



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:32 PM UTC

PDB ID : 4N9F / pdb_00004n9f
Title : Crystal structure of the Vif-CBFbeta-CUL5-ElOB-ElOC pentameric complex
Authors : Guo, Y.Y.; Dong, L.Y.; Huang, Z.W.
Deposited on : 2013-10-21
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

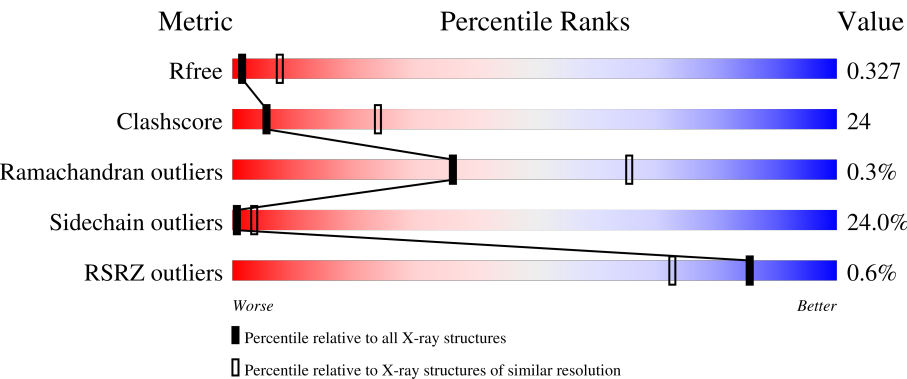
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	3	311	43%41%9%• 5%
1	9	311	50%33%11%5%
1	C	311	42%39%14%• 5%
1	I	311	% 37%44%14%• 5%
1	O	311	38%42%13%• •

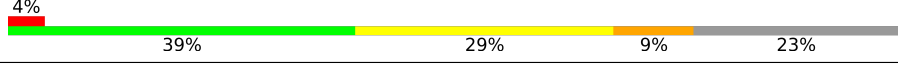
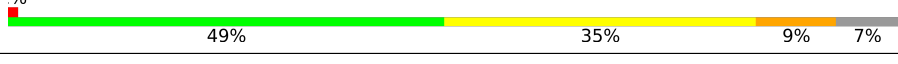
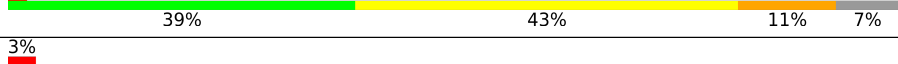
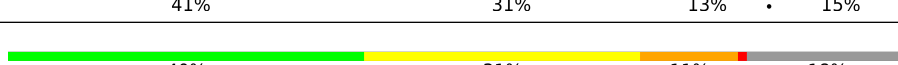
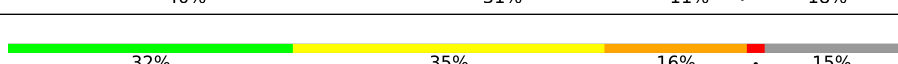
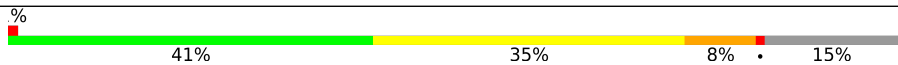
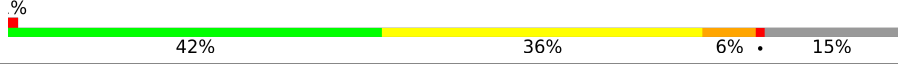
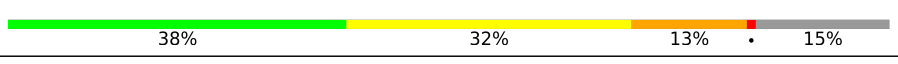
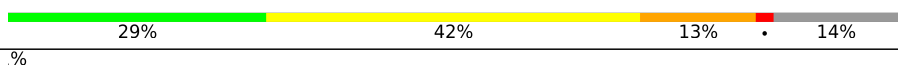
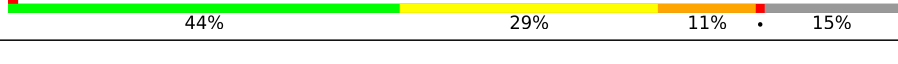
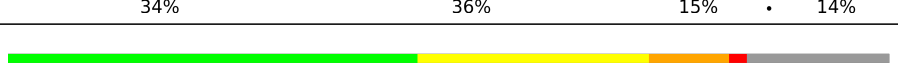
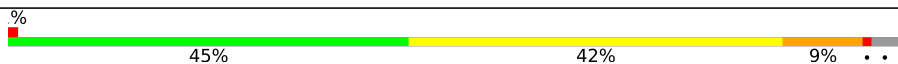
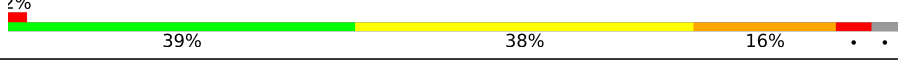
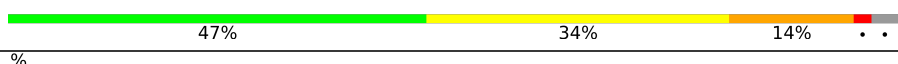
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Mol	Chain	Length	Quality of chain
1	U	311	
1	V	311	
1	f	311	
1	l	311	
1	r	311	
1	w	311	
1	x	311	
2	5	96	
2	B	96	
2	E	96	
2	K	96	
2	Q	96	
2	T	96	
2	Y	96	
2	Z	96	
2	h	96	
2	n	96	
2	t	96	
2	z	96	
3	4	102	
3	D	102	
3	H	102	
3	J	102	
3	P	102	
3	W	102	

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Mol	Chain	Length	Quality of chain
3	X	102	
3	e	102	
3	g	102	
3	m	102	
3	s	102	
3	y	102	
4	0	170	
4	6	170	
4	F	170	
4	L	170	
4	N	170	
4	R	170	
4	a	170	
4	c	170	
4	i	170	
4	k	170	
4	o	170	
4	u	170	
5	1	176	
5	2	176	
5	7	176	
5	G	176	
5	M	176	
5	S	176	
5	b	176	

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Mol	Chain	Length	Quality of chain
5	d	176	41%40%15%.
5	j	176	% 45%38%14%. .
5	p	176	39%44%11%. .
5	q	176	% 40%33%21%. .
5	v	176	% 41%42%13%. .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 77274 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 Cullin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	299	Total	C	N	O	S	0	2	0
			2469	1567	420	465	17			
1	C	297	Total	C	N	O	S	0	1	0
			2446	1555	417	457	17			
1	I	296	Total	C	N	O	S	0	1	0
			2441	1552	416	456	17			
1	O	298	Total	C	N	O	S	0	1	0
			2451	1558	418	458	17			
1	V	296	Total	C	N	O	S	0	1	0
			2441	1552	416	456	17			
1	f	296	Total	C	N	O	S	0	1	0
			2441	1552	416	456	17			
1	l	297	Total	C	N	O	S	0	0	0
			2444	1555	416	456	17			
1	r	296	Total	C	N	O	S	0	1	0
			2441	1552	416	456	17			
1	x	294	Total	C	N	O	S	0	0	0
			2419	1540	410	452	17			
1	3	295	Total	C	N	O	S	0	1	0
			2435	1549	415	454	17			
1	9	295	Total	C	N	O	S	0	1	0
			2435	1549	415	454	17			
1	w	296	Total	C	N	O	S	0	1	0
			2440	1552	416	455	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	11	ALA	-	expression tag	UNP Q93034
C	11	ALA	-	expression tag	UNP Q93034
I	11	ALA	-	expression tag	UNP Q93034
O	11	ALA	-	expression tag	UNP Q93034
V	11	ALA	-	expression tag	UNP Q93034

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Chain	Residue	Modelled	Actual	Comment	Reference
f	11	ALA	-	expression tag	UNP Q93034
l	11	ALA	-	expression tag	UNP Q93034
r	11	ALA	-	expression tag	UNP Q93034
x	11	ALA	-	expression tag	UNP Q93034
3	11	ALA	-	expression tag	UNP Q93034
9	11	ALA	-	expression tag	UNP Q93034
w	11	ALA	-	expression tag	UNP Q93034

- Molecule 2 is a protein called Transcription elongation factor B polypeptide 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	E	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	K	86	Total 683	C 442	N 110	O 127	S 4	0	0	0
2	Q	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	Z	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	h	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	n	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	t	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	z	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	5	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	T	87	Total 691	C 447	N 111	O 128	S 5	0	0	0
2	B	87	Total 691	C 447	N 111	O 128	S 5	0	0	0

- Molecule 3 is a protein called Transcription elongation factor B polypeptide 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	95	Total 748	C 474	N 125	O 146	S 3	0	0	0
3	D	95	Total 748	C 474	N 125	O 146	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	90	Total	C	N	O	S	0	0	0
			711	449	120	139	3			
3	P	94	Total	C	N	O	S	0	0	0
			740	470	124	143	3			
3	W	91	Total	C	N	O	S	0	0	0
			717	454	121	139	3			
3	g	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	m	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	s	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	y	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	4	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			
3	e	79	Total	C	N	O	S	0	0	0
			624	394	109	119	2			
3	H	95	Total	C	N	O	S	0	0	0
			748	474	125	146	3			

- Molecule 4 is a protein called Core-binding factor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	a	146	Total	C	N	O	S	0	0	0
			1193	745	217	225	6			
4	F	145	Total	C	N	O	S	0	0	0
			1185	741	216	222	6			
4	L	144	Total	C	N	O	S	0	0	0
			1154	723	211	214	6			
4	R	144	Total	C	N	O	S	0	0	0
			1175	734	212	223	6			
4	c	145	Total	C	N	O	S	0	0	0
			1180	737	213	224	6			
4	i	155	Total	C	N	O	S	0	0	0
			1271	790	232	243	6			
4	o	143	Total	C	N	O	S	0	0	0
			1167	730	211	220	6			
4	u	143	Total	C	N	O	S	0	0	0
			1167	730	211	220	6			
4	0	144	Total	C	N	O	S	0	0	0
			1175	734	212	223	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	6	140	Total	C	N	O	S	0	0	0
			1147	718	208	215	6			
4	k	147	Total	C	N	O	S	0	0	0
			1196	746	215	229	6			
4	N	145	Total	C	N	O	S	0	0	0
			1173	734	213	220	6			

- Molecule 5 is a protein called Virion infectivity factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	b	172	Total	C	N	O	S	0	0	0
			1414	908	258	243	5			
5	G	170	Total	C	N	O	S	0	0	0
			1397	898	256	239	4			
5	M	171	Total	C	N	O	S	0	0	0
			1402	901	257	240	4			
5	S	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			
5	d	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			
5	j	170	Total	C	N	O	S	0	0	0
			1397	898	256	239	4			
5	p	169	Total	C	N	O	S	0	0	0
			1380	887	251	238	4			
5	v	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			
5	1	170	Total	C	N	O	S	0	0	0
			1385	890	252	239	4			
5	7	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			
5	q	169	Total	C	N	O	S	0	0	0
			1386	892	252	238	4			
5	2	170	Total	C	N	O	S	0	0	0
			1391	895	253	239	4			

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	b	1	Total	Zn	0	0
			1	1		
6	G	1	Total	Zn	0	0
			1	1		

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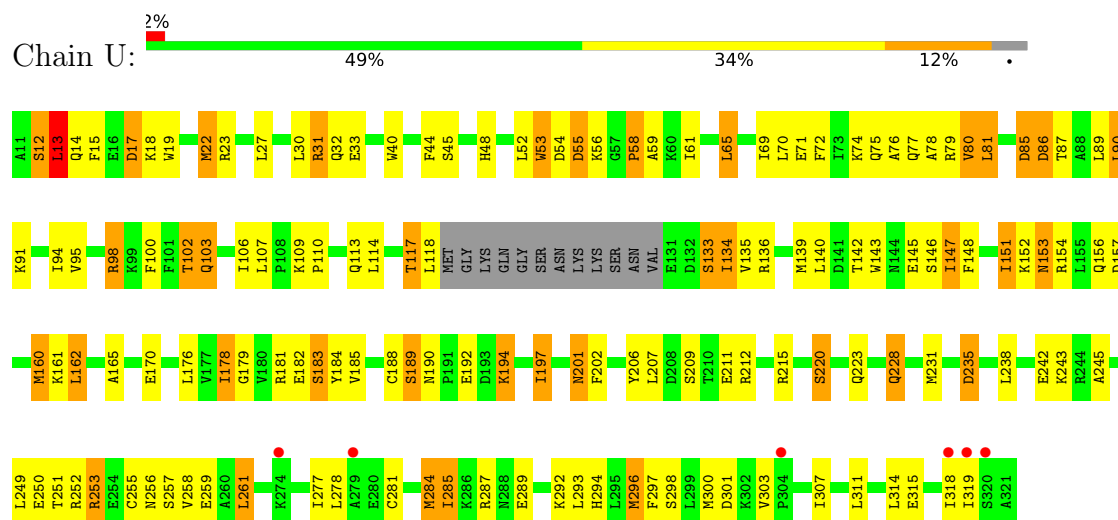
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total 1	Zn 1	0	0
6	S	1	Total 1	Zn 1	0	0
6	d	1	Total 1	Zn 1	0	0
6	j	1	Total 1	Zn 1	0	0
6	p	1	Total 1	Zn 1	0	0
6	v	1	Total 1	Zn 1	0	0
6	1	1	Total 1	Zn 1	0	0
6	7	1	Total 1	Zn 1	0	0
6	q	1	Total 1	Zn 1	0	0
6	2	1	Total 1	Zn 1	0	0

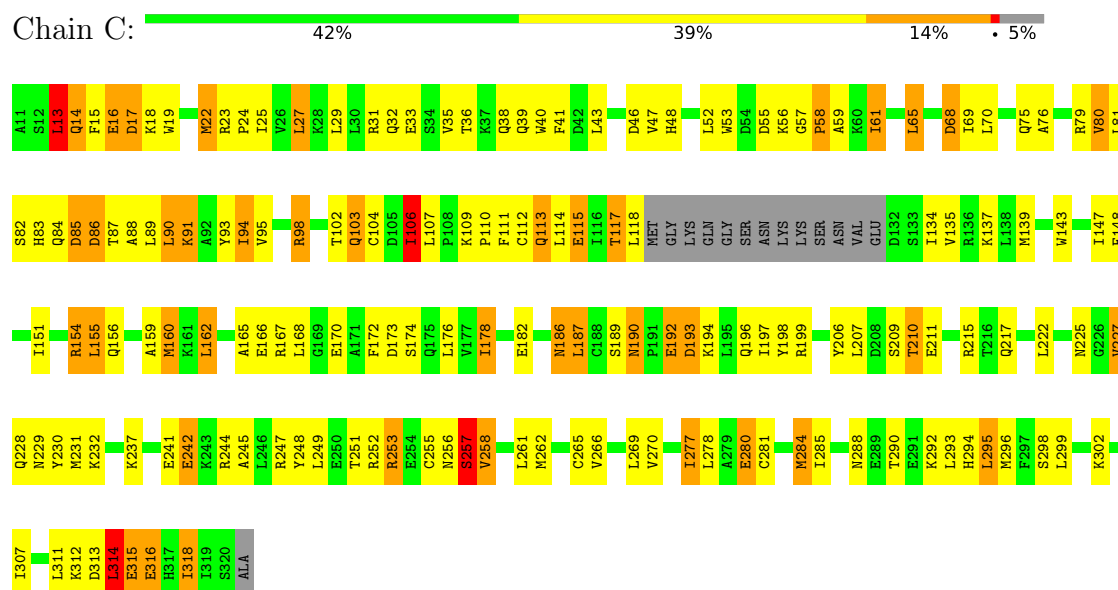
3 Residue-property plots

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

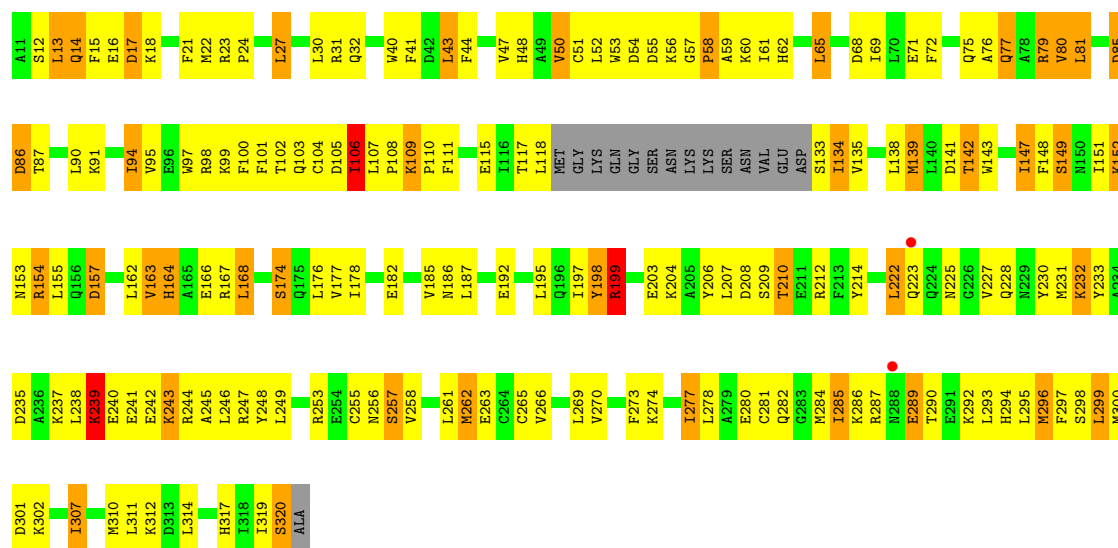
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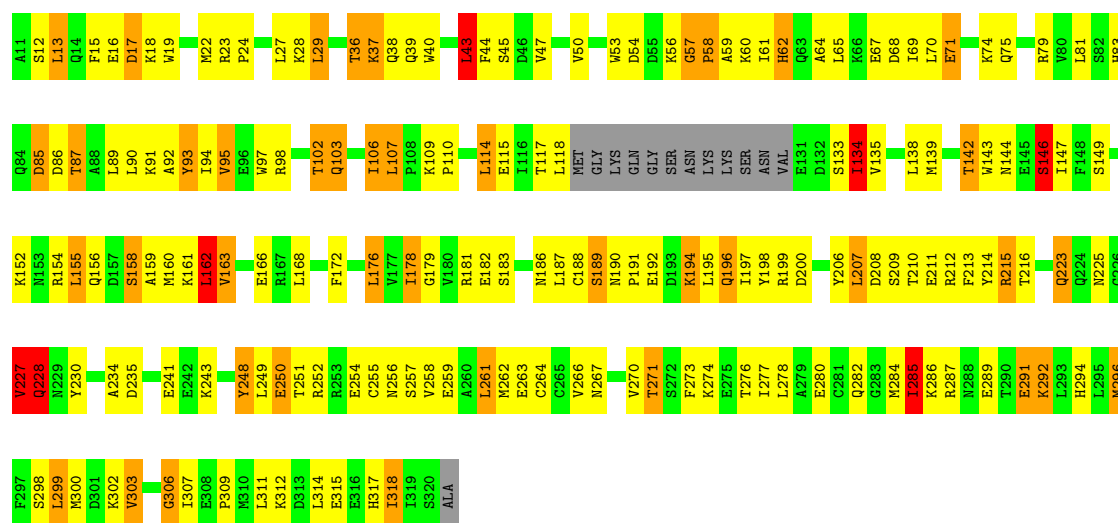
• Molecule 1: Cullin-5



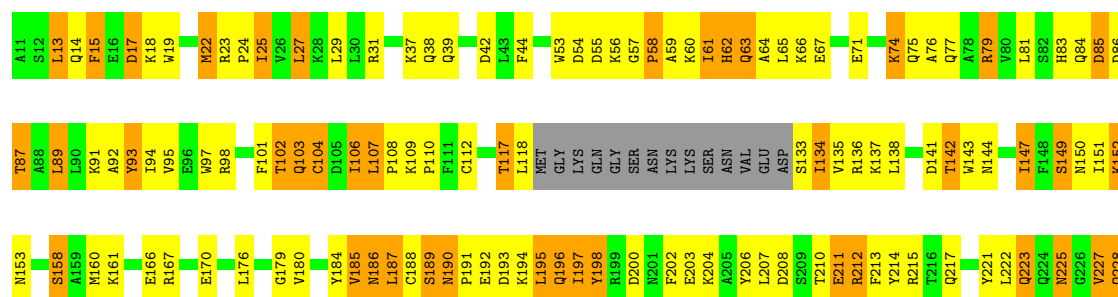
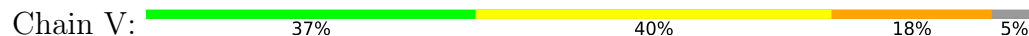
• Molecule 1: Cullin-5

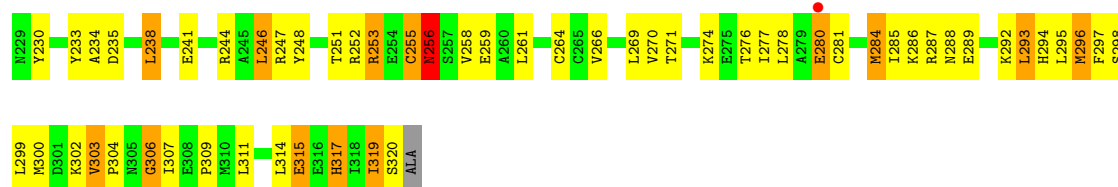


• Molecule 1: Cullin-5

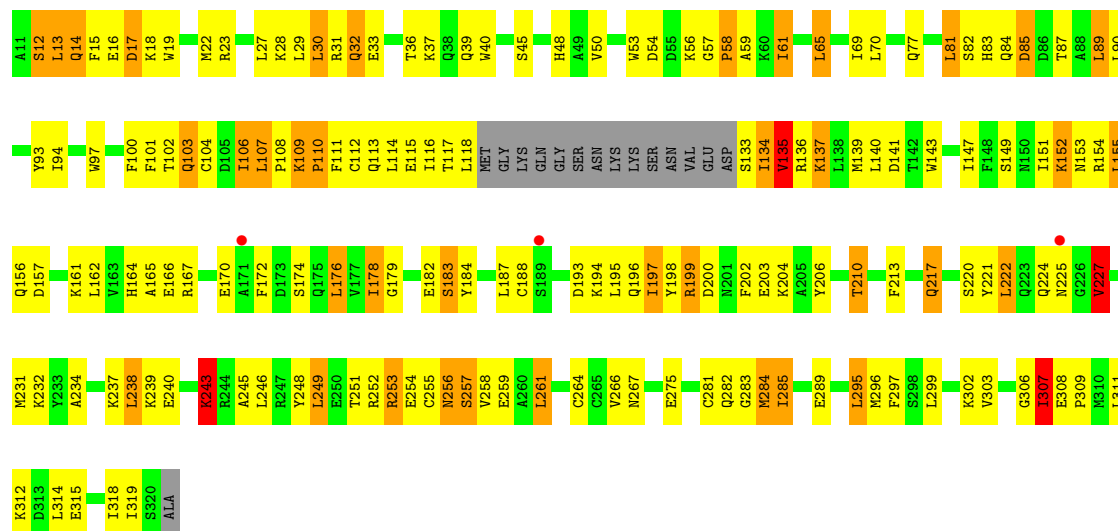
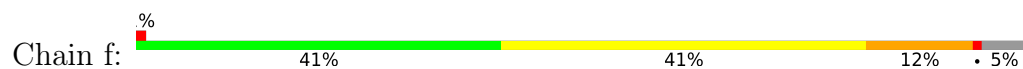


• Molecule 1: Cullin-5

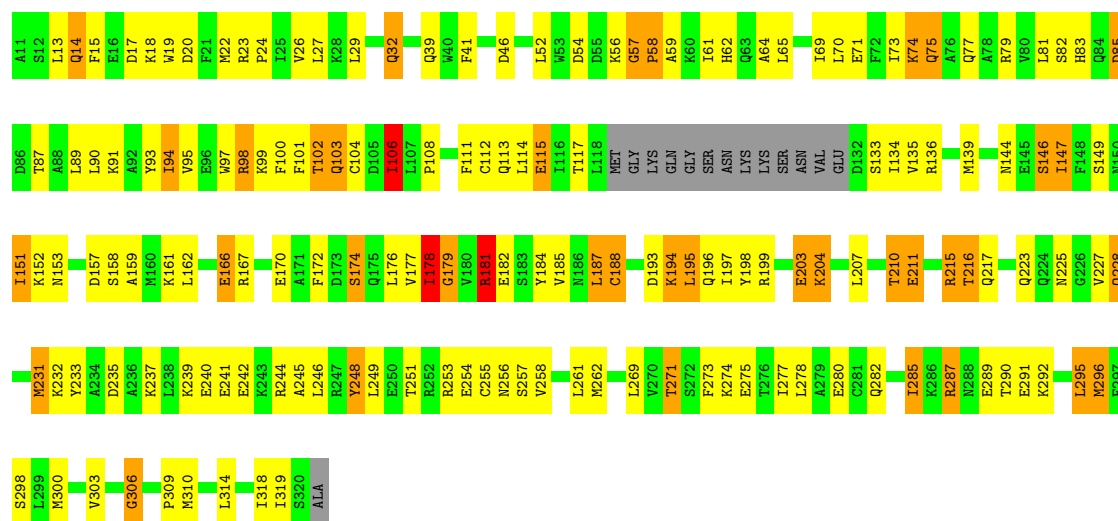




• Molecule 1: Cullin-5

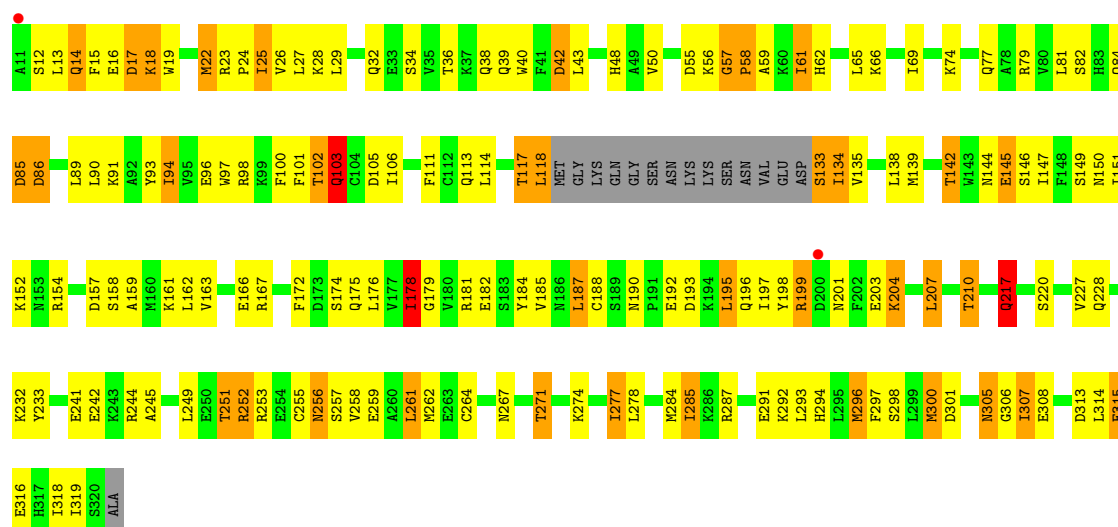


• Molecule 1: Cullin-5

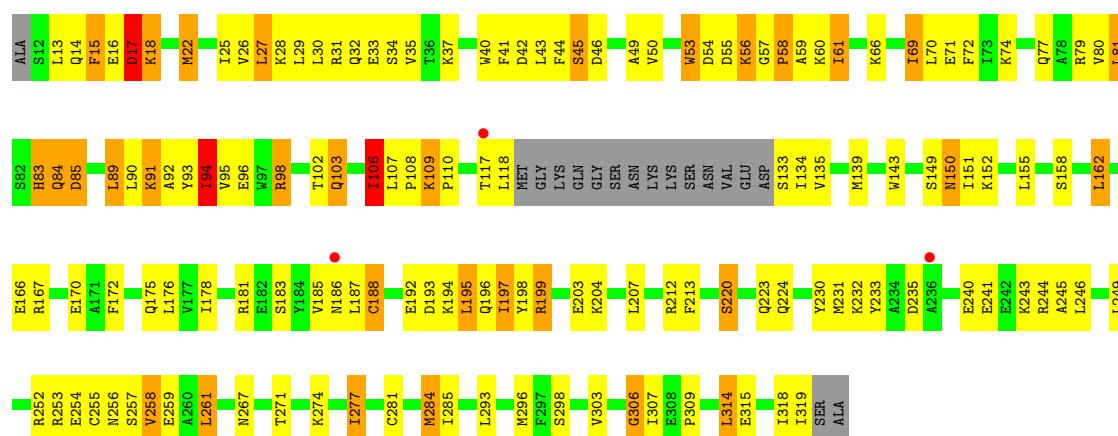


• Molecule 1: Cullin-5

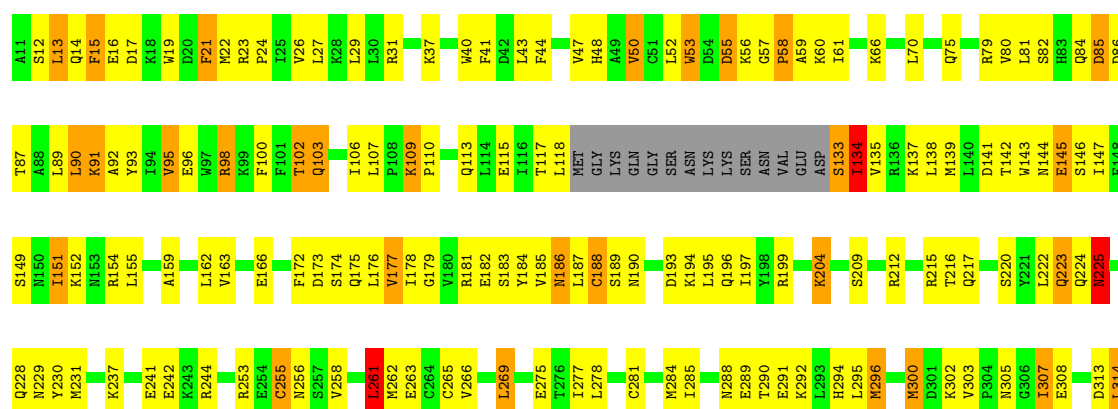




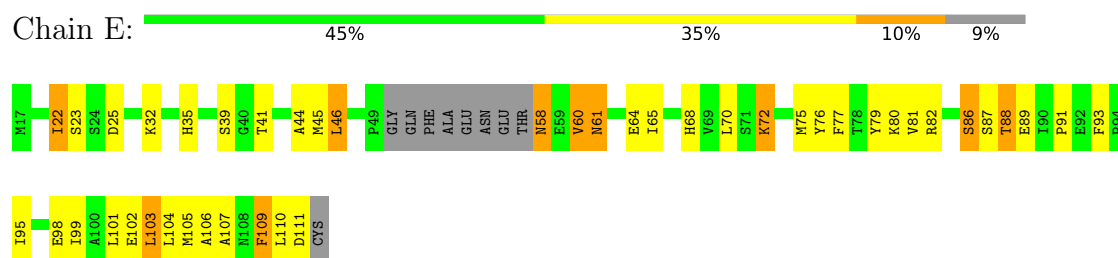
• Molecule 1: Cullin-5



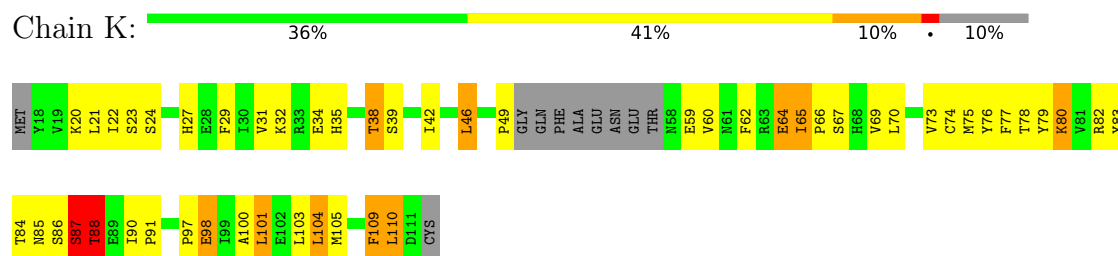
• Molecule 1: Cullin-5



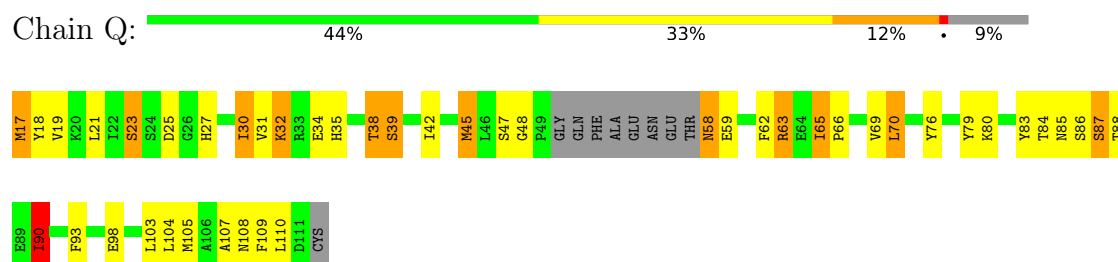
- Molecule 2: Transcription elongation factor B polypeptide 1



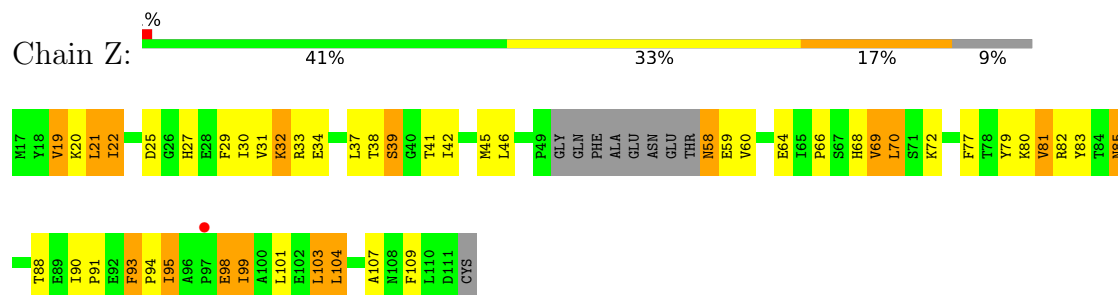
- Molecule 2: Transcription elongation factor B polypeptide 1



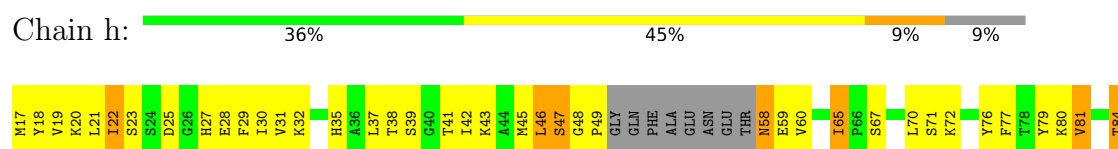
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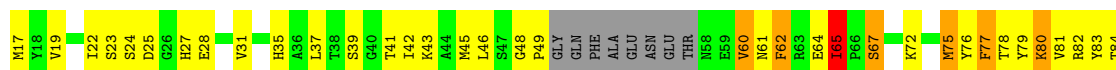


- Molecule 2: Transcription elongation factor B polypeptide 1

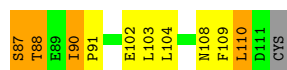
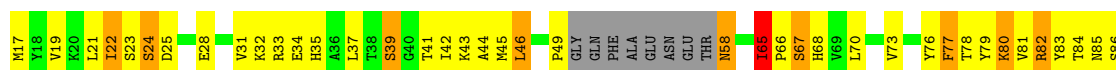




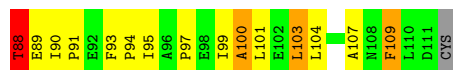
- Molecule 2: Transcription elongation factor B polypeptide 1



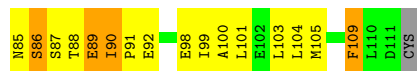
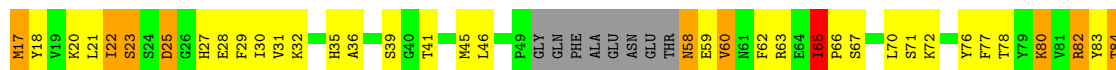
- Molecule 2: Transcription elongation factor B polypeptide 1



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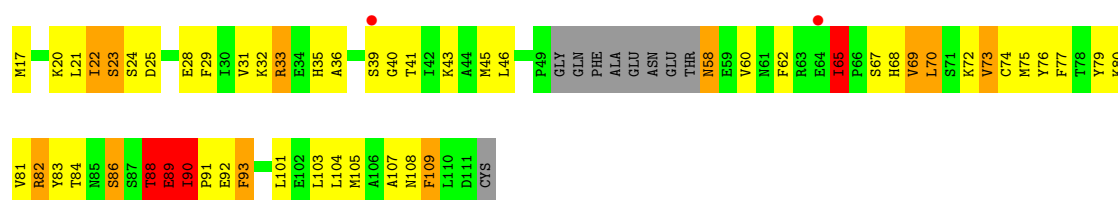


- Molecule 2: Transcription elongation factor B polypeptide 1

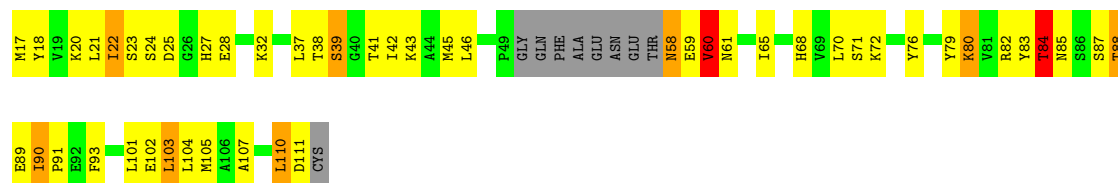


- Molecule 2: Transcription elongation factor B polypeptide 1

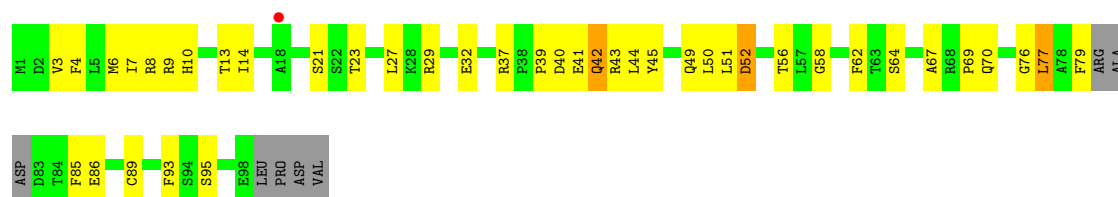




• Molecule 2: Transcription elongation factor B polypeptide 1



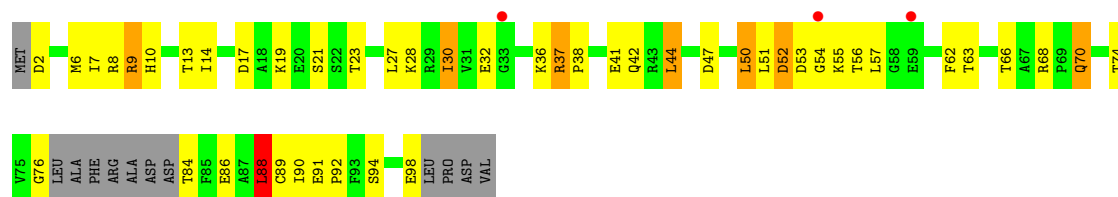
• Molecule 3: Transcription elongation factor B polypeptide 2



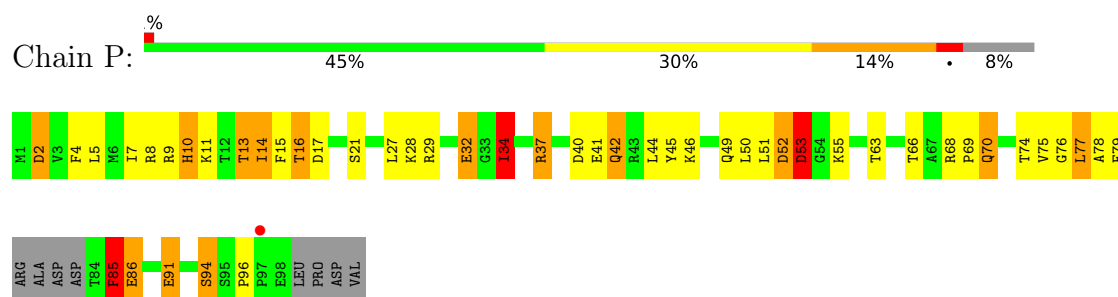
• Molecule 3: Transcription elongation factor B polypeptide 2



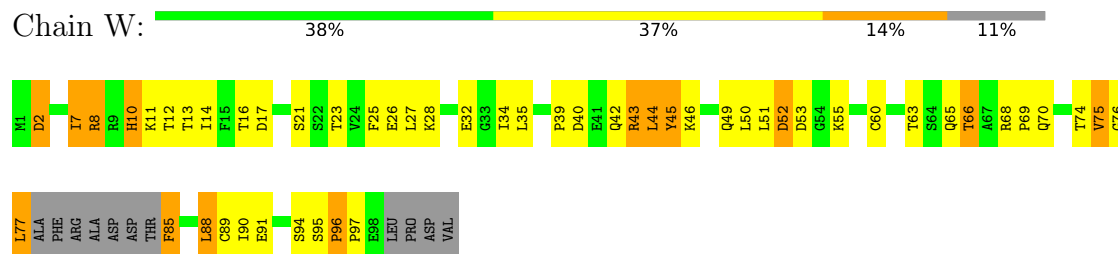
• Molecule 3: Transcription elongation factor B polypeptide 2



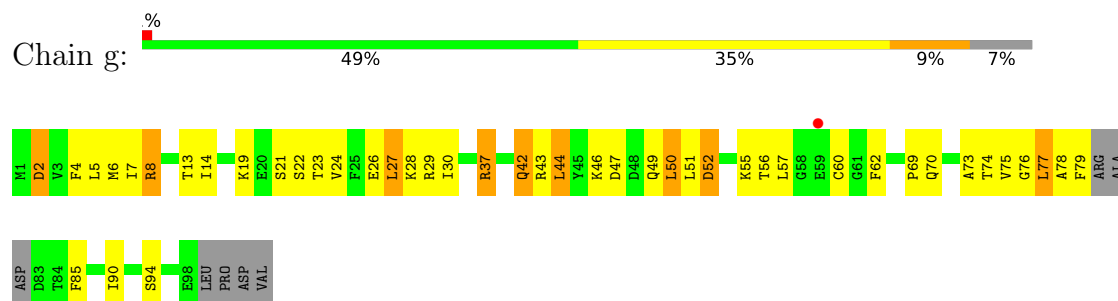
• Molecule 3: Transcription elongation factor B polypeptide 2



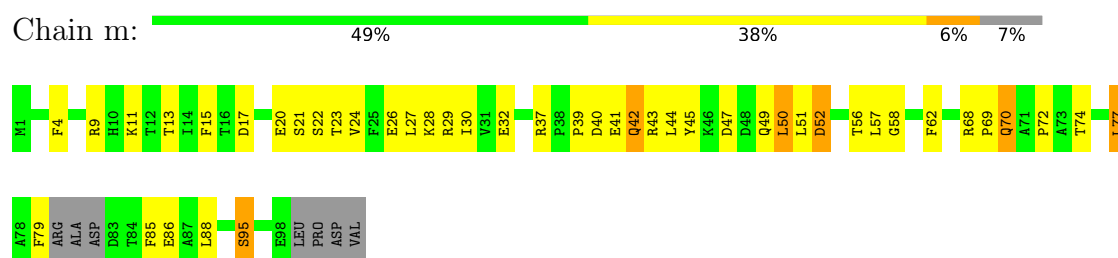
- Molecule 3: Transcription elongation factor B polypeptide 2



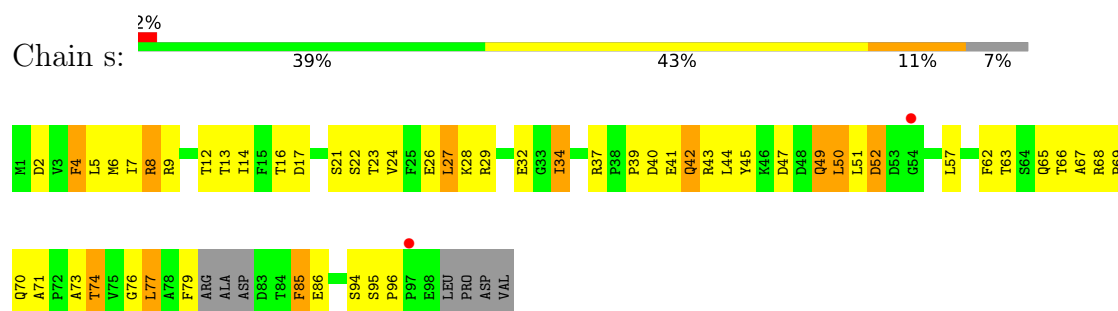
- Molecule 3: Transcription elongation factor B polypeptide 2



- Molecule 3: Transcription elongation factor B polypeptide 2

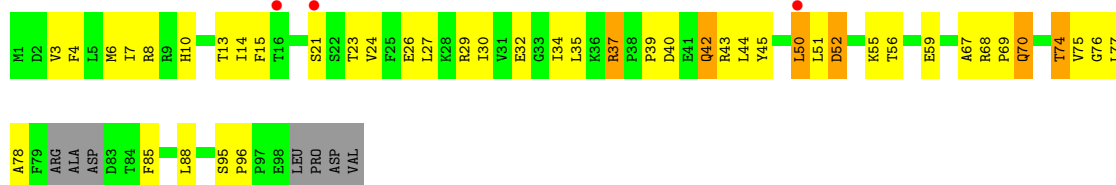


- Molecule 3: Transcription elongation factor B polypeptide 2



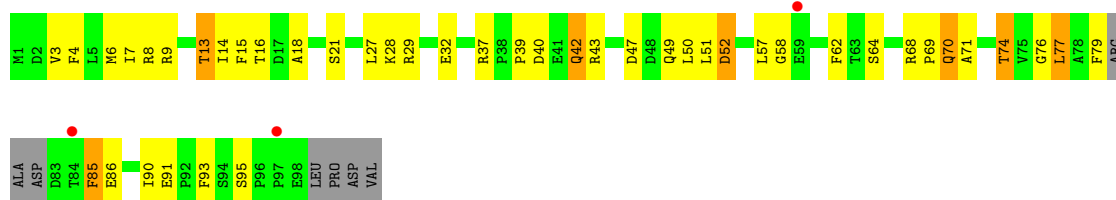
- Molecule 3: Transcription elongation factor B polypeptide 2

Chain y: 

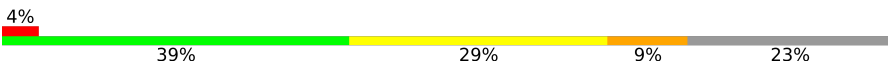


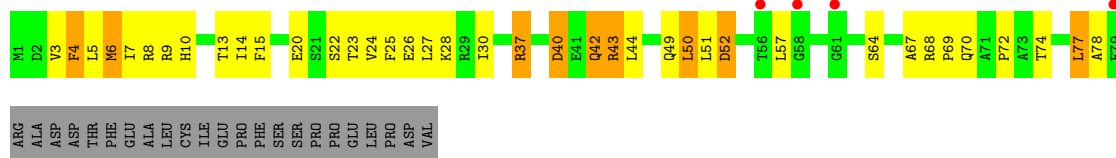
- Molecule 3: Transcription elongation factor B polypeptide 2

Chain 4: 



- Molecule 3: Transcription elongation factor B polypeptide 2

Chain e: 

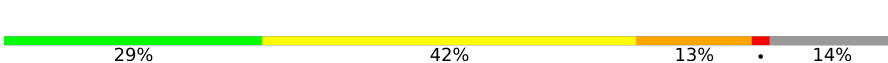


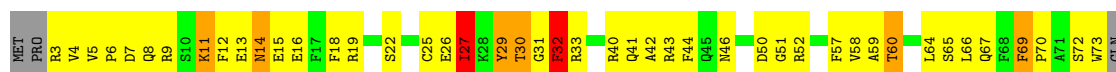
- Molecule 3: Transcription elongation factor B polypeptide 2

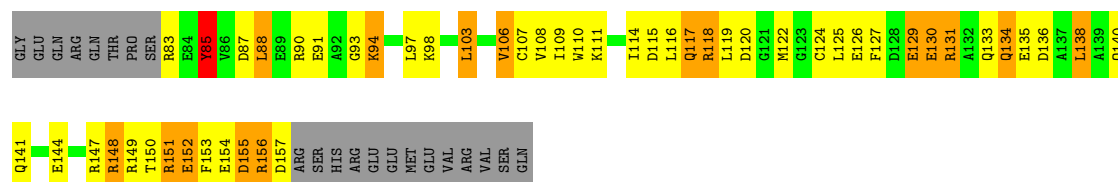
Chain H: 



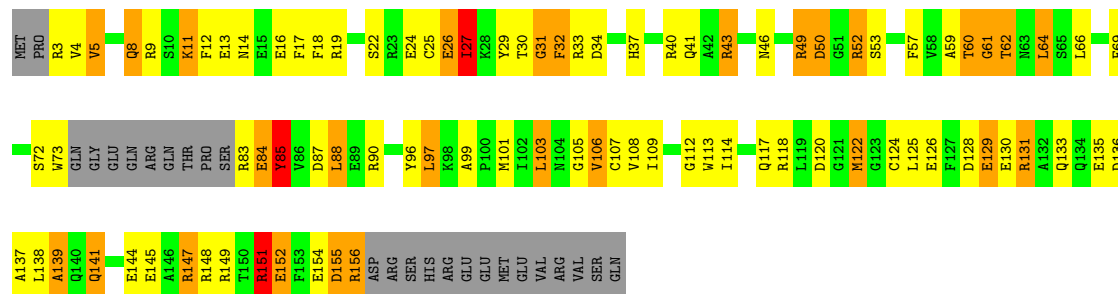
- Molecule 4: Core-binding factor subunit beta

Chain a: 

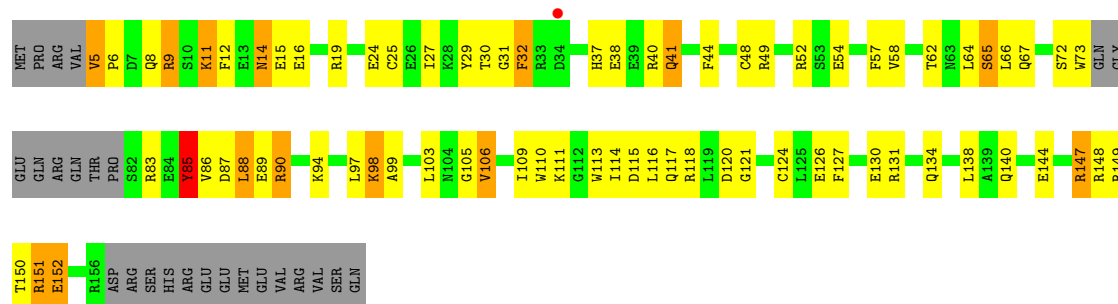




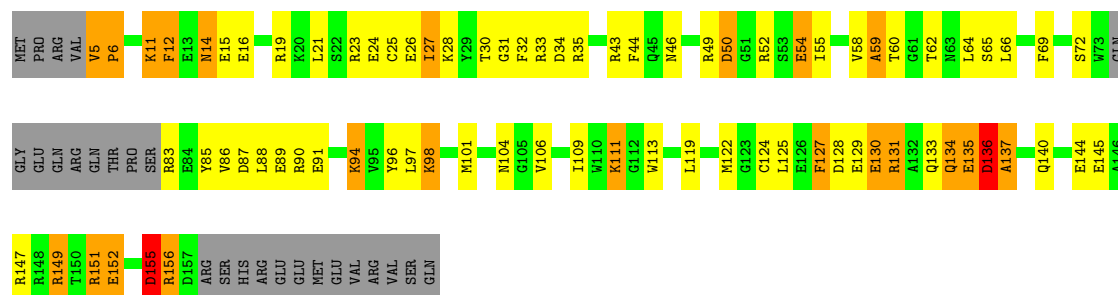
• Molecule 4: Core-binding factor subunit beta



• Molecule 4: Core-binding factor subunit beta

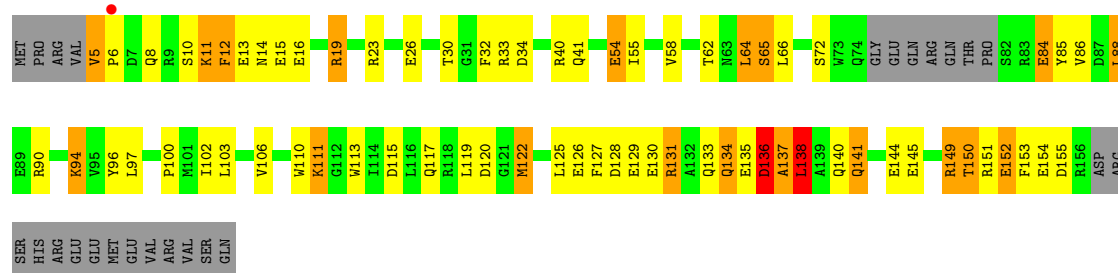


• Molecule 4: Core-binding factor subunit beta

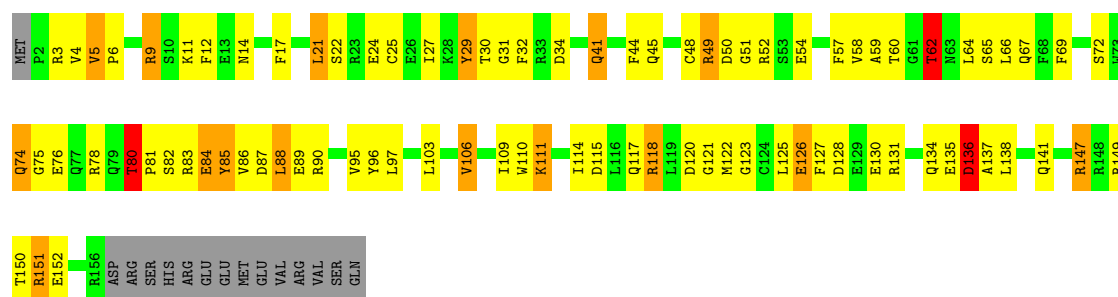


• Molecule 4: Core-binding factor subunit beta

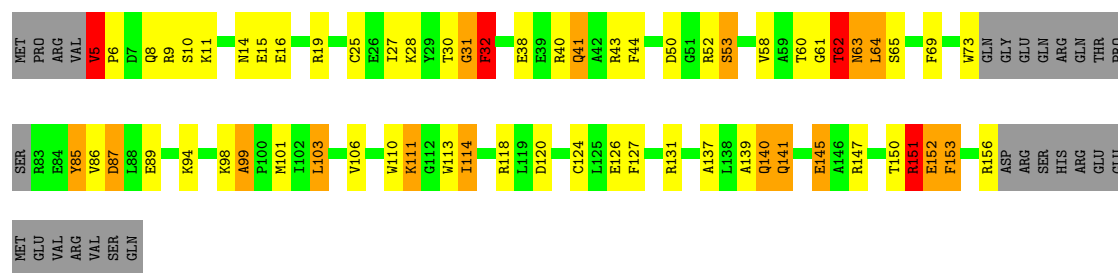




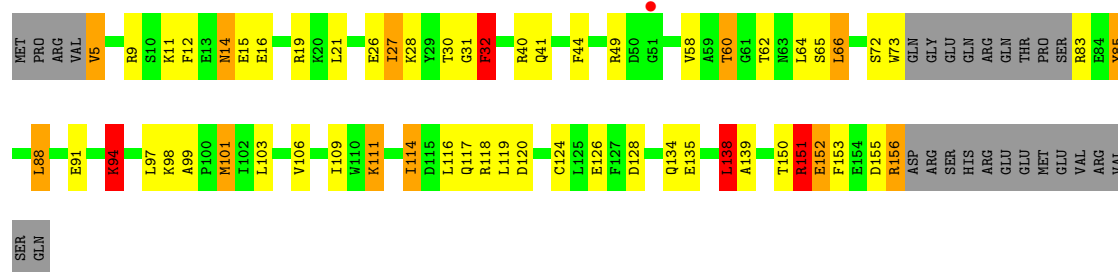
• Molecule 4: Core-binding factor subunit beta



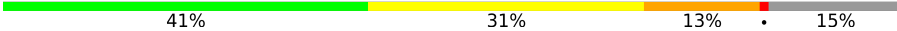
• Molecule 4: Core-binding factor subunit beta

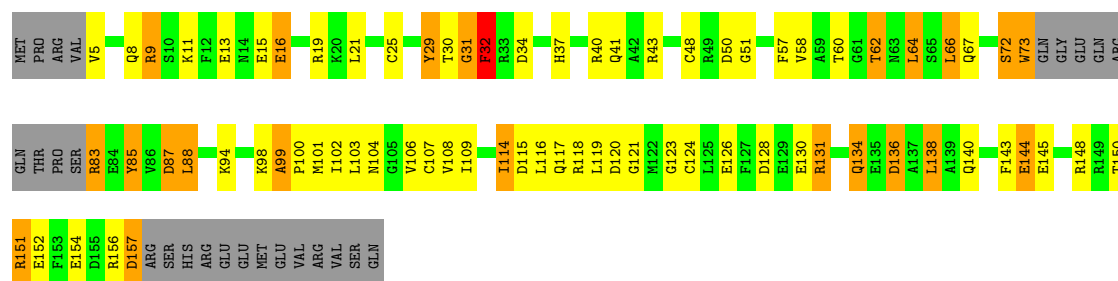


• Molecule 4: Core-binding factor subunit beta

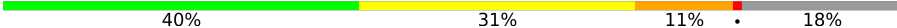


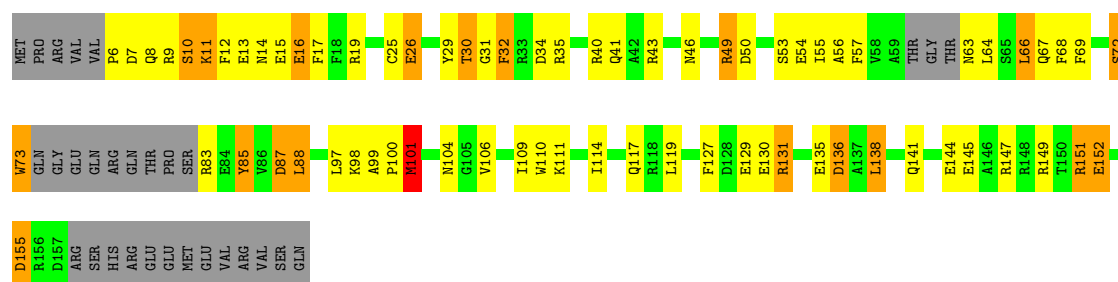
• Molecule 4: Core-binding factor subunit beta

Chain 0: 

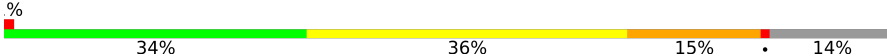


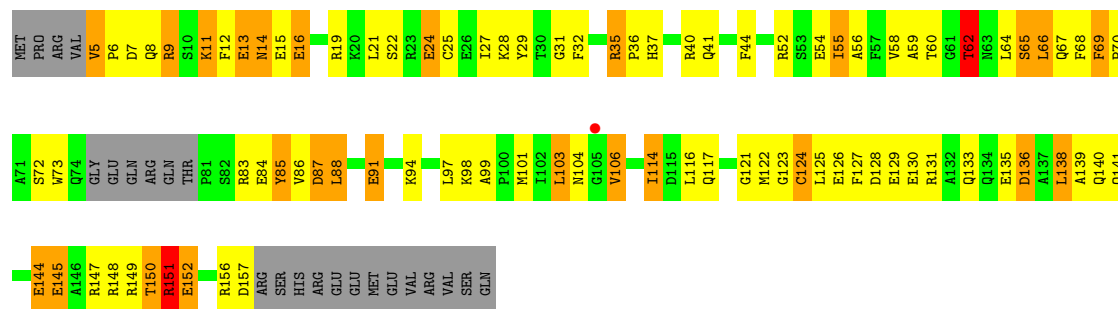
• Molecule 4: Core-binding factor subunit beta

Chain 6: 



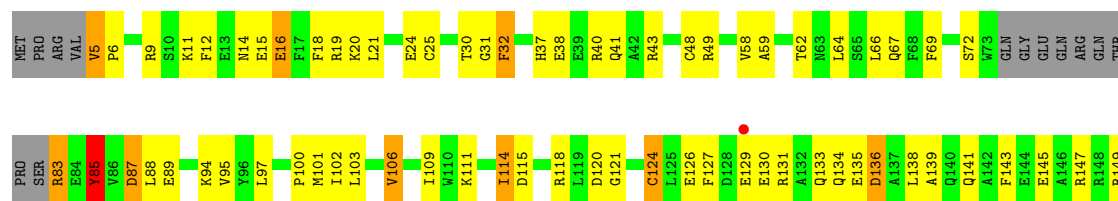
• Molecule 4: Core-binding factor subunit beta

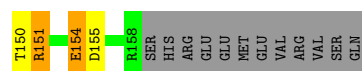
Chain k: 



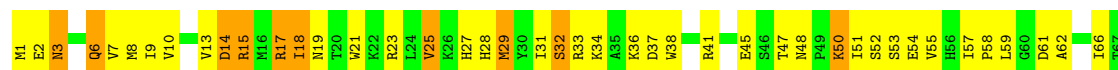
• Molecule 4: Core-binding factor subunit beta

Chain N: 

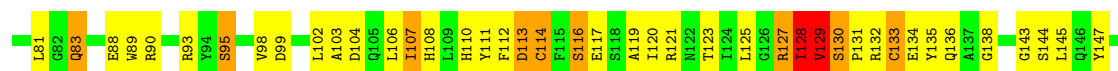
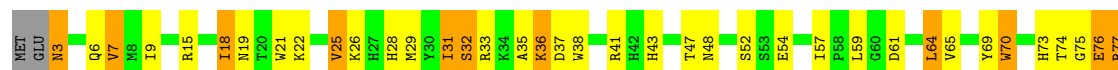




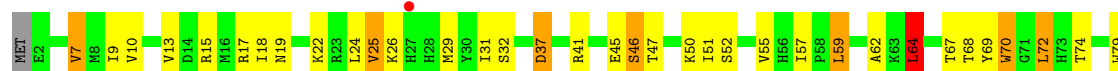
• Molecule 5: Virion infectivity factor



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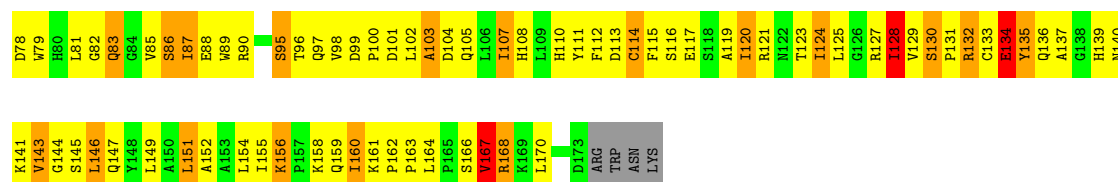


• Molecule 5: Virion infectivity factor

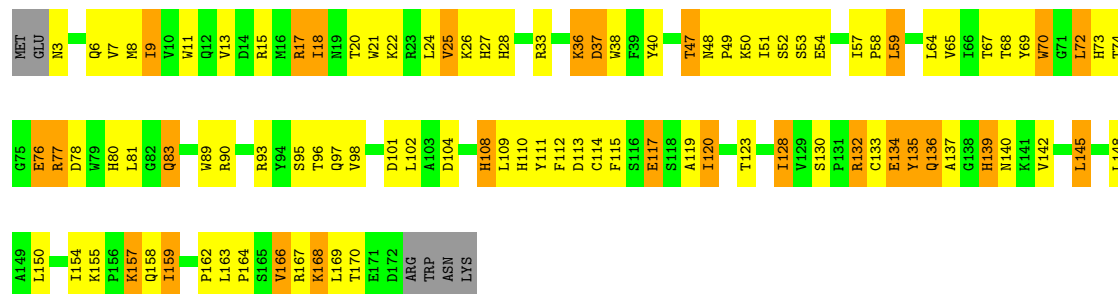


• Molecule 5: Virion infectivity factor

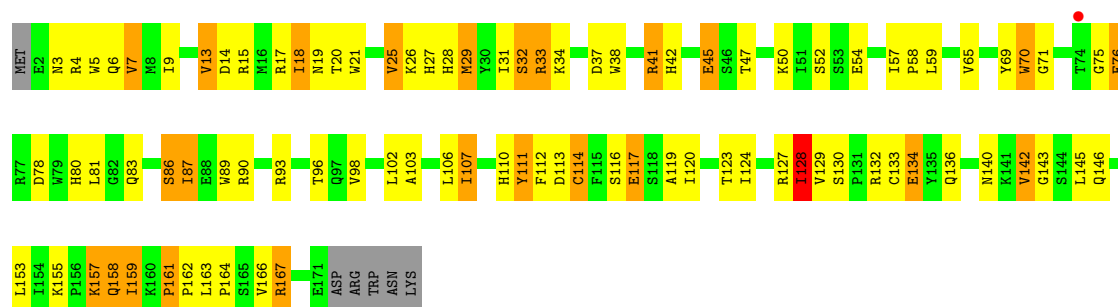




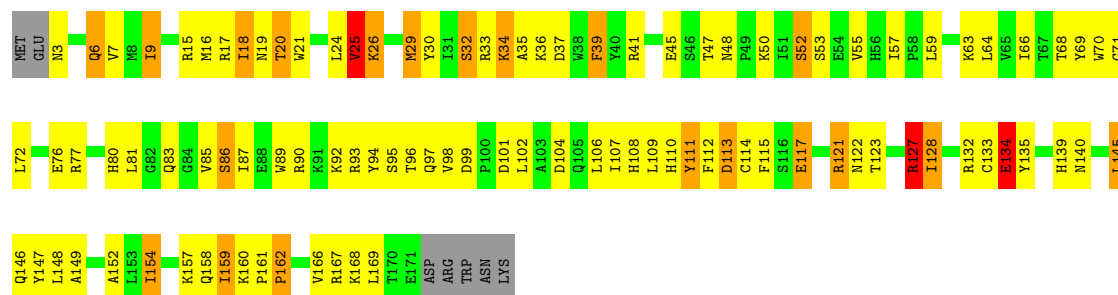
• Molecule 5: Virion infectivity factor



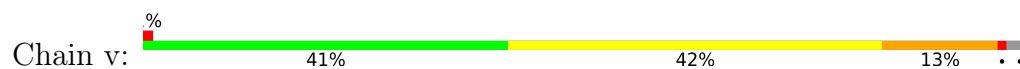
• Molecule 5: Virion infectivity factor

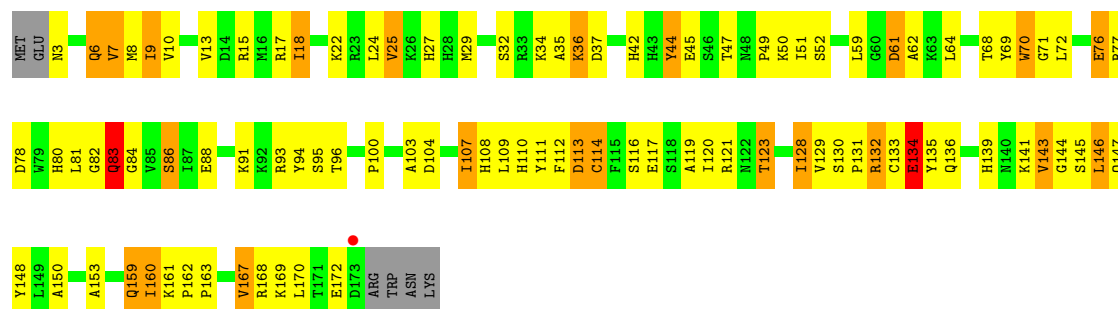


• Molecule 5: Virion infectivity factor

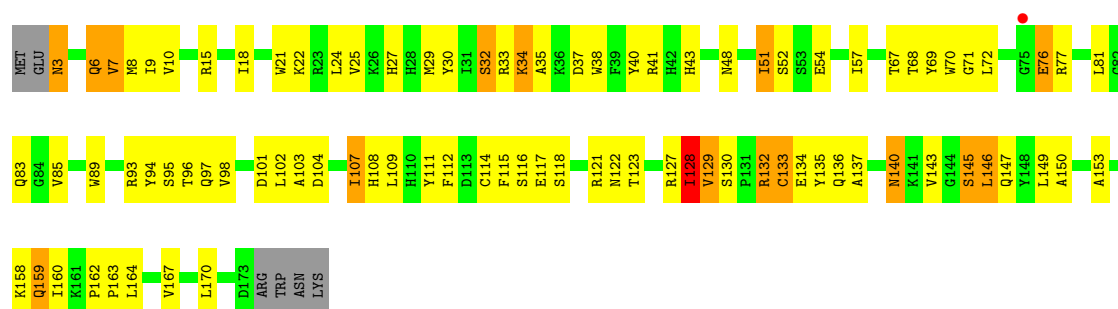
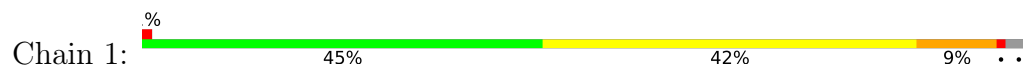


• Molecule 5: Virion infectivity factor

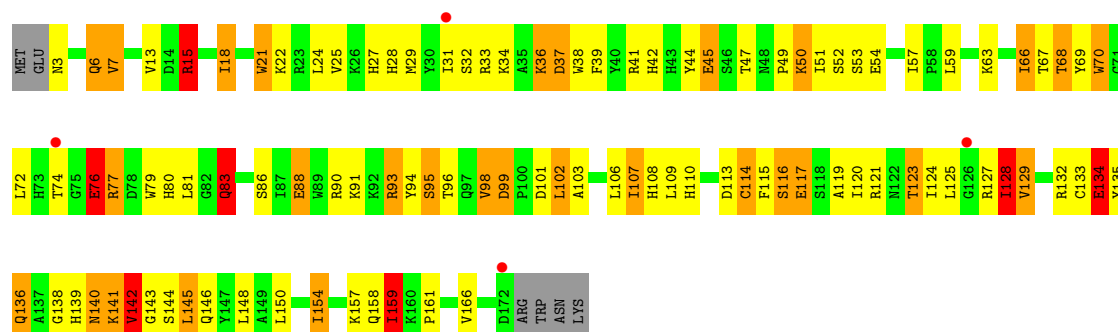




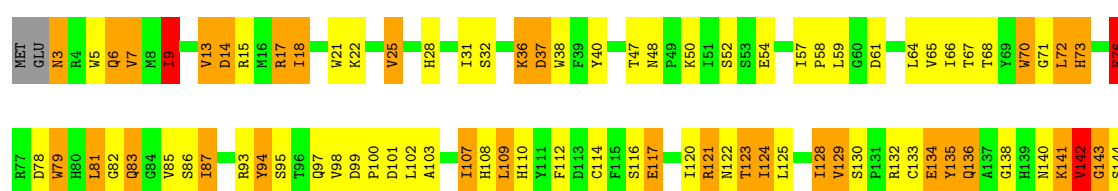
• Molecule 5: Virion infectivity factor

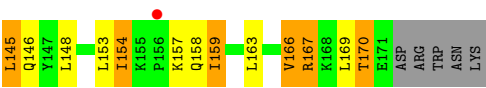


• Molecule 5: Virion infectivity factor

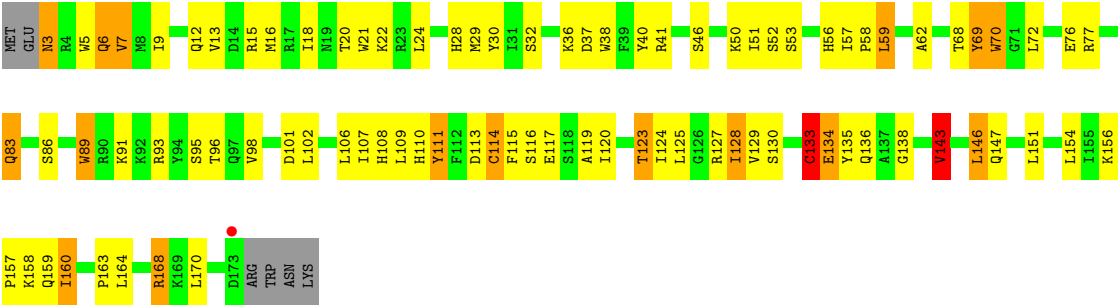


• Molecule 5: Virion infectivity factor





• Molecule 5: Virion infectivity factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.92Å 204.00Å 247.87Å 65.51° 90.28° 90.50°	Depositor
Resolution (Å)	49.53 – 3.30 49.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.53-3.30) 93.0 (49.53-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.262 , 0.324 0.266 , 0.327	Depositor DCC
R_{free} test set	14295 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	100.1	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l 0.327 for -h,k,k-l 0.196 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	77274	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	3	0.76	0/2480	1.25	18/3340 (0.5%)
1	9	0.62	0/2480	1.19	16/3340 (0.5%)
1	C	0.77	0/2491	1.26	21/3355 (0.6%)
1	I	0.73	0/2486	1.32	26/3348 (0.8%)
1	O	0.81	1/2496 (0.0%)	1.29	27/3362 (0.8%)
1	U	0.72	1/2514 (0.0%)	1.27	22/3386 (0.6%)
1	V	0.82	2/2486 (0.1%)	1.33	27/3348 (0.8%)
1	f	0.71	0/2486	1.31	27/3348 (0.8%)
1	l	0.80	0/2489	1.30	21/3352 (0.6%)
1	r	0.78	0/2486	1.29	24/3348 (0.7%)
1	w	0.73	1/2485 (0.0%)	1.31	22/3347 (0.7%)
1	x	0.62	0/2464	1.12	11/3319 (0.3%)
2	5	0.73	0/706	1.28	7/954 (0.7%)
2	B	0.73	0/706	1.19	3/954 (0.3%)
2	E	0.73	0/706	1.13	1/954 (0.1%)
2	K	0.78	0/698	1.30	10/944 (1.1%)
2	Q	0.75	0/706	1.37	7/954 (0.7%)
2	T	0.63	0/706	1.30	8/954 (0.8%)
2	Y	0.73	0/706	1.31	7/954 (0.7%)
2	Z	0.69	0/706	1.14	2/954 (0.2%)
2	h	0.82	0/706	1.32	8/954 (0.8%)
2	n	0.83	0/706	1.35	6/954 (0.6%)
2	t	0.77	0/706	1.29	9/954 (0.9%)
2	z	0.70	0/706	1.19	6/954 (0.6%)
3	4	0.60	0/762	1.13	5/1029 (0.5%)
3	D	0.61	0/762	1.07	3/1029 (0.3%)
3	H	0.57	0/762	1.17	10/1029 (1.0%)
3	J	0.73	0/724	1.28	6/977 (0.6%)
3	P	0.68	0/754	1.26	9/1018 (0.9%)
3	W	0.65	0/730	1.21	4/985 (0.4%)
3	X	0.62	0/762	1.07	0/1029
3	e	0.58	0/634	1.17	5/854 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	g	0.62	0/762	1.12	4/1029 (0.4%)
3	m	0.66	0/762	1.17	4/1029 (0.4%)
3	s	0.71	0/762	1.25	11/1029 (1.1%)
3	y	0.58	0/762	1.02	3/1029 (0.3%)
4	0	0.77	0/1198	1.21	10/1610 (0.6%)
4	6	0.77	0/1169	1.14	5/1567 (0.3%)
4	F	0.84	0/1208	1.37	14/1623 (0.9%)
4	L	0.80	1/1177 (0.1%)	1.31	9/1583 (0.6%)
4	N	0.72	0/1196	1.17	5/1608 (0.3%)
4	R	0.84	0/1198	1.41	15/1610 (0.9%)
4	a	0.82	0/1216	1.28	10/1634 (0.6%)
4	c	0.87	0/1203	1.29	9/1616 (0.6%)
4	i	0.78	0/1297	1.33	15/1744 (0.9%)
4	k	0.79	0/1220	1.23	12/1639 (0.7%)
4	o	0.84	0/1190	1.28	16/1599 (1.0%)
4	u	0.90	0/1190	1.29	10/1599 (0.6%)
5	1	0.77	0/1427	1.19	8/1942 (0.4%)
5	2	0.73	0/1433	1.17	10/1949 (0.5%)
5	7	0.71	0/1433	1.20	10/1949 (0.5%)
5	G	0.80	0/1439	1.31	15/1956 (0.8%)
5	M	0.80	0/1444	1.22	7/1963 (0.4%)
5	S	0.88	0/1433	1.31	11/1949 (0.6%)
5	b	0.87	1/1456 (0.1%)	1.35	16/1978 (0.8%)
5	d	0.88	1/1433 (0.1%)	1.34	12/1949 (0.6%)
5	j	0.82	0/1439	1.25	6/1956 (0.3%)
5	p	0.91	2/1422 (0.1%)	1.35	13/1935 (0.7%)
5	q	0.84	1/1428 (0.1%)	1.22	11/1942 (0.6%)
5	v	0.89	0/1433	1.28	10/1949 (0.5%)
All	All	0.76	11/78927 (0.0%)	1.26	659/106546 (0.6%)

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	3	0	1
2	T	0	1
2	Y	0	1
4	R	0	1
5	j	0	1
5	q	0	1
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	q	9	ILE	CA-CB	-6.71	1.46	1.54
5	b	129	VAL	CA-CB	6.50	1.62	1.55
1	V	270	VAL	CA-CB	-6.16	1.49	1.55
1	w	227	VAL	CA-CB	6.06	1.62	1.54
5	d	59	LEU	CA-C	-5.97	1.45	1.52
1	U	58	PRO	N-CD	5.47	1.55	1.47
4	L	27	ILE	CA-CB	-5.39	1.47	1.54
1	O	163	VAL	CA-CB	5.30	1.61	1.54
5	p	107	ILE	CA-CB	-5.09	1.48	1.54
5	p	154	ILE	CA-CB	5.09	1.60	1.53
1	V	248	TYR	CA-C	5.04	1.59	1.52

All (659) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	90	ILE	CA-C-N	12.62	133.52	120.14
2	Q	90	ILE	C-N-CA	12.62	133.52	120.14
1	w	151	ILE	N-CA-C	12.41	125.11	112.83
5	p	111	TYR	N-CA-C	12.25	129.65	113.72
1	f	227	VAL	N-CA-C	11.98	121.92	110.42
4	R	136	ASP	N-CA-C	11.78	128.60	109.40
2	Y	90	ILE	CA-C-N	11.54	134.27	119.84
2	Y	90	ILE	C-N-CA	11.54	134.27	119.84
1	I	147	ILE	CB-CA-C	-11.31	102.10	111.71
5	j	111	TYR	N-CA-C	11.11	128.16	113.72
1	3	151	ILE	N-CA-C	10.88	123.60	112.83
2	n	65	ILE	N-CA-C	10.76	120.75	108.05
2	z	65	ILE	N-CA-C	10.71	119.76	107.77
1	r	306	GLY	N-CA-C	10.53	125.37	112.73
1	l	106	ILE	N-CA-C	10.14	120.65	110.82
4	o	32	PHE	N-CA-C	-10.09	93.03	108.67
5	b	142	VAL	N-CA-C	-10.07	88.40	109.34
1	V	106	ILE	N-CA-C	10.00	120.52	110.82
2	T	88	THR	N-CA-C	9.92	122.04	111.03
1	I	257	SER	N-CA-C	9.90	121.66	111.07
1	w	306	GLY	N-CA-C	9.79	124.48	112.73
1	l	57	GLY	O-C-N	9.66	124.55	121.07
5	G	83	GLN	N-CA-C	9.60	121.99	108.74
1	V	306	GLY	N-CA-C	9.60	125.05	112.77
1	U	58	PRO	CA-N-CD	-9.58	98.58	112.00
1	O	106	ILE	N-CA-C	9.49	120.03	110.82
4	F	138	LEU	N-CA-C	9.42	121.62	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	90	ILE	CA-C-N	9.40	131.59	119.84
2	T	90	ILE	C-N-CA	9.40	131.59	119.84
1	f	58	PRO	CA-N-CD	-9.35	98.90	112.00
4	L	90	ARG	N-CA-C	9.26	121.30	111.03
1	V	58	PRO	CA-N-CD	-9.25	99.04	112.00
1	r	58	PRO	CA-N-CD	-9.24	99.07	112.00
5	b	111	TYR	N-CA-C	9.21	124.45	112.12
1	U	134	ILE	N-CA-C	-9.16	99.64	111.09
1	U	148	PHE	N-CA-C	9.16	121.26	111.28
1	w	190	ASN	CA-C-N	9.10	128.77	118.85
1	w	190	ASN	C-N-CA	9.10	128.77	118.85
1	O	306	GLY	N-CA-C	9.06	123.61	112.73
1	U	106	ILE	N-CA-C	9.05	119.60	110.82
4	0	99	ALA	CA-C-N	9.01	132.50	120.79
4	0	99	ALA	C-N-CA	9.01	132.50	120.79
1	9	58	PRO	CA-N-CD	-8.93	99.50	112.00
1	C	314	LEU	N-CA-C	-8.88	101.56	111.07
2	Z	93	PHE	CA-C-N	8.82	130.86	119.84
2	Z	93	PHE	C-N-CA	8.82	130.86	119.84
1	l	58	PRO	CA-N-CD	-8.81	99.66	112.00
5	G	48	ASN	CA-C-N	8.77	128.41	119.56
5	G	48	ASN	C-N-CA	8.77	128.41	119.56
1	C	106	ILE	N-CA-C	8.74	120.52	111.00
5	G	155	LYS	CA-C-N	8.68	129.21	119.92
5	G	155	LYS	C-N-CA	8.68	129.21	119.92
1	O	58	PRO	CA-N-CD	-8.65	99.89	112.00
1	x	58	PRO	CA-N-CD	-8.59	99.97	112.00
2	Q	65	ILE	CA-C-N	8.56	128.43	120.21
2	Q	65	ILE	C-N-CA	8.56	128.43	120.21
4	o	151	ARG	N-CA-C	8.56	121.56	111.71
1	x	94	ILE	N-CA-C	8.56	118.64	110.42
1	3	58	PRO	CA-N-CD	-8.54	100.04	112.00
1	I	58	PRO	CA-N-CD	-8.54	100.05	112.00
1	C	58	PRO	CA-N-CD	-8.52	100.08	112.00
2	n	65	ILE	CA-C-N	8.48	128.35	120.21
2	n	65	ILE	C-N-CA	8.48	128.35	120.21
1	V	190	ASN	CA-C-N	8.43	128.04	118.85
1	V	190	ASN	C-N-CA	8.43	128.04	118.85
4	F	151	ARG	N-CA-C	8.40	120.52	111.36
5	7	144	SER	N-CA-C	-8.35	98.12	110.48
4	i	31	GLY	N-CA-C	-8.27	101.06	112.13
1	I	227	VAL	N-CA-C	8.24	119.02	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	LEU	N-CA-C	8.22	122.66	108.02
4	L	138	LEU	N-CA-C	-8.20	103.25	113.18
2	n	86	SER	N-CA-C	8.20	119.85	111.07
1	r	106	ILE	N-CA-C	8.17	118.74	110.82
1	3	134	ILE	N-CA-C	8.17	118.21	110.53
4	a	32	PHE	N-CA-C	-8.16	96.02	108.67
1	I	225	ASN	N-CA-C	8.14	123.39	113.38
4	R	135	GLU	CA-C-N	-8.13	110.74	122.94
4	R	135	GLU	C-N-CA	-8.13	110.74	122.94
5	q	144	SER	N-CA-C	-8.13	98.25	110.28
1	w	58	PRO	CA-N-CD	-8.11	100.65	112.00
5	S	167	VAL	CB-CA-C	-8.06	99.20	112.26
4	F	62	THR	N-CA-C	8.04	119.83	108.74
1	I	53	TRP	N-CA-C	8.01	122.82	112.89
1	f	53	TRP	N-CA-C	7.97	122.27	112.23
3	P	37	ARG	CA-C-N	7.97	128.59	120.38
3	P	37	ARG	C-N-CA	7.97	128.59	120.38
4	N	154	GLU	N-CA-C	7.95	122.24	112.54
5	b	83	GLN	N-CA-C	7.92	119.07	108.38
5	G	111	TYR	N-CA-C	7.89	123.10	111.34
3	W	10	HIS	CB-CA-C	-7.86	107.51	116.63
4	i	80	THR	CA-C-N	-7.79	112.64	120.98
4	i	80	THR	C-N-CA	-7.79	112.64	120.98
2	Q	65	ILE	N-CA-C	7.79	117.24	108.05
1	O	257	SER	N-CA-C	7.78	120.45	111.11
4	c	54	GLU	N-CA-C	-7.75	96.94	109.96
1	V	248	TYR	N-CA-C	7.75	123.22	112.45
1	f	107	LEU	N-CA-C	7.73	122.71	112.35
4	u	32	PHE	N-CA-C	-7.71	94.96	108.23
1	f	116	ILE	N-CA-C	-7.71	102.93	110.72
3	e	10	HIS	CB-CA-C	-7.69	107.72	116.63
3	4	47	ASP	CB-CA-C	-7.66	107.75	116.63
1	l	306	GLY	N-CA-C	7.64	121.90	112.73
2	5	65	ILE	N-CA-C	7.64	117.06	108.05
2	h	65	ILE	CA-C-N	7.62	129.36	119.84
2	h	65	ILE	C-N-CA	7.62	129.36	119.84
1	U	31	ARG	N-CA-C	7.59	122.54	113.28
1	V	227	VAL	N-CA-C	7.58	117.65	110.30
1	C	186	ASN	N-CA-C	7.55	121.75	112.23
1	r	178	ILE	N-CA-C	7.55	118.34	110.72
1	r	256	ASN	N-CA-C	7.53	122.66	113.17
5	S	168	ARG	N-CA-C	-7.53	103.02	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	64	LEU	N-CA-C	-7.52	97.48	109.59
5	q	143	GLY	N-CA-C	7.50	130.96	113.18
1	r	151	ILE	N-CA-C	7.50	120.25	112.83
5	v	143	VAL	CB-CA-C	-7.50	104.14	112.68
4	F	69	PHE	CA-C-N	-7.48	112.28	119.76
4	F	69	PHE	C-N-CA	-7.48	112.28	119.76
4	c	138	LEU	N-CA-C	-7.42	103.13	111.07
4	L	85	TYR	N-CA-C	7.41	120.47	108.76
1	I	261	LEU	N-CA-C	-7.38	103.18	111.07
5	p	127	ARG	N-CA-C	7.36	120.36	111.82
1	x	53	TRP	N-CA-C	7.35	121.49	112.23
5	S	151	LEU	N-CA-C	-7.35	103.27	111.28
1	V	87	THR	N-CA-C	-7.34	103.28	111.28
1	f	134	ILE	N-CA-CB	-7.33	99.13	111.23
4	i	51	GLY	CA-C-N	-7.33	111.92	122.77
4	i	51	GLY	C-N-CA	-7.33	111.92	122.77
1	I	240	GLU	N-CA-C	7.33	119.06	111.14
3	s	71	ALA	CA-C-N	7.32	127.75	119.92
3	s	71	ALA	C-N-CA	7.32	127.75	119.92
1	I	270	VAL	N-CA-C	7.31	118.35	111.48
2	T	93	PHE	CA-C-N	-7.30	111.89	120.13
2	T	93	PHE	C-N-CA	-7.30	111.89	120.13
3	g	37	ARG	CA-C-N	7.29	127.89	120.38
3	g	37	ARG	C-N-CA	7.29	127.89	120.38
1	f	225	ASN	N-CA-C	7.28	122.34	113.17
5	2	143	VAL	N-CA-C	-7.27	102.10	112.35
1	C	148	PHE	N-CA-C	7.22	119.16	111.28
5	l	34	LYS	N-CA-C	7.22	118.80	111.07
3	P	34	ILE	N-CA-C	7.22	117.31	110.74
2	t	88	THR	N-CA-C	7.22	120.21	111.40
1	O	225	ASN	N-CA-C	7.20	122.25	113.17
2	t	80	LYS	N-CA-C	-7.19	103.37	111.07
5	v	83	GLN	N-CA-C	7.19	119.38	109.18
4	k	85	TYR	N-CA-C	7.18	120.27	108.99
1	U	303	VAL	N-CA-C	-7.17	101.92	108.95
3	P	53	ASP	N-CA-C	7.16	119.17	111.36
1	O	248	TYR	N-CA-C	7.16	122.01	113.28
1	V	186	ASN	N-CA-C	7.15	120.11	111.82
1	l	151	ILE	N-CA-C	7.13	119.89	112.83
1	x	42	ASP	N-CA-C	-7.13	103.51	111.28
4	a	85	TYR	N-CA-C	7.12	120.01	108.76
1	V	225	ASN	N-CA-C	7.12	122.14	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	69	PHE	CA-C-N	7.11	127.10	119.78
4	R	69	PHE	C-N-CA	7.11	127.10	119.78
5	b	129	VAL	N-CA-C	7.10	117.15	108.06
1	V	53	TRP	N-CA-C	7.10	121.18	112.23
4	F	31	GLY	N-CA-C	-7.08	102.64	112.13
4	u	124	CYS	N-CA-C	7.08	117.94	108.38
5	v	76	GLU	N-CA-C	7.07	120.08	108.99
4	o	124	CYS	N-CA-C	7.03	117.79	107.88
3	W	96	PRO	CA-C-N	7.03	127.47	120.52
3	W	96	PRO	C-N-CA	7.03	127.47	120.52
4	u	151	ARG	N-CA-C	6.99	119.75	111.71
1	w	225	ASN	N-CA-C	6.98	121.96	113.17
1	f	16	GLU	N-CA-C	-6.97	103.61	111.14
1	C	187	LEU	N-CA-C	6.97	119.91	111.82
1	I	106	ILE	N-CA-C	6.97	118.60	111.00
4	0	31	GLY	N-CA-C	-6.95	102.82	112.13
1	f	14	GLN	N-CA-C	6.94	122.60	113.30
4	c	23	ARG	N-CA-C	6.94	121.41	113.15
4	a	41	GLN	N-CA-C	-6.93	103.65	111.07
4	L	86	VAL	N-CA-C	-6.92	96.28	107.28
3	W	8	ARG	N-CA-C	6.92	119.69	108.34
3	H	40	ASP	N-CA-C	-6.91	102.67	112.13
1	r	12	SER	N-CA-C	-6.90	103.81	111.82
4	c	134	GLN	N-CA-C	6.89	121.44	112.89
5	S	6	GLN	N-CA-C	-6.89	98.17	109.40
5	7	76	GLU	N-CA-C	6.88	119.31	108.79
1	f	257	SER	N-CA-C	6.87	118.77	111.28
1	O	68	ASP	N-CA-C	6.86	118.83	111.36
1	U	190	ASN	CA-C-N	6.86	126.32	118.85
1	U	190	ASN	C-N-CA	6.86	126.32	118.85
5	S	77	ARG	N-CA-C	-6.85	104.54	113.17
1	V	13	LEU	N-CA-C	6.84	120.32	108.76
5	7	15	ARG	N-CA-C	6.84	118.82	111.36
5	M	111	TYR	N-CA-C	6.84	121.28	112.12
1	O	87	THR	N-CA-C	-6.84	103.83	111.28
4	i	14	ASN	N-CA-C	6.84	121.95	112.45
4	k	31	GLY	N-CA-C	-6.83	102.97	112.13
1	O	285	ILE	N-CA-C	-6.83	103.65	110.62
1	3	255	CYS	N-CA-C	6.83	120.26	109.81
1	r	313	ASP	N-CA-C	-6.82	103.85	111.28
5	S	76	GLU	N-CA-C	6.81	119.53	108.76
4	k	62	THR	N-CA-C	-6.81	98.62	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	144	SER	N-CA-C	-6.81	100.36	110.23
5	b	140	ASN	N-CA-C	6.80	121.35	111.02
1	l	146	SER	N-CA-C	6.74	119.98	111.69
1	l	181	ARG	N-CA-C	-6.73	103.94	111.28
1	3	147	ILE	N-CA-C	6.70	117.78	111.48
5	2	5	TRP	N-CA-C	6.69	119.89	109.52
1	U	12	SER	N-CA-C	6.67	121.17	112.89
1	f	187	LEU	N-CA-C	6.67	120.64	112.23
4	N	37	HIS	N-CA-C	6.65	118.32	111.14
5	S	134	GLU	N-CA-C	-6.63	99.53	109.94
2	5	90	ILE	N-CA-C	6.62	123.19	108.88
3	4	71	ALA	CA-C-N	6.61	126.58	120.03
3	4	71	ALA	C-N-CA	6.61	126.58	120.03
1	w	161	LYS	N-CA-C	-6.61	104.08	111.28
4	R	23	ARG	N-CA-C	6.60	121.19	113.20
1	r	217	GLN	N-CA-C	6.60	118.27	111.14
3	4	91	GLU	CA-C-N	6.59	126.57	119.78
3	4	91	GLU	C-N-CA	6.59	126.57	119.78
3	m	95	SER	CA-C-N	6.59	124.41	119.66
3	m	95	SER	C-N-CA	6.59	124.41	119.66
1	r	103	GLN	N-CA-C	6.59	118.54	111.36
1	V	303	VAL	CA-C-N	6.57	126.34	119.05
1	V	303	VAL	C-N-CA	6.57	126.34	119.05
1	f	106	ILE	N-CA-C	6.56	117.18	110.82
1	l	248	TYR	N-CA-C	6.55	121.28	113.28
4	0	85	TYR	N-CA-C	6.55	119.11	108.76
1	w	106	ILE	N-CA-C	6.55	116.69	110.53
5	b	157	LYS	N-CA-C	6.55	119.24	111.71
5	p	20	THR	N-CA-C	-6.54	104.07	111.07
1	9	190	ASN	CA-C-N	6.54	125.97	118.85
1	9	190	ASN	C-N-CA	6.54	125.97	118.85
3	P	10	HIS	CB-CA-C	-6.53	109.05	116.63
5	1	111	TYR	N-CA-C	6.53	121.07	111.34
1	l	285	ILE	N-CA-C	-6.53	104.40	110.53
1	r	190	ASN	CA-C-N	6.53	125.76	118.97
1	r	190	ASN	C-N-CA	6.53	125.76	118.97
4	R	149	ARG	N-CA-C	6.51	119.34	110.55
1	C	137	LYS	N-CA-C	-6.50	104.19	111.28
1	V	134	ILE	N-CA-C	6.50	117.13	110.82
3	s	47	ASP	CB-CA-C	-6.50	109.09	116.63
5	d	76	GLU	N-CA-C	6.49	119.01	108.76
5	1	76	GLU	N-CA-C	6.48	118.71	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	53	TRP	N-CA-C	6.47	120.38	112.23
1	I	174	SER	N-CA-C	6.46	119.14	111.71
1	3	269	LEU	N-CA-C	6.45	119.62	111.69
4	o	85	TYR	N-CA-C	6.45	119.11	108.99
4	c	19	ARG	N-CA-C	-6.44	104.18	111.07
1	f	307	ILE	N-CA-C	6.43	117.22	110.72
3	H	5	LEU	N-CA-C	6.43	119.20	109.23
4	0	123	GLY	N-CA-C	6.43	120.49	110.91
1	l	271	THR	N-CA-C	6.43	118.29	111.28
1	3	53	TRP	N-CA-C	6.43	120.33	112.23
4	R	137	ALA	N-CA-C	-6.43	100.06	109.63
1	f	109	LYS	CA-C-N	-6.43	113.19	119.87
1	f	109	LYS	C-N-CA	-6.43	113.19	119.87
5	2	69	TYR	N-CA-C	6.43	119.18	109.41
1	U	189	SER	N-CA-C	6.42	119.24	111.40
3	H	71	ALA	CA-C-N	6.41	126.38	120.03
3	H	71	ALA	C-N-CA	6.41	126.38	120.03
1	f	12	SER	N-CA-C	6.41	120.71	113.02
1	w	28	LYS	N-CA-C	-6.40	104.30	111.28
1	U	78	ALA	N-CA-C	-6.40	104.22	111.07
4	a	69	PHE	CA-C-N	-6.40	113.36	119.76
4	a	69	PHE	C-N-CA	-6.40	113.36	119.76
2	Y	96	ALA	CA-C-N	6.39	126.89	119.47
2	Y	96	ALA	C-N-CA	6.39	126.89	119.47
3	e	37	ARG	CA-C-N	6.39	126.96	120.38
3	e	37	ARG	C-N-CA	6.39	126.96	120.38
5	q	79	TRP	N-CA-C	6.38	118.32	111.36
1	I	243	LYS	N-CA-C	-6.37	104.33	111.28
1	3	134	ILE	CB-CA-C	-6.37	103.67	112.02
1	9	257	SER	N-CA-C	6.37	118.22	111.28
1	3	261	LEU	N-CA-C	-6.36	104.35	111.28
1	O	57	GLY	O-C-N	6.34	123.35	121.07
4	F	61	GLY	N-CA-C	-6.34	104.77	115.62
5	S	103	ALA	N-CA-C	-6.34	104.28	111.07
1	I	187	LEU	N-CA-C	6.33	120.73	112.89
2	t	77	PHE	N-CA-C	-6.32	104.30	111.07
4	R	14	ASN	N-CA-C	6.32	119.46	111.69
5	p	25	VAL	CB-CA-C	-6.32	103.75	112.02
1	9	80	VAL	N-CA-C	6.32	116.49	110.74
2	K	90	ILE	CA-C-N	6.31	126.83	120.14
2	K	90	ILE	C-N-CA	6.31	126.83	120.14
1	w	277	ILE	N-CA-C	-6.30	104.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	133	CYS	N-CA-C	6.29	119.40	109.96
1	C	190	ASN	CA-C-N	6.29	125.70	118.85
1	C	190	ASN	C-N-CA	6.29	125.70	118.85
5	q	136	GLN	N-CA-C	-6.28	104.72	112.38
2	K	110	LEU	N-CA-C	6.28	117.92	111.14
1	3	303	VAL	CA-C-N	6.28	125.50	118.97
1	3	303	VAL	C-N-CA	6.28	125.50	118.97
1	w	263	GLU	N-CA-C	-6.27	104.36	111.07
4	o	53	SER	N-CA-C	-6.26	98.87	108.76
1	V	147	ILE	N-CA-C	6.26	116.30	110.42
5	1	48	ASN	CA-C-N	6.26	125.88	119.56
5	1	48	ASN	C-N-CA	6.26	125.88	119.56
1	9	217	GLN	N-CA-C	6.25	119.38	111.69
4	c	141	GLN	N-CA-C	-6.25	104.47	111.28
3	D	71	ALA	CA-C-N	6.24	126.60	119.92
3	D	71	ALA	C-N-CA	6.24	126.60	119.92
3	g	8	ARG	N-CA-C	6.24	118.58	108.41
1	I	195	LEU	N-CA-C	6.23	120.50	113.02
1	9	109	LYS	CA-C-N	-6.21	113.28	119.56
1	9	109	LYS	C-N-CA	-6.21	113.28	119.56
4	L	105	GLY	CA-C-N	-6.21	115.48	123.19
4	L	105	GLY	C-N-CA	-6.21	115.48	123.19
1	x	18	LYS	N-CA-C	6.20	118.04	111.28
5	d	20	THR	N-CA-C	-6.20	104.52	111.28
2	K	80	LYS	N-CA-C	-6.19	104.45	111.07
4	i	69	PHE	CA-C-N	-6.19	113.57	119.76
4	i	69	PHE	C-N-CA	-6.19	113.57	119.76
1	O	162	LEU	CB-CG-CD2	-6.18	92.16	110.70
5	7	134	GLU	N-CA-C	-6.18	100.24	109.94
3	J	53	ASP	N-CA-C	6.18	118.99	111.82
3	s	65	GLN	N-CA-C	6.17	119.28	111.69
4	6	101	MET	N-CA-C	6.17	119.03	109.60
2	t	87	SER	N-CA-C	6.16	118.07	111.36
5	d	136	GLN	N-CA-C	-6.16	104.87	112.38
2	5	65	ILE	CA-C-N	6.15	127.53	119.84
2	5	65	ILE	C-N-CA	6.15	127.53	119.84
1	V	137	LYS	N-CA-C	-6.14	104.59	111.28
4	a	134	GLN	N-CA-C	6.13	119.96	112.23
2	K	87	SER	N-CA-C	6.13	120.77	113.16
1	r	287	ARG	N-CA-C	-6.13	105.77	113.18
3	P	42	GLN	N-CA-C	6.12	118.72	109.23
4	N	20	LYS	N-CA-C	6.12	118.03	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	k	35	ARG	CA-C-N	6.12	126.08	120.21
4	k	35	ARG	C-N-CA	6.12	126.08	120.21
1	3	186	ASN	N-CA-C	6.11	118.90	111.82
5	p	48	ASN	CA-C-N	-6.09	112.73	119.19
5	p	48	ASN	C-N-CA	-6.09	112.73	119.19
1	w	191	PRO	N-CA-C	6.09	121.56	113.40
2	K	86	SER	N-CA-C	6.08	119.40	109.06
5	v	111	TYR	N-CA-C	6.08	120.40	111.34
1	r	57	GLY	O-C-N	6.07	123.26	121.07
1	C	315	GLU	N-CA-C	6.07	117.97	111.36
1	C	316	GLU	N-CA-C	-6.06	104.68	111.28
5	q	124	ILE	N-CA-C	6.05	116.83	110.72
4	k	151	ARG	N-CA-C	6.05	117.95	111.36
4	N	85	TYR	N-CA-C	6.04	118.31	108.76
4	F	27	ILE	N-CA-C	6.04	117.29	108.53
4	a	27	ILE	N-CA-C	6.04	118.07	108.89
4	o	62	THR	N-CA-C	6.04	120.35	112.92
1	f	114	LEU	N-CA-C	6.04	117.66	111.14
4	F	85	TYR	N-CA-C	6.03	118.29	108.76
1	l	39	GLN	N-CA-C	-6.03	104.70	111.28
5	2	168	ARG	N-CA-C	-6.02	104.72	111.28
5	G	143	GLY	N-CA-C	6.01	120.24	112.54
1	O	53	TRP	N-CA-C	6.01	120.34	112.89
4	6	85	TYR	N-CA-C	6.00	117.97	108.79
1	f	283	GLY	N-CA-C	-5.99	105.55	112.50
1	3	106	ILE	N-CA-C	5.99	117.53	111.00
4	k	124	CYS	N-CA-C	5.99	116.32	107.88
1	U	53	TRP	N-CA-C	5.98	119.77	112.23
5	d	72	LEU	N-CA-C	-5.98	102.64	110.53
1	l	178	ILE	N-CA-C	5.97	116.75	110.72
1	w	68	ASP	N-CA-C	5.97	117.87	111.36
4	R	31	GLY	N-CA-C	-5.97	104.14	112.13
2	B	84	THR	N-CA-C	-5.97	104.90	111.82
1	r	305	ASN	N-CA-C	5.96	120.68	113.17
1	x	303	VAL	N-CA-C	-5.96	103.48	109.02
2	T	65	ILE	N-CA-C	5.95	115.07	108.05
1	r	294	HIS	N-CA-C	-5.95	104.80	111.28
4	o	137	ALA	N-CA-C	5.95	117.44	111.07
4	u	138	LEU	N-CA-C	5.95	117.56	111.14
1	O	134	ILE	N-CA-C	-5.94	104.94	110.53
2	h	87	SER	N-CA-C	5.94	119.71	112.23
5	b	153	LEU	N-CA-C	5.93	117.55	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	p	34	LYS	N-CA-C	5.93	117.44	110.97
5	d	9	ILE	CB-CA-C	-5.93	103.72	111.25
1	U	13	LEU	N-CA-C	5.93	118.39	108.02
5	p	162	PRO	CA-C-O	-5.93	114.68	121.56
3	J	88	LEU	N-CA-C	5.92	118.38	108.73
4	a	13	GLU	N-CA-C	5.92	117.54	111.14
3	s	37	ARG	CA-C-N	5.92	126.48	120.38
3	s	37	ARG	C-N-CA	5.92	126.48	120.38
4	k	69	PHE	CA-C-N	5.92	125.68	119.76
4	k	69	PHE	C-N-CA	5.92	125.68	119.76
1	9	106	ILE	N-CA-C	5.91	116.12	110.74
2	T	73	VAL	N-CA-C	5.91	116.69	110.72
1	O	37	LYS	N-CA-C	5.90	118.47	111.33
4	L	31	GLY	N-CA-C	-5.89	104.23	112.13
1	O	43	LEU	N-CA-C	-5.89	104.94	111.36
5	M	110	HIS	CA-C-N	-5.89	113.10	122.17
5	M	110	HIS	C-N-CA	-5.89	113.10	122.17
4	o	99	ALA	CA-C-N	-5.88	113.64	119.99
4	o	99	ALA	C-N-CA	-5.88	113.64	119.99
5	S	69	TYR	N-CA-C	5.88	119.14	109.85
5	q	76	GLU	N-CA-C	5.88	118.04	108.76
1	9	303	VAL	N-CA-C	-5.87	103.56	109.02
4	c	85	TYR	N-CA-C	5.86	117.76	108.79
3	m	40	ASP	N-CA-C	-5.86	104.10	112.13
2	t	90	ILE	N-CA-C	5.86	121.53	108.88
5	7	34	LYS	N-CA-C	5.86	117.34	111.07
1	V	18	LYS	N-CA-C	5.85	118.89	111.69
4	0	16	GLU	N-CA-C	5.85	118.60	111.82
1	w	14	GLN	N-CA-C	5.84	120.11	112.92
1	3	217	GLN	N-CA-C	5.84	117.72	111.36
2	K	75	MET	N-CA-C	-5.82	104.84	111.07
5	2	160	ILE	N-CA-C	5.82	117.55	109.80
1	r	147	ILE	CB-CA-C	-5.81	106.77	111.71
4	L	52	ARG	N-CA-C	5.81	119.07	107.62
1	f	178	ILE	CB-CA-C	-5.81	104.45	111.88
1	3	187	LEU	N-CA-C	5.80	119.54	112.23
2	B	110	LEU	N-CA-C	5.80	118.48	111.40
4	u	5	VAL	CA-C-N	-5.80	113.05	119.19
4	u	5	VAL	C-N-CA	-5.80	113.05	119.19
4	i	141	GLN	N-CA-C	-5.79	104.97	111.28
1	x	17	ASP	N-CA-C	-5.79	104.89	111.14
1	C	22	MET	CA-C-N	5.78	128.22	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	MET	C-N-CA	5.78	128.22	120.58
4	o	86	VAL	N-CA-CB	-5.78	104.70	112.10
1	V	227	VAL	CB-CA-C	-5.78	104.58	111.81
5	2	111	TYR	N-CA-C	5.78	119.86	112.12
4	u	94	LYS	N-CA-C	5.78	117.57	108.96
4	6	16	GLU	N-CA-C	5.78	118.52	111.82
5	G	127	ARG	N-CA-C	5.77	120.02	113.15
1	U	56	LYS	N-CA-C	-5.77	106.01	113.16
1	x	106	ILE	N-CA-C	5.77	117.29	111.00
5	2	76	GLU	N-CA-C	5.77	117.87	108.76
4	i	52	ARG	N-CA-C	5.77	118.76	107.57
4	F	84	GLU	N-CA-C	-5.76	101.88	110.23
3	P	16	THR	N-CA-C	5.76	116.16	108.38
1	f	147	ILE	CB-CA-C	-5.76	101.85	111.29
1	w	39	GLN	N-CA-C	-5.76	105.00	111.28
2	T	89	GLU	N-CA-C	5.75	120.37	113.23
5	7	154	ILE	N-CA-C	5.75	116.14	107.80
5	2	12	GLN	N-CA-C	-5.75	101.77	110.28
1	x	56	LYS	N-CA-C	-5.75	106.04	113.16
5	p	169	LEU	CA-CB-CG	5.74	136.38	116.30
3	s	96	PRO	CA-C-N	-5.74	114.35	120.03
3	s	96	PRO	C-N-CA	-5.74	114.35	120.03
4	o	31	GLY	N-CA-C	-5.73	104.46	112.13
2	Y	93	PHE	CA-C-N	5.72	126.60	120.13
2	Y	93	PHE	C-N-CA	5.72	126.60	120.13
1	C	13	LEU	CA-C-N	-5.72	114.71	122.95
1	C	13	LEU	C-N-CA	-5.72	114.71	122.95
1	l	179	GLY	N-CA-C	-5.71	105.87	112.73
1	C	80	VAL	N-CA-C	5.70	116.35	110.82
2	5	67	SER	N-CA-C	5.70	117.58	111.36
3	P	85	PHE	N-CA-C	-5.70	100.40	109.07
1	V	198	TYR	N-CA-C	-5.70	104.97	111.07
3	H	53	ASP	N-CA-C	5.69	118.25	111.71
5	1	30	TYR	N-CA-C	5.69	120.36	112.45
2	z	88	THR	N-CA-C	5.68	117.95	111.02
4	0	124	CYS	N-CA-C	5.68	116.05	108.38
5	j	142	VAL	N-CA-C	5.67	116.45	110.72
2	h	47	SER	N-CA-C	5.66	117.83	110.53
4	0	32	PHE	N-CA-C	-5.66	99.90	108.67
3	y	10	HIS	CB-CA-C	-5.66	110.07	116.63
2	z	65	ILE	CA-C-N	5.66	126.91	119.84
2	z	65	ILE	C-N-CA	5.66	126.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	128	ILE	CA-C-N	5.65	132.13	121.97
5	G	128	ILE	C-N-CA	5.65	132.13	121.97
1	O	292	LYS	N-CA-C	5.65	118.29	111.40
4	R	155	ASP	N-CA-C	5.64	117.89	109.25
3	H	10	HIS	CB-CA-C	-5.64	110.08	116.63
4	u	85	TYR	N-CA-C	5.63	117.41	108.79
5	d	69	TYR	N-CA-C	5.63	118.75	109.85
1	w	249	LEU	CA-C-N	-5.63	113.60	121.99
1	w	249	LEU	C-N-CA	-5.63	113.60	121.99
1	V	187	LEU	N-CA-C	5.63	118.35	111.82
1	r	86	ASP	N-CA-C	5.63	117.50	111.36
1	U	142	THR	N-CA-C	-5.63	105.15	111.28
1	I	294	HIS	N-CA-C	-5.62	105.15	111.28
1	I	22	MET	N-CA-C	5.62	118.34	111.82
5	b	10	VAL	N-CA-C	5.61	115.94	107.75
1	x	84	GLN	N-CA-C	-5.61	106.28	113.23
5	b	14	ASP	N-CA-C	-5.60	102.61	110.50
5	d	142	VAL	N-CA-C	-5.59	100.95	109.78
5	7	21	TRP	N-CA-C	-5.59	105.19	111.28
4	N	124	CYS	N-CA-C	5.58	116.75	108.60
4	i	29	TYR	CA-C-N	-5.58	115.58	122.84
4	i	29	TYR	C-N-CA	-5.58	115.58	122.84
1	I	43	LEU	N-CA-C	-5.58	105.20	111.28
1	O	227	VAL	CB-CA-C	-5.57	104.74	112.04
2	h	109	PHE	N-CA-C	-5.57	105.12	111.14
1	U	147	ILE	CB-CA-C	-5.56	106.98	111.71
4	c	149	ARG	N-CA-C	5.56	118.06	110.55
2	t	110	LEU	N-CA-C	5.56	117.42	111.36
2	z	100	ALA	N-CA-C	5.56	117.34	111.28
4	i	62	THR	N-CA-C	5.55	118.05	110.55
4	0	87	ASP	N-CA-C	5.55	118.13	108.76
2	z	83	TYR	N-CA-C	5.54	120.04	113.28
5	j	110	HIS	CA-C-N	-5.54	113.46	122.26
5	j	110	HIS	C-N-CA	-5.54	113.46	122.26
5	b	97	GLN	N-CA-C	-5.53	103.08	110.55
2	K	84	THR	N-CA-C	-5.52	105.41	111.82
1	3	215	ARG	N-CA-C	-5.52	105.26	111.28
1	3	225	ASN	N-CA-C	5.52	120.13	113.17
1	V	288	ASN	CA-C-N	-5.52	115.18	122.85
1	V	288	ASN	C-N-CA	-5.52	115.18	122.85
4	R	134	GLN	N-CA-C	5.51	119.17	112.23
3	H	22	SER	N-CA-C	-5.50	102.74	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	47	ASP	CB-CA-C	-5.49	110.26	116.63
5	S	79	TRP	N-CA-C	5.49	117.34	111.36
1	l	74	LYS	N-CA-C	-5.49	104.94	111.69
1	O	294	HIS	N-CA-C	-5.49	105.30	111.28
1	w	26	VAL	N-CA-C	5.48	115.68	110.42
1	9	186	ASN	N-CA-C	5.48	118.18	111.82
1	V	76	ALA	N-CA-C	-5.48	105.31	111.28
5	q	94	TYR	N-CA-C	-5.47	100.78	109.59
1	r	39	GLN	N-CA-C	-5.47	105.22	111.07
1	V	107	LEU	N-CA-C	5.47	121.90	109.81
5	l	140	ASN	N-CA-C	5.47	122.45	110.80
4	a	52	ARG	N-CA-C	5.47	118.45	107.41
1	l	231	MET	N-CA-C	-5.46	105.32	111.28
5	G	144	SER	N-CA-C	-5.46	102.19	110.28
1	C	257	SER	N-CA-C	5.46	116.91	111.07
1	l	287	ARG	N-CA-C	-5.46	106.60	113.20
5	v	34	LYS	N-CA-C	5.46	116.92	110.97
5	b	123	THR	N-CA-C	-5.46	105.33	111.28
2	t	65	ILE	N-CA-C	5.46	120.66	108.88
5	b	134	GLU	N-CA-C	-5.45	101.39	109.94
5	p	29	MET	N-CA-C	-5.44	104.99	111.03
1	I	263	GLU	N-CA-C	-5.44	105.25	111.07
4	o	53	SER	CA-C-N	-5.44	114.54	122.65
4	o	53	SER	C-N-CA	-5.44	114.54	122.65
1	U	220	SER	N-CA-C	5.44	117.02	111.14
1	O	146	SER	N-CA-C	5.42	118.36	111.69
5	v	82	GLY	N-CA-C	5.42	122.15	112.22
5	q	154	ILE	N-CA-C	5.42	115.91	107.99
1	f	243	LYS	N-CA-C	-5.42	105.27	111.07
1	C	227	VAL	N-CA-C	5.42	115.62	110.42
1	x	306	GLY	N-CA-C	5.42	120.33	113.24
3	g	47	ASP	CB-CA-C	-5.41	110.35	116.63
5	G	48	ASN	N-CA-C	5.41	116.47	109.65
5	b	107	ILE	CB-CA-C	-5.41	105.04	111.97
3	H	95	SER	CA-C-N	5.41	123.56	119.66
3	H	95	SER	C-N-CA	5.41	123.56	119.66
2	E	64	GLU	N-CA-C	5.41	117.25	111.36
3	D	34	ILE	N-CA-C	5.41	115.66	110.74
4	o	87	ASP	N-CA-C	5.41	117.89	108.76
5	v	25	VAL	CB-CA-C	-5.41	105.05	111.97
5	M	119	ALA	N-CA-C	5.40	116.85	111.07
1	9	196	GLN	N-CA-C	5.40	117.59	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	133	SER	N-CA-C	-5.40	103.41	110.53
2	Y	41	THR	N-CA-C	-5.40	105.29	111.07
2	Q	38	THR	N-CA-C	-5.40	105.40	111.28
1	r	227	VAL	N-CA-C	5.40	115.60	110.42
2	K	64	GLU	N-CA-C	5.39	117.16	111.28
1	C	86	ASP	N-CA-C	5.39	116.96	111.14
4	F	53	SER	N-CA-C	-5.39	100.54	108.79
5	G	110	HIS	CA-C-N	-5.39	115.11	121.90
5	G	110	HIS	C-N-CA	-5.39	115.11	121.90
2	h	29	PHE	CA-C-N	-5.38	116.09	123.14
2	h	29	PHE	C-N-CA	-5.38	116.09	123.14
3	J	54	GLY	N-CA-C	-5.38	106.42	115.62
1	f	110	PRO	N-CA-C	-5.38	107.42	114.03
4	R	6	PRO	N-CA-C	-5.38	107.14	113.86
1	l	199	ARG	N-CA-C	-5.37	105.42	111.28
1	C	40	TRP	CA-CB-CG	5.34	123.74	113.60
2	n	77	PHE	N-CA-C	-5.34	105.15	110.97
5	p	76	GLU	N-CA-C	5.34	116.96	108.79
5	S	24	LEU	N-CA-C	5.33	117.09	111.28
3	s	40	ASP	N-CA-C	-5.32	104.84	112.13
3	J	37	ARG	CA-C-N	5.32	125.86	120.38
3	J	37	ARG	C-N-CA	5.32	125.86	120.38
3	s	2	ASP	N-CA-C	5.31	118.34	110.48
5	2	89	TRP	N-CA-C	-5.31	99.87	108.52
1	U	235	ASP	N-CA-C	-5.30	105.50	111.28
1	O	114	LEU	N-CA-C	-5.30	105.50	111.28
1	9	107	LEU	N-CA-C	5.29	120.68	113.16
1	I	186	ASN	N-CA-C	5.29	118.89	112.23
1	U	257	SER	N-CA-C	5.28	116.72	111.07
5	q	121	ARG	N-CA-C	-5.28	105.61	111.36
4	6	87	ASP	N-CA-C	5.27	117.67	108.76
4	k	144	GLU	N-CA-C	-5.27	105.54	111.28
1	f	217	GLN	N-CA-C	5.26	116.83	111.14
1	I	178	ILE	CB-CA-C	-5.26	105.13	112.02
1	r	187	LEU	N-CA-C	5.26	117.92	111.82
5	1	51	ILE	N-CA-C	5.26	115.67	107.99
1	w	261	LEU	N-CA-C	-5.25	105.45	111.07
4	F	139	ALA	N-CA-C	5.25	117.08	111.36
1	I	148	PHE	N-CA-C	5.25	116.69	111.07
1	V	256	ASN	N-CA-C	5.24	119.66	113.16
5	p	69	TYR	N-CA-C	5.24	118.13	109.85
1	O	190	ASN	CA-C-N	5.24	124.56	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	190	ASN	C-N-CA	5.24	124.56	118.85
2	5	100	ALA	N-CA-C	5.24	116.99	111.28
1	I	12	SER	N-CA-C	5.23	117.43	108.90
1	O	228	GLN	N-CA-C	5.23	117.06	111.36
2	5	25	ASP	N-CA-C	-5.23	106.67	113.16
5	b	103	ALA	N-CA-C	-5.23	105.47	111.07
5	v	134	GLU	N-CA-C	-5.23	101.73	109.94
5	M	107	ILE	CB-CA-C	-5.22	105.29	111.97
4	R	27	ILE	N-CA-C	5.22	115.99	108.48
1	f	135	VAL	N-CA-C	-5.22	105.31	111.00
1	9	107	LEU	CA-C-N	-5.22	114.24	119.56
1	9	107	LEU	C-N-CA	-5.22	114.24	119.56
1	O	235	ASP	N-CA-C	-5.21	105.61	111.28
4	k	123	GLY	N-CA-C	5.21	118.67	110.91
3	J	86	GLU	N-CA-C	5.20	117.58	109.52
5	d	120	ILE	N-CA-C	5.20	115.97	110.72
3	P	96	PRO	N-CA-C	-5.20	104.36	110.70
1	l	235	ASP	N-CA-C	-5.19	105.52	111.07
2	K	88	THR	N-CA-C	5.19	116.74	111.14
5	G	157	LYS	N-CA-C	5.18	118.70	112.38
1	V	37	LYS	N-CA-C	5.18	117.32	111.11
5	v	143	VAL	N-CA-C	-5.17	99.05	106.55
3	y	37	ARG	CA-C-N	5.17	125.70	120.38
3	y	37	ARG	C-N-CA	5.17	125.70	120.38
1	r	251	THR	CA-C-N	5.16	127.45	120.38
1	r	251	THR	C-N-CA	5.16	127.45	120.38
4	R	59	ALA	N-CA-C	5.15	119.04	112.34
2	Q	110	LEU	N-CA-C	5.15	116.71	111.14
5	7	44	TYR	N-CA-C	5.15	119.28	112.89
4	u	134	GLN	N-CA-C	5.15	116.75	111.03
1	l	225	ASN	N-CA-C	5.15	119.71	113.38
3	e	40	ASP	N-CA-C	-5.15	105.08	112.13
4	i	138	LEU	N-CA-C	5.13	116.96	111.36
4	u	14	ASN	N-CA-C	5.13	119.41	111.56
1	l	290	THR	N-CA-C	-5.13	105.38	111.69
1	U	242	GLU	N-CA-C	-5.13	105.77	111.36
4	o	5	VAL	CA-C-N	-5.13	114.38	119.56
4	o	5	VAL	C-N-CA	-5.13	114.38	119.56
1	w	16	GLU	N-CA-C	-5.12	105.78	111.36
4	F	29	TYR	N-CA-C	-5.12	100.82	108.96
5	j	161	PRO	CA-C-N	5.11	125.11	119.89
5	j	161	PRO	C-N-CA	5.11	125.11	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	7	159	ILE	N-CA-C	5.11	117.86	109.78
1	l	15	PHE	N-CA-C	5.11	118.29	111.75
5	v	51	ILE	N-CA-C	5.11	115.66	108.36
1	f	240	GLU	N-CA-C	5.10	116.53	111.07
1	3	300	MET	N-CA-C	5.10	117.57	111.71
3	m	47	ASP	CB-CA-C	-5.10	110.72	116.63
5	q	123	THR	N-CA-C	-5.10	105.73	111.28
1	I	199	ARG	N-CA-C	-5.09	105.64	111.14
5	d	65	VAL	N-CA-C	5.09	115.38	107.28
3	e	8	ARG	N-CA-C	5.09	116.70	108.41
1	O	291	GLU	N-CA-C	-5.08	105.18	111.33
3	s	34	ILE	N-CA-C	5.08	115.36	110.74
4	L	14	ASN	N-CA-C	5.07	119.50	112.45
5	M	74	THR	N-CA-C	5.07	117.66	109.40
2	n	60	VAL	N-CA-C	5.07	115.96	108.45
5	p	134	GLU	N-CA-C	-5.07	102.51	110.17
2	t	32	LYS	N-CA-C	-5.07	102.55	110.10
4	0	29	TYR	N-CA-C	-5.07	101.50	109.25
1	w	134	ILE	CB-CA-C	-5.06	105.34	111.87
4	c	110	TRP	N-CA-C	-5.06	100.99	109.24
5	q	36	LYS	N-CA-C	5.06	117.45	111.33
2	h	96	ALA	N-CA-C	-5.06	103.69	110.07
4	F	52	ARG	N-CA-C	5.05	117.15	107.75
1	O	250	GLU	N-CA-C	5.05	116.98	109.25
1	I	239	LYS	N-CA-C	-5.05	105.67	111.07
1	I	262	MET	CG-SD-CE	-5.05	89.80	100.90
5	b	85	VAL	CB-CA-C	-5.04	102.89	110.55
4	6	130	GLU	N-CA-C	5.04	116.46	110.97
5	d	157	LYS	N-CA-C	5.04	117.66	111.82
1	r	16	GLU	N-CA-C	-5.03	105.71	111.14
4	a	119	LEU	N-CA-C	-5.03	107.10	113.23
1	f	261	LEU	N-CA-C	-5.03	105.69	111.07
4	i	85	TYR	N-CA-C	5.03	116.88	108.99
1	9	135	VAL	N-CA-C	5.03	115.26	110.53
5	d	108	HIS	CA-C-N	-5.02	113.55	120.28
5	d	108	HIS	C-N-CA	-5.02	113.55	120.28
4	k	14	ASN	N-CA-C	5.02	117.52	111.40
1	U	152	LYS	N-CA-C	5.02	116.75	111.28
1	I	86	ASP	N-CA-C	-5.02	105.89	111.36
1	O	107	LEU	N-CA-C	5.01	120.89	109.81
5	7	83	GLN	N-CA-C	5.01	115.93	108.86
2	t	24	SER	N-CA-C	-5.01	105.90	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	204	LYS	N-CA-C	-5.00	105.83	111.28
2	B	60	VAL	N-CA-C	5.00	115.85	108.45

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	253	ARG	Peptide
4	R	155	ASP	Peptide
2	T	89	GLU	Peptide
2	Y	91	PRO	Peptide
5	j	33	ARG	Peptide
5	q	142	VAL	Peptide

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	3	2435	0	2426	134	0
1	9	2435	0	2426	94	0
1	C	2446	0	2433	130	0
1	I	2441	0	2431	127	0
1	O	2451	0	2435	144	0
1	U	2469	0	2450	84	0
1	V	2441	0	2431	146	1
1	f	2441	0	2431	127	0
1	l	2444	0	2441	112	0
1	r	2441	0	2431	110	1
1	w	2440	0	2428	120	0
1	x	2419	0	2409	104	0
2	5	691	0	693	37	0
2	B	691	0	693	49	0
2	E	691	0	693	32	0
2	K	683	0	684	33	0
2	Q	691	0	693	30	0
2	T	691	0	693	44	0
2	Y	691	0	693	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	691	0	693	38	0
2	h	691	0	693	34	0
2	n	691	0	693	53	0
2	t	691	0	693	41	0
2	z	691	0	693	43	0
3	4	748	0	741	27	0
3	D	748	0	741	24	0
3	H	748	0	741	26	0
3	J	711	0	707	28	0
3	P	740	0	737	44	0
3	W	717	0	716	32	0
3	X	748	0	741	29	0
3	e	624	0	632	21	0
3	g	748	0	741	29	0
3	m	748	0	741	31	0
3	s	748	0	741	35	0
3	y	748	0	741	27	0
4	0	1175	0	1091	59	0
4	6	1147	0	1065	78	0
4	F	1185	0	1111	70	0
4	L	1154	0	1066	54	0
4	N	1173	0	1089	55	0
4	R	1175	0	1093	70	0
4	a	1193	0	1115	70	0
4	c	1180	0	1096	58	0
4	i	1271	0	1193	55	0
4	k	1196	0	1111	69	0
4	o	1167	0	1089	55	0
4	u	1167	0	1089	55	0
5	1	1385	0	1344	62	0
5	2	1391	0	1362	69	0
5	7	1391	0	1363	86	0
5	G	1397	0	1373	75	0
5	M	1402	0	1375	53	0
5	S	1391	0	1362	95	0
5	b	1414	0	1391	83	0
5	d	1391	0	1362	71	3
5	j	1397	0	1373	69	0
5	p	1380	0	1343	74	2
5	q	1386	0	1361	84	0
5	v	1391	0	1363	81	1
6	1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	2	1	0	0	0	0
6	7	1	0	0	0	0
6	G	1	0	0	0	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
6	b	1	0	0	0	0
6	d	1	0	0	0	0
6	j	1	0	0	0	0
6	p	1	0	0	0	0
6	q	1	0	0	0	0
6	v	1	0	0	0	0
All	All	77274	0	75779	3598	4

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 24.

All (3598) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:19:TRP:CD1	1:3:23:ARG:HE	0.99	1.68
1:3:19:TRP:NE1	1:3:23:ARG:HE	1.08	1.51
1:w:19:TRP:CD1	1:w:23:ARG:HE	1.32	1.47
4:R:14:ASN:O	4:R:19:ARG:CZ	1.67	1.41
4:R:14:ASN:CA	4:R:19:ARG:HH21	1.34	1.41
1:O:19:TRP:NE1	1:O:23:ARG:HE	1.20	1.40
1:O:19:TRP:CD1	1:O:23:ARG:HE	1.41	1.38
1:3:19:TRP:CD1	1:3:23:ARG:NE	1.75	1.38
4:u:14:ASN:O	4:u:19:ARG:NE	1.57	1.37
1:V:19:TRP:CE3	1:V:23:ARG:NE	1.99	1.31
4:R:14:ASN:HA	4:R:19:ARG:NH2	1.44	1.28
1:f:19:TRP:NE1	1:f:23:ARG:CG	1.94	1.23
1:O:19:TRP:CD1	1:O:23:ARG:NE	2.09	1.20
1:l:23:ARG:CG	1:l:24:PRO:HD3	1.73	1.19
1:O:19:TRP:NE1	1:O:23:ARG:NE	1.94	1.15
1:f:19:TRP:NE1	1:f:23:ARG:HG2	1.45	1.15
1:l:58:PRO:HD2	1:l:59:ALA:H	1.13	1.14
1:w:19:TRP:CD1	1:w:23:ARG:NE	2.14	1.13
4:R:14:ASN:CA	4:R:19:ARG:NH2	2.05	1.12
5:b:50:LYS:NZ	5:b:70:TRP:O	1.82	1.12
1:I:58:PRO:HD2	1:I:59:ALA:H	1.10	1.12
1:f:58:PRO:HD2	1:f:59:ALA:H	1.12	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:58:PRO:HD2	1:3:59:ALA:H	1.13	1.12
1:x:58:PRO:HD2	1:x:59:ALA:H	1.03	1.11
1:O:58:PRO:HD2	1:O:59:ALA:H	1.16	1.10
4:o:14:ASN:O	4:o:19:ARG:CZ	1.99	1.10
1:3:19:TRP:NE1	1:3:23:ARG:NE	1.79	1.09
1:3:56:LYS:C	1:3:58:PRO:HD3	1.77	1.09
1:V:58:PRO:HD2	1:V:59:ALA:H	1.01	1.08
1:U:19:TRP:CE2	1:U:23:ARG:HG2	1.87	1.08
1:C:58:PRO:HD2	1:C:59:ALA:H	1.06	1.08
1:9:56:LYS:C	1:9:58:PRO:HD3	1.78	1.08
4:6:14:ASN:O	4:6:19:ARG:CZ	2.01	1.08
1:w:58:PRO:HD2	1:w:59:ALA:H	1.10	1.08
4:u:14:ASN:O	4:u:19:ARG:CZ	2.03	1.07
1:r:58:PRO:HD2	1:r:59:ALA:H	1.18	1.06
4:R:14:ASN:O	4:R:19:ARG:NE	1.87	1.05
4:c:14:ASN:HA	4:c:19:ARG:HH21	1.16	1.05
1:w:19:TRP:NE1	1:w:23:ARG:HE	1.54	1.05
1:9:19:TRP:CE2	1:9:23:ARG:HG2	1.91	1.04
1:O:19:TRP:HE1	1:O:23:ARG:NE	1.53	1.03
1:l:23:ARG:HG2	1:l:24:PRO:CD	1.86	1.03
4:6:14:ASN:O	4:6:19:ARG:NE	1.91	1.03
2:n:108:ASN:HA	5:p:146:GLN:HE22	1.23	1.01
1:f:19:TRP:CE2	1:f:23:ARG:HG2	1.95	1.01
4:R:156:ARG:HH21	4:R:156:ARG:HG3	1.25	1.00
1:O:188:CYS:SG	1:O:194:LYS:NZ	2.36	0.99
1:9:19:TRP:O	1:9:23:ARG:HG3	1.61	0.98
1:U:58:PRO:HD2	1:U:59:ALA:H	1.26	0.98
1:l:23:ARG:HG2	1:l:24:PRO:HD3	0.99	0.98
1:3:19:TRP:HE1	1:3:23:ARG:NE	1.61	0.97
3:W:44:LEU:HD21	3:W:75:VAL:HG13	1.44	0.96
4:0:118:ARG:HE	4:0:120:ASP:HB2	1.27	0.96
5:p:50:LYS:NZ	5:p:71:GLY:O	1.98	0.96
1:9:56:LYS:C	1:9:58:PRO:CD	2.38	0.96
1:C:19:TRP:O	1:C:23:ARG:HG3	1.63	0.96
1:3:56:LYS:C	1:3:58:PRO:CD	2.38	0.95
4:6:14:ASN:HA	4:6:19:ARG:HH21	1.30	0.95
4:o:14:ASN:O	4:o:19:ARG:NE	1.99	0.95
1:9:58:PRO:HD2	1:9:59:ALA:H	1.28	0.95
1:C:19:TRP:CE2	1:C:23:ARG:HG2	2.00	0.95
4:R:15:GLU:O	4:R:19:ARG:HG3	1.67	0.94
5:S:36:LYS:NZ	5:S:37:ASP:OD1	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:19:TRP:NE1	1:O:23:ARG:CG	2.30	0.94
3:J:28:LYS:HE2	3:J:44:LEU:HD23	1.47	0.94
1:r:77:GLN:NE2	1:r:146:SER:O	2.02	0.93
4:R:14:ASN:C	4:R:19:ARG:CZ	2.42	0.93
1:r:32:GLN:HE21	1:r:103:GLN:HE22	1.12	0.92
5:b:140:ASN:OD1	5:b:167:ARG:NH1	2.02	0.92
1:9:57:GLY:N	1:9:58:PRO:HD3	1.82	0.92
4:R:14:ASN:HA	4:R:19:ARG:HH21	0.74	0.91
1:3:19:TRP:CD1	1:3:23:ARG:CZ	2.52	0.91
1:l:178:ILE:HG22	1:l:181:ARG:HH12	1.35	0.90
4:0:151:ARG:NH2	5:1:112:PHE:O	2.03	0.90
1:V:58:PRO:HD2	1:V:59:ALA:N	1.81	0.90
4:R:14:ASN:C	4:R:19:ARG:NE	2.29	0.90
1:V:58:PRO:CD	1:V:59:ALA:H	1.83	0.90
1:3:19:TRP:HD1	1:3:23:ARG:NE	1.51	0.90
1:w:167:ARG:NH2	1:w:241:GLU:OE1	2.04	0.90
4:u:151:ARG:HG2	5:v:109:LEU:HA	1.54	0.90
1:r:19:TRP:CE2	1:r:23:ARG:HG2	2.07	0.90
1:x:58:PRO:CD	1:x:59:ALA:H	1.85	0.90
1:3:19:TRP:HD1	1:3:23:ARG:CZ	1.85	0.90
1:f:109:LYS:NZ	2:h:47:SER:OG	2.05	0.89
4:6:14:ASN:CA	4:6:19:ARG:HH21	1.85	0.89
4:N:14:ASN:O	4:N:19:ARG:NE	2.05	0.89
1:r:19:TRP:O	1:r:23:ARG:HG3	1.73	0.89
4:0:99:ALA:HB1	5:1:7:VAL:HG11	1.55	0.89
4:k:41:GLN:NE2	4:k:117:GLN:O	2.05	0.88
4:c:15:GLU:O	4:c:19:ARG:HG3	1.73	0.88
2:n:108:ASN:HA	5:p:146:GLN:NE2	1.87	0.88
1:f:133:SER:OG	1:f:134:ILE:N	1.99	0.88
4:o:14:ASN:HA	4:o:19:ARG:HH21	1.37	0.88
1:3:144:ASN:O	1:3:149:SER:OG	1.91	0.88
5:2:134:GLU:HG2	5:2:158:LYS:HB2	1.54	0.88
4:k:136:ASP:OD1	4:k:139:ALA:N	2.07	0.88
5:b:112:PHE:HE2	5:b:163:LEU:HD22	1.37	0.88
1:V:19:TRP:O	1:V:23:ARG:HG3	1.74	0.87
4:F:8:GLN:NE2	4:F:105:GLY:O	2.07	0.87
1:r:48:HIS:HD1	2:t:109:PHE:HD1	1.22	0.87
1:x:58:PRO:HD2	1:x:59:ALA:N	1.82	0.87
1:V:19:TRP:HA	1:V:22:MET:HG3	1.57	0.87
1:l:23:ARG:CG	1:l:24:PRO:CD	2.49	0.87
1:l:228:GLN:OE1	1:l:292:LYS:NZ	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:57:GLY:N	1:3:58:PRO:HD3	1.89	0.87
1:I:58:PRO:HD2	1:I:59:ALA:N	1.87	0.87
1:l:58:PRO:HD2	1:l:59:ALA:N	1.89	0.87
1:w:58:PRO:HD2	1:w:59:ALA:N	1.87	0.87
4:6:15:GLU:O	4:6:19:ARG:HG3	1.76	0.86
5:b:134:GLU:OE1	5:b:135:TYR:N	2.07	0.86
1:3:56:LYS:O	1:3:58:PRO:HD2	1.75	0.86
1:f:19:TRP:HE1	1:f:23:ARG:HG2	1.36	0.86
1:9:19:TRP:CE2	1:9:23:ARG:CG	2.57	0.86
1:O:37:LYS:NZ	2:Q:58:ASN:OD1	2.09	0.86
4:F:14:ASN:HA	4:F:19:ARG:HH21	1.40	0.85
4:R:14:ASN:HA	4:R:19:ARG:CZ	2.06	0.85
1:x:56:LYS:HB2	1:x:60:LYS:HE3	1.57	0.85
1:U:19:TRP:O	1:U:23:ARG:HG3	1.77	0.85
4:N:15:GLU:OE2	4:N:147:ARG:NH2	2.08	0.85
1:C:38:GLN:OE1	2:E:61:ASN:ND2	2.08	0.85
3:W:50:LEU:HD12	3:W:51:LEU:H	1.41	0.85
1:f:58:PRO:HD2	1:f:59:ALA:N	1.90	0.85
1:U:19:TRP:HE3	1:U:22:MET:HE2	1.42	0.85
1:I:242:GLU:HB2	1:I:262:MET:HE1	1.58	0.85
1:O:58:PRO:HD2	1:O:59:ALA:N	1.91	0.85
1:3:86:ASP:OD1	1:3:154:ARG:NH1	2.10	0.85
1:C:154:ARG:HH11	1:C:154:ARG:HG2	1.41	0.85
1:V:17:ASP:OD1	1:V:17:ASP:N	2.10	0.85
5:G:128:ILE:HG13	5:G:129:VAL:H	1.40	0.84
4:R:26:GLU:HG3	4:R:122:MET:HE3	1.59	0.84
4:k:151:ARG:NH2	5:q:112:PHE:O	2.09	0.84
1:l:77:GLN:NE2	1:l:146:SER:O	2.09	0.84
2:Q:23:SER:OG	2:Q:25:ASP:OD1	1.93	0.84
4:o:14:ASN:O	4:o:19:ARG:NH2	2.09	0.84
1:C:58:PRO:HD2	1:C:59:ALA:N	1.85	0.84
4:R:32:PHE:HE2	4:R:43:ARG:HD2	1.40	0.84
1:w:277:ILE:HG22	1:w:296:MET:HE3	1.59	0.84
4:R:14:ASN:O	4:R:19:ARG:NH2	2.10	0.84
4:k:14:ASN:O	4:k:19:ARG:NE	2.11	0.83
4:a:8:GLN:NE2	4:a:140:GLN:OE1	2.11	0.83
4:o:14:ASN:CA	4:o:19:ARG:HH21	1.91	0.83
1:O:162:LEU:HD21	1:O:172:PHE:CD1	2.13	0.83
1:x:245:ALA:HB2	1:x:261:LEU:HD12	1.61	0.83
5:b:3:ASN:H	5:b:3:ASN:HD22	1.23	0.83
4:i:5:VAL:HG13	4:i:6:PRO:HD3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:43:ARG:HG3	3:H:50:LEU:HD21	1.61	0.83
4:a:11:LYS:HD2	4:a:147:ARG:HH12	1.44	0.83
2:K:35:HIS:O	2:K:38:THR:OG1	1.95	0.83
1:O:19:TRP:HE1	1:O:23:ARG:HE	1.07	0.83
5:d:17:ARG:HH11	5:d:17:ARG:HG3	1.43	0.82
4:N:15:GLU:O	4:N:19:ARG:HG3	1.78	0.82
1:f:19:TRP:HE1	1:f:23:ARG:CG	1.86	0.82
4:O:136:ASP:N	4:O:136:ASP:OD1	2.06	0.82
5:q:13:VAL:O	5:q:83:GLN:NE2	2.13	0.82
1:3:255:CYS:SG	1:3:256:ASN:N	2.47	0.82
4:R:14:ASN:C	4:R:19:ARG:NH2	2.38	0.82
1:l:77:GLN:HG3	1:l:147:ILE:HG12	1.62	0.82
1:C:58:PRO:CD	1:C:59:ALA:H	1.89	0.82
1:f:166:GLU:OE2	1:f:248:TYR:OH	1.97	0.82
4:i:41:GLN:NE2	4:i:117:GLN:O	2.12	0.82
5:M:59:LEU:HD11	5:M:64:LEU:HB2	1.61	0.82
1:f:90:LEU:HD22	1:f:176:LEU:HD23	1.62	0.82
5:S:58:PRO:O	5:S:111:TYR:OH	1.97	0.82
2:Z:21:LEU:HD12	2:Z:29:PHE:HB2	1.62	0.82
1:O:62:HIS:HB2	1:O:114:LEU:HD21	1.62	0.81
1:I:167:ARG:HE	1:I:244:ARG:HH12	1.26	0.81
2:K:74:CYS:HA	2:K:77:PHE:HD1	1.45	0.81
3:P:9:ARG:HB2	3:P:77:LEU:HB3	1.63	0.81
4:k:14:ASN:O	4:k:19:ARG:CZ	2.28	0.81
1:O:115:GLU:OE2	1:O:134:ILE:N	2.14	0.81
5:S:9:ILE:H	5:S:97:GLN:HE22	1.27	0.81
5:q:108:HIS:NE2	5:q:114:CYS:SG	2.50	0.81
2:Z:107:ALA:HB2	5:d:145:LEU:HD13	1.62	0.81
5:7:119:ALA:HA	5:7:129:VAL:HG21	1.63	0.81
1:3:58:PRO:HD2	1:3:59:ALA:N	1.90	0.81
1:I:90:LEU:HD22	1:I:176:LEU:HD23	1.63	0.80
1:3:56:LYS:O	1:3:58:PRO:CD	2.28	0.80
1:C:255:CYS:HG	1:C:257:SER:HG	1.21	0.80
5:d:36:LYS:NZ	5:d:37:ASP:OD1	2.14	0.80
4:N:31:GLY:H	4:N:40:ARG:HH22	1.27	0.80
3:P:52:ASP:N	3:P:52:ASP:OD1	2.14	0.80
1:I:17:ASP:OD1	1:I:17:ASP:N	2.15	0.80
1:3:19:TRP:NE1	1:3:23:ARG:CG	2.45	0.80
3:W:39:PRO:HA	3:W:42:GLN:HG2	1.62	0.80
1:9:266:VAL:HG11	1:9:302:LYS:HB3	1.62	0.80
1:w:58:PRO:CD	1:w:59:ALA:H	1.93	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:303:VAL:HG22	1:w:304:PRO:HD2	1.64	0.80
1:O:19:TRP:NE1	1:O:23:ARG:HG2	1.96	0.80
5:b:120:ILE:HD11	5:b:146:GLN:HB3	1.64	0.79
3:s:43:ARG:HG3	3:s:50:LEU:HD21	1.64	0.79
1:U:19:TRP:NE1	1:U:23:ARG:HG2	1.97	0.79
1:I:58:PRO:CD	1:I:59:ALA:H	1.94	0.79
4:R:14:ASN:CB	4:R:19:ARG:HH21	1.94	0.79
1:x:94:ILE:HG13	1:x:176:LEU:HD23	1.63	0.79
1:O:15:PHE:HE2	1:O:60:LYS:HD2	1.48	0.79
1:O:71:GLU:OE2	1:O:75:GLN:NE2	2.15	0.79
4:i:114:ILE:HD13	4:i:121:GLY:HA3	1.64	0.79
2:E:88:THR:OG1	2:E:89:GLU:N	2.12	0.79
4:c:151:ARG:HG2	5:d:108:HIS:CE1	2.18	0.79
1:f:56:LYS:C	1:f:58:PRO:HD3	2.06	0.79
4:O:15:GLU:O	4:O:19:ARG:HG3	1.81	0.79
2:n:96:ALA:H	2:n:99:ILE:HD11	1.47	0.79
5:b:158:GLN:HG3	5:b:158:GLN:O	1.80	0.79
5:q:28:HIS:HD2	5:q:163:LEU:HD23	1.47	0.79
4:N:11:LYS:HB2	4:N:15:GLU:HG3	1.65	0.79
4:L:118:ARG:HE	4:L:120:ASP:HB2	1.46	0.78
5:j:13:VAL:HG21	5:j:18:ILE:HG13	1.64	0.78
1:C:14:GLN:NE2	1:C:14:GLN:O	2.16	0.78
1:f:193:ASP:OD2	1:f:199:ARG:NH1	2.16	0.78
4:a:138:LEU:H	4:a:138:LEU:HD12	1.49	0.78
4:O:151:ARG:NH2	5:p:112:PHE:O	2.16	0.78
4:k:11:LYS:HE2	4:k:147:ARG:HH12	1.48	0.78
1:w:19:TRP:NE1	1:w:23:ARG:NE	2.27	0.78
1:w:19:TRP:HD1	1:w:23:ARG:NE	1.81	0.78
5:d:18:ILE:HD13	5:d:169:LEU:HD11	1.65	0.78
1:3:19:TRP:CE2	1:3:23:ARG:HG2	2.19	0.78
5:G:112:PHE:CE1	5:G:163:LEU:HD22	2.19	0.78
4:i:27:ILE:HG22	4:i:59:ALA:HA	1.65	0.78
3:y:24:VAL:HG13	3:y:44:LEU:HD12	1.65	0.78
2:5:88:THR:N	4:6:16:GLU:OE1	2.17	0.78
4:R:5:VAL:HG13	4:R:6:PRO:HD3	1.66	0.78
2:n:31:VAL:HG12	3:m:15:PHE:HB2	1.66	0.78
1:r:58:PRO:HD2	1:r:59:ALA:N	1.92	0.78
5:b:58:PRO:O	5:b:111:TYR:OH	2.01	0.78
4:R:33:ARG:C	5:S:77:ARG:HH12	1.91	0.78
1:V:266:VAL:HG21	1:V:302:LYS:HG2	1.67	0.78
1:f:206:TYR:O	1:f:210:THR:OG1	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:37:ARG:O	3:J:42:GLN:NE2	2.16	0.77
1:9:17:ASP:OD1	1:9:17:ASP:N	2.16	0.77
1:U:19:TRP:CE2	1:U:23:ARG:CG	2.65	0.77
1:V:19:TRP:CE3	1:V:23:ARG:CZ	2.68	0.77
1:x:108:PRO:HB3	1:x:135:VAL:HB	1.65	0.77
1:3:40:TRP:HD1	1:3:41:PHE:HD1	1.31	0.77
1:9:56:LYS:O	1:9:58:PRO:HD2	1.84	0.77
1:l:58:PRO:CD	1:l:59:ALA:H	1.94	0.77
4:i:151:ARG:NH2	5:j:112:PHE:O	2.17	0.77
4:6:155:ASP:OD1	4:6:155:ASP:N	2.16	0.77
3:H:6:MET:HE3	3:H:74:THR:HG23	1.66	0.77
4:a:15:GLU:O	4:a:19:ARG:HG3	1.83	0.77
5:v:50:LYS:NZ	5:v:71:GLY:O	2.15	0.77
4:N:24:GLU:HA	4:N:124:CYS:HB3	1.67	0.77
4:a:155:ASP:OD1	4:a:155:ASP:N	2.18	0.77
3:s:28:LYS:HB3	3:s:39:PRO:HB3	1.66	0.77
4:k:14:ASN:HA	4:k:19:ARG:HH21	1.48	0.77
4:u:103:LEU:HD21	5:v:9:ILE:HD11	1.67	0.77
2:B:88:THR:HG23	2:B:89:GLU:OE1	1.84	0.77
5:j:45:GLU:OE1	5:1:41:ARG:NH2	2.18	0.76
1:3:228:GLN:HE22	1:3:292:LYS:HD3	1.50	0.76
3:J:2:ASP:OD1	3:J:19:LYS:NZ	2.17	0.76
1:w:19:TRP:HD1	1:w:23:ARG:HE	1.24	0.76
5:d:52:SER:HG	5:d:70:TRP:CD1	2.03	0.76
3:m:9:ARG:NH1	3:m:86:GLU:OE2	2.18	0.76
5:p:15:ARG:HB3	5:p:83:GLN:HE22	1.50	0.76
5:2:36:LYS:NZ	5:2:37:ASP:OD1	2.13	0.76
1:f:58:PRO:CD	1:f:59:ALA:H	1.95	0.76
1:w:245:ALA:HB1	1:w:249:LEU:HD12	1.68	0.76
1:l:233:TYR:CE1	1:l:237:LYS:HE3	2.21	0.76
1:V:166:GLU:CD	1:V:244:ARG:HH22	1.94	0.76
4:0:144:GLU:OE2	4:0:148:ARG:NH1	2.19	0.76
5:G:41:ARG:NH1	5:7:45:GLU:OE1	2.19	0.75
2:K:105:MET:HE2	5:M:124:ILE:HG23	1.68	0.75
1:9:56:LYS:O	1:9:58:PRO:CD	2.33	0.75
1:V:85:ASP:OD1	1:V:85:ASP:N	2.17	0.75
5:d:134:GLU:OE1	5:d:135:TYR:N	2.16	0.75
3:s:24:VAL:HG13	3:s:44:LEU:HD12	1.67	0.75
1:3:19:TRP:NE1	1:3:23:ARG:CD	2.49	0.75
1:U:19:TRP:CE3	1:U:22:MET:HE2	2.21	0.75
4:c:136:ASP:OD1	4:c:138:LEU:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:58:PRO:HD2	1:9:59:ALA:N	1.98	0.75
1:C:19:TRP:CE2	1:C:23:ARG:CG	2.70	0.75
4:c:14:ASN:HA	4:c:19:ARG:NH2	1.97	0.75
2:T:76:TYR:OH	5:q:143:GLY:O	2.05	0.75
1:V:19:TRP:CZ3	1:V:23:ARG:NE	2.54	0.75
1:3:58:PRO:CD	1:3:59:ALA:H	1.97	0.75
1:w:286:LYS:HG2	1:w:317:HIS:CD2	2.22	0.75
1:r:32:GLN:NE2	1:r:103:GLN:HE22	1.85	0.75
1:U:58:PRO:HD2	1:U:59:ALA:N	1.99	0.74
2:E:23:SER:OG	2:E:25:ASP:OD1	2.05	0.74
4:c:14:ASN:O	4:c:19:ARG:CZ	2.35	0.74
5:p:20:THR:HG22	5:p:24:LEU:HD11	1.69	0.74
1:r:19:TRP:CE2	1:r:23:ARG:CG	2.70	0.74
3:D:9:ARG:HD3	3:D:77:LEU:HD23	1.68	0.74
5:S:104:ASP:HA	5:S:107:ILE:HG13	1.70	0.74
4:u:85:TYR:HE2	4:u:98:LYS:HD3	1.52	0.74
1:w:19:TRP:O	1:w:23:ARG:HG3	1.88	0.74
2:B:17:MET:HG3	2:B:18:TYR:HD1	1.51	0.74
1:V:19:TRP:HE3	1:V:23:ARG:HE	1.23	0.74
1:r:167:ARG:NH2	1:r:210:THR:OG1	2.19	0.74
1:3:16:GLU:OE2	1:3:60:LYS:NZ	2.20	0.74
1:3:159:ALA:HB1	1:3:177:VAL:HG23	1.70	0.74
5:p:90:ARG:HG2	5:p:95:SER:HB2	1.67	0.74
2:t:76:TYR:OH	5:v:144:GLY:O	2.05	0.74
4:F:50:ASP:OD1	4:F:52:ARG:N	2.21	0.74
1:l:85:ASP:OD1	1:l:85:ASP:N	2.20	0.74
4:0:41:GLN:NE2	4:0:117:GLN:O	2.19	0.74
3:X:9:ARG:HD3	3:X:77:LEU:HD23	1.67	0.74
5:d:54:GLU:HG2	5:d:67:THR:HG23	1.70	0.74
1:l:57:GLY:N	1:l:58:PRO:HD3	2.03	0.74
4:0:83:ARG:HH22	4:0:131:ARG:HG3	1.53	0.74
4:a:88:LEU:HD23	4:a:88:LEU:H	1.53	0.74
1:O:58:PRO:CD	1:O:59:ALA:H	1.97	0.74
3:m:28:LYS:HB3	3:m:39:PRO:HB3	1.70	0.74
1:I:85:ASP:OD1	1:I:85:ASP:N	2.19	0.74
4:c:14:ASN:CA	4:c:19:ARG:HH21	1.98	0.74
4:0:151:ARG:HG2	5:1:109:LEU:HA	1.70	0.74
5:S:101:ASP:O	5:S:140:ASN:ND2	2.21	0.73
4:6:11:LYS:HD3	4:6:147:ARG:HH12	1.53	0.73
3:D:9:ARG:NH1	3:D:86:GLU:OE2	2.21	0.73
1:I:103:GLN:O	1:I:106:ILE:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:8:ARG:NH2	3:P:91:GLU:O	2.21	0.73
1:9:57:GLY:N	1:9:58:PRO:CD	2.50	0.73
1:l:287:ARG:NE	1:l:289:GLU:OE2	2.21	0.73
5:d:48:ASN:HB3	5:d:51:ILE:HG13	1.69	0.73
1:w:41:PHE:HE2	2:B:61:ASN:H	1.35	0.73
2:Y:25:ASP:OD1	2:Y:67:SER:N	2.22	0.73
1:V:83:HIS:CD2	1:V:92:ALA:HB2	2.24	0.73
5:v:134:GLU:OE2	5:v:159:GLN:N	2.21	0.73
1:V:19:TRP:HE3	1:V:23:ARG:HH21	1.35	0.73
1:U:17:ASP:N	1:U:17:ASP:OD1	2.22	0.73
1:O:85:ASP:N	1:O:85:ASP:OD1	2.22	0.73
5:p:20:THR:O	5:p:24:LEU:HD12	1.88	0.73
2:t:83:TYR:CZ	2:t:91:PRO:HG3	2.23	0.73
2:E:61:ASN:OD1	2:E:61:ASN:N	2.20	0.73
1:r:77:GLN:HG2	1:r:81:LEU:HD22	1.70	0.73
1:U:90:LEU:HD21	1:U:176:LEU:HB3	1.71	0.72
3:g:24:VAL:HG13	3:g:44:LEU:HD12	1.71	0.72
5:q:54:GLU:HG2	5:q:67:THR:HG23	1.69	0.72
4:0:114:ILE:HG12	4:0:121:GLY:HA3	1.71	0.72
1:I:174:SER:OG	1:I:247:ARG:NH1	2.23	0.72
1:f:57:GLY:N	1:f:58:PRO:HD3	2.04	0.72
5:p:134:GLU:CD	5:p:135:TYR:H	1.97	0.72
5:G:114:CYS:HA	5:G:133:CYS:HA	1.71	0.72
1:3:19:TRP:NE1	1:3:23:ARG:HG2	2.05	0.72
2:K:88:THR:OG1	4:L:16:GLU:OE2	2.07	0.72
4:a:11:LYS:HD2	4:a:147:ARG:NH1	2.04	0.72
5:M:113:ASP:OD1	5:M:113:ASP:N	2.20	0.72
3:W:25:PHE:HB2	3:W:53:ASP:HB3	1.71	0.72
1:w:138:LEU:O	1:w:142:THR:OG1	2.08	0.72
2:B:107:ALA:O	5:2:147:GLN:NE2	2.22	0.72
4:F:14:ASN:O	4:F:19:ARG:NE	2.23	0.72
4:L:151:ARG:NH2	5:M:112:PHE:O	2.22	0.72
5:d:17:ARG:HH22	5:d:168:LYS:HE2	1.53	0.72
4:k:15:GLU:O	4:k:19:ARG:HG3	1.90	0.72
4:c:151:ARG:NH1	5:d:112:PHE:O	2.23	0.72
4:o:31:GLY:H	4:o:40:ARG:HH12	1.38	0.72
5:v:134:GLU:CD	5:v:135:TYR:H	1.97	0.72
4:6:49:ARG:HG2	4:6:49:ARG:HH11	1.55	0.72
4:6:151:ARG:HG2	5:7:109:LEU:HA	1.72	0.72
5:j:25:VAL:O	5:j:29:MET:HG2	1.89	0.72
1:C:85:ASP:OD1	1:C:85:ASP:N	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:8:GLN:NE2	4:L:140:GLN:OE1	2.23	0.71
4:L:152:GLU:HG3	5:M:139:HIS:CE1	2.23	0.71
1:O:15:PHE:CE2	1:O:60:LYS:HD2	2.25	0.71
1:O:94:ILE:HG13	1:O:176:LEU:HD13	1.73	0.71
2:n:42:ILE:HD11	2:n:62:PHE:HZ	1.53	0.71
2:B:111:ASP:HB2	5:2:147:GLN:NE2	2.06	0.71
5:d:58:PRO:O	5:d:111:TYR:OH	2.07	0.71
3:X:9:ARG:NH1	3:X:86:GLU:OE2	2.23	0.71
3:X:43:ARG:HG3	3:X:50:LEU:HD21	1.71	0.71
1:O:19:TRP:NE1	1:O:23:ARG:CD	2.53	0.71
1:l:144:ASN:HD22	1:l:187:LEU:HB3	1.55	0.71
1:U:19:TRP:HA	1:U:22:MET:HG3	1.72	0.71
1:C:18:LYS:NZ	1:C:46:ASP:OD1	2.24	0.71
5:d:22:LYS:HE2	5:d:53:SER:HB3	1.71	0.71
4:u:14:ASN:HA	4:u:19:ARG:HH21	1.56	0.71
3:e:37:ARG:O	3:e:42:GLN:NE2	2.24	0.71
4:k:8:GLN:OE1	4:k:106:VAL:HA	1.90	0.71
2:t:86:SER:OG	4:u:16:GLU:OE2	2.09	0.70
5:7:119:ALA:O	5:7:123:THR:OG1	2.09	0.70
1:I:278:LEU:HD21	1:I:300:MET:HE2	1.72	0.70
1:l:167:ARG:HH21	1:l:241:GLU:CD	1.99	0.70
1:C:17:ASP:OD1	1:C:17:ASP:N	2.23	0.70
1:O:19:TRP:CE2	1:O:23:ARG:HG2	2.26	0.70
1:V:19:TRP:HE3	1:V:23:ARG:NH2	1.89	0.70
4:6:14:ASN:O	4:6:19:ARG:NH2	2.25	0.70
2:T:76:TYR:HA	2:T:93:PHE:HE2	1.56	0.70
1:U:228:GLN:HA	1:U:228:GLN:HE21	1.55	0.70
5:b:159:ILE:HG21	5:b:163:LEU:HG	1.74	0.70
1:r:14:GLN:O	1:r:15:PHE:HB3	1.91	0.70
3:s:39:PRO:HA	3:s:42:GLN:HG3	1.74	0.70
1:r:58:PRO:CD	1:r:59:ALA:H	1.98	0.70
4:o:141:GLN:O	4:o:145:GLU:HG2	1.90	0.70
1:r:181:ARG:O	1:r:185:VAL:HG23	1.92	0.70
4:L:151:ARG:HG2	5:M:109:LEU:HA	1.73	0.70
1:r:32:GLN:HE21	1:r:103:GLN:NE2	1.88	0.70
1:3:178:ILE:O	1:3:182:GLU:HG3	1.92	0.70
4:k:114:ILE:HG12	4:k:121:GLY:HA3	1.73	0.70
1:C:192:GLU:OE2	1:x:199:ARG:NH2	2.25	0.70
4:c:137:ALA:HA	4:c:140:GLN:HB2	1.73	0.70
2:z:83:TYR:CE2	2:z:91:PRO:HD2	2.26	0.70
1:f:108:PRO:HB3	1:f:135:VAL:HB	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:105:MET:HG2	5:j:124:ILE:HG12	1.74	0.70
1:3:166:GLU:HG2	1:3:244:ARG:HH21	1.57	0.70
1:9:111:PHE:HD2	1:9:114:LEU:HD22	1.57	0.70
2:B:111:ASP:HB2	5:2:147:GLN:HE22	1.56	0.70
5:G:134:GLU:HG3	5:G:159:ILE:HD12	1.74	0.69
1:f:107:LEU:O	1:f:110:PRO:HD2	1.90	0.69
1:f:165:ALA:HB1	1:f:170:GLU:HB3	1.74	0.69
1:C:61:ILE:HD11	1:C:111:PHE:HE1	1.56	0.69
1:l:14:GLN:HB2	1:l:54:ASP:HB2	1.74	0.69
1:U:255:CYS:SG	1:U:256:ASN:N	2.66	0.69
5:G:125:LEU:HD13	5:G:127:ARG:NH1	2.07	0.69
5:S:88:GLU:OE1	5:S:90:ARG:NE	2.25	0.69
2:T:79:TYR:OH	2:T:91:PRO:O	2.10	0.69
1:U:197:ILE:O	1:U:201:ASN:ND2	2.23	0.69
5:d:50:LYS:O	5:d:70:TRP:N	2.22	0.69
1:x:80:VAL:HA	1:x:92:ALA:HB1	1.75	0.69
1:9:162:LEU:HD23	1:9:172:PHE:CD2	2.27	0.69
2:B:23:SER:OG	2:B:25:ASP:OD1	2.08	0.69
1:V:14:GLN:HB2	1:V:54:ASP:HB2	1.75	0.69
5:d:108:HIS:HD2	5:d:135:TYR:HB3	1.57	0.69
2:n:35:HIS:HD2	2:n:78:THR:HG22	1.57	0.69
3:m:43:ARG:HG3	3:m:50:LEU:HD21	1.73	0.69
1:3:19:TRP:CE3	1:3:22:MET:HE2	2.28	0.69
1:f:57:GLY:O	1:f:61:ILE:HG22	1.92	0.69
4:F:99:ALA:HB1	5:G:7:VAL:HG11	1.74	0.69
1:O:19:TRP:HD1	1:O:23:ARG:NE	1.84	0.69
1:V:63:GLN:NE2	1:V:67:GLU:OE2	2.26	0.69
1:r:56:LYS:C	1:r:58:PRO:HD3	2.18	0.69
4:u:151:ARG:NH1	4:u:155:ASP:OD1	2.26	0.69
5:7:36:LYS:NZ	5:7:37:ASP:OD1	2.25	0.69
5:q:28:HIS:CD2	5:q:163:LEU:HD23	2.26	0.69
5:q:101:ASP:O	5:q:140:ASN:ND2	2.26	0.69
1:w:14:GLN:O	1:w:15:PHE:HB3	1.93	0.69
1:O:19:TRP:HE1	1:O:23:ARG:CD	2.06	0.69
1:r:188:CYS:HB2	1:r:197:ILE:HG12	1.75	0.69
5:q:21:TRP:O	5:q:25:VAL:HG22	1.93	0.69
1:I:58:PRO:CD	1:I:59:ALA:N	2.55	0.69
1:f:85:ASP:OD1	1:f:85:ASP:N	2.26	0.69
4:6:14:ASN:HA	4:6:19:ARG:NH2	2.06	0.69
1:w:84:GLN:O	1:w:154:ARG:NH2	2.25	0.69
5:b:134:GLU:HG3	5:b:159:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:6:MET:HE3	3:4:74:THR:HG23	1.74	0.68
4:k:101:MET:HE1	5:q:9:ILE:HD11	1.75	0.68
5:b:159:ILE:HG22	5:b:162:PRO:HA	1.75	0.68
1:l:178:ILE:HG22	1:l:181:ARG:NH1	2.08	0.68
1:w:58:PRO:CD	1:w:59:ALA:N	2.54	0.68
1:w:288:ASN:O	1:w:288:ASN:ND2	2.26	0.68
1:C:277:ILE:HG22	1:C:296:MET:HE3	1.74	0.68
4:6:41:GLN:NE2	4:6:117:GLN:O	2.25	0.68
2:T:73:VAL:HG12	2:T:77:PHE:HE1	1.57	0.68
4:N:14:ASN:O	4:N:19:ARG:CZ	2.41	0.68
3:X:42:GLN:HB3	3:X:77:LEU:HD11	1.74	0.68
5:G:134:GLU:CD	5:G:135:TYR:H	2.01	0.68
1:l:56:LYS:C	1:l:58:PRO:HD3	2.18	0.68
3:g:37:ARG:O	3:g:42:GLN:NE2	2.27	0.68
5:q:50:LYS:NZ	5:q:71:GLY:O	2.26	0.68
1:C:13:LEU:HD23	1:C:18:LYS:HE3	1.76	0.68
5:G:41:ARG:NH2	5:7:45:GLU:OE2	2.26	0.68
5:S:59:LEU:HB3	5:S:110:HIS:ND1	2.09	0.68
4:o:152:GLU:OE1	5:p:139:HIS:ND1	2.27	0.68
5:G:125:LEU:HD13	5:G:127:ARG:HH11	1.57	0.68
1:O:214:TYR:OH	1:O:241:GLU:OE2	2.08	0.68
2:T:25:ASP:OD1	2:T:67:SER:HB3	1.94	0.68
4:k:37:HIS:CE1	4:k:41:GLN:HE21	2.11	0.68
4:a:14:ASN:O	4:a:19:ARG:NE	2.27	0.68
1:V:287:ARG:NE	1:V:289:GLU:OE2	2.25	0.68
5:j:50:LYS:NZ	5:j:71:GLY:O	2.27	0.68
5:G:15:ARG:NH2	1:f:318:ILE:HD13	2.09	0.67
5:S:98:VAL:HG13	5:S:102:LEU:HD23	1.75	0.67
1:f:115:GLU:OE2	1:f:135:VAL:HG23	1.94	0.67
1:U:19:TRP:NE1	1:U:23:ARG:CG	2.45	0.67
1:I:138:LEU:O	1:I:142:THR:OG1	2.11	0.67
1:l:227:VAL:HG11	1:l:280:GLU:HG3	1.75	0.67
1:3:40:TRP:HD1	1:3:41:PHE:CD1	2.11	0.67
1:9:150:ASN:OD1	1:9:150:ASN:N	2.26	0.67
1:I:135:VAL:O	1:I:139:MET:HG3	1.94	0.67
1:O:89:LEU:HD22	1:O:154:ARG:HE	1.59	0.67
1:f:61:ILE:HD11	1:f:111:PHE:HE1	1.58	0.67
1:x:240:GLU:OE2	1:x:244:ARG:NH2	2.17	0.67
4:a:14:ASN:O	4:a:19:ARG:NH2	2.28	0.67
1:V:255:CYS:SG	1:V:256:ASN:N	2.67	0.67
5:d:8:MET:HA	5:d:97:GLN:HE22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:i:88:LEU:HD22	4:i:95:VAL:HG23	1.75	0.67
1:x:255:CYS:SG	1:x:256:ASN:N	2.67	0.67
1:3:57:GLY:N	1:3:58:PRO:CD	2.57	0.67
1:l:61:ILE:HD11	1:l:111:PHE:HE1	1.59	0.67
5:S:76:GLU:OE2	5:S:77:ARG:N	2.27	0.67
4:c:129:GLU:O	4:c:133:GLN:HG3	1.93	0.67
5:7:36:LYS:HG3	5:7:37:ASP:N	2.09	0.67
1:l:167:ARG:NH2	1:l:210:THR:OG1	2.27	0.67
2:T:83:TYR:HD2	2:T:90:ILE:HG22	1.60	0.67
5:p:114:CYS:HA	5:p:133:CYS:HA	1.76	0.67
3:H:79:PHE:H	3:H:86:GLU:HG3	1.60	0.67
5:M:51:ILE:HG12	5:M:69:TYR:CE1	2.30	0.66
5:j:13:VAL:CG2	5:j:18:ILE:HG13	2.24	0.66
5:q:141:LYS:HD2	5:q:142:VAL:HG13	1.77	0.66
5:G:121:ARG:HE	5:G:125:LEU:HD11	1.59	0.66
5:G:128:ILE:CG1	5:G:129:VAL:H	2.06	0.66
1:I:167:ARG:HE	1:I:244:ARG:NH1	1.94	0.66
1:O:306:GLY:O	1:O:309:PRO:HD2	1.95	0.66
4:R:46:ASN:O	4:R:49:ARG:N	2.28	0.66
4:i:131:ARG:O	4:i:135:GLU:N	2.26	0.66
4:k:11:LYS:CE	4:k:147:ARG:HH12	2.07	0.66
1:U:278:LEU:HD21	1:U:300:MET:HE2	1.77	0.66
4:R:14:ASN:CB	4:R:19:ARG:NH2	2.55	0.66
2:n:79:TYR:HE1	2:n:91:PRO:HG2	1.59	0.66
2:z:83:TYR:HE2	2:z:91:PRO:HD2	1.60	0.66
5:7:142:VAL:HG23	5:7:143:GLY:H	1.59	0.66
4:N:21:LEU:HD21	4:N:64:LEU:HD11	1.76	0.66
1:U:52:LEU:O	5:b:121:ARG:NH1	2.29	0.66
1:I:57:GLY:O	1:I:61:ILE:HG22	1.94	0.66
2:K:23:SER:OG	2:K:24:SER:N	2.28	0.66
4:u:98:LYS:HZ1	4:u:109:ILE:HD13	1.61	0.66
2:5:23:SER:OG	2:5:25:ASP:OD1	2.14	0.66
1:V:15:PHE:CE2	1:V:60:LYS:HB3	2.30	0.66
3:m:22:SER:HB2	3:m:57:LEU:HD12	1.77	0.66
1:C:61:ILE:HD11	1:C:111:PHE:CE1	2.31	0.66
1:C:167:ARG:NE	1:C:241:GLU:OE2	2.28	0.66
4:k:150:THR:OG1	4:k:152:GLU:OE1	2.13	0.66
4:a:14:ASN:O	4:a:19:ARG:CZ	2.44	0.66
4:F:14:ASN:O	4:F:19:ARG:CZ	2.43	0.66
5:j:158:GLN:O	5:j:158:GLN:NE2	2.28	0.66
3:s:22:SER:HB2	3:s:57:LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:37:ARG:NH2	3:P:41:GLU:OE1	2.26	0.66
1:l:198:TYR:OH	1:l:249:LEU:HD22	1.96	0.66
4:N:145:GLU:O	4:N:149:ARG:HG3	1.95	0.66
1:O:196:GLN:HE22	1:O:199:ARG:CZ	2.09	0.66
1:r:277:ILE:HG22	1:r:296:MET:HE2	1.77	0.66
2:B:107:ALA:C	5:2:147:GLN:HE21	2.03	0.66
4:F:32:PHE:N	4:F:32:PHE:CD1	2.64	0.65
4:R:151:ARG:NH1	4:R:155:ASP:OD1	2.29	0.65
2:n:83:TYR:CZ	2:n:91:PRO:HG3	2.32	0.65
1:x:55:ASP:HA	5:1:121:ARG:HH22	1.61	0.65
1:I:52:LEU:O	5:M:121:ARG:NH1	2.29	0.65
1:I:57:GLY:N	1:I:58:PRO:HD3	2.12	0.65
5:p:66:ILE:HG12	5:p:87:ILE:HD12	1.77	0.65
5:v:134:GLU:OE1	5:v:135:TYR:N	2.24	0.65
5:v:168:ARG:O	5:v:172:GLU:HG3	1.96	0.65
5:M:51:ILE:HG12	5:M:69:TYR:HE1	1.61	0.65
1:C:27:LEU:O	1:C:31:ARG:HD2	1.97	0.65
1:O:71:GLU:O	1:O:75:GLN:HG3	1.97	0.65
1:l:58:PRO:CD	1:l:59:ALA:N	2.56	0.65
1:9:58:PRO:CD	1:9:59:ALA:H	2.06	0.65
1:w:85:ASP:OD1	1:w:85:ASP:N	2.30	0.65
4:a:9:ARG:NH1	4:L:90:ARG:HG3	2.12	0.65
4:F:32:PHE:N	4:F:32:PHE:HD1	1.94	0.65
1:I:77:GLN:HG3	1:I:81:LEU:HD13	1.78	0.65
1:O:56:LYS:C	1:O:58:PRO:HD3	2.21	0.65
4:u:85:TYR:CE2	4:u:98:LYS:HD3	2.31	0.65
2:z:72:LYS:HZ1	2:z:95:ILE:HG12	1.62	0.65
1:w:53:TRP:CZ3	5:2:125:LEU:HD22	2.32	0.65
1:O:57:GLY:N	1:O:58:PRO:HD3	2.12	0.65
4:i:136:ASP:CG	4:i:137:ALA:N	2.54	0.65
3:s:42:GLN:HB3	3:s:77:LEU:HD11	1.77	0.65
1:3:58:PRO:CD	1:3:59:ALA:N	2.58	0.65
5:q:143:GLY:HA2	5:q:148:LEU:HG	1.79	0.65
2:Y:79:TYR:CE2	2:Y:93:PHE:HB2	2.32	0.65
5:d:108:HIS:HE1	5:d:114:CYS:HB2	1.62	0.65
2:t:76:TYR:CD2	5:v:146:LEU:HG	2.31	0.65
4:i:78:ARG:NH2	4:i:84:GLU:OE1	2.30	0.65
1:r:274:LYS:HG3	1:r:278:LEU:HD12	1.78	0.65
1:x:93:TYR:OH	1:x:143:TRP:NE1	2.26	0.65
1:3:138:LEU:O	1:3:142:THR:OG1	2.07	0.65
1:w:255:CYS:SG	1:w:256:ASN:N	2.67	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:42:ILE:HD11	2:Y:62:PHE:HZ	1.61	0.64
5:d:78:ASP:HB3	5:d:80:HIS:CE1	2.31	0.64
3:g:23:THR:HG22	3:g:56:THR:HG22	1.79	0.64
4:i:118:ARG:HH11	4:i:120:ASP:HB2	1.62	0.64
1:l:188:CYS:O	1:l:194:LYS:NZ	2.28	0.64
1:l:231:MET:SD	1:l:296:MET:HG3	2.37	0.64
1:C:98:ARG:O	1:C:102:THR:OG1	2.08	0.64
1:I:32:GLN:NE2	1:I:103:GLN:OE1	2.27	0.64
2:K:74:CYS:HA	2:K:77:PHE:CD1	2.30	0.64
2:T:31:VAL:HG12	3:e:15:PHE:HB2	1.79	0.64
2:K:67:SER:OG	3:J:94:SER:N	2.26	0.64
4:R:14:ASN:C	4:R:19:ARG:HE	2.05	0.64
1:r:178:ILE:O	1:r:182:GLU:HG3	1.97	0.64
2:z:77:PHE:O	2:z:81:VAL:HG23	1.97	0.64
2:T:62:PHE:CG	2:T:65:ILE:HD11	2.32	0.64
1:U:245:ALA:HB2	1:U:261:LEU:HD12	1.80	0.64
1:f:56:LYS:C	1:f:58:PRO:CD	2.71	0.64
1:f:93:TYR:HE1	1:f:143:TRP:HZ2	1.43	0.64
4:6:155:ASP:HB2	5:7:116:SER:HB3	1.79	0.64
5:7:134:GLU:CD	5:7:135:TYR:H	2.05	0.64
4:N:151:ARG:NH1	4:N:155:ASP:OD1	2.30	0.64
1:C:19:TRP:HE3	1:C:22:MET:HE2	1.63	0.64
5:S:33:ARG:O	5:S:36:LYS:HG2	1.97	0.64
1:V:196:GLN:HG3	1:V:197:ILE:N	2.11	0.64
3:W:50:LEU:HD12	3:W:51:LEU:N	2.13	0.64
1:3:52:LEU:O	5:7:121:ARG:NH1	2.30	0.64
2:E:79:TYR:CE2	2:E:93:PHE:HB2	2.33	0.64
3:W:52:ASP:OD1	3:W:55:LYS:HE2	1.97	0.64
2:5:63:ARG:NE	2:5:63:ARG:HA	2.11	0.64
4:6:73:TRP:N	4:6:73:TRP:CD1	2.64	0.64
1:C:104:CYS:SG	1:C:139:MET:HE2	2.38	0.64
4:F:49:ARG:CZ	4:F:49:ARG:HB2	2.28	0.64
3:m:50:LEU:HD22	3:m:51:LEU:H	1.63	0.64
5:b:112:PHE:CD2	5:b:163:LEU:HD13	2.33	0.64
3:P:42:GLN:CD	3:P:77:LEU:HG	2.23	0.64
2:Z:21:LEU:CD1	2:Z:29:PHE:HB2	2.27	0.64
5:d:17:ARG:HG3	5:d:17:ARG:NH1	2.12	0.64
4:k:12:PHE:CD2	4:k:127:PHE:HB2	2.33	0.64
1:w:15:PHE:CE2	1:w:60:LYS:HB3	2.32	0.64
3:X:37:ARG:NH2	3:X:41:GLU:OE1	2.30	0.64
1:f:152:LYS:HA	1:f:155:LEU:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:28:HIS:HA	5:7:32:SER:HB3	1.80	0.64
5:7:108:HIS:CD2	5:7:138:GLY:HA3	2.33	0.64
1:9:85:ASP:HB2	1:9:88:ALA:HB3	1.80	0.64
1:C:151:ILE:HG13	1:C:155:LEU:HD22	1.79	0.64
2:E:79:TYR:OH	2:E:91:PRO:O	2.13	0.64
4:c:5:VAL:HG13	4:c:6:PRO:HD3	1.78	0.63
1:f:167:ARG:HH22	1:f:206:TYR:HE1	1.43	0.63
4:o:103:LEU:HD11	5:p:9:ILE:HD13	1.80	0.63
1:r:69:ILE:HD12	1:r:138:LEU:HD23	1.79	0.63
1:U:44:PHE:CE1	1:U:110:PRO:HA	2.33	0.63
1:I:192:GLU:OE2	1:w:192:GLU:HB3	1.97	0.63
2:Y:77:PHE:O	2:Y:81:VAL:HG23	1.98	0.63
1:O:69:ILE:HD13	1:O:139:MET:HG2	1.81	0.63
1:f:19:TRP:CE2	1:f:23:ARG:CG	2.68	0.63
3:4:58:GLY:HA2	3:4:62:PHE:O	1.97	0.63
5:7:41:ARG:HB3	5:7:45:GLU:HG3	1.80	0.63
4:R:104:ASN:HB3	4:R:147:ARG:HH21	1.62	0.63
5:S:59:LEU:HB3	5:S:110:HIS:CE1	2.33	0.63
1:f:152:LYS:HA	1:f:155:LEU:HD11	1.80	0.63
1:l:75:GLN:O	1:l:79:ARG:HG3	1.99	0.63
4:u:98:LYS:NZ	4:u:109:ILE:HD13	2.14	0.63
1:x:107:LEU:O	1:x:110:PRO:HD2	1.97	0.63
2:5:86:SER:OG	2:5:89:GLU:HG2	1.99	0.63
4:L:94:LYS:HG2	4:L:115:ASP:HA	1.81	0.63
1:O:58:PRO:CD	1:O:59:ALA:N	2.58	0.63
4:i:151:ARG:HH21	5:j:113:ASP:HA	1.63	0.63
5:q:21:TRP:CD1	5:q:169:LEU:HD22	2.34	0.63
1:w:287:ARG:NH2	1:w:289:GLU:OE2	2.23	0.63
1:I:206:TYR:O	1:I:210:THR:OG1	2.16	0.63
1:f:17:ASP:OD1	1:f:17:ASP:N	2.22	0.63
2:h:76:TYR:HA	2:h:93:PHE:CE2	2.34	0.63
4:u:66:LEU:HD21	4:u:101:MET:HE1	1.80	0.63
1:w:58:PRO:O	1:w:61:ILE:HG22	1.99	0.63
1:U:76:ALA:O	1:U:80:VAL:HG23	1.98	0.63
4:a:85:TYR:CE2	4:a:98:LYS:HD3	2.33	0.63
5:b:108:HIS:CD2	5:b:138:GLY:HA3	2.33	0.63
5:b:112:PHE:CE2	5:b:163:LEU:HD22	2.27	0.63
4:R:32:PHE:CE2	4:R:43:ARG:HD2	2.29	0.63
4:R:85:TYR:CE2	4:R:98:LYS:HB3	2.34	0.63
5:S:66:ILE:HG12	5:S:87:ILE:HG23	1.78	0.63
2:n:77:PHE:O	2:n:81:VAL:HG23	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:p:15:ARG:HB3	5:p:83:GLN:NE2	2.12	0.63
4:0:8:GLN:NE2	4:0:140:GLN:OE1	2.27	0.63
1:3:193:ASP:OD1	1:3:196:GLN:N	2.32	0.63
4:i:151:ARG:HE	5:j:114:CYS:HB2	1.63	0.63
5:j:128:ILE:HD12	5:j:129:VAL:H	1.64	0.63
4:u:28:LYS:HG3	4:u:60:THR:HG22	1.79	0.63
2:z:72:LYS:NZ	2:z:95:ILE:HG12	2.13	0.63
4:0:32:PHE:N	4:0:32:PHE:CD1	2.67	0.63
5:1:38:TRP:CE2	5:1:57:ILE:HG12	2.34	0.63
1:9:281:CYS:O	1:9:284:MET:HG2	1.99	0.63
2:h:20:LYS:HD3	2:h:59:GLU:OE2	1.99	0.62
3:m:24:VAL:HG13	3:m:44:LEU:HD12	1.81	0.62
2:5:88:THR:H	4:6:16:GLU:CD	2.07	0.62
1:U:315:GLU:O	1:U:318:ILE:HG22	1.99	0.62
1:V:15:PHE:CD1	1:V:15:PHE:C	2.77	0.62
1:C:231:MET:HB3	1:C:295:LEU:HD23	1.81	0.62
2:E:41:THR:HG21	2:E:109:PHE:HE1	1.64	0.62
2:t:108:ASN:HA	5:v:147:GLN:NE2	2.14	0.62
5:2:113:ASP:O	5:2:133:CYS:HA	1.99	0.62
4:R:129:GLU:O	4:R:133:GLN:HG3	1.98	0.62
2:Z:85:ASN:OD1	2:Z:85:ASN:N	2.20	0.62
1:r:98:ARG:O	1:r:102:THR:OG1	2.16	0.62
5:1:71:GLY:HA2	5:1:81:LEU:HB2	1.81	0.62
1:3:37:LYS:NZ	2:5:58:ASN:HB3	2.14	0.62
1:V:44:PHE:HE1	1:V:112:CYS:HG	1.46	0.62
5:7:25:VAL:O	5:7:29:MET:HG3	1.99	0.62
3:H:7:ILE:HA	3:H:75:VAL:HB	1.80	0.62
1:V:19:TRP:CD1	1:V:22:MET:HB2	2.34	0.62
2:t:22:ILE:HD11	2:t:28:GLU:HG2	1.80	0.62
1:3:92:ALA:O	1:3:95:VAL:HG23	1.99	0.62
4:6:141:GLN:NE2	4:6:145:GLU:OE2	2.32	0.62
2:B:89:GLU:O	2:B:90:ILE:HG13	1.98	0.62
5:G:134:GLU:OE1	5:G:135:TYR:N	2.30	0.62
4:0:107:CYS:SG	4:0:131:ARG:HB3	2.39	0.62
5:1:43:HIS:ND1	1:3:308:GLU:OE1	2.32	0.62
1:V:135:VAL:O	1:V:138:LEU:HB3	1.99	0.62
2:Z:66:PRO:HD2	2:Z:69:VAL:HG21	1.80	0.62
5:v:61:ASP:OD1	5:v:61:ASP:N	2.32	0.62
2:T:20:LYS:HD3	2:T:28:GLU:CD	2.25	0.62
1:w:54:ASP:HB3	1:w:57:GLY:HA3	1.81	0.62
1:3:19:TRP:HD1	1:3:23:ARG:NH2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:85:ASP:N	1:U:85:ASP:OD1	2.33	0.62
4:a:33:ARG:HA	4:a:40:ARG:HH11	1.63	0.62
2:K:73:VAL:HG12	2:K:77:PHE:HE1	1.65	0.62
3:m:39:PRO:HA	3:m:42:GLN:HG3	1.82	0.62
2:B:104:LEU:HD12	5:2:154:LEU:HD12	1.81	0.62
5:b:134:GLU:CD	5:b:135:TYR:H	2.05	0.61
3:D:52:ASP:OD1	3:D:52:ASP:N	2.32	0.61
1:I:284:MET:HE2	1:I:293:LEU:HG	1.81	0.61
3:W:28:LYS:HG2	3:W:42:GLN:OE1	1.98	0.61
5:v:120:ILE:HD11	5:v:147:GLN:HB3	1.82	0.61
3:P:44:LEU:O	3:P:50:LEU:HD12	2.00	0.61
5:d:77:ARG:HH11	5:d:77:ARG:HB2	1.66	0.61
1:f:58:PRO:CD	1:f:59:ALA:N	2.58	0.61
1:3:19:TRP:CD1	1:3:23:ARG:NH2	2.68	0.61
1:9:149:SER:HA	1:9:152:LYS:HD3	1.82	0.61
3:W:8:ARG:NH2	3:W:91:GLU:O	2.32	0.61
2:t:77:PHE:O	2:t:81:VAL:HG23	2.00	0.61
4:0:32:PHE:N	4:0:32:PHE:HD1	1.98	0.61
5:1:38:TRP:CD2	5:1:57:ILE:HG12	2.34	0.61
5:b:21:TRP:O	5:b:25:VAL:HG22	2.01	0.61
1:C:36:THR:OG1	1:C:39:GLN:HG3	2.00	0.61
1:V:238:LEU:HG	1:V:269:LEU:HD12	1.81	0.61
1:f:61:ILE:HD11	1:f:111:PHE:CE1	2.34	0.61
1:l:32:GLN:HE21	1:l:103:GLN:NE2	1.98	0.61
1:9:91:LYS:O	1:9:95:VAL:HG23	1.99	0.61
5:d:15:ARG:HD2	5:d:83:GLN:NE2	2.15	0.61
4:u:152:GLU:HG2	5:v:148:TYR:CE1	2.35	0.61
4:0:109:ILE:HG13	4:0:128:ASP:HB2	1.82	0.61
4:k:54:GLU:OE1	4:k:54:GLU:N	2.33	0.61
1:l:245:ALA:O	1:l:249:LEU:N	2.33	0.61
3:y:8:ARG:HD3	3:y:74:THR:HG22	1.81	0.61
5:G:36:LYS:NZ	5:G:37:ASP:OD1	2.24	0.61
1:I:77:GLN:HB2	1:I:147:ILE:HG12	1.82	0.61
2:z:86:SER:OG	4:0:16:GLU:OE2	2.18	0.61
1:C:56:LYS:C	1:C:58:PRO:HD3	2.25	0.61
1:C:311:LEU:HD13	5:j:70:TRP:CD2	2.36	0.61
1:I:287:ARG:NH2	1:I:289:GLU:OE2	2.29	0.61
3:P:52:ASP:HB2	3:P:55:LYS:HB2	1.82	0.61
3:W:77:LEU:C	3:W:88:LEU:HD23	2.26	0.61
1:l:181:ARG:HE	1:l:249:LEU:C	2.09	0.61
3:4:52:ASP:OD1	3:4:52:ASP:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:MET:HG3	2:B:18:TYR:CD1	2.35	0.61
4:N:5:VAL:HG13	4:N:6:PRO:HD3	1.83	0.61
1:I:198:TYR:C	1:I:198:TYR:CD1	2.79	0.61
1:r:57:GLY:N	1:r:58:PRO:HD3	2.16	0.61
1:r:84:GLN:O	1:r:154:ARG:NH2	2.33	0.61
1:r:162:LEU:HD23	1:r:172:PHE:CD2	2.36	0.61
4:c:88:LEU:H	4:c:88:LEU:HD23	1.65	0.61
5:v:69:TYR:O	5:v:83:GLN:HB3	2.01	0.61
1:3:31:ARG:NH2	1:3:75:GLN:OE1	2.33	0.61
1:3:107:LEU:O	1:3:110:PRO:HD2	2.00	0.61
5:q:112:PHE:CE1	5:q:163:LEU:HD22	2.36	0.61
1:w:193:ASP:OD2	1:w:199:ARG:NH1	2.34	0.61
5:b:38:TRP:CD2	5:b:57:ILE:HG12	2.35	0.60
1:C:242:GLU:HG3	1:C:262:MET:SD	2.41	0.60
5:M:50:LYS:HD2	5:M:72:LEU:HD23	1.83	0.60
5:b:134:GLU:OE2	5:b:158:GLN:N	2.33	0.60
5:S:20:THR:O	5:S:24:LEU:HD12	2.01	0.60
2:n:22:ILE:HG13	2:n:28:GLU:HG2	1.83	0.60
1:U:52:LEU:HD23	1:U:53:TRP:NE1	2.16	0.60
5:b:17:ARG:NH1	5:b:168:LYS:HE2	2.16	0.60
1:I:245:ALA:O	1:I:249:LEU:HB2	2.01	0.60
5:b:15:ARG:NH1	5:b:19:ASN:HD21	1.99	0.60
2:E:106:ALA:O	2:E:110:LEU:HG	2.01	0.60
1:O:138:LEU:O	1:O:142:THR:OG1	2.19	0.60
4:c:136:ASP:OD1	4:c:137:ALA:N	2.34	0.60
1:x:90:LEU:HD23	1:x:91:LYS:H	1.65	0.60
1:9:230:TYR:OH	1:9:269:LEU:O	2.15	0.60
2:B:22:ILE:HD13	2:B:28:GLU:HG2	1.82	0.60
5:2:114:CYS:SG	5:2:133:CYS:HB2	2.42	0.60
5:S:134:GLU:CD	5:S:135:TYR:H	2.09	0.60
1:r:133:SER:OG	1:r:134:ILE:N	2.33	0.60
1:3:98:ARG:NH1	1:3:175:GLN:OE1	2.33	0.60
1:9:19:TRP:CZ2	1:9:23:ARG:HG2	2.36	0.60
3:e:3:VAL:HG12	3:e:64:SER:HA	1.83	0.60
3:H:28:LYS:HB3	3:H:39:PRO:HB3	1.84	0.60
5:S:24:LEU:HD23	5:S:163:PRO:O	2.02	0.60
4:i:109:ILE:HG13	4:i:128:ASP:HB2	1.82	0.60
5:j:28:HIS:CD2	5:j:163:LEU:HA	2.37	0.60
1:r:58:PRO:CD	1:r:59:ALA:N	2.60	0.60
1:x:44:PHE:CE2	1:x:110:PRO:HA	2.37	0.60
4:0:130:GLU:O	4:0:134:GLN:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:37:LYS:HZ3	2:5:58:ASN:HB3	1.65	0.60
1:3:141:ASP:O	1:3:145:GLU:HG3	2.02	0.60
3:4:37:ARG:O	3:4:42:GLN:NE2	2.34	0.60
5:G:114:CYS:SG	5:G:133:CYS:HB2	2.41	0.60
1:O:19:TRP:HE3	1:O:22:MET:HE2	1.65	0.60
4:R:14:ASN:HA	4:R:19:ARG:NE	2.17	0.60
2:n:96:ALA:O	2:n:99:ILE:HG13	2.01	0.60
4:o:151:ARG:HG3	5:p:108:HIS:O	2.01	0.60
1:r:19:TRP:CZ2	1:r:23:ARG:HG2	2.37	0.60
4:F:8:GLN:NE2	4:F:106:VAL:HA	2.17	0.60
4:F:151:ARG:NH2	5:G:112:PHE:O	2.27	0.60
2:Q:31:VAL:HG12	3:P:15:PHE:HB2	1.83	0.60
1:f:137:LYS:HE2	1:f:141:ASP:OD2	2.02	0.60
1:f:255:CYS:SG	1:f:256:ASN:N	2.75	0.60
3:m:44:LEU:HB3	3:m:51:LEU:HD12	1.82	0.60
5:b:119:ALA:O	5:b:123:THR:OG1	2.19	0.60
4:F:3:ARG:NH1	4:i:89:GLU:O	2.35	0.60
1:O:15:PHE:H	1:O:50:VAL:HG22	1.67	0.60
1:O:93:TYR:HD1	1:O:93:TYR:C	2.10	0.60
1:V:58:PRO:O	1:V:61:ILE:HG22	2.02	0.60
1:f:203:GLU:OE1	1:f:257:SER:OG	2.14	0.60
5:p:24:LEU:HD23	5:p:162:PRO:O	2.00	0.60
5:p:122:ASN:OD1	5:p:127:ARG:NH1	2.35	0.60
2:5:105:MET:HE2	5:7:124:ILE:HG23	1.84	0.60
1:C:284:MET:HE2	1:C:293:LEU:HG	1.84	0.60
1:O:223:GLN:OE1	1:O:223:GLN:HA	2.02	0.60
4:R:59:ALA:HB3	4:R:62:THR:HB	1.84	0.60
2:h:47:SER:OG	2:h:48:GLY:N	2.34	0.60
5:7:38:TRP:CD2	5:7:57:ILE:HG12	2.36	0.60
1:9:179:GLY:O	1:9:183:SER:OG	2.18	0.60
1:w:19:TRP:CD1	1:w:23:ARG:CZ	2.84	0.60
5:j:37:ASP:HB2	5:j:111:TYR:HE2	1.66	0.59
2:t:79:TYR:HE1	2:t:91:PRO:HG2	1.67	0.59
3:s:57:LEU:O	3:s:62:PHE:HB2	2.02	0.59
2:5:88:THR:OG1	4:6:16:GLU:OE2	2.18	0.59
1:9:240:GLU:OE2	1:9:244:ARG:NH1	2.35	0.59
1:U:19:TRP:CZ2	1:U:23:ARG:HG2	2.36	0.59
1:I:100:PHE:CD2	1:I:143:TRP:CE3	2.91	0.59
2:n:96:ALA:N	2:n:99:ILE:HD11	2.16	0.59
5:7:103:ALA:O	5:7:107:ILE:HG13	2.01	0.59
1:O:19:TRP:NE1	1:O:23:ARG:HG3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:108:HIS:CD2	5:d:135:TYR:HB3	2.36	0.59
5:v:134:GLU:HG2	5:v:160:ILE:HD12	1.84	0.59
4:k:21:LEU:HB3	4:k:125:LEU:CD1	2.32	0.59
1:w:19:TRP:HD1	1:w:23:ARG:NH2	2.01	0.59
2:Y:62:PHE:CG	2:Y:65:ILE:HD11	2.37	0.59
5:b:41:ARG:NE	5:b:54:GLU:OE1	2.36	0.59
1:C:90:LEU:HD21	1:C:176:LEU:HB3	1.84	0.59
3:J:57:LEU:O	3:J:62:PHE:HB2	2.03	0.59
4:L:149:ARG:HG3	5:M:109:LEU:HD11	1.82	0.59
4:R:149:ARG:O	5:S:105:GLN:NE2	2.36	0.59
5:d:22:LYS:HD3	5:d:40:TYR:OH	2.03	0.59
4:k:141:GLN:HG2	4:k:145:GLU:OE2	2.02	0.59
1:w:18:LYS:O	1:w:22:MET:HG3	2.03	0.59
1:w:148:PHE:CD2	1:w:187:LEU:HD12	2.37	0.59
2:B:105:MET:HE3	5:2:124:ILE:HG23	1.84	0.59
5:2:38:TRP:CD2	5:2:57:ILE:HG12	2.37	0.59
1:C:230:TYR:OH	1:C:269:LEU:O	2.21	0.59
2:E:86:SER:HB2	4:F:16:GLU:HB2	1.85	0.59
4:R:83:ARG:O	4:R:98:LYS:NZ	2.21	0.59
1:f:65:LEU:O	1:f:69:ILE:HG13	2.01	0.59
3:s:67:ALA:HB2	3:s:73:ALA:HB2	1.85	0.59
1:x:85:ASP:OD1	1:x:85:ASP:N	2.28	0.59
1:x:246:LEU:HD23	1:x:258:VAL:HG11	1.85	0.59
1:3:41:PHE:HE2	2:5:60:VAL:HA	1.66	0.59
4:6:9:ARG:O	4:6:12:PHE:HB3	2.03	0.59
4:6:11:LYS:HD3	4:6:147:ARG:NH1	2.16	0.59
2:B:76:TYR:CD1	5:2:146:LEU:HG	2.37	0.59
1:O:103:GLN:OE1	1:O:103:GLN:HA	2.02	0.59
2:Z:33:ARG:O	2:Z:37:LEU:HG	2.02	0.59
5:d:15:ARG:HD2	5:d:83:GLN:HE22	1.67	0.59
1:f:315:GLU:HA	1:f:318:ILE:HG22	1.83	0.59
5:j:21:TRP:O	5:j:25:VAL:HG22	2.03	0.59
2:t:19:VAL:HG12	2:t:58:ASN:HB2	1.84	0.59
4:0:94:LYS:HG2	4:0:115:ASP:HA	1.85	0.59
1:3:19:TRP:CD1	1:3:23:ARG:CD	2.81	0.59
4:a:151:ARG:NH2	5:b:112:PHE:O	2.29	0.59
1:C:154:ARG:HG2	1:C:154:ARG:NH1	2.13	0.59
4:F:41:GLN:NE2	4:F:117:GLN:O	2.36	0.59
4:F:156:ARG:HB3	5:G:117:GLU:OE1	2.02	0.59
5:G:129:VAL:HG22	5:G:130:SER:H	1.68	0.59
1:V:93:TYR:CD1	1:V:93:TYR:C	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:306:GLY:O	1:V:309:PRO:HD2	2.02	0.59
5:j:28:HIS:HD2	5:j:164:PRO:HD3	1.68	0.59
2:t:83:TYR:CE2	2:t:91:PRO:HG3	2.37	0.59
1:x:231:MET:HG2	1:x:277:ILE:HD13	1.85	0.59
4:6:14:ASN:C	4:6:19:ARG:NE	2.61	0.59
1:U:136:ARG:O	1:U:140:LEU:HD12	2.03	0.59
1:I:41:PHE:O	1:I:44:PHE:HB2	2.03	0.59
5:M:112:PHE:CE1	5:M:163:LEU:HD22	2.38	0.59
1:O:166:GLU:OE2	1:O:248:TYR:OH	2.14	0.59
3:s:63:THR:HG1	3:s:66:THR:H	1.49	0.59
1:3:19:TRP:CE2	1:3:23:ARG:CG	2.85	0.59
5:G:65:VAL:HG21	5:G:90:ARG:NH2	2.18	0.59
1:O:19:TRP:CE2	1:O:23:ARG:CG	2.86	0.59
1:O:255:CYS:SG	1:O:256:ASN:N	2.75	0.59
4:i:74:GLN:NE2	4:i:74:GLN:O	2.36	0.59
5:1:114:CYS:HA	5:1:133:CYS:HA	1.85	0.59
1:w:15:PHE:HB2	1:w:50:VAL:HG13	1.84	0.59
3:H:52:ASP:OD1	3:H:52:ASP:N	2.30	0.59
1:V:297:PHE:HE2	1:V:311:LEU:HD21	1.68	0.58
1:f:19:TRP:NE1	1:f:23:ARG:HG3	2.08	0.58
1:f:184:TYR:CD2	1:f:202:PHE:HB2	2.38	0.58
3:g:52:ASP:OD1	3:g:52:ASP:N	2.32	0.58
1:l:296:MET:HE3	1:l:310:MET:SD	2.42	0.58
5:p:59:LEU:HD11	5:p:64:LEU:HB2	1.85	0.58
1:x:18:LYS:NZ	1:x:46:ASP:OD2	2.21	0.58
3:y:52:ASP:OD1	3:y:52:ASP:N	2.35	0.58
1:3:89:LEU:HD22	1:3:154:ARG:HH21	1.68	0.58
1:C:56:LYS:O	1:C:58:PRO:CD	2.51	0.58
1:C:206:TYR:O	1:C:210:THR:OG1	2.21	0.58
3:D:57:LEU:O	3:D:62:PHE:HB2	2.03	0.58
5:M:98:VAL:HG13	5:M:102:LEU:HB3	1.84	0.58
1:O:250:GLU:OE2	1:O:252:ARG:N	2.35	0.58
1:V:19:TRP:HE3	1:V:23:ARG:CZ	2.12	0.58
1:V:138:LEU:O	1:V:142:THR:OG1	2.20	0.58
3:W:43:ARG:HB2	3:W:85:PHE:CZ	2.38	0.58
3:4:42:GLN:HB3	3:4:77:LEU:HD11	1.84	0.58
1:9:262:MET:O	1:9:266:VAL:HG23	2.02	0.58
4:k:11:LYS:NZ	4:k:147:ARG:HH22	2.01	0.58
2:B:87:SER:O	2:B:87:SER:OG	2.20	0.58
5:2:53:SER:OG	5:2:68:THR:OG1	2.21	0.58
3:D:43:ARG:HG3	3:D:50:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:156:ARG:HA	5:G:117:GLU:HG2	1.85	0.58
1:V:317:HIS:C	1:V:317:HIS:CD2	2.81	0.58
3:W:7:ILE:HB	3:W:14:ILE:HB	1.84	0.58
1:f:19:TRP:O	1:f:23:ARG:HG3	2.02	0.58
1:9:58:PRO:CD	1:9:59:ALA:N	2.63	0.58
1:9:174:SER:HA	1:9:248:TYR:OH	2.03	0.58
1:O:278:LEU:HG	1:O:300:MET:HE2	1.86	0.58
5:S:66:ILE:HD13	5:S:167:VAL:HG13	1.84	0.58
1:V:57:GLY:N	1:V:58:PRO:HD3	2.18	0.58
1:V:213:PHE:HD1	1:V:214:TYR:CD1	2.21	0.58
5:d:101:ASP:O	5:d:140:ASN:ND2	2.36	0.58
1:f:312:LYS:O	1:f:312:LYS:HD2	2.04	0.58
1:r:193:ASP:OD1	1:r:196:GLN:N	2.36	0.58
4:0:72:SER:HB2	4:0:73:TRP:HD1	1.68	0.58
1:C:91:LYS:O	1:C:95:VAL:HG23	2.04	0.58
2:K:42:ILE:O	2:K:46:LEU:HD22	2.02	0.58
1:l:162:LEU:HD23	1:l:172:PHE:CD2	2.38	0.58
1:x:45:SER:HA	2:z:109:PHE:CE2	2.39	0.58
4:k:136:ASP:OD2	4:k:138:LEU:HD12	2.04	0.58
5:2:3:ASN:HD22	5:2:3:ASN:N	2.01	0.58
4:a:12:PHE:CD2	4:a:127:PHE:HB2	2.37	0.58
1:I:231:MET:HG2	1:I:277:ILE:HD11	1.85	0.58
1:O:90:LEU:O	1:O:94:ILE:HG12	2.04	0.58
4:R:14:ASN:CA	4:R:19:ARG:HE	2.15	0.58
4:c:26:GLU:HG3	4:c:122:MET:HE2	1.84	0.58
1:l:41:PHE:HD1	2:n:45:MET:HE2	1.68	0.58
1:r:241:GLU:OE2	1:r:244:ARG:NH1	2.36	0.58
1:3:57:GLY:O	1:3:61:ILE:HG22	2.03	0.58
1:U:178:ILE:O	1:U:182:GLU:HG3	2.04	0.58
3:J:32:GLU:HB2	3:J:38:PRO:HA	1.86	0.58
1:V:19:TRP:CH2	1:V:64:ALA:HB1	2.39	0.58
1:V:63:GLN:O	1:V:66:LYS:N	2.37	0.58
4:c:111:LYS:HG3	4:c:126:GLU:OE2	2.03	0.58
5:j:98:VAL:HG13	5:j:102:LEU:HB3	1.85	0.58
5:j:117:GLU:N	5:j:117:GLU:OE1	2.36	0.58
2:B:88:THR:HG22	4:N:16:GLU:OE2	2.03	0.58
1:O:93:TYR:C	1:O:93:TYR:CD1	2.82	0.58
5:p:72:LEU:O	5:p:81:LEU:HB3	2.04	0.58
1:3:27:LEU:O	1:3:31:ARG:HD2	2.03	0.58
2:B:41:THR:O	2:B:45:MET:HG3	2.04	0.58
2:B:68:HIS:NE2	2:B:102:GLU:OE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:136:ASP:OD1	4:F:139:ALA:N	2.37	0.58
2:h:76:TYR:HA	2:h:93:PHE:HE2	1.68	0.58
4:i:80:THR:HG22	4:i:81:PRO:HD3	1.86	0.58
2:n:41:THR:O	2:n:45:MET:HG3	2.04	0.58
1:r:252:ARG:HH11	1:r:252:ARG:HG3	1.68	0.58
5:2:128:ILE:HG12	5:2:129:VAL:H	1.68	0.58
1:U:188:CYS:SG	1:U:197:ILE:HG23	2.44	0.58
3:X:23:THR:HA	3:X:56:THR:HA	1.86	0.58
5:b:3:ASN:HD22	5:b:3:ASN:N	1.99	0.58
1:I:56:LYS:C	1:I:58:PRO:HD3	2.29	0.58
1:I:76:ALA:O	1:I:80:VAL:HG22	2.04	0.58
1:I:255:CYS:SG	1:I:256:ASN:N	2.77	0.58
3:P:63:THR:OG1	3:P:66:THR:HG23	2.04	0.58
3:W:43:ARG:NH2	3:W:53:ASP:OD1	2.36	0.58
5:j:157:LYS:O	5:j:158:GLN:HG3	2.02	0.58
1:l:166:GLU:HA	1:l:170:GLU:O	2.04	0.58
1:3:222:LEU:O	1:3:222:LEU:HD23	2.03	0.58
1:9:241:GLU:O	1:9:245:ALA:N	2.37	0.58
1:w:36:THR:N	1:w:39:GLN:OE1	2.37	0.58
1:O:162:LEU:HD21	1:O:172:PHE:CG	2.38	0.57
4:R:151:ARG:HG3	5:S:108:HIS:O	2.04	0.57
5:j:103:ALA:O	5:j:107:ILE:HG13	2.04	0.57
4:6:14:ASN:CA	4:6:19:ARG:NH2	2.63	0.57
4:6:31:GLY:N	4:6:40:ARG:HH22	2.01	0.57
4:u:15:GLU:O	4:u:19:ARG:HG3	2.03	0.57
2:z:35:HIS:HD2	2:z:78:THR:HG22	1.69	0.57
1:w:19:TRP:HD1	1:w:23:ARG:CZ	2.15	0.57
1:w:55:ASP:OD1	1:w:55:ASP:N	2.37	0.57
5:b:108:HIS:HD2	5:b:138:GLY:HA3	1.68	0.57
1:C:178:ILE:O	1:C:182:GLU:HG3	2.03	0.57
1:C:266:VAL:HG21	1:C:302:LYS:HG2	1.86	0.57
1:I:86:ASP:OD1	1:I:154:ARG:NH1	2.33	0.57
4:L:130:GLU:O	4:L:134:GLN:HG3	2.04	0.57
3:P:37:ARG:HD3	3:P:79:PHE:CZ	2.40	0.57
1:V:107:LEU:O	1:V:110:PRO:HD2	2.04	0.57
1:V:266:VAL:HG11	1:V:302:LYS:HB3	1.86	0.57
1:r:255:CYS:SG	1:r:256:ASN:N	2.78	0.57
1:3:288:ASN:ND2	1:3:288:ASN:O	2.37	0.57
4:6:32:PHE:N	4:6:32:PHE:CD1	2.69	0.57
4:k:99:ALA:HB1	5:q:7:VAL:HG11	1.86	0.57
1:w:319:ILE:H	1:w:319:ILE:HD12	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:SER:OG	2:B:24:SER:N	2.36	0.57
5:2:158:LYS:O	5:2:159:GLN:HG3	2.04	0.57
4:a:67:GLN:NE2	5:b:72:LEU:HG	2.19	0.57
3:J:52:ASP:OD1	3:J:52:ASP:N	2.37	0.57
1:O:278:LEU:HA	1:O:296:MET:HE1	1.85	0.57
4:R:21:LEU:HB3	4:R:125:LEU:HD12	1.87	0.57
3:4:8:ARG:HE	3:4:13:THR:HB	1.69	0.57
4:6:14:ASN:CB	4:6:19:ARG:HH21	2.17	0.57
5:7:53:SER:HG	5:7:68:THR:HG1	1.49	0.57
4:N:31:GLY:H	4:N:40:ARG:NH2	2.01	0.57
3:s:50:LEU:HD22	3:s:51:LEU:H	1.68	0.57
1:x:30:LEU:HD21	1:x:69:ILE:HA	1.86	0.57
1:w:94:ILE:HG13	1:w:176:LEU:HA	1.86	0.57
2:B:17:MET:HE3	2:B:18:TYR:HE1	1.69	0.57
4:i:22:SER:O	4:i:22:SER:OG	2.22	0.57
5:j:32:SER:OG	5:j:34:LYS:HG2	2.04	0.57
5:j:42:HIS:O	5:j:45:GLU:HG3	2.05	0.57
2:z:86:SER:OG	2:z:88:THR:HG22	2.04	0.57
4:6:49:ARG:HG2	4:6:49:ARG:NH1	2.17	0.57
4:k:9:ARG:O	4:k:13:GLU:HG2	2.04	0.57
1:w:90:LEU:HD21	1:w:176:LEU:HB3	1.85	0.57
1:C:58:PRO:CD	1:C:59:ALA:N	2.53	0.57
1:V:19:TRP:CE3	1:V:23:ARG:NH2	2.70	0.57
3:m:42:GLN:HB3	3:m:77:LEU:HD11	1.85	0.57
2:t:22:ILE:CD1	2:t:28:GLU:HG2	2.35	0.57
5:v:59:LEU:HB3	5:v:110:HIS:ND1	2.20	0.57
5:7:109:LEU:HB2	5:7:110:HIS:HD2	1.70	0.57
4:k:11:LYS:HZ3	4:k:147:ARG:HH22	1.51	0.57
1:w:233:TYR:CE2	1:w:237:LYS:HE3	2.38	0.57
2:E:109:PHE:C	2:E:109:PHE:HD1	2.12	0.57
5:d:59:LEU:HD11	5:d:64:LEU:HB2	1.86	0.57
1:r:157:ASP:O	1:r:161:LYS:HG3	2.05	0.57
1:x:195:LEU:HD21	1:x:255:CYS:HB2	1.86	0.57
3:H:42:GLN:HB3	3:H:77:LEU:HD11	1.87	0.57
5:b:69:TYR:O	5:b:83:GLN:HB2	2.04	0.57
5:S:134:GLU:HG2	5:S:160:ILE:HD13	1.86	0.57
4:c:86:VAL:HG22	4:c:97:LEU:HD23	1.87	0.57
4:c:151:ARG:HG2	5:d:108:HIS:HE1	1.68	0.57
5:p:99:ASP:OD1	5:p:102:LEU:N	2.31	0.57
2:t:109:PHE:HD2	2:t:110:LEU:HD23	1.68	0.57
1:x:28:LYS:HG2	1:x:33:GLU:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:56:ALA:HB2	4:6:67:GLN:NE2	2.19	0.57
1:U:65:LEU:O	1:U:69:ILE:HG13	2.04	0.57
1:U:281:CYS:HA	1:U:284:MET:SD	2.45	0.57
1:I:297:PHE:CE2	1:I:307:ILE:HD11	2.40	0.57
4:i:59:ALA:HB3	4:i:62:THR:OG1	2.05	0.57
2:n:83:TYR:CE2	2:n:91:PRO:HG3	2.39	0.57
1:r:144:ASN:HB2	1:r:187:LEU:HD13	1.87	0.57
3:s:6:MET:HE3	3:s:74:THR:HG23	1.86	0.57
1:9:255:CYS:SG	1:9:256:ASN:N	2.77	0.57
2:T:88:THR:OG1	2:T:89:GLU:N	2.36	0.57
4:N:69:PHE:HB2	5:2:6:GLN:HG2	1.86	0.57
5:2:21:TRP:CD1	5:2:170:LEU:HD22	2.40	0.57
1:C:65:LEU:O	1:C:69:ILE:HG13	2.05	0.56
1:I:222:LEU:HG	1:I:230:TYR:CD2	2.39	0.56
4:R:14:ASN:CA	4:R:19:ARG:NE	2.68	0.56
5:j:28:HIS:CD2	5:j:164:PRO:HD3	2.40	0.56
1:l:71:GLU:O	1:l:75:GLN:NE2	2.38	0.56
4:6:30:THR:HG21	5:7:74:THR:HA	1.87	0.56
5:7:141:LYS:HG2	5:7:142:VAL:HG22	1.86	0.56
5:b:15:ARG:HH12	5:b:19:ASN:HD21	1.52	0.56
1:V:212:ARG:HG2	1:V:212:ARG:HH11	1.71	0.56
1:f:32:GLN:HG3	1:f:32:GLN:O	2.05	0.56
1:l:41:PHE:HD1	2:n:45:MET:CE	2.18	0.56
1:l:242:GLU:HB2	1:l:262:MET:SD	2.46	0.56
4:o:152:GLU:HG3	5:p:139:HIS:CE1	2.40	0.56
5:7:15:ARG:HB3	5:7:83:GLN:HE22	1.68	0.56
1:9:58:PRO:HB2	1:9:118:LEU:HD21	1.85	0.56
1:w:19:TRP:CD1	1:w:23:ARG:HH21	2.23	0.56
1:w:284:MET:O	1:w:288:ASN:N	2.37	0.56
1:U:58:PRO:CD	1:U:59:ALA:N	2.69	0.56
3:X:58:GLY:HA2	3:X:62:PHE:O	2.06	0.56
1:C:166:GLU:HB2	1:C:172:PHE:HE2	1.69	0.56
1:C:255:CYS:SG	1:C:257:SER:OG	2.48	0.56
5:G:70:TRP:CG	1:f:311:LEU:HD13	2.40	0.56
4:L:14:ASN:HA	4:L:19:ARG:HH21	1.70	0.56
4:R:127:PHE:CD1	4:R:127:PHE:C	2.83	0.56
5:S:134:GLU:OE1	5:S:135:TYR:N	2.19	0.56
1:V:58:PRO:CD	1:V:59:ALA:N	2.50	0.56
1:f:172:PHE:CD1	1:f:172:PHE:C	2.82	0.56
1:l:215:ARG:HH22	4:u:156:ARG:HH11	1.51	0.56
5:p:20:THR:HG22	5:p:24:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:p:98:VAL:HG13	5:p:102:LEU:HD23	1.87	0.56
4:u:151:ARG:NH2	5:v:112:PHE:O	2.31	0.56
2:z:35:HIS:CD2	2:z:78:THR:HG22	2.41	0.56
1:3:44:PHE:CE1	1:3:110:PRO:HA	2.40	0.56
1:3:278:LEU:HA	1:3:296:MET:CE	2.35	0.56
5:7:120:ILE:HD11	5:7:146:GLN:HB3	1.86	0.56
4:N:31:GLY:N	4:N:40:ARG:HH22	2.00	0.56
2:E:77:PHE:O	2:E:81:VAL:HG23	2.05	0.56
5:G:113:ASP:N	5:G:113:ASP:OD1	2.32	0.56
3:J:88:LEU:HG	3:J:89:CYS:N	2.20	0.56
1:f:179:GLY:O	1:f:183:SER:OG	2.24	0.56
5:p:113:ASP:OD1	5:p:113:ASP:N	2.34	0.56
2:T:107:ALA:HB1	5:q:145:LEU:HB3	1.86	0.56
4:L:12:PHE:CD2	4:L:127:PHE:HB2	2.40	0.56
4:L:115:ASP:HB3	4:L:118:ARG:HB2	1.88	0.56
4:R:15:GLU:O	4:R:19:ARG:CG	2.47	0.56
1:V:143:TRP:CD1	1:V:187:LEU:HD11	2.40	0.56
1:r:55:ASP:OD1	5:v:121:ARG:NH2	2.38	0.56
3:s:9:ARG:NH1	3:s:86:GLU:OE2	2.38	0.56
4:u:65:SER:OG	4:u:66:LEU:N	2.37	0.56
5:7:76:GLU:OE2	5:7:77:ARG:N	2.38	0.56
1:C:312:LYS:HG2	1:C:316:GLU:OE1	2.06	0.56
4:L:14:ASN:O	4:L:19:ARG:NE	2.39	0.56
1:f:282:GLN:O	1:f:285:ILE:HG22	2.06	0.56
5:1:27:HIS:CE1	5:1:162:PRO:HG2	2.40	0.56
1:3:29:LEU:O	1:3:103:GLN:HG3	2.05	0.56
1:U:61:ILE:O	1:U:65:LEU:HB2	2.05	0.56
2:Y:61:ASN:OD1	2:Y:63:ARG:NH2	2.39	0.56
4:a:33:ARG:HA	4:a:40:ARG:NH1	2.21	0.56
1:C:107:LEU:O	1:C:110:PRO:HD2	2.06	0.56
1:I:91:LYS:HG2	1:I:176:LEU:HD21	1.88	0.56
5:M:64:LEU:HD22	5:M:88:GLU:O	2.06	0.56
1:f:196:GLN:O	1:f:200:ASP:HB2	2.05	0.56
4:i:130:GLU:O	4:i:134:GLN:HG3	2.05	0.56
5:j:50:LYS:HD2	5:j:70:TRP:O	2.06	0.56
2:n:62:PHE:CD2	2:n:65:ILE:HD11	2.40	0.56
4:0:100:PRO:HA	4:0:109:ILE:HA	1.87	0.56
1:3:237:LYS:O	1:3:241:GLU:HG2	2.06	0.56
1:9:94:ILE:HG13	1:9:176:LEU:HA	1.88	0.56
1:U:156:GLN:O	1:U:160:MET:HE2	2.05	0.56
4:a:152:GLU:HG2	5:b:147:TYR:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:115:PHE:CE1	5:b:132:ARG:HA	2.41	0.56
2:E:109:PHE:C	2:E:109:PHE:CD1	2.83	0.56
5:G:69:TYR:O	5:G:83:GLN:HB2	2.06	0.56
4:L:5:VAL:HG13	4:L:6:PRO:HD3	1.87	0.56
5:S:22:LYS:HD3	5:S:40:TYR:OH	2.06	0.56
4:c:136:ASP:CG	4:c:137:ALA:H	2.13	0.56
1:x:98:ARG:O	1:x:102:THR:HG23	2.06	0.56
2:z:42:ILE:HA	2:z:45:MET:HG3	1.88	0.56
5:q:166:VAL:O	5:q:170:THR:HG22	2.06	0.56
5:2:59:LEU:HB3	5:2:110:HIS:ND1	2.20	0.56
1:C:312:LYS:C	1:C:316:GLU:OE1	2.49	0.56
5:G:104:ASP:OD2	5:G:167:ARG:HG3	2.05	0.56
5:M:25:VAL:O	5:M:29:MET:HG3	2.06	0.56
1:f:93:TYR:HE1	1:f:143:TRP:CZ2	2.24	0.56
1:l:255:CYS:SG	1:l:256:ASN:N	2.78	0.56
2:z:72:LYS:HZ2	2:z:93:PHE:HE1	1.51	0.56
1:9:52:LEU:O	5:q:121:ARG:NH1	2.39	0.56
2:B:104:LEU:HD21	5:2:120:ILE:HG13	1.88	0.56
1:O:15:PHE:CE2	1:O:60:LYS:HB3	2.41	0.56
4:c:14:ASN:O	4:c:19:ARG:NE	2.39	0.56
4:k:29:TYR:CE2	4:k:44:PHE:HB2	2.41	0.56
4:k:144:GLU:O	4:k:148:ARG:HG3	2.06	0.56
5:b:25:VAL:O	5:b:29:MET:HG2	2.06	0.55
1:C:288:ASN:O	1:C:288:ASN:ND2	2.39	0.55
3:W:23:THR:H	3:W:26:GLU:HG3	1.70	0.55
2:t:82:ARG:NH1	2:t:83:TYR:CE1	2.73	0.55
1:U:13:LEU:HD22	1:U:18:LYS:HE2	1.87	0.55
1:C:19:TRP:CE3	1:C:22:MET:HE2	2.40	0.55
1:C:48:HIS:HB2	1:C:113:GLN:NE2	2.21	0.55
2:K:60:VAL:HG12	2:K:62:PHE:CE1	2.41	0.55
4:L:11:LYS:HD3	4:L:147:ARG:NH2	2.22	0.55
1:V:227:VAL:HG11	1:V:280:GLU:HG3	1.86	0.55
4:c:84:GLU:HB3	4:c:100:PRO:HD2	1.88	0.55
1:l:193:ASP:OD1	1:l:195:LEU:HD12	2.06	0.55
4:o:32:PHE:CE2	4:o:43:ARG:HD2	2.41	0.55
4:o:118:ARG:HE	4:o:120:ASP:HB2	1.69	0.55
5:7:15:ARG:CB	5:7:83:GLN:HE22	2.19	0.55
5:7:52:SER:HG	5:7:70:TRP:CD1	2.23	0.55
2:T:28:GLU:C	2:T:29:PHE:HD1	2.14	0.55
5:b:13:VAL:O	5:b:83:GLN:NE2	2.40	0.55
1:I:242:GLU:CB	1:I:262:MET:HE1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:91:GLU:CD	4:R:94:LYS:HE2	2.31	0.55
4:c:153:PHE:HE2	5:d:120:ILE:HB	1.72	0.55
4:k:140:GLN:HG2	5:q:94:TYR:CE2	2.41	0.55
5:2:106:LEU:HA	5:2:109:LEU:HG	1.88	0.55
1:C:166:GLU:HB2	1:C:172:PHE:CE2	2.42	0.55
1:C:193:ASP:OD2	1:C:196:GLN:HB2	2.05	0.55
2:K:83:TYR:CZ	2:K:91:PRO:HG3	2.41	0.55
5:p:127:ARG:O	5:p:128:ILE:HB	2.07	0.55
1:r:166:GLU:HG2	1:r:244:ARG:HE	1.71	0.55
5:v:114:CYS:SG	5:v:133:CYS:HB2	2.47	0.55
5:v:119:ALA:HB2	5:v:129:VAL:HG21	1.87	0.55
1:x:181:ARG:O	1:x:185:VAL:HG23	2.06	0.55
2:5:22:ILE:HD13	2:5:28:GLU:HG2	1.87	0.55
2:5:88:THR:HG23	4:6:16:GLU:OE1	2.05	0.55
5:q:134:GLU:OE1	5:q:135:TYR:N	2.34	0.55
5:d:134:GLU:HG2	5:d:159:ILE:HD13	1.88	0.55
1:f:31:ARG:O	1:f:32:GLN:HB3	2.06	0.55
1:r:17:ASP:N	1:r:17:ASP:OD1	2.35	0.55
2:t:68:HIS:NE2	2:t:102:GLU:OE1	2.36	0.55
1:x:90:LEU:HD23	1:x:91:LYS:N	2.22	0.55
2:B:71:SER:OG	2:B:72:LYS:N	2.38	0.55
2:B:72:LYS:HE3	2:B:93:PHE:CE1	2.41	0.55
2:B:80:LYS:O	2:B:84:THR:HB	2.07	0.55
1:U:98:ARG:O	1:U:102:THR:OG1	2.25	0.55
1:C:57:GLY:O	1:C:61:ILE:HG22	2.05	0.55
1:O:15:PHE:O	1:O:18:LYS:N	2.40	0.55
4:R:12:PHE:CD1	4:R:12:PHE:C	2.84	0.55
2:Z:77:PHE:O	2:Z:81:VAL:HG23	2.07	0.55
2:h:35:HIS:CE1	2:h:81:VAL:HG21	2.42	0.55
1:l:23:ARG:HG3	1:l:24:PRO:HD3	1.81	0.55
5:1:21:TRP:NE1	5:1:170:LEU:HD22	2.21	0.55
1:3:179:GLY:O	1:3:183:SER:OG	2.23	0.55
5:b:51:ILE:HD13	5:b:54:GLU:OE2	2.06	0.55
5:G:73:HIS:O	5:G:74:THR:OG1	2.21	0.55
5:M:46:SER:OG	5:M:51:ILE:HD12	2.06	0.55
1:f:97:TRP:CZ2	1:f:101:PHE:CD2	2.94	0.55
2:n:22:ILE:HG22	2:n:23:SER:N	2.21	0.55
5:q:170:THR:O	5:q:170:THR:OG1	2.24	0.55
4:N:149:ARG:NH1	4:N:154:GLU:OE2	2.40	0.55
5:b:17:ARG:HH12	5:b:168:LYS:HD2	1.71	0.55
4:F:12:PHE:HA	4:F:18:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:44:LEU:HD23	3:W:45:TYR:N	2.22	0.55
1:r:22:MET:HE1	1:r:61:ILE:HD11	1.88	0.55
5:1:104:ASP:OD1	5:1:135:TYR:OH	2.21	0.55
1:w:40:TRP:HD1	1:w:41:PHE:CD1	2.24	0.55
4:N:32:PHE:N	4:N:32:PHE:CD1	2.74	0.55
2:E:79:TYR:CD2	2:E:93:PHE:HD2	2.25	0.55
3:D:77:LEU:HG	3:D:78:ALA:N	2.22	0.55
4:L:14:ASN:HA	4:L:19:ARG:HE	1.71	0.55
4:L:48:CYS:HB3	4:L:88:LEU:HD21	1.88	0.55
5:S:144:GLY:HA3	5:S:149:LEU:HD21	1.88	0.55
1:f:245:ALA:HA	1:f:249:LEU:HD12	1.88	0.55
2:h:17:MET:HG2	2:h:18:TYR:CD1	2.41	0.55
2:h:77:PHE:O	2:h:81:VAL:HG22	2.06	0.55
4:o:152:GLU:HG2	5:p:147:TYR:CE1	2.42	0.55
5:p:86:SER:C	5:p:87:ILE:HD13	2.32	0.55
3:y:8:ARG:O	3:y:76:GLY:HA2	2.07	0.55
5:7:115:PHE:HB3	5:7:119:ALA:HB3	1.89	0.55
1:9:27:LEU:O	1:9:31:ARG:HD2	2.06	0.55
5:q:13:VAL:HG21	5:q:18:ILE:HD12	1.89	0.55
3:P:7:ILE:HG12	3:P:75:VAL:HG11	1.89	0.55
3:P:37:ARG:HD3	3:P:79:PHE:CE1	2.42	0.55
1:l:56:LYS:C	1:l:58:PRO:CD	2.80	0.55
3:s:14:ILE:HD13	3:s:34:ILE:HD13	1.89	0.55
4:k:91:GLU:OE2	4:k:94:LYS:HD2	2.07	0.55
2:E:41:THR:O	2:E:45:MET:HG3	2.07	0.54
5:G:128:ILE:O	5:G:129:VAL:HG12	2.06	0.54
1:V:281:CYS:HB2	1:V:296:MET:HE1	1.88	0.54
4:c:149:ARG:HD2	4:c:154:GLU:OE2	2.07	0.54
1:f:107:LEU:HD23	1:f:139:MET:SD	2.47	0.54
1:f:197:ILE:HG13	1:f:198:TYR:N	2.21	0.54
1:l:22:MET:HE1	1:l:61:ILE:HD12	1.88	0.54
1:U:245:ALA:O	1:U:249:LEU:HB2	2.07	0.54
3:X:52:ASP:OD1	3:X:52:ASP:N	2.40	0.54
4:a:51:GLY:HA2	5:b:3:ASN:OD1	2.06	0.54
5:G:121:ARG:HH21	5:G:127:ARG:HH12	1.54	0.54
4:R:14:ASN:CA	4:R:19:ARG:CZ	2.69	0.54
1:V:167:ARG:HH12	1:V:210:THR:HA	1.72	0.54
2:T:40:GLY:O	2:T:43:LYS:HB3	2.07	0.54
4:N:151:ARG:HD2	5:2:114:CYS:HB2	1.89	0.54
2:K:87:SER:O	2:K:87:SER:OG	2.25	0.54
3:J:6:MET:HA	3:J:14:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:207:LEU:HD22	1:O:261:LEU:HD12	1.89	0.54
2:Q:84:THR:HA	5:S:143:VAL:HG11	1.89	0.54
2:Z:20:LYS:HA	2:Z:29:PHE:O	2.07	0.54
2:n:25:ASP:CG	2:n:67:SER:HG	2.15	0.54
4:u:151:ARG:HH12	4:u:155:ASP:CG	2.15	0.54
2:z:23:SER:OG	2:z:24:SER:N	2.40	0.54
4:6:15:GLU:CD	4:6:147:ARG:HH22	2.15	0.54
4:k:5:VAL:HG13	4:k:6:PRO:HD3	1.90	0.54
4:F:5:VAL:O	4:F:8:GLN:HB2	2.07	0.54
4:F:26:GLU:HA	4:F:122:MET:HE3	1.89	0.54
3:P:68:ARG:HB3	3:P:69:PRO:HD2	1.89	0.54
5:S:28:HIS:CE1	5:S:164:LEU:HD23	2.43	0.54
1:V:27:LEU:O	1:V:31:ARG:HD2	2.07	0.54
2:n:37:LEU:HD13	2:n:43:LYS:HE2	1.90	0.54
4:6:14:ASN:C	4:6:19:ARG:HE	2.15	0.54
2:T:90:ILE:HD12	5:q:142:VAL:HG12	1.89	0.54
5:q:48:ASN:OD1	5:q:50:LYS:N	2.28	0.54
1:w:12:SER:O	1:w:13:LEU:HD23	2.07	0.54
5:G:121:ARG:NE	5:G:125:LEU:HD11	2.20	0.54
1:I:61:ILE:HD11	1:I:111:PHE:HE1	1.71	0.54
1:O:315:GLU:HA	1:O:318:ILE:HG23	1.89	0.54
5:j:119:ALA:O	5:j:123:THR:OG1	2.24	0.54
3:m:68:ARG:HB3	3:m:69:PRO:HD2	1.90	0.54
5:1:158:LYS:C	5:1:159:GLN:HG3	2.32	0.54
1:9:181:ARG:HG2	1:9:198:TYR:HE2	1.73	0.54
1:w:20:ASP:OD1	1:w:23:ARG:CZ	2.56	0.54
5:2:15:ARG:CB	5:2:83:GLN:HE22	2.20	0.54
1:I:231:MET:SD	1:I:296:MET:HG3	2.48	0.54
5:M:41:ARG:HD2	5:M:45:GLU:OE1	2.08	0.54
3:W:16:THR:OG1	3:W:17:ASP:N	2.41	0.54
4:u:14:ASN:C	4:u:19:ARG:HE	2.13	0.54
1:3:41:PHE:CE2	2:5:60:VAL:HA	2.42	0.54
1:3:228:GLN:HE22	1:3:292:LYS:CD	2.21	0.54
1:9:237:LYS:O	1:9:240:GLU:HB3	2.08	0.54
2:T:74:CYS:HA	2:T:77:PHE:CD1	2.43	0.54
4:k:32:PHE:HA	5:q:73:HIS:HE1	1.71	0.54
4:k:136:ASP:OD1	4:k:138:LEU:N	2.41	0.54
1:w:178:ILE:O	1:w:182:GLU:HG3	2.08	0.54
4:N:129:GLU:O	4:N:133:GLN:HG3	2.08	0.54
1:I:199:ARG:O	1:I:203:GLU:HB3	2.08	0.54
1:O:19:TRP:HA	1:O:22:MET:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:4:PHE:O	3:P:5:LEU:HD23	2.07	0.54
1:V:167:ARG:HH22	1:V:210:THR:HG23	1.71	0.54
4:c:64:LEU:HD23	4:c:65:SER:N	2.22	0.54
1:f:134:ILE:HG22	1:f:135:VAL:N	2.23	0.54
1:l:90:LEU:HD12	1:l:158:SER:HB3	1.90	0.54
1:9:184:TYR:CD2	1:9:202:PHE:HB2	2.42	0.54
3:e:50:LEU:HD13	3:e:51:LEU:N	2.23	0.54
5:q:38:TRP:CD2	5:q:57:ILE:HG12	2.42	0.54
1:w:19:TRP:HD1	1:w:23:ARG:HH21	1.54	0.54
1:w:19:TRP:CE3	1:w:22:MET:HE2	2.42	0.54
4:N:149:ARG:NH2	5:2:109:LEU:HD13	2.22	0.54
1:C:162:LEU:HD22	1:C:172:PHE:CD1	2.42	0.54
1:I:204:LYS:HG2	1:I:208:ASP:OD2	2.08	0.54
2:Z:79:TYR:OH	2:Z:91:PRO:O	2.13	0.54
1:l:19:TRP:HE3	1:l:22:MET:HE2	1.73	0.54
5:7:88:GLU:HG2	5:7:95:SER:OG	2.08	0.54
1:9:178:ILE:O	1:9:182:GLU:HG3	2.08	0.54
2:B:37:LEU:HD13	2:B:43:LYS:HE2	1.89	0.54
1:U:135:VAL:O	1:U:139:MET:HG3	2.08	0.54
1:U:281:CYS:O	1:U:284:MET:HG2	2.08	0.54
1:O:109:LYS:HD2	2:Q:47:SER:OG	2.07	0.54
1:O:278:LEU:HA	1:O:296:MET:CE	2.38	0.54
4:c:127:PHE:HE1	4:c:129:GLU:HA	1.73	0.54
4:i:136:ASP:CG	4:i:137:ALA:H	2.15	0.54
1:r:135:VAL:O	1:r:139:MET:HG3	2.08	0.54
2:5:80:LYS:O	2:5:84:THR:HB	2.08	0.54
4:6:9:ARG:HB3	4:6:127:PHE:CE2	2.43	0.54
1:9:65:LEU:O	1:9:69:ILE:HG13	2.07	0.54
3:e:3:VAL:HG12	3:e:64:SER:CA	2.38	0.54
1:C:57:GLY:N	1:C:58:PRO:HD3	2.23	0.54
3:D:24:VAL:HB	3:D:53:ASP:HA	1.90	0.54
4:F:108:VAL:HB	4:F:125:LEU:HD22	1.90	0.54
5:G:121:ARG:HE	5:G:125:LEU:CD1	2.21	0.54
1:O:266:VAL:HG21	1:O:302:LYS:HG2	1.90	0.54
3:P:42:GLN:HG3	3:P:78:ALA:O	2.08	0.54
5:S:135:TYR:CE1	5:S:137:ALA:HB3	2.43	0.54
3:W:63:THR:OG1	3:W:65:GLN:HG2	2.08	0.54
4:c:151:ARG:HB2	5:d:109:LEU:HA	1.89	0.54
1:l:57:GLY:N	1:l:58:PRO:CD	2.72	0.54
1:r:25:ILE:HA	1:r:28:LYS:HD3	1.89	0.54
4:u:152:GLU:CB	4:u:153:PHE:HD1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:v:161:LYS:HA	5:v:162:PRO:C	2.32	0.54
1:O:56:LYS:C	1:O:58:PRO:CD	2.81	0.53
5:j:120:ILE:HD11	5:j:146:GLN:HB3	1.90	0.53
1:r:217:GLN:OE1	1:r:233:TYR:OH	2.14	0.53
4:O:138:LEU:HD13	4:O:138:LEU:H	1.73	0.53
2:5:83:TYR:CE2	2:5:91:PRO:HG3	2.42	0.53
2:B:23:SER:HB3	2:B:27:HIS:HB2	1.89	0.53
1:U:48:HIS:HB2	1:U:113:GLN:HE21	1.73	0.53
1:I:241:GLU:OE1	1:I:244:ARG:NH1	2.41	0.53
1:O:85:ASP:O	1:O:89:LEU:N	2.41	0.53
5:S:128:ILE:HG12	5:S:129:VAL:N	2.22	0.53
5:v:44:TYR:HD1	5:v:45:GLU:N	2.06	0.53
1:x:49:ALA:O	1:x:53:TRP:CD1	2.61	0.53
1:3:278:LEU:HD23	1:3:296:MET:HE2	1.90	0.53
2:B:23:SER:N	2:B:27:HIS:O	2.37	0.53
2:B:88:THR:HG23	2:B:89:GLU:CD	2.32	0.53
4:N:49:ARG:NH1	4:N:89:GLU:OE2	2.38	0.53
1:U:179:GLY:O	1:U:183:SER:OG	2.27	0.53
5:b:148:LEU:O	5:b:151:ALA:HB3	2.08	0.53
1:C:19:TRP:CZ2	1:C:23:ARG:HG2	2.41	0.53
1:C:56:LYS:O	1:C:58:PRO:HD2	2.09	0.53
5:S:59:LEU:HD11	5:S:64:LEU:HB2	1.89	0.53
1:x:54:ASP:HB3	1:x:57:GLY:HA3	1.90	0.53
2:z:62:PHE:HB3	2:z:65:ILE:CG1	2.39	0.53
5:7:132:ARG:HD2	5:7:154:ILE:HG23	1.90	0.53
3:D:42:GLN:HA	3:D:78:ALA:O	2.08	0.53
1:I:56:LYS:C	1:I:58:PRO:CD	2.81	0.53
1:O:107:LEU:O	1:O:110:PRO:HD2	2.08	0.53
1:f:29:LEU:O	1:f:103:GLN:HG3	2.09	0.53
5:j:25:VAL:HG12	5:j:38:TRP:CZ3	2.43	0.53
2:T:28:GLU:O	2:T:29:PHE:HD1	1.92	0.53
5:q:54:GLU:CG	5:q:67:THR:HG23	2.39	0.53
1:I:166:GLU:OE2	1:I:248:TYR:HE2	1.90	0.53
1:I:167:ARG:HH22	1:I:206:TYR:HE1	1.54	0.53
4:R:104:ASN:HD22	4:R:104:ASN:N	2.05	0.53
1:V:235:ASP:HB2	1:V:295:LEU:HD11	1.90	0.53
1:f:93:TYR:CE1	1:f:143:TRP:HZ2	2.25	0.53
3:g:52:ASP:CG	3:g:55:LYS:HD3	2.34	0.53
4:u:152:GLU:HG3	5:v:139:HIS:CE1	2.43	0.53
5:2:46:SER:OG	5:2:51:ILE:HB	2.08	0.53
1:U:94:ILE:HG13	1:U:176:LEU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:22:SER:O	4:a:22:SER:OG	2.26	0.53
1:I:238:LEU:HG	1:I:269:LEU:HD13	1.89	0.53
3:J:7:ILE:HB	3:J:14:ILE:HB	1.91	0.53
5:d:72:LEU:O	5:d:81:LEU:HB3	2.09	0.53
3:g:28:LYS:HG3	3:g:44:LEU:HG	1.90	0.53
5:j:128:ILE:HD12	5:j:129:VAL:N	2.23	0.53
1:r:203:GLU:OE1	1:r:257:SER:OG	2.12	0.53
4:k:11:LYS:NZ	4:k:147:ARG:HH12	2.06	0.53
4:N:32:PHE:N	4:N:32:PHE:HD1	2.07	0.53
5:2:51:ILE:HG12	5:2:69:TYR:HE1	1.74	0.53
1:U:284:MET:HG3	1:U:293:LEU:HG	1.89	0.53
1:I:27:LEU:HD12	1:I:30:LEU:HD12	1.90	0.53
1:V:222:LEU:HD11	1:V:276:THR:HG21	1.91	0.53
1:l:93:TYR:CD2	1:l:151:ILE:HD11	2.43	0.53
1:l:98:ARG:HG3	1:l:99:LYS:N	2.23	0.53
3:H:39:PRO:HA	3:H:42:GLN:HG3	1.91	0.53
5:G:41:ARG:HB2	5:G:54:GLU:HB2	1.91	0.53
2:Z:34:GLU:HA	2:Z:37:LEU:HD12	1.91	0.53
5:j:41:ARG:HB2	5:j:54:GLU:HB2	1.90	0.53
3:m:52:ASP:OD1	3:m:52:ASP:N	2.42	0.53
5:p:37:ASP:HB2	5:p:111:TYR:HE2	1.72	0.53
1:x:17:ASP:N	1:x:17:ASP:OD1	2.40	0.53
1:3:19:TRP:CD1	1:3:23:ARG:HH21	2.26	0.53
2:T:22:ILE:HD13	2:T:28:GLU:HG2	1.91	0.53
1:w:65:LEU:O	1:w:69:ILE:HG13	2.09	0.53
1:w:148:PHE:O	1:w:152:LYS:HG2	2.08	0.53
4:a:70:PRO:HD2	4:a:73:TRP:CE3	2.44	0.53
1:l:71:GLU:HG3	1:l:75:GLN:HE22	1.73	0.53
4:6:73:TRP:N	4:6:73:TRP:HD1	2.06	0.53
4:k:37:HIS:CE1	4:k:41:GLN:NE2	2.75	0.53
3:H:27:LEU:HD12	3:H:57:LEU:HD21	1.91	0.53
5:b:112:PHE:HD2	5:b:163:LEU:HD13	1.73	0.53
4:L:149:ARG:CZ	5:M:109:LEU:HD12	2.39	0.53
5:d:135:TYR:OH	5:d:164:PRO:O	2.18	0.53
1:9:281:CYS:HB2	1:9:296:MET:HE1	1.91	0.53
4:k:41:GLN:OE1	4:k:117:GLN:HA	2.08	0.53
5:q:37:ASP:OD1	5:q:37:ASP:N	2.42	0.53
5:q:70:TRP:O	5:q:72:LEU:HD23	2.09	0.53
1:U:55:ASP:OD1	1:U:55:ASP:N	2.41	0.52
2:E:22:ILE:HB	2:E:61:ASN:HA	1.91	0.52
4:F:73:TRP:N	4:F:73:TRP:CD1	2.76	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:297:PHE:CD2	1:I:307:ILE:HD11	2.42	0.52
1:O:13:LEU:HD22	1:O:18:LYS:HE2	1.91	0.52
2:Z:83:TYR:CE1	2:Z:91:PRO:HD2	2.44	0.52
2:n:35:HIS:CD2	2:n:78:THR:HG22	2.42	0.52
5:p:104:ASP:OD2	5:p:167:ARG:HB3	2.09	0.52
1:r:32:GLN:HB2	1:r:103:GLN:NE2	2.24	0.52
3:e:52:ASP:OD1	3:e:52:ASP:N	2.41	0.52
1:w:84:GLN:H	1:w:84:GLN:CD	2.11	0.52
3:D:43:ARG:CG	3:D:50:LEU:HD21	2.39	0.52
4:R:12:PHE:C	4:R:12:PHE:HD1	2.16	0.52
1:V:246:LEU:CD2	1:V:258:VAL:HG11	2.39	0.52
5:d:109:LEU:HD12	5:d:110:HIS:N	2.24	0.52
5:j:25:VAL:HG12	5:j:38:TRP:HZ3	1.73	0.52
1:l:41:PHE:CE1	2:n:60:VAL:HG22	2.44	0.52
1:9:107:LEU:HD23	1:9:139:MET:SD	2.49	0.52
4:k:83:ARG:NH2	4:k:128:ASP:OD2	2.39	0.52
1:w:162:LEU:HD23	1:w:172:PHE:CD1	2.44	0.52
1:w:244:ARG:HG2	1:w:248:TYR:CD2	2.44	0.52
2:Y:19:VAL:HG13	2:Y:33:ARG:HD2	1.90	0.52
4:a:29:TYR:CD1	4:a:29:TYR:C	2.87	0.52
1:C:13:LEU:H	1:C:13:LEU:HD12	1.75	0.52
2:t:109:PHE:CD2	2:t:110:LEU:HD23	2.43	0.52
1:x:29:LEU:O	1:x:103:GLN:HG3	2.10	0.52
5:1:15:ARG:CB	5:1:83:GLN:HE22	2.22	0.52
1:3:100:PHE:CD2	1:3:143:TRP:CE3	2.97	0.52
4:N:102:ILE:HD11	4:N:135:GLU:OE2	2.09	0.52
1:C:58:PRO:O	1:C:61:ILE:HG23	2.09	0.52
3:D:46:LYS:HB3	3:D:51:LEU:HD21	1.92	0.52
1:I:164:HIS:ND1	1:I:164:HIS:C	2.68	0.52
2:Q:42:ILE:HA	2:Q:45:MET:CE	2.39	0.52
3:P:75:VAL:HG13	3:P:76:GLY:H	1.75	0.52
4:c:14:ASN:O	4:c:19:ARG:NH2	2.41	0.52
5:d:24:LEU:HD22	5:d:162:PRO:O	2.09	0.52
4:i:54:GLU:OE1	4:i:54:GLU:N	2.38	0.52
2:t:108:ASN:HD22	5:v:147:GLN:NE2	2.07	0.52
2:z:62:PHE:HB3	2:z:65:ILE:HG13	1.90	0.52
2:5:17:MET:HG3	2:5:18:TYR:HD1	1.74	0.52
1:U:86:ASP:OD1	1:U:154:ARG:NH1	2.43	0.52
4:F:14:ASN:HA	4:F:19:ARG:NH2	2.19	0.52
1:I:214:TYR:OH	1:I:237:LYS:HD3	2.09	0.52
4:R:28:LYS:HG2	4:R:60:THR:OG1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:303:VAL:HG13	1:V:304:PRO:HD2	1.91	0.52
1:f:245:ALA:O	1:f:249:LEU:HB2	2.08	0.52
1:l:94:ILE:HG13	1:l:176:LEU:HA	1.92	0.52
1:r:48:HIS:ND1	2:t:109:PHE:HD1	2.01	0.52
1:3:278:LEU:HG	1:3:300:MET:HE3	1.92	0.52
4:F:17:PHE:HD1	4:F:18:PHE:CD1	2.27	0.52
1:O:230:TYR:O	1:O:234:ALA:N	2.39	0.52
1:f:178:ILE:O	1:f:182:GLU:HG3	2.09	0.52
1:l:18:LYS:O	1:l:22:MET:HG3	2.10	0.52
2:n:27:HIS:CE1	3:m:11:LYS:HG2	2.45	0.52
5:p:29:MET:HG2	5:p:35:ALA:O	2.09	0.52
3:s:16:THR:OG1	3:s:17:ASP:N	2.39	0.52
1:x:79:ARG:NH2	1:x:96:GLU:OE1	2.39	0.52
3:y:43:ARG:HH21	3:y:50:LEU:HD11	1.73	0.52
3:4:79:PHE:H	3:4:86:GLU:HG3	1.74	0.52
1:O:93:TYR:CD2	1:O:155:LEU:HD11	2.45	0.52
1:O:267:ASN:HA	1:O:271:THR:OG1	2.09	0.52
5:S:145:SER:O	5:S:149:LEU:HG	2.09	0.52
1:r:159:ALA:O	1:r:163:VAL:HG23	2.08	0.52
1:9:231:MET:HG2	1:9:277:ILE:HD13	1.92	0.52
3:e:3:VAL:HB	3:e:67:ALA:HB3	1.92	0.52
5:G:158:GLN:HG3	5:G:158:GLN:O	2.08	0.52
2:K:109:PHE:C	2:K:109:PHE:CD1	2.87	0.52
4:R:14:ASN:HA	4:R:19:ARG:HE	1.75	0.52
1:V:101:PHE:HE1	1:V:136:ARG:NH2	2.07	0.52
2:Z:19:VAL:HG12	2:Z:58:ASN:O	2.10	0.52
1:f:151:ILE:HG13	1:f:155:LEU:HD21	1.92	0.52
5:v:52:SER:HB2	5:v:68:THR:OG1	2.10	0.52
2:5:62:PHE:CG	2:5:65:ILE:HD11	2.45	0.52
4:6:32:PHE:N	4:6:32:PHE:HD1	2.05	0.52
5:7:39:PHE:HE1	5:7:41:ARG:HE	1.58	0.52
5:G:119:ALA:HA	5:G:129:VAL:HG11	1.91	0.52
1:I:14:GLN:HG3	1:I:15:PHE:H	1.74	0.52
2:K:66:PRO:HG2	2:K:69:VAL:HG23	1.92	0.52
3:J:23:THR:HG22	3:J:56:THR:HG22	1.92	0.52
1:V:98:ARG:O	1:V:102:THR:OG1	2.27	0.52
4:c:32:PHE:CE1	5:d:73:HIS:CE1	2.98	0.52
2:h:80:LYS:O	2:h:84:THR:HG22	2.10	0.52
4:o:69:PHE:HB2	5:p:6:GLN:HG2	1.91	0.52
1:r:25:ILE:HG13	1:r:26:VAL:N	2.23	0.52
3:s:45:TYR:CZ	3:s:50:LEU:HD23	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:203:GLU:O	1:x:207:LEU:HG	2.10	0.52
1:9:19:TRP:CE3	1:9:22:MET:HE2	2.45	0.52
2:Y:35:HIS:HD2	2:Y:78:THR:HG22	1.74	0.52
4:L:29:TYR:CE2	4:L:44:PHE:HB2	2.45	0.52
1:O:75:GLN:C	1:O:79:ARG:HE	2.18	0.52
1:l:65:LEU:O	1:l:69:ILE:HG13	2.10	0.52
4:o:32:PHE:CD1	4:o:32:PHE:N	2.76	0.52
1:r:58:PRO:O	1:r:61:ILE:HG22	2.10	0.52
3:s:29:ARG:HD3	3:s:32:GLU:OE1	2.10	0.52
4:u:14:ASN:O	4:u:19:ARG:CD	2.53	0.52
4:N:118:ARG:HE	4:N:120:ASP:HB2	1.75	0.52
1:C:112:CYS:HA	1:C:115:GLU:HG3	1.92	0.51
3:J:9:ARG:HH11	3:J:10:HIS:CE1	2.28	0.51
1:O:92:ALA:O	1:O:95:VAL:HG23	2.10	0.51
3:P:9:ARG:NH2	3:P:10:HIS:CD2	2.78	0.51
4:R:127:PHE:CD1	4:R:128:ASP:N	2.78	0.51
5:S:18:ILE:HD12	5:S:83:GLN:HB2	1.91	0.51
1:V:160:MET:HE1	1:V:206:TYR:HD2	1.74	0.51
2:Z:20:LYS:HG2	2:Z:59:GLU:HG3	1.92	0.51
1:f:231:MET:HE1	1:f:296:MET:HB2	1.91	0.51
1:f:231:MET:HE3	1:f:295:LEU:HG	1.92	0.51
1:l:23:ARG:HG3	1:l:24:PRO:CD	2.37	0.51
1:l:32:GLN:HE21	1:l:103:GLN:HE22	1.58	0.51
1:l:306:GLY:O	1:l:309:PRO:HD2	2.09	0.51
3:m:41:GLU:O	3:m:79:PHE:HA	2.10	0.51
1:r:40:TRP:CD2	2:t:49:PRO:C	2.88	0.51
1:r:94:ILE:HG13	1:r:176:LEU:HA	1.92	0.51
4:6:69:PHE:HB2	5:7:6:GLN:HG2	1.90	0.51
5:7:98:VAL:HG13	5:7:102:LEU:HB3	1.92	0.51
2:K:109:PHE:C	2:K:109:PHE:HD1	2.18	0.51
1:O:29:LEU:O	1:O:103:GLN:NE2	2.42	0.51
1:O:102:THR:O	1:O:106:ILE:HG12	2.10	0.51
1:f:14:GLN:O	1:f:15:PHE:HB3	2.08	0.51
1:l:203:GLU:OE1	1:l:257:SER:OG	2.27	0.51
1:x:188:CYS:SG	1:x:197:ILE:HG23	2.50	0.51
4:6:55:ILE:HB	4:6:68:PHE:HB2	1.92	0.51
4:F:37:HIS:O	4:F:41:GLN:HG3	2.11	0.51
4:F:155:ASP:OD1	4:F:155:ASP:N	2.43	0.51
5:S:103:ALA:HB3	5:S:167:VAL:HG21	1.91	0.51
1:f:90:LEU:O	1:f:94:ILE:HG12	2.10	0.51
1:x:49:ALA:O	1:x:53:TRP:HD1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:79:ARG:NH2	1:3:96:GLU:OE2	2.42	0.51
5:q:129:VAL:HG22	5:q:130:SER:H	1.76	0.51
4:N:151:ARG:HG3	5:2:108:HIS:O	2.10	0.51
1:C:160:MET:N	1:C:160:MET:SD	2.83	0.51
2:E:41:THR:HG21	2:E:109:PHE:CE1	2.44	0.51
1:V:143:TRP:HD1	1:V:187:LEU:HD11	1.74	0.51
2:h:23:SER:OG	2:h:27:HIS:HB2	2.10	0.51
3:g:43:ARG:HG2	3:g:50:LEU:HD21	1.93	0.51
4:i:115:ASP:HB3	4:i:118:ARG:HB2	1.91	0.51
1:l:91:LYS:O	1:l:95:VAL:HG23	2.11	0.51
1:r:48:HIS:CE1	2:t:109:PHE:HA	2.45	0.51
5:v:27:HIS:CE1	5:v:162:PRO:HD2	2.45	0.51
5:v:59:LEU:HD11	5:v:64:LEU:HB2	1.93	0.51
3:4:50:LEU:HD13	3:4:51:LEU:N	2.26	0.51
2:T:35:HIS:O	2:T:77:PHE:HD2	1.93	0.51
4:k:88:LEU:H	4:k:88:LEU:HD22	1.74	0.51
1:w:267:ASN:HA	1:w:271:THR:HB	1.91	0.51
3:H:50:LEU:HD22	3:H:51:LEU:H	1.74	0.51
1:U:90:LEU:HD23	1:U:90:LEU:C	2.36	0.51
4:a:27:ILE:HD11	4:a:122:MET:O	2.10	0.51
1:C:14:GLN:C	1:C:16:GLU:H	2.18	0.51
4:F:8:GLN:HE22	4:F:106:VAL:HA	1.73	0.51
4:F:109:ILE:HG12	4:F:128:ASP:HB2	1.93	0.51
4:L:118:ARG:NE	4:L:120:ASP:HB2	2.22	0.51
3:P:28:LYS:NZ	3:P:53:ASP:OD1	2.39	0.51
1:f:14:GLN:O	1:f:14:GLN:HG3	2.10	0.51
1:l:100:PHE:CE1	1:l:104:CYS:SG	3.04	0.51
3:s:52:ASP:OD1	3:s:52:ASP:N	2.39	0.51
5:1:54:GLU:HG2	5:1:67:THR:HG23	1.92	0.51
5:q:15:ARG:O	5:q:18:ILE:HG22	2.10	0.51
1:w:44:PHE:CZ	1:w:110:PRO:HA	2.46	0.51
1:w:92:ALA:O	1:w:95:VAL:HG23	2.10	0.51
4:N:67:GLN:NE2	5:2:72:LEU:HD13	2.25	0.51
4:N:83:ARG:HB3	4:N:100:PRO:HG3	1.92	0.51
1:U:153:ASN:OD1	1:U:153:ASN:N	2.39	0.51
4:a:118:ARG:NH2	4:a:120:ASP:OD2	2.44	0.51
4:a:153:PHE:CE2	5:b:120:ILE:HD12	2.46	0.51
5:G:41:ARG:HH22	5:7:45:GLU:CD	2.18	0.51
1:I:235:ASP:O	1:I:239:LYS:HB2	2.10	0.51
4:L:32:PHE:CD1	4:L:32:PHE:N	2.77	0.51
1:O:159:ALA:O	1:O:163:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:100:PHE:O	1:f:103:GLN:HB2	2.10	0.51
5:j:112:PHE:CD2	5:j:163:LEU:HD13	2.45	0.51
2:n:72:LYS:O	2:n:75:MET:HB2	2.10	0.51
3:s:23:THR:O	3:s:26:GLU:HB2	2.10	0.51
5:v:128:ILE:HG12	5:v:129:VAL:H	1.76	0.51
1:x:162:LEU:HD23	1:x:172:PHE:CD2	2.46	0.51
2:z:31:VAL:HG12	3:y:15:PHE:HB2	1.93	0.51
2:z:82:ARG:HD2	2:z:83:TYR:CD1	2.46	0.51
5:1:25:VAL:O	5:1:29:MET:HG3	2.10	0.51
1:3:225:ASN:OD1	1:3:225:ASN:N	2.44	0.51
1:3:242:GLU:HB2	1:3:262:MET:HE2	1.92	0.51
4:k:55:ILE:HG13	4:k:68:PHE:HB2	1.92	0.51
5:q:98:VAL:HG13	5:q:102:LEU:HB3	1.92	0.51
5:2:24:LEU:HD22	5:2:163:PRO:O	2.10	0.51
1:U:289:GLU:OE1	1:U:292:LYS:HG3	2.10	0.51
3:X:50:LEU:HD13	3:X:51:LEU:N	2.26	0.51
4:F:155:ASP:O	5:G:117:GLU:N	2.38	0.51
5:G:15:ARG:HH21	1:f:318:ILE:HD13	1.76	0.51
2:K:35:HIS:CE1	2:K:78:THR:HG22	2.45	0.51
3:J:28:LYS:HZ3	3:J:44:LEU:N	2.09	0.51
4:L:118:ARG:HH21	4:L:120:ASP:HB2	1.76	0.51
5:M:103:ALA:O	5:M:107:ILE:HG12	2.11	0.51
3:P:44:LEU:HD22	3:P:75:VAL:HG22	1.93	0.51
1:V:103:GLN:NE2	1:V:106:ILE:HD12	2.26	0.51
4:o:14:ASN:HA	4:o:19:ARG:NH2	2.16	0.51
1:r:228:GLN:HG2	1:r:292:LYS:NZ	2.25	0.51
1:x:245:ALA:HB1	1:x:249:LEU:HD12	1.92	0.51
4:6:104:ASN:ND2	5:7:99:ASP:OD1	2.42	0.51
1:w:112:CYS:HA	1:w:115:GLU:HG3	1.92	0.51
1:I:23:ARG:HB3	1:I:24:PRO:HD3	1.92	0.51
1:I:167:ARG:NH2	1:I:206:TYR:HE1	2.07	0.51
2:Z:88:THR:CG2	4:c:16:GLU:OE1	2.59	0.51
1:f:57:GLY:N	1:f:58:PRO:CD	2.73	0.51
1:r:178:ILE:HG22	1:r:181:ARG:NH1	2.25	0.51
2:t:28:GLU:OE1	3:s:12:THR:OG1	2.29	0.51
2:5:35:HIS:HD2	2:5:78:THR:HG22	1.76	0.51
5:7:38:TRP:CD1	5:7:57:ILE:HG23	2.46	0.51
1:C:55:ASP:OD1	5:G:121:ARG:NH2	2.41	0.51
1:I:99:LYS:O	1:I:103:GLN:HG2	2.11	0.51
1:l:23:ARG:HG3	1:l:24:PRO:N	2.26	0.51
5:p:160:LYS:HA	5:p:161:PRO:C	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:16:GLU:HA	4:u:19:ARG:HB2	1.92	0.51
4:u:32:PHE:N	4:u:32:PHE:CD1	2.79	0.51
4:u:152:GLU:C	4:u:153:PHE:HD1	2.19	0.51
1:3:228:GLN:NE2	1:3:292:LYS:HD3	2.22	0.51
4:N:48:CYS:HB3	4:N:88:LEU:HD21	1.92	0.51
1:U:109:LYS:HB2	1:U:110:PRO:HD3	1.93	0.51
3:X:43:ARG:CG	3:X:50:LEU:HD21	2.41	0.51
1:I:292:LYS:O	1:I:295:LEU:HB3	2.11	0.51
1:I:320:SER:O	1:I:320:SER:OG	2.21	0.51
5:M:52:SER:HB2	5:M:68:THR:OG1	2.11	0.51
1:O:43:LEU:HD22	1:O:47:VAL:HG23	1.93	0.51
4:i:147:ARG:HG3	5:j:102:LEU:HD21	1.92	0.51
1:r:15:PHE:CD2	1:r:19:TRP:HB2	2.46	0.51
4:u:118:ARG:HE	4:u:120:ASP:CG	2.19	0.51
5:v:128:ILE:HG12	5:v:129:VAL:N	2.26	0.51
4:0:102:ILE:HG12	4:0:107:CYS:SG	2.51	0.51
1:9:22:MET:O	1:9:26:VAL:HG23	2.11	0.51
1:w:57:GLY:O	1:w:60:LYS:HB2	2.11	0.51
5:2:16:MET:O	5:2:20:THR:OG1	2.27	0.51
3:D:29:ARG:NH1	3:D:32:GLU:OE1	2.39	0.50
1:I:21:PHE:CZ	1:V:286:LYS:HB3	2.45	0.50
2:K:82:ARG:O	2:K:85:ASN:HB2	2.11	0.50
1:V:19:TRP:CE2	1:V:23:ARG:HG2	2.46	0.50
2:Z:107:ALA:HB1	5:d:145:LEU:HB3	1.93	0.50
1:r:62:HIS:O	1:r:66:LYS:HB2	2.11	0.50
2:t:85:ASN:OD1	2:t:86:SER:N	2.45	0.50
2:z:83:TYR:HE2	2:z:91:PRO:CD	2.24	0.50
3:y:23:THR:HG22	3:y:56:THR:HG22	1.94	0.50
5:1:15:ARG:HB3	5:1:83:GLN:HE22	1.76	0.50
1:C:258:VAL:O	1:C:262:MET:HG2	2.11	0.50
4:F:3:ARG:HH11	4:i:89:GLU:HB3	1.76	0.50
1:I:167:ARG:NH2	1:I:210:THR:HG23	2.27	0.50
2:K:83:TYR:CE1	2:K:91:PRO:HG3	2.46	0.50
4:L:14:ASN:O	4:L:19:ARG:CZ	2.60	0.50
5:S:113:ASP:HB2	5:S:131:PRO:HG2	1.92	0.50
1:V:86:ASP:OD1	1:V:86:ASP:N	2.45	0.50
2:Z:64:GLU:O	2:Z:66:PRO:HD3	2.11	0.50
4:c:152:GLU:C	4:c:153:PHE:HD1	2.17	0.50
1:f:154:ARG:HA	1:f:157:ASP:OD1	2.11	0.50
3:m:26:GLU:O	3:m:30:ILE:HD13	2.11	0.50
5:p:9:ILE:HG22	5:p:9:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:p:104:ASP:OD2	5:p:167:ARG:N	2.40	0.50
5:p:106:LEU:O	5:p:109:LEU:HB2	2.11	0.50
1:r:79:ARG:NE	1:r:96:GLU:OE2	2.44	0.50
1:r:85:ASP:OD1	1:r:85:ASP:N	2.41	0.50
2:z:22:ILE:HD11	2:z:59:GLU:OE2	2.11	0.50
5:1:51:ILE:HG12	5:1:69:TYR:HE1	1.76	0.50
3:4:57:LEU:O	3:4:62:PHE:HB2	2.11	0.50
3:H:23:THR:HG22	3:H:56:THR:HG22	1.93	0.50
5:2:3:ASN:N	5:2:3:ASN:ND2	2.59	0.50
2:Y:105:MET:HE3	5:b:124:ILE:HG23	1.93	0.50
5:b:50:LYS:HZ2	5:b:72:LEU:HD12	1.76	0.50
2:n:22:ILE:HG22	2:n:23:SER:H	1.75	0.50
4:u:73:TRP:CE3	5:v:49:PRO:HD2	2.47	0.50
4:u:151:ARG:NH2	5:v:113:ASP:HA	2.26	0.50
5:v:104:ASP:OD2	5:v:167:VAL:N	2.45	0.50
1:x:40:TRP:NE1	1:x:44:PHE:HE1	2.10	0.50
3:y:45:TYR:CD1	3:y:88:LEU:HD13	2.47	0.50
4:0:118:ARG:HE	4:0:120:ASP:CB	2.13	0.50
5:1:34:LYS:HB3	5:1:112:PHE:HE1	1.76	0.50
4:6:41:GLN:HE22	4:6:117:GLN:HG3	1.75	0.50
1:9:19:TRP:HE3	1:9:22:MET:HE2	1.76	0.50
2:T:41:THR:O	2:T:45:MET:HG3	2.11	0.50
3:e:6:MET:HA	3:e:14:ILE:O	2.12	0.50
2:Y:71:SER:OG	2:Y:72:LYS:N	2.40	0.50
4:a:117:GLN:HG2	4:a:118:ARG:HG2	1.94	0.50
1:C:22:MET:SD	1:C:46:ASP:HB3	2.52	0.50
1:C:113:GLN:O	1:C:117:THR:OG1	2.27	0.50
1:C:192:GLU:CD	1:x:199:ARG:HH22	2.19	0.50
4:F:43:ARG:HH11	4:F:43:ARG:CG	2.24	0.50
4:R:111:LYS:NZ	4:R:111:LYS:HB3	2.25	0.50
1:V:184:TYR:CD2	1:V:202:PHE:HB2	2.46	0.50
4:c:102:ILE:C	4:c:103:LEU:HD23	2.36	0.50
1:r:56:LYS:C	1:r:58:PRO:CD	2.84	0.50
2:z:79:TYR:OH	2:z:91:PRO:O	2.22	0.50
1:9:109:LYS:HB2	1:9:110:PRO:HD3	1.91	0.50
3:H:8:ARG:O	3:H:76:GLY:HA2	2.12	0.50
5:b:8:MET:HA	5:b:97:GLN:HE22	1.75	0.50
3:D:5:LEU:HD23	3:D:73:ALA:HB3	1.94	0.50
4:L:151:ARG:HE	5:M:114:CYS:HB2	1.76	0.50
1:O:178:ILE:O	1:O:182:GLU:HG3	2.12	0.50
5:d:76:GLU:OE2	5:d:77:ARG:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:p:134:GLU:CD	5:p:135:TYR:N	2.67	0.50
1:r:94:ILE:HD12	1:r:179:GLY:HA3	1.93	0.50
1:r:158:SER:HA	1:r:161:LYS:HD3	1.94	0.50
2:z:109:PHE:CD1	2:z:109:PHE:C	2.90	0.50
1:3:44:PHE:CZ	1:3:110:PRO:HA	2.46	0.50
1:U:91:LYS:O	1:U:95:VAL:HG23	2.12	0.50
5:b:128:ILE:HG23	5:b:129:VAL:N	2.26	0.50
1:C:56:LYS:C	1:C:58:PRO:CD	2.85	0.50
4:F:12:PHE:HA	4:F:18:PHE:HD2	1.76	0.50
4:F:96:TYR:C	4:F:97:LEU:HG	2.35	0.50
1:I:109:LYS:HB2	1:I:110:PRO:HD3	1.94	0.50
1:O:196:GLN:NE2	1:O:199:ARG:CZ	2.75	0.50
1:r:66:LYS:HA	1:r:138:LEU:HD21	1.91	0.50
3:s:8:ARG:O	3:s:76:GLY:HA2	2.12	0.50
3:s:43:ARG:CG	3:s:50:LEU:HD21	2.39	0.50
5:v:6:GLN:O	5:v:6:GLN:HG3	2.08	0.50
1:x:72:PHE:HE1	1:x:79:ARG:HH22	1.60	0.50
4:0:13:GLU:O	4:0:19:ARG:NE	2.44	0.50
5:1:21:TRP:CD1	5:1:170:LEU:HD22	2.47	0.50
4:6:11:LYS:NZ	4:6:147:ARG:HH12	2.09	0.50
1:9:186:ASN:HD22	1:9:186:ASN:N	2.09	0.50
1:w:13:LEU:HA	1:w:17:ASP:OD2	2.11	0.50
1:w:26:VAL:O	1:w:29:LEU:HB2	2.11	0.50
1:C:165:ALA:HB1	1:C:170:GLU:HB2	1.93	0.50
5:G:155:LYS:N	5:G:155:LYS:HD2	2.27	0.50
1:O:19:TRP:CD1	1:O:23:ARG:HG3	2.46	0.50
1:V:228:GLN:NE2	1:V:292:LYS:HD2	2.26	0.50
2:Z:27:HIS:ND1	3:W:11:LYS:O	2.32	0.50
4:u:14:ASN:CA	4:u:19:ARG:HH21	2.23	0.50
1:x:271:THR:O	1:x:274:LYS:HB3	2.11	0.50
3:y:32:GLU:CD	3:y:39:PRO:HD3	2.37	0.50
2:5:87:SER:N	4:6:16:GLU:OE1	2.44	0.50
4:6:66:LEU:HD13	4:6:110:TRP:CE2	2.47	0.50
5:q:103:ALA:HB3	5:q:166:VAL:HG21	1.94	0.50
1:U:75:GLN:O	1:U:79:ARG:HG3	2.11	0.50
1:U:287:ARG:NE	1:U:289:GLU:OE2	2.38	0.50
2:Y:79:TYR:CZ	2:Y:93:PHE:HB2	2.46	0.50
4:a:144:GLU:O	4:a:148:ARG:HB2	2.12	0.50
4:F:24:GLU:HA	4:F:124:CYS:HB3	1.94	0.50
1:O:75:GLN:HB2	1:O:79:ARG:HH11	1.77	0.50
4:R:156:ARG:HG3	4:R:156:ARG:NH2	2.02	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:52:SER:HB2	5:S:68:THR:OG1	2.12	0.50
1:V:149:SER:HA	1:V:152:LYS:HE3	1.93	0.50
1:V:193:ASP:OD1	1:V:195:LEU:HD12	2.12	0.50
3:W:75:VAL:HG12	3:W:76:GLY:N	2.26	0.50
4:c:94:LYS:HD3	4:c:113:TRP:CE3	2.47	0.50
5:1:3:ASN:N	5:1:3:ASN:HD22	2.07	0.50
5:1:29:MET:N	5:1:35:ALA:HB3	2.26	0.50
1:3:85:ASP:OD1	1:3:85:ASP:N	2.35	0.50
4:6:99:ALA:HB1	5:7:7:VAL:HG11	1.93	0.50
5:7:15:ARG:O	5:7:18:ILE:N	2.45	0.50
5:q:120:ILE:HD11	5:q:146:GLN:HG2	1.94	0.50
1:w:19:TRP:CD1	1:w:23:ARG:NH2	2.79	0.50
4:a:69:PHE:HZ	5:b:69:TYR:HE2	1.60	0.50
5:b:113:ASP:N	5:b:113:ASP:OD1	2.32	0.50
1:C:284:MET:O	1:C:288:ASN:N	2.45	0.50
3:D:50:LEU:HD13	3:D:51:LEU:N	2.27	0.50
1:I:40:TRP:CE3	2:K:49:PRO:HG2	2.47	0.50
3:J:8:ARG:O	3:J:76:GLY:HA2	2.11	0.50
1:V:97:TRP:NE1	1:V:179:GLY:O	2.42	0.50
1:V:230:TYR:CD1	1:V:233:TYR:HD2	2.29	0.50
1:f:40:TRP:CE3	2:h:49:PRO:HG2	2.47	0.50
5:j:38:TRP:CD2	5:j:57:ILE:HG12	2.47	0.50
3:m:23:THR:O	3:m:26:GLU:N	2.43	0.50
5:p:89:TRP:O	5:p:95:SER:HA	2.11	0.50
4:u:44:PHE:HE2	4:u:114:ILE:HG21	1.75	0.50
1:x:241:GLU:OE2	1:x:244:ARG:NH1	2.45	0.50
3:y:42:GLN:HB3	3:y:77:LEU:HD11	1.94	0.50
5:1:103:ALA:O	5:1:107:ILE:HG13	2.11	0.50
3:4:29:ARG:HD3	3:4:32:GLU:OE1	2.12	0.50
1:9:250:GLU:OE2	1:9:253:ARG:HB2	2.11	0.50
1:I:163:VAL:HG23	1:I:177:VAL:HG21	1.93	0.49
1:I:262:MET:O	1:I:266:VAL:HG23	2.12	0.49
5:M:135:TYR:CE2	5:M:137:ALA:HB3	2.47	0.49
1:O:228:GLN:CA	1:O:228:GLN:HE21	2.24	0.49
5:S:21:TRP:O	5:S:25:VAL:HG22	2.12	0.49
5:S:38:TRP:CD2	5:S:57:ILE:HG12	2.47	0.49
1:V:293:LEU:HA	1:V:296:MET:HB2	1.94	0.49
2:Z:95:ILE:HD11	5:d:148:LEU:HB3	1.93	0.49
4:c:12:PHE:C	4:c:12:PHE:HD1	2.20	0.49
4:c:12:PHE:C	4:c:12:PHE:CD1	2.90	0.49
1:f:281:CYS:HB2	1:f:296:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:o:28:LYS:HG3	4:o:60:THR:HG22	1.94	0.49
2:t:35:HIS:HD2	2:t:78:THR:HG22	1.77	0.49
4:u:41:GLN:OE1	4:u:117:GLN:HA	2.12	0.49
4:u:99:ALA:HB1	5:v:7:VAL:HG11	1.94	0.49
5:v:24:LEU:HD22	5:v:163:PRO:O	2.11	0.49
5:v:78:ASP:HB3	5:v:80:HIS:CE1	2.46	0.49
5:7:18:ILE:HD13	5:7:68:THR:HG22	1.94	0.49
2:T:73:VAL:CG1	2:T:77:PHE:HE1	2.22	0.49
4:k:131:ARG:HG2	4:k:135:GLU:HG3	1.92	0.49
5:q:134:GLU:OE2	5:q:159:ILE:HG22	2.12	0.49
2:B:83:TYR:HE2	2:B:89:GLU:HB2	1.76	0.49
1:C:23:ARG:N	1:C:24:PRO:HD2	2.26	0.49
1:I:57:GLY:N	1:I:58:PRO:CD	2.75	0.49
4:R:44:PHE:HD2	4:R:119:LEU:HD22	1.77	0.49
1:f:213:PHE:CD1	1:f:213:PHE:C	2.90	0.49
4:o:153:PHE:N	4:o:153:PHE:CD1	2.79	0.49
1:x:14:GLN:O	1:x:16:GLU:N	2.39	0.49
1:x:55:ASP:HA	5:1:121:ARG:NH2	2.26	0.49
1:3:19:TRP:HE1	1:3:23:ARG:CD	2.18	0.49
1:3:182:GLU:O	1:3:186:ASN:ND2	2.28	0.49
4:k:37:HIS:O	4:k:41:GLN:HG2	2.12	0.49
5:q:38:TRP:CE2	5:q:57:ILE:HG12	2.47	0.49
1:C:190:ASN:ND2	1:C:193:ASP:O	2.45	0.49
1:I:108:PRO:HB3	1:I:135:VAL:HB	1.94	0.49
1:I:198:TYR:C	1:I:198:TYR:HD1	2.20	0.49
1:V:180:VAL:HG12	1:V:202:PHE:HE2	1.77	0.49
3:g:8:ARG:O	3:g:90:ILE:HG12	2.11	0.49
1:l:23:ARG:CG	1:l:24:PRO:N	2.71	0.49
1:x:28:LYS:O	1:x:32:GLN:N	2.45	0.49
4:a:32:PHE:N	4:a:32:PHE:CD1	2.78	0.49
4:F:88:LEU:H	4:F:88:LEU:CD2	2.26	0.49
2:Q:63:ARG:HA	2:Q:63:ARG:HE	1.77	0.49
5:d:89:TRP:O	5:d:95:SER:HA	2.13	0.49
1:l:179:GLY:O	1:l:182:GLU:HB2	2.12	0.49
1:r:97:TRP:CZ2	1:r:101:PHE:HD2	2.30	0.49
1:r:113:GLN:O	1:r:117:THR:OG1	2.30	0.49
2:z:40:GLY:O	2:z:43:LYS:HB3	2.11	0.49
3:y:3:VAL:HB	3:y:67:ALA:HB3	1.93	0.49
4:0:48:CYS:HB3	4:0:88:LEU:HD21	1.94	0.49
2:T:17:MET:O	2:T:33:ARG:HB2	2.11	0.49
3:X:8:ARG:O	3:X:76:GLY:HA2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:129:GLU:O	4:a:133:GLN:HG3	2.12	0.49
5:b:52:SER:N	5:b:68:THR:O	2.44	0.49
3:D:22:SER:HB2	3:D:57:LEU:HD12	1.94	0.49
4:F:136:ASP:CG	4:F:137:ALA:N	2.70	0.49
5:G:133:CYS:SG	5:G:134:GLU:O	2.70	0.49
2:Q:108:ASN:HA	5:S:147:GLN:OE1	2.11	0.49
2:h:58:ASN:OD1	2:h:58:ASN:N	2.45	0.49
2:n:25:ASP:OD2	2:n:67:SER:OG	2.30	0.49
4:u:98:LYS:HZ3	4:u:109:ILE:HG21	1.77	0.49
1:3:281:CYS:O	1:3:285:ILE:HD12	2.12	0.49
2:5:88:THR:HG23	4:6:16:GLU:CD	2.37	0.49
1:w:192:GLU:HG3	1:w:193:ASP:N	2.28	0.49
2:B:83:TYR:HE1	3:H:69:PRO:HG3	1.77	0.49
4:F:103:LEU:O	4:F:106:VAL:HG13	2.13	0.49
1:I:13:LEU:HD23	1:I:18:LYS:HG2	1.95	0.49
1:O:19:TRP:CD1	1:O:23:ARG:CG	2.96	0.49
1:V:66:LYS:HE2	1:V:138:LEU:HD11	1.94	0.49
2:h:41:THR:O	2:h:45:MET:HG3	2.13	0.49
1:l:159:ALA:HB1	1:l:177:VAL:HG22	1.95	0.49
4:o:153:PHE:N	4:o:153:PHE:HD1	2.10	0.49
3:y:4:PHE:O	3:y:67:ALA:HB1	2.12	0.49
1:3:266:VAL:HG21	1:3:302:LYS:HG2	1.94	0.49
1:U:31:ARG:HD3	1:U:33:GLU:OE2	2.12	0.49
3:X:37:ARG:HH21	3:X:41:GLU:HB3	1.77	0.49
4:F:50:ASP:OD1	4:F:50:ASP:C	2.55	0.49
5:G:18:ILE:HD12	5:G:83:GLN:HG3	1.95	0.49
3:g:50:LEU:HD13	3:g:51:LEU:N	2.27	0.49
3:g:55:LYS:HE2	3:g:60:CYS:SG	2.52	0.49
2:n:41:THR:OG1	2:n:110:LEU:O	2.31	0.49
5:p:20:THR:C	5:p:24:LEU:HD12	2.37	0.49
2:z:23:SER:OG	2:z:25:ASP:OD1	2.28	0.49
4:6:100:PRO:HA	4:6:109:ILE:HA	1.94	0.49
4:6:147:ARG:HG3	5:7:102:LEU:HD21	1.95	0.49
1:w:72:PHE:CD1	1:w:72:PHE:C	2.90	0.49
1:C:43:LEU:O	1:C:47:VAL:HG23	2.11	0.49
5:S:69:TYR:HE1	5:S:86:SER:HB3	1.76	0.49
4:c:151:ARG:HH21	4:c:155:ASP:CG	2.20	0.49
2:h:79:TYR:OH	2:h:91:PRO:O	2.20	0.49
4:i:48:CYS:HB3	4:i:88:LEU:HD21	1.94	0.49
1:l:303:VAL:HG12	1:l:306:GLY:H	1.78	0.49
1:r:316:GLU:O	1:r:319:ILE:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:v:120:ILE:CD1	5:v:147:GLN:HB3	2.43	0.49
4:0:13:GLU:C	4:0:19:ARG:HE	2.18	0.49
1:3:19:TRP:HE3	1:3:22:MET:HE2	1.76	0.49
2:5:82:ARG:O	2:5:85:ASN:HB2	2.12	0.49
5:7:127:ARG:O	5:7:128:ILE:HG22	2.12	0.49
1:w:93:TYR:CE1	1:w:143:TRP:HZ2	2.30	0.49
4:N:136:ASP:C	4:N:136:ASP:OD1	2.56	0.49
4:a:69:PHE:CZ	5:b:69:TYR:HE2	2.29	0.49
5:G:127:ARG:O	5:G:128:ILE:HG13	2.13	0.49
1:I:97:TRP:NE1	1:I:182:GLU:OE1	2.46	0.49
3:P:7:ILE:HG12	3:P:75:VAL:CG1	2.43	0.49
1:V:75:GLN:O	1:V:79:ARG:HG2	2.12	0.49
4:i:17:PHE:O	4:i:21:LEU:HG	2.13	0.49
5:p:26:LYS:HD2	5:p:30:TYR:CE2	2.48	0.49
4:u:44:PHE:CE2	4:u:114:ILE:HG21	2.48	0.49
5:1:101:ASP:O	5:1:140:ASN:ND2	2.46	0.49
5:1:115:PHE:HE1	5:1:132:ARG:HA	1.77	0.49
5:7:54:GLU:HG2	5:7:67:THR:HG23	1.95	0.49
5:7:134:GLU:HG2	5:7:157:LYS:HB2	1.94	0.49
5:q:13:VAL:CG2	5:q:18:ILE:HD12	2.43	0.49
1:w:253:ARG:HD2	1:w:253:ARG:HA	1.44	0.49
4:N:143:PHE:HB2	5:2:89:TRP:CZ3	2.48	0.49
3:X:42:GLN:HB3	3:X:77:LEU:CD1	2.43	0.49
1:C:114:LEU:O	1:C:118:LEU:HG	2.13	0.49
1:C:284:MET:CE	1:C:293:LEU:HG	2.43	0.49
1:I:23:ARG:HB3	1:I:24:PRO:CD	2.43	0.49
5:S:158:LYS:O	5:S:159:GLN:HG2	2.13	0.49
2:h:30:ILE:HB	3:g:14:ILE:HG12	1.95	0.49
1:l:23:ARG:O	1:l:26:VAL:N	2.46	0.49
1:l:108:PRO:HB3	1:l:135:VAL:HB	1.94	0.49
2:t:37:LEU:HD22	2:t:43:LYS:HE3	1.95	0.49
4:u:109:ILE:HG13	4:u:128:ASP:HB2	1.93	0.49
5:v:139:HIS:CD2	5:v:139:HIS:N	2.80	0.49
4:0:85:TYR:OH	4:6:129:GLU:OE2	2.30	0.49
4:6:6:PRO:O	4:6:10:SER:OG	2.30	0.49
5:7:157:LYS:O	5:7:158:GLN:HG3	2.13	0.49
1:w:19:TRP:HE1	1:w:23:ARG:NE	2.08	0.49
2:B:20:LYS:O	2:B:60:VAL:N	2.40	0.49
2:Y:62:PHE:HB3	2:Y:65:ILE:HG12	1.95	0.48
4:a:90:ARG:HG3	4:L:9:ARG:NH1	2.28	0.48
4:F:129:GLU:O	4:F:133:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:103:LEU:O	4:L:106:VAL:HG13	2.12	0.48
5:M:24:LEU:HD22	5:M:162:PRO:O	2.13	0.48
1:V:230:TYR:CE1	1:V:233:TYR:HD2	2.30	0.48
4:c:90:ARG:HD2	4:c:96:TYR:CD1	2.48	0.48
5:j:58:PRO:O	5:j:59:LEU:HD23	2.13	0.48
3:m:4:PHE:CE1	3:m:69:PRO:HD3	2.48	0.48
3:s:7:ILE:HD11	3:s:27:LEU:HD21	1.95	0.48
1:x:15:PHE:CD2	1:x:60:LYS:HD2	2.48	0.48
1:9:193:ASP:HB3	1:9:196:GLN:HB2	1.95	0.48
2:T:75:MET:HG2	3:e:72:PRO:HD2	1.95	0.48
2:T:88:THR:HG22	4:k:16:GLU:OE1	2.13	0.48
4:k:56:ALA:HB2	4:k:67:GLN:OE1	2.12	0.48
5:2:115:PHE:HB3	5:2:119:ALA:CB	2.43	0.48
1:U:14:GLN:HB2	1:U:54:ASP:HB2	1.95	0.48
2:Y:88:THR:OG1	4:a:16:GLU:HG2	2.12	0.48
5:b:55:VAL:HG12	5:b:57:ILE:HG13	1.95	0.48
1:C:311:LEU:HD13	5:j:70:TRP:CG	2.47	0.48
3:J:8:ARG:H	3:J:76:GLY:HA2	1.77	0.48
5:M:50:LYS:O	5:M:70:TRP:N	2.46	0.48
3:W:8:ARG:O	3:W:76:GLY:HA2	2.14	0.48
5:d:83:GLN:CD	5:d:83:GLN:N	2.71	0.48
1:f:14:GLN:NE2	1:f:54:ASP:OD1	2.46	0.48
5:j:128:ILE:HG23	5:j:129:VAL:N	2.28	0.48
4:u:14:ASN:O	4:u:19:ARG:NH2	2.44	0.48
5:v:169:LYS:O	5:v:172:GLU:HB2	2.14	0.48
5:1:103:ALA:HB3	5:1:167:VAL:HG21	1.95	0.48
1:3:90:LEU:HD23	1:3:91:LYS:N	2.28	0.48
5:2:114:CYS:HA	5:2:133:CYS:HB2	1.95	0.48
1:C:41:PHE:CZ	2:E:60:VAL:HG22	2.49	0.48
1:O:270:VAL:HG22	1:O:299:LEU:HD13	1.94	0.48
2:Q:79:TYR:CD2	2:Q:93:PHE:HD2	2.31	0.48
3:P:14:ILE:HD11	3:P:34:ILE:HG21	1.94	0.48
1:V:104:CYS:HB3	1:V:136:ARG:HG3	1.96	0.48
2:h:20:LYS:HE2	2:h:28:GLU:CD	2.37	0.48
4:o:27:ILE:HD13	4:o:110:TRP:CH2	2.48	0.48
1:w:69:ILE:HD13	1:w:139:MET:HG2	1.94	0.48
1:U:107:LEU:O	1:U:110:PRO:HD2	2.14	0.48
1:I:154:ARG:HA	1:I:157:ASP:OD2	2.13	0.48
2:Z:41:THR:O	2:Z:45:MET:HG3	2.13	0.48
5:j:78:ASP:HB3	5:j:80:HIS:CE1	2.48	0.48
5:j:127:ARG:O	5:j:128:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:146:SER:HA	1:r:150:ASN:OD1	2.14	0.48
2:n:62:PHE:CD1	2:n:62:PHE:N	2.82	0.48
4:o:103:LEU:HD11	5:p:9:ILE:CD1	2.42	0.48
5:p:32:SER:OG	5:p:33:ARG:N	2.45	0.48
2:t:19:VAL:HG22	2:t:33:ARG:HA	1.95	0.48
4:u:91:GLU:CD	4:u:94:LYS:HE2	2.38	0.48
2:z:41:THR:HG22	2:z:45:MET:SD	2.54	0.48
1:9:245:ALA:O	1:9:249:LEU:HB2	2.14	0.48
4:N:12:PHE:CD2	4:N:127:PHE:HB2	2.49	0.48
4:N:87:ASP:C	4:N:87:ASP:OD1	2.57	0.48
5:2:50:LYS:O	5:2:70:TRP:N	2.47	0.48
1:U:297:PHE:O	1:U:301:ASP:HB2	2.12	0.48
4:a:91:GLU:OE1	4:a:94:LYS:HE2	2.14	0.48
4:F:17:PHE:HD1	4:F:18:PHE:CE1	2.31	0.48
4:F:59:ALA:C	4:F:61:GLY:H	2.20	0.48
3:P:41:GLU:O	3:P:85:PHE:HE1	1.97	0.48
1:V:117:THR:C	1:V:118:LEU:HD23	2.39	0.48
5:d:21:TRP:O	5:d:25:VAL:HG22	2.14	0.48
1:l:211:GLU:OE1	1:l:215:ARG:NH1	2.47	0.48
5:v:50:LYS:O	5:v:70:TRP:N	2.40	0.48
5:v:132:ARG:NH2	1:x:84:GLN:OE1	2.47	0.48
4:6:12:PHE:CD2	4:6:127:PHE:HB2	2.48	0.48
5:q:28:HIS:CD2	5:q:163:LEU:HA	2.48	0.48
5:q:87:ILE:HG22	5:q:98:VAL:HB	1.95	0.48
1:U:30:LEU:HB3	1:U:72:PHE:CD2	2.49	0.48
3:X:37:ARG:NH2	3:X:41:GLU:HB3	2.29	0.48
4:a:29:TYR:CE2	4:a:44:PHE:CD1	3.02	0.48
5:b:127:ARG:O	5:b:128:ILE:HG22	2.13	0.48
1:C:14:GLN:O	1:C:16:GLU:N	2.42	0.48
4:L:32:PHE:N	4:L:32:PHE:HD1	2.11	0.48
4:c:90:ARG:HD2	4:c:96:TYR:CE1	2.49	0.48
5:j:142:VAL:HG23	5:j:143:GLY:N	2.29	0.48
5:1:32:SER:OG	5:1:33:ARG:N	2.46	0.48
1:3:135:VAL:O	1:3:139:MET:HG3	2.13	0.48
4:6:151:ARG:HH21	5:7:113:ASP:HA	1.78	0.48
1:9:25:ILE:HD13	1:9:39:GLN:HB3	1.96	0.48
3:X:43:ARG:HE	3:X:50:LEU:HD11	1.78	0.48
1:C:93:TYR:CE1	1:C:143:TRP:HZ2	2.31	0.48
1:C:228:GLN:CD	1:C:292:LYS:HD3	2.38	0.48
1:I:214:TYR:CE1	1:I:237:LYS:HD3	2.49	0.48
1:O:57:GLY:N	1:O:58:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:103:GLN:O	1:V:106:ILE:N	2.47	0.48
1:f:115:GLU:HG2	1:f:118:LEU:HD12	1.96	0.48
4:i:86:VAL:HG23	4:i:97:LEU:CD2	2.43	0.48
5:p:149:ALA:O	5:p:152:ALA:HB3	2.12	0.48
1:r:300:MET:CB	1:r:307:ILE:HD12	2.44	0.48
3:s:49:GLN:HG3	3:s:50:LEU:N	2.27	0.48
5:v:42:HIS:HB2	5:v:44:TYR:CE1	2.48	0.48
5:v:69:TYR:HE1	5:v:86:SER:HB3	1.79	0.48
4:0:72:SER:HB2	4:0:73:TRP:CD1	2.48	0.48
4:0:85:TYR:CE1	4:0:98:LYS:HB3	2.49	0.48
5:1:22:LYS:HD3	5:1:40:TYR:OH	2.12	0.48
3:4:8:ARG:O	3:4:76:GLY:HA2	2.13	0.48
1:9:113:GLN:HE21	1:9:116:ILE:HD12	1.79	0.48
5:G:28:HIS:C	5:G:35:ALA:HB3	2.39	0.48
1:I:75:GLN:O	1:I:79:ARG:HG2	2.14	0.48
1:I:90:LEU:HD23	1:I:90:LEU:O	2.14	0.48
1:I:199:ARG:HG2	1:I:203:GLU:CD	2.38	0.48
4:L:54:GLU:O	4:L:54:GLU:HG2	2.13	0.48
1:O:188:CYS:SG	1:O:194:LYS:O	2.64	0.48
5:S:86:SER:C	5:S:87:ILE:HG13	2.38	0.48
1:V:85:ASP:O	1:V:89:LEU:N	2.47	0.48
1:f:19:TRP:CE3	1:f:22:MET:HE3	2.49	0.48
1:r:94:ILE:CD1	1:r:179:GLY:HA3	2.44	0.48
1:r:245:ALA:HB2	1:r:261:LEU:HD12	1.96	0.48
1:3:14:GLN:O	1:3:16:GLU:N	2.45	0.48
1:9:14:GLN:HB2	1:9:54:ASP:HB2	1.95	0.48
5:q:108:HIS:CE1	5:q:112:PHE:HB2	2.49	0.48
4:a:32:PHE:N	4:a:32:PHE:HD1	2.12	0.48
1:C:314:LEU:HD13	5:j:15:ARG:CZ	2.44	0.48
2:E:72:LYS:HD3	2:E:72:LYS:HA	1.68	0.48
4:F:9:ARG:O	4:F:13:GLU:HG3	2.13	0.48
1:I:14:GLN:CG	1:I:15:PHE:H	2.26	0.48
1:I:151:ILE:HG13	1:I:155:LEU:CD1	2.44	0.48
2:K:83:TYR:CE2	2:K:91:PRO:HG3	2.49	0.48
1:O:19:TRP:HE1	1:O:23:ARG:CG	2.15	0.48
5:S:116:SER:H	5:S:119:ALA:HB2	1.78	0.48
1:V:97:TRP:CZ3	1:V:101:PHE:HB2	2.48	0.48
5:d:108:HIS:ND1	5:d:108:HIS:O	2.47	0.48
1:f:100:PHE:CD2	1:f:143:TRP:CE3	3.02	0.48
4:o:14:ASN:C	4:o:19:ARG:NH2	2.71	0.48
5:p:86:SER:O	5:p:87:ILE:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:p:157:LYS:O	5:p:158:GLN:HG3	2.14	0.48
2:t:41:THR:O	2:t:44:ALA:HB3	2.14	0.48
3:s:68:ARG:HB3	3:s:69:PRO:HD2	1.96	0.48
2:5:65:ILE:HA	2:5:66:PRO:HD3	1.73	0.48
4:a:157:ASP:HB2	5:b:118:SER:HB3	1.96	0.48
1:C:167:ARG:CZ	1:C:241:GLU:OE1	2.62	0.48
1:I:230:TYR:HD1	1:I:233:TYR:HD2	1.59	0.48
1:O:86:ASP:OD1	1:O:154:ARG:NH2	2.47	0.48
4:R:27:ILE:O	4:R:27:ILE:HG13	2.13	0.48
5:S:85:VAL:HG21	5:S:170:LEU:HG	1.94	0.48
1:V:62:HIS:C	1:V:62:HIS:ND1	2.72	0.48
1:V:280:GLU:N	1:V:280:GLU:OE1	2.46	0.48
2:Z:22:ILE:HG12	2:Z:60:VAL:O	2.12	0.48
1:r:38:GLN:NE2	1:r:42:ASP:OD1	2.28	0.48
2:t:39:SER:OG	2:t:42:ILE:HG13	2.14	0.48
1:x:315:GLU:O	1:x:319:ILE:HG13	2.14	0.48
2:z:74:CYS:O	2:z:77:PHE:HB2	2.12	0.48
4:0:31:GLY:H	4:0:40:ARG:HH12	1.62	0.48
4:N:94:LYS:HG2	4:N:115:ASP:HA	1.95	0.48
4:a:59:ALA:O	4:a:60:THR:HG22	2.13	0.47
5:G:43:HIS:HB3	5:G:52:SER:O	2.14	0.47
1:I:115:GLU:OE2	1:I:134:ILE:HB	2.14	0.47
1:I:185:VAL:HG22	1:I:198:TYR:CD2	2.49	0.47
1:I:282:GLN:O	1:I:286:LYS:HG2	2.13	0.47
3:P:16:THR:OG1	3:P:17:ASP:N	2.46	0.47
4:R:127:PHE:HE1	4:R:129:GLU:HA	1.77	0.47
5:S:139:HIS:CD2	5:S:139:HIS:N	2.82	0.47
4:i:32:PHE:H	4:i:32:PHE:HD1	1.62	0.47
5:j:140:ASN:OD1	5:j:167:ARG:HD3	2.14	0.47
2:n:89:GLU:HG3	2:n:89:GLU:O	2.13	0.47
5:1:149:LEU:HA	5:1:149:LEU:HD23	1.73	0.47
1:3:230:TYR:OH	1:3:269:LEU:O	2.25	0.47
2:T:73:VAL:O	2:T:76:TYR:HB3	2.14	0.47
3:e:20:GLU:OE2	3:e:64:SER:N	2.44	0.47
3:e:43:ARG:HG3	3:e:50:LEU:HD21	1.95	0.47
1:w:144:ASN:O	1:w:149:SER:OG	2.24	0.47
4:N:21:LEU:CD2	4:N:64:LEU:HD11	2.44	0.47
1:U:147:ILE:HG22	1:U:151:ILE:HD11	1.96	0.47
5:b:3:ASN:H	5:b:3:ASN:ND2	1.98	0.47
2:E:72:LYS:O	2:E:75:MET:HB2	2.15	0.47
4:F:62:THR:HG21	4:F:64:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:15:PHE:CD1	1:O:15:PHE:C	2.91	0.47
1:O:142:THR:O	1:O:146:SER:HB3	2.14	0.47
5:S:104:ASP:CG	5:S:167:VAL:HG23	2.39	0.47
1:V:193:ASP:OD1	1:V:196:GLN:N	2.46	0.47
4:c:84:GLU:OE1	4:c:84:GLU:N	2.44	0.47
5:d:52:SER:OG	5:d:70:TRP:CD1	2.67	0.47
4:i:54:GLU:OE2	5:j:50:LYS:NZ	2.46	0.47
3:m:57:LEU:O	3:m:62:PHE:HB2	2.14	0.47
3:m:70:GLN:H	3:m:70:GLN:HG3	1.18	0.47
5:v:119:ALA:O	5:v:123:THR:HG23	2.14	0.47
2:z:90:ILE:HG23	2:z:90:ILE:O	2.15	0.47
4:k:13:GLU:HG2	4:k:13:GLU:H	1.52	0.47
1:U:114:LEU:O	1:U:118:LEU:HG	2.14	0.47
4:a:12:PHE:HA	4:a:18:PHE:CD2	2.49	0.47
5:M:62:ALA:HB2	5:M:91:LYS:HB2	1.97	0.47
3:W:88:LEU:HD22	3:W:89:CYS:N	2.29	0.47
5:d:33:ARG:O	5:d:36:LYS:HB3	2.13	0.47
5:j:134:GLU:OE2	5:j:163:LEU:HD11	2.13	0.47
1:r:97:TRP:CZ2	1:r:101:PHE:CD2	3.02	0.47
4:0:73:TRP:CD1	4:0:73:TRP:N	2.81	0.47
3:4:7:ILE:HD11	3:4:16:THR:HG21	1.95	0.47
1:9:111:PHE:O	1:9:114:LEU:HB3	2.14	0.47
1:9:267:ASN:HA	1:9:271:THR:OG1	2.14	0.47
2:T:107:ALA:CB	5:q:145:LEU:HB3	2.44	0.47
5:q:76:GLU:OE2	5:q:78:ASP:N	2.47	0.47
4:a:156:ARG:HA	5:b:117:GLU:HG3	1.97	0.47
1:C:166:GLU:OE2	1:C:248:TYR:OH	2.15	0.47
1:O:109:LYS:HB2	1:O:110:PRO:HD3	1.96	0.47
5:S:125:LEU:HD13	5:S:127:ARG:NH1	2.29	0.47
1:f:303:VAL:HG12	1:f:306:GLY:H	1.79	0.47
4:i:11:LYS:HE2	4:i:147:ARG:CZ	2.45	0.47
2:n:107:ALA:C	5:p:146:GLN:HE21	2.22	0.47
5:p:101:ASP:O	5:p:140:ASN:ND2	2.48	0.47
1:r:167:ARG:HH22	1:r:210:THR:HG1	1.56	0.47
4:0:103:LEU:HD23	4:0:108:VAL:HG21	1.96	0.47
1:3:113:GLN:O	1:3:117:THR:HG23	2.14	0.47
2:5:17:MET:HG3	2:5:18:TYR:CD1	2.50	0.47
2:5:86:SER:HB2	4:6:16:GLU:OE2	2.14	0.47
1:9:55:ASP:HA	5:q:121:ARG:HH22	1.79	0.47
1:9:90:LEU:HD13	1:9:158:SER:HB3	1.96	0.47
1:9:144:ASN:HD22	1:9:145:GLU:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:k:59:ALA:O	4:k:60:THR:HG22	2.14	0.47
1:w:160:MET:HE2	1:w:160:MET:HA	1.96	0.47
3:X:37:ARG:HD3	3:X:79:PHE:CZ	2.49	0.47
1:I:65:LEU:O	1:I:69:ILE:HG12	2.15	0.47
3:P:2:ASP:N	3:P:2:ASP:OD1	2.47	0.47
4:R:131:ARG:HG2	4:R:135:GLU:HG2	1.97	0.47
1:V:101:PHE:HA	1:V:104:CYS:SG	2.55	0.47
1:l:41:PHE:CD1	2:n:45:MET:HE2	2.49	0.47
2:n:75:MET:HE2	3:m:72:PRO:HD2	1.96	0.47
2:n:76:TYR:CG	5:p:145:LEU:HG	2.49	0.47
4:o:85:TYR:CE2	4:o:98:LYS:HD2	2.49	0.47
1:r:86:ASP:OD1	1:r:154:ARG:NH2	2.47	0.47
3:4:42:GLN:HB3	3:4:77:LEU:CD1	2.43	0.47
2:T:58:ASN:HD22	2:T:58:ASN:N	2.13	0.47
2:T:76:TYR:CD2	5:q:145:LEU:HG	2.49	0.47
4:k:55:ILE:HD11	4:k:86:VAL:HG21	1.97	0.47
5:q:79:TRP:O	5:q:81:LEU:HD23	2.15	0.47
1:w:117:THR:C	1:w:118:LEU:HD23	2.39	0.47
1:w:303:VAL:CG2	1:w:304:PRO:HD2	2.41	0.47
4:a:88:LEU:H	4:a:88:LEU:CD2	2.25	0.47
5:b:53:SER:O	5:b:54:GLU:HG3	2.15	0.47
5:b:70:TRP:O	5:b:72:LEU:N	2.47	0.47
2:E:102:GLU:O	2:E:105:MET:HB2	2.15	0.47
4:L:97:LEU:O	4:L:111:LYS:HA	2.14	0.47
1:O:97:TRP:NE1	1:O:179:GLY:O	2.47	0.47
3:W:63:THR:H	3:W:66:THR:HG23	1.80	0.47
5:d:38:TRP:CD2	5:d:57:ILE:HG12	2.50	0.47
2:h:35:HIS:O	2:h:38:THR:OG1	2.24	0.47
4:u:152:GLU:HG3	5:v:139:HIS:HE1	1.79	0.47
4:k:67:GLN:NE2	5:q:72:LEU:HD13	2.30	0.47
4:N:114:ILE:HA	4:N:121:GLY:HA3	1.96	0.47
2:Y:109:PHE:C	2:Y:109:PHE:CD1	2.93	0.47
5:b:13:VAL:HG21	5:b:18:ILE:HG13	1.97	0.47
5:b:28:HIS:NE2	5:b:161:PRO:O	2.45	0.47
1:I:243:LYS:HB2	1:I:243:LYS:HE3	1.66	0.47
1:I:246:LEU:HD23	1:I:258:VAL:HG11	1.97	0.47
1:O:13:LEU:HA	1:O:17:ASP:OD2	2.14	0.47
1:O:19:TRP:O	1:O:23:ARG:HG3	2.14	0.47
1:O:172:PHE:CD1	1:O:172:PHE:C	2.92	0.47
1:O:307:ILE:O	1:O:311:LEU:HG	2.15	0.47
1:V:223:GLN:NE2	1:V:223:GLN:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:68:ARG:HB3	3:W:69:PRO:HD2	1.97	0.47
1:l:93:TYR:HD2	1:l:151:ILE:HD11	1.80	0.47
1:l:274:LYS:HG2	1:l:275:GLU:N	2.30	0.47
3:m:23:THR:HA	3:m:56:THR:HA	1.97	0.47
5:p:64:LEU:HD23	5:p:66:ILE:HD11	1.97	0.47
1:r:178:ILE:HG22	1:r:181:ARG:HH12	1.80	0.47
1:x:14:GLN:O	1:x:14:GLN:HG3	2.15	0.47
1:x:106:ILE:HA	1:x:109:LYS:HD2	1.97	0.47
3:y:50:LEU:HD13	3:y:51:LEU:N	2.30	0.47
4:0:67:GLN:NE2	5:1:72:LEU:HD22	2.29	0.47
1:3:66:LYS:HA	1:3:138:LEU:HD21	1.95	0.47
2:5:98:GLU:HG2	2:5:99:ILE:N	2.29	0.47
4:6:9:ARG:HB3	4:6:127:PHE:CZ	2.50	0.47
3:e:42:GLN:HB3	3:e:77:LEU:HD11	1.96	0.47
4:k:37:HIS:HE1	4:k:41:GLN:NE2	2.11	0.47
4:k:85:TYR:CE2	4:k:98:LYS:HD3	2.50	0.47
5:2:29:MET:HE2	5:2:30:TYR:CE1	2.50	0.47
5:2:134:GLU:OE1	5:2:135:TYR:N	2.34	0.47
4:L:152:GLU:HG3	5:M:139:HIS:HE1	1.78	0.47
1:f:77:GLN:HG2	1:f:81:LEU:HD22	1.96	0.47
2:h:72:LYS:HE3	2:h:93:PHE:HE1	1.80	0.47
2:n:109:PHE:C	2:n:109:PHE:CD1	2.92	0.47
5:p:111:TYR:O	5:p:112:PHE:CD1	2.68	0.47
1:x:58:PRO:CD	1:x:59:ALA:N	2.50	0.47
1:x:267:ASN:O	1:x:271:THR:HB	2.15	0.47
5:1:137:ALA:O	5:1:140:ASN:OD1	2.33	0.47
2:5:23:SER:N	2:5:27:HIS:O	2.43	0.47
2:T:77:PHE:O	2:T:81:VAL:HG22	2.14	0.47
4:k:73:TRP:O	5:q:47:THR:HG23	2.14	0.47
3:H:37:ARG:HH21	3:H:41:GLU:HB3	1.78	0.47
5:2:22:LYS:HD3	5:2:40:TYR:OH	2.15	0.47
3:X:37:ARG:HH21	3:X:41:GLU:CD	2.22	0.47
1:C:174:SER:OG	1:C:247:ARG:NH1	2.48	0.47
2:E:46:LEU:HD13	2:E:46:LEU:HA	1.72	0.47
4:F:17:PHE:CD1	4:F:18:PHE:CE1	3.03	0.47
5:G:114:CYS:O	5:G:131:PRO:HG2	2.14	0.47
1:I:48:HIS:O	1:I:51:CYS:HB2	2.14	0.47
3:J:63:THR:OG1	3:J:66:THR:HG23	2.15	0.47
1:O:86:ASP:O	1:O:89:LEU:HB3	2.15	0.47
1:O:211:GLU:O	1:O:215:ARG:HB2	2.15	0.47
2:Q:25:ASP:O	3:P:11:LYS:NZ	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7:ILE:CG2	3:P:77:LEU:HD13	2.45	0.47
2:Z:104:LEU:HD11	5:d:150:LEU:HD13	1.97	0.47
1:f:135:VAL:HG12	1:f:136:ARG:N	2.29	0.47
1:f:167:ARG:NH2	1:f:210:THR:CG2	2.78	0.47
3:g:42:GLN:HB3	3:g:77:LEU:HD11	1.96	0.47
1:l:194:LYS:HA	1:l:194:LYS:HD2	1.59	0.47
4:o:11:LYS:O	4:o:15:GLU:HB2	2.14	0.47
5:p:39:PHE:N	5:p:39:PHE:CD1	2.83	0.47
1:U:113:GLN:O	1:U:117:THR:OG1	2.20	0.47
1:U:194:LYS:HA	1:U:194:LYS:HD2	1.45	0.47
2:Y:109:PHE:C	2:Y:109:PHE:HD1	2.23	0.47
5:M:17:ARG:HD3	5:M:168:LYS:O	2.15	0.47
5:M:104:ASP:OD1	5:M:135:TYR:OH	2.33	0.47
5:M:117:GLU:H	5:M:117:GLU:HG3	1.56	0.47
1:O:57:GLY:O	1:O:61:ILE:HG22	2.15	0.47
5:S:128:ILE:HG12	5:S:129:VAL:H	1.80	0.47
1:V:180:VAL:HG12	1:V:202:PHE:CE2	2.50	0.47
4:c:8:GLN:OE1	4:c:106:VAL:HA	2.15	0.47
5:d:104:ASP:OD1	5:d:166:VAL:HG13	2.14	0.47
1:f:28:LYS:O	1:f:32:GLN:N	2.48	0.47
3:g:77:LEU:HD21	3:g:79:PHE:CZ	2.50	0.47
4:i:34:ASP:N	4:i:34:ASP:OD1	2.48	0.47
4:i:83:ARG:NH2	4:i:128:ASP:OD2	2.48	0.47
3:m:23:THR:O	3:m:26:GLU:HB2	2.15	0.47
3:s:8:ARG:HE	3:s:8:ARG:HB3	1.53	0.47
1:x:109:LYS:HB2	1:x:110:PRO:HD3	1.96	0.47
2:z:82:ARG:HD2	2:z:83:TYR:CE1	2.50	0.47
3:y:26:GLU:O	3:y:29:ARG:HB3	2.15	0.47
4:6:11:LYS:CD	4:6:147:ARG:HH12	2.26	0.47
4:6:101:MET:H	4:6:101:MET:HG2	1.51	0.47
4:k:7:ASP:O	4:k:11:LYS:HG2	2.15	0.47
3:H:8:ARG:HE	3:H:13:THR:HB	1.80	0.47
5:b:104:ASP:OD2	5:b:167:ARG:HG3	2.15	0.46
4:F:31:GLY:H	4:F:40:ARG:HH12	1.62	0.46
1:I:281:CYS:O	1:I:285:ILE:HD12	2.14	0.46
5:S:8:MET:SD	5:S:97:GLN:NE2	2.88	0.46
5:S:115:PHE:HB3	5:S:119:ALA:CB	2.45	0.46
5:S:120:ILE:O	5:S:124:ILE:HD12	2.15	0.46
1:V:74:LYS:HE2	1:V:74:LYS:HB2	1.68	0.46
1:l:93:TYR:CD1	1:l:93:TYR:C	2.93	0.46
2:n:60:VAL:HG12	2:n:62:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:37:ARG:NH2	3:m:41:GLU:OE1	2.34	0.46
5:p:29:MET:HE2	5:p:30:TYR:CE1	2.51	0.46
1:r:278:LEU:HA	1:r:296:MET:HE1	1.97	0.46
3:s:45:TYR:CE2	3:s:50:LEU:HD23	2.50	0.46
4:u:111:LYS:HE3	4:u:111:LYS:HB3	1.50	0.46
1:x:188:CYS:HB2	1:x:197:ILE:HG12	1.98	0.46
1:w:242:GLU:O	1:w:246:LEU:HG	2.14	0.46
5:2:62:ALA:HB2	5:2:91:LYS:HB2	1.97	0.46
2:Y:62:PHE:CD2	2:Y:65:ILE:HD11	2.50	0.46
4:F:85:TYR:CD1	4:F:85:TYR:C	2.93	0.46
5:G:32:SER:OG	5:G:33:ARG:N	2.49	0.46
4:L:24:GLU:HA	4:L:124:CYS:HB3	1.97	0.46
5:M:37:ASP:OD1	5:M:37:ASP:N	2.48	0.46
3:s:4:PHE:N	3:s:4:PHE:CD1	2.83	0.46
3:s:23:THR:OG1	3:s:26:GLU:HG3	2.15	0.46
4:u:31:GLY:H	4:u:40:ARG:HH12	1.62	0.46
2:5:41:THR:O	2:5:45:MET:HG3	2.15	0.46
3:4:6:MET:HA	3:4:14:ILE:O	2.14	0.46
5:7:69:TYR:HB3	5:7:72:LEU:HD11	1.96	0.46
1:9:190:ASN:OD1	1:9:192:GLU:N	2.48	0.46
1:w:31:ARG:NH1	1:w:75:GLN:HE22	2.12	0.46
1:w:237:LYS:HA	1:w:237:LYS:HD3	1.77	0.46
5:2:51:ILE:HG12	5:2:69:TYR:CE1	2.49	0.46
5:2:134:GLU:CG	5:2:158:LYS:HB2	2.37	0.46
2:E:88:THR:HG22	4:F:16:GLU:OE2	2.14	0.46
5:G:112:PHE:HE1	5:G:163:LEU:HD22	1.76	0.46
1:I:115:GLU:CD	1:I:134:ILE:H	2.23	0.46
4:R:152:GLU:HG3	5:S:139:HIS:CE1	2.50	0.46
1:V:206:TYR:HE1	1:V:261:LEU:HD12	1.80	0.46
2:Z:58:ASN:HD22	2:Z:58:ASN:N	2.13	0.46
4:o:141:GLN:NE2	4:o:145:GLU:OE1	2.48	0.46
1:3:98:ARG:O	1:3:102:THR:OG1	2.33	0.46
4:6:141:GLN:O	4:6:144:GLU:HB3	2.14	0.46
5:7:33:ARG:O	5:7:36:LYS:HB3	2.15	0.46
1:9:186:ASN:HD22	1:9:186:ASN:H	1.63	0.46
5:q:122:ASN:HB3	5:q:128:ILE:O	2.15	0.46
5:2:77:ARG:HA	5:2:77:ARG:HD3	1.80	0.46
4:L:114:ILE:HD13	4:L:121:GLY:HA3	1.98	0.46
5:M:133:CYS:SG	5:M:134:GLU:O	2.74	0.46
1:V:29:LEU:HA	1:V:29:LEU:HD23	1.64	0.46
1:V:86:ASP:C	1:V:89:LEU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:83:TYR:CE1	2:t:91:PRO:HD3	2.51	0.46
5:v:52:SER:HB2	5:v:68:THR:HG1	1.79	0.46
1:3:181:ARG:O	1:3:185:VAL:HG23	2.15	0.46
5:7:91:LYS:O	5:7:94:TYR:HB3	2.16	0.46
1:9:266:VAL:HG11	1:9:302:LYS:CB	2.40	0.46
2:B:104:LEU:HD22	5:2:124:ILE:HD11	1.97	0.46
4:N:21:LEU:HA	4:N:21:LEU:HD23	1.75	0.46
1:U:231:MET:SD	1:U:296:MET:HG2	2.56	0.46
4:a:116:LEU:HD23	4:a:116:LEU:HA	1.80	0.46
5:M:106:LEU:O	5:M:109:LEU:HB2	2.16	0.46
5:S:59:LEU:HD23	5:S:110:HIS:ND1	2.31	0.46
2:Z:98:GLU:HG2	2:Z:99:ILE:N	2.30	0.46
3:W:2:ASP:OD1	3:W:2:ASP:N	2.48	0.46
3:W:45:TYR:N	3:W:45:TYR:CD1	2.84	0.46
3:g:4:PHE:CE2	3:g:69:PRO:HB3	2.51	0.46
4:i:90:ARG:HD2	4:i:96:TYR:CE1	2.50	0.46
5:j:86:SER:C	5:j:87:ILE:HG12	2.40	0.46
4:u:32:PHE:N	4:u:32:PHE:HD1	2.14	0.46
2:z:65:ILE:H	2:z:65:ILE:HG12	1.44	0.46
3:4:43:ARG:HB2	3:4:85:PHE:CZ	2.50	0.46
4:6:57:PHE:CE2	4:6:97:LEU:HD13	2.51	0.46
4:6:141:GLN:O	4:6:145:GLU:HG3	2.14	0.46
1:9:271:THR:O	1:9:274:LYS:HB3	2.15	0.46
5:q:100:PRO:CG	5:q:170:THR:HG21	2.45	0.46
1:U:181:ARG:HB2	1:U:202:PHE:CE2	2.51	0.46
4:a:42:ALA:O	4:a:46:ASN:ND2	2.49	0.46
1:I:16:GLU:OE1	1:I:16:GLU:N	2.48	0.46
1:O:195:LEU:HD21	1:O:255:CYS:HB2	1.98	0.46
1:O:314:LEU:O	1:O:318:ILE:HG23	2.15	0.46
2:Q:42:ILE:HA	2:Q:45:MET:HE2	1.98	0.46
3:P:4:PHE:C	3:P:5:LEU:HD23	2.41	0.46
2:Z:32:LYS:HB2	2:Z:32:LYS:HE3	1.64	0.46
5:d:119:ALA:O	5:d:123:THR:OG1	2.29	0.46
3:g:27:LEU:HD12	3:g:57:LEU:HD21	1.98	0.46
3:g:52:ASP:HB2	3:g:55:LYS:HB2	1.96	0.46
1:l:97:TRP:HE1	1:l:182:GLU:HB2	1.81	0.46
2:n:48:GLY:HA3	2:n:49:PRO:HD2	1.82	0.46
1:r:138:LEU:O	1:r:142:THR:OG1	2.24	0.46
1:x:306:GLY:O	1:x:309:PRO:HD2	2.15	0.46
4:0:50:ASP:OD1	4:0:51:GLY:N	2.48	0.46
1:3:12:SER:HB2	1:3:13:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:29:TYR:HD2	4:6:119:LEU:HD13	1.81	0.46
5:7:117:GLU:H	5:7:117:GLU:HG3	1.39	0.46
4:k:69:PHE:O	5:q:6:GLN:N	2.39	0.46
5:q:129:VAL:HG22	5:q:130:SER:N	2.30	0.46
1:C:103:GLN:O	1:C:106:ILE:N	2.48	0.46
1:C:211:GLU:OE1	1:C:215:ARG:NH2	2.49	0.46
4:F:155:ASP:HB2	5:G:116:SER:HA	1.97	0.46
1:I:104:CYS:SG	1:I:139:MET:HE2	2.55	0.46
3:J:91:GLU:HA	3:J:92:PRO:HD3	1.83	0.46
4:L:118:ARG:HE	4:L:120:ASP:CB	2.24	0.46
1:f:13:LEU:HB3	1:f:18:LYS:HE2	1.97	0.46
1:r:111:PHE:O	1:r:114:LEU:N	2.45	0.46
5:v:100:PRO:HB3	5:v:167:VAL:HG23	1.98	0.46
1:x:15:PHE:CE2	1:x:60:LYS:HD2	2.51	0.46
2:z:58:ASN:N	2:z:58:ASN:HD22	2.14	0.46
4:0:9:ARG:O	4:0:13:GLU:HG3	2.16	0.46
1:9:166:GLU:HB2	1:9:172:PHE:CE1	2.51	0.46
2:T:73:VAL:HG12	2:T:77:PHE:CE1	2.46	0.46
5:q:3:ASN:HD22	5:q:3:ASN:N	2.13	0.46
4:N:87:ASP:OD1	4:N:89:GLU:N	2.48	0.46
1:U:211:GLU:O	1:U:215:ARG:HB2	2.16	0.46
3:X:39:PRO:HA	3:X:42:GLN:HG3	1.96	0.46
4:a:29:TYR:HE1	4:a:31:GLY:HA3	1.80	0.46
2:E:58:ASN:HD22	2:E:58:ASN:N	2.13	0.46
3:P:46:LYS:HB2	3:P:51:LEU:HD21	1.98	0.46
5:S:156:LYS:HA	5:S:156:LYS:HD2	1.58	0.46
1:V:167:ARG:NH2	1:V:210:THR:HG23	2.31	0.46
4:c:130:GLU:O	4:c:134:GLN:HG3	2.16	0.46
1:f:198:TYR:CD1	1:f:198:TYR:C	2.93	0.46
1:f:222:LEU:HD21	1:f:227:VAL:HG13	1.97	0.46
1:f:246:LEU:HD23	1:f:258:VAL:HG11	1.98	0.46
1:x:109:LYS:HE3	2:z:47:SER:OG	2.16	0.46
1:x:220:SER:O	1:x:224:GLN:HG3	2.16	0.46
2:5:30:ILE:HB	3:4:14:ILE:HG12	1.98	0.46
3:D:27:LEU:HD12	3:D:57:LEU:HD21	1.98	0.46
1:I:15:PHE:HA	1:I:50:VAL:HG22	1.98	0.46
1:I:100:PHE:HE2	1:I:143:TRP:HB2	1.80	0.46
2:K:73:VAL:O	2:K:77:PHE:CD1	2.69	0.46
1:O:207:LEU:O	1:O:210:THR:HB	2.16	0.46
3:P:7:ILE:O	3:P:13:THR:HA	2.16	0.46
5:S:24:LEU:CD2	5:S:163:PRO:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:63:GLN:HG3	1:V:64:ALA:N	2.31	0.46
5:d:134:GLU:OE2	5:d:158:GLN:N	2.49	0.46
1:l:152:LYS:HE3	1:l:184:TYR:OH	2.15	0.46
1:r:23:ARG:HB2	1:r:24:PRO:HD3	1.98	0.46
4:u:26:GLU:O	4:u:60:THR:HG23	2.16	0.46
1:x:30:LEU:HD23	1:x:72:PHE:HD2	1.81	0.46
1:3:231:MET:HE3	1:3:295:LEU:HD23	1.98	0.46
4:6:56:ALA:HB2	4:6:67:GLN:HE22	1.79	0.46
4:6:111:LYS:HE3	4:6:111:LYS:HB3	1.57	0.46
5:7:27:HIS:O	5:7:31:ILE:N	2.47	0.46
1:9:44:PHE:CZ	1:9:110:PRO:HA	2.50	0.46
4:k:129:GLU:O	4:k:133:GLN:HG3	2.16	0.46
2:B:107:ALA:CB	5:2:147:GLN:HG3	2.46	0.46
5:2:58:PRO:O	5:2:111:TYR:OH	2.26	0.46
4:F:43:ARG:HH11	4:F:43:ARG:HG3	1.80	0.46
1:I:13:LEU:C	1:I:13:LEU:HD22	2.41	0.46
1:I:31:ARG:HH21	1:I:75:GLN:HE22	1.63	0.46
5:S:130:SER:HA	5:S:131:PRO:HA	1.63	0.46
1:V:77:GLN:HB2	1:V:147:ILE:HG12	1.97	0.46
1:f:153:ASN:O	1:f:157:ASP:OD1	2.34	0.46
1:l:41:PHE:HE1	2:n:60:VAL:HG22	1.80	0.46
2:n:23:SER:OG	2:n:24:SER:N	2.49	0.46
3:m:43:ARG:CG	3:m:50:LEU:HD21	2.42	0.46
1:r:100:PHE:CZ	1:r:139:MET:HE2	2.51	0.46
2:t:84:THR:HA	5:v:143:VAL:HG21	1.96	0.46
1:x:167:ARG:HB3	1:x:213:PHE:CZ	2.51	0.46
5:1:52:SER:HB2	5:1:68:THR:OG1	2.16	0.46
5:7:6:GLN:O	5:7:6:GLN:HG3	2.13	0.46
4:k:59:ALA:HB3	4:k:62:THR:OG1	2.16	0.46
1:w:83:HIS:HB2	1:w:89:LEU:HB2	1.96	0.46
1:w:157:ASP:OD1	1:w:157:ASP:N	2.48	0.46
1:I:151:ILE:HG13	1:I:155:LEU:HD11	1.98	0.45
3:J:32:GLU:O	3:J:36:LYS:HA	2.16	0.45
1:O:89:LEU:CD2	1:O:154:ARG:HE	2.28	0.45
1:O:194:LYS:HE3	1:O:194:LYS:HB3	1.47	0.45
3:P:9:ARG:HB2	3:P:77:LEU:CB	2.41	0.45
1:V:103:GLN:HE22	1:V:106:ILE:HD12	1.81	0.45
1:f:167:ARG:HH22	1:f:210:THR:CG2	2.29	0.45
4:i:151:ARG:NE	5:j:114:CYS:HB2	2.30	0.45
5:j:15:ARG:O	5:j:19:ASN:ND2	2.42	0.45
1:l:52:LEU:O	5:p:121:ARG:NH2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:166:GLU:OE1	1:l:244:ARG:NE	2.36	0.45
2:t:90:ILE:HG23	2:t:90:ILE:O	2.16	0.45
1:x:57:GLY:N	1:x:58:PRO:HD3	2.31	0.45
5:1:128:ILE:HG23	5:1:129:VAL:N	2.31	0.45
1:3:172:PHE:CD1	1:3:172:PHE:C	2.94	0.45
3:4:28:LYS:HB3	3:4:39:PRO:HB3	1.99	0.45
4:6:16:GLU:HA	4:6:19:ARG:HD2	1.97	0.45
1:9:19:TRP:HA	1:9:22:MET:HG3	1.98	0.45
1:w:41:PHE:CZ	2:B:60:VAL:HG22	2.51	0.45
1:w:144:ASN:HB2	1:w:187:LEU:HD13	1.98	0.45
4:N:59:ALA:HB3	4:N:62:THR:CG2	2.46	0.45
1:C:29:LEU:HA	1:C:29:LEU:HD23	1.69	0.45
1:C:85:ASP:HB2	1:C:88:ALA:HB3	1.98	0.45
1:C:245:ALA:O	1:C:249:LEU:HB2	2.16	0.45
4:F:109:ILE:HD11	4:F:128:ASP:CG	2.41	0.45
5:G:103:ALA:O	5:G:107:ILE:HG13	2.15	0.45
1:I:23:ARG:NH1	1:I:68:ASP:OD2	2.48	0.45
5:M:86:SER:C	5:M:87:ILE:HG13	2.40	0.45
5:M:105:GLN:O	5:M:109:LEU:HD23	2.16	0.45
1:V:56:LYS:C	1:V:58:PRO:HD3	2.41	0.45
4:c:64:LEU:HD23	4:c:64:LEU:C	2.41	0.45
2:t:23:SER:OG	2:t:24:SER:N	2.48	0.45
2:t:58:ASN:HD22	2:t:58:ASN:N	2.14	0.45
2:z:72:LYS:NZ	2:z:94:PRO:O	2.49	0.45
4:6:131:ARG:NH2	4:6:135:GLU:OE2	2.49	0.45
1:9:21:PHE:O	1:9:24:PRO:HD2	2.17	0.45
5:q:72:LEU:O	5:q:81:LEU:HB3	2.16	0.45
4:L:113:TRP:HZ3	4:L:115:ASP:HB2	1.81	0.45
5:d:17:ARG:HH22	5:d:168:LYS:CE	2.27	0.45
5:j:32:SER:OG	5:j:33:ARG:N	2.48	0.45
4:o:27:ILE:HD13	4:o:110:TRP:HH2	1.81	0.45
2:t:76:TYR:CG	5:v:146:LEU:HG	2.51	0.45
5:v:62:ALA:HB2	5:v:91:LYS:HB2	1.98	0.45
2:z:99:ILE:O	2:z:103:LEU:HB2	2.17	0.45
3:e:68:ARG:HB3	3:e:69:PRO:HD2	1.98	0.45
2:B:23:SER:HB3	2:B:27:HIS:N	2.31	0.45
5:2:41:ARG:NH2	5:2:56:HIS:CE1	2.85	0.45
3:D:37:ARG:NH2	3:D:41:GLU:OE1	2.48	0.45
1:I:97:TRP:CZ2	1:I:101:PHE:CG	3.05	0.45
1:I:273:PHE:N	1:I:273:PHE:CD1	2.82	0.45
1:O:181:ARG:HD2	1:O:181:ARG:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:18:ILE:O	5:S:21:TRP:HB3	2.16	0.45
5:S:158:LYS:HB3	5:S:160:ILE:HD13	1.99	0.45
1:V:23:ARG:N	1:V:24:PRO:HD2	2.32	0.45
1:V:44:PHE:HE1	1:V:112:CYS:SG	2.40	0.45
5:d:11:TRP:CD1	5:d:11:TRP:N	2.84	0.45
4:i:29:TYR:HB2	4:i:57:PHE:CE1	2.51	0.45
3:m:23:THR:H	3:m:26:GLU:CD	2.24	0.45
3:y:4:PHE:H	3:y:67:ALA:HB1	1.82	0.45
3:y:42:GLN:HA	3:y:78:ALA:O	2.17	0.45
4:0:151:ARG:HE	5:1:108:HIS:CE1	2.35	0.45
2:5:71:SER:OG	2:5:72:LYS:N	2.49	0.45
5:q:68:THR:HG22	5:q:85:VAL:HG22	1.98	0.45
1:w:29:LEU:O	1:w:103:GLN:NE2	2.49	0.45
2:E:76:TYR:HA	2:E:93:PHE:CE2	2.52	0.45
4:F:59:ALA:O	4:F:60:THR:HG22	2.16	0.45
4:R:50:ASP:OD1	4:R:50:ASP:N	2.44	0.45
1:V:306:GLY:C	1:V:309:PRO:HD2	2.42	0.45
1:l:135:VAL:O	1:l:139:MET:HG3	2.15	0.45
4:o:111:LYS:HE3	4:o:111:LYS:HB3	1.31	0.45
5:v:114:CYS:HA	5:v:133:CYS:HA	1.98	0.45
1:3:133:SER:OG	1:3:134:ILE:N	2.49	0.45
1:3:196:GLN:C	1:3:196:GLN:CD	2.84	0.45
1:9:166:GLU:HB2	1:9:172:PHE:HE1	1.81	0.45
2:T:23:SER:OG	2:T:24:SER:N	2.49	0.45
3:H:41:GLU:O	3:H:79:PHE:HA	2.16	0.45
5:b:62:ALA:HB2	5:b:91:LYS:HB2	1.99	0.45
5:G:121:ARG:HH21	5:G:127:ARG:NH1	2.14	0.45
1:I:15:PHE:HB3	1:I:16:GLU:OE1	2.17	0.45
2:K:67:SER:HG	3:J:94:SER:H	1.57	0.45
2:K:73:VAL:HG11	2:K:110:LEU:HD13	1.97	0.45
4:L:57:PHE:CE1	4:L:114:ILE:HG13	2.52	0.45
2:Z:93:PHE:HA	2:Z:94:PRO:HD3	1.88	0.45
4:c:137:ALA:HA	4:c:140:GLN:CB	2.44	0.45
1:f:101:PHE:O	1:f:104:CYS:N	2.49	0.45
4:i:32:PHE:CD1	4:i:32:PHE:N	2.84	0.45
5:j:15:ARG:NE	5:j:83:GLN:HE22	2.15	0.45
1:l:29:LEU:HD23	1:l:29:LEU:HA	1.72	0.45
2:n:41:THR:HG21	2:n:109:PHE:CE1	2.52	0.45
2:n:88:THR:HG23	2:n:89:GLU:H	1.81	0.45
1:r:242:GLU:HB2	1:r:262:MET:SD	2.57	0.45
4:u:27:ILE:O	4:u:27:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:77:GLN:O	1:x:81:LEU:HB2	2.15	0.45
2:z:23:SER:HB2	2:z:70:LEU:HD12	1.98	0.45
1:3:284:MET:HE1	1:3:292:LYS:HB3	1.98	0.45
1:w:20:ASP:OD1	1:w:23:ARG:NH1	2.49	0.45
3:J:52:ASP:CG	3:J:55:LYS:HD3	2.42	0.45
1:O:29:LEU:HD11	1:O:40:TRP:HZ3	1.81	0.45
3:P:44:LEU:HD22	3:P:75:VAL:CG2	2.47	0.45
4:c:32:PHE:N	4:c:32:PHE:CD1	2.85	0.45
1:r:114:LEU:O	1:r:118:LEU:HD12	2.16	0.45
3:s:26:GLU:O	3:s:29:ARG:HB3	2.17	0.45
1:3:222:LEU:HD23	1:3:222:LEU:C	2.41	0.45
4:6:85:TYR:CE2	4:6:98:LYS:HD3	2.51	0.45
5:7:27:HIS:CE1	5:7:161:PRO:HG2	2.52	0.45
5:7:93:ARG:HG3	5:7:93:ARG:O	2.16	0.45
2:T:46:LEU:HD13	2:T:46:LEU:HA	1.84	0.45
2:T:69:VAL:O	2:T:72:LYS:N	2.50	0.45
2:B:39:SER:HB2	2:B:110:LEU:HB3	1.97	0.45
4:N:62:THR:HG23	4:N:64:LEU:HB2	1.99	0.45
4:N:67:GLN:O	5:2:7:VAL:HA	2.17	0.45
4:a:118:ARG:HE	4:a:118:ARG:HB3	1.32	0.45
3:J:9:ARG:NH1	3:J:10:HIS:CE1	2.84	0.45
1:O:90:LEU:HG	1:O:176:LEU:CD1	2.47	0.45
1:O:156:GLN:O	1:O:160:MET:HG2	2.16	0.45
2:Q:76:TYR:HA	2:Q:93:PHE:HE2	1.81	0.45
4:R:34:ASP:OD1	4:R:35:ARG:N	2.49	0.45
5:S:89:TRP:O	5:S:95:SER:HA	2.17	0.45
1:V:190:ASN:HA	1:V:191:PRO:HD2	1.77	0.45
4:c:136:ASP:CG	4:c:137:ALA:N	2.74	0.45
5:d:98:VAL:HG13	5:d:102:LEU:HD23	1.98	0.45
4:u:88:LEU:N	4:u:88:LEU:HD23	2.31	0.45
4:u:139:ALA:HB1	5:v:94:TYR:HD2	1.81	0.45
5:v:13:VAL:HG21	5:v:18:ILE:HG13	1.99	0.45
4:0:104:ASN:OD1	5:1:98:VAL:HA	2.17	0.45
1:9:144:ASN:HB2	1:9:187:LEU:HB3	1.99	0.45
1:9:282:GLN:O	1:9:285:ILE:HB	2.16	0.45
4:k:84:GLU:OE2	5:q:5:TRP:O	2.34	0.45
5:q:135:TYR:O	5:q:138:GLY:N	2.45	0.45
1:C:91:LYS:O	1:C:91:LYS:HD2	2.17	0.45
1:C:182:GLU:O	1:C:186:ASN:ND2	2.28	0.45
4:F:152:GLU:HG2	5:G:147:TYR:CD1	2.52	0.45
1:I:90:LEU:HD23	1:I:90:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:HIS:O	1:I:168:LEU:HD23	2.17	0.45
1:O:54:ASP:HB3	1:O:57:GLY:HA3	1.98	0.45
3:P:8:ARG:HG2	3:P:13:THR:HB	1.98	0.45
5:S:101:ASP:OD1	5:S:168:ARG:HD2	2.16	0.45
5:S:114:CYS:SG	5:S:133:CYS:HB2	2.57	0.45
5:S:149:LEU:O	5:S:152:ALA:HB3	2.16	0.45
2:h:101:LEU:HD23	5:j:153:LEU:HD11	1.99	0.45
1:l:98:ARG:O	1:l:102:THR:OG1	2.34	0.45
5:v:128:ILE:HG23	5:v:129:VAL:H	1.82	0.45
5:v:130:SER:HA	5:v:131:PRO:HA	1.71	0.45
1:x:284:MET:HE3	1:x:284:MET:HB3	1.79	0.45
4:6:16:GLU:O	4:6:19:ARG:HB2	2.17	0.45
5:7:77:ARG:HD3	5:7:77:ARG:HA	1.51	0.45
5:7:134:GLU:OE2	5:7:157:LYS:HB2	2.17	0.45
2:T:109:PHE:CD1	2:T:109:PHE:C	2.95	0.45
5:q:87:ILE:CG2	5:q:98:VAL:HB	2.47	0.45
2:B:79:TYR:CE2	2:B:93:PHE:HB2	2.52	0.45
2:B:85:ASN:OD1	4:N:19:ARG:NH2	2.50	0.45
4:a:93:GLY:O	4:a:116:LEU:HB2	2.17	0.45
4:a:115:ASP:OD2	4:a:118:ARG:HG3	2.17	0.45
1:C:35:VAL:HG13	1:C:39:GLN:HB2	1.99	0.45
5:G:21:TRP:O	5:G:25:VAL:HG22	2.17	0.45
4:L:87:ASP:OD1	4:L:89:GLU:N	2.50	0.45
5:M:127:ARG:O	5:M:128:ILE:HG12	2.18	0.45
3:P:75:VAL:HG13	3:P:76:GLY:N	2.32	0.45
4:R:152:GLU:HG3	5:S:139:HIS:HE1	1.82	0.45
5:S:127:ARG:O	5:S:128:ILE:HB	2.16	0.45
2:Z:66:PRO:O	2:Z:69:VAL:HG23	2.17	0.45
5:d:22:LYS:O	5:d:25:VAL:HG23	2.17	0.45
1:f:30:LEU:HG	1:f:107:LEU:HD22	1.99	0.45
2:h:67:SER:OG	3:g:94:SER:N	2.39	0.45
4:i:82:SER:OG	5:j:4:ARG:NH1	2.50	0.45
1:l:172:PHE:CZ	1:l:248:TYR:OH	2.70	0.45
4:o:99:ALA:HB3	4:o:110:TRP:HB3	1.98	0.45
5:p:18:ILE:HG22	5:p:19:ASN:N	2.32	0.45
1:r:267:ASN:OD1	1:r:271:THR:HG21	2.17	0.45
5:v:133:CYS:SG	5:v:134:GLU:O	2.57	0.45
5:1:8:MET:HA	5:1:97:GLN:HE22	1.82	0.45
1:3:162:LEU:HD23	1:3:172:PHE:CD1	2.52	0.45
5:7:21:TRP:O	5:7:25:VAL:HG22	2.17	0.45
5:7:128:ILE:HG23	5:7:129:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:143:GLY:HA3	5:7:148:LEU:HG	1.98	0.45
1:U:165:ALA:HB1	1:U:170:GLU:HB2	1.99	0.44
2:Q:62:PHE:CE2	2:Q:70:LEU:HD11	2.52	0.44
5:S:59:LEU:O	5:S:60:GLY:C	2.59	0.44
1:V:152:LYS:HG3	1:V:184:TYR:OH	2.17	0.44
1:f:152:LYS:HA	1:f:155:LEU:HD12	2.00	0.44
1:f:256:ASN:OD1	1:f:256:ASN:C	2.59	0.44
3:g:5:LEU:HD13	3:g:75:VAL:HG21	1.99	0.44
3:g:22:SER:HB2	3:g:57:LEU:HD12	1.98	0.44
1:l:188:CYS:HB2	1:l:197:ILE:HG12	1.98	0.44
1:3:159:ALA:O	1:3:162:LEU:N	2.50	0.44
1:9:18:LYS:O	1:9:22:MET:HG3	2.17	0.44
2:T:82:ARG:NH1	2:T:83:TYR:CZ	2.86	0.44
1:w:104:CYS:SG	1:w:139:MET:HE2	2.57	0.44
3:H:79:PHE:H	3:H:86:GLU:CG	2.28	0.44
4:N:111:LYS:HB3	4:N:111:LYS:HE3	1.42	0.44
5:2:133:CYS:SG	5:2:134:GLU:O	2.74	0.44
1:U:100:PHE:O	1:U:103:GLN:HB2	2.16	0.44
1:C:31:ARG:O	1:C:32:GLN:HB3	2.17	0.44
1:C:52:LEU:HD23	1:C:53:TRP:NE1	2.32	0.44
4:F:11:LYS:HE2	4:F:147:ARG:NH2	2.32	0.44
2:Q:30:ILE:HB	3:P:14:ILE:HG12	1.99	0.44
2:Q:39:SER:OG	2:Q:42:ILE:HG13	2.17	0.44
2:h:37:LEU:HD22	2:h:43:LYS:HG2	1.98	0.44
1:r:93:TYR:CD1	1:r:93:TYR:C	2.96	0.44
1:r:103:GLN:OE1	1:r:103:GLN:HA	2.17	0.44
2:t:41:THR:O	2:t:45:MET:HG3	2.17	0.44
5:v:139:HIS:ND1	5:v:148:TYR:OH	2.50	0.44
2:z:68:HIS:CD2	3:y:96:PRO:HD3	2.51	0.44
4:0:11:LYS:HB2	4:0:15:GLU:HG3	1.98	0.44
1:3:55:ASP:OD2	5:7:127:ARG:NH1	2.41	0.44
1:3:278:LEU:HA	1:3:296:MET:HE1	1.99	0.44
4:k:116:LEU:HD23	4:k:116:LEU:HA	1.53	0.44
5:q:38:TRP:CZ3	5:q:57:ILE:HD11	2.52	0.44
3:X:44:LEU:O	3:X:50:LEU:HD22	2.17	0.44
4:a:69:PHE:HB2	5:b:6:GLN:HG2	1.99	0.44
1:C:189:SER:O	1:C:189:SER:OG	2.35	0.44
4:F:84:GLU:O	4:F:85:TYR:HB3	2.18	0.44
1:I:249:LEU:HD22	1:I:257:SER:HB2	1.99	0.44
1:V:109:LYS:HB2	1:V:110:PRO:HD3	1.99	0.44
2:Z:38:THR:HB	2:Z:77:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:11:TRP:CD1	5:d:11:TRP:H	2.35	0.44
5:d:139:HIS:N	5:d:139:HIS:CD2	2.84	0.44
3:g:46:LYS:HD2	3:g:62:PHE:CE1	2.53	0.44
5:j:98:VAL:CG1	5:j:102:LEU:HB3	2.47	0.44
1:r:174:SER:O	1:r:178:ILE:HG13	2.17	0.44
5:v:128:ILE:HG23	5:v:129:VAL:N	2.33	0.44
5:v:132:ARG:H	5:v:132:ARG:HG2	1.58	0.44
1:x:151:ILE:HG13	1:x:155:LEU:CD1	2.48	0.44
1:x:151:ILE:HG13	1:x:155:LEU:HD11	1.98	0.44
1:x:195:LEU:O	1:x:198:TYR:HB3	2.18	0.44
3:4:6:MET:HG2	3:4:15:PHE:CE1	2.53	0.44
5:7:106:LEU:HA	5:7:109:LEU:HG	1.99	0.44
3:e:4:PHE:CE1	3:e:69:PRO:N	2.85	0.44
3:e:4:PHE:HE1	3:e:68:ARG:HA	1.82	0.44
5:q:36:LYS:HG3	5:q:37:ASP:OD1	2.17	0.44
2:B:83:TYR:CE2	2:B:91:PRO:HD3	2.52	0.44
5:b:17:ARG:NH1	5:b:168:LYS:O	2.50	0.44
1:C:91:LYS:HD2	1:C:91:LYS:C	2.40	0.44
1:C:253:ARG:HA	1:C:253:ARG:HD2	1.66	0.44
1:O:19:TRP:CD1	1:O:23:ARG:CD	2.97	0.44
1:O:285:ILE:HG21	1:O:317:HIS:CG	2.53	0.44
3:P:9:ARG:NH1	3:P:86:GLU:OE1	2.50	0.44
5:S:18:ILE:CD1	5:S:83:GLN:HB2	2.46	0.44
5:S:160:ILE:HG21	5:S:164:LEU:HG	2.00	0.44
1:V:141:ASP:OD1	1:V:189:SER:OG	2.12	0.44
1:V:144:ASN:HB2	1:V:187:LEU:HD22	1.99	0.44
1:V:246:LEU:N	1:V:246:LEU:HD23	2.31	0.44
4:c:11:LYS:HB2	4:c:11:LYS:NZ	2.32	0.44
1:f:65:LEU:HD21	1:f:111:PHE:CZ	2.52	0.44
1:f:104:CYS:HA	1:f:139:MET:HE1	1.99	0.44
1:f:174:SER:HB3	1:f:248:TYR:HE1	1.83	0.44
5:j:27:HIS:CE1	5:j:161:PRO:HG2	2.52	0.44
5:v:76:GLU:OE2	5:v:77:ARG:N	2.50	0.44
1:x:314:LEU:HD22	1:x:314:LEU:HA	1.76	0.44
5:1:98:VAL:HG13	5:1:102:LEU:HB3	1.99	0.44
1:3:15:PHE:CD1	1:3:15:PHE:C	2.95	0.44
1:3:269:LEU:HD23	1:3:269:LEU:HA	1.82	0.44
1:9:231:MET:SD	1:9:296:MET:HG2	2.57	0.44
2:T:24:SER:HB3	2:T:65:ILE:O	2.18	0.44
3:e:24:VAL:HG13	3:e:44:LEU:HD12	1.99	0.44
5:q:98:VAL:HG12	5:q:99:ASP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:88:LEU:HD23	4:a:88:LEU:N	2.28	0.44
1:C:94:ILE:HG12	1:C:176:LEU:HA	1.99	0.44
3:D:37:ARG:HH21	3:D:41:GLU:HB3	1.82	0.44
1:O:189:SER:O	1:O:191:PRO:HD3	2.17	0.44
1:O:195:LEU:O	1:O:198:TYR:HB3	2.17	0.44
5:S:34:LYS:HB3	5:S:112:PHE:CE1	2.52	0.44
5:S:104:ASP:OD2	5:S:168:ARG:HB2	2.17	0.44
1:V:19:TRP:HD1	1:V:22:MET:HB2	1.80	0.44
4:c:86:VAL:HG22	4:c:97:LEU:CD2	2.46	0.44
1:l:215:ARG:NH2	4:u:156:ARG:HH11	2.15	0.44
1:l:269:LEU:HD23	1:l:269:LEU:HA	1.63	0.44
4:o:38:GLU:HA	4:o:41:GLN:HG3	1.99	0.44
4:o:147:ARG:HG3	5:p:102:LEU:HD11	1.98	0.44
1:r:261:LEU:O	1:r:264:CYS:HB3	2.17	0.44
4:0:138:LEU:HD13	4:0:138:LEU:N	2.32	0.44
4:6:72:SER:C	4:6:73:TRP:HD1	2.26	0.44
2:T:107:ALA:HB2	5:q:145:LEU:HD13	1.99	0.44
2:B:23:SER:CB	2:B:27:HIS:HB2	2.46	0.44
4:a:138:LEU:H	4:a:138:LEU:CD1	2.16	0.44
1:I:199:ARG:HA	1:I:203:GLU:HB3	1.98	0.44
1:O:158:SER:O	1:O:161:LYS:HB2	2.18	0.44
4:R:136:ASP:CG	4:R:140:GLN:H	2.26	0.44
3:W:34:ILE:HG22	3:W:35:LEU:HD23	2.00	0.44
4:c:33:ARG:HA	4:c:40:ARG:NH1	2.32	0.44
5:d:47:THR:O	5:d:49:PRO:HD3	2.18	0.44
1:f:234:ALA:O	1:f:238:LEU:HD12	2.18	0.44
2:h:17:MET:HG2	2:h:18:TYR:CE1	2.52	0.44
2:h:25:ASP:OD2	2:h:67:SER:HB3	2.17	0.44
3:s:41:GLU:O	3:s:79:PHE:HA	2.18	0.44
1:x:29:LEU:HD23	1:x:29:LEU:HA	1.82	0.44
3:y:8:ARG:HH11	3:y:74:THR:CG2	2.31	0.44
4:0:116:LEU:HD23	4:0:116:LEU:HA	1.79	0.44
3:4:3:VAL:HG22	3:4:18:ALA:O	2.16	0.44
5:7:21:TRP:CH2	5:7:66:ILE:HG21	2.53	0.44
2:T:86:SER:OG	2:T:88:THR:HG23	2.17	0.44
2:Y:76:TYR:CD2	5:b:145:LEU:HG	2.52	0.44
4:a:149:ARG:HD2	4:a:154:GLU:OE2	2.18	0.44
5:b:48:ASN:HB3	5:b:51:ILE:HG13	1.99	0.44
5:b:70:TRP:CG	1:I:311:LEU:HD13	2.53	0.44
1:C:168:LEU:HA	1:C:168:LEU:HD23	1.70	0.44
1:C:311:LEU:HA	1:C:311:LEU:HD23	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:296:MET:HB3	1:I:310:MET:HE1	1.99	0.44
2:K:27:HIS:HB3	2:K:29:PHE:HE1	1.83	0.44
2:K:104:LEU:HD21	5:M:120:ILE:HG13	1.98	0.44
3:J:38:PRO:O	3:J:42:GLN:HG3	2.18	0.44
4:L:98:LYS:HA	4:L:110:TRP:O	2.17	0.44
1:O:64:ALA:HA	1:O:67:GLU:HG2	2.00	0.44
3:P:29:ARG:NH1	3:P:32:GLU:OE1	2.36	0.44
5:S:59:LEU:O	5:S:62:ALA:N	2.46	0.44
5:S:101:ASP:C	5:S:140:ASN:ND2	2.74	0.44
2:h:42:ILE:O	2:h:46:LEU:HD22	2.18	0.44
3:g:2:ASP:OD2	3:g:19:LYS:HE2	2.18	0.44
3:g:77:LEU:HG	3:g:78:ALA:N	2.33	0.44
1:l:153:ASN:ND2	1:r:145:GLU:OE1	2.51	0.44
4:o:118:ARG:HH21	4:o:120:ASP:CB	2.31	0.44
1:r:297:PHE:O	1:r:297:PHE:HD1	2.01	0.44
5:v:13:VAL:CG2	5:v:18:ILE:HG13	2.48	0.44
1:x:243:LYS:HA	1:x:243:LYS:HD2	1.79	0.44
5:1:6:GLN:O	5:1:6:GLN:HG3	2.15	0.44
5:1:150:ALA:O	5:1:153:ALA:HB3	2.18	0.44
2:T:70:LEU:HA	2:T:70:LEU:HD23	1.69	0.44
2:B:22:ILE:HG12	2:B:60:VAL:O	2.18	0.44
3:H:42:GLN:HB3	3:H:77:LEU:CD1	2.46	0.44
3:H:43:ARG:HE	3:H:50:LEU:HD11	1.83	0.44
5:2:72:LEU:HA	5:2:72:LEU:HD23	1.50	0.44
3:X:3:VAL:HB	3:X:67:ALA:HB3	2.00	0.44
1:C:48:HIS:CG	1:C:113:GLN:OE1	2.71	0.44
5:G:75:GLY:C	5:G:76:GLU:HG2	2.42	0.44
5:G:128:ILE:HG13	5:G:129:VAL:N	2.22	0.44
1:I:14:GLN:HG3	1:I:54:ASP:HB2	1.99	0.44
3:J:30:ILE:HD12	3:J:30:ILE:HA	1.85	0.44
4:L:85:TYR:CE1	4:L:98:LYS:HB3	2.53	0.44
3:P:52:ASP:OD2	3:P:55:LYS:HD3	2.17	0.44
1:V:107:LEU:N	1:V:108:PRO:HD2	2.32	0.44
1:V:166:GLU:CD	1:V:244:ARG:NH2	2.70	0.44
1:V:221:TYR:CE1	1:V:225:ASN:HB2	2.52	0.44
1:V:253:ARG:NE	1:V:253:ARG:HA	2.33	0.44
1:l:75:GLN:HB3	1:l:79:ARG:NH1	2.33	0.44
2:n:80:LYS:NZ	2:n:84:THR:OG1	2.46	0.44
4:o:73:TRP:N	4:o:73:TRP:CD1	2.86	0.44
2:t:22:ILE:HD13	2:t:22:ILE:HA	1.64	0.44
1:x:80:VAL:HG22	1:x:92:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:135:VAL:O	1:x:139:MET:HG3	2.18	0.44
5:7:51:ILE:HG12	5:7:69:TYR:CE1	2.53	0.44
4:k:87:ASP:OD1	4:k:87:ASP:C	2.60	0.44
5:q:117:GLU:H	5:q:117:GLU:HG3	1.55	0.44
1:w:31:ARG:HH12	1:w:75:GLN:HE22	1.66	0.44
4:N:14:ASN:O	4:N:19:ARG:NH2	2.51	0.44
4:N:138:LEU:O	4:N:141:GLN:HG3	2.17	0.44
2:Y:23:SER:OG	2:Y:25:ASP:OD1	2.30	0.44
2:Y:109:PHE:HD1	2:Y:109:PHE:O	2.01	0.44
1:C:193:ASP:OD1	1:C:196:GLN:N	2.51	0.44
1:C:318:ILE:HD13	1:C:318:ILE:HA	1.78	0.44
4:L:15:GLU:O	4:L:19:ARG:HG3	2.18	0.44
1:O:143:TRP:CD1	1:O:187:LEU:HD11	2.53	0.44
1:O:284:MET:HE2	1:O:292:LYS:HB3	1.98	0.44
1:f:65:LEU:HD13	1:f:65:LEU:HA	1.69	0.44
1:f:101:PHE:O	1:f:104:CYS:HB2	2.18	0.44
1:f:112:CYS:SG	1:f:113:GLN:N	2.91	0.44
1:r:65:LEU:O	1:r:69:ILE:HG13	2.18	0.44
1:r:86:ASP:O	1:r:89:LEU:HB3	2.18	0.44
5:v:15:ARG:HA	5:v:83:GLN:HE22	1.83	0.44
5:v:36:LYS:NZ	5:v:37:ASP:OD1	2.45	0.44
1:x:94:ILE:HD13	1:x:94:ILE:HA	1.82	0.44
1:x:277:ILE:HG22	1:x:296:MET:HE3	2.00	0.44
1:9:113:GLN:O	1:9:117:THR:OG1	2.32	0.44
5:q:61:ASP:OD1	5:q:61:ASP:N	2.50	0.44
1:w:12:SER:C	1:w:13:LEU:HD23	2.42	0.44
1:w:43:LEU:HA	1:w:43:LEU:HD12	1.79	0.44
1:w:164:HIS:CE1	1:w:168:LEU:HD21	2.53	0.44
5:b:122:ASN:HB3	5:b:128:ILE:O	2.18	0.43
4:F:141:GLN:O	4:F:145:GLU:HG3	2.18	0.43
1:O:117:THR:C	1:O:118:LEU:HD23	2.43	0.43
2:Q:27:HIS:CD2	3:P:11:LYS:HG2	2.53	0.43
1:V:284:MET:HE2	1:V:284:MET:HB3	1.62	0.43
4:c:153:PHE:N	4:c:153:PHE:CD1	2.86	0.43
1:f:37:LYS:O	1:f:40:TRP:HB3	2.18	0.43
2:h:89:GLU:OE1	2:h:89:GLU:HA	2.18	0.43
5:p:117:GLU:H	5:p:117:GLU:HG3	1.45	0.43
1:r:94:ILE:HD13	1:r:94:ILE:HA	1.79	0.43
4:0:32:PHE:CE2	4:0:43:ARG:HD2	2.52	0.43
1:9:195:LEU:O	1:9:198:TYR:HB3	2.18	0.43
1:w:40:TRP:HD1	1:w:41:PHE:HD1	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:62:HIS:HE1	1:w:66:LYS:HD2	1.83	0.43
1:w:137:LYS:HE2	1:w:141:ASP:OD2	2.18	0.43
4:N:38:GLU:O	4:N:41:GLN:HB2	2.18	0.43
1:U:71:GLU:HG2	1:U:75:GLN:NE2	2.32	0.43
2:Y:20:LYS:HE2	2:Y:28:GLU:OE1	2.18	0.43
3:X:4:PHE:N	3:X:4:PHE:CD1	2.86	0.43
3:X:4:PHE:CE1	3:X:69:PRO:HD3	2.53	0.43
5:b:112:PHE:N	5:b:112:PHE:CD1	2.86	0.43
1:I:43:LEU:O	1:I:47:VAL:HG23	2.17	0.43
5:M:57:ILE:HG21	5:M:107:ILE:HD12	2.00	0.43
5:j:14:ASP:N	5:j:14:ASP:OD1	2.47	0.43
5:j:58:PRO:O	5:j:111:TYR:HE1	2.01	0.43
1:l:77:GLN:HG2	1:l:81:LEU:HD11	1.99	0.43
1:l:83:HIS:ND1	1:l:83:HIS:N	2.65	0.43
3:m:20:GLU:O	3:m:58:GLY:N	2.43	0.43
1:r:139:MET:HE2	1:r:139:MET:HB3	1.77	0.43
5:v:8:MET:HE1	5:v:88:GLU:OE2	2.18	0.43
5:v:81:LEU:HA	5:v:81:LEU:HD23	1.78	0.43
1:x:89:LEU:O	1:x:92:ALA:N	2.51	0.43
1:3:19:TRP:CZ2	1:3:23:ARG:HG2	2.53	0.43
1:9:106:ILE:O	1:9:109:LYS:HG3	2.17	0.43
4:k:21:LEU:HB3	4:k:125:LEU:HD12	1.98	0.43
4:k:138:LEU:H	4:k:138:LEU:HG	1.15	0.43
1:w:148:PHE:HD2	1:w:187:LEU:HD12	1.83	0.43
4:a:153:PHE:N	4:a:153:PHE:CD1	2.83	0.43
4:F:62:THR:CB	4:F:64:LEU:H	2.31	0.43
5:G:38:TRP:CD2	5:G:57:ILE:HG12	2.54	0.43
1:I:31:ARG:O	1:I:32:GLN:HB3	2.18	0.43
3:J:70:GLN:H	3:J:70:GLN:HG3	1.37	0.43
4:i:67:GLN:O	5:j:7:VAL:HA	2.18	0.43
1:r:249:LEU:HD23	1:r:249:LEU:HA	1.76	0.43
2:5:76:TYR:CD1	5:7:145:LEU:HG	2.53	0.43
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.72	0.43
1:C:255:CYS:SG	1:C:256:ASN:N	2.92	0.43
1:I:94:ILE:O	1:I:98:ARG:HB2	2.18	0.43
1:V:160:MET:SD	1:V:206:TYR:HA	2.59	0.43
5:j:42:HIS:H	5:j:45:GLU:CD	2.20	0.43
5:p:59:LEU:HB3	5:p:110:HIS:ND1	2.34	0.43
1:r:300:MET:HB2	1:r:307:ILE:HD12	2.00	0.43
1:x:40:TRP:O	1:x:43:LEU:HB3	2.19	0.43
1:x:56:LYS:HE3	1:x:60:LYS:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:83:HIS:N	1:x:83:HIS:ND1	2.66	0.43
2:z:65:ILE:HA	2:z:66:PRO:HD3	1.65	0.43
4:0:51:GLY:HA2	5:1:3:ASN:OD1	2.18	0.43
4:6:15:GLU:OE2	4:6:147:ARG:NH2	2.38	0.43
1:w:166:GLU:HB2	1:w:172:PHE:CE2	2.54	0.43
4:N:11:LYS:HB3	4:N:11:LYS:HE2	1.43	0.43
5:2:101:ASP:OD1	5:2:168:ARG:HG3	2.18	0.43
5:2:156:LYS:HD2	5:2:157:PRO:HD2	2.00	0.43
1:U:30:LEU:HD22	1:U:72:PHE:CD2	2.53	0.43
2:Y:63:ARG:NE	2:Y:63:ARG:HA	2.33	0.43
4:a:29:TYR:HE1	4:a:31:GLY:CA	2.31	0.43
4:a:110:TRP:HA	4:a:124:CYS:O	2.17	0.43
3:D:96:PRO:HA	3:D:97:PRO:HD3	1.88	0.43
4:F:57:PHE:CE2	4:F:97:LEU:HD22	2.54	0.43
5:M:102:LEU:HD12	5:M:102:LEU:HA	1.81	0.43
2:Z:20:LYS:CG	2:Z:59:GLU:HG3	2.49	0.43
2:Z:72:LYS:HD2	2:Z:72:LYS:HA	1.76	0.43
4:c:33:ARG:HA	4:c:40:ARG:HH11	1.83	0.43
5:d:135:TYR:CE1	5:d:137:ALA:HB3	2.53	0.43
1:l:19:TRP:CZ2	1:l:64:ALA:HB1	2.53	0.43
3:m:4:PHE:CD1	3:m:4:PHE:N	2.86	0.43
4:o:85:TYR:HE2	4:o:98:LYS:HD2	1.83	0.43
1:r:101:PHE:O	1:r:101:PHE:HD1	2.01	0.43
1:r:195:LEU:O	1:r:199:ARG:N	2.42	0.43
5:v:25:VAL:O	5:v:29:MET:HG3	2.18	0.43
1:x:14:GLN:O	1:x:16:GLU:HG2	2.18	0.43
4:0:118:ARG:NE	4:0:120:ASP:HB2	2.11	0.43
4:0:143:PHE:HB2	5:1:89:TRP:CZ3	2.53	0.43
1:9:227:VAL:O	1:9:230:TYR:HB3	2.18	0.43
2:B:80:LYS:HZ2	5:2:143:VAL:HG21	1.82	0.43
2:Y:98:GLU:HG2	2:Y:99:ILE:N	2.34	0.43
5:G:3:ASN:HD22	5:G:3:ASN:N	2.17	0.43
5:G:31:ILE:O	5:G:31:ILE:HG22	2.18	0.43
1:I:31:ARG:NH2	1:I:75:GLN:HE22	2.17	0.43
1:I:102:THR:O	1:I:105:ASP:HB2	2.19	0.43
4:L:38:GLU:HA	4:L:41:GLN:HG3	2.01	0.43
1:O:43:LEU:HD13	1:O:110:PRO:CB	2.48	0.43
1:O:208:ASP:O	1:O:212:ARG:HG3	2.19	0.43
2:Q:83:TYR:HE2	3:P:69:PRO:HG2	1.83	0.43
1:V:93:TYR:C	1:V:93:TYR:HD1	2.26	0.43
1:V:101:PHE:CE1	1:V:136:ARG:NH2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:206:TYR:HE1	1:V:261:LEU:CD1	2.32	0.43
5:j:89:TRP:HB3	5:j:96:THR:HG22	2.00	0.43
1:l:20:ASP:HA	1:l:23:ARG:HD2	2.01	0.43
2:n:99:ILE:HG13	2:n:99:ILE:H	1.66	0.43
5:v:72:LEU:O	5:v:81:LEU:HB3	2.18	0.43
1:x:245:ALA:O	1:x:249:LEU:HB2	2.18	0.43
4:0:57:PHE:O	4:0:66:LEU:N	2.50	0.43
5:1:127:ARG:O	5:1:128:ILE:HG22	2.18	0.43
1:9:135:VAL:O	1:9:139:MET:HG3	2.19	0.43
1:9:203:GLU:O	1:9:207:LEU:HG	2.18	0.43
4:k:69:PHE:HA	4:k:70:PRO:HD3	1.84	0.43
5:q:14:ASP:HB3	5:q:17:ARG:HD2	1.99	0.43
5:b:27:HIS:O	5:b:31:ILE:HB	2.18	0.43
1:C:68:ASP:OD1	1:C:68:ASP:N	2.52	0.43
1:C:109:LYS:HB3	2:E:44:ALA:HB1	2.00	0.43
4:F:151:ARG:HH11	4:F:151:ARG:HD3	1.68	0.43
2:Q:70:LEU:HD23	2:Q:70:LEU:HA	1.76	0.43
1:V:234:ALA:HB3	1:V:299:LEU:HD11	1.99	0.43
2:Z:39:SER:OG	2:Z:42:ILE:HG13	2.19	0.43
2:Z:95:ILE:HG23	2:Z:103:LEU:HD12	2.00	0.43
5:d:117:GLU:H	5:d:117:GLU:HG3	1.51	0.43
4:i:29:TYR:CE2	4:i:44:PHE:HB2	2.54	0.43
1:l:295:LEU:HD12	1:l:295:LEU:O	2.17	0.43
2:n:76:TYR:CD2	5:p:145:LEU:HG	2.54	0.43
2:n:109:PHE:C	2:n:109:PHE:HD1	2.26	0.43
5:p:26:LYS:HD2	5:p:30:TYR:HE2	1.82	0.43
1:r:267:ASN:O	1:r:271:THR:HG22	2.18	0.43
3:y:75:VAL:HG12	3:y:76:GLY:N	2.34	0.43
5:1:21:TRP:CD1	5:1:170:LEU:HB2	2.53	0.43
5:1:81:LEU:HD23	5:1:81:LEU:HA	1.74	0.43
4:k:14:ASN:HA	4:k:19:ARG:NH2	2.24	0.43
5:q:114:CYS:HA	5:q:133:CYS:HA	2.00	0.43
1:w:37:LYS:O	1:w:40:TRP:HB3	2.19	0.43
3:H:9:ARG:NH1	3:H:86:GLU:OE2	2.52	0.43
5:2:134:GLU:OE2	5:2:159:GLN:N	2.51	0.43
1:U:278:LEU:HD11	1:U:300:MET:HE2	2.00	0.43
1:C:280:GLU:O	1:C:284:MET:HG3	2.19	0.43
2:E:107:ALA:O	2:E:111:ASP:HB2	2.19	0.43
4:F:12:PHE:CD1	4:F:18:PHE:HB3	2.53	0.43
5:G:81:LEU:HA	5:G:81:LEU:HD23	1.64	0.43
1:I:90:LEU:CD2	1:I:94:ILE:HG12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:232:LYS:HB2	1:I:232:LYS:HE3	1.71	0.43
3:J:52:ASP:O	3:J:55:LYS:HB2	2.19	0.43
5:M:79:TRP:CD1	5:M:79:TRP:H	2.35	0.43
1:O:19:TRP:CD1	1:O:23:ARG:CZ	2.93	0.43
2:n:22:ILE:CG2	2:n:23:SER:H	2.32	0.43
2:n:79:TYR:CE1	2:n:91:PRO:HG2	2.47	0.43
1:x:230:TYR:CE1	1:x:233:TYR:HD2	2.36	0.43
1:x:281:CYS:HB2	1:x:296:MET:HE1	2.00	0.43
1:3:21:PHE:N	1:3:21:PHE:CD1	2.87	0.43
3:4:9:ARG:HD3	3:4:77:LEU:HD23	2.00	0.43
4:6:88:LEU:H	4:6:88:LEU:HG	1.41	0.43
3:e:77:LEU:HG	3:e:78:ALA:N	2.33	0.43
1:w:196:GLN:O	1:w:200:ASP:N	2.47	0.43
1:U:40:TRP:NE1	1:U:44:PHE:HE2	2.17	0.43
5:G:65:VAL:HG21	5:G:90:ARG:CZ	2.49	0.43
4:L:32:PHE:O	4:L:40:ARG:HD2	2.18	0.43
4:L:99:ALA:HB1	5:M:7:VAL:HG11	2.01	0.43
5:M:15:ARG:CZ	5:M:15:ARG:HB3	2.48	0.43
2:Q:25:ASP:OD2	3:P:94:SER:OG	2.32	0.43
4:R:32:PHE:N	4:R:32:PHE:CD1	2.82	0.43
4:R:89:GLU:OE1	4:R:89:GLU:HA	2.19	0.43
5:S:132:ARG:NH1	1:w:82:SER:HB2	2.34	0.43
1:V:213:PHE:CD1	1:V:214:TYR:CE1	3.06	0.43
1:V:241:GLU:O	1:V:244:ARG:HB3	2.17	0.43
3:W:96:PRO:HA	3:W:97:PRO:HD3	1.81	0.43
1:f:199:ARG:HA	1:f:203:GLU:HB3	2.01	0.43
2:h:105:MET:CG	5:j:124:ILE:HG12	2.46	0.43
4:i:88:LEU:HD22	4:i:95:VAL:CG2	2.45	0.43
4:o:94:LYS:HE3	4:o:113:TRP:CE3	2.53	0.43
1:r:22:MET:HB3	1:r:43:LEU:HD11	2.01	0.43
1:x:204:LYS:HB2	1:x:204:LYS:HE3	1.86	0.43
1:x:293:LEU:HD13	5:7:79:TRP:CZ2	2.54	0.43
4:0:134:GLN:HG2	4:0:134:GLN:H	1.59	0.43
5:1:122:ASN:HB3	5:1:128:ILE:O	2.18	0.43
1:3:23:ARG:N	1:3:24:PRO:HD2	2.34	0.43
1:3:223:GLN:HE21	1:3:223:GLN:HB2	1.55	0.43
4:6:14:ASN:C	4:6:19:ARG:NH2	2.77	0.43
4:6:67:GLN:NE2	5:7:72:LEU:HD22	2.34	0.43
5:7:22:LYS:HA	5:7:25:VAL:HG22	2.01	0.43
2:T:36:ALA:HA	2:T:77:PHE:CE2	2.54	0.43
3:H:58:GLY:HA2	3:H:62:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:79:PHE:N	3:H:86:GLU:HG3	2.32	0.43
3:X:3:VAL:HG12	3:X:64:SER:HA	2.01	0.43
5:b:21:TRP:CH2	5:b:66:ILE:HD13	2.54	0.43
1:C:173:ASP:HB3	1:C:176:LEU:HD11	2.01	0.43
4:F:27:ILE:HD11	4:F:122:MET:C	2.44	0.43
5:G:74:THR:HG22	5:G:75:GLY:N	2.34	0.43
4:L:41:GLN:NE2	4:L:116:LEU:O	2.52	0.43
4:L:87:ASP:OD1	4:L:87:ASP:C	2.62	0.43
1:O:44:PHE:CZ	1:O:110:PRO:HA	2.54	0.43
1:O:262:MET:O	1:O:266:VAL:HG23	2.18	0.43
4:R:130:GLU:O	4:R:134:GLN:HG3	2.18	0.43
5:S:151:LEU:HD12	5:S:151:LEU:HA	1.84	0.43
1:V:166:GLU:HB3	1:V:244:ARG:NH2	2.34	0.43
2:Z:109:PHE:CD1	2:Z:109:PHE:C	2.96	0.43
2:n:85:ASN:OD1	4:o:15:GLU:HA	2.19	0.43
1:r:19:TRP:CE3	1:r:22:MET:HE2	2.54	0.43
2:t:65:ILE:HA	2:t:66:PRO:HD3	1.92	0.43
1:x:175:GLN:HA	1:x:178:ILE:HD12	2.01	0.43
2:z:88:THR:HG23	2:z:89:GLU:OE1	2.19	0.43
2:z:109:PHE:C	2:z:109:PHE:HD1	2.26	0.43
3:y:37:ARG:O	3:y:42:GLN:NE2	2.52	0.43
4:0:29:TYR:O	4:0:40:ARG:NH2	2.50	0.43
4:0:157:ASP:OD2	5:1:118:SER:HB3	2.19	0.43
5:1:24:LEU:HD22	5:1:163:PRO:O	2.19	0.43
5:1:112:PHE:CE1	5:1:164:LEU:HD22	2.54	0.43
5:1:132:ARG:H	5:1:132:ARG:HG2	1.60	0.43
4:6:136:ASP:OD1	4:6:136:ASP:C	2.62	0.43
1:9:107:LEU:O	1:9:110:PRO:HD2	2.19	0.43
4:k:35:ARG:HA	4:k:36:PRO:HD3	1.86	0.43
5:q:58:PRO:O	5:q:59:LEU:HD23	2.19	0.43
4:N:32:PHE:O	4:N:40:ARG:NH1	2.47	0.43
1:U:162:LEU:HD12	1:U:162:LEU:HA	1.84	0.42
1:U:245:ALA:HB1	1:U:249:LEU:HD12	1.99	0.42
2:Y:62:PHE:HD2	2:Y:70:LEU:HD11	1.83	0.42
4:a:30:THR:HB	5:b:73:HIS:O	2.18	0.42
5:G:19:ASN:ND2	1:f:318:ILE:HG12	2.33	0.42
1:I:284:MET:HE2	1:I:284:MET:HB3	1.72	0.42
5:M:140:ASN:OD1	5:M:167:ARG:HD3	2.19	0.42
1:O:24:PRO:O	1:O:28:LYS:HG3	2.19	0.42
1:O:176:LEU:N	1:O:176:LEU:HD23	2.32	0.42
1:O:299:LEU:HD22	1:O:299:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:25:ILE:CD1	1:V:39:GLN:HB3	2.49	0.42
1:V:138:LEU:HD12	1:V:138:LEU:HA	1.89	0.42
3:W:52:ASP:OD1	3:W:52:ASP:N	2.45	0.42
5:d:27:HIS:ND1	5:d:28:HIS:N	2.67	0.42
5:d:59:LEU:CD1	5:d:64:LEU:HB2	2.49	0.42
1:f:172:PHE:C	1:f:172:PHE:HD1	2.25	0.42
1:l:157:ASP:O	1:l:161:LYS:HG3	2.19	0.42
1:l:278:LEU:HG	1:l:300:MET:HE3	2.00	0.42
2:z:76:TYR:CG	5:1:146:LEU:HG	2.54	0.42
3:y:34:ILE:HG22	3:y:35:LEU:HD23	2.00	0.42
3:y:55:LYS:HG2	3:y:59:GLU:OE1	2.19	0.42
4:0:13:GLU:O	4:0:19:ARG:HG2	2.19	0.42
4:0:140:GLN:HG2	5:1:94:TYR:OH	2.18	0.42
4:0:151:ARG:HG3	5:1:108:HIS:O	2.19	0.42
1:3:19:TRP:CD1	1:3:23:ARG:CG	3.00	0.42
1:3:29:LEU:HA	1:3:29:LEU:HD23	1.68	0.42
1:3:109:LYS:HB2	1:3:110:PRO:HD3	2.00	0.42
1:9:94:ILE:HG13	1:9:176:LEU:HD23	2.01	0.42
1:9:220:SER:O	1:9:224:GLN:HG3	2.19	0.42
1:9:318:ILE:HG21	5:2:15:ARG:HH22	1.83	0.42
1:w:135:VAL:O	1:w:139:MET:HG3	2.18	0.42
5:2:50:LYS:HD2	5:2:70:TRP:O	2.19	0.42
1:U:77:GLN:HE21	1:U:81:LEU:HD22	1.82	0.42
4:a:107:CYS:SG	4:a:131:ARG:HB3	2.58	0.42
1:C:237:LYS:HD3	1:C:237:LYS:HA	1.76	0.42
1:C:312:LYS:O	1:C:315:GLU:N	2.52	0.42
2:E:68:HIS:ND1	3:D:94:SER:O	2.52	0.42
4:L:73:TRP:N	4:L:73:TRP:CD1	2.83	0.42
1:O:15:PHE:HE2	1:O:60:LYS:HB3	1.83	0.42
1:O:36:THR:HG23	1:O:39:GLN:OE1	2.19	0.42
1:O:144:ASN:ND2	1:O:187:LEU:O	2.51	0.42
4:R:136:ASP:OD1	4:R:137:ALA:N	2.52	0.42
1:V:57:GLY:N	1:V:58:PRO:CD	2.83	0.42
1:V:184:TYR:O	1:V:197:ILE:HD11	2.18	0.42
5:d:83:GLN:N	5:d:83:GLN:OE1	2.52	0.42
4:i:75:GLY:O	5:1:93:ARG:HD3	2.19	0.42
3:m:45:TYR:CD2	3:m:88:LEU:HD22	2.54	0.42
5:p:52:SER:HB3	5:p:68:THR:OG1	2.19	0.42
5:p:122:ASN:O	5:p:127:ARG:N	2.51	0.42
2:5:27:HIS:CD2	3:4:93:PHE:HE1	2.36	0.42
5:7:49:PRO:HB2	5:7:50:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:k:40:ARG:HE	4:k:40:ARG:HB3	1.61	0.42
1:w:24:PRO:O	1:w:28:LYS:HG3	2.20	0.42
1:w:162:LEU:CD2	1:w:172:PHE:CD1	3.02	0.42
5:2:15:ARG:HA	5:2:83:GLN:HE22	1.84	0.42
4:a:135:GLU:O	4:a:136:ASP:HB2	2.18	0.42
1:I:30:LEU:HD13	1:I:72:PHE:HB3	2.01	0.42
4:L:149:ARG:NH1	5:M:109:LEU:HD12	2.34	0.42
2:Q:66:PRO:HG2	2:Q:69:VAL:HB	2.01	0.42
2:Q:109:PHE:CD1	2:Q:109:PHE:C	2.96	0.42
4:R:33:ARG:CB	5:S:77:ARG:HH12	2.31	0.42
1:V:213:PHE:CD1	1:V:214:TYR:CD1	3.04	0.42
2:Z:88:THR:HG21	4:c:16:GLU:OE1	2.19	0.42
1:f:36:THR:HG23	1:f:39:GLN:OE1	2.19	0.42
3:g:2:ASP:OD1	3:g:2:ASP:N	2.52	0.42
3:g:8:ARG:H	3:g:76:GLY:HA2	1.83	0.42
4:i:44:PHE:CE1	4:i:48:CYS:SG	3.12	0.42
4:o:14:ASN:C	4:o:19:ARG:HH21	2.26	0.42
1:r:152:LYS:HB2	1:r:184:TYR:OH	2.19	0.42
2:t:25:ASP:OD2	2:t:67:SER:OG	2.37	0.42
2:t:46:LEU:HD13	2:t:46:LEU:HA	1.73	0.42
5:v:134:GLU:CD	5:v:135:TYR:N	2.71	0.42
1:3:40:TRP:HE1	2:5:45:MET:HA	1.84	0.42
3:4:8:ARG:HB2	3:4:90:ILE:HD13	2.01	0.42
5:7:53:SER:OG	5:7:68:THR:OG1	2.20	0.42
1:9:19:TRP:O	1:9:23:ARG:CG	2.50	0.42
1:9:94:ILE:HA	1:9:94:ILE:HD13	1.75	0.42
4:k:104:ASN:OD1	5:q:98:VAL:HA	2.19	0.42
1:w:173:ASP:HB3	1:w:176:LEU:HG	2.01	0.42
1:w:306:GLY:O	1:w:309:PRO:HD2	2.19	0.42
4:N:88:LEU:HD23	4:N:95:VAL:HG23	2.01	0.42
5:2:115:PHE:HB3	5:2:119:ALA:HB3	2.01	0.42
1:C:82:SER:OG	1:C:83:HIS:ND1	2.52	0.42
1:C:109:LYS:HB2	1:C:110:PRO:HD3	2.01	0.42
1:I:280:GLU:O	1:I:284:MET:HG3	2.19	0.42
1:O:40:TRP:CZ2	2:Q:48:GLY:HA3	2.54	0.42
1:O:243:LYS:HA	1:O:243:LYS:HD2	1.88	0.42
2:Q:80:LYS:O	2:Q:84:THR:HB	2.19	0.42
3:P:7:ILE:HA	3:P:75:VAL:HG12	2.02	0.42
1:V:66:LYS:HG3	1:V:138:LEU:HD21	2.00	0.42
1:V:107:LEU:HA	1:V:107:LEU:HD12	1.81	0.42
1:V:204:LYS:HB2	1:V:204:LYS:HE3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:68:HIS:HB3	3:W:94:SER:O	2.19	0.42
5:d:28:HIS:CE1	5:d:163:LEU:HD23	2.54	0.42
1:f:82:SER:OG	1:f:83:HIS:ND1	2.50	0.42
1:f:156:GLN:HB2	1:f:184:TYR:OH	2.19	0.42
5:j:120:ILE:CD1	5:j:146:GLN:HB3	2.49	0.42
1:l:22:MET:SD	1:l:46:ASP:HB3	2.60	0.42
4:o:152:GLU:HG2	5:p:147:TYR:CD1	2.55	0.42
1:3:159:ALA:O	1:3:162:LEU:HB2	2.19	0.42
1:3:242:GLU:HB2	1:3:262:MET:CE	2.49	0.42
2:5:20:LYS:HA	2:5:29:PHE:O	2.18	0.42
5:7:15:ARG:HB3	5:7:83:GLN:NE2	2.33	0.42
5:7:27:HIS:HA	5:7:31:ILE:HD12	2.01	0.42
3:e:24:VAL:HG22	3:e:57:LEU:HD23	2.00	0.42
4:k:24:GLU:HA	4:k:124:CYS:HB3	2.01	0.42
4:k:131:ARG:NE	4:k:135:GLU:OE2	2.50	0.42
5:q:167:ARG:HE	5:q:167:ARG:HB3	1.41	0.42
2:Y:37:LEU:HA	2:Y:37:LEU:HD23	1.58	0.42
4:a:3:ARG:C	4:a:6:PRO:HD2	2.45	0.42
4:a:57:PHE:CE2	4:a:97:LEU:HD13	2.55	0.42
1:C:227:VAL:O	1:C:230:TYR:HB3	2.20	0.42
4:F:88:LEU:H	4:F:88:LEU:HD22	1.85	0.42
4:L:41:GLN:HE22	4:L:117:GLN:C	2.27	0.42
5:S:98:VAL:HG12	5:S:99:ASP:O	2.20	0.42
1:V:15:PHE:HB3	1:V:60:LYS:HE3	2.02	0.42
1:V:103:GLN:CD	1:V:106:ILE:HD12	2.45	0.42
4:c:115:ASP:O	4:c:119:LEU:N	2.45	0.42
1:f:48:HIS:HA	1:f:113:GLN:HG2	2.01	0.42
1:f:243:LYS:C	1:f:243:LYS:HD3	2.45	0.42
2:h:72:LYS:HD2	2:h:72:LYS:HA	1.65	0.42
4:i:27:ILE:HD13	4:i:110:TRP:HZ2	1.84	0.42
4:i:84:GLU:H	4:i:84:GLU:HG3	1.40	0.42
4:o:14:ASN:CA	4:o:19:ARG:NH2	2.71	0.42
5:p:41:ARG:HG2	5:p:45:GLU:OE1	2.19	0.42
5:p:98:VAL:HG12	5:p:99:ASP:O	2.20	0.42
1:r:285:ILE:HD12	1:r:293:LEU:HD21	2.00	0.42
5:v:129:VAL:HG22	5:v:130:SER:N	2.33	0.42
1:3:91:LYS:O	1:3:95:VAL:HG22	2.19	0.42
3:4:70:GLN:H	3:4:70:GLN:HG3	1.46	0.42
5:7:128:ILE:O	5:7:129:VAL:HB	2.19	0.42
5:q:103:ALA:O	5:q:107:ILE:HG13	2.20	0.42
2:Y:62:PHE:CD2	2:Y:70:LEU:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:10:HIS:ND1	3:X:89:CYS:SG	2.91	0.42
5:b:81:LEU:HD23	5:b:81:LEU:HA	1.84	0.42
1:C:151:ILE:O	1:C:154:ARG:HB2	2.19	0.42
2:E:76:TYR:HA	2:E:93:PHE:HE2	1.84	0.42
1:I:307:ILE:HD13	1:I:307:ILE:HA	1.68	0.42
2:K:98:GLU:H	2:K:98:GLU:HG2	1.54	0.42
4:R:86:VAL:O	4:R:86:VAL:HG12	2.20	0.42
1:V:79:ARG:HG2	1:V:79:ARG:H	1.49	0.42
4:c:141:GLN:O	4:c:144:GLU:HG2	2.18	0.42
4:c:152:GLU:C	4:c:153:PHE:CD1	2.98	0.42
2:h:37:LEU:HD22	2:h:43:LYS:CG	2.50	0.42
2:h:104:LEU:HD21	5:j:120:ILE:HD11	2.00	0.42
1:l:181:ARG:HB3	1:l:181:ARG:HH11	1.84	0.42
5:p:92:LYS:O	5:p:93:ARG:HB2	2.20	0.42
1:x:54:ASP:HB3	1:x:57:GLY:CA	2.49	0.42
1:3:174:SER:O	1:3:178:ILE:HG13	2.19	0.42
1:3:314:LEU:C	1:3:314:LEU:HD22	2.45	0.42
4:6:11:LYS:HE2	4:6:11:LYS:HB2	1.48	0.42
4:N:58:VAL:HG23	4:N:64:LEU:O	2.20	0.42
1:U:285:ILE:HD11	5:M:79:TRP:CH2	2.55	0.42
1:C:156:GLN:O	1:C:159:ALA:HB3	2.20	0.42
2:E:35:HIS:O	2:E:77:PHE:CD2	2.73	0.42
4:F:96:TYR:HA	4:F:113:TRP:HA	2.01	0.42
5:G:108:HIS:CD2	5:G:138:GLY:HA3	2.55	0.42
1:O:286:LYS:HG2	1:O:317:HIS:CD2	2.55	0.42
3:P:70:GLN:H	3:P:70:GLN:HG3	1.36	0.42
5:S:25:VAL:O	5:S:29:MET:HG3	2.20	0.42
5:S:34:LYS:HB3	5:S:112:PHE:HE1	1.85	0.42
1:f:221:TYR:CD1	1:f:221:TYR:C	2.98	0.42
1:f:281:CYS:HA	1:f:284:MET:HG3	2.01	0.42
4:i:24:GLU:HA	4:i:123:GLY:O	2.19	0.42
2:n:22:ILE:CG2	2:n:23:SER:N	2.83	0.42
4:o:139:ALA:HB1	5:p:94:TYR:HD2	1.85	0.42
3:s:4:PHE:CE2	3:s:69:PRO:HB3	2.55	0.42
3:s:43:ARG:HD3	3:s:85:PHE:CE2	2.55	0.42
4:u:138:LEU:HD13	4:u:138:LEU:HA	1.87	0.42
1:x:72:PHE:HE1	1:x:79:ARG:NH2	2.18	0.42
1:x:83:HIS:O	1:x:89:LEU:HD23	2.20	0.42
4:0:103:LEU:HD11	5:1:9:ILE:HD12	2.01	0.42
2:5:72:LYS:HA	2:5:72:LYS:HD2	1.85	0.42
5:7:115:PHE:CE1	5:7:132:ARG:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:69:VAL:O	2:T:72:LYS:HB2	2.20	0.42
5:q:22:LYS:HD3	5:q:40:TYR:OH	2.20	0.42
5:q:98:VAL:CG1	5:q:102:LEU:HB3	2.50	0.42
1:U:100:PHE:CD2	1:U:143:TRP:CE3	3.08	0.42
2:Y:39:SER:HB3	2:Y:42:ILE:HB	2.02	0.42
5:b:91:LYS:O	5:b:94:TYR:HB3	2.20	0.42
1:C:315:GLU:HA	1:C:318:ILE:HB	2.01	0.42
4:F:90:ARG:HG3	4:i:9:ARG:NH1	2.34	0.42
4:F:144:GLU:HG3	4:F:148:ARG:HD2	2.01	0.42
4:L:65:SER:OG	4:L:67:GLN:HG2	2.19	0.42
1:O:155:LEU:N	1:O:155:LEU:HD23	2.34	0.42
4:R:16:GLU:O	4:R:16:GLU:HG2	2.20	0.42
4:R:24:GLU:HA	4:R:124:CYS:HB3	2.01	0.42
5:S:22:LYS:HE2	5:S:53:SER:HB3	2.02	0.42
5:S:104:ASP:OD2	5:S:168:ARG:N	2.41	0.42
5:S:121:ARG:HE	5:S:125:LEU:HD11	1.84	0.42
1:f:15:PHE:CD1	1:f:15:PHE:C	2.97	0.42
1:f:308:GLU:HB2	1:f:309:PRO:HD3	2.02	0.42
4:i:86:VAL:HG12	5:j:5:TRP:HE1	1.84	0.42
1:l:204:LYS:HE2	1:l:204:LYS:HB2	1.58	0.42
2:n:83:TYR:CE1	2:n:91:PRO:HG3	2.55	0.42
3:m:29:ARG:O	3:m:32:GLU:HB3	2.20	0.42
4:o:5:VAL:HG13	4:o:6:PRO:HD3	2.01	0.42
4:o:6:PRO:O	4:o:10:SER:OG	2.31	0.42
4:o:139:ALA:O	4:o:140:GLN:C	2.62	0.42
1:r:18:LYS:HA	1:r:18:LYS:HD2	1.68	0.42
1:r:228:GLN:HG2	1:r:292:LYS:HZ3	1.84	0.42
5:v:150:ALA:O	5:v:153:ALA:HB3	2.20	0.42
3:y:43:ARG:HE	3:y:50:LEU:HD21	1.85	0.42
1:3:19:TRP:CZ3	1:3:22:MET:HE2	2.54	0.42
1:3:48:HIS:HD2	1:3:48:HIS:O	2.02	0.42
4:6:26:GLU:H	4:6:26:GLU:HG3	1.59	0.42
4:6:152:GLU:HG3	5:7:139:HIS:CE1	2.54	0.42
1:9:260:ALA:O	1:9:263:GLU:HB2	2.19	0.42
3:e:25:PHE:CD1	3:e:25:PHE:C	2.97	0.42
5:q:72:LEU:HD22	5:q:72:LEU:HA	1.90	0.42
5:q:114:CYS:SG	5:q:133:CYS:SG	3.18	0.42
5:2:108:HIS:CD2	5:2:138:GLY:HA3	2.55	0.42
1:I:149:SER:HA	1:I:152:LYS:HD3	2.01	0.42
2:K:76:TYR:O	2:K:80:LYS:HB2	2.20	0.42
5:S:120:ILE:O	5:S:120:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:167:VAL:O	5:S:168:ARG:C	2.63	0.42
5:d:115:PHE:CE1	5:d:133:CYS:HB3	2.55	0.42
5:d:135:TYR:HD1	5:d:135:TYR:HA	1.62	0.42
1:f:89:LEU:HD23	1:f:89:LEU:C	2.45	0.42
1:f:281:CYS:O	1:f:284:MET:HG3	2.19	0.42
1:l:112:CYS:HA	1:l:115:GLU:HG3	2.02	0.42
1:r:25:ILE:O	1:r:28:LYS:HB2	2.20	0.42
1:r:197:ILE:HG13	1:r:198:TYR:N	2.34	0.42
1:r:204:LYS:HE3	1:r:204:LYS:HB2	1.67	0.42
5:v:103:ALA:O	5:v:107:ILE:HG13	2.20	0.42
5:v:169:LYS:HA	5:v:172:GLU:CD	2.44	0.42
1:x:255:CYS:SG	1:x:257:SER:N	2.91	0.42
2:z:97:PRO:HA	2:z:100:ALA:HB2	2.01	0.42
3:y:68:ARG:HB3	3:y:69:PRO:HD2	2.01	0.42
4:6:54:GLU:O	4:6:54:GLU:HG2	2.19	0.42
1:9:318:ILE:HD13	5:2:15:ARG:HH12	1.84	0.42
5:2:36:LYS:HE3	5:2:36:LYS:HB3	1.85	0.42
4:a:67:GLN:HE22	5:b:72:LEU:HG	1.85	0.42
4:a:130:GLU:O	4:a:134:GLN:HG3	2.20	0.42
5:b:114:CYS:O	5:b:131:PRO:HG2	2.20	0.42
5:b:134:GLU:HG2	5:b:157:LYS:HB3	2.02	0.42
1:C:75:GLN:O	1:C:79:ARG:HG3	2.20	0.42
5:G:98:VAL:HG13	5:G:102:LEU:HD23	2.01	0.42
1:I:297:PHE:CD1	1:I:297:PHE:C	2.98	0.42
1:I:317:HIS:O	1:I:320:SER:HB3	2.19	0.42
2:K:79:TYR:OH	2:K:91:PRO:O	2.35	0.42
5:S:52:SER:HG	5:S:70:TRP:CD1	2.37	0.42
1:V:54:ASP:OD1	1:V:55:ASP:N	2.53	0.42
1:f:302:LYS:HD3	1:f:302:LYS:HA	1.93	0.42
3:g:5:LEU:HA	3:g:73:ALA:O	2.19	0.42
4:i:111:LYS:NZ	4:i:126:GLU:OE1	2.47	0.42
5:j:28:HIS:HE2	5:j:162:PRO:C	2.28	0.42
5:j:58:PRO:O	5:j:111:TYR:CE1	2.72	0.42
2:n:108:ASN:CA	5:p:146:GLN:NE2	2.70	0.42
5:p:16:MET:O	5:p:20:THR:OG1	2.29	0.42
5:p:57:ILE:O	5:p:59:LEU:HD12	2.20	0.42
5:v:72:LEU:HA	5:v:72:LEU:HD23	1.66	0.42
5:1:108:HIS:HB2	5:1:135:TYR:HD2	1.84	0.42
1:3:14:GLN:C	1:3:16:GLU:H	2.25	0.42
1:3:53:TRP:CZ3	5:7:125:LEU:HD22	2.55	0.42
5:7:52:SER:HB2	5:7:68:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:63:LYS:NZ	5:7:90:ARG:HD2	2.34	0.42
5:7:69:TYR:CB	5:7:72:LEU:HD11	2.49	0.42
5:7:136:GLN:H	5:7:136:GLN:HG3	1.41	0.42
1:9:181:ARG:O	1:9:185:VAL:HG23	2.20	0.42
1:w:278:LEU:HG	1:w:300:MET:HE2	2.02	0.42
2:B:58:ASN:HD22	2:B:58:ASN:N	2.18	0.42
2:B:107:ALA:HB1	5:2:147:GLN:HG3	2.02	0.42
1:U:315:GLU:OE2	5:M:22:LYS:NZ	2.53	0.41
1:U:318:ILE:HG12	5:M:19:ASN:OD1	2.20	0.41
2:Y:23:SER:HB2	2:Y:67:SER:HA	2.02	0.41
1:C:278:LEU:HA	1:C:296:MET:CE	2.49	0.41
5:G:128:ILE:CG1	5:G:129:VAL:N	2.81	0.41
1:I:15:PHE:CE2	1:I:60:LYS:HB3	2.54	0.41
1:I:103:GLN:O	1:I:104:CYS:C	2.63	0.41
4:L:88:LEU:N	4:L:88:LEU:HD23	2.35	0.41
2:Q:87:SER:HA	2:Q:90:ILE:HD11	2.01	0.41
4:R:11:LYS:HE2	4:R:11:LYS:HB3	1.56	0.41
4:R:90:ARG:HD2	4:R:96:TYR:CD1	2.55	0.41
1:V:227:VAL:HG11	1:V:280:GLU:CG	2.49	0.41
4:c:127:PHE:C	4:c:127:PHE:CD1	2.98	0.41
4:i:29:TYR:HE2	4:i:44:PHE:HB2	1.85	0.41
5:j:69:TYR:HE2	5:j:86:SER:HB3	1.85	0.41
1:3:26:VAL:O	1:3:29:LEU:HB2	2.20	0.41
1:3:258:VAL:O	1:3:261:LEU:HB3	2.20	0.41
1:U:235:ASP:O	1:U:238:LEU:HB2	2.19	0.41
3:X:9:ARG:HB2	3:X:77:LEU:HB3	2.02	0.41
4:a:43:ARG:HA	4:a:43:ARG:HD3	1.82	0.41
4:a:106:VAL:O	4:a:108:VAL:HG13	2.20	0.41
5:b:72:LEU:O	5:b:81:LEU:HB3	2.20	0.41
1:C:25:ILE:HD13	1:C:39:GLN:HB3	2.02	0.41
5:G:35:ALA:O	5:G:38:TRP:HB2	2.20	0.41
1:I:97:TRP:CE2	1:I:101:PHE:HB2	2.54	0.41
5:M:99:ASP:C	5:M:99:ASP:OD1	2.62	0.41
1:O:19:TRP:CZ3	1:O:61:ILE:HG13	2.56	0.41
2:Q:27:HIS:HD2	3:P:11:LYS:O	2.03	0.41
5:S:125:LEU:HB2	5:S:127:ARG:HG3	2.01	0.41
1:V:77:GLN:HB2	1:V:147:ILE:CD1	2.49	0.41
1:V:101:PHE:HZ	1:V:186:ASN:OD1	2.03	0.41
1:f:297:PHE:CE2	1:f:307:ILE:HD11	2.54	0.41
1:f:307:ILE:HD13	1:f:307:ILE:HA	1.61	0.41
1:l:289:GLU:OE1	1:l:292:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:37:LEU:HB3	2:n:43:LYS:HE2	2.02	0.41
2:n:88:THR:OG1	2:n:89:GLU:N	2.48	0.41
4:o:16:GLU:O	4:o:16:GLU:HG2	2.21	0.41
4:o:141:GLN:NE2	4:o:145:GLU:CD	2.78	0.41
5:p:72:LEU:HD23	5:p:72:LEU:HA	1.83	0.41
5:v:29:MET:HA	5:v:35:ALA:C	2.45	0.41
1:x:183:SER:HB3	1:x:187:LEU:HD12	2.02	0.41
4:0:144:GLU:HG3	4:0:145:GLU:N	2.34	0.41
2:5:36:ALA:HA	2:5:77:PHE:CE2	2.56	0.41
4:6:14:ASN:HA	4:6:19:ARG:HE	1.86	0.41
5:7:42:HIS:O	5:7:45:GLU:HG2	2.20	0.41
2:B:103:LEU:HD23	2:B:103:LEU:HA	1.83	0.41
5:2:134:GLU:HG2	5:2:158:LYS:CB	2.38	0.41
1:U:31:ARG:O	1:U:32:GLN:HB3	2.21	0.41
1:U:94:ILE:HD13	1:U:94:ILE:HA	1.84	0.41
2:Y:29:PHE:HZ	3:X:93:PHE:CE1	2.38	0.41
1:C:90:LEU:HD23	1:C:90:LEU:C	2.46	0.41
1:C:94:ILE:HD12	1:C:94:ILE:HA	1.81	0.41
1:C:197:ILE:HG13	1:C:198:TYR:N	2.35	0.41
5:G:74:THR:O	5:G:76:GLU:N	2.54	0.41
2:K:62:PHE:CD2	2:K:65:ILE:HD11	2.55	0.41
3:J:76:GLY:HA3	3:J:90:ILE:HD11	2.03	0.41
1:O:160:MET:SD	1:O:206:TYR:HA	2.61	0.41
1:O:287:ARG:NH2	1:O:289:GLU:OE2	2.53	0.41
5:S:76:GLU:OE2	5:S:78:ASP:N	2.54	0.41
4:i:45:GLN:O	4:i:49:ARG:HB2	2.20	0.41
1:l:101:PHE:HE1	1:l:136:ARG:NH2	2.19	0.41
4:o:64:LEU:O	4:o:64:LEU:HD13	2.20	0.41
5:p:80:HIS:H	5:p:80:HIS:HD1	1.68	0.41
1:r:207:LEU:HD22	1:r:261:LEU:HD23	2.03	0.41
2:t:22:ILE:HG22	2:t:23:SER:O	2.20	0.41
3:s:50:LEU:HD22	3:s:51:LEU:N	2.34	0.41
4:u:152:GLU:CB	4:u:153:PHE:CD1	3.02	0.41
1:x:199:ARG:HA	1:x:203:GLU:HB3	2.02	0.41
1:3:22:MET:HG2	1:3:43:LEU:HD12	2.01	0.41
1:3:225:ASN:O	1:3:229:ASN:ND2	2.50	0.41
4:6:43:ARG:HD3	4:6:43:ARG:HA	1.82	0.41
5:7:115:PHE:HB3	5:7:119:ALA:CB	2.49	0.41
1:w:250:GLU:O	1:w:250:GLU:HG3	2.18	0.41
2:B:39:SER:OG	2:B:42:ILE:HG13	2.20	0.41
2:B:70:LEU:HD23	2:B:70:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:5:LEU:HD23	3:H:73:ALA:HB3	2.02	0.41
4:N:11:LYS:HD3	4:N:15:GLU:OE2	2.20	0.41
5:G:38:TRP:NE1	5:G:57:ILE:HG23	2.35	0.41
5:G:59:LEU:HD11	5:G:64:LEU:HB2	2.03	0.41
5:G:106:LEU:HD23	5:G:106:LEU:HA	1.89	0.41
5:G:166:VAL:O	5:G:170:THR:HG23	2.20	0.41
1:I:199:ARG:HA	1:I:203:GLU:CB	2.51	0.41
1:O:19:TRP:HE1	1:O:23:ARG:HG2	1.77	0.41
1:O:135:VAL:O	1:O:139:MET:HG3	2.20	0.41
1:O:168:LEU:HD21	1:O:213:PHE:HE2	1.86	0.41
1:O:278:LEU:HD23	1:O:296:MET:HE1	2.02	0.41
4:R:94:LYS:HD3	4:R:113:TRP:CE3	2.56	0.41
5:S:132:ARG:NH1	5:S:158:LYS:HE3	2.36	0.41
1:V:19:TRP:CD2	1:V:23:ARG:CG	3.03	0.41
1:V:185:VAL:HG23	1:V:198:TYR:CG	2.54	0.41
1:V:211:GLU:O	1:V:215:ARG:HB2	2.20	0.41
1:l:166:GLU:OE2	1:l:172:PHE:HE1	2.03	0.41
4:o:44:PHE:HE2	4:o:114:ILE:HG21	1.85	0.41
5:v:50:LYS:HD2	5:v:70:TRP:O	2.19	0.41
1:x:193:ASP:HB3	1:x:196:GLN:HB2	2.01	0.41
5:1:76:GLU:OE2	5:1:77:ARG:N	2.48	0.41
1:3:19:TRP:O	1:3:23:ARG:HG3	2.20	0.41
1:3:230:TYR:CD1	1:3:230:TYR:C	2.98	0.41
1:3:307:ILE:HD13	1:3:307:ILE:HA	1.70	0.41
1:9:76:ALA:O	1:9:80:VAL:HG23	2.20	0.41
1:w:50:VAL:HG11	1:w:61:ILE:HD12	2.03	0.41
1:w:62:HIS:CE1	1:w:66:LYS:HD2	2.56	0.41
4:N:32:PHE:CZ	4:N:43:ARG:HD2	2.56	0.41
3:X:3:VAL:HG12	3:X:64:SER:CA	2.50	0.41
4:a:108:VAL:HB	4:a:125:LEU:HD22	2.02	0.41
5:b:18:ILE:HG22	5:b:19:ASN:HD22	1.85	0.41
5:G:159:ILE:HG21	5:G:163:LEU:HG	2.02	0.41
1:I:94:ILE:HD12	1:I:94:ILE:HA	1.84	0.41
1:O:271:THR:HG23	1:O:303:VAL:HG22	2.01	0.41
1:V:214:TYR:HE2	1:V:241:GLU:HG3	1.85	0.41
1:f:315:GLU:O	1:f:318:ILE:HG22	2.21	0.41
3:g:23:THR:HA	3:g:56:THR:HA	2.02	0.41
5:j:75:GLY:O	5:j:76:GLU:CD	2.63	0.41
1:l:174:SER:O	1:l:178:ILE:HG13	2.20	0.41
4:o:103:LEU:HD12	4:o:103:LEU:HA	1.66	0.41
1:r:144:ASN:OD1	1:r:144:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:152:GLU:HG2	5:v:148:TYR:CD1	2.54	0.41
1:x:41:PHE:O	1:x:45:SER:OG	2.35	0.41
1:x:56:LYS:HB2	1:x:60:LYS:CE	2.40	0.41
1:x:249:LEU:HD23	1:x:249:LEU:HA	1.89	0.41
3:y:7:ILE:HA	3:y:75:VAL:HB	2.03	0.41
4:0:37:HIS:O	4:0:41:GLN:HG2	2.21	0.41
5:1:98:VAL:HG13	5:1:102:LEU:HD23	2.02	0.41
1:3:224:GLN:HB2	1:3:225:ASN:OD1	2.20	0.41
5:7:80:HIS:O	5:7:81:LEU:HB2	2.20	0.41
5:7:157:LYS:HE2	5:7:159:ILE:HD12	2.02	0.41
1:9:24:PRO:O	1:9:28:LYS:HG3	2.20	0.41
1:w:57:GLY:N	1:w:58:PRO:HD3	2.35	0.41
1:w:244:ARG:HD3	1:w:248:TYR:HE2	1.86	0.41
1:U:253:ARG:HD2	1:U:253:ARG:HA	1.66	0.41
5:b:59:LEU:HB3	5:b:110:HIS:ND1	2.36	0.41
3:D:8:ARG:O	3:D:76:GLY:HA2	2.21	0.41
5:G:25:VAL:O	5:G:29:MET:HG3	2.21	0.41
1:O:266:VAL:HG11	1:O:302:LYS:HB3	2.02	0.41
2:Q:17:MET:HG2	2:Q:18:TYR:CD1	2.56	0.41
5:S:146:LEU:HD23	5:S:146:LEU:HA	1.79	0.41
1:V:158:SER:O	1:V:161:LYS:HB2	2.20	0.41
1:V:278:LEU:HD22	1:V:309:PRO:HB2	2.03	0.41
5:d:15:ARG:HG2	5:d:83:GLN:CD	2.46	0.41
5:d:80:HIS:O	5:d:81:LEU:HB2	2.19	0.41
1:f:19:TRP:HE3	1:f:22:MET:HE3	1.85	0.41
5:j:81:LEU:HD23	5:j:81:LEU:HA	1.86	0.41
1:l:103:GLN:HA	1:l:106:ILE:HB	2.03	0.41
1:l:162:LEU:HD23	1:l:172:PHE:HD2	1.85	0.41
1:l:181:ARG:NH1	1:l:181:ARG:HB3	2.36	0.41
5:p:25:VAL:O	5:p:29:MET:HG3	2.21	0.41
1:r:175:GLN:HA	1:r:178:ILE:HG13	2.02	0.41
2:t:108:ASN:HD22	5:v:147:GLN:HE21	1.68	0.41
5:v:10:VAL:CG1	5:v:84:GLY:HA3	2.50	0.41
1:x:166:GLU:HB2	1:x:172:PHE:CE1	2.56	0.41
4:0:41:GLN:HE21	4:0:119:LEU:HG	1.85	0.41
1:3:173:ASP:HB3	1:3:176:LEU:HG	2.03	0.41
1:w:81:LEU:HD11	1:w:151:ILE:HG21	2.01	0.41
1:U:311:LEU:HD13	5:M:70:TRP:CD2	2.56	0.41
2:Y:41:THR:O	2:Y:45:MET:HG3	2.20	0.41
1:C:167:ARG:NH1	1:C:210:THR:HG23	2.35	0.41
1:C:244:ARG:HG2	1:C:248:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:70:GLN:H	3:D:70:GLN:HG3	1.46	0.41
5:G:43:HIS:ND1	1:f:308:GLU:OE2	2.47	0.41
1:I:107:LEU:HD23	1:I:139:MET:SD	2.61	0.41
2:K:20:LYS:HD2	2:K:59:GLU:CD	2.45	0.41
1:O:75:GLN:HB2	1:O:79:ARG:NH1	2.36	0.41
1:O:83:HIS:ND1	1:O:83:HIS:N	2.68	0.41
1:O:97:TRP:CZ2	1:O:183:SER:HA	2.56	0.41
5:S:98:VAL:CG1	5:S:102:LEU:HB3	2.51	0.41
3:W:23:THR:O	3:W:26:GLU:N	2.53	0.41
2:h:104:LEU:O	2:h:104:LEU:HD22	2.21	0.41
5:j:34:LYS:HE3	5:j:159:ILE:CD1	2.50	0.41
3:m:22:SER:HB2	3:m:57:LEU:CD1	2.50	0.41
1:r:193:ASP:OD1	1:r:195:LEU:N	2.53	0.41
4:u:118:ARG:HE	4:u:120:ASP:HB2	1.86	0.41
5:v:29:MET:N	5:v:35:ALA:HB3	2.36	0.41
2:z:107:ALA:HB1	5:1:147:GLN:HG3	2.02	0.41
4:0:62:THR:CG2	4:0:64:LEU:HB3	2.50	0.41
1:3:15:PHE:HA	1:3:50:VAL:HG22	2.02	0.41
3:e:23:THR:O	3:e:26:GLU:HB2	2.20	0.41
3:H:8:ARG:HE	3:H:8:ARG:HB3	1.74	0.41
1:U:206:TYR:O	1:U:209:SER:HB3	2.21	0.41
1:U:296:MET:HE2	1:U:296:MET:HB3	1.58	0.41
4:a:27:ILE:HD11	4:a:122:MET:C	2.45	0.41
1:C:281:CYS:HB3	1:C:296:MET:HE1	2.01	0.41
4:F:97:LEU:HD12	4:F:112:GLY:C	2.45	0.41
1:O:273:PHE:O	1:O:274:LYS:C	2.64	0.41
5:S:72:LEU:O	5:S:81:LEU:HB3	2.20	0.41
5:S:125:LEU:CB	5:S:127:ARG:HG3	2.51	0.41
1:V:94:ILE:HG13	1:V:176:LEU:HA	2.03	0.41
1:V:103:GLN:OE1	1:V:106:ILE:HD12	2.21	0.41
1:V:106:ILE:O	1:V:109:LYS:HG3	2.21	0.41
1:V:297:PHE:CE2	1:V:311:LEU:HD21	2.52	0.41
3:g:6:MET:HA	3:g:14:ILE:O	2.21	0.41
4:o:14:ASN:C	4:o:19:ARG:HE	2.29	0.41
5:v:113:ASP:OD1	5:v:113:ASP:N	2.32	0.41
1:x:31:ARG:O	1:x:32:GLN:HB2	2.21	0.41
1:x:166:GLU:HA	1:x:170:GLU:O	2.21	0.41
1:3:151:ILE:HB	1:3:155:LEU:CD1	2.51	0.41
4:6:147:ARG:HG3	5:7:102:LEU:HD11	2.01	0.41
1:9:167:ARG:NH2	1:9:210:THR:OG1	2.45	0.41
1:9:188:CYS:SG	1:9:197:ILE:HG23	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:307:ILE:HD13	1:9:307:ILE:HA	1.71	0.41
2:T:83:TYR:HE2	2:T:89:GLU:HB3	1.85	0.41
3:e:28:LYS:NZ	3:e:43:ARG:HA	2.36	0.41
4:k:117:GLN:O	4:k:117:GLN:HG3	2.20	0.41
5:q:17:ARG:HB3	5:q:169:LEU:HD12	2.02	0.41
1:w:14:GLN:O	1:w:15:PHE:CB	2.67	0.41
1:w:114:LEU:O	1:w:118:LEU:HG	2.20	0.41
2:B:104:LEU:HD11	5:2:151:LEU:HD13	2.03	0.41
3:H:23:THR:O	3:H:26:GLU:HB2	2.21	0.41
3:H:85:PHE:HD1	3:H:85:PHE:HA	1.75	0.41
2:Y:107:ALA:O	2:Y:111:ASP:HB2	2.21	0.41
3:X:6:MET:HA	3:X:14:ILE:O	2.21	0.41
3:X:29:ARG:O	3:X:32:GLU:HB3	2.21	0.41
4:a:111:LYS:HE3	4:a:111:LYS:HB3	1.50	0.41
5:b:32:SER:OG	5:b:33:ARG:N	2.52	0.41
5:b:117:GLU:HG3	5:b:117:GLU:H	1.64	0.41
1:C:135:VAL:O	1:C:139:MET:HG3	2.20	0.41
1:C:193:ASP:CG	1:C:196:GLN:HB2	2.46	0.41
2:E:68:HIS:HB3	3:D:94:SER:O	2.21	0.41
2:E:103:LEU:HD23	2:E:103:LEU:HA	1.85	0.41
3:D:9:ARG:HB2	3:D:77:LEU:HB3	2.01	0.41
1:I:299:LEU:HD23	1:I:299:LEU:HA	1.83	0.41
2:K:79:TYR:HD2	3:J:70:GLN:HB3	1.86	0.41
4:L:116:LEU:HD23	4:L:116:LEU:HA	1.90	0.41
4:L:144:GLU:O	4:L:148:ARG:HG3	2.21	0.41
5:M:98:VAL:CG1	5:M:102:LEU:HB3	2.48	0.41
5:M:135:TYR:CZ	5:M:137:ALA:HB3	2.56	0.41
1:O:227:VAL:HG11	1:O:280:GLU:CG	2.51	0.41
1:O:273:PHE:N	1:O:273:PHE:CD1	2.86	0.41
2:Q:58:ASN:HB3	2:Q:59:GLU:H	1.64	0.41
3:P:52:ASP:CG	3:P:55:LYS:HD3	2.46	0.41
1:V:15:PHE:CD2	1:V:60:LYS:HB3	2.55	0.41
3:W:46:LYS:HB3	3:W:51:LEU:HD21	2.03	0.41
5:d:18:ILE:HD12	5:d:68:THR:HG21	2.03	0.41
1:f:82:SER:HG	1:f:83:HIS:HD1	1.68	0.41
2:h:101:LEU:HD23	2:h:101:LEU:HA	1.85	0.41
3:g:7:ILE:HA	3:g:75:VAL:HB	2.02	0.41
4:i:118:ARG:NH1	4:i:120:ASP:HB2	2.33	0.41
4:i:151:ARG:NH2	5:j:113:ASP:HA	2.34	0.41
1:l:101:PHE:O	1:l:104:CYS:HB2	2.21	0.41
2:n:61:ASN:OD1	2:n:61:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:o:62:THR:C	4:o:63:ASN:CG	2.89	0.41
2:t:68:HIS:HB3	3:s:94:SER:O	2.21	0.41
1:x:22:MET:O	1:x:26:VAL:HG23	2.21	0.41
1:x:30:LEU:HD22	1:x:72:PHE:HB3	2.03	0.41
1:x:44:PHE:CZ	1:x:110:PRO:HA	2.55	0.41
2:z:83:TYR:CD2	2:z:91:PRO:HD2	2.56	0.41
3:y:6:MET:HA	3:y:14:ILE:O	2.21	0.41
1:3:21:PHE:N	1:3:21:PHE:HD1	2.19	0.41
3:4:4:PHE:CE1	3:4:69:PRO:HD3	2.56	0.41
3:4:43:ARG:HD2	3:4:43:ARG:HA	1.97	0.41
3:4:68:ARG:HB3	3:4:69:PRO:HD2	2.03	0.41
5:7:108:HIS:NE2	5:7:114:CYS:SG	2.94	0.41
4:k:69:PHE:HB2	5:q:6:GLN:HG2	2.03	0.41
4:k:103:LEU:HD21	5:q:9:ILE:CD1	2.50	0.41
5:q:109:LEU:HB2	5:q:110:HIS:HD2	1.86	0.41
1:w:15:PHE:HE1	1:w:19:TRP:CE3	2.39	0.41
1:w:39:GLN:O	1:w:42:ASP:HB2	2.20	0.41
1:w:267:ASN:HA	1:w:271:THR:CB	2.51	0.41
1:w:303:VAL:CG1	1:w:306:GLY:HA3	2.51	0.41
4:N:18:PHE:HE2	4:N:106:VAL:CG1	2.34	0.41
4:N:136:ASP:OD1	4:N:139:ALA:N	2.43	0.41
5:2:28:HIS:HA	5:2:32:SER:HB3	2.02	0.41
5:2:127:ARG:O	5:2:128:ILE:HG22	2.21	0.41
4:a:73:TRP:CD1	4:a:73:TRP:N	2.88	0.41
1:C:225:ASN:HB3	1:C:229:ASN:HB2	2.02	0.41
4:F:107:CYS:SG	4:F:131:ARG:HB3	2.61	0.41
5:G:98:VAL:HG12	5:G:99:ASP:O	2.21	0.41
1:I:274:LYS:O	1:I:277:ILE:HG22	2.21	0.41
4:L:113:TRP:HH2	4:L:118:ARG:HH22	1.68	0.41
1:O:227:VAL:HG11	1:O:280:GLU:HG3	2.03	0.41
2:Q:42:ILE:HA	2:Q:45:MET:HE3	2.03	0.41
4:R:54:GLU:OE1	5:S:50:LYS:HE3	2.21	0.41
5:S:81:LEU:HB3	5:S:82:GLY:H	1.60	0.41
2:Z:70:LEU:HD23	2:Z:70:LEU:HA	1.65	0.41
5:d:9:ILE:H	5:d:97:GLN:HE22	1.69	0.41
1:f:299:LEU:HD23	1:f:299:LEU:HA	1.88	0.41
4:i:103:LEU:O	4:i:106:VAL:HG13	2.21	0.41
4:i:149:ARG:HH11	4:i:149:ARG:HD2	1.71	0.41
4:o:16:GLU:HA	4:o:19:ARG:HD2	2.01	0.41
1:r:57:GLY:N	1:r:58:PRO:CD	2.83	0.41
4:0:21:LEU:HD23	4:0:21:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:10:VAL:HG11	5:1:69:TYR:HD2	1.86	0.41
1:3:93:TYR:CD1	1:3:93:TYR:C	2.97	0.41
2:T:65:ILE:H	2:T:65:ILE:HG12	1.57	0.41
5:q:82:GLY:HA2	5:q:83:GLN:OE1	2.20	0.41
1:w:183:SER:O	1:w:187:LEU:HG	2.21	0.41
2:B:22:ILE:HB	2:B:61:ASN:CG	2.46	0.41
5:2:98:VAL:HG13	5:2:102:LEU:HB3	2.03	0.41
1:U:185:VAL:HG21	1:U:250:GLU:OE1	2.21	0.40
4:a:103:LEU:HD12	5:b:97:GLN:HB2	2.02	0.40
4:a:157:ASP:CB	5:b:118:SER:HB3	2.51	0.40
5:b:153:LEU:HA	5:b:153:LEU:HD23	1.82	0.40
4:F:149:ARG:NH1	4:F:154:GLU:OE2	2.51	0.40
5:G:89:TRP:O	5:G:95:SER:HA	2.21	0.40
2:K:97:PRO:HA	2:K:100:ALA:HB2	2.03	0.40
5:M:168:LYS:O	5:M:171:GLU:HG3	2.21	0.40
4:R:98:LYS:HZ2	4:R:98:LYS:HG2	1.32	0.40
5:S:9:ILE:N	5:S:97:GLN:HE22	2.05	0.40
5:S:100:PRO:O	5:S:101:ASP:C	2.63	0.40
1:V:253:ARG:C	1:V:255:CYS:H	2.27	0.40
4:c:127:PHE:CD1	4:c:128:ASP:N	2.90	0.40
5:d:132:ARG:HH11	5:d:157:LYS:HE2	1.86	0.40
1:l:152:LYS:HE3	1:l:184:TYR:CE1	2.56	0.40
1:r:50:VAL:HG11	1:r:61:ILE:HD12	2.03	0.40
4:u:11:LYS:HE2	4:u:11:LYS:HB3	1.58	0.40
4:u:118:ARG:O	4:u:119:LEU:HB2	2.21	0.40
4:u:151:ARG:HG3	5:v:108:HIS:O	2.21	0.40
1:x:61:ILE:HD12	1:x:61:ILE:O	2.21	0.40
2:z:76:TYR:OH	5:1:145:SER:HA	2.21	0.40
1:3:75:GLN:O	1:3:79:ARG:HG3	2.21	0.40
1:9:149:SER:HA	1:9:152:LYS:CD	2.50	0.40
1:w:113:GLN:O	1:w:117:THR:OG1	2.31	0.40
1:w:148:PHE:CD2	1:w:152:LYS:HD3	2.56	0.40
4:N:85:TYR:CD1	4:N:85:TYR:C	2.99	0.40
5:2:164:LEU:H	5:2:164:LEU:HD12	1.85	0.40
1:C:228:GLN:OE1	1:C:292:LYS:HD3	2.21	0.40
2:E:87:SER:O	2:E:87:SER:OG	2.33	0.40
4:F:33:ARG:CB	5:G:77:ARG:HD2	2.52	0.40
1:O:306:GLY:C	1:O:309:PRO:HD2	2.46	0.40
2:Q:32:LYS:O	2:Q:35:HIS:HB2	2.21	0.40
4:R:46:ASN:O	4:R:50:ASP:OD1	2.38	0.40
1:V:152:LYS:HG2	1:V:153:ASN:N	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:22:ILE:HG12	2:Z:22:ILE:H	1.71	0.40
3:W:85:PHE:HD1	3:W:85:PHE:HA	1.75	0.40
1:f:234:ALA:HB3	1:f:299:LEU:HD11	2.02	0.40
2:h:22:ILE:HA	2:h:27:HIS:O	2.21	0.40
1:l:167:ARG:NH2	1:l:241:GLU:OE1	2.54	0.40
4:o:60:THR:OG1	4:o:61:GLY:N	2.55	0.40
5:p:134:GLU:HG2	5:p:159:ILE:HD12	2.03	0.40
2:z:79:TYR:HD2	3:y:70:GLN:HG2	1.85	0.40
1:3:48:HIS:O	1:3:48:HIS:CD2	2.74	0.40
1:3:48:HIS:CD2	1:3:48:HIS:C	2.97	0.40
5:q:15:ARG:HG2	5:q:83:GLN:CD	2.46	0.40
5:q:21:TRP:HZ2	5:q:66:ILE:HG21	1.87	0.40
1:w:193:ASP:OD1	1:w:196:GLN:N	2.54	0.40
1:w:195:LEU:O	1:w:196:GLN:C	2.64	0.40
1:w:215:ARG:HB2	1:w:215:ARG:NH1	2.37	0.40
5:2:119:ALA:O	5:2:123:THR:OG1	2.39	0.40
4:L:37:HIS:O	4:L:41:GLN:HG2	2.20	0.40
5:S:133:CYS:SG	5:S:134:GLU:O	2.80	0.40
5:S:161:LYS:HA	5:S:162:PRO:C	2.46	0.40
1:V:319:ILE:H	1:V:319:ILE:HG12	1.44	0.40
2:Z:88:THR:HG23	4:c:16:GLU:OE1	2.21	0.40
2:Z:90:ILE:HG23	2:Z:90:ILE:O	2.21	0.40
4:c:150:THR:OG1	4:c:152:GLU:OE1	2.35	0.40
5:d:111:TYR:HB3	5:d:112:PHE:CD1	2.56	0.40
1:f:140:LEU:HD23	1:f:140:LEU:HA	1.84	0.40
2:h:19:VAL:O	2:h:30:ILE:HG23	2.21	0.40
3:g:26:GLU:O	3:g:29:ARG:HB3	2.20	0.40
1:l:195:LEU:O	1:l:198:TYR:HB3	2.21	0.40
3:m:50:LEU:HD22	3:m:51:LEU:N	2.32	0.40
4:o:8:GLN:HB3	4:o:127:PHE:HE2	1.87	0.40
4:o:50:ASP:OD1	4:o:52:ARG:N	2.52	0.40
5:p:134:GLU:HG2	5:p:159:ILE:CD1	2.51	0.40
1:x:27:LEU:HD12	1:x:27:LEU:HA	1.91	0.40
1:x:150:ASN:OD1	1:x:150:ASN:N	2.53	0.40
4:0:41:GLN:HE22	4:0:117:GLN:C	2.20	0.40
3:4:3:VAL:HG12	3:4:64:SER:HA	2.04	0.40
4:6:34:ASP:OD1	4:6:35:ARG:N	2.54	0.40
4:6:136:ASP:OD1	4:6:138:LEU:N	2.55	0.40
5:7:68:THR:O	5:7:69:TYR:CG	2.74	0.40
1:9:98:ARG:HD2	1:9:98:ARG:HA	1.91	0.40
2:T:72:LYS:HA	2:T:72:LYS:HD2	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:q:100:PRO:HB3	5:q:170:THR:HG21	2.03	0.40
5:q:121:ARG:O	5:q:124:ILE:HB	2.21	0.40
5:b:1:MET:O	5:b:2:GLU:HB3	2.21	0.40
1:C:76:ALA:O	1:C:80:VAL:HG23	2.22	0.40
3:D:51:LEU:HD22	3:D:60:CYS:SG	2.61	0.40
4:F:12:PHE:CZ	4:F:22:SER:HB2	2.57	0.40
3:J:50:LEU:HD13	3:J:51:LEU:H	1.87	0.40
5:M:98:VAL:HG12	5:M:99:ASP:O	2.22	0.40
2:Q:107:ALA:HB2	5:S:146:LEU:HD13	2.03	0.40
1:V:93:TYR:HD2	1:V:151:ILE:HD11	1.87	0.40
5:d:38:TRP:CH2	5:d:164:PRO:HG2	2.56	0.40
1:f:253:ARG:HA	1:f:253:ARG:HD2	1.74	0.40
1:f:297:PHE:CD1	1:f:297:PHE:C	2.99	0.40
4:i:12:PHE:CD2	4:i:127:PHE:HB2	2.57	0.40
1:x:232:LYS:O	1:x:235:ASP:HB3	2.21	0.40
1:3:58:PRO:HA	1:3:61:ILE:CG2	2.51	0.40
1:3:152:LYS:HB2	1:3:184:TYR:OH	2.21	0.40
1:3:188:CYS:SG	1:3:190:ASN:HB3	2.62	0.40
1:3:204:LYS:HB3	1:3:204:LYS:HE3	1.84	0.40
2:5:109:PHE:CD1	2:5:109:PHE:C	2.99	0.40
5:7:140:ASN:ND2	5:7:140:ASN:N	2.69	0.40
4:k:14:ASN:CA	4:k:19:ARG:HH21	2.26	0.40
1:U:243:LYS:HD2	1:U:243:LYS:HA	1.78	0.40
2:Y:76:TYR:CD1	2:Y:76:TYR:C	2.99	0.40
4:a:29:TYR:CE1	4:a:31:GLY:CA	3.05	0.40
5:b:17:ARG:HH12	5:b:168:LYS:HE2	1.85	0.40
1:C:113:GLN:HE21	1:C:113:GLN:HB2	1.63	0.40
4:F:118:ARG:NH2	4:F:120:ASP:CB	2.85	0.40
2:K:101:LEU:HD23	5:M:153:LEU:HD11	2.04	0.40
4:R:151:ARG:NE	5:S:114:CYS:HB2	2.37	0.40
1:V:15:PHE:C	1:V:15:PHE:HD1	2.25	0.40
3:W:10:HIS:HB3	3:W:11:LYS:H	1.57	0.40
4:c:131:ARG:HG2	4:c:135:GLU:OE2	2.22	0.40
4:c:152:GLU:CB	4:c:153:PHE:HD1	2.34	0.40
1:f:134:ILE:HD12	1:f:134:ILE:HG23	1.77	0.40
1:f:157:ASP:OD1	1:f:157:ASP:N	2.55	0.40
5:j:65:VAL:HG21	5:j:90:ARG:NH1	2.37	0.40
1:l:216:THR:HG22	1:l:217:GLN:N	2.36	0.40
1:l:273:PHE:O	1:l:274:LYS:C	2.65	0.40
5:p:115:PHE:CE2	5:p:133:CYS:HB2	2.57	0.40
3:s:43:ARG:HD3	3:s:85:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:12:PHE:C	4:u:12:PHE:CD1	3.00	0.40
4:0:31:GLY:H	4:0:40:ARG:NH1	2.18	0.40
2:5:17:MET:CG	2:5:18:TYR:HD1	2.34	0.40
1:9:156:GLN:HE21	1:9:205:ALA:CB	2.34	0.40
2:T:62:PHE:HB3	2:T:65:ILE:CG1	2.51	0.40
4:k:65:SER:OG	4:k:66:LEU:N	2.53	0.40
4:k:84:GLU:H	4:k:84:GLU:HG2	1.52	0.40
5:q:15:ARG:HH22	1:w:318:ILE:HG13	1.86	0.40
4:N:16:GLU:HA	4:N:19:ARG:HD2	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:93:ARG:NH2	5:p:93:ARG:NH2[1_545]	2.01	0.19
1:V:315:GLU:OE2	5:v:22:LYS:NZ[1_545]	2.08	0.12
5:d:93:ARG:NH2	5:p:93:ARG:CZ[1_545]	2.09	0.11
5:d:22:LYS:NZ	1:r:315:GLU:OE2[1_545]	2.19	0.01

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	3	292/311 (94%)	289 (99%)	2 (1%)	1 (0%)	36	65
1	9	292/311 (94%)	279 (96%)	13 (4%)	0	100	100
1	C	294/311 (94%)	290 (99%)	3 (1%)	1 (0%)	36	65
1	I	293/311 (94%)	288 (98%)	5 (2%)	0	100	100
1	O	295/311 (95%)	291 (99%)	4 (1%)	0	100	100
1	U	297/311 (96%)	290 (98%)	6 (2%)	1 (0%)	36	65
1	V	293/311 (94%)	288 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	f	293/311 (94%)	287 (98%)	6 (2%)	0	100	100
1	l	293/311 (94%)	287 (98%)	6 (2%)	0	100	100
1	r	293/311 (94%)	287 (98%)	6 (2%)	0	100	100
1	w	293/311 (94%)	289 (99%)	4 (1%)	0	100	100
1	x	290/311 (93%)	287 (99%)	2 (1%)	1 (0%)	36	65
2	5	83/96 (86%)	82 (99%)	1 (1%)	0	100	100
2	B	83/96 (86%)	82 (99%)	1 (1%)	0	100	100
2	E	83/96 (86%)	81 (98%)	2 (2%)	0	100	100
2	K	82/96 (85%)	81 (99%)	1 (1%)	0	100	100
2	Q	83/96 (86%)	82 (99%)	1 (1%)	0	100	100
2	T	83/96 (86%)	82 (99%)	1 (1%)	0	100	100
2	Y	83/96 (86%)	77 (93%)	6 (7%)	0	100	100
2	Z	83/96 (86%)	79 (95%)	4 (5%)	0	100	100
2	h	83/96 (86%)	81 (98%)	2 (2%)	0	100	100
2	n	83/96 (86%)	81 (98%)	2 (2%)	0	100	100
2	t	83/96 (86%)	81 (98%)	2 (2%)	0	100	100
2	z	83/96 (86%)	79 (95%)	4 (5%)	0	100	100
3	4	91/102 (89%)	86 (94%)	5 (6%)	0	100	100
3	D	91/102 (89%)	87 (96%)	4 (4%)	0	100	100
3	H	91/102 (89%)	85 (93%)	6 (7%)	0	100	100
3	J	86/102 (84%)	83 (96%)	3 (4%)	0	100	100
3	P	90/102 (88%)	87 (97%)	3 (3%)	0	100	100
3	W	87/102 (85%)	84 (97%)	3 (3%)	0	100	100
3	X	91/102 (89%)	85 (93%)	6 (7%)	0	100	100
3	e	77/102 (76%)	72 (94%)	5 (6%)	0	100	100
3	g	91/102 (89%)	85 (93%)	6 (7%)	0	100	100
3	m	91/102 (89%)	86 (94%)	5 (6%)	0	100	100
3	s	91/102 (89%)	85 (93%)	6 (7%)	0	100	100
3	y	91/102 (89%)	86 (94%)	5 (6%)	0	100	100
4	0	140/170 (82%)	137 (98%)	2 (1%)	1 (1%)	18	49
4	6	134/170 (79%)	130 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	141/170 (83%)	137 (97%)	4 (3%)	0	100	100
4	L	140/170 (82%)	136 (97%)	4 (3%)	0	100	100
4	N	141/170 (83%)	136 (96%)	5 (4%)	0	100	100
4	R	140/170 (82%)	135 (96%)	5 (4%)	0	100	100
4	a	142/170 (84%)	138 (97%)	4 (3%)	0	100	100
4	c	141/170 (83%)	135 (96%)	4 (3%)	2 (1%)	9	33
4	i	153/170 (90%)	148 (97%)	4 (3%)	1 (1%)	18	49
4	k	143/170 (84%)	140 (98%)	3 (2%)	0	100	100
4	o	139/170 (82%)	136 (98%)	3 (2%)	0	100	100
4	u	139/170 (82%)	136 (98%)	3 (2%)	0	100	100
5	1	168/176 (96%)	161 (96%)	4 (2%)	3 (2%)	6	29
5	2	168/176 (96%)	162 (96%)	5 (3%)	1 (1%)	21	52
5	7	168/176 (96%)	160 (95%)	4 (2%)	4 (2%)	4	24
5	G	168/176 (96%)	159 (95%)	7 (4%)	2 (1%)	10	37
5	M	169/176 (96%)	161 (95%)	7 (4%)	1 (1%)	21	52
5	S	168/176 (96%)	162 (96%)	5 (3%)	1 (1%)	21	52
5	b	170/176 (97%)	161 (95%)	6 (4%)	3 (2%)	6	29
5	d	168/176 (96%)	162 (96%)	5 (3%)	1 (1%)	21	52
5	j	168/176 (96%)	163 (97%)	4 (2%)	1 (1%)	21	52
5	p	167/176 (95%)	164 (98%)	2 (1%)	1 (1%)	21	52
5	q	167/176 (95%)	161 (96%)	4 (2%)	2 (1%)	10	37
5	v	168/176 (96%)	161 (96%)	6 (4%)	1 (1%)	21	52
All	All	9291/10260 (91%)	9012 (97%)	250 (3%)	29 (0%)	36	65

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	b	128	ILE
5	G	129	VAL
5	M	128	ILE
5	j	128	ILE
5	p	128	ILE
5	1	128	ILE
5	1	143	VAL

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Mol	Chain	Res	Type
5	7	128	ILE
5	b	142	VAL
5	G	128	ILE
5	S	128	ILE
4	c	137	ALA
5	q	128	ILE
5	q	129	VAL
5	2	128	ILE
1	U	15	PHE
1	C	15	PHE
4	i	136	ASP
5	v	128	ILE
1	x	15	PHE
4	0	60	THR
5	b	141	LYS
4	c	136	ASP
5	d	128	ILE
5	7	129	VAL
5	7	141	LYS
1	3	15	PHE
5	7	142	VAL
5	1	129	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	3	269/283 (95%)	212 (79%)	57 (21%)	1	5
1	9	269/283 (95%)	220 (82%)	49 (18%)	2	8
1	C	270/283 (95%)	206 (76%)	64 (24%)	1	4
1	I	270/283 (95%)	207 (77%)	63 (23%)	1	4
1	O	270/283 (95%)	200 (74%)	70 (26%)	0	2
1	U	273/283 (96%)	214 (78%)	59 (22%)	1	5
1	V	270/283 (95%)	191 (71%)	79 (29%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	270/283 (95%)	204 (76%)	66 (24%)	1	3
1	l	271/283 (96%)	205 (76%)	66 (24%)	1	3
1	r	270/283 (95%)	210 (78%)	60 (22%)	1	5
1	w	269/283 (95%)	208 (77%)	61 (23%)	1	4
1	x	268/283 (95%)	209 (78%)	59 (22%)	1	5
2	5	78/85 (92%)	54 (69%)	24 (31%)	0	1
2	B	78/85 (92%)	61 (78%)	17 (22%)	1	5
2	E	78/85 (92%)	57 (73%)	21 (27%)	0	2
2	K	77/85 (91%)	59 (77%)	18 (23%)	1	4
2	Q	78/85 (92%)	55 (70%)	23 (30%)	0	2
2	T	78/85 (92%)	53 (68%)	25 (32%)	0	1
2	Y	78/85 (92%)	53 (68%)	25 (32%)	0	1
2	Z	78/85 (92%)	56 (72%)	22 (28%)	0	2
2	h	78/85 (92%)	60 (77%)	18 (23%)	1	4
2	n	78/85 (92%)	60 (77%)	18 (23%)	1	4
2	t	78/85 (92%)	60 (77%)	18 (23%)	1	4
2	z	78/85 (92%)	59 (76%)	19 (24%)	1	3
3	4	83/90 (92%)	71 (86%)	12 (14%)	3	14
3	D	83/90 (92%)	70 (84%)	13 (16%)	2	12
3	H	83/90 (92%)	72 (87%)	11 (13%)	4	17
3	J	80/90 (89%)	63 (79%)	17 (21%)	1	5
3	P	82/90 (91%)	63 (77%)	19 (23%)	1	4
3	W	80/90 (89%)	57 (71%)	23 (29%)	0	2
3	X	83/90 (92%)	70 (84%)	13 (16%)	2	12
3	e	68/90 (76%)	50 (74%)	18 (26%)	0	2
3	g	83/90 (92%)	69 (83%)	14 (17%)	2	10
3	m	83/90 (92%)	70 (84%)	13 (16%)	2	12
3	s	83/90 (92%)	68 (82%)	15 (18%)	2	8
3	y	83/90 (92%)	71 (86%)	12 (14%)	3	14
4	0	118/149 (79%)	88 (75%)	30 (25%)	0	3
4	6	114/149 (76%)	82 (72%)	32 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	119/149 (80%)	80 (67%)	39 (33%)	0	1
4	L	112/149 (75%)	86 (77%)	26 (23%)	1	4
4	N	116/149 (78%)	92 (79%)	24 (21%)	1	6
4	R	118/149 (79%)	86 (73%)	32 (27%)	0	2
4	a	120/149 (80%)	79 (66%)	41 (34%)	0	1
4	c	118/149 (79%)	88 (75%)	30 (25%)	0	3
4	i	130/149 (87%)	95 (73%)	35 (27%)	0	2
4	k	121/149 (81%)	84 (69%)	37 (31%)	0	1
4	o	117/149 (78%)	88 (75%)	29 (25%)	1	3
4	u	117/149 (78%)	88 (75%)	29 (25%)	1	3
5	1	145/160 (91%)	121 (83%)	24 (17%)	2	11
5	2	147/160 (92%)	121 (82%)	26 (18%)	2	8
5	7	147/160 (92%)	104 (71%)	43 (29%)	0	2
5	G	148/160 (92%)	110 (74%)	38 (26%)	0	2
5	M	148/160 (92%)	113 (76%)	35 (24%)	1	4
5	S	147/160 (92%)	109 (74%)	38 (26%)	0	2
5	b	150/160 (94%)	111 (74%)	39 (26%)	0	2
5	d	147/160 (92%)	113 (77%)	34 (23%)	1	4
5	j	148/160 (92%)	108 (73%)	40 (27%)	0	2
5	p	145/160 (91%)	108 (74%)	37 (26%)	0	3
5	q	147/160 (92%)	100 (68%)	47 (32%)	0	1
5	v	147/160 (92%)	114 (78%)	33 (22%)	1	5
All	All	8334/9204 (90%)	6335 (76%)	1999 (24%)	1	3

All (1999) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	12	SER
1	U	13	LEU
1	U	17	ASP
1	U	22	MET
1	U	27	LEU
1	U	45	SER
1	U	55	ASP

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Mol	Chain	Res	Type
1	U	65	LEU
1	U	70	LEU
1	U	74	LYS
1	U	80	VAL
1	U	81	LEU
1	U	85	ASP
1	U	86	ASP
1	U	87	THR
1	U	89	LEU
1	U	90	LEU
1	U	98	ARG
1	U	102	THR
1	U	103	GLN
1	U	117	THR
1	U	133	SER
1	U	134	ILE
1	U	145	GLU
1	U	146	SER
1	U	151	ILE
1	U	153	ASN
1	U	157	ASP
1	U	160	MET
1	U	161	LYS
1	U	162	LEU
1	U	178	ILE
1	U	183	SER
1	U	184	TYR
1	U	189	SER
1	U	192	GLU
1	U	194	LYS
1	U	197	ILE
1	U	201	ASN
1	U	207	LEU
1	U	212	ARG
1	U	220	SER
1	U	223	GLN
1	U	228	GLN
1	U	251	THR
1	U	252	ARG
1	U	253	ARG
1	U	258	VAL
1	U	259	GLU

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Mol	Chain	Res	Type
1	U	261	LEU
1	U	277	ILE
1	U	284	MET
1	U	285	ILE
1	U	294	HIS
1	U	296	MET
1	U	298	SER
1	U	307	ILE
1	U	314	LEU
1	U	319	ILE
2	Y	17	MET
2	Y	21	LEU
2	Y	22	ILE
2	Y	23	SER
2	Y	25	ASP
2	Y	32	LYS
2	Y	34	GLU
2	Y	38	THR
2	Y	42	ILE
2	Y	46	LEU
2	Y	58	ASN
2	Y	59	GLU
2	Y	60	VAL
2	Y	65	ILE
2	Y	70	LEU
2	Y	80	LYS
2	Y	82	ARG
2	Y	86	SER
2	Y	87	SER
2	Y	88	THR
2	Y	90	ILE
2	Y	101	LEU
2	Y	103	LEU
2	Y	104	LEU
2	Y	109	PHE
3	X	7	ILE
3	X	13	THR
3	X	21	SER
3	X	27	LEU
3	X	40	ASP
3	X	42	GLN
3	X	45	TYR

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Mol	Chain	Res	Type
3	X	49	GLN
3	X	52	ASP
3	X	70	GLN
3	X	77	LEU
3	X	85	PHE
3	X	95	SER
4	a	4	VAL
4	a	5	VAL
4	a	7	ASP
4	a	11	LYS
4	a	14	ASN
4	a	25	CYS
4	a	26	GLU
4	a	27	ILE
4	a	29	TYR
4	a	30	THR
4	a	32	PHE
4	a	50	ASP
4	a	58	VAL
4	a	60	THR
4	a	64	LEU
4	a	65	SER
4	a	66	LEU
4	a	72	SER
4	a	83	ARG
4	a	85	TYR
4	a	87	ASP
4	a	88	LEU
4	a	94	LYS
4	a	103	LEU
4	a	106	VAL
4	a	109	ILE
4	a	114	ILE
4	a	117	GLN
4	a	118	ARG
4	a	126	GLU
4	a	129	GLU
4	a	130	GLU
4	a	131	ARG
4	a	138	LEU
4	a	141	GLN
4	a	148	ARG

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Mol	Chain	Res	Type
4	a	150	THR
4	a	151	ARG
4	a	152	GLU
4	a	155	ASP
4	a	156	ARG
5	b	3	ASN
5	b	6	GLN
5	b	7	VAL
5	b	9	ILE
5	b	14	ASP
5	b	15	ARG
5	b	17	ARG
5	b	18	ILE
5	b	23	ARG
5	b	25	VAL
5	b	29	MET
5	b	32	SER
5	b	34	LYS
5	b	36	LYS
5	b	37	ASP
5	b	45	GLU
5	b	47	THR
5	b	50	LYS
5	b	61	ASP
5	b	70	TRP
5	b	85	VAL
5	b	95	SER
5	b	105	GLN
5	b	113	ASP
5	b	114	CYS
5	b	116	SER
5	b	117	GLU
5	b	123	THR
5	b	128	ILE
5	b	129	VAL
5	b	130	SER
5	b	132	ARG
5	b	134	GLU
5	b	136	GLN
5	b	142	VAL
5	b	145	LEU
5	b	158	GLN

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Mol	Chain	Res	Type
5	b	159	ILE
5	b	166	VAL
1	C	13	LEU
1	C	14	GLN
1	C	16	GLU
1	C	17	ASP
1	C	27	LEU
1	C	33	GLU
1	C	61	ILE
1	C	65	LEU
1	C	68	ASP
1	C	70	LEU
1	C	81	LEU
1	C	84	GLN
1	C	85	ASP
1	C	86	ASP
1	C	87	THR
1	C	89	LEU
1	C	90	LEU
1	C	91	LYS
1	C	94	ILE
1	C	98	ARG
1	C	103	GLN
1	C	106	ILE
1	C	113	GLN
1	C	115	GLU
1	C	117	THR
1	C	134	ILE
1	C	147	ILE
1	C	154	ARG
1	C	155	LEU
1	C	160	MET
1	C	162	LEU
1	C	178	ILE
1	C	192	GLU
1	C	193	ASP
1	C	194	LYS
1	C	199	ARG
1	C	207	LEU
1	C	209	SER
1	C	210	THR
1	C	217	GLN

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Mol	Chain	Res	Type
1	C	222	LEU
1	C	232	LYS
1	C	242	GLU
1	C	251	THR
1	C	252	ARG
1	C	253	ARG
1	C	257	SER
1	C	258	VAL
1	C	261	LEU
1	C	265	CYS
1	C	270	VAL
1	C	277	ILE
1	C	280	GLU
1	C	284	MET
1	C	285	ILE
1	C	290	THR
1	C	294	HIS
1	C	295	LEU
1	C	298	SER
1	C	299	LEU
1	C	307	ILE
1	C	313	ASP
1	C	314	LEU
1	C	318	ILE
2	E	22	ILE
2	E	32	LYS
2	E	39	SER
2	E	46	LEU
2	E	58	ASN
2	E	60	VAL
2	E	61	ASN
2	E	65	ILE
2	E	70	LEU
2	E	72	LYS
2	E	80	LYS
2	E	82	ARG
2	E	86	SER
2	E	88	THR
2	E	95	ILE
2	E	98	GLU
2	E	99	ILE
2	E	101	LEU

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Mol	Chain	Res	Type
2	E	103	LEU
2	E	104	LEU
2	E	109	PHE
3	D	13	THR
3	D	21	SER
3	D	27	LEU
3	D	36	LYS
3	D	40	ASP
3	D	45	TYR
3	D	49	GLN
3	D	50	LEU
3	D	52	ASP
3	D	70	GLN
3	D	74	THR
3	D	85	PHE
3	D	95	SER
4	F	4	VAL
4	F	5	VAL
4	F	8	GLN
4	F	11	LYS
4	F	25	CYS
4	F	26	GLU
4	F	27	ILE
4	F	30	THR
4	F	32	PHE
4	F	34	ASP
4	F	43	ARG
4	F	46	ASN
4	F	49	ARG
4	F	50	ASP
4	F	60	THR
4	F	64	LEU
4	F	66	LEU
4	F	72	SER
4	F	83	ARG
4	F	85	TYR
4	F	87	ASP
4	F	88	LEU
4	F	97	LEU
4	F	101	MET
4	F	103	LEU
4	F	106	VAL

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Mol	Chain	Res	Type
4	F	114	ILE
4	F	122	MET
4	F	126	GLU
4	F	129	GLU
4	F	130	GLU
4	F	131	ARG
4	F	135	GLU
4	F	141	GLN
4	F	147	ARG
4	F	151	ARG
4	F	152	GLU
4	F	155	ASP
4	F	156	ARG
5	G	3	ASN
5	G	6	GLN
5	G	7	VAL
5	G	9	ILE
5	G	18	ILE
5	G	22	LYS
5	G	25	VAL
5	G	26	LYS
5	G	31	ILE
5	G	32	SER
5	G	36	LYS
5	G	47	THR
5	G	61	ASP
5	G	64	LEU
5	G	70	TRP
5	G	76	GLU
5	G	77	ARG
5	G	88	GLU
5	G	93	ARG
5	G	95	SER
5	G	107	ILE
5	G	113	ASP
5	G	114	CYS
5	G	116	SER
5	G	120	ILE
5	G	123	THR
5	G	129	VAL
5	G	130	SER
5	G	132	ARG

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Mol	Chain	Res	Type
5	G	133	CYS
5	G	136	GLN
5	G	145	LEU
5	G	155	LYS
5	G	157	LYS
5	G	158	GLN
5	G	159	ILE
5	G	166	VAL
5	G	167	ARG
1	I	13	LEU
1	I	14	GLN
1	I	17	ASP
1	I	27	LEU
1	I	50	VAL
1	I	55	ASP
1	I	62	HIS
1	I	65	LEU
1	I	71	GLU
1	I	77	GLN
1	I	79	ARG
1	I	80	VAL
1	I	81	LEU
1	I	85	ASP
1	I	87	THR
1	I	94	ILE
1	I	95	VAL
1	I	106	ILE
1	I	109	LYS
1	I	117	THR
1	I	118	LEU
1	I	133	SER
1	I	134	ILE
1	I	139	MET
1	I	141	ASP
1	I	142	THR
1	I	149	SER
1	I	152	LYS
1	I	153	ASN
1	I	154	ARG
1	I	157	ASP
1	I	162	LEU
1	I	163	VAL

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Mol	Chain	Res	Type
1	I	164	HIS
1	I	168	LEU
1	I	197	ILE
1	I	198	TYR
1	I	199	ARG
1	I	207	LEU
1	I	209	SER
1	I	210	THR
1	I	212	ARG
1	I	222	LEU
1	I	223	GLN
1	I	228	GLN
1	I	232	LYS
1	I	239	LYS
1	I	253	ARG
1	I	265	CYS
1	I	277	ILE
1	I	285	ILE
1	I	289	GLU
1	I	290	THR
1	I	296	MET
1	I	298	SER
1	I	299	LEU
1	I	301	ASP
1	I	302	LYS
1	I	307	ILE
1	I	312	LYS
1	I	314	LEU
1	I	319	ILE
1	I	320	SER
2	K	21	LEU
2	K	22	ILE
2	K	31	VAL
2	K	32	LYS
2	K	34	GLU
2	K	38	THR
2	K	39	SER
2	K	46	LEU
2	K	64	GLU
2	K	65	ILE
2	K	70	LEU
2	K	87	SER

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Mol	Chain	Res	Type
2	K	88	THR
2	K	98	GLU
2	K	101	LEU
2	K	103	LEU
2	K	104	LEU
2	K	109	PHE
3	J	9	ARG
3	J	13	THR
3	J	17	ASP
3	J	21	SER
3	J	27	LEU
3	J	30	ILE
3	J	41	GLU
3	J	44	LEU
3	J	47	ASP
3	J	50	LEU
3	J	52	ASP
3	J	68	ARG
3	J	70	GLN
3	J	74	THR
3	J	84	THR
3	J	88	LEU
3	J	98	GLU
4	L	5	VAL
4	L	9	ARG
4	L	11	LYS
4	L	25	CYS
4	L	30	THR
4	L	32	PHE
4	L	41	GLN
4	L	49	ARG
4	L	58	VAL
4	L	62	THR
4	L	64	LEU
4	L	65	SER
4	L	66	LEU
4	L	72	SER
4	L	83	ARG
4	L	85	TYR
4	L	88	LEU
4	L	98	LYS
4	L	106	VAL

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Mol	Chain	Res	Type
4	L	109	ILE
4	L	126	GLU
4	L	131	ARG
4	L	147	ARG
4	L	150	THR
4	L	151	ARG
4	L	152	GLU
5	M	7	VAL
5	M	9	ILE
5	M	10	VAL
5	M	13	VAL
5	M	18	ILE
5	M	25	VAL
5	M	26	LYS
5	M	31	ILE
5	M	32	SER
5	M	37	ASP
5	M	46	SER
5	M	47	THR
5	M	55	VAL
5	M	59	LEU
5	M	64	LEU
5	M	67	THR
5	M	70	TRP
5	M	72	LEU
5	M	86	SER
5	M	90	ARG
5	M	95	SER
5	M	113	ASP
5	M	114	CYS
5	M	116	SER
5	M	117	GLU
5	M	123	THR
5	M	128	ILE
5	M	132	ARG
5	M	134	GLU
5	M	136	GLN
5	M	145	LEU
5	M	154	ILE
5	M	159	ILE
5	M	166	VAL
5	M	167	ARG

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Mol	Chain	Res	Type
1	O	12	SER
1	O	13	LEU
1	O	16	GLU
1	O	17	ASP
1	O	27	LEU
1	O	29	LEU
1	O	36	THR
1	O	38	GLN
1	O	43	LEU
1	O	45	SER
1	O	62	HIS
1	O	65	LEU
1	O	70	LEU
1	O	71	GLU
1	O	74	LYS
1	O	81	LEU
1	O	85	ASP
1	O	87	THR
1	O	91	LYS
1	O	93	TYR
1	O	95	VAL
1	O	98	ARG
1	O	102	THR
1	O	103	GLN
1	O	133	SER
1	O	134	ILE
1	O	142	THR
1	O	146	SER
1	O	147	ILE
1	O	149	SER
1	O	152	LYS
1	O	155	LEU
1	O	158	SER
1	O	162	LEU
1	O	176	LEU
1	O	178	ILE
1	O	186	ASN
1	O	189	SER
1	O	192	GLU
1	O	194	LYS
1	O	196	GLN
1	O	197	ILE

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Mol	Chain	Res	Type
1	O	200	ASP
1	O	207	LEU
1	O	209	SER
1	O	215	ARG
1	O	216	THR
1	O	223	GLN
1	O	227	VAL
1	O	228	GLN
1	O	249	LEU
1	O	251	THR
1	O	254	GLU
1	O	258	VAL
1	O	259	GLU
1	O	261	LEU
1	O	263	GLU
1	O	264	CYS
1	O	271	THR
1	O	276	THR
1	O	277	ILE
1	O	282	GLN
1	O	285	ILE
1	O	291	GLU
1	O	296	MET
1	O	298	SER
1	O	299	LEU
1	O	303	VAL
1	O	312	LYS
1	O	318	ILE
2	Q	17	MET
2	Q	19	VAL
2	Q	21	LEU
2	Q	23	SER
2	Q	30	ILE
2	Q	32	LYS
2	Q	34	GLU
2	Q	38	THR
2	Q	39	SER
2	Q	45	MET
2	Q	58	ASN
2	Q	63	ARG
2	Q	65	ILE
2	Q	70	LEU

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Mol	Chain	Res	Type
2	Q	85	ASN
2	Q	86	SER
2	Q	87	SER
2	Q	88	THR
2	Q	90	ILE
2	Q	98	GLU
2	Q	103	LEU
2	Q	104	LEU
2	Q	105	MET
3	P	2	ASP
3	P	13	THR
3	P	14	ILE
3	P	21	SER
3	P	27	LEU
3	P	32	GLU
3	P	34	ILE
3	P	40	ASP
3	P	45	TYR
3	P	49	GLN
3	P	52	ASP
3	P	53	ASP
3	P	70	GLN
3	P	74	THR
3	P	77	LEU
3	P	85	PHE
3	P	86	GLU
3	P	91	GLU
3	P	94	SER
4	R	5	VAL
4	R	11	LYS
4	R	12	PHE
4	R	25	CYS
4	R	30	THR
4	R	50	ASP
4	R	52	ARG
4	R	54	GLU
4	R	55	ILE
4	R	58	VAL
4	R	64	LEU
4	R	65	SER
4	R	66	LEU
4	R	72	SER

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Mol	Chain	Res	Type
4	R	87	ASP
4	R	88	LEU
4	R	94	LYS
4	R	97	LEU
4	R	98	LYS
4	R	101	MET
4	R	106	VAL
4	R	109	ILE
4	R	111	LYS
4	R	127	PHE
4	R	130	GLU
4	R	131	ARG
4	R	136	ASP
4	R	144	GLU
4	R	145	GLU
4	R	151	ARG
4	R	152	GLU
4	R	156	ARG
5	S	3	ASN
5	S	6	GLN
5	S	7	VAL
5	S	15	ARG
5	S	17	ARG
5	S	23	ARG
5	S	24	LEU
5	S	25	VAL
5	S	32	SER
5	S	36	LYS
5	S	47	THR
5	S	70	TRP
5	S	83	GLN
5	S	86	SER
5	S	87	ILE
5	S	95	SER
5	S	96	THR
5	S	107	ILE
5	S	114	CYS
5	S	117	GLU
5	S	120	ILE
5	S	123	THR
5	S	124	ILE
5	S	128	ILE

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Mol	Chain	Res	Type
5	S	130	SER
5	S	132	ARG
5	S	134	GLU
5	S	135	TYR
5	S	136	GLN
5	S	141	LYS
5	S	143	VAL
5	S	146	LEU
5	S	154	LEU
5	S	155	ILE
5	S	156	LYS
5	S	160	ILE
5	S	166	SER
5	S	167	VAL
1	V	13	LEU
1	V	15	PHE
1	V	17	ASP
1	V	22	MET
1	V	25	ILE
1	V	27	LEU
1	V	38	GLN
1	V	42	ASP
1	V	61	ILE
1	V	62	HIS
1	V	63	GLN
1	V	65	LEU
1	V	71	GLU
1	V	74	LYS
1	V	79	ARG
1	V	81	LEU
1	V	84	GLN
1	V	85	ASP
1	V	87	THR
1	V	89	LEU
1	V	91	LYS
1	V	93	TYR
1	V	95	VAL
1	V	102	THR
1	V	103	GLN
1	V	104	CYS
1	V	117	THR
1	V	133	SER

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Mol	Chain	Res	Type
1	V	134	ILE
1	V	142	THR
1	V	149	SER
1	V	150	ASN
1	V	152	LYS
1	V	158	SER
1	V	170	GLU
1	V	185	VAL
1	V	188	CYS
1	V	189	SER
1	V	192	GLU
1	V	194	LYS
1	V	195	LEU
1	V	196	GLN
1	V	197	ILE
1	V	200	ASP
1	V	203	GLU
1	V	207	LEU
1	V	208	ASP
1	V	211	GLU
1	V	212	ARG
1	V	217	GLN
1	V	223	GLN
1	V	228	GLN
1	V	238	LEU
1	V	246	LEU
1	V	247	ARG
1	V	251	THR
1	V	252	ARG
1	V	253	ARG
1	V	255	CYS
1	V	256	ASN
1	V	259	GLU
1	V	264	CYS
1	V	271	THR
1	V	274	LYS
1	V	277	ILE
1	V	280	GLU
1	V	284	MET
1	V	285	ILE
1	V	293	LEU
1	V	294	HIS

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Mol	Chain	Res	Type
1	V	296	MET
1	V	298	SER
1	V	300	MET
1	V	307	ILE
1	V	314	LEU
1	V	315	GLU
1	V	317	HIS
1	V	319	ILE
1	V	320	SER
2	Z	19	VAL
2	Z	21	LEU
2	Z	22	ILE
2	Z	25	ASP
2	Z	30	ILE
2	Z	31	VAL
2	Z	32	LYS
2	Z	39	SER
2	Z	46	LEU
2	Z	58	ASN
2	Z	69	VAL
2	Z	70	LEU
2	Z	80	LYS
2	Z	81	VAL
2	Z	82	ARG
2	Z	85	ASN
2	Z	95	ILE
2	Z	98	GLU
2	Z	99	ILE
2	Z	101	LEU
2	Z	103	LEU
2	Z	104	LEU
3	W	2	ASP
3	W	7	ILE
3	W	12	THR
3	W	13	THR
3	W	21	SER
3	W	27	LEU
3	W	32	GLU
3	W	40	ASP
3	W	43	ARG
3	W	44	LEU
3	W	45	TYR

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Mol	Chain	Res	Type
3	W	49	GLN
3	W	52	ASP
3	W	60	CYS
3	W	66	THR
3	W	70	GLN
3	W	74	THR
3	W	75	VAL
3	W	77	LEU
3	W	85	PHE
3	W	88	LEU
3	W	90	ILE
3	W	95	SER
4	c	5	VAL
4	c	10	SER
4	c	11	LYS
4	c	12	PHE
4	c	13	GLU
4	c	30	THR
4	c	34	ASP
4	c	41	GLN
4	c	54	GLU
4	c	55	ILE
4	c	58	VAL
4	c	62	THR
4	c	64	LEU
4	c	65	SER
4	c	66	LEU
4	c	72	SER
4	c	84	GLU
4	c	88	LEU
4	c	94	LYS
4	c	111	LYS
4	c	117	GLN
4	c	120	ASP
4	c	122	MET
4	c	125	LEU
4	c	131	ARG
4	c	136	ASP
4	c	138	LEU
4	c	145	GLU
4	c	150	THR
4	c	152	GLU

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Mol	Chain	Res	Type
5	d	3	ASN
5	d	6	GLN
5	d	7	VAL
5	d	13	VAL
5	d	17	ARG
5	d	18	ILE
5	d	25	VAL
5	d	26	LYS
5	d	36	LYS
5	d	37	ASP
5	d	47	THR
5	d	70	TRP
5	d	74	THR
5	d	77	ARG
5	d	83	GLN
5	d	90	ARG
5	d	96	THR
5	d	113	ASP
5	d	117	GLU
5	d	128	ILE
5	d	130	SER
5	d	132	ARG
5	d	134	GLU
5	d	135	TYR
5	d	136	GLN
5	d	139	HIS
5	d	145	LEU
5	d	154	ILE
5	d	155	LYS
5	d	159	ILE
5	d	166	VAL
5	d	167	ARG
5	d	168	LYS
5	d	170	THR
1	f	12	SER
1	f	13	LEU
1	f	17	ASP
1	f	27	LEU
1	f	30	LEU
1	f	32	GLN
1	f	33	GLU
1	f	45	SER

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Mol	Chain	Res	Type
1	f	50	VAL
1	f	61	ILE
1	f	65	LEU
1	f	70	LEU
1	f	81	LEU
1	f	84	GLN
1	f	85	ASP
1	f	87	THR
1	f	89	LEU
1	f	102	THR
1	f	103	GLN
1	f	106	ILE
1	f	117	THR
1	f	135	VAL
1	f	137	LYS
1	f	149	SER
1	f	152	LYS
1	f	155	LEU
1	f	161	LYS
1	f	162	LEU
1	f	164	HIS
1	f	176	LEU
1	f	183	SER
1	f	188	CYS
1	f	194	LYS
1	f	195	LEU
1	f	197	ILE
1	f	199	ARG
1	f	210	THR
1	f	217	GLN
1	f	220	SER
1	f	222	LEU
1	f	224	GLN
1	f	227	VAL
1	f	232	LYS
1	f	237	LYS
1	f	238	LEU
1	f	239	LYS
1	f	243	LYS
1	f	249	LEU
1	f	251	THR
1	f	252	ARG

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Mol	Chain	Res	Type
1	f	253	ARG
1	f	254	GLU
1	f	256	ASN
1	f	259	GLU
1	f	261	LEU
1	f	264	CYS
1	f	266	VAL
1	f	267	ASN
1	f	275	GLU
1	f	284	MET
1	f	285	ILE
1	f	289	GLU
1	f	295	LEU
1	f	307	ILE
1	f	314	LEU
1	f	319	ILE
2	h	21	LEU
2	h	22	ILE
2	h	31	VAL
2	h	32	LYS
2	h	39	SER
2	h	46	LEU
2	h	58	ASN
2	h	60	VAL
2	h	65	ILE
2	h	70	LEU
2	h	71	SER
2	h	81	VAL
2	h	84	THR
2	h	90	ILE
2	h	98	GLU
2	h	101	LEU
2	h	103	LEU
2	h	104	LEU
3	g	2	ASP
3	g	13	THR
3	g	21	SER
3	g	27	LEU
3	g	30	ILE
3	g	42	GLN
3	g	44	LEU
3	g	49	GLN

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Mol	Chain	Res	Type
3	g	50	LEU
3	g	52	ASP
3	g	70	GLN
3	g	74	THR
3	g	77	LEU
3	g	85	PHE
4	i	3	ARG
4	i	4	VAL
4	i	5	VAL
4	i	9	ARG
4	i	21	LEU
4	i	25	CYS
4	i	30	THR
4	i	41	GLN
4	i	49	ARG
4	i	50	ASP
4	i	58	VAL
4	i	60	THR
4	i	62	THR
4	i	64	LEU
4	i	65	SER
4	i	66	LEU
4	i	72	SER
4	i	74	GLN
4	i	76	GLU
4	i	80	THR
4	i	84	GLU
4	i	85	TYR
4	i	87	ASP
4	i	88	LEU
4	i	106	VAL
4	i	111	LYS
4	i	118	ARG
4	i	122	MET
4	i	125	LEU
4	i	126	GLU
4	i	136	ASP
4	i	147	ARG
4	i	150	THR
4	i	151	ARG
4	i	152	GLU
5	j	3	ASN

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Mol	Chain	Res	Type
5	j	6	GLN
5	j	7	VAL
5	j	9	ILE
5	j	13	VAL
5	j	17	ARG
5	j	18	ILE
5	j	20	THR
5	j	25	VAL
5	j	26	LYS
5	j	29	MET
5	j	31	ILE
5	j	32	SER
5	j	41	ARG
5	j	45	GLU
5	j	47	THR
5	j	52	SER
5	j	70	TRP
5	j	76	GLU
5	j	86	SER
5	j	87	ILE
5	j	93	ARG
5	j	106	LEU
5	j	107	ILE
5	j	114	CYS
5	j	116	SER
5	j	117	GLU
5	j	128	ILE
5	j	130	SER
5	j	132	ARG
5	j	133	CYS
5	j	134	GLU
5	j	136	GLN
5	j	145	LEU
5	j	155	LYS
5	j	157	LYS
5	j	158	GLN
5	j	159	ILE
5	j	166	VAL
5	j	167	ARG
1	l	13	LEU
1	l	14	GLN
1	l	17	ASP

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Mol	Chain	Res	Type
1	1	27	LEU
1	1	32	GLN
1	1	62	HIS
1	1	70	LEU
1	1	73	ILE
1	1	74	LYS
1	1	75	GLN
1	1	82	SER
1	1	85	ASP
1	1	87	THR
1	1	89	LEU
1	1	94	ILE
1	1	98	ARG
1	1	102	THR
1	1	103	GLN
1	1	106	ILE
1	1	113	GLN
1	1	114	LEU
1	1	115	GLU
1	1	117	THR
1	1	133	SER
1	1	134	ILE
1	1	147	ILE
1	1	149	SER
1	1	166	GLU
1	1	174	SER
1	1	178	ILE
1	1	181	ARG
1	1	185	VAL
1	1	187	LEU
1	1	188	CYS
1	1	194	LYS
1	1	195	LEU
1	1	196	GLN
1	1	203	GLU
1	1	204	LYS
1	1	207	LEU
1	1	210	THR
1	1	211	GLU
1	1	215	ARG
1	1	216	THR
1	1	223	GLN

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Mol	Chain	Res	Type
1	l	228	GLN
1	l	232	LYS
1	l	239	LYS
1	l	240	GLU
1	l	246	LEU
1	l	251	THR
1	l	253	ARG
1	l	254	GLU
1	l	258	VAL
1	l	261	LEU
1	l	271	THR
1	l	277	ILE
1	l	282	GLN
1	l	285	ILE
1	l	291	GLU
1	l	295	LEU
1	l	296	MET
1	l	298	SER
1	l	314	LEU
1	l	318	ILE
1	l	319	ILE
2	n	17	MET
2	n	19	VAL
2	n	39	SER
2	n	46	LEU
2	n	62	PHE
2	n	64	GLU
2	n	65	ILE
2	n	67	SER
2	n	75	MET
2	n	80	LYS
2	n	82	ARG
2	n	88	THR
2	n	90	ILE
2	n	92	GLU
2	n	99	ILE
2	n	103	LEU
2	n	104	LEU
2	n	109	PHE
3	m	13	THR
3	m	17	ASP
3	m	21	SER

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Mol	Chain	Res	Type
3	m	27	LEU
3	m	42	GLN
3	m	49	GLN
3	m	50	LEU
3	m	52	ASP
3	m	70	GLN
3	m	74	THR
3	m	77	LEU
3	m	85	PHE
3	m	95	SER
4	o	5	VAL
4	o	9	ARG
4	o	25	CYS
4	o	30	THR
4	o	32	PHE
4	o	41	GLN
4	o	53	SER
4	o	58	VAL
4	o	62	THR
4	o	63	ASN
4	o	64	LEU
4	o	65	SER
4	o	87	ASP
4	o	89	GLU
4	o	101	MET
4	o	103	LEU
4	o	106	VAL
4	o	111	LYS
4	o	114	ILE
4	o	126	GLU
4	o	131	ARG
4	o	140	GLN
4	o	141	GLN
4	o	145	GLU
4	o	150	THR
4	o	151	ARG
4	o	152	GLU
4	o	153	PHE
4	o	156	ARG
5	p	3	ASN
5	p	6	GLN
5	p	7	VAL

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Mol	Chain	Res	Type
5	p	9	ILE
5	p	17	ARG
5	p	18	ILE
5	p	21	TRP
5	p	25	VAL
5	p	26	LYS
5	p	32	SER
5	p	34	LYS
5	p	36	LYS
5	p	39	PHE
5	p	47	THR
5	p	52	SER
5	p	53	SER
5	p	55	VAL
5	p	63	LYS
5	p	70	TRP
5	p	77	ARG
5	p	85	VAL
5	p	86	SER
5	p	96	THR
5	p	97	GLN
5	p	113	ASP
5	p	117	GLU
5	p	121	ARG
5	p	123	THR
5	p	127	ARG
5	p	132	ARG
5	p	134	GLU
5	p	145	LEU
5	p	148	LEU
5	p	154	ILE
5	p	159	ILE
5	p	166	VAL
5	p	168	LYS
1	r	13	LEU
1	r	14	GLN
1	r	17	ASP
1	r	18	LYS
1	r	22	MET
1	r	25	ILE
1	r	27	LEU
1	r	29	LEU

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Mol	Chain	Res	Type
1	r	34	SER
1	r	36	THR
1	r	42	ASP
1	r	61	ILE
1	r	74	LYS
1	r	82	SER
1	r	85	ASP
1	r	90	LEU
1	r	91	LYS
1	r	94	ILE
1	r	102	THR
1	r	103	GLN
1	r	105	ASP
1	r	117	THR
1	r	118	LEU
1	r	133	SER
1	r	134	ILE
1	r	142	THR
1	r	145	GLU
1	r	149	SER
1	r	178	ILE
1	r	192	GLU
1	r	195	LEU
1	r	199	ARG
1	r	201	ASN
1	r	204	LYS
1	r	207	LEU
1	r	210	THR
1	r	217	GLN
1	r	220	SER
1	r	232	LYS
1	r	251	THR
1	r	252	ARG
1	r	253	ARG
1	r	258	VAL
1	r	259	GLU
1	r	261	LEU
1	r	271	THR
1	r	277	ILE
1	r	284	MET
1	r	285	ILE
1	r	291	GLU

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Mol	Chain	Res	Type
1	r	296	MET
1	r	298	SER
1	r	300	MET
1	r	301	ASP
1	r	305	ASN
1	r	307	ILE
1	r	308	GLU
1	r	314	LEU
1	r	315	GLU
1	r	318	ILE
2	t	17	MET
2	t	21	LEU
2	t	22	ILE
2	t	31	VAL
2	t	34	GLU
2	t	39	SER
2	t	46	LEU
2	t	58	ASN
2	t	65	ILE
2	t	67	SER
2	t	70	LEU
2	t	73	VAL
2	t	80	LYS
2	t	82	ARG
2	t	87	SER
2	t	88	THR
2	t	103	LEU
2	t	104	LEU
3	s	4	PHE
3	s	5	LEU
3	s	8	ARG
3	s	13	THR
3	s	21	SER
3	s	27	LEU
3	s	42	GLN
3	s	49	GLN
3	s	50	LEU
3	s	52	ASP
3	s	70	GLN
3	s	74	THR
3	s	77	LEU
3	s	85	PHE

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Mol	Chain	Res	Type
3	s	95	SER
4	u	5	VAL
4	u	9	ARG
4	u	21	LEU
4	u	27	ILE
4	u	30	THR
4	u	32	PHE
4	u	49	ARG
4	u	58	VAL
4	u	60	THR
4	u	62	THR
4	u	64	LEU
4	u	66	LEU
4	u	72	SER
4	u	83	ARG
4	u	88	LEU
4	u	94	LYS
4	u	97	LEU
4	u	101	MET
4	u	106	VAL
4	u	111	LYS
4	u	114	ILE
4	u	116	LEU
4	u	126	GLU
4	u	135	GLU
4	u	138	LEU
4	u	150	THR
4	u	151	ARG
4	u	152	GLU
4	u	156	ARG
5	v	3	ASN
5	v	6	GLN
5	v	7	VAL
5	v	9	ILE
5	v	17	ARG
5	v	18	ILE
5	v	32	SER
5	v	36	LYS
5	v	44	TYR
5	v	47	THR
5	v	61	ASP
5	v	70	TRP

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Mol	Chain	Res	Type
5	v	83	GLN
5	v	86	SER
5	v	93	ARG
5	v	95	SER
5	v	96	THR
5	v	107	ILE
5	v	113	ASP
5	v	114	CYS
5	v	116	SER
5	v	117	GLU
5	v	123	THR
5	v	132	ARG
5	v	134	GLU
5	v	136	GLN
5	v	141	LYS
5	v	145	SER
5	v	146	LEU
5	v	159	GLN
5	v	160	ILE
5	v	167	VAL
5	v	170	LEU
1	x	13	LEU
1	x	17	ASP
1	x	22	MET
1	x	25	ILE
1	x	27	LEU
1	x	34	SER
1	x	35	VAL
1	x	37	LYS
1	x	45	SER
1	x	50	VAL
1	x	61	ILE
1	x	66	LYS
1	x	69	ILE
1	x	70	LEU
1	x	71	GLU
1	x	74	LYS
1	x	81	LEU
1	x	83	HIS
1	x	85	ASP
1	x	89	LEU
1	x	91	LYS

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Mol	Chain	Res	Type
1	x	94	ILE
1	x	95	VAL
1	x	98	ARG
1	x	103	GLN
1	x	106	ILE
1	x	109	LYS
1	x	117	THR
1	x	118	LEU
1	x	133	SER
1	x	134	ILE
1	x	149	SER
1	x	150	ASN
1	x	152	LYS
1	x	158	SER
1	x	162	LEU
1	x	186	ASN
1	x	188	CYS
1	x	192	GLU
1	x	194	LYS
1	x	195	LEU
1	x	197	ILE
1	x	199	ARG
1	x	212	ARG
1	x	220	SER
1	x	223	GLN
1	x	252	ARG
1	x	253	ARG
1	x	254	GLU
1	x	258	VAL
1	x	259	GLU
1	x	261	LEU
1	x	277	ILE
1	x	284	MET
1	x	285	ILE
1	x	298	SER
1	x	307	ILE
1	x	314	LEU
1	x	318	ILE
2	z	22	ILE
2	z	23	SER
2	z	32	LYS
2	z	39	SER

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Mol	Chain	Res	Type
2	z	45	MET
2	z	46	LEU
2	z	58	ASN
2	z	59	GLU
2	z	60	VAL
2	z	65	ILE
2	z	70	LEU
2	z	80	LYS
2	z	82	ARG
2	z	84	THR
2	z	88	THR
2	z	101	LEU
2	z	103	LEU
2	z	104	LEU
2	z	109	PHE
3	y	13	THR
3	y	21	SER
3	y	27	LEU
3	y	30	ILE
3	y	40	ASP
3	y	42	GLN
3	y	50	LEU
3	y	52	ASP
3	y	70	GLN
3	y	74	THR
3	y	85	PHE
3	y	95	SER
4	0	5	VAL
4	0	9	ARG
4	0	25	CYS
4	0	30	THR
4	0	32	PHE
4	0	34	ASP
4	0	58	VAL
4	0	62	THR
4	0	64	LEU
4	0	66	LEU
4	0	72	SER
4	0	73	TRP
4	0	83	ARG
4	0	87	ASP
4	0	88	LEU

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Mol	Chain	Res	Type
4	0	101	MET
4	0	106	VAL
4	0	114	ILE
4	0	126	GLU
4	0	131	ARG
4	0	134	GLN
4	0	136	ASP
4	0	138	LEU
4	0	144	GLU
4	0	150	THR
4	0	151	ARG
4	0	152	GLU
4	0	154	GLU
4	0	156	ARG
4	0	157	ASP
5	1	3	ASN
5	1	6	GLN
5	1	7	VAL
5	1	18	ILE
5	1	32	SER
5	1	37	ASP
5	1	70	TRP
5	1	85	VAL
5	1	95	SER
5	1	96	THR
5	1	107	ILE
5	1	116	SER
5	1	117	GLU
5	1	123	THR
5	1	128	ILE
5	1	130	SER
5	1	132	ARG
5	1	133	CYS
5	1	134	GLU
5	1	136	GLN
5	1	145	SER
5	1	146	LEU
5	1	159	GLN
5	1	160	ILE
1	3	13	LEU
1	3	17	ASP
1	3	21	PHE

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Mol	Chain	Res	Type
1	3	47	VAL
1	3	50	VAL
1	3	55	ASP
1	3	70	LEU
1	3	80	VAL
1	3	81	LEU
1	3	82	SER
1	3	84	GLN
1	3	85	ASP
1	3	87	THR
1	3	90	LEU
1	3	91	LYS
1	3	95	VAL
1	3	98	ARG
1	3	102	THR
1	3	103	GLN
1	3	109	LYS
1	3	115	GLU
1	3	118	LEU
1	3	133	SER
1	3	134	ILE
1	3	137	LYS
1	3	145	GLU
1	3	146	SER
1	3	163	VAL
1	3	177	VAL
1	3	188	CYS
1	3	189	SER
1	3	194	LYS
1	3	195	LEU
1	3	197	ILE
1	3	199	ARG
1	3	204	LYS
1	3	209	SER
1	3	212	ARG
1	3	216	THR
1	3	220	SER
1	3	223	GLN
1	3	225	ASN
1	3	261	LEU
1	3	263	GLU
1	3	265	CYS

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Mol	Chain	Res	Type
1	3	275	GLU
1	3	277	ILE
1	3	289	GLU
1	3	290	THR
1	3	291	GLU
1	3	294	HIS
1	3	296	MET
1	3	305	ASN
1	3	307	ILE
1	3	313	ASP
1	3	314	LEU
1	3	318	ILE
2	5	17	MET
2	5	21	LEU
2	5	22	ILE
2	5	23	SER
2	5	31	VAL
2	5	32	LYS
2	5	39	SER
2	5	46	LEU
2	5	58	ASN
2	5	59	GLU
2	5	60	VAL
2	5	65	ILE
2	5	70	LEU
2	5	80	LYS
2	5	82	ARG
2	5	84	THR
2	5	86	SER
2	5	89	GLU
2	5	90	ILE
2	5	92	GLU
2	5	101	LEU
2	5	103	LEU
2	5	104	LEU
2	5	109	PHE
3	4	13	THR
3	4	21	SER
3	4	27	LEU
3	4	40	ASP
3	4	42	GLN
3	4	49	GLN

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Mol	Chain	Res	Type
3	4	52	ASP
3	4	70	GLN
3	4	74	THR
3	4	77	LEU
3	4	85	PHE
3	4	95	SER
4	6	7	ASP
4	6	8	GLN
4	6	10	SER
4	6	11	LYS
4	6	13	GLU
4	6	17	PHE
4	6	25	CYS
4	6	26	GLU
4	6	30	THR
4	6	32	PHE
4	6	46	ASN
4	6	49	ARG
4	6	50	ASP
4	6	53	SER
4	6	63	ASN
4	6	64	LEU
4	6	66	LEU
4	6	72	SER
4	6	73	TRP
4	6	83	ARG
4	6	87	ASP
4	6	88	LEU
4	6	101	MET
4	6	106	VAL
4	6	114	ILE
4	6	131	ARG
4	6	136	ASP
4	6	138	LEU
4	6	149	ARG
4	6	151	ARG
4	6	152	GLU
4	6	155	ASP
5	7	3	ASN
5	7	6	GLN
5	7	7	VAL
5	7	13	VAL

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Mol	Chain	Res	Type
5	7	15	ARG
5	7	18	ILE
5	7	24	LEU
5	7	36	LYS
5	7	37	ASP
5	7	45	GLU
5	7	47	THR
5	7	50	LYS
5	7	59	LEU
5	7	66	ILE
5	7	68	THR
5	7	70	TRP
5	7	76	GLU
5	7	77	ARG
5	7	83	GLN
5	7	86	SER
5	7	88	GLU
5	7	93	ARG
5	7	95	SER
5	7	96	THR
5	7	98	VAL
5	7	99	ASP
5	7	101	ASP
5	7	102	LEU
5	7	107	ILE
5	7	114	CYS
5	7	116	SER
5	7	117	GLU
5	7	123	THR
5	7	128	ILE
5	7	133	CYS
5	7	134	GLU
5	7	136	GLN
5	7	140	ASN
5	7	142	VAL
5	7	145	LEU
5	7	150	LEU
5	7	159	ILE
5	7	166	VAL
1	9	13	LEU
1	9	17	ASP
1	9	18	LYS

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Mol	Chain	Res	Type
1	9	34	SER
1	9	50	VAL
1	9	70	LEU
1	9	81	LEU
1	9	85	ASP
1	9	90	LEU
1	9	91	LYS
1	9	94	ILE
1	9	102	THR
1	9	103	GLN
1	9	117	THR
1	9	118	LEU
1	9	133	SER
1	9	134	ILE
1	9	144	ASN
1	9	147	ILE
1	9	149	SER
1	9	150	ASN
1	9	162	LEU
1	9	186	ASN
1	9	188	CYS
1	9	194	LYS
1	9	195	LEU
1	9	197	ILE
1	9	199	ARG
1	9	212	ARG
1	9	220	SER
1	9	223	GLN
1	9	232	LYS
1	9	235	ASP
1	9	246	LEU
1	9	252	ARG
1	9	253	ARG
1	9	255	CYS
1	9	259	GLU
1	9	261	LEU
1	9	262	MET
1	9	266	VAL
1	9	267	ASN
1	9	271	THR
1	9	277	ILE
1	9	285	ILE

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Mol	Chain	Res	Type
1	9	298	SER
1	9	307	ILE
1	9	314	LEU
1	9	318	ILE
2	T	21	LEU
2	T	22	ILE
2	T	23	SER
2	T	32	LYS
2	T	33	ARG
2	T	39	SER
2	T	58	ASN
2	T	60	VAL
2	T	65	ILE
2	T	68	HIS
2	T	69	VAL
2	T	70	LEU
2	T	80	LYS
2	T	82	ARG
2	T	84	THR
2	T	86	SER
2	T	88	THR
2	T	90	ILE
2	T	92	GLU
2	T	101	LEU
2	T	103	LEU
2	T	104	LEU
2	T	105	MET
2	T	108	ASN
2	T	109	PHE
3	e	4	PHE
3	e	5	LEU
3	e	6	MET
3	e	7	ILE
3	e	9	ARG
3	e	13	THR
3	e	22	SER
3	e	27	LEU
3	e	30	ILE
3	e	40	ASP
3	e	42	GLN
3	e	43	ARG
3	e	49	GLN

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Mol	Chain	Res	Type
3	e	50	LEU
3	e	52	ASP
3	e	70	GLN
3	e	74	THR
3	e	77	LEU
4	k	5	VAL
4	k	9	ARG
4	k	11	LYS
4	k	13	GLU
4	k	16	GLU
4	k	22	SER
4	k	24	GLU
4	k	25	CYS
4	k	27	ILE
4	k	28	LYS
4	k	52	ARG
4	k	55	ILE
4	k	58	VAL
4	k	62	THR
4	k	64	LEU
4	k	65	SER
4	k	66	LEU
4	k	72	SER
4	k	87	ASP
4	k	88	LEU
4	k	91	GLU
4	k	97	LEU
4	k	103	LEU
4	k	106	VAL
4	k	114	ILE
4	k	122	MET
4	k	126	GLU
4	k	130	GLU
4	k	136	ASP
4	k	138	LEU
4	k	145	GLU
4	k	149	ARG
4	k	150	THR
4	k	151	ARG
4	k	152	GLU
4	k	156	ARG
4	k	157	ASP

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Mol	Chain	Res	Type
5	q	3	ASN
5	q	6	GLN
5	q	7	VAL
5	q	9	ILE
5	q	13	VAL
5	q	14	ASP
5	q	17	ARG
5	q	18	ILE
5	q	25	VAL
5	q	31	ILE
5	q	32	SER
5	q	37	ASP
5	q	52	SER
5	q	64	LEU
5	q	65	VAL
5	q	70	TRP
5	q	72	LEU
5	q	73	HIS
5	q	76	GLU
5	q	81	LEU
5	q	83	GLN
5	q	86	SER
5	q	87	ILE
5	q	93	ARG
5	q	95	SER
5	q	97	GLN
5	q	107	ILE
5	q	109	LEU
5	q	116	SER
5	q	117	GLU
5	q	123	THR
5	q	125	LEU
5	q	132	ARG
5	q	134	GLU
5	q	135	TYR
5	q	136	GLN
5	q	141	LYS
5	q	142	VAL
5	q	145	LEU
5	q	153	LEU
5	q	154	ILE
5	q	157	LYS

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Mol	Chain	Res	Type
5	q	158	GLN
5	q	159	ILE
5	q	166	VAL
5	q	167	ARG
5	q	170	THR
1	w	14	GLN
1	w	17	ASP
1	w	22	MET
1	w	27	LEU
1	w	31	ARG
1	w	50	VAL
1	w	55	ASP
1	w	71	GLU
1	w	74	LYS
1	w	79	ARG
1	w	81	LEU
1	w	84	GLN
1	w	85	ASP
1	w	87	THR
1	w	89	LEU
1	w	90	LEU
1	w	91	LYS
1	w	95	VAL
1	w	98	ARG
1	w	106	ILE
1	w	118	LEU
1	w	142	THR
1	w	149	SER
1	w	152	LYS
1	w	154	ARG
1	w	157	ASP
1	w	162	LEU
1	w	168	LEU
1	w	187	LEU
1	w	188	CYS
1	w	196	GLN
1	w	197	ILE
1	w	199	ARG
1	w	204	LYS
1	w	207	LEU
1	w	210	THR
1	w	215	ARG

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Mol	Chain	Res	Type
1	w	217	GLN
1	w	220	SER
1	w	223	GLN
1	w	228	GLN
1	w	250	GLU
1	w	251	THR
1	w	252	ARG
1	w	253	ARG
1	w	254	GLU
1	w	259	GLU
1	w	261	LEU
1	w	275	GLU
1	w	277	ILE
1	w	280	GLU
1	w	284	MET
1	w	285	ILE
1	w	289	GLU
1	w	290	THR
1	w	294	HIS
1	w	298	SER
1	w	303	VAL
1	w	307	ILE
1	w	314	LEU
1	w	318	ILE
2	B	21	LEU
2	B	22	ILE
2	B	32	LYS
2	B	38	THR
2	B	39	SER
2	B	46	LEU
2	B	58	ASN
2	B	59	GLU
2	B	60	VAL
2	B	65	ILE
2	B	80	LYS
2	B	82	ARG
2	B	84	THR
2	B	88	THR
2	B	90	ILE
2	B	101	LEU
2	B	103	LEU
3	H	13	THR

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Mol	Chain	Res	Type
3	H	21	SER
3	H	27	LEU
3	H	40	ASP
3	H	42	GLN
3	H	50	LEU
3	H	52	ASP
3	H	70	GLN
3	H	74	THR
3	H	85	PHE
3	H	95	SER
4	N	5	VAL
4	N	9	ARG
4	N	16	GLU
4	N	25	CYS
4	N	30	THR
4	N	32	PHE
4	N	66	LEU
4	N	72	SER
4	N	83	ARG
4	N	85	TYR
4	N	87	ASP
4	N	97	LEU
4	N	101	MET
4	N	103	LEU
4	N	106	VAL
4	N	109	ILE
4	N	114	ILE
4	N	126	GLU
4	N	130	GLU
4	N	131	ARG
4	N	134	GLN
4	N	136	ASP
4	N	150	THR
4	N	151	ARG
5	2	3	ASN
5	2	6	GLN
5	2	7	VAL
5	2	9	ILE
5	2	13	VAL
5	2	18	ILE
5	2	52	SER
5	2	59	LEU

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Mol	Chain	Res	Type
5	2	70	TRP
5	2	83	GLN
5	2	86	SER
5	2	93	ARG
5	2	95	SER
5	2	96	THR
5	2	107	ILE
5	2	114	CYS
5	2	116	SER
5	2	117	GLU
5	2	123	THR
5	2	130	SER
5	2	133	CYS
5	2	134	GLU
5	2	136	GLN
5	2	143	VAL
5	2	146	LEU
5	2	160	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	32	GLN
1	U	77	GLN
1	U	103	GLN
1	U	156	GLN
1	U	228	GLN
2	Y	35	HIS
4	a	41	GLN
5	b	3	ASN
5	b	19	ASN
1	C	14	GLN
1	C	48	HIS
1	C	156	GLN
1	C	228	GLN
1	C	282	GLN
3	D	10	HIS
4	F	14	ASN
4	F	134	GLN
5	G	42	HIS
1	I	75	GLN
1	I	153	ASN

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Mol	Chain	Res	Type
1	I	156	GLN
1	I	196	GLN
4	L	41	GLN
4	L	63	ASN
4	L	67	GLN
5	M	73	HIS
1	O	38	GLN
1	O	84	GLN
1	O	150	ASN
1	O	153	ASN
1	O	156	GLN
1	O	217	GLN
1	O	317	HIS
2	Q	27	HIS
3	P	42	GLN
4	R	104	ASN
4	R	133	GLN
5	S	3	ASN
5	S	73	HIS
5	S	105	GLN
5	S	139	HIS
1	V	75	GLN
1	V	228	GLN
1	V	305	ASN
4	c	37	HIS
4	c	41	GLN
4	c	134	GLN
5	d	97	GLN
1	f	77	GLN
1	f	201	ASN
1	f	217	GLN
1	f	223	GLN
1	f	294	HIS
2	h	35	HIS
5	j	73	HIS
1	l	32	GLN
1	l	39	GLN
1	l	75	GLN
1	l	144	ASN
1	l	317	HIS
2	n	35	HIS
2	n	58	ASN

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Mol	Chain	Res	Type
2	n	108	ASN
4	o	140	GLN
5	p	42	HIS
5	p	140	ASN
5	p	146	GLN
1	r	14	GLN
1	r	32	GLN
1	r	77	GLN
5	v	27	HIS
5	v	73	HIS
5	v	140	ASN
5	v	147	GLN
1	x	75	GLN
1	x	156	GLN
1	x	186	ASN
1	x	256	ASN
1	x	267	ASN
1	x	317	HIS
3	y	10	HIS
3	y	42	GLN
4	0	67	GLN
5	1	42	HIS
5	1	140	ASN
1	3	48	HIS
1	3	196	GLN
1	3	228	GLN
2	5	35	HIS
4	6	37	HIS
4	6	41	GLN
5	7	110	HIS
5	7	139	HIS
1	9	84	GLN
1	9	113	GLN
1	9	144	ASN
1	9	164	HIS
1	9	186	ASN
1	9	201	ASN
1	9	217	GLN
4	k	37	HIS
4	k	41	GLN
5	q	28	HIS
5	q	42	HIS

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Mol	Chain	Res	Type
5	q	73	HIS
5	q	110	HIS
1	w	32	GLN
1	w	62	HIS
1	w	75	GLN
1	w	103	GLN
1	w	201	ASN
1	w	317	HIS
2	B	108	ASN
4	N	67	GLN
5	2	73	HIS
5	2	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	3	295/311 (94%)	-0.81	0 100 100	20, 60, 139, 214	1 (0%)
1	9	295/311 (94%)	-0.51	1 (0%) 90 82	42, 104, 191, 306	1 (0%)
1	C	297/311 (95%)	-0.73	0 100 100	23, 57, 124, 228	1 (0%)
1	I	296/311 (95%)	-0.83	2 (0%) 84 70	24, 69, 144, 252	1 (0%)
1	O	298/311 (95%)	-0.87	0 100 100	20, 60, 126, 207	1 (0%)
1	U	299/311 (96%)	-0.71	6 (2%) 65 46	20, 59, 129, 219	2 (0%)
1	V	296/311 (95%)	-0.86	1 (0%) 90 82	17, 60, 125, 228	1 (0%)
1	f	296/311 (95%)	-0.72	3 (1%) 79 63	26, 67, 147, 223	1 (0%)
1	l	297/311 (95%)	-0.93	0 100 100	19, 47, 105, 176	0
1	r	296/311 (95%)	-0.94	2 (0%) 84 70	13, 48, 118, 195	1 (0%)
1	w	296/311 (95%)	-0.84	1 (0%) 90 82	4, 60, 145, 197	1 (0%)
1	x	294/311 (94%)	-0.45	3 (1%) 79 63	41, 107, 198, 297	0
2	5	87/96 (90%)	-0.53	0 100 100	44, 76, 172, 193	0
2	B	87/96 (90%)	-0.59	0 100 100	45, 76, 169, 246	0
2	E	87/96 (90%)	-0.89	0 100 100	23, 46, 121, 189	0
2	K	86/96 (89%)	-0.75	0 100 100	32, 54, 134, 201	0
2	Q	87/96 (90%)	-0.77	0 100 100	36, 61, 138, 195	0
2	T	87/96 (90%)	-0.54	2 (2%) 61 42	60, 92, 168, 226	0
2	Y	87/96 (90%)	-0.79	1 (1%) 78 60	23, 49, 129, 184	0
2	Z	87/96 (90%)	-0.85	1 (1%) 78 60	34, 61, 143, 184	0
2	h	87/96 (90%)	-0.79	0 100 100	35, 63, 141, 175	0
2	n	87/96 (90%)	-0.83	0 100 100	24, 51, 110, 176	0
2	t	87/96 (90%)	-0.85	0 100 100	28, 51, 127, 198	0
2	z	87/96 (90%)	-0.46	0 100 100	55, 91, 168, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	4	95/102 (93%)	-0.38	3 (3%) 50 34	61, 115, 212, 286	0
3	D	95/102 (93%)	-0.45	0 100 100	51, 86, 177, 225	0
3	H	95/102 (93%)	-0.43	1 (1%) 78 60	71, 107, 209, 248	0
3	J	90/102 (88%)	-0.30	3 (3%) 49 33	62, 87, 171, 260	0
3	P	94/102 (92%)	-0.68	1 (1%) 78 60	38, 79, 151, 174	0
3	W	91/102 (89%)	-0.79	0 100 100	41, 72, 141, 208	0
3	X	95/102 (93%)	-0.64	1 (1%) 78 60	44, 80, 177, 216	0
3	e	79/102 (77%)	-0.19	4 (5%) 33 22	79, 106, 177, 210	0
3	g	95/102 (93%)	-0.49	1 (1%) 78 60	73, 99, 210, 260	0
3	m	95/102 (93%)	-0.76	0 100 100	45, 78, 164, 226	0
3	s	95/102 (93%)	-0.73	2 (2%) 63 44	42, 68, 142, 188	0
3	y	95/102 (93%)	-0.17	3 (3%) 50 34	76, 106, 219, 290	0
4	0	144/170 (84%)	-0.74	0 100 100	26, 56, 122, 194	0
4	6	140/170 (82%)	-0.79	0 100 100	33, 66, 121, 195	0
4	F	145/170 (85%)	-0.95	0 100 100	22, 49, 101, 164	0
4	L	144/170 (84%)	-0.88	1 (0%) 84 70	20, 52, 114, 170	0
4	N	145/170 (85%)	-0.75	1 (0%) 84 70	34, 70, 135, 198	0
4	R	144/170 (84%)	-0.94	0 100 100	16, 45, 99, 223	0
4	a	146/170 (85%)	-0.87	0 100 100	20, 48, 96, 214	0
4	c	145/170 (85%)	-0.89	1 (0%) 84 70	22, 43, 97, 160	0
4	i	155/170 (91%)	-0.90	0 100 100	24, 55, 120, 177	0
4	k	147/170 (86%)	-0.71	1 (0%) 84 70	32, 58, 128, 183	0
4	o	143/170 (84%)	-0.81	0 100 100	18, 46, 103, 149	0
4	u	143/170 (84%)	-0.84	1 (0%) 84 70	20, 48, 105, 152	0
5	1	170/176 (96%)	-0.72	1 (0%) 85 73	36, 62, 141, 239	0
5	2	170/176 (96%)	-0.67	1 (0%) 85 73	34, 67, 151, 221	0
5	7	170/176 (96%)	-0.69	4 (2%) 59 40	30, 65, 158, 254	0
5	G	170/176 (96%)	-0.94	0 100 100	16, 41, 95, 173	0
5	M	171/176 (97%)	-0.81	1 (0%) 85 73	24, 46, 103, 189	0
5	S	170/176 (96%)	-0.87	0 100 100	21, 36, 106, 233	0
5	b	172/176 (97%)	-0.91	1 (0%) 85 73	22, 41, 93, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	d	170/176 (96%)	-0.82	0 100 100	18, 39, 106, 172	0
5	j	170/176 (96%)	-0.82	1 (0%) 85 73	19, 42, 108, 180	0
5	p	169/176 (96%)	-0.85	0 100 100	21, 38, 83, 138	0
5	q	169/176 (96%)	-0.67	1 (0%) 85 73	33, 59, 125, 190	0
5	v	170/176 (96%)	-0.87	1 (0%) 85 73	21, 37, 105, 186	0
All	All	9494/10260 (92%)	-0.75	58 (0%) 85 73	4, 62, 151, 306	11 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	279	ALA	4.7
2	T	39	SER	4.6
5	2	173	ASP	4.3
4	k	105	GLY	4.3
5	b	158	GLN	3.9
2	Z	97	PRO	3.8
3	4	97	PRO	3.5
5	1	75	GLY	3.4
3	y	50	LEU	3.2
3	X	18	ALA	3.2
1	r	11	ALA	3.1
3	y	16	THR	3.1
3	e	58	GLY	3.0
5	7	126	GLY	3.0
3	4	84	THR	3.0
3	J	33	GLY	2.9
3	P	97	PRO	2.9
3	e	56	THR	2.8
4	N	129	GLU	2.8
4	c	6	PRO	2.8
3	y	21	SER	2.8
3	H	84	THR	2.7
1	x	186	ASN	2.6
3	4	59	GLU	2.6
5	M	27	HIS	2.5
1	f	189	SER	2.5
5	7	74	THR	2.5
5	q	156	PRO	2.5
5	v	173	ASP	2.5
1	x	117	THR	2.5

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Mol	Chain	Res	Type	RSRZ
5	j	74	THR	2.5
1	U	274	LYS	2.4
5	7	172	ASP	2.4
1	w	170	GLU	2.4
1	f	225	ASN	2.3
1	U	320[A]	SER	2.3
1	I	223	GLN	2.3
3	g	59	GLU	2.3
3	s	97	PRO	2.3
1	f	171	ALA	2.3
1	V	280	GLU	2.2
3	J	54	GLY	2.2
3	J	59	GLU	2.2
4	L	34	ASP	2.2
2	Y	92	GLU	2.2
5	7	31	ILE	2.2
4	u	51	GLY	2.2
1	9	189	SER	2.1
3	e	79	PHE	2.1
1	r	200	ASP	2.1
1	I	288	ASN	2.1
1	U	318	ILE	2.1
1	U	304	PRO	2.1
1	U	319	ILE	2.1
3	e	61	GLY	2.1
1	x	236	ALA	2.0
3	s	54	GLY	2.0
2	T	64	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ZN	b	201	1/1	0.99	0.02	33,33,33,33	0
6	ZN	G	201	1/1	1.00	0.01	47,47,47,47	0
6	ZN	M	201	1/1	1.00	0.02	25,25,25,25	0
6	ZN	S	201	1/1	1.00	0.02	32,32,32,32	0
6	ZN	d	201	1/1	1.00	0.01	25,25,25,25	0
6	ZN	j	201	1/1	1.00	0.01	24,24,24,24	0
6	ZN	p	201	1/1	1.00	0.02	19,19,19,19	0
6	ZN	v	201	1/1	1.00	0.01	24,24,24,24	0
6	ZN	1	201	1/1	1.00	0.02	65,65,65,65	0
6	ZN	7	201	1/1	1.00	0.02	51,51,51,51	0
6	ZN	q	201	1/1	1.00	0.04	50,50,50,50	0
6	ZN	2	201	1/1	1.00	0.01	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.