:B:68:TYR:CD1	3.02	0.47
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.78	0.47
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.48	0.47
3:D:515:ARG:O	3:D:545:HIS:HB3	2.14	0.47
4:E:21:LEU:HD12	4:E:21:LEU:HA	1.74	0.47
5:F:532:LEU:O	5:F:536:THR:HG23	2.14	0.47
1:G:155:ALA:H	1:G:174:ASP:CG	2.16	0.47
2:I:996:ARG:HD2	2:I:999:GLU:OE1	2.13	0.47
3:J:334:LYS:HA	3:J:335:GLN:HA	1.58	0.47
3:J:369:PRO:HB3	3:J:444:GLY:O	2.15	0.47
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.96	0.47
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.96	0.47
2:C:1131:MET:HE2	2:C:1141:LEU:HA	1.95	0.47
2:C:169:LYS:O	2:C:170:VAL:HG22	2.14	0.47
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.50	0.47
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.68	0.47
3:J:317:THR:CG2	3:J:320:ASN:HB3	2.44	0.47
2:I:808:ASN:H	3:J:633:ALA:HB2	1.79	0.47
1:B:79:LEU:HD11	3:D:526:VAL:HG11	1.96	0.47
4:E:3:ARG:HB2	4:E:48:VAL:HG13	1.96	0.47
1:G:166:ARG:O	1:G:167:PRO:C	2.52	0.47
1:G:185:TYR:HH	2:I:1087:TYR:HH	1.62	0.47
1:G:228:LEU:HG	1:H:221:ALA:HB1	1.97	0.47
2:I:1148:ALA:HA	2:I:1201:LEU:CD2	2.43	0.47
3:J:810:THR:HG23	3:J:811:GLU:H	1.80	0.47
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.96	0.47
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.96	0.47
4:E:82:ALA:O	4:E:85:ALA:HB3	2.13	0.47
1:H:55:ALA:HB3	1:H:177:TYR:HD1	1.78	0.47
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.95	0.47
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.14	0.47
2:C:859:GLU:O	2:C:863:SER:N	2.47	0.47
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.97	0.47
3:D:652:GLU:O	3:D:656:GLU:HG3	2.14	0.47
3:D:810:THR:HG23	3:D:811:GLU:H	1.79	0.47
1:G:62:ASP:OD1	1:G:141:SER:OG	2.32	0.47
2:C:229:ILE:HD13	2:C:334:GLU:HG2	1.97	0.47
2:I:1312:ASN:ND2	2:I:1314:GLN:HE21	2.08	0.47
2:I:60:GLN:O	2:I:476:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:343:LEU:HD12	3:J:344:GLY:CA	2.45	0.47
5:L:606:VAL:HG13	5:L:607:LEU:HD12	1.96	0.47
1:A:230:ALA:O	1:A:233:ASP:O	2.33	0.47
2:C:138:ILE:HG22	2:C:139:ASN:N	2.30	0.47
2:C:180:ARG:CZ	2:C:465:ARG:HH12	2.28	0.47
2:C:494:ASN:HB3	2:C:497:PRO:HD2	1.95	0.47
3:D:244:VAL:HA	3:D:269:TYR:OH	2.14	0.47
2:C:812:PHE:HZ	3:D:503:SER:HB2	1.79	0.47
2:I:47:TYR:OH	2:I:398:SER:HB2	2.14	0.47
3:J:58:CYS:SG	3:J:60:ARG:HB3	2.55	0.47
3:J:594:GLN:HG3	3:J:596:LEU:HD22	1.97	0.47
3:J:748:ALA:O	3:J:777:HIS:HD2	1.98	0.47
3:J:793:SER:O	3:J:797:THR:HG23	2.14	0.47
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.72	0.47
1:B:201:LEU:HG	1:B:203:ILE:CD1	2.45	0.47
2:C:698:PRO:HG3	2:C:1231:TYR:CE2	2.49	0.47
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.15	0.47
2:C:183:TRP:HB2	2:C:199:ASP:HA	1.97	0.47
2:C:371:ARG:HD3	2:C:374:GLU:OE2	2.15	0.47
3:D:290:ILE:HD12	3:D:290:ILE:H	1.80	0.47
3:D:801:VAL:O	3:D:805:GLN:HB2	2.15	0.47
3:D:914:ALA:O	3:D:918:ILE:HG23	2.14	0.47
5:F:139:GLU:HG2	5:F:351:THR:HA	1.97	0.47
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.96	0.47
1:H:192:VAL:HB	1:H:195:ARG:HB2	1.96	0.47
2:I:9:LYS:O	2:I:1172:LEU:HA	2.15	0.47
3:J:514:THR:CB	3:J:576:ARG:HG2	2.45	0.47
3:J:598:LYS:O	3:J:601:ILE:HG22	2.15	0.47
4:K:59:ILE:HD12	4:K:64:LEU:HD21	1.97	0.47
2:C:615:VAL:HG13	2:C:651:ASP:N	2.30	0.47
2:C:67:GLU:HB3	2:C:103:VAL:CG2	2.44	0.47
3:D:1176:VAL:HA	3:D:1186:TYR:O	2.15	0.47
2:C:1326:LEU:HD21	3:D:337:ARG:CZ	2.45	0.47
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.96	0.47
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.50	0.47
2:I:979:LEU:HA	2:I:1002:LEU:CD1	2.44	0.47
2:I:1272:GLU:HG2	2:I:1276:TRP:CZ2	2.50	0.47
2:I:149:LEU:HD12	2:I:452:ARG:O	2.15	0.47
2:I:519:ASN:ND2	2:I:796:LEU:HD23	2.30	0.47
3:J:1170:LYS:C	3:J:1172:LYS:H	2.18	0.47
3:J:649:LYS:O	3:J:653:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:OG1	1:B:207:THR:O	2.32	0.46
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.97	0.46
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.96	0.46
1:G:45:ARG:HH12	1:H:38:THR:N	2.11	0.46
2:I:208:ILE:HG12	2:I:362:ALA:HB1	1.97	0.46
2:I:62:TYR:C	2:I:64:GLY:H	2.19	0.46
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.95	0.46
3:J:74:LYS:NZ	3:J:86:GLU:OE1	2.43	0.46
5:L:388:ILE:O	5:L:392:LYS:HG3	2.16	0.46
2:C:106:GLU:HG3	2:C:107:ARG:N	2.30	0.46
2:C:98:VAL:O	2:C:121:GLU:HA	2.15	0.46
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.45	0.46
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.96	0.46
3:D:789:LYS:HE3	3:D:931:THR:C	2.35	0.46
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.59	0.46
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.15	0.46
3:J:516:ASP:HA	3:J:545:HIS:HB2	1.97	0.46
3:J:544:LEU:O	3:J:574:VAL:HB	2.15	0.46
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.96	0.46
3:J:615:LYS:HZ3	4:K:7:GLN:HG2	1.80	0.46
1:B:158:ARG:HG2	1:B:172:LEU:HD23	1.97	0.46
2:C:299:LYS:HG2	2:C:334:GLU:OE1	2.15	0.46
1:G:79:LEU:HD11	2:I:693:LEU:HD21	1.96	0.46
1:H:173:VAL:HG12	1:H:174:ASP:H	1.80	0.46
1:H:34:GLY:N	1:H:199:ASP:OD2	2.49	0.46
2:I:214:ASN:HB2	2:I:359:ARG:HD2	1.97	0.46
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.58	0.46
2:I:499:SER:O	2:I:503:LYS:HB2	2.16	0.46
2:I:720:ARG:NE	2:I:736:VAL:HG11	2.30	0.46
3:J:364:HIS:CD2	4:K:4:VAL:HG23	2.50	0.46
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.16	0.46
5:L:342:GLN:OE1	5:L:345:GLN:NE2	2.48	0.46
5:L:583:THR:HG22	5:L:584:ARG:H	1.79	0.46
1:A:234:LEU:H	1:B:218:ARG:HH12	1.63	0.46
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.96	0.46
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.50	0.46
5:F:147:GLN:HE22	5:F:150:ARG:NH1	2.13	0.46
1:G:197:ASP:O	1:G:198:LEU:HD23	2.14	0.46
2:I:232:ILE:HD13	2:I:326:SER:OG	2.15	0.46
3:J:930:LEU:HD23	3:J:1244:GLN:HG3	1.98	0.46
3:J:1297:LYS:HG3	3:J:1299:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:297:ARG:HB3	5:L:97:PRO:HB3	1.97	0.46
3:J:518:VAL:HG12	3:J:707:ILE:HD13	1.98	0.46
3:J:504:GLN:OE1	3:J:731:ARG:NH1	2.49	0.46
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.51	0.46
2:C:606:LEU:HD21	2:C:614:TYR:HD1	1.81	0.46
2:C:906:PHE:CE2	5:F:608:ARG:HD3	2.50	0.46
3:D:253:VAL:HG21	5:F:523:ILE:HG21	1.98	0.46
3:D:733:SER:O	3:D:737:ILE:HG12	2.14	0.46
5:F:418:LYS:HD2	5:F:434:TRP:CZ2	2.50	0.46
2:I:1327:LEU:HG	2:I:1337:ILE:HG23	1.96	0.46
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.98	0.46
2:I:703:GLY:N	2:I:705:GLU:OE2	2.47	0.46
1:G:152:TYR:CZ	2:I:824:GLN:HA	2.51	0.46
3:J:34:SER:HG	3:J:104:HIS:HD1	1.58	0.46
3:J:583:VAL:HG21	3:J:592:VAL:HG11	1.97	0.46
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.98	0.46
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.58	0.46
2:C:1059:ARG:O	2:C:1234:LYS:NZ	2.43	0.46
2:C:169:LYS:O	2:C:169:LYS:HG2	2.15	0.46
2:C:301:TYR:CE2	2:C:333:ILE:HA	2.50	0.46
3:J:30:ILE:HD13	3:J:243:PRO:HD3	1.97	0.46
3:J:290:ILE:HD12	3:J:290:ILE:H	1.80	0.46
3:J:53:ARG:HB2	3:J:54:ASP:OD1	2.16	0.46
1:A:61:ILE:HG22	1:A:62:ASP:H	1.80	0.46
3:D:140:TYR:O	3:D:297:ARG:NH1	2.48	0.46
3:D:45:ASN:O	3:D:46:TYR:HB3	2.15	0.46
3:D:77:ARG:HH21	5:F:568:ASN:HA	1.80	0.46
5:F:96:ASP:O	5:F:98:VAL:N	2.48	0.46
1:G:45:ARG:NH1	1:H:38:THR:N	2.63	0.46
2:I:786:GLY:N	2:I:789:THR:OG1	2.48	0.46
3:D:1301:THR:HG23	3:J:1301:THR:CG2	2.45	0.46
3:J:848:VAL:O	3:J:857:LEU:HD12	2.15	0.46
5:L:108:VAL:HG11	5:L:381:GLU:O	2.16	0.46
2:C:1191:LYS:O	2:C:1195:ILE:HG13	2.16	0.46
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.30	0.46
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.16	0.46
3:D:416:ILE:HA	3:D:416:ILE:HD13	1.75	0.46
3:D:93:THR:HG22	3:D:94:GLN:H	1.80	0.46
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.57	0.46
2:I:1101:LEU:HB3	3:J:731:ARG:HD3	1.97	0.46
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.77	0.46
3:J:462:ASP:CG	3:J:464:ASP:OD2	2.54	0.46
3:J:85:CYS:HB3	3:J:88:CYS:O	2.16	0.46
5:L:248:GLU:O	5:L:252:LEU:N	2.37	0.46
2:C:1291:LEU:HD11	3:D:1354:GLY:HA2	1.97	0.46
2:C:1312:ASN:OD1	2:C:1314:GLN:HG3	2.15	0.46
2:C:323:ALA:O	2:C:327:GLN:HG3	2.16	0.46
2:C:57:PHE:HD1	2:C:58:PRO:HA	1.81	0.46
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.50	0.46
2:C:734:ILE:O	2:C:748:ILE:HB	2.15	0.46
3:D:744:ARG:O	3:D:759:ILE:HB	2.16	0.46
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.97	0.46
1:H:74:VAL:HG22	1:H:133:LEU:HD12	1.96	0.46
1:H:211:ILE:HD11	1:H:215:GLU:CD	2.36	0.46
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.98	0.46
3:J:1168:GLU:OE1	3:J:1173:ARG:HG3	2.15	0.46
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.98	0.46
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.63	0.46
5:L:557:LYS:O	5:L:561:MET:HB2	2.16	0.46
1:B:110:VAL:O	1:B:130:ILE:HB	2.15	0.46
2:C:211:ARG:HB2	2:C:362:ALA:HB2	1.96	0.46
2:C:617:ALA:HA	2:C:636:CYS:SG	2.56	0.46
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.30	0.46
3:D:609:TYR:OH	3:D:905:ARG:HA	2.16	0.46
3:D:877:VAL:O	3:D:877:VAL:HG13	2.16	0.46
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.98	0.46
5:F:507:MET:HG2	5:F:520:GLY:CA	2.45	0.46
1:H:67:GLU:OE1	1:H:67:GLU:N	2.49	0.46
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.98	0.46
2:I:57:PHE:HD1	2:I:58:PRO:HA	1.81	0.46
2:I:886:LYS:CE	2:I:916:SER:HB3	2.45	0.46
3:J:1205:GLU:N	3:J:1208:ASP:OD2	2.49	0.46
3:J:631:TYR:O	3:J:635:SER:N	2.49	0.46
3:J:694:SER:O	3:J:698:MET:HB2	2.16	0.46
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.98	0.46
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.97	0.46
1:B:74:VAL:HG12	1:B:76:GLU:HB2	1.98	0.45
2:C:263:VAL:HG21	2:C:273:HIS:CD2	2.51	0.45
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.74	0.45
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.16	0.45
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:871:VAL:O	2:C:944:ARG:NH1	2.48	0.45
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.99	0.45
5:F:507:MET:HG2	5:F:520:GLY:HA3	1.98	0.45
2:C:1248:THR:HG21	5:F:531:PRO:CG	2.45	0.45
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.98	0.45
2:I:1331:ARG:HA	2:I:1335:ILE:O	2.15	0.45
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.15	0.45
2:I:672:GLU:HB3	2:I:1187:PHE:CD2	2.51	0.45
3:J:515:ARG:NH2	3:J:717:VAL:O	2.49	0.45
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.51	0.45
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.52	0.45
2:C:730:SER:O	2:C:753:LEU:HB2	2.16	0.45
2:C:896:THR:HB	2:C:897:PRO:HD2	1.98	0.45
2:C:725:GLN:HE22	2:C:966:ILE:HG23	1.81	0.45
3:D:1141:VAL:HG13	3:D:1237:VAL:HG23	1.98	0.45
3:D:814:CYS:SG	3:D:816:THR:HG22	2.56	0.45
5:F:562:ARG:HA	5:F:562:ARG:HD2	1.77	0.45
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.16	0.45
2:I:115:LYS:HD3	2:I:116:ASP:N	2.30	0.45
2:I:494:ASN:HB3	2:I:497:PRO:CD	2.46	0.45
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.98	0.45
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.98	0.45
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.51	0.45
3:J:746:LEU:CD2	3:J:758:PRO:HG3	2.46	0.45
3:J:860:ARG:HB3	3:J:861:ASN:H	1.68	0.45
5:L:601:PRO:O	5:L:602:SER:OG	2.21	0.45
1:A:177:TYR:O	1:A:178:SER:HB2	2.17	0.45
2:C:615:VAL:HG22	2:C:650:VAL:HA	1.99	0.45
3:D:42:GLU:OE1	3:D:42:GLU:N	2.47	0.45
5:F:227:GLN:HE22	5:F:251:LYS:HZ2	1.60	0.45
5:F:372:ALA:O	5:F:376:LYS:HG3	2.17	0.45
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.99	0.45
2:I:91:THR:HB	2:I:138:ILE:O	2.16	0.45
2:I:734:ILE:O	2:I:748:ILE:HB	2.17	0.45
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.82	0.45
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	1.97	0.45
3:J:1327:GLU:OE2	3:J:1329:THR:HB	2.17	0.45
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.52	0.45
3:J:363:LEU:O	3:J:363:LEU:HG	2.16	0.45
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.63	0.45
5:L:481:GLU:O	5:L:484:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.97	0.45
1:A:91:ARG:HH21	1:A:122:GLU:CD	2.20	0.45
1:A:179:PRO:HA	1:A:208:ASN:ND2	2.31	0.45
1:A:223:ILE:HD13	1:B:8:PHE:HE1	1.81	0.45
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.65	0.45
2:C:298:ALA:HB3	2:C:334:GLU:CB	2.47	0.45
2:C:516:VAL:HG23	2:C:526:HIS:HD2	1.82	0.45
2:C:18:ARG:NH1	2:C:622:ASN:OD1	2.40	0.45
3:D:1171:GLY:HA2	3:D:1193:TRP:CH2	2.51	0.45
5:F:306:PHE:CE1	5:F:315:TRP:CG	3.02	0.45
5:F:320:ILE:HG21	5:F:331:HIS:NE2	2.30	0.45
5:F:354:THR:O	5:F:358:VAL:HG23	2.16	0.45
2:I:1285:TYR:CE2	3:J:1356:LEU:HD11	2.52	0.45
2:I:37:LYS:HA	2:I:37:LYS:HD3	1.65	0.45
3:J:884:SER:OG	3:J:1254:GLU:OE1	2.15	0.45
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.80	0.45
3:J:749:LYS:HG3	3:J:751:ASP:HB3	1.97	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.45
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.17	0.45
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.99	0.45
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.31	0.45
3:D:109:SER:HB2	3:D:296:LYS:HE2	1.99	0.45
3:D:347:VAL:HG12	3:D:348:ASP:O	2.16	0.45
2:C:1313:HIS:N	4:E:31:GLN:OE1	2.40	0.45
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.14	0.45
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.32	0.45
3:J:689:ALA:O	3:J:693:VAL:HG23	2.16	0.45
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.98	0.45
2:C:733:VAL:CG1	2:C:748:ILE:HG13	2.47	0.45
3:D:1167:LYS:HB3	3:D:1167:LYS:HE3	1.63	0.45
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.66	0.45
3:D:320:ASN:OD1	3:D:322:ARG:HB3	2.16	0.45
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.51	0.45
3:D:695:LYS:HD3	3:D:695:LYS:HA	1.60	0.45
1:H:214:GLU:O	1:H:218:ARG:HG3	2.16	0.45
1:H:74:VAL:CG1	1:H:76:GLU:HB2	2.47	0.45
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.99	0.45
2:I:854:ILE:O	2:I:857:VAL:HG22	2.16	0.45
3:J:214:ARG:HA	3:J:217:LEU:HB3	1.99	0.45
3:J:650:LYS:O	3:J:654:ILE:HG13	2.17	0.45
5:L:596:ARG:HG3	5:L:599:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.47	0.45
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.15	0.45
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.19	0.45
3:D:849:LEU:H	3:D:849:LEU:HD22	1.82	0.45
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.97	0.45
1:G:211:ILE:CG2	1:G:216:ALA:HB2	2.45	0.45
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.52	0.45
2:I:465:ARG:O	2:I:469:VAL:HG13	2.17	0.45
2:I:524:ILE:HD13	2:I:708:VAL:HG13	1.97	0.45
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.81	0.45
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.98	0.45
5:L:128:ASN:HA	5:L:131:GLN:NE2	2.21	0.45
5:L:354:THR:O	5:L:358:VAL:HG23	2.17	0.45
5:L:465:ARG:HG2	5:L:465:ARG:H	1.37	0.45
1:B:25:LYS:HE2	1:B:202:VAL:HG11	1.99	0.45
3:D:1297:LYS:N	3:D:1298:VAL:HA	2.30	0.45
3:D:268:LEU:HA	3:D:268:LEU:HD23	1.83	0.45
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.97	0.45
3:D:432:LEU:HD21	3:D:489:ASN:CB	2.47	0.45
2:I:80:PHE:HB3	2:I:84:GLU:CB	2.44	0.45
3:J:749:LYS:HG2	3:J:753:SER:O	2.17	0.45
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.99	0.45
5:L:603:ARG:HH11	5:L:603:ARG:HA	1.82	0.45
1:A:117:HIS:CE1	1:A:118:ASP:O	2.69	0.45
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.65	0.45
2:C:480:SER:HB3	2:C:481:LEU:HD22	1.99	0.45
3:D:114:ILE:HD11	3:D:311:ARG:CB	2.37	0.45
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.82	0.45
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.99	0.45
3:D:504:GLN:OE1	3:D:731:ARG:NH1	2.50	0.45
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.98	0.45
5:F:306:PHE:HE1	5:F:315:TRP:CD2	2.35	0.45
1:G:74:VAL:CG2	1:G:76:GLU:HB2	2.47	0.45
2:I:208:ILE:HG12	2:I:362:ALA:CB	2.47	0.45
2:I:74:ARG:HG2	2:I:75:LEU:N	2.31	0.45
2:I:4:SER:HB2	2:I:7:GLU:HG3	1.99	0.45
3:J:1266:ILE:HG13	3:J:1276:GLU:O	2.17	0.45
3:J:245:LEU:O	3:J:250:ARG:NH2	2.50	0.45
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.51	0.45
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.17	0.45
1:B:112:ALA:O	1:B:115:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:432:LEU:HD21	3:D:489:ASN:HB2	1.98	0.45
3:D:62:PHE:O	3:D:101:ARG:HD2	2.17	0.45
5:F:101:TYR:HE2	5:F:388:ILE:HD11	1.82	0.45
1:H:31:LEU:HA	1:H:31:LEU:HD13	1.75	0.45
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.99	0.45
2:I:402:ARG:HG2	2:I:416:GLY:H	1.82	0.45
2:I:411:ARG:NH2	2:I:427:ASP:OD2	2.43	0.45
3:J:733:SER:O	3:J:737:ILE:HG12	2.17	0.45
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.71	0.45
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.99	0.44
2:C:53:PHE:O	2:C:57:PHE:HB2	2.17	0.44
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.32	0.44
2:C:1281:TYR:OH	3:D:434:ILE:O	2.35	0.44
1:G:51:MET:HE1	1:G:216:ALA:HA	1.99	0.44
1:G:13:LEU:HD22	1:H:231:PHE:CD1	2.52	0.44
1:G:154:PRO:HB2	2:I:1059:ARG:HH21	1.83	0.44
2:I:1262:LYS:HD3	2:I:1262:LYS:HA	1.68	0.44
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.18	0.44
2:I:810:TYR:HE2	3:J:359:PRO:HD2	1.82	0.44
3:J:1236:GLU:O	3:J:1239:ASP:HB2	2.17	0.44
3:J:838:ARG:NH1	3:J:1250:ASP:OD1	2.50	0.44
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.32	0.44
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.78	0.44
5:L:483:LEU:HA	5:L:486:ARG:NH1	2.32	0.44
2:C:517:GLN:HE21	2:C:759:SER:HB2	1.83	0.44
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.52	0.44
2:I:1198:LEU:HA	2:I:1198:LEU:HD22	1.74	0.44
2:I:1312:ASN:HD21	2:I:1314:GLN:NE2	2.09	0.44
3:J:122:SER:O	3:J:126:LEU:HG	2.17	0.44
3:J:1290:ARG:HD3	3:J:1294:ALA:CB	2.48	0.44
2:I:1271:GLY:C	3:J:343:LEU:HD11	2.36	0.44
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.17	0.44
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.58	0.44
1:A:176:CYS:O	1:A:177:TYR:C	2.55	0.44
2:C:1161:LEU:HD21	2:C:1165:SER:HB3	1.99	0.44
2:C:159:SER:O	2:C:160:ASP:HB2	2.16	0.44
3:D:1273:ASP:OD1	3:D:1273:ASP:N	2.47	0.44
3:D:901:ARG:HA	3:D:908:ILE:HA	2.00	0.44
4:E:83:VAL:HA	4:E:86:ILE:HG12	1.98	0.44
5:F:157:ARG:HB3	5:F:160:ASP:OD2	2.17	0.44
5:F:166:VAL:O	5:F:258:GLN:NE2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:580:PHE:C	5:F:582:VAL:H	2.21	0.44
1:H:40:GLY:HA3	1:H:185:TYR:CG	2.53	0.44
1:H:224:LEU:HD12	1:H:224:LEU:HA	1.63	0.44
2:I:156:PHE:CD1	2:I:443:ASP:HB2	2.52	0.44
3:J:264:ASP:OD2	5:L:506:SER:OG	2.24	0.44
3:J:850:LYS:HB3	3:J:851:PRO:HD2	1.99	0.44
1:A:115:ILE:HG22	1:A:116:THR:H	1.81	0.44
1:A:45:ARG:NH1	1:B:38:THR:H	2.14	0.44
1:B:57:THR:O	1:B:173:VAL:N	2.46	0.44
2:C:17:LYS:NZ	2:C:1154:ASP:O	2.37	0.44
2:C:1142:ARG:CD	2:C:1161:LEU:HD22	2.46	0.44
2:C:210:LEU:O	2:C:215:TYR:HB2	2.18	0.44
2:C:692:THR:OG1	2:C:693:LEU:N	2.50	0.44
2:C:703:GLY:N	2:C:705:GLU:OE2	2.37	0.44
2:C:828:PHE:HA	2:C:828:PHE:HD1	1.60	0.44
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.75	0.44
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.98	0.44
1:H:211:ILE:CD1	1:H:215:GLU:HG2	2.46	0.44
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.72	0.44
2:I:588:GLU:HG3	2:I:605:TYR:HD1	1.82	0.44
3:J:29:MET:HG3	3:J:29:MET:O	2.18	0.44
3:J:739:GLN:HA	3:J:744:ARG:HB3	1.99	0.44
1:A:175:ALA:HB1	1:A:177:TYR:CE1	2.53	0.44
2:C:685:MET:SD	2:C:1073:LYS:HG3	2.57	0.44
3:D:26:SER:HB2	3:D:236:TRP:CE2	2.52	0.44
3:D:342:LEU:HA	3:D:343:LEU:HA	1.82	0.44
3:D:748:ALA:O	3:D:777:HIS:CD2	2.70	0.44
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.99	0.44
1:H:197:ASP:OD1	1:H:197:ASP:N	2.50	0.44
2:I:1072:ASN:N	2:I:1072:ASN:OD1	2.32	0.44
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.83	0.44
2:I:462:ASN:O	2:I:466:VAL:HG23	2.17	0.44
3:J:218:THR:HG21	3:J:1275:LEU:HD21	1.99	0.44
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.98	0.44
3:J:430:HIS:HA	3:J:921:GLN:HB3	2.00	0.44
5:L:462:LYS:O	5:L:466:ILE:HG13	2.17	0.44
1:A:23:HIS:CE1	1:A:204:GLU:HG3	2.53	0.44
2:C:878:THR:OG1	2:C:879:GLY:N	2.50	0.44
1:H:41:ASN:HA	1:H:44:ARG:NH1	2.33	0.44
2:I:145:ILE:HB	2:I:456:VAL:HG22	1.99	0.44
2:I:74:ARG:NH2	2:I:97:ARG:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:268:LEU:HG	3:J:324:LEU:HD22	1.99	0.44
3:J:908:ILE:HD13	3:J:909:ILE:O	2.17	0.44
5:L:139:GLU:HG2	5:L:351:THR:HA	2.00	0.44
1:A:13:LEU:H	1:A:13:LEU:HD23	1.83	0.44
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.52	0.44
3:D:1145:PHE:O	3:D:1309:ILE:HG12	2.17	0.44
2:I:566:GLY:O	2:I:569:ILE:HG13	2.18	0.44
3:J:1263:LYS:CE	3:J:1279:GLN:HE21	2.26	0.44
5:L:96:ASP:O	5:L:98:VAL:N	2.51	0.44
2:C:10:ARG:HA	2:C:1172:LEU:HD23	2.00	0.44
2:C:263:VAL:HG12	2:C:264:GLU:O	2.18	0.44
2:C:46:GLN:OE1	2:C:47:TYR:N	2.49	0.44
3:D:1172:LYS:HB3	3:D:1189:MET:HB3	2.00	0.44
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.38	0.44
5:F:138:PRO:HD2	5:F:353:LEU:HD11	2.00	0.44
2:I:11:ILE:HA	2:I:11:ILE:HD13	1.89	0.44
2:I:62:TYR:O	2:I:64:GLY:N	2.50	0.44
3:D:1302:TYR:CD1	3:J:1297:LYS:HD3	2.52	0.44
5:L:515:GLU:HG2	5:L:516:ASP:H	1.83	0.44
2:C:226:GLU:HB3	2:C:245:ARG:HH22	1.82	0.44
2:C:500:ALA:O	2:C:504:GLU:HB2	2.16	0.44
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.53	0.44
3:D:126:LEU:HD13	3:D:223:LEU:HD21	2.00	0.44
5:F:548:LEU:HD22	5:F:556:ALA:HA	1.98	0.44
5:F:557:LYS:O	5:F:561:MET:HB2	2.18	0.44
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.48	0.44
2:I:75:LEU:HD13	2:I:75:LEU:HA	1.59	0.44
3:J:1243:LEU:HA	3:J:1243:LEU:HD12	1.70	0.44
3:D:1284:ARG:NH2	3:J:1292:LEU:HD11	2.33	0.44
3:J:425:ARG:NH1	3:J:464:ASP:CG	2.71	0.44
3:J:75:TYR:N	3:J:75:TYR:CD1	2.85	0.44
5:L:115:GLY:HA2	5:L:118:ASP:HB2	2.00	0.44
5:L:157:ARG:HB3	5:L:160:ASP:OD2	2.18	0.44
2:C:486:THR:HG23	2:C:487:LEU:H	1.81	0.43
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.99	0.43
3:D:45:ASN:O	3:D:46:TYR:CD2	2.70	0.43
3:D:598:LYS:O	3:D:601:ILE:HG22	2.18	0.43
3:D:613:GLY:O	3:D:617:THR:OG1	2.25	0.43
2:I:13:LYS:NZ	2:I:1148:ALA:O	2.51	0.43
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	1.99	0.43
5:L:390:ILE:O	5:L:393:LYS:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:HB3	1:A:163:GLU:H	1.58	0.43
1:A:50:SER:HB2	1:B:8:PHE:CZ	2.53	0.43
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.52	0.43
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	2.00	0.43
2:C:124:MET:O	2:C:124:MET:HG3	2.18	0.43
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.99	0.43
2:C:62:TYR:C	2:C:64:GLY:H	2.21	0.43
3:D:891:ASP:OD2	3:D:1285:VAL:HG12	2.19	0.43
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.53	0.43
3:D:356:THR:OG1	3:D:357:VAL:N	2.48	0.43
3:D:516:ASP:HA	3:D:545:HIS:CB	2.48	0.43
3:D:646:ILE:HG22	3:D:647:PRO:HD2	1.99	0.43
3:D:843:VAL:CG1	3:D:897:HIS:O	2.66	0.43
4:E:86:ILE:C	4:E:88:GLU:H	2.20	0.43
2:I:102:LEU:O	2:I:116:ASP:HA	2.18	0.43
2:I:169:LYS:O	2:I:170:VAL:HG22	2.18	0.43
2:I:212:ALA:HA	2:I:359:ARG:HG3	1.99	0.43
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.53	0.43
2:I:593:LYS:HB3	2:I:602:GLU:HG3	1.99	0.43
3:J:215:LYS:HD2	3:J:216:LYS:HG3	1.99	0.43
5:L:266:PHE:O	5:L:270:VAL:HG23	2.18	0.43
2:C:214:ASN:CB	2:C:359:ARG:HD2	2.48	0.43
3:D:189:LEU:HB3	3:D:234:PRO:HB2	2.01	0.43
3:D:606:ASN:OD1	3:D:610:ARG:NE	2.51	0.43
3:D:94:GLN:O	3:D:97:VAL:HG22	2.18	0.43
5:F:343:LYS:O	5:F:347:ILE:HG13	2.17	0.43
5:F:533:ASP:O	5:F:536:THR:N	2.51	0.43
1:G:219:ARG:HA	1:G:222:THR:HB	2.00	0.43
1:H:175:ALA:HB1	1:H:177:TYR:CE1	2.52	0.43
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.17	0.43
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.32	0.43
2:I:828:PHE:HZ	2:I:1232:MET:O	2.01	0.43
2:I:596:ASP:C	2:I:648:ASP:OD1	2.57	0.43
3:J:1162:ILE:O	3:J:1178:THR:N	2.51	0.43
3:J:294:ASN:HD22	5:L:406:GLN:HE21	1.66	0.43
3:J:425:ARG:HH11	3:J:425:ARG:HD2	1.47	0.43
3:J:591:ILE:HG23	3:J:604:MET:HE2	2.00	0.43
3:J:842:ARG:HB3	3:J:882:VAL:HG11	2.00	0.43
5:L:137:TYR:O	5:L:141:ILE:HG12	2.18	0.43
5:L:309:ASN:HB3	5:L:310:GLU:H	1.69	0.43
1:A:132:HIS:O	1:A:133:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.81	0.43
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.01	0.43
3:D:264:ASP:OD2	5:F:506:SER:OG	2.31	0.43
5:F:515:GLU:HG2	5:F:515:GLU:O	2.18	0.43
1:H:115:ILE:HG22	1:H:116:THR:H	1.82	0.43
2:I:119:GLU:HG3	2:I:489:PRO:CD	2.47	0.43
2:I:803:ALA:HB2	2:I:1094:VAL:HG21	2.00	0.43
3:J:1168:GLU:OE1	3:J:1173:ARG:NH1	2.51	0.43
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	2.00	0.43
3:J:804:ALA:O	3:J:806:ASP:N	2.52	0.43
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.65	0.43
1:A:207:THR:HG22	1:A:209:GLY:H	1.84	0.43
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.99	0.43
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.63	0.43
3:D:248:ASP:O	3:D:251:PRO:HG3	2.19	0.43
1:H:183:ILE:CD1	1:H:205:MET:HG3	2.48	0.43
2:I:339:ASN:HB3	2:I:343:HIS:H	1.82	0.43
2:I:890:LYS:HE2	2:I:891:GLY:H	1.84	0.43
1:B:31:LEU:HA	1:B:31:LEU:HD13	1.92	0.43
2:C:1008:GLN:O	2:C:1012:GLU:HB2	2.17	0.43
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.53	0.43
2:C:20:GLN:HG3	2:C:20:GLN:O	2.19	0.43
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.90	0.43
3:D:179:LYS:HB2	3:D:184:ALA:CB	2.46	0.43
5:F:127:ILE:O	5:F:130:VAL:HG22	2.18	0.43
5:F:561:MET:HG2	5:F:576:VAL:CG2	2.47	0.43
1:H:134:THR:HG23	1:H:135:ASP:N	2.33	0.43
2:I:560:PRO:HB3	3:J:776:THR:HG21	1.99	0.43
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.65	0.43
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.54	0.43
5:L:127:ILE:O	5:L:130:VAL:HG22	2.18	0.43
1:B:153:VAL:N	1:B:175:ALA:O	2.49	0.43
2:C:996:ARG:HA	2:C:996:ARG:HD3	1.46	0.43
1:G:44:ARG:HA	1:G:183:ILE:HG21	2.00	0.43
2:I:1126:ASP:O	2:I:1130:ALA:N	2.48	0.43
2:I:239:MET:O	2:I:284:LEU:HD12	2.18	0.43
2:I:71:VAL:HB	2:I:99:LYS:HB2	2.00	0.43
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.84	0.43
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.53	0.43
3:J:322:ARG:HB2	3:J:322:ARG:NH1	2.34	0.43
2:I:1272:GLU:H	3:J:343:LEU:CD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:342:LEU:HA	3:J:343:LEU:HD12	1.99	0.43
3:J:436:ALA:N	3:J:484:MET:O	2.31	0.43
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.53	0.43
3:J:642:ASP:HA	3:J:764:ARG:NH2	2.34	0.43
1:B:23:HIS:HD1	1:B:206:GLU:HG2	1.83	0.43
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.34	0.43
2:C:148:GLN:O	2:C:453:ILE:HA	2.18	0.43
2:C:488:MET:C	2:C:490:GLN:H	2.21	0.43
2:C:718:ALA:HB2	2:C:783:LEU:HD23	2.01	0.43
2:C:941:LYS:HB2	2:C:946:LEU:HG	2.00	0.43
3:D:328:ALA:O	3:D:332:LYS:HB2	2.19	0.43
3:D:343:LEU:HD13	3:D:344:GLY:CA	2.48	0.43
1:H:51:MET:C	1:H:150:ARG:HG2	2.39	0.43
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.99	0.43
2:I:808:ASN:HA	3:J:629:PHE:HB3	2.00	0.43
2:I:820:GLU:N	2:I:1080:ASN:O	2.52	0.43
2:I:86:GLN:HA	2:I:140:GLY:HA2	2.00	0.43
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.22	0.43
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.65	0.43
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.57	0.43
3:J:683:ILE:HD13	3:J:683:ILE:HG21	1.83	0.43
3:J:650:LYS:HZ1	3:J:762:ASN:HD22	1.66	0.43
5:L:515:GLU:C	5:L:517:SER:N	2.72	0.43
1:A:231:PHE:HE2	1:B:39:LEU:HD13	1.82	0.43
1:A:238:ARG:HA	1:B:13:LEU:HA	1.99	0.43
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.01	0.43
2:C:1220:GLN:HG2	2:C:1221:PHE:H	1.84	0.43
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.18	0.43
2:C:221:LEU:HD11	2:C:314:ASN:HB2	2.00	0.43
3:D:18:ASP:HB2	3:D:1373:ARG:NH2	2.34	0.43
3:D:605:LEU:HD23	3:D:605:LEU:HA	1.72	0.43
5:F:166:VAL:HG23	5:F:258:GLN:O	2.18	0.43
2:I:1212:LEU:O	2:I:1221:PHE:N	2.52	0.43
2:I:968:GLU:OE2	2:I:1022:LYS:NZ	2.39	0.43
3:J:527:LEU:HD21	3:J:536:LEU:HG	2.01	0.43
3:J:761:ALA:H	3:J:771:GLN:NE2	2.16	0.43
1:B:18:GLN:HG3	1:B:20:SER:O	2.17	0.43
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.31	0.43
2:C:209:ILE:O	2:C:213:LEU:N	2.52	0.43
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.49	0.43
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1278:GLU:HG3	3:D:1279:GLN:N	2.33	0.43
3:D:807:LEU:HD23	3:D:915:ILE:HG13	2.01	0.43
1:G:166:ARG:N	1:G:167:PRO:HD2	2.34	0.43
1:G:223:ILE:HD13	1:H:8:PHE:CZ	2.54	0.43
1:G:23:HIS:HB2	1:G:206:GLU:HA	2.01	0.43
1:G:32:GLU:HA	1:G:198:LEU:CD2	2.48	0.43
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	2.01	0.43
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.01	0.43
2:I:213:LEU:HD23	2:I:213:LEU:HA	1.76	0.43
2:I:232:ILE:HD12	2:I:330:HIS:O	2.19	0.43
3:J:356:THR:OG1	3:J:357:VAL:N	2.48	0.43
3:J:358:GLY:N	3:J:359:PRO:HD3	2.34	0.43
3:J:683:ILE:HD11	3:J:754:ILE:HG23	2.01	0.43
3:J:810:THR:HG21	3:J:893:GLY:HA3	2.00	0.43
2:I:1313:HIS:O	4:K:28:ARG:NH1	2.52	0.43
1:A:45:ARG:NH1	1:B:38:THR:N	2.67	0.42
1:B:53:GLY:HA3	1:B:177:TYR:C	2.39	0.42
2:C:109:ALA:HB1	2:C:110:PRO:O	2.19	0.42
2:C:943:LYS:O	2:C:947:GLU:HG3	2.19	0.42
3:D:1307:LEU:HB3	3:D:1312:ALA:HB2	2.01	0.42
2:C:1270:PHE:N	3:D:343:LEU:HD11	2.34	0.42
5:F:137:TYR:O	5:F:141:ILE:HG12	2.19	0.42
2:I:1149:TYR:N	2:I:1149:TYR:CD2	2.87	0.42
2:I:1191:LYS:O	2:I:1195:ILE:HG13	2.19	0.42
3:J:342:LEU:HA	3:J:343:LEU:HA	1.33	0.42
5:L:248:GLU:HA	5:L:251:LYS:HZ2	1.84	0.42
5:L:465:ARG:HB3	5:L:468:ARG:HH22	1.84	0.42
5:L:483:LEU:N	5:L:483:LEU:HD12	2.29	0.42
5:L:561:MET:HA	5:L:567:MET:HE1	2.01	0.42
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.54	0.42
2:C:1151:LEU:HD12	2:C:1151:LEU:HA	1.70	0.42
2:C:211:ARG:O	2:C:359:ARG:HA	2.19	0.42
2:C:55:SER:OG	2:C:56:VAL:N	2.51	0.42
3:D:1267:VAL:O	3:D:1274:PHE:CE1	2.72	0.42
3:D:609:TYR:HD1	3:D:610:ARG:HH11	1.67	0.42
5:F:396:ASN:C	5:F:398:GLY:H	2.22	0.42
1:H:118:ASP:HB2	1:H:121:VAL:CG2	2.49	0.42
1:H:102:LEU:O	1:H:141:SER:HA	2.19	0.42
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.19	0.42
2:I:194:LEU:HD11	2:I:432:LEU:HD23	2.02	0.42
2:I:629:PHE:O	2:I:647:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:331:ILE:O	3:J:337:ARG:HA	2.19	0.42
3:J:522:GLY:O	3:J:525:MET:HG2	2.19	0.42
5:L:166:VAL:HG23	5:L:258:GLN:O	2.19	0.42
5:L:544:THR:O	5:L:547:VAL:HG12	2.19	0.42
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.84	0.42
1:A:90:VAL:HG22	1:A:91:ARG:H	1.84	0.42
1:B:175:ALA:HB1	1:B:177:TYR:CZ	2.53	0.42
1:B:211:ILE:HD11	1:B:215:GLU:CD	2.39	0.42
1:B:48:LEU:HD11	3:D:538:ARG:HB2	1.99	0.42
1:B:64:VAL:HG11	1:B:69:SER:HB2	2.00	0.42
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.54	0.42
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.19	0.42
2:C:292:ILE:HG23	2:C:295:LYS:HB2	2.00	0.42
2:C:619:ALA:HB1	2:C:657:THR:HA	2.00	0.42
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	2.01	0.42
3:D:1298:VAL:CB	3:D:1299:GLY:HA3	2.49	0.42
3:D:746:LEU:CD2	3:D:758:PRO:HG3	2.49	0.42
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.00	0.42
5:F:320:ILE:HG12	5:F:330:LEU:HB2	2.02	0.42
5:F:456:MET:CE	5:F:497:VAL:HG13	2.49	0.42
5:F:547:VAL:CG2	5:F:598:LEU:HD22	2.50	0.42
1:G:22:THR:O	1:G:207:THR:HB	2.19	0.42
2:I:362:ALA:O	2:I:366:ILE:HG13	2.19	0.42
2:I:379:GLU:H	2:I:379:GLU:CD	2.22	0.42
2:I:397:LEU:HB3	2:I:401:GLY:HA3	2.00	0.42
2:I:891:GLY:C	2:I:892:GLU:HG3	2.39	0.42
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.85	0.42
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.52	0.42
3:J:483:LEU:HD22	4:K:17:PHE:HE1	1.85	0.42
3:J:54:ASP:OD1	3:J:54:ASP:N	2.51	0.42
3:J:51:PRO:HB2	3:J:57:PHE:O	2.19	0.42
4:K:60:ASN:OD1	4:K:62:GLN:HB3	2.18	0.42
1:A:166:ARG:O	1:A:167:PRO:C	2.58	0.42
1:A:166:ARG:N	1:A:167:PRO:HD2	2.34	0.42
3:D:268:LEU:HG	3:D:324:LEU:HD22	2.01	0.42
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.92	0.42
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.19	0.42
4:E:51:LEU:HD23	4:E:51:LEU:HA	1.88	0.42
2:I:1158:LYS:HG3	2:I:1159:VAL:N	2.34	0.42
2:I:702:THR:HA	2:I:1184:THR:O	2.20	0.42
2:I:14:ASP:OD2	2:I:1156:ARG:NE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:279:LYS:HB3	2:I:279:LYS:HE3	1.74	0.42
3:J:18:ASP:HB2	3:J:1373:ARG:HH21	1.84	0.42
3:J:518:VAL:HA	3:J:547:ARG:CZ	2.49	0.42
3:J:682:VAL:HA	3:J:685:ILE:HD13	2.01	0.42
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.79	0.42
2:C:553:THR:O	2:C:557:ARG:HD2	2.19	0.42
2:C:887:VAL:HB	2:C:913:VAL:HG22	2.01	0.42
3:D:252:LEU:HD23	3:D:262:THR:HB	2.01	0.42
3:D:516:ASP:N	3:D:516:ASP:OD1	2.50	0.42
3:D:797:THR:O	3:D:801:VAL:HG12	2.18	0.42
5:F:556:ALA:O	5:F:560:ARG:HG3	2.20	0.42
1:H:136:GLU:CG	1:H:137:ASN:H	2.31	0.42
2:I:795:ALA:HB1	2:I:1231:TYR:OH	2.19	0.42
2:I:538:LEU:H	2:I:538:LEU:HG	1.44	0.42
3:J:480:ALA:O	3:J:485:MET:N	2.52	0.42
5:L:567:MET:HE2	5:L:567:MET:HB2	1.93	0.42
1:B:64:VAL:HG11	1:B:69:SER:HB3	2.02	0.42
1:B:96:ASP:O	1:B:97:GLU:HG2	2.20	0.42
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.85	0.42
2:C:136:PHE:O	2:C:142:GLU:HA	2.19	0.42
2:C:48:GLY:N	2:C:461:GLU:OE1	2.53	0.42
2:C:494:ASN:HD22	2:C:497:PRO:HD3	1.84	0.42
3:D:546:ALA:O	3:D:573:THR:HA	2.19	0.42
3:D:749:LYS:HB2	3:D:750:PRO:HD2	2.01	0.42
1:G:23:HIS:CB	1:G:206:GLU:HA	2.49	0.42
1:G:11:PRO:HA	1:G:30:PRO:HB2	2.02	0.42
1:H:59:VAL:HG12	1:H:61:ILE:HD13	2.01	0.42
2:I:1065:LYS:CD	2:I:1235:LEU:HD12	2.50	0.42
2:I:139:ASN:O	2:I:141:THR:HG23	2.20	0.42
2:I:301:TYR:HB2	2:I:311:CYS:SG	2.60	0.42
2:I:387:ASN:HA	2:I:391:SER:HB2	2.02	0.42
2:I:890:LYS:HE2	2:I:891:GLY:N	2.34	0.42
3:J:930:LEU:HD11	3:J:1241:TYR:CZ	2.55	0.42
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.54	0.42
5:L:134:VAL:HG22	5:L:273:MET:HE3	2.02	0.42
5:L:134:VAL:HA	5:L:273:MET:HE1	2.02	0.42
1:B:201:LEU:HG	1:B:203:ILE:HD13	2.01	0.42
2:C:367:TYR:CD1	2:C:384:LEU:HD22	2.55	0.42
2:C:7:GLU:HG2	2:C:706:ARG:NH1	2.35	0.42
3:D:1158:GLU:HG3	3:D:1186:TYR:OH	2.19	0.42
3:D:850:LYS:HB3	3:D:851:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:70:CYS:SG	3:D:85:CYS:HB2	2.60	0.42
3:D:839:VAL:HG13	3:D:882:VAL:HG21	2.02	0.42
2:I:1064:ASP:O	2:I:1076:ILE:HG22	2.19	0.42
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.86	0.42
2:I:367:TYR:HD1	2:I:384:LEU:HD22	1.83	0.42
2:I:52:ALA:HB2	2:I:461:GLU:HG3	2.01	0.42
2:I:673:HIS:O	2:I:1109:ILE:HG22	2.19	0.42
3:J:232:ASN:HA	3:J:236:TRP:CZ3	2.54	0.42
3:D:1372:ARG:HG3	3:J:854:ALA:HB2	2.02	0.42
5:L:161:LEU:HD12	5:L:161:LEU:HA	1.69	0.42
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.86	0.42
2:C:716:ALA:O	2:C:783:LEU:HB2	2.20	0.42
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.84	0.42
2:C:840:SER:O	2:C:1047:LEU:N	2.43	0.42
2:C:92:TYR:O	2:C:128:PRO:HA	2.20	0.42
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.82	0.42
3:D:220:ARG:NH1	3:D:224:LEU:HD11	2.35	0.42
3:D:343:LEU:HA	3:D:343:LEU:HD22	1.35	0.42
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.81	0.42
4:E:15:ASN:O	4:E:16:ARG:HB3	2.19	0.42
5:F:390:ILE:O	5:F:393:LYS:HB2	2.19	0.42
5:F:488:LEU:H	5:F:488:LEU:HG	1.47	0.42
1:G:102:LEU:HB3	1:G:142:MET:HG2	2.01	0.42
1:G:58:GLU:CD	1:G:145:LYS:HE3	2.40	0.42
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.45	0.42
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.55	0.42
2:I:204:LEU:HA	2:I:204:LEU:HD23	1.84	0.42
3:J:425:ARG:HD2	3:J:459:ALA:HA	2.02	0.42
5:L:580:PHE:C	5:L:582:VAL:H	2.23	0.42
1:A:67:GLU:HB3	1:A:82:LEU:HD11	2.01	0.42
2:C:1192:GLU:O	2:C:1196:LYS:N	2.31	0.42
2:C:28:LEU:HD21	2:C:524:ILE:HD12	2.02	0.42
2:C:468:LEU:O	2:C:471:VAL:HG12	2.20	0.42
2:C:849:GLU:HB2	2:C:887:VAL:HG23	2.01	0.42
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.35	0.42
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	2.02	0.42
3:D:560:ASN:ND2	3:D:560:ASN:O	2.53	0.42
3:D:683:ILE:HD11	3:D:754:ILE:CG2	2.50	0.42
3:D:291:ILE:HD13	5:F:409:ASN:HB3	2.02	0.42
5:F:470:MET:CE	5:F:486:ARG:HH11	2.33	0.42
1:G:86:LYS:HE3	1:G:86:LYS:HB2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:ALA:HB3	1:H:124:VAL:HG12	2.02	0.42
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.34	0.42
1:H:71:LYS:HD2	1:H:71:LYS:HA	1.85	0.42
2:I:528:ARG:NH1	2:I:576:SER:O	2.52	0.42
2:I:734:ILE:HD11	2:I:783:LEU:HD11	2.01	0.42
2:I:81:ASP:HA	2:I:92:TYR:HE1	1.85	0.42
3:J:1158:GLU:O	3:J:1206:ARG:NH1	2.52	0.42
3:J:325:LYS:HE2	3:J:330:MET:HA	2.02	0.42
1:A:40:GLY:HA3	1:A:185:TYR:CD2	2.55	0.42
1:A:236:ASP:HA	1:B:14:VAL:HG13	2.02	0.42
2:C:117:ILE:HD12	2:C:488:MET:HG2	2.01	0.42
3:D:1243:LEU:HA	3:D:1243:LEU:HD12	1.81	0.42
3:D:420:PRO:O	3:D:471:PRO:HD2	2.20	0.42
3:D:833:GLU:HA	3:D:834:PRO:HD3	1.85	0.42
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.02	0.42
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.84	0.42
2:I:237:LEU:HD13	2:I:237:LEU:HA	1.64	0.42
3:J:1231:ARG:HG3	3:J:1235:ASN:OD1	2.20	0.42
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.50	0.42
3:D:1375:ALA:CB	3:J:853:THR:HG21	2.50	0.42
4:K:66:VAL:HG22	4:K:69:ARG:NH2	2.29	0.42
5:L:110:LEU:HD23	5:L:110:LEU:HA	1.83	0.42
5:L:288:MET:SD	5:L:299:LYS:HE2	2.60	0.42
1:A:236:ASP:HA	1:B:14:VAL:O	2.20	0.41
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.85	0.41
1:B:7:GLU:O	1:B:8:PHE:CD2	2.72	0.41
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	2.02	0.41
5:F:383:ASN:HB2	5:F:412:LEU:HD21	2.03	0.41
2:I:1106:ARG:NE	3:J:731:ARG:HH21	2.17	0.41
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.20	0.41
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.52	0.41
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	2.02	0.41
3:J:165:TYR:O	3:J:169:LEU:HB2	2.20	0.41
3:J:506:VAL:H	3:J:506:VAL:HG12	1.59	0.41
3:J:510:LEU:HG	3:J:513:MET:HE2	2.01	0.41
5:L:374:ARG:HH11	5:L:374:ARG:HD2	1.69	0.41
1:A:93:GLN:H	1:A:120:ASP:HB3	1.84	0.41
2:C:810:TYR:CD1	2:C:1078:LYS:HD2	2.52	0.41
2:C:1253:LEU:CD1	3:D:253:VAL:HG11	2.50	0.41
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	2.01	0.41
2:C:325:LEU:O	2:C:330:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:SER:OG	2:C:455:SER:HB3	2.20	0.41
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.35	0.41
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.56	0.41
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.50	0.41
4:E:86:ILE:O	4:E:88:GLU:N	2.53	0.41
5:F:348:GLU:HG2	5:F:354:THR:HA	2.01	0.41
5:F:580:PHE:HD1	5:F:580:PHE:HA	1.51	0.41
1:G:115:ILE:HG22	1:G:116:THR:H	1.85	0.41
1:H:175:ALA:HB1	1:H:177:TYR:CZ	2.55	0.41
1:H:53:GLY:HA3	1:H:177:TYR:C	2.40	0.41
2:I:1060:ILE:HD11	2:I:1066:MET:SD	2.60	0.41
2:I:606:LEU:HD21	2:I:614:TYR:HD1	1.85	0.41
2:I:796:LEU:O	2:I:1233:LEU:HD12	2.19	0.41
3:J:1261:LEU:HA	3:J:1305:ASP:O	2.20	0.41
3:J:172:PHE:HB3	3:J:175:GLU:OE2	2.20	0.41
3:J:355:ILE:HG21	3:J:466:MET:HG3	2.01	0.41
2:I:1276:TRP:CZ2	3:J:801:VAL:HG11	2.55	0.41
5:L:315:TRP:CZ2	5:L:341:LEU:HD11	2.55	0.41
5:L:483:LEU:H	5:L:483:LEU:CD1	2.28	0.41
1:B:100:LEU:O	1:B:144:ILE:HG22	2.19	0.41
2:C:786:GLY:N	2:C:789:THR:OG1	2.51	0.41
3:D:278:ARG:HH11	3:D:295:GLU:CD	2.22	0.41
3:D:647:PRO:HG3	3:D:697:MET:CB	2.43	0.41
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.51	0.41
4:E:77:ALA:O	4:E:80:LEU:HB2	2.19	0.41
1:G:67:GLU:H	1:G:67:GLU:HG2	1.66	0.41
2:I:409:LEU:HD13	2:I:427:ASP:HB3	2.01	0.41
3:J:218:THR:HG21	3:J:1275:LEU:HD11	2.02	0.41
3:J:201:LEU:HD22	3:J:217:LEU:HD11	2.02	0.41
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.20	0.41
3:J:797:THR:HG22	3:J:924:GLY:CA	2.46	0.41
3:J:79:LYS:O	3:J:81:ARG:HG2	2.20	0.41
1:A:50:SER:CB	1:B:8:PHE:CZ	3.03	0.41
1:B:14:VAL:HG23	1:B:27:THR:O	2.19	0.41
1:B:6:THR:OG1	1:B:7:GLU:N	2.48	0.41
2:C:799:ASN:HA	2:C:1231:TYR:HA	2.02	0.41
2:C:1246:ARG:HG2	2:C:1247:SER:N	2.35	0.41
2:C:139:ASN:O	2:C:141:THR:HG23	2.20	0.41
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.45	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.86	0.41
3:D:490:ILE:HD13	3:D:490:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:GLU:HG3	1:H:143:ARG:O	2.20	0.41
2:I:803:ALA:CB	2:I:1094:VAL:HG21	2.50	0.41
3:J:34:SER:HB2	3:J:104:HIS:HB3	2.01	0.41
3:J:186:GLN:HB2	3:J:238:ILE:HG21	2.01	0.41
2:I:1313:HIS:HB2	3:J:474:LEU:HD13	2.02	0.41
1:B:173:VAL:HG12	1:B:174:ASP:N	2.35	0.41
1:B:155:ALA:N	1:B:174:ASP:OD1	2.45	0.41
1:B:190:ALA:O	1:B:198:LEU:HB2	2.19	0.41
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.20	0.41
2:C:1107:MET:HG2	3:D:740:LEU:HD11	2.02	0.41
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.02	0.41
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.35	0.41
3:D:322:ARG:HB2	3:D:322:ARG:CZ	2.50	0.41
5:F:584:ARG:HH11	5:F:584:ARG:HA	1.84	0.41
1:G:89:ALA:HB1	1:G:210:THR:CG2	2.51	0.41
3:J:1262:ARG:HD2	3:J:1279:GLN:HE22	1.86	0.41
3:J:481:ARG:O	3:J:485:MET:HB2	2.20	0.41
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.54	0.41
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.85	0.41
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	2.02	0.41
2:C:1241:ASP:O	2:C:1244:HIS:CE1	2.74	0.41
2:C:230:PHE:CE1	2:C:239:MET:HB2	2.55	0.41
2:C:478:ARG:CG	2:C:492:MET:HG2	2.40	0.41
3:D:1332:LEU:HD13	3:D:1332:LEU:HA	1.85	0.41
3:D:281:ARG:HH11	3:D:281:ARG:HD3	1.68	0.41
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.53	0.41
1:G:176:CYS:O	1:G:177:TYR:C	2.59	0.41
2:I:1070:HIS:CD2	2:I:1111:GLN:HA	2.55	0.41
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.86	0.41
2:I:213:LEU:HB3	2:I:422:LYS:HD2	2.02	0.41
3:J:1165:PHE:HD2	3:J:1173:ARG:NE	2.18	0.41
3:J:746:LEU:HG	3:J:758:PRO:HB3	2.02	0.41
1:A:187:VAL:HG23	1:A:187:VAL:O	2.20	0.41
1:A:207:THR:HG22	1:A:208:ASN:N	2.34	0.41
1:A:8:PHE:O	1:A:9:LEU:HD23	2.19	0.41
1:B:211:ILE:HD12	1:B:211:ILE:HA	1.67	0.41
2:C:1152:GLY:O	2:C:1153:ALA:CB	2.68	0.41
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.66	0.41
2:C:75:LEU:HA	2:C:75:LEU:HD13	1.79	0.41
3:D:903:LEU:HA	3:D:903:LEU:HD12	1.86	0.41
5:F:467:SER:O	5:F:471:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:PRO:HA	1:G:208:ASN:ND2	2.36	0.41
1:G:76:GLU:OE2	1:G:76:GLU:N	2.54	0.41
2:I:696:ASP:HB2	2:I:798:GLN:CG	2.40	0.41
2:I:696:ASP:HB3	2:I:697:LYS:H	1.62	0.41
2:I:701:GLY:O	2:I:1184:THR:N	2.37	0.41
3:J:416:ILE:HG12	3:J:441:LEU:CD2	2.49	0.41
5:L:476:ARG:HG3	5:L:477:GLU:HG2	2.01	0.41
1:B:178:SER:HB2	1:B:180:VAL:HG22	2.01	0.41
1:B:211:ILE:HD11	1:B:215:GLU:CG	2.51	0.41
2:C:1066:MET:HG2	2:C:1234:LYS:HA	2.03	0.41
2:C:1283:ALA:HB1	2:C:1286:THR:HB	2.02	0.41
2:C:1301:ARG:HG3	2:C:1302:THR:H	1.85	0.41
2:C:13:LYS:O	2:C:1183:ALA:N	2.43	0.41
2:C:516:VAL:H	2:C:526:HIS:HD2	1.69	0.41
2:C:146:VAL:HG13	2:C:529:ARG:HB3	2.02	0.41
2:C:618:GLN:CG	3:D:770:LEU:HD21	2.50	0.41
2:C:62:TYR:O	2:C:64:GLY:N	2.53	0.41
3:D:1347:LEU:HG	3:D:1357:ILE:HG23	2.02	0.41
3:D:169:LEU:HD23	3:D:173:GLY:HA2	2.01	0.41
3:D:683:ILE:HG21	3:D:683:ILE:HD13	1.84	0.41
3:D:85:CYS:HB3	3:D:88:CYS:O	2.20	0.41
5:F:402:LEU:HA	5:F:405:ILE:HG12	2.02	0.41
1:H:90:VAL:HG12	1:H:91:ARG:H	1.86	0.41
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.89	0.41
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.62	0.41
2:I:231:GLU:HG2	2:I:332:ARG:NH2	2.36	0.41
2:I:799:ASN:HA	2:I:1231:TYR:HA	2.03	0.41
3:J:580:TRP:HH2	3:J:587:LEU:O	2.03	0.41
3:J:591:ILE:HG23	3:J:592:VAL:HG13	2.02	0.41
3:J:814:CYS:SG	3:J:816:THR:HG22	2.61	0.41
3:J:93:THR:HG22	3:J:94:GLN:H	1.86	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.03	0.41
1:A:189:ALA:HB1	1:A:191:ARG:HH12	1.84	0.41
1:A:187:VAL:CG1	1:A:201:LEU:HD13	2.51	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.21	0.41
1:B:182:ARG:HD2	3:D:581:MET:HE3	2.02	0.41
2:C:136:PHE:O	2:C:143:ARG:N	2.43	0.41
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.50	0.41
2:C:972:PHE:HB2	2:C:994:ARG:HH21	1.86	0.41
3:D:1154:ALA:N	3:D:1214:PRO:O	2.46	0.41
3:D:860:ARG:HB3	3:D:861:ASN:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:281:ARG:HA	5:F:284:GLU:OE1	2.21	0.41
5:F:575:GLU:O	5:F:579:GLN:HG2	2.21	0.41
1:H:116:THR:HG23	1:H:116:THR:O	2.21	0.41
1:H:67:GLU:HA	1:H:78:ILE:HG21	2.03	0.41
2:I:1046:VAL:HG21	2:I:1049:ILE:HD11	2.02	0.41
2:I:1149:TYR:N	2:I:1149:TYR:HD2	2.19	0.41
2:I:1157:GLN:HG3	2:I:1158:LYS:O	2.20	0.41
2:I:1270:PHE:CE1	2:I:1290:MET:HG2	2.56	0.41
2:I:149:LEU:HD11	2:I:451:ARG:HB3	2.03	0.41
3:J:1192:LYS:HB2	3:J:1192:LYS:HE3	1.99	0.41
3:J:215:LYS:O	3:J:218:THR:HG22	2.21	0.41
2:I:620:ASN:OD1	3:J:769:VAL:HG23	2.21	0.41
3:J:825:VAL:C	3:J:826:ILE:HG13	2.41	0.41
1:B:140:ILE:HD11	1:B:142:MET:CE	2.51	0.41
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.88	0.41
3:D:429:LEU:HA	3:D:429:LEU:HD13	1.85	0.41
3:D:705:THR:OG1	3:D:718:SER:HA	2.21	0.41
5:F:391:ALA:HB3	5:F:405:ILE:HG22	2.03	0.41
5:F:512:GLY:C	5:F:514:ASP:H	2.24	0.41
1:G:13:LEU:HD23	1:G:13:LEU:H	1.85	0.41
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.40	0.41
2:I:211:ARG:HD3	2:I:357:ASN:O	2.20	0.41
2:I:409:LEU:HD11	2:I:428:VAL:HG23	2.03	0.41
2:I:540:ARG:H	2:I:540:ARG:HG3	1.64	0.41
2:I:726:TYR:CE2	2:I:728:ASP:HB2	2.56	0.41
2:I:924:VAL:HG12	2:I:1058:ARG:NH2	2.35	0.41
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.86	0.41
3:J:521:LYS:HD2	3:J:541:LEU:O	2.21	0.41
3:J:549:LYS:HA	3:J:570:LYS:O	2.21	0.41
3:J:620:PHE:CE1	3:J:624:ILE:HD11	2.55	0.41
5:L:324:LYS:HB3	5:L:325:PRO:HD2	2.03	0.41
3:J:291:ILE:HD13	5:L:409:ASN:HB3	2.03	0.41
1:A:118:ASP:HB3	1:A:121:VAL:CG2	2.50	0.41
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.95	0.41
1:B:113:ALA:HB2	1:B:126:PRO:HB3	2.02	0.41
2:C:279:LYS:HB3	2:C:279:LYS:HE3	1.88	0.41
2:C:91:THR:HA	2:C:138:ILE:O	2.21	0.41
3:D:805:GLN:OE1	3:D:1348:LYS:HD3	2.21	0.41
5:F:584:ARG:HA	5:F:584:ARG:NH1	2.36	0.41
1:G:11:PRO:HD2	1:H:227:GLN:HA	2.03	0.41
1:G:195:ARG:HG2	1:G:198:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:LEU:HA	1:H:39:LEU:HD23	1.95	0.41
2:I:1151:LEU:HD22	2:I:1197:GLU:OE2	2.20	0.41
3:J:833:GLU:OE1	3:J:1242:ARG:HD3	2.20	0.41
2:I:1281:TYR:OH	3:J:431:ARG:O	2.36	0.41
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	2.04	0.41
3:J:620:PHE:O	3:J:624:ILE:HG13	2.21	0.41
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.36	0.41
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.90	0.41
1:A:166:ARG:NH1	1:A:168:ILE:HG12	2.36	0.40
1:A:60:GLU:HB2	1:A:170:ARG:HD3	2.03	0.40
1:B:82:LEU:HD22	1:B:173:VAL:HG22	2.03	0.40
2:C:578:TYR:HB3	2:C:590:PRO:HG2	2.02	0.40
2:C:719:LYS:O	2:C:779:ARG:HG3	2.21	0.40
2:C:898:GLU:N	2:C:898:GLU:OE1	2.50	0.40
3:D:46:TYR:CD1	5:F:452:ILE:HG22	2.56	0.40
3:D:594:GLN:HG3	3:D:596:LEU:HD22	2.04	0.40
4:E:50:ALA:O	4:E:54:ILE:HG12	2.21	0.40
5:F:601:PRO:CA	5:F:604:SER:HB3	2.49	0.40
1:G:232:VAL:C	1:H:218:ARG:HH12	2.24	0.40
1:H:205:MET:HG2	1:H:206:GLU:H	1.86	0.40
2:I:18:ARG:HH12	2:I:622:ASN:HA	1.85	0.40
2:I:230:PHE:CE1	2:I:239:MET:HB2	2.56	0.40
3:J:1144:LEU:HA	3:J:1144:LEU:HD23	1.89	0.40
3:J:473:THR:HG23	3:J:476:ALA:N	2.33	0.40
4:K:7:GLN:NE2	4:K:7:GLN:O	2.54	0.40
5:L:111:LEU:HA	5:L:111:LEU:HD23	1.77	0.40
2:C:1341:ASP:HB3	3:D:18:ASP:OD2	2.21	0.40
2:C:720:ARG:NH2	2:C:736:VAL:HG21	2.36	0.40
5:F:357:GLN:HG3	5:F:357:GLN:H	1.71	0.40
2:I:10:ARG:HA	2:I:1172:LEU:CD2	2.37	0.40
2:I:953:LEU:HD12	2:I:953:LEU:HA	1.94	0.40
2:I:1225:VAL:HA	3:J:638:SER:CB	2.51	0.40
5:L:161:LEU:O	5:L:262:VAL:HG23	2.21	0.40
1:A:54:CYS:HB3	1:A:148:ARG:HG3	2.04	0.40
2:C:1104:PRO:HG2	3:D:725:MET:SD	2.62	0.40
2:C:213:LEU:HD23	2:C:385:PHE:HE2	1.87	0.40
2:C:401:GLY:O	2:C:405:PHE:HB2	2.21	0.40
2:C:516:VAL:HG23	2:C:526:HIS:CD2	2.56	0.40
1:A:83:LEU:CD2	2:C:694:ARG:HE	2.23	0.40
2:C:754:THR:O	2:C:755:LYS:HD2	2.21	0.40
3:D:521:LYS:HB3	3:D:541:LEU:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:111:LEU:HD23	5:F:111:LEU:HA	1.83	0.40
3:J:338:PHE:O	3:J:340:GLN:N	2.54	0.40
3:J:650:LYS:NZ	3:J:762:ASN:HD22	2.19	0.40
3:J:481:ARG:NH1	4:K:3:ARG:O	2.54	0.40
2:C:1013:GLN:NE2	2:C:1016:GLU:OE2	2.55	0.40
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.21	0.40
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.53	0.40
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.89	0.40
3:D:461:PHE:HD2	3:D:461:PHE:HA	1.70	0.40
3:D:591:ILE:HG23	3:D:592:VAL:HG13	2.03	0.40
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.54	0.40
1:G:207:THR:HG22	1:G:208:ASN:N	2.36	0.40
1:H:177:TYR:O	1:H:178:SER:C	2.59	0.40
2:I:23:ASP:OD1	2:I:23:ASP:N	2.51	0.40
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	2.04	0.40
3:J:1173:ARG:N	3:J:1190:ILE:O	2.51	0.40
3:J:557:LYS:HB2	3:J:557:LYS:HE3	1.76	0.40
4:K:26:ARG:O	4:K:29:GLN:HB2	2.22	0.40
5:L:481:GLU:OE1	5:L:495:ARG:NH2	2.53	0.40
1:A:57:THR:O	1:A:173:VAL:HG22	2.21	0.40
1:A:181:GLU:HB3	1:A:206:GLU:HG3	2.03	0.40
1:A:234:LEU:H	1:B:218:ARG:NH1	2.19	0.40
1:A:45:ARG:HH21	2:C:1216:ARG:HA	1.83	0.40
2:C:388:LEU:HA	2:C:388:LEU:HD23	1.84	0.40
2:C:61:SER:HB3	2:C:479:LEU:HB3	2.04	0.40
2:C:631:GLU:OE1	2:C:631:GLU:N	2.53	0.40
2:C:674:ASP:OD1	2:C:1110:GLY:N	2.45	0.40
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	2.02	0.40
3:D:480:ALA:O	3:D:485:MET:N	2.55	0.40
3:D:697:MET:HG3	3:D:698:MET:N	2.36	0.40
2:C:1276:TRP:CH2	3:D:801:VAL:HG11	2.56	0.40
5:F:465:ARG:H	5:F:465:ARG:HG2	1.42	0.40
1:H:8:PHE:HB2	1:H:10:LYS:HZ2	1.85	0.40
2:I:835:GLU:OE2	2:I:1051:LYS:HD3	2.21	0.40
2:I:1301:ARG:HG3	2:I:1302:THR:H	1.86	0.40
2:I:227:LYS:HZ3	2:I:298:ALA:HB1	1.84	0.40
2:I:757:THR:O	2:I:833:ILE:HD12	2.21	0.40
3:J:647:PRO:HG3	3:J:697:MET:HB3	2.04	0.40
3:J:652:GLU:O	3:J:656:GLU:HG3	2.21	0.40
5:L:380:VAL:HG22	5:L:416:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/320 (72%)	201 (87%)	25 (11%)	5 (2%)	6	29
1	B	213/320 (67%)	186 (87%)	24 (11%)	3 (1%)	11	37
1	G	225/320 (70%)	193 (86%)	26 (12%)	6 (3%)	5	26
1	H	212/320 (66%)	189 (89%)	19 (9%)	4 (2%)	8	31
2	C	1338/1342 (100%)	1229 (92%)	99 (7%)	10 (1%)	22	55
2	I	1338/1342 (100%)	1227 (92%)	100 (8%)	11 (1%)	19	51
3	D	1163/1407 (83%)	1067 (92%)	86 (7%)	10 (1%)	17	49
3	J	1151/1407 (82%)	1054 (92%)	81 (7%)	16 (1%)	11	37
4	E	87/90 (97%)	82 (94%)	5 (6%)	0	100	100
4	K	77/90 (86%)	72 (94%)	3 (4%)	2 (3%)	5	26
5	F	462/613 (75%)	421 (91%)	36 (8%)	5 (1%)	14	44
5	L	463/613 (76%)	422 (91%)	39 (8%)	2 (0%)	34	67
All	All	6960/8184 (85%)	6343 (91%)	543 (8%)	74 (1%)	14	44

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	GLU
1	A	232	VAL
2	C	170	VAL
2	C	484	LEU
2	C	1137	GLU
2	C	1153	ALA
2	C	1159	VAL
3	D	10	ALA
3	D	1274	PHE
3	D	1294	ALA
5	F	512	GLY
5	F	569	THR

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Mol	Chain	Res	Type
1	G	162	GLU
1	G	167	PRO
1	G	229	GLU
1	G	231	PHE
2	I	170	VAL
2	I	484	LEU
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	332	LYS
3	J	1169	THR
4	K	15	ASN
5	L	512	GLY
1	A	167	PRO
2	C	697	LYS
2	C	1158	LYS
3	D	19	ALA
3	D	332	LYS
3	D	712	GLN
3	D	1169	THR
1	H	178	SER
2	I	697	LYS
2	I	1154	ASP
3	J	19	ALA
3	J	334	LYS
3	J	339	ARG
3	J	341	ASN
3	J	712	GLN
5	F	515	GLU
1	G	9	LEU
1	H	193	GLU
2	I	1158	LYS
3	J	333	GLY
3	J	1167	LYS
1	A	14	VAL
1	A	162	GLU
1	B	13	LEU
1	B	138	ALA
1	H	177	TYR
3	J	338	PHE
2	C	63	SER

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Mol	Chain	Res	Type
2	C	573	ASN
3	D	806	ASP
1	G	196	THR
2	I	63	SER
3	J	710	ASP
5	L	166	VAL
5	F	516	ASP
1	H	138	ALA
3	J	806	ASP
3	J	344	GLY
3	J	826	ILE
3	J	831	VAL
4	K	14	GLY
3	D	826	ILE
3	D	831	VAL
1	B	178	SER
3	J	336	GLY
2	C	1186	VAL
5	F	166	VAL
2	I	1186	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/279 (72%)	192 (96%)	9 (4%)	27	58
1	B	186/279 (67%)	173 (93%)	13 (7%)	15	44
1	G	193/279 (69%)	182 (94%)	11 (6%)	20	50
1	H	183/279 (66%)	172 (94%)	11 (6%)	19	49
2	C	1155/1157 (100%)	1066 (92%)	89 (8%)	13	40
2	I	1154/1157 (100%)	1063 (92%)	91 (8%)	12	39
3	D	962/1168 (82%)	885 (92%)	77 (8%)	12	38
3	J	960/1168 (82%)	881 (92%)	79 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	72/74 (97%)	64 (89%)	8 (11%)	6	22
4	K	67/74 (90%)	63 (94%)	4 (6%)	19	49
5	F	417/540 (77%)	381 (91%)	36 (9%)	10	35
5	L	418/540 (77%)	382 (91%)	36 (9%)	10	35
All	All	5968/6994 (85%)	5504 (92%)	464 (8%)	12	39

All (464) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	13	LEU
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	231	PHE
1	B	7	GLU
1	B	8	PHE
1	B	9	LEU
1	B	33	ARG
1	B	50	SER
1	B	61	ILE
1	B	68	TYR
1	B	91	ARG
1	B	103	ASN
1	B	115	ILE
1	B	133	LEU
1	B	176	CYS
1	B	198	LEU
2	C	11	ILE
2	C	39	ILE
2	C	60	GLN
2	C	70	TYR
2	C	82	VAL
2	C	90	VAL
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU

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Mol	Chain	Res	Type
2	C	120	GLN
2	C	132	ASP
2	C	189	ASP
2	C	285	ILE
2	C	299	LYS
2	C	320	ASP
2	C	369	MET
2	C	377	THR
2	C	394	ARG
2	C	419	ILE
2	C	423	ASP
2	C	445	ILE
2	C	485	ASP
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	496	LYS
2	C	518	ASN
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	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	672	GLU
2	C	680	LEU
2	C	684	ASN
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	791	LEU
2	C	799	ASN
2	C	800	MET
2	C	814	ASP

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Mol	Chain	Res	Type
2	C	817	LEU
2	C	826	ASP
2	C	828	PHE
2	C	840	SER
2	C	878	THR
2	C	890	LYS
2	C	895	LEU
2	C	919	ARG
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	1073	LYS
2	C	1076	ILE
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1146	GLN
2	C	1156	ARG
2	C	1159	VAL
2	C	1160	ASP
2	C	1198	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1238	LEU
2	C	1253	LEU
2	C	1264	GLN
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1341	ASP
2	C	1342	GLU
3	D	11	GLN
3	D	12	THR
3	D	18	ASP
3	D	26	SER
3	D	46	TYR

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Mol	Chain	Res	Type
3	D	54	ASP
3	D	79	LYS
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	97	VAL
3	D	98	ARG
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	252	LEU
3	D	312	ARG
3	D	324	LEU
3	D	343	LEU
3	D	394	ILE
3	D	416	ILE
3	D	425	ARG
3	D	454	CYS
3	D	462	ASP
3	D	490	ILE
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	568	SER
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	678	ARG
3	D	680	ASN
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	704	GLU
3	D	707	ILE
3	D	708	ASN

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Mol	Chain	Res	Type
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	746	LEU
3	D	754	ILE
3	D	770	LEU
3	D	805	GLN
3	D	807	LEU
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	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	21	LEU
4	E	28	ARG
4	E	39	VAL
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	154	GLU
5	F	264	LYS

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Mol	Chain	Res	Type
5	F	267	ASP
5	F	301	ASN
5	F	306	PHE
5	F	310	GLU
5	F	335	GLU
5	F	341	LEU
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
5	F	471	LEU
5	F	472	GLN
5	F	476	ARG
5	F	479	THR
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	530	LEU
5	F	547	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	580	PHE
5	F	587	ILE
5	F	599	ARG
5	F	600	HIS
5	F	606	VAL
1	G	9	LEU
1	G	13	LEU
1	G	18	GLN
1	G	50	SER
1	G	61	ILE
1	G	74	VAL
1	G	115	ILE
1	G	133	LEU
1	G	145	LYS
1	G	166	ARG

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Mol	Chain	Res	Type
1	G	231	PHE
1	H	15	ASP
1	H	50	SER
1	H	61	ILE
1	H	68	TYR
1	H	91	ARG
1	H	103	ASN
1	H	115	ILE
1	H	143	ARG
1	H	176	CYS
1	H	198	LEU
1	H	231	PHE
2	I	11	ILE
2	I	60	GLN
2	I	70	TYR
2	I	82	VAL
2	I	90	VAL
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	132	ASP
2	I	189	ASP
2	I	285	ILE
2	I	299	LYS
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	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	510	GLN
2	I	518	ASN
2	I	538	LEU
2	I	542	ARG

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Mol	Chain	Res	Type
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	623	LEU
2	I	633	LEU
2	I	639	LYS
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	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	817	LEU
2	I	826	ASP
2	I	840	SER
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	919	ARG
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	1073	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE

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Mol	Chain	Res	Type
2	I	1114	GLU
2	I	1134	GLN
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1160	ASP
2	I	1198	LEU
2	I	1210	ILE
2	I	1231	TYR
2	I	1237	HIS
2	I	1238	LEU
2	I	1253	LEU
2	I	1264	GLN
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	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	97	VAL
3	J	98	ARG
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	233	LYS
3	J	252	LEU
3	J	312	ARG
3	J	324	LEU
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	425	ARG
3	J	454	CYS

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Mol	Chain	Res	Type
3	J	462	ASP
3	J	506	VAL
3	J	507	VAL
3	J	513	MET
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	568	SER
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	678	ARG
3	J	680	ASN
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	704	GLU
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	746	LEU
3	J	754	ILE
3	J	798	ARG
3	J	805	GLN
3	J	810	THR
3	J	844	THR
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	860	ARG
3	J	908	ILE
3	J	918	ILE
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS

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Mol	Chain	Res	Type
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	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1298	VAL
3	J	1333	THR
3	J	1343	GLU
4	K	3	ARG
4	K	13	ILE
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	264	LYS
5	L	267	ASP
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	445	ASP
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	479	THR
5	L	482	GLU
5	L	486	ARG
5	L	491	GLU
5	L	508	GLU

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Mol	Chain	Res	Type
5	L	530	LEU
5	L	547	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 (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	GLN
1	B	66	HIS
1	B	75	GLN
1	B	186	ASN
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	568	ASN
2	C	618	GLN
2	C	659	GLN
2	C	1013	GLN
2	C	1116	HIS
2	C	1146	GLN
2	C	1220	GLN
2	C	1288	GLN
2	C	1313	HIS
2	C	1314	GLN
2	C	1336	ASN
3	D	94	GLN
3	D	200	GLN
3	D	294	ASN
3	D	419	HIS
3	D	424	ASN

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Mol	Chain	Res	Type
3	D	450	HIS
3	D	594	GLN
3	D	702	GLN
3	D	777	HIS
3	D	792	ASN
3	D	817	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1218	HIS
3	D	1227	HIS
3	D	1366	HIS
4	E	7	GLN
5	F	129	GLN
5	F	131	GLN
5	F	147	GLN
5	F	227	GLN
5	F	301	ASN
5	F	309	ASN
5	F	446	GLN
5	F	455	HIS
5	F	469	GLN
5	F	600	HIS
1	G	84	ASN
1	H	128	HIS
2	I	69	GLN
2	I	139	ASN
2	I	327	GLN
2	I	343	HIS
2	I	494	ASN
2	I	673	HIS
2	I	688	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1220	GLN
2	I	1313	HIS
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	206	ASN
3	J	364	HIS
3	J	365	GLN

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Mol	Chain	Res	Type
3	J	419	HIS
3	J	424	ASN
3	J	450	HIS
3	J	465	GLN
3	J	702	GLN
3	J	716	GLN
3	J	777	HIS
3	J	910	ASN
3	J	929	GLN
3	J	1227	HIS
3	J	1244	GLN
3	J	1279	GLN
4	K	7	GLN
5	L	131	GLN
5	L	301	ASN
5	L	345	GLN
5	L	406	GLN
5	L	446	GLN
5	L	455	HIS
5	L	518	HIS
5	L	600	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	233/320 (72%)	-0.03	4 (1%) 70 68	105, 144, 198, 236	0
1	B	217/320 (67%)	0.49	23 (10%) 6 7	121, 192, 243, 265	0
1	G	227/320 (70%)	0.25	10 (4%) 34 34	162, 195, 234, 271	0
1	H	216/320 (67%)	0.61	23 (10%) 6 7	175, 215, 240, 264	0
2	C	1340/1342 (99%)	0.07	52 (3%) 39 38	78, 133, 242, 297	0
2	I	1340/1342 (99%)	0.33	93 (6%) 16 18	104, 171, 269, 334	0
3	D	1167/1407 (82%)	0.09	32 (2%) 54 53	83, 120, 204, 261	0
3	J	1155/1407 (82%)	0.24	60 (5%) 27 27	99, 146, 228, 277	0
4	E	89/90 (98%)	-0.03	3 (3%) 45 44	118, 156, 179, 198	0
4	K	79/90 (87%)	1.24	20 (25%) 0 0	211, 251, 298, 305	0
5	F	468/613 (76%)	0.17	24 (5%) 28 28	115, 167, 295, 326	0
5	L	469/613 (76%)	0.20	25 (5%) 26 27	130, 181, 301, 320	0
All	All	7000/8184 (85%)	0.21	369 (5%) 26 27	78, 156, 252, 334	0

All (369) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	7.7
2	C	319	LEU	7.0
2	I	1005	GLU	6.7
2	I	1000	LEU	6.6
2	I	999	GLU	6.5
2	I	983	GLY	6.4
5	F	314	THR	6.4
2	C	251	ALA	5.8
4	K	40	PRO	5.7
2	C	1002	LEU	5.6
1	H	135	ASP	5.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	1001	GLY	5.3
2	I	1006	GLU	5.3
3	J	1203	ARG	5.2
2	I	998	LEU	5.2
2	I	981	ALA	5.2
2	C	317	LEU	5.1
5	L	489	MET	5.1
5	L	290	LEU	5.1
2	I	1002	LEU	5.0
2	I	988	LYS	5.0
1	B	172	LEU	4.9
3	D	1202	GLU	4.9
5	L	319	ALA	4.7
3	J	1198	VAL	4.7
2	I	1003	THR	4.7
2	I	1007	LYS	4.6
2	I	979	LEU	4.6
3	J	542	ALA	4.6
5	F	305	LEU	4.6
5	L	488	LEU	4.6
1	H	97	GLU	4.6
3	J	521	LYS	4.6
5	F	313	ASP	4.5
4	K	58	LEU	4.4
5	L	321	ALA	4.4
3	J	1187	GLU	4.4
2	I	1008	GLN	4.3
5	L	322	MET	4.3
1	H	14	VAL	4.3
5	F	322	MET	4.3
4	K	33	GLY	4.3
2	I	987	GLU	4.2
1	H	106	GLY	4.2
5	F	326	TRP	4.2
3	J	849	LEU	4.2
4	K	2	ALA	4.1
5	F	319	ALA	4.1
3	J	1161	GLY	4.1
5	F	315	TRP	4.1
3	J	674	THR	4.1
5	L	315	TRP	4.1
2	I	603	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	98	VAL	4.0
3	J	830	ASP	4.0
2	I	1154	ASP	4.0
3	J	707	ILE	4.0
5	F	323	ASN	4.0
3	J	208	THR	4.0
2	I	720	ARG	3.9
5	L	421	TYR	3.9
2	I	725	GLN	3.9
2	I	1011	LEU	3.9
5	L	483	LEU	3.9
4	K	39	VAL	3.9
2	I	1022	LYS	3.9
5	L	490	PRO	3.9
5	L	317	ASN	3.9
2	I	1001	GLY	3.8
1	H	28	LEU	3.8
5	L	344	LEU	3.8
2	I	986	ALA	3.8
1	B	147	GLN	3.8
1	H	96	ASP	3.8
2	C	1003	THR	3.8
4	K	36	ASP	3.7
4	K	41	GLU	3.7
2	I	978	VAL	3.7
1	B	160	HIS	3.7
3	D	1172	LYS	3.7
2	C	311	CYS	3.7
2	I	989	LEU	3.7
2	I	414	ILE	3.7
1	H	27	THR	3.6
2	I	984	VAL	3.6
3	J	212	THR	3.6
2	I	67	GLU	3.6
2	I	727	VAL	3.5
2	I	300	ASP	3.5
3	J	668	PHE	3.5
2	I	1004	ASP	3.5
3	D	208	THR	3.5
1	H	124	VAL	3.5
3	J	218	THR	3.4
4	K	56	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	I	103	VAL	3.4
1	H	148	ARG	3.4
1	B	95	LYS	3.4
3	J	1249	ASN	3.3
1	G	193	GLU	3.3
2	C	231	GLU	3.3
2	I	111	GLU	3.3
5	F	337	VAL	3.3
2	I	234	ASP	3.3
2	C	254	ASP	3.3
3	D	1161	GLY	3.3
2	C	271	ALA	3.3
3	D	857	LEU	3.3
2	I	985	GLU	3.2
5	F	301	ASN	3.2
2	C	257	ALA	3.2
5	L	318	ALA	3.2
3	J	92	VAL	3.2
2	I	1020	GLU	3.2
4	K	75	GLN	3.2
2	C	265	LYS	3.2
4	K	74	GLU	3.2
1	H	107	ILE	3.2
2	I	169	LYS	3.2
1	B	159	ILE	3.1
3	J	826	ILE	3.1
2	I	190	PRO	3.1
5	F	310	GLU	3.1
2	C	246	LEU	3.1
1	B	24	ALA	3.1
2	I	773	LEU	3.1
3	J	857	LEU	3.1
1	H	204	GLU	3.1
1	B	143	ARG	3.1
2	I	376	PRO	3.0
3	J	1199	PHE	3.0
2	C	1000	LEU	3.0
1	H	94	GLY	3.0
3	J	708	ASN	3.0
3	J	1162	ILE	3.0
2	I	486	THR	3.0
2	C	45	GLY	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	D	477	GLN	3.0
2	C	164	THR	3.0
1	B	65	LEU	3.0
4	K	68	GLU	3.0
1	B	105	SER	3.0
2	C	283	LYS	3.0
3	D	218	THR	3.0
2	C	243	PRO	3.0
1	G	184	ALA	3.0
2	C	165	HIS	3.0
1	H	18	GLN	3.0
3	J	314	ARG	2.9
2	I	975	ILE	2.9
3	D	212	THR	2.9
1	B	62	ASP	2.9
2	C	234	ASP	2.9
4	E	34	GLY	2.9
5	F	167	ASP	2.9
2	I	1017	GLN	2.9
1	B	97	GLU	2.9
3	J	217	LEU	2.9
3	J	892	PHE	2.9
2	I	1010	GLN	2.9
5	F	421	TYR	2.9
3	J	528	THR	2.9
2	I	442	VAL	2.9
3	D	1302	TYR	2.8
2	C	745	GLU	2.8
1	B	70	THR	2.8
2	I	593	LYS	2.8
2	I	584	TYR	2.8
1	H	98	VAL	2.8
2	I	413	GLU	2.8
3	J	675	ALA	2.8
2	I	745	GLU	2.8
2	C	305	SER	2.8
2	C	114	VAL	2.8
2	I	604	HIS	2.8
3	J	732	GLY	2.7
3	D	1171	GLY	2.7
4	K	64	LEU	2.7
2	C	981	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	25	LYS	2.7
3	J	518	VAL	2.7
3	J	747	MET	2.7
1	H	72	GLU	2.7
2	C	113	THR	2.7
3	D	69	GLU	2.7
2	I	319	LEU	2.7
2	I	1015	ALA	2.7
2	I	13	LYS	2.7
2	I	1025	PHE	2.7
3	J	300	GLN	2.7
2	I	1012	GLU	2.7
3	J	564	VAL	2.7
1	B	158	ARG	2.7
1	G	133	LEU	2.7
2	I	972	PHE	2.7
2	C	373	GLY	2.7
3	D	471	PRO	2.7
5	L	312	SER	2.6
2	I	264	GLU	2.6
2	C	262	TYR	2.6
1	B	69	SER	2.6
1	G	205	MET	2.6
1	H	233	ASP	2.6
3	J	214	ARG	2.6
3	J	1169	THR	2.6
3	D	518	VAL	2.6
1	B	96	ASP	2.6
2	I	308	GLU	2.6
2	I	267	ARG	2.6
2	I	1018	TYR	2.6
3	J	894	VAL	2.6
5	F	355	ILE	2.6
2	I	311	CYS	2.6
2	C	978	VAL	2.6
3	J	661	VAL	2.6
3	J	175	GLU	2.6
2	I	107	ARG	2.6
3	D	888	CYS	2.6
2	I	165	HIS	2.6
1	H	145	LYS	2.5
3	J	827	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	238	GLN	2.5
4	K	26	ARG	2.5
1	B	67	GLU	2.5
1	B	204	GLU	2.5
3	J	1202	GLU	2.5
5	L	337	VAL	2.5
5	L	328	GLU	2.5
5	F	300	LYS	2.5
5	F	321	ALA	2.5
3	J	563	LEU	2.5
1	H	202	VAL	2.5
2	C	282	VAL	2.5
3	J	1252	HIS	2.5
1	B	25	LYS	2.5
1	H	147	GLN	2.5
1	G	54	CYS	2.5
1	G	160	HIS	2.5
1	G	192	VAL	2.5
2	I	259	GLY	2.5
2	C	485	ASP	2.5
2	I	117	ILE	2.4
3	D	207	GLU	2.4
3	J	856	ILE	2.4
1	B	178	SER	2.4
1	H	13	LEU	2.4
4	E	2	ALA	2.4
2	C	250	THR	2.4
3	J	811	GLU	2.4
1	B	121	VAL	2.4
4	K	35	LYS	2.4
3	D	1177	ILE	2.4
2	I	992	LEU	2.4
3	D	92	VAL	2.4
3	J	931	THR	2.4
2	I	289	VAL	2.4
2	C	77	GLU	2.4
5	F	155	GLU	2.4
2	C	237	LEU	2.4
3	J	682	VAL	2.4
5	L	111	LEU	2.4
3	D	830	ASP	2.4
2	C	103	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	181	GLU	2.4
2	C	67	GLU	2.4
5	L	320	ILE	2.4
2	I	101	ARG	2.3
1	A	162	GLU	2.3
2	C	241	LEU	2.3
3	J	80	HIS	2.3
5	F	303	ILE	2.3
2	I	236	LYS	2.3
2	I	991	LYS	2.3
3	D	217	LEU	2.3
2	C	247	ARG	2.3
5	L	316	PHE	2.3
3	D	1375	ALA	2.3
3	D	419	HIS	2.3
5	L	289	LYS	2.3
5	L	422	ARG	2.3
3	J	1297	LYS	2.3
4	E	35	LYS	2.3
2	C	332	ARG	2.3
2	I	913	VAL	2.3
3	J	69	GLU	2.3
1	G	194	GLN	2.3
2	I	1136	GLN	2.3
5	L	599	ARG	2.3
2	I	726	TYR	2.3
5	F	234	THR	2.3
3	D	205	LEU	2.2
3	D	420	PRO	2.2
2	I	980	VAL	2.2
4	K	32	VAL	2.2
2	C	268	ARG	2.2
1	H	29	GLU	2.2
2	C	258	ASN	2.2
3	D	1166	GLY	2.2
1	G	209	GLY	2.2
1	H	137	ASN	2.2
4	K	77	ALA	2.2
2	I	1070	HIS	2.2
2	I	147	SER	2.2
3	D	1203	ARG	2.2
2	C	266	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	2.2
3	J	714	GLU	2.2
3	J	667	GLN	2.2
2	I	1023	HIS	2.2
2	I	1068	GLY	2.2
2	I	906	PHE	2.2
2	I	1072	ASN	2.2
2	I	322	LEU	2.2
2	I	633	LEU	2.2
3	J	154	LEU	2.2
2	C	169	LYS	2.2
3	D	469	HIS	2.2
2	I	187	GLU	2.1
2	I	265	LYS	2.1
3	D	209	ASN	2.1
5	F	158	LEU	2.1
3	J	712	GLN	2.1
3	J	266	ASN	2.1
3	J	1186	TYR	2.1
2	I	1144	PHE	2.1
1	B	139	SER	2.1
3	D	319	SER	2.1
3	D	826	ILE	2.1
2	I	895	LEU	2.1
3	D	68	TYR	2.1
3	J	176	PHE	2.1
2	I	1014	LEU	2.1
2	C	909	LYS	2.1
4	K	71	GLU	2.1
4	K	34	GLY	2.1
2	I	590	PRO	2.1
4	K	37	PRO	2.1
5	F	483	LEU	2.1
2	C	374	GLU	2.1
2	C	163	LYS	2.1
1	B	173	VAL	2.1
5	L	338	HIS	2.1
2	I	969	ALA	2.1
5	F	318	ALA	2.1
3	J	829	GLY	2.1
2	C	492	MET	2.1
3	J	209	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	101	ARG	2.1
2	I	1069	ARG	2.1
3	J	1171	GLY	2.1
5	L	513	ASP	2.1
5	L	613	ASP	2.1
2	C	316	GLU	2.1
2	I	105	TYR	2.1
1	A	237	VAL	2.1
3	D	1376	GLY	2.1
3	J	677	GLU	2.1
2	C	414	ILE	2.1
3	J	1204	VAL	2.0
5	F	304	THR	2.0
5	F	325	PRO	2.0
2	C	300	ASP	2.0
3	J	554	GLU	2.0
2	I	536	GLY	2.0
2	C	584	TYR	2.0
2	I	247	ARG	2.0
4	K	13	ILE	2.0
1	G	94	GLY	2.0
3	D	547	ARG	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ZN	D	2003	1/1	0.70	0.20	189,189,189,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	2001	1/1	0.71	0.27	189,189,189,189	0
7	ZN	D	2004	1/1	0.74	0.29	189,189,189,189	0
6	MG	D	2002	1/1	0.78	0.29	189,189,189,189	0
6	MG	J	2001	1/1	0.85	0.29	189,189,189,189	0
6	MG	I	1401	1/1	0.85	0.30	189,189,189,189	0
7	ZN	J	2003	1/1	0.88	0.22	189,189,189,189	0
7	ZN	J	2002	1/1	0.94	0.13	310,310,310,310	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.