



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:00 am GMT

PDB ID : 3PJS
Title : Mechanism of Activation Gating in the Full-Length KcsA K⁺ Channel
Authors : Uysal, S.; Cuello, L.G.; Kossiakoff, A.; Perozo, E.
Deposited on : 2010-11-10
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

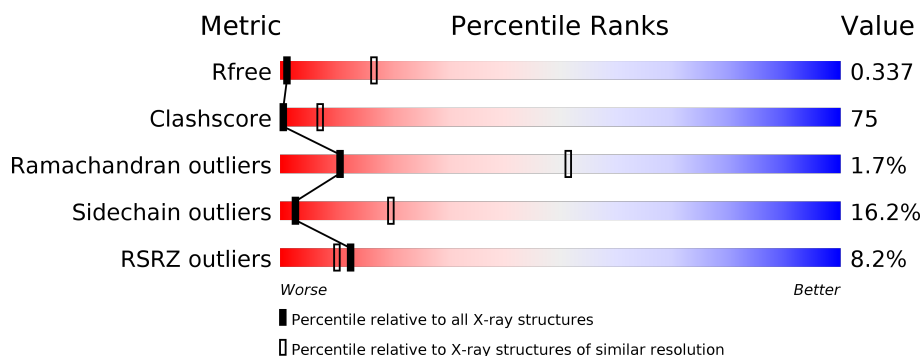
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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

Mol	Chain	Length	Quality of chain
1	A	215	<div> <div>4%</div> <div>27%</div> <div>53%</div> <div>17%</div> <div>•</div> </div>
1	C	215	<div> <div>%</div> <div>28%</div> <div>53%</div> <div>17%</div> <div>•</div> </div>
2	B	224	<div> <div>4%</div> <div>31%</div> <div>51%</div> <div>13%</div> <div>• •</div> </div>
2	D	224	<div> <div>30%</div> <div>52%</div> <div>13%</div> <div>• •</div> </div>
3	K	166	<div> <div>15%</div> <div>21%</div> <div>54%</div> <div>8%</div> <div>•</div> <div>16%</div> </div>
3	L	166	<div> <div>8%</div> <div>18%</div> <div>58%</div> <div>8%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
3	M	166	<p>19% 22% 55% 7% 16%</p>
3	N	166	<p>14% 23% 54% 7% 16%</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10982 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 FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1658	1038	276	339	5			
1	C	215	Total	C	N	O	S	0	0	0
			1658	1038	276	339	5			

- Molecule 2 is a protein called FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1653	1050	272	325	6			
2	D	219	Total	C	N	O	S	0	0	0
			1653	1050	272	325	6			

- Molecule 3 is a protein called Voltage-gated potassium channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	139	Total	C	N	O	S	0	0	0
			1090	697	195	196	2			
3	L	139	Total	C	N	O	S	0	0	0
			1090	697	195	196	2			
3	M	139	Total	C	N	O	S	0	0	0
			1090	697	195	196	2			
3	N	139	Total	C	N	O	S	0	0	0
			1090	697	195	196	2			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	MET	-	EXPRESSION TAG	UNP P0A334
K	-4	HIS	-	EXPRESSION TAG	UNP P0A334
K	-3	HIS	-	EXPRESSION TAG	UNP P0A334
K	-2	HIS	-	EXPRESSION TAG	UNP P0A334

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	EXPRESSION TAG	UNP P0A334
K	0	HIS	-	EXPRESSION TAG	UNP P0A334
K	1	HIS	-	EXPRESSION TAG	UNP P0A334
K	2	PRO	-	EXPRESSION TAG	UNP P0A334
K	3	PRO	-	EXPRESSION TAG	UNP P0A334
K	4	MET	-	EXPRESSION TAG	UNP P0A334
K	5	LEU	-	EXPRESSION TAG	UNP P0A334
K	6	SER	-	EXPRESSION TAG	UNP P0A334
K	7	GLY	-	EXPRESSION TAG	UNP P0A334
K	8	LEU	-	EXPRESSION TAG	UNP P0A334
K	9	LEU	-	EXPRESSION TAG	UNP P0A334
K	10	ALA	-	EXPRESSION TAG	UNP P0A334
K	11	ARG	-	EXPRESSION TAG	UNP P0A334
K	12	LEU	-	EXPRESSION TAG	UNP P0A334
K	13	VAL	-	EXPRESSION TAG	UNP P0A334
K	14	LYS	-	EXPRESSION TAG	UNP P0A334
K	15	LEU	-	EXPRESSION TAG	UNP P0A334
K	16	LEU	-	EXPRESSION TAG	UNP P0A334
K	17	LEU	-	EXPRESSION TAG	UNP P0A334
K	18	GLY	-	EXPRESSION TAG	UNP P0A334
K	19	ARG	-	EXPRESSION TAG	UNP P0A334
K	20	HIS	-	EXPRESSION TAG	UNP P0A334
K	21	GLY	-	EXPRESSION TAG	UNP P0A334
K	25	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
K	117	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
K	120	GLN	GLU	ENGINEERED MUTATION	UNP P0A334
K	121	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
K	122	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
K	123	GLN	GLY	ENGINEERED MUTATION	UNP P0A334
K	124	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
L	-5	MET	-	EXPRESSION TAG	UNP P0A334
L	-4	HIS	-	EXPRESSION TAG	UNP P0A334
L	-3	HIS	-	EXPRESSION TAG	UNP P0A334
L	-2	HIS	-	EXPRESSION TAG	UNP P0A334
L	-1	HIS	-	EXPRESSION TAG	UNP P0A334
L	0	HIS	-	EXPRESSION TAG	UNP P0A334
L	1	HIS	-	EXPRESSION TAG	UNP P0A334
L	2	PRO	-	EXPRESSION TAG	UNP P0A334
L	3	PRO	-	EXPRESSION TAG	UNP P0A334
L	4	MET	-	EXPRESSION TAG	UNP P0A334
L	5	LEU	-	EXPRESSION TAG	UNP P0A334
L	6	SER	-	EXPRESSION TAG	UNP P0A334

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Chain	Residue	Modelled	Actual	Comment	Reference
L	7	GLY	-	EXPRESSION TAG	UNP P0A334
L	8	LEU	-	EXPRESSION TAG	UNP P0A334
L	9	LEU	-	EXPRESSION TAG	UNP P0A334
L	10	ALA	-	EXPRESSION TAG	UNP P0A334
L	11	ARG	-	EXPRESSION TAG	UNP P0A334
L	12	LEU	-	EXPRESSION TAG	UNP P0A334
L	13	VAL	-	EXPRESSION TAG	UNP P0A334
L	14	LYS	-	EXPRESSION TAG	UNP P0A334
L	15	LEU	-	EXPRESSION TAG	UNP P0A334
L	16	LEU	-	EXPRESSION TAG	UNP P0A334
L	17	LEU	-	EXPRESSION TAG	UNP P0A334
L	18	GLY	-	EXPRESSION TAG	UNP P0A334
L	19	ARG	-	EXPRESSION TAG	UNP P0A334
L	20	HIS	-	EXPRESSION TAG	UNP P0A334
L	21	GLY	-	EXPRESSION TAG	UNP P0A334
L	25	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
L	117	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
L	120	GLN	GLU	ENGINEERED MUTATION	UNP P0A334
L	121	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
L	122	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
L	123	GLN	GLY	ENGINEERED MUTATION	UNP P0A334
L	124	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
M	-5	MET	-	EXPRESSION TAG	UNP P0A334
M	-4	HIS	-	EXPRESSION TAG	UNP P0A334
M	-3	HIS	-	EXPRESSION TAG	UNP P0A334
M	-2	HIS	-	EXPRESSION TAG	UNP P0A334
M	-1	HIS	-	EXPRESSION TAG	UNP P0A334
M	0	HIS	-	EXPRESSION TAG	UNP P0A334
M	1	HIS	-	EXPRESSION TAG	UNP P0A334
M	2	PRO	-	EXPRESSION TAG	UNP P0A334
M	3	PRO	-	EXPRESSION TAG	UNP P0A334
M	4	MET	-	EXPRESSION TAG	UNP P0A334
M	5	LEU	-	EXPRESSION TAG	UNP P0A334
M	6	SER	-	EXPRESSION TAG	UNP P0A334
M	7	GLY	-	EXPRESSION TAG	UNP P0A334
M	8	LEU	-	EXPRESSION TAG	UNP P0A334
M	9	LEU	-	EXPRESSION TAG	UNP P0A334
M	10	ALA	-	EXPRESSION TAG	UNP P0A334
M	11	ARG	-	EXPRESSION TAG	UNP P0A334
M	12	LEU	-	EXPRESSION TAG	UNP P0A334
M	13	VAL	-	EXPRESSION TAG	UNP P0A334
M	14	LYS	-	EXPRESSION TAG	UNP P0A334

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Chain	Residue	Modelled	Actual	Comment	Reference
M	15	LEU	-	EXPRESSION TAG	UNP P0A334
M	16	LEU	-	EXPRESSION TAG	UNP P0A334
M	17	LEU	-	EXPRESSION TAG	UNP P0A334
M	18	GLY	-	EXPRESSION TAG	UNP P0A334
M	19	ARG	-	EXPRESSION TAG	UNP P0A334
M	20	HIS	-	EXPRESSION TAG	UNP P0A334
M	21	GLY	-	EXPRESSION TAG	UNP P0A334
M	25	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
M	117	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
M	120	GLN	GLU	ENGINEERED MUTATION	UNP P0A334
M	121	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
M	122	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
M	123	GLN	GLY	ENGINEERED MUTATION	UNP P0A334
M	124	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
N	-5	MET	-	EXPRESSION TAG	UNP P0A334
N	-4	HIS	-	EXPRESSION TAG	UNP P0A334
N	-3	HIS	-	EXPRESSION TAG	UNP P0A334
N	-2	HIS	-	EXPRESSION TAG	UNP P0A334
N	-1	HIS	-	EXPRESSION TAG	UNP P0A334
N	0	HIS	-	EXPRESSION TAG	UNP P0A334
N	1	HIS	-	EXPRESSION TAG	UNP P0A334
N	2	PRO	-	EXPRESSION TAG	UNP P0A334
N	3	PRO	-	EXPRESSION TAG	UNP P0A334
N	4	MET	-	EXPRESSION TAG	UNP P0A334
N	5	LEU	-	EXPRESSION TAG	UNP P0A334
N	6	SER	-	EXPRESSION TAG	UNP P0A334
N	7	GLY	-	EXPRESSION TAG	UNP P0A334
N	8	LEU	-	EXPRESSION TAG	UNP P0A334
N	9	LEU	-	EXPRESSION TAG	UNP P0A334
N	10	ALA	-	EXPRESSION TAG	UNP P0A334
N	11	ARG	-	EXPRESSION TAG	UNP P0A334
N	12	LEU	-	EXPRESSION TAG	UNP P0A334
N	13	VAL	-	EXPRESSION TAG	UNP P0A334
N	14	LYS	-	EXPRESSION TAG	UNP P0A334
N	15	LEU	-	EXPRESSION TAG	UNP P0A334
N	16	LEU	-	EXPRESSION TAG	UNP P0A334
N	17	LEU	-	EXPRESSION TAG	UNP P0A334
N	18	GLY	-	EXPRESSION TAG	UNP P0A334
N	19	ARG	-	EXPRESSION TAG	UNP P0A334
N	20	HIS	-	EXPRESSION TAG	UNP P0A334
N	21	GLY	-	EXPRESSION TAG	UNP P0A334
N	25	GLN	HIS	ENGINEERED MUTATION	UNP P0A334

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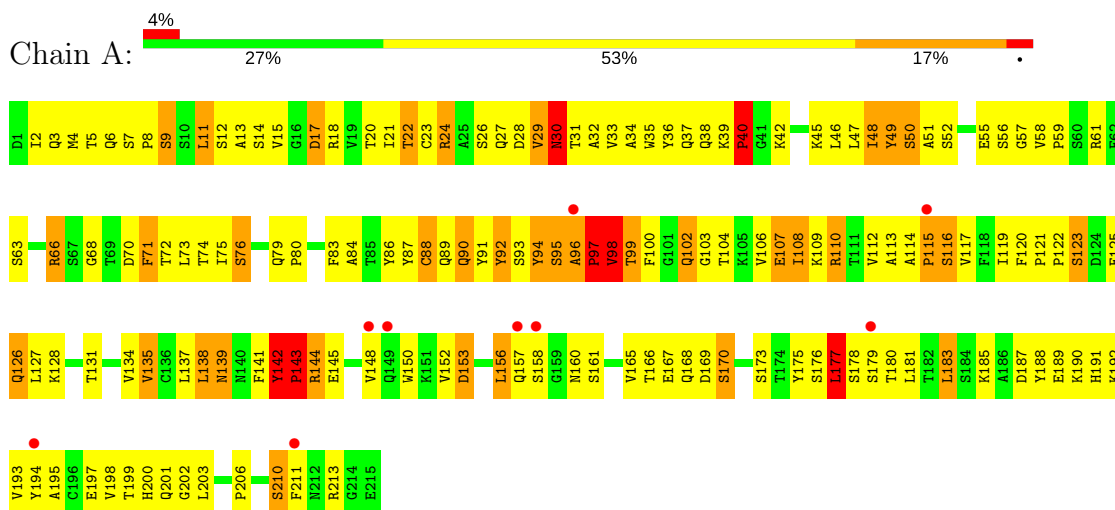
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Chain	Residue	Modelled	Actual	Comment	Reference
N	117	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
N	120	GLN	GLU	ENGINEERED MUTATION	UNP P0A334
N	121	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
N	122	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
N	123	GLN	GLY	ENGINEERED MUTATION	UNP P0A334
N	124	GLN	HIS	ENGINEERED MUTATION	UNP P0A334

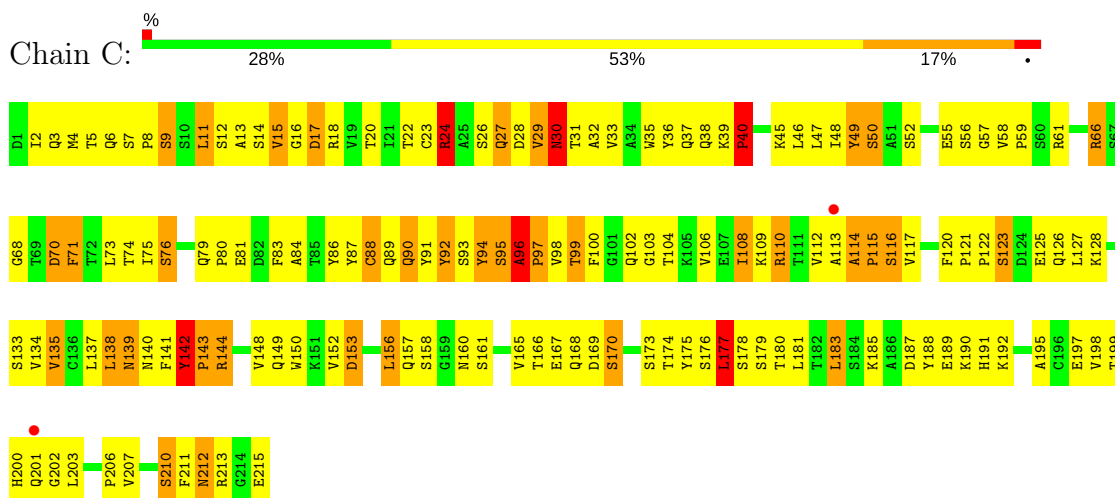
3 Residue-property plots

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

• Molecule 1: FAB light chain

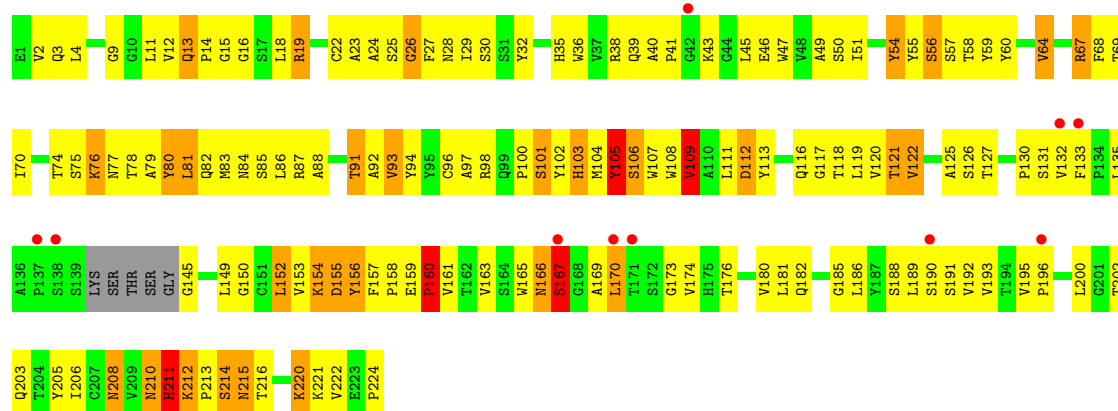


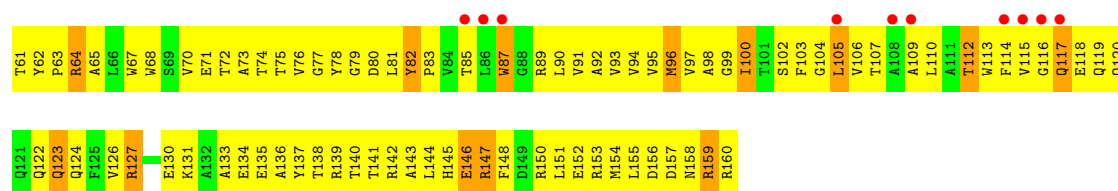
• Molecule 1: FAB light chain



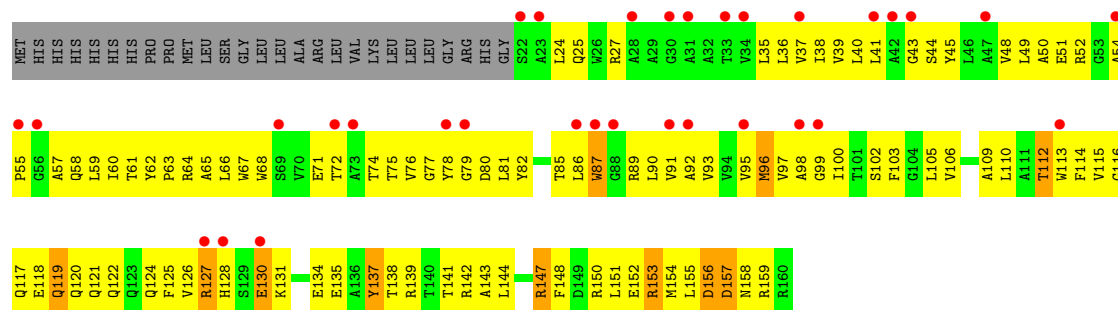
• Molecule 2: FAB heavy chain



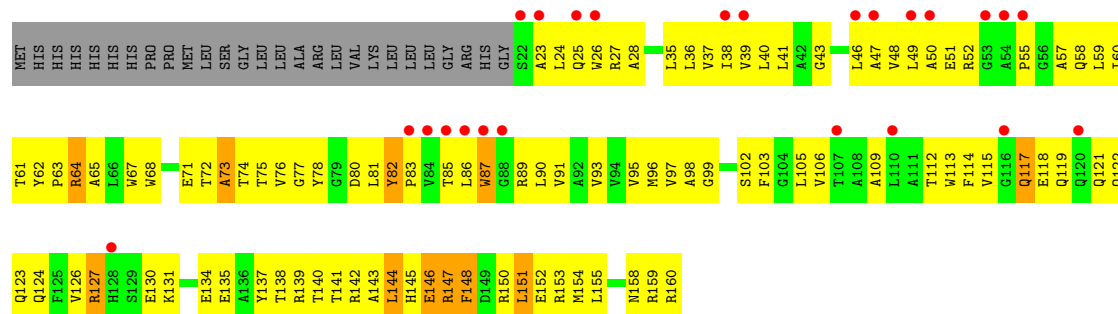




• Molecule 3: Voltage-gated potassium channel



• Molecule 3: Voltage-gated potassium channel



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.27Å 176.72Å 340.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.80 39.17 – 3.70	Depositor EDS
% Data completeness (in resolution range)	82.4 (40.00-3.80) 80.9 (39.17-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.66Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.281 , 0.332 0.289 , 0.337	Depositor DCC
R_{free} test set	1358 reflections (4.63%)	DCC
Wilson B-factor (Å ²)	135.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 163.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10982	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	6/1694 (0.4%)	1.41	25/2300 (1.1%)
1	C	0.68	0/1694	1.26	24/2300 (1.0%)
2	B	0.78	3/1698 (0.2%)	1.09	16/2319 (0.7%)
2	D	0.74	0/1698	1.17	18/2319 (0.8%)
3	K	0.59	0/1113	0.84	3/1517 (0.2%)
3	L	0.63	0/1113	0.75	0/1517
3	M	0.57	0/1113	0.75	2/1517 (0.1%)
3	N	0.60	0/1113	0.76	0/1517
All	All	0.69	9/11236 (0.1%)	1.08	88/15306 (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	A	0	2
1	C	0	1
3	K	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	PRO	N-CD	-12.23	1.30	1.47
1	A	115	PRO	CA-C	6.68	1.66	1.52
2	B	166	ASN	C-O	-6.56	1.10	1.23
2	B	154	LYS	C-O	-6.42	1.11	1.23
1	A	116	SER	N-CA	5.69	1.57	1.46
1	A	142	TYR	C-N	5.68	1.45	1.34
2	B	109	VAL	CB-CG1	-5.25	1.41	1.52
1	A	142	TYR	CD2-CE2	5.22	1.47	1.39
1	A	142	TYR	CB-CG	5.13	1.59	1.51

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	TYR	C-N-CD	-26.37	62.58	120.60
1	A	96	ALA	CB-CA-C	-18.99	81.62	110.10
1	A	96	ALA	C-N-CD	-17.89	81.25	120.60
1	A	96	ALA	N-CA-C	16.27	154.93	111.00
1	C	116	SER	N-CA-CB	-16.25	86.13	110.50
1	C	142	TYR	C-N-CD	-13.56	90.77	120.60
3	K	156	ASP	N-CA-CB	13.36	134.64	110.60
1	C	29	VAL	N-CA-C	-13.13	75.55	111.00
2	D	154	LYS	CB-CA-C	-12.91	84.58	110.40
2	D	154	LYS	N-CA-C	12.24	144.04	111.00
1	C	114	ALA	C-N-CD	-11.90	94.42	120.60
1	A	95	SER	N-CA-C	-11.69	79.43	111.00
2	D	109	VAL	N-CA-C	-11.62	79.62	111.00
1	A	29	VAL	N-CA-C	-11.48	80.00	111.00
1	C	95	SER	CB-CA-C	11.13	131.25	110.10
1	C	177	LEU	CB-CA-C	-10.47	90.31	110.20
1	A	142	TYR	C-N-CA	10.23	164.97	122.00
1	A	50	SER	N-CA-C	-9.99	84.02	111.00
1	A	29	VAL	CB-CA-C	9.97	130.34	111.40
1	C	50	SER	N-CA-C	-9.74	84.69	111.00
2	D	155	ASP	N-CA-C	-9.68	84.87	111.00
1	C	23	CYS	CB-CA-C	9.45	129.30	110.40
1	C	96	ALA	N-CA-C	-9.41	85.59	111.00
2	D	214	SER	N-CA-C	-9.33	85.81	111.00
2	D	109	VAL	CB-CA-C	9.26	129.00	111.40
1	A	66	ARG	CG-CD-NE	9.16	131.03	111.80
1	C	66	ARG	CG-CD-NE	9.15	131.03	111.80
1	C	142	TYR	C-N-CA	9.05	160.01	122.00
1	A	97	PRO	CA-N-CD	8.32	123.34	111.70
1	A	23	CYS	N-CA-CB	-8.27	95.71	110.60
1	A	22	THR	CB-CA-C	-8.25	89.32	111.60
2	B	166	ASN	CB-CA-C	-8.19	94.03	110.40
1	C	178	SER	N-CA-CB	-8.04	98.45	110.50
1	C	29	VAL	CB-CA-C	7.99	126.58	111.40
2	D	110	ALA	N-CA-CB	7.92	121.19	110.10
2	D	111	LEU	N-CA-C	-7.69	90.23	111.00
1	A	177	LEU	CB-CA-C	-7.58	95.79	110.20
1	C	23	CYS	N-CA-C	-7.54	90.64	111.00
2	B	167	SER	N-CA-CB	7.50	121.75	110.50
2	D	105	TYR	N-CA-CB	7.42	123.96	110.60
2	B	153	VAL	N-CA-C	-7.33	91.19	111.00
2	B	214	SER	N-CA-C	-7.33	91.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	HIS	N-CA-C	7.31	130.74	111.00
2	D	55	TYR	N-CA-C	-7.20	91.57	111.00
2	B	55	TYR	N-CA-C	-7.12	91.76	111.00
1	A	102	GLN	N-CA-C	-7.11	91.81	111.00
2	D	211	HIS	N-CA-C	-6.96	92.20	111.00
1	C	30	ASN	N-CA-CB	-6.91	98.17	110.60
3	K	156	ASP	N-CA-C	-6.67	92.98	111.00
1	C	102	GLN	N-CA-C	-6.67	92.99	111.00
1	A	97	PRO	N-CA-CB	-6.46	95.49	102.60
2	B	154	LYS	CA-C-N	6.42	131.34	117.20
2	B	155	ASP	N-CA-C	-6.42	93.67	111.00
2	B	154	LYS	N-CA-C	6.35	128.15	111.00
2	B	57	SER	N-CA-C	6.30	128.01	111.00
1	C	30	ASN	N-CA-C	-6.30	94.00	111.00
1	C	143	PRO	CA-N-CD	-6.25	102.75	111.50
2	B	109	VAL	N-CA-C	-6.24	94.14	111.00
2	D	110	ALA	CB-CA-C	-6.23	100.75	110.10
2	D	105	TYR	N-CA-C	-6.23	94.19	111.00
2	B	211	HIS	N-CA-C	-6.22	94.21	111.00
1	A	178	SER	N-CA-CB	-6.19	101.22	110.50
1	C	114	ALA	CB-CA-C	6.13	119.30	110.10
1	A	143	PRO	N-CA-C	-6.04	96.41	112.10
2	D	170	LEU	N-CA-C	-5.99	94.83	111.00
2	D	57	SER	N-CA-C	5.92	126.99	111.00
2	D	76	LYS	N-CA-C	-5.87	95.16	111.00
2	B	76	LYS	N-CA-C	-5.84	95.22	111.00
1	A	30	ASN	N-CA-CB	-5.79	100.19	110.60
1	A	138	LEU	N-CA-C	-5.75	95.49	111.00
2	B	154	LYS	O-C-N	-5.74	113.52	122.70
1	A	98	VAL	N-CA-C	-5.73	95.53	111.00
1	C	138	LEU	N-CA-C	-5.62	95.81	111.00
1	C	24	ARG	N-CA-CB	5.61	120.70	110.60
1	A	30	ASN	N-CA-C	-5.59	95.90	111.00
2	D	103	HIS	N-CA-C	5.57	126.04	111.00
1	C	95	SER	N-CA-C	-5.44	96.32	111.00
3	M	156	ASP	N-CA-C	-5.37	96.49	111.00
1	A	66	ARG	CB-CG-CD	-5.34	97.72	111.60
3	M	156	ASP	CB-CA-C	5.27	120.94	110.40
1	C	27	GLN	CB-CA-C	5.27	120.94	110.40
3	K	155	LEU	N-CA-C	5.27	125.22	111.00
1	C	139	ASN	N-CA-C	5.22	125.10	111.00
2	B	156	TYR	N-CA-CB	5.17	119.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASN	N-CA-C	5.15	124.90	111.00
2	B	105	TYR	N-CA-CB	5.14	119.86	110.60
2	D	110	ALA	N-CA-C	5.14	124.89	111.00
1	A	116	SER	CB-CA-C	-5.12	100.38	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	TYR	Mainchain
1	A	92	TYR	Sidechain
1	C	92	TYR	Sidechain
3	K	155	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1658	0	1606	299	0
1	C	1658	0	1606	248	0
2	B	1653	0	1597	285	0
2	D	1653	0	1597	274	0
3	K	1090	0	1093	185	0
3	L	1090	0	1093	193	0
3	M	1090	0	1093	181	0
3	N	1090	0	1093	167	0
All	All	10982	0	10778	1632	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 75.

All (1632) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:TRP:HE1	2:B:174:VAL:CG2	1.04	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:TRP:CH2	2:B:193:VAL:HG11	1.39	1.54
2:B:130:PRO:CB	2:B:155:ASP:O	1.64	1.45
1:C:115:PRO:CB	1:C:141:PHE:HB3	1.47	1.45
2:B:165:TRP:CH2	2:B:193:VAL:CG1	1.97	1.43
1:C:49:TYR:CD2	2:D:109:VAL:HG12	1.57	1.39
2:B:165:TRP:NE1	2:B:174:VAL:CG2	1.86	1.37
2:B:130:PRO:CG	2:B:156:TYR:HB3	1.59	1.33
1:C:115:PRO:CG	1:C:141:PHE:HB3	1.58	1.32
2:B:130:PRO:HB3	2:B:155:ASP:C	1.51	1.30
3:N:71:GLU:OE1	3:N:76:VAL:CG1	1.79	1.29
1:C:115:PRO:HG3	1:C:141:PHE:CB	1.63	1.28
2:B:165:TRP:HZ2	2:B:193:VAL:CB	1.47	1.27
2:B:165:TRP:CZ2	2:B:193:VAL:HB	1.69	1.25
2:B:165:TRP:CZ2	2:B:193:VAL:CB	2.21	1.22
3:N:71:GLU:OE1	3:N:76:VAL:CB	1.88	1.22
2:B:165:TRP:CZ2	2:B:193:VAL:CG1	2.22	1.20
3:N:71:GLU:OE1	3:N:76:VAL:HB	1.42	1.19
2:B:130:PRO:HG3	2:B:156:TYR:CB	1.74	1.18
3:L:46:LEU:HB2	3:L:91:VAL:HG11	1.21	1.16
1:C:98:VAL:HG21	2:D:47:TRP:CD1	1.82	1.14
2:B:130:PRO:HB3	2:B:155:ASP:O	0.95	1.12
1:A:32:ALA:O	1:A:91:TYR:CD1	2.02	1.12
2:B:39:GLN:O	2:B:92:ALA:HB1	1.49	1.12
2:D:99:GLN:HB2	2:D:110:ALA:O	1.50	1.12
3:N:61:THR:HG22	3:N:63:PRO:HD2	1.22	1.12
2:D:154:LYS:O	2:D:154:LYS:HG2	1.36	1.11
3:N:143:ALA:HA	3:N:146:GLU:HB2	1.28	1.11
2:B:165:TRP:HH2	2:B:193:VAL:HG12	1.13	1.11
3:M:153:ARG:NE	3:M:157:ASP:OD2	1.83	1.11
3:L:150:ARG:HD3	3:M:152:GLU:OE2	1.50	1.10
2:B:165:TRP:CZ2	2:B:193:VAL:HG11	1.82	1.10
1:A:113:ALA:HB3	1:A:142:TYR:H	1.16	1.10
1:C:89:GLN:HE22	2:D:111:LEU:HD23	0.97	1.10
2:B:165:TRP:NE1	2:B:174:VAL:HG22	1.57	1.09
1:C:4:MET:CE	1:C:90:GLN:HB3	1.82	1.09
2:D:157:PHE:CE2	2:D:158:PRO:HB3	1.86	1.09
2:B:165:TRP:NE1	2:B:174:VAL:HG21	1.52	1.08
2:B:165:TRP:HE1	2:B:174:VAL:HG21	0.97	1.08
1:A:98:VAL:HG21	2:B:47:TRP:CD1	1.87	1.08
1:C:115:PRO:HG3	1:C:141:PHE:HB2	1.34	1.07
2:B:165:TRP:HH2	2:B:193:VAL:CG1	1.49	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:THR:CG2	2:B:122:VAL:H	1.67	1.06
1:C:115:PRO:HB3	1:C:141:PHE:HB3	1.31	1.06
1:C:4:MET:HE2	1:C:90:GLN:HB3	1.36	1.05
1:A:30:ASN:ND2	1:A:31:THR:HG23	1.71	1.05
1:C:89:GLN:NE2	2:D:111:LEU:HD23	1.73	1.04
3:M:153:ARG:CG	3:M:153:ARG:HH11	1.72	1.03
2:B:165:TRP:HE1	2:B:174:VAL:HG22	0.88	1.03
1:C:89:GLN:HE22	2:D:111:LEU:CD2	1.70	1.03
3:L:147:ARG:HH11	3:L:147:ARG:HB3	1.17	1.02
2:D:39:GLN:O	2:D:92:ALA:HB1	1.60	1.01
3:M:153:ARG:NH1	3:M:153:ARG:HG2	1.56	1.01
1:C:110:ARG:HD3	1:C:173:SER:HB2	1.41	1.01
3:K:61:THR:HG22	3:K:63:PRO:HD2	1.42	1.00
1:C:11:LEU:HD21	1:C:106:VAL:HG13	1.44	1.00
3:L:61:THR:HB	3:L:64:ARG:HG2	1.39	1.00
1:C:38:GLN:HE22	2:D:39:GLN:HE22	1.04	0.99
1:C:49:TYR:CD2	2:D:109:VAL:CG1	2.44	0.99
2:D:154:LYS:O	2:D:154:LYS:CG	2.05	0.99
1:C:91:TYR:HA	1:C:97:PRO:O	1.62	0.99
1:A:112:VAL:HG11	1:A:201:GLN:HG3	1.43	0.99
1:C:115:PRO:CB	1:C:141:PHE:CB	2.41	0.98
1:C:115:PRO:HG3	1:C:141:PHE:HB3	1.28	0.98
1:A:142:TYR:HD1	1:A:142:TYR:O	1.46	0.98
2:D:165:TRP:CD1	2:D:170:LEU:HB3	2.00	0.97
1:A:38:GLN:HE22	2:B:39:GLN:HE22	1.03	0.97
3:N:147:ARG:HH11	3:N:147:ARG:HB3	1.28	0.97
2:B:119:LEU:HD21	2:B:121:THR:HG23	1.44	0.97
2:D:91:THR:HG22	2:D:121:THR:HA	1.46	0.96
3:M:25:GLN:NE2	3:M:113:TRP:HE1	1.62	0.96
1:A:114:ALA:HA	1:A:200:HIS:CD2	2.00	0.96
1:A:144:ARG:HG2	1:A:144:ARG:O	1.64	0.96
1:A:115:PRO:HD3	1:A:200:HIS:CD2	2.00	0.96
2:B:91:THR:HG22	2:B:121:THR:HA	1.47	0.96
1:A:115:PRO:HD3	1:A:200:HIS:CG	2.00	0.95
1:A:4:MET:CE	1:A:90:GLN:HB3	1.96	0.95
1:C:49:TYR:HD1	1:C:50:SER:N	1.64	0.95
1:C:144:ARG:O	1:C:144:ARG:HG2	1.65	0.95
3:M:153:ARG:HG2	3:M:153:ARG:HH11	0.80	0.95
1:C:2:ILE:CD1	1:C:29:VAL:HG22	1.97	0.95
1:A:108:ILE:HG22	1:A:168:GLN:NE2	1.81	0.95
2:D:119:LEU:HD21	2:D:121:THR:HG23	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:52:ARG:HA	3:K:60:ILE:HG22	1.48	0.94
3:M:61:THR:HG22	3:M:63:PRO:HD2	1.48	0.94
2:B:212:LYS:HD3	2:B:212:LYS:H	1.33	0.94
1:A:49:TYR:HD1	1:A:50:SER:N	1.64	0.94
2:D:99:GLN:CB	2:D:110:ALA:O	2.16	0.94
3:L:52:ARG:HA	3:L:60:ILE:HG22	1.49	0.94
2:B:165:TRP:HZ2	2:B:193:VAL:HB	0.77	0.94
2:B:104:MET:O	3:M:153:ARG:NE	2.00	0.94
2:D:91:THR:CG2	2:D:122:VAL:H	1.81	0.94
1:C:115:PRO:CG	1:C:141:PHE:CB	2.31	0.94
1:A:98:VAL:HG21	2:B:47:TRP:CG	2.03	0.93
2:D:87:ARG:O	2:D:122:VAL:HG11	1.69	0.93
3:L:159:ARG:HB2	3:M:159:ARG:NH1	1.84	0.93
1:C:137:LEU:HD11	2:D:192:VAL:HG21	1.51	0.92
3:N:109:ALA:O	3:N:113:TRP:CD1	2.21	0.92
2:B:130:PRO:HD3	2:B:156:TYR:HA	1.50	0.92
2:D:86:LEU:HB3	2:D:122:VAL:HG21	1.51	0.92
1:C:30:ASN:ND2	1:C:31:THR:HG23	1.84	0.92
1:A:114:ALA:HA	1:A:200:HIS:HD2	1.34	0.91
3:L:46:LEU:CB	3:L:91:VAL:HG11	1.99	0.91
3:L:60:ILE:HG13	3:L:61:THR:H	1.36	0.91
1:A:142:TYR:O	1:A:142:TYR:CD1	2.23	0.91
1:C:115:PRO:HB3	1:C:141:PHE:CB	2.00	0.91
1:C:168:GLN:HE21	1:C:173:SER:HB3	1.34	0.91
1:C:49:TYR:HD1	1:C:50:SER:H	0.98	0.91
3:L:43:GLY:O	3:L:68:TRP:CZ3	2.24	0.90
3:K:155:LEU:HD13	3:N:154:MET:HB3	1.54	0.90
3:K:152:GLU:O	3:K:155:LEU:HB2	1.71	0.90
3:N:71:GLU:OE1	3:N:76:VAL:HG11	1.68	0.89
1:C:166:THR:HG22	1:C:176:SER:H	1.38	0.89
3:M:127:ARG:HD3	3:M:127:ARG:O	1.72	0.89
3:M:52:ARG:HA	3:M:60:ILE:HG22	1.55	0.89
3:M:153:ARG:CD	3:M:157:ASP:OD2	2.21	0.88
1:A:168:GLN:HE21	1:A:173:SER:HB3	1.38	0.88
1:A:49:TYR:HD1	1:A:50:SER:H	0.92	0.88
2:B:91:THR:HG23	2:B:122:VAL:H	1.34	0.88
2:B:130:PRO:HG3	2:B:156:TYR:HB3	0.90	0.88
3:L:61:THR:HG22	3:L:63:PRO:HD2	1.54	0.88
1:C:59:PRO:HB3	1:C:61:ARG:NH1	1.89	0.88
2:B:86:LEU:HB3	2:B:122:VAL:HG21	1.56	0.88
2:B:165:TRP:CD1	2:B:174:VAL:HG21	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ALA:HA	2:B:122:VAL:CG1	2.02	0.88
3:K:51:GLU:HG3	3:K:59:LEU:HD23	1.56	0.87
1:A:11:LEU:HD21	1:A:106:VAL:HG13	1.55	0.87
3:L:39:VAL:HG12	3:L:95:VAL:HA	1.56	0.87
3:N:59:LEU:HD12	3:N:65:ALA:HB1	1.56	0.87
3:M:74:THR:HB	3:N:75:THR:HG21	1.57	0.87
1:A:110:ARG:HE	1:A:142:TYR:HB3	1.39	0.87
1:A:32:ALA:O	1:A:91:TYR:CE1	2.27	0.87
3:L:109:ALA:O	3:L:113:TRP:HD1	1.56	0.87
1:A:144:ARG:HB3	1:A:144:ARG:HH11	1.39	0.87
1:C:144:ARG:HB3	1:C:144:ARG:HH11	1.38	0.87
3:M:35:LEU:HD12	3:M:38:ILE:HD12	1.57	0.86
2:B:87:ARG:O	2:B:122:VAL:HG11	1.75	0.86
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.57	0.86
1:C:66:ARG:NH1	1:C:68:GLY:HA2	1.90	0.86
3:K:151:LEU:HD22	3:N:151:LEU:HD13	1.56	0.86
1:A:113:ALA:O	1:A:200:HIS:CD2	2.28	0.86
2:B:166:ASN:HD22	2:B:169:ALA:HB3	1.37	0.86
3:N:58:GLN:O	3:N:64:ARG:HD2	1.76	0.86
1:A:166:THR:HG22	1:A:176:SER:H	1.38	0.85
3:L:58:GLN:O	3:L:64:ARG:HD2	1.76	0.85
3:M:151:LEU:HD23	3:M:151:LEU:O	1.75	0.85
1:A:35:TRP:CZ3	1:A:88:CYS:HB2	2.11	0.85
1:C:110:ARG:CD	1:C:173:SER:HB2	2.06	0.85
1:C:89:GLN:HG2	1:C:90:GLN:N	1.90	0.85
3:K:29:ALA:HA	3:K:105:LEU:HD23	1.59	0.85
3:L:138:THR:O	3:L:141:THR:HG22	1.76	0.85
2:D:40:ALA:HB3	2:D:43:LYS:HB2	1.56	0.85
2:B:166:ASN:HB2	2:B:169:ALA:CB	2.07	0.85
2:B:165:TRP:CH2	2:B:193:VAL:HG12	1.91	0.84
1:A:108:ILE:HG22	1:A:168:GLN:HE22	1.40	0.84
1:A:4:MET:HE2	1:A:90:GLN:HB3	1.59	0.84
1:C:35:TRP:CZ3	1:C:88:CYS:HB2	2.12	0.84
3:L:135:GLU:O	3:L:139:ARG:HG3	1.76	0.84
1:A:137:LEU:HD12	2:B:192:VAL:HG11	1.58	0.84
2:B:130:PRO:CG	2:B:155:ASP:O	2.26	0.84
3:N:49:LEU:HB2	3:N:62:TYR:OH	1.76	0.84
3:L:147:ARG:HB3	3:L:147:ARG:NH1	1.92	0.84
1:C:2:ILE:HD13	1:C:29:VAL:HG22	1.57	0.84
3:L:32:ALA:HB3	3:L:105:LEU:HD21	1.59	0.84
1:A:49:TYR:CD2	2:B:109:VAL:HG12	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PRO:HB3	1:A:61:ARG:NH1	1.92	0.83
1:C:98:VAL:HG21	2:D:47:TRP:CG	2.13	0.83
2:D:145:GLY:O	2:D:196:PRO:HA	1.78	0.83
3:N:52:ARG:HG2	3:N:60:ILE:O	1.77	0.83
2:B:130:PRO:CG	2:B:156:TYR:CB	2.46	0.83
2:D:91:THR:HG23	2:D:122:VAL:H	1.43	0.83
2:D:88:ALA:HA	2:D:122:VAL:CG1	2.09	0.83
1:A:13:ALA:O	1:A:108:ILE:HG12	1.78	0.82
1:A:89:GLN:HG2	1:A:90:GLN:N	1.94	0.82
1:C:108:ILE:HG22	1:C:168:GLN:HE22	1.44	0.82
1:A:89:GLN:HE22	2:B:111:LEU:HD23	1.42	0.82
1:A:112:VAL:CG1	1:A:201:GLN:HG3	2.09	0.82
1:C:13:ALA:O	1:C:108:ILE:HG12	1.80	0.82
3:L:150:ARG:CD	3:M:152:GLU:OE2	2.27	0.82
2:D:11:LEU:HD11	2:D:157:PHE:HE2	1.43	0.82
3:K:158:ASN:HD22	3:L:159:ARG:NH1	1.77	0.82
3:M:62:TYR:HB2	3:M:63:PRO:HD3	1.60	0.82
2:B:145:GLY:O	2:B:196:PRO:HA	1.80	0.81
3:K:35:LEU:HD12	3:K:38:ILE:HD12	1.61	0.81
2:B:130:PRO:CB	2:B:155:ASP:H	1.92	0.81
3:N:159:ARG:HD2	3:N:160:ARG:HG3	1.60	0.81
2:D:130:PRO:HB2	2:D:153:VAL:HG12	1.63	0.81
3:N:51:GLU:HG3	3:N:59:LEU:HD23	1.63	0.81
1:A:142:TYR:C	1:A:142:TYR:CD1	2.53	0.81
3:K:62:TYR:HB2	3:K:63:PRO:HD3	1.63	0.81
3:N:155:LEU:HD22	3:N:159:ARG:HH21	1.44	0.81
2:D:149:LEU:HD12	2:D:222:VAL:HG11	1.63	0.80
3:K:157:ASP:OD1	3:K:157:ASP:N	2.13	0.80
1:A:2:ILE:CD1	1:A:29:VAL:HG22	2.10	0.80
1:A:11:LEU:CD2	1:A:106:VAL:HA	2.11	0.80
2:B:166:ASN:HB2	2:B:169:ALA:HB3	1.63	0.80
3:K:43:GLY:O	3:K:68:TRP:CZ3	2.34	0.80
1:A:115:PRO:HD3	1:A:200:HIS:CB	2.12	0.80
2:D:162:THR:HG23	2:D:212:LYS:HE2	1.62	0.80
3:M:51:GLU:HG3	3:M:59:LEU:HD23	1.63	0.80
1:A:115:PRO:CG	1:A:200:HIS:HB2	2.10	0.80
2:D:11:LEU:CD1	2:D:157:PHE:HE2	1.94	0.80
3:K:37:VAL:O	3:K:41:LEU:HG	1.81	0.80
1:A:137:LEU:HD11	2:B:192:VAL:HG21	1.63	0.80
3:K:74:THR:OG1	3:K:76:VAL:HG23	1.82	0.80
3:L:150:ARG:HD3	3:M:152:GLU:CD	2.01	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:147:ARG:HG3	3:K:147:ARG:HH11	1.45	0.79
1:A:112:VAL:CG1	1:A:201:GLN:CG	2.60	0.79
3:L:50:ALA:O	3:L:85:THR:HG21	1.83	0.79
2:B:152:LEU:HD21	2:B:154:LYS:HD2	1.63	0.79
2:B:165:TRP:CD1	2:B:170:LEU:O	2.35	0.79
1:C:11:LEU:CD2	1:C:106:VAL:HA	2.13	0.79
2:B:165:TRP:O	2:B:206:ILE:O	2.01	0.79
2:D:99:GLN:CG	2:D:110:ALA:O	2.31	0.79
2:B:105:TYR:O	2:B:105:TYR:HD1	1.66	0.79
1:C:20:THR:HG22	1:C:74:THR:OG1	1.83	0.79
3:L:109:ALA:O	3:L:113:TRP:CD1	2.36	0.79
1:A:89:GLN:HE22	2:B:111:LEU:CD2	1.95	0.79
1:C:66:ARG:HH11	1:C:68:GLY:HA2	1.45	0.79
3:N:52:ARG:HA	3:N:60:ILE:HG22	1.63	0.78
1:C:49:TYR:CE2	2:D:109:VAL:HG12	2.19	0.78
1:A:93:SER:O	1:A:97:PRO:HB3	1.83	0.78
3:K:70:VAL:HG12	3:L:96:MET:SD	2.23	0.78
1:A:120:PHE:HB2	1:A:135:VAL:HG13	1.65	0.78
3:M:153:ARG:HD3	3:M:157:ASP:OD2	1.83	0.78
3:M:150:ARG:HD3	3:N:152:GLU:OE2	1.82	0.78
3:K:159:ARG:HH12	3:N:159:ARG:HB2	1.49	0.78
1:A:122:PRO:HB2	1:A:127:LEU:HD11	1.63	0.78
2:B:54:TYR:HD1	2:B:54:TYR:O	1.67	0.78
1:C:90:GLN:O	1:C:97:PRO:O	2.00	0.77
3:M:147:ARG:HE	3:N:145:HIS:CD2	2.03	0.77
2:B:104:MET:O	3:M:153:ARG:CD	2.31	0.77
3:L:154:MET:HB3	3:M:156:ASP:OD2	1.84	0.77
1:A:12:SER:OG	1:A:109:LYS:HB2	1.84	0.77
3:N:114:PHE:O	3:N:117:GLN:HG2	1.83	0.77
1:C:12:SER:OG	1:C:109:LYS:HB2	1.85	0.77
2:D:157:PHE:CD2	2:D:158:PRO:N	2.52	0.77
3:L:159:ARG:HD2	3:L:160:ARG:HG3	1.67	0.77
3:M:158:ASN:HB3	3:N:159:ARG:NH1	2.00	0.77
3:N:126:VAL:O	3:N:130:GLU:HB2	1.85	0.77
1:C:122:PRO:HB2	1:C:127:LEU:HD11	1.67	0.77
1:C:49:TYR:CE2	2:D:109:VAL:CG1	2.67	0.77
3:K:67:TRP:HH2	3:L:68:TRP:HZ2	1.33	0.77
3:N:67:TRP:HB3	3:N:81:LEU:HD12	1.66	0.77
3:M:120:GLN:O	3:M:124:GLN:HG3	1.85	0.77
2:B:104:MET:O	3:M:153:ARG:HD2	1.85	0.76
2:D:220:LYS:HD3	2:D:221:LYS:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:28:ALA:O	3:K:105:LEU:HD21	1.84	0.76
1:A:89:GLN:HB2	1:A:100:PHE:CD1	2.20	0.76
1:C:32:ALA:HB3	1:C:92:TYR:HB2	1.65	0.76
2:D:220:LYS:HD3	2:D:221:LYS:H	1.49	0.76
3:N:35:LEU:HD12	3:N:38:ILE:HD12	1.67	0.76
3:N:74:THR:OG1	3:N:76:VAL:HG23	1.85	0.76
1:A:79:GLN:HB3	1:A:80:PRO:HD2	1.66	0.76
1:A:123:SER:O	1:A:127:LEU:HD13	1.84	0.76
1:A:4:MET:HE1	1:A:90:GLN:HB3	1.67	0.76
2:B:130:PRO:HB2	2:B:155:ASP:H	1.49	0.76
3:M:158:ASN:HB3	3:N:159:ARG:HH12	1.46	0.76
2:D:99:GLN:HG3	2:D:110:ALA:HA	1.65	0.76
3:L:153:ARG:O	3:L:157:ASP:CB	2.34	0.76
3:N:71:GLU:OE1	3:N:76:VAL:HG12	1.81	0.76
3:L:43:GLY:O	3:L:68:TRP:CE3	2.37	0.76
3:K:127:ARG:HH11	3:K:130:GLU:HG3	1.51	0.76
3:L:43:GLY:O	3:L:68:TRP:HZ3	1.66	0.75
3:L:158:ASN:ND2	3:M:159:ARG:HD2	2.01	0.75
3:N:143:ALA:CA	3:N:146:GLU:HB2	2.11	0.75
1:A:110:ARG:HG2	1:A:142:TYR:CD2	2.20	0.75
1:C:191:HIS:O	1:C:213:ARG:HD3	1.86	0.75
1:C:137:LEU:HD12	2:D:192:VAL:HG11	1.65	0.75
3:L:143:ALA:HA	3:L:146:GLU:HB2	1.68	0.75
1:A:110:ARG:NE	1:A:142:TYR:HB3	2.01	0.75
3:K:32:ALA:HB3	3:K:105:LEU:CD2	2.17	0.75
3:N:51:GLU:HB3	3:N:59:LEU:O	1.87	0.75
2:B:130:PRO:CA	2:B:155:ASP:O	2.34	0.75
1:C:2:ILE:HD13	1:C:29:VAL:CG2	2.16	0.75
1:A:192:LYS:HA	1:A:213:ARG:CD	2.16	0.75
2:B:130:PRO:CD	2:B:156:TYR:CB	2.65	0.75
1:C:79:GLN:HB3	1:C:80:PRO:HD2	1.69	0.75
1:A:113:ALA:O	1:A:200:HIS:NE2	2.20	0.74
1:A:112:VAL:HG13	1:A:201:GLN:CG	2.17	0.74
2:D:11:LEU:HD11	2:D:157:PHE:CE2	2.21	0.74
1:A:143:PRO:O	1:A:143:PRO:HD2	1.85	0.74
1:C:32:ALA:O	1:C:91:TYR:N	2.19	0.74
2:D:165:TRP:CZ3	2:D:207:CYS:HB3	2.22	0.74
3:M:158:ASN:HD21	3:N:160:ARG:HD2	1.50	0.74
3:L:67:TRP:HZ3	3:M:89:ARG:HA	1.50	0.74
1:A:91:TYR:HA	1:A:97:PRO:O	1.87	0.74
1:C:49:TYR:HD2	2:D:109:VAL:HG12	1.46	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:60:ILE:HG13	3:L:61:THR:N	2.02	0.74
3:L:87:TRP:CZ3	3:L:90:LEU:HD12	2.22	0.74
1:A:83:PHE:CE1	1:A:108:ILE:HB	2.22	0.74
2:B:208:ASN:HD22	2:B:208:ASN:N	1.85	0.74
2:D:165:TRP:HZ3	2:D:207:CYS:HB3	1.50	0.74
3:L:46:LEU:HB2	3:L:91:VAL:CG1	2.10	0.74
3:N:135:GLU:O	3:N:139:ARG:HG3	1.87	0.74
3:N:37:VAL:O	3:N:41:LEU:HG	1.87	0.74
3:L:74:THR:OG1	3:L:76:VAL:HG23	1.88	0.74
3:N:59:LEU:CD1	3:N:65:ALA:HB1	2.18	0.74
1:A:195:ALA:HA	1:A:210:SER:HB2	1.69	0.73
2:D:16:GLY:O	2:D:84:ASN:O	2.05	0.73
3:K:102:SER:O	3:K:106:VAL:HG23	1.88	0.73
3:N:137:TYR:O	3:N:140:THR:HG22	1.88	0.73
1:C:123:SER:O	1:C:127:LEU:HD13	1.88	0.73
3:M:61:THR:HB	3:M:64:ARG:HG2	1.68	0.73
3:M:76:VAL:HG22	3:N:75:THR:HA	1.70	0.73
2:D:154:LYS:HG3	2:D:188:SER:OG	1.87	0.73
2:B:165:TRP:CE2	2:B:174:VAL:HG22	2.23	0.73
2:B:60:TYR:HE2	2:B:70:ILE:H	1.34	0.73
2:B:193:VAL:HG13	2:B:193:VAL:O	1.88	0.73
1:C:36:TYR:OH	2:D:111:LEU:HB2	1.88	0.73
2:D:165:TRP:O	2:D:206:ILE:O	2.07	0.73
3:M:151:LEU:HD23	3:M:151:LEU:C	2.07	0.73
3:N:93:VAL:O	3:N:97:VAL:HG23	1.87	0.73
1:C:195:ALA:HA	1:C:210:SER:HB2	1.69	0.73
1:C:49:TYR:CD1	1:C:50:SER:N	2.53	0.72
1:A:89:GLN:HE21	1:A:98:VAL:HG12	1.54	0.72
3:K:23:ALA:O	3:K:27:ARG:HD3	1.89	0.72
1:A:165:VAL:HG12	1:A:177:LEU:HD22	1.70	0.72
2:B:97:ALA:HB3	2:B:111:LEU:HD12	1.71	0.72
3:K:67:TRP:HB3	3:K:81:LEU:HD12	1.72	0.72
3:L:76:VAL:HA	3:M:75:THR:HB	1.71	0.72
2:B:16:GLY:O	2:B:84:ASN:O	2.07	0.72
1:C:165:VAL:HG12	1:C:177:LEU:HD22	1.70	0.72
2:D:60:TYR:HE2	2:D:70:ILE:H	1.38	0.72
2:B:130:PRO:CD	2:B:156:TYR:HB3	2.19	0.72
3:M:48:VAL:HG11	3:M:62:TYR:HA	1.71	0.72
3:N:109:ALA:O	3:N:113:TRP:HD1	1.72	0.72
1:A:114:ALA:HB1	1:A:203:LEU:CD2	2.19	0.72
1:C:89:GLN:HE21	1:C:98:VAL:HG12	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:GLY:O	2:D:193:VAL:HA	1.90	0.72
1:A:112:VAL:HG13	1:A:201:GLN:HG2	1.71	0.72
3:K:60:ILE:HG13	3:K:61:THR:H	1.55	0.72
2:B:211:HIS:ND1	2:B:213:PRO:HD2	2.05	0.72
2:D:64:VAL:HG21	2:D:68:PHE:CG	2.25	0.71
1:C:212:ASN:N	1:C:212:ASN:HD22	1.85	0.71
3:N:124:GLN:HA	3:N:127:ARG:HG2	1.72	0.71
1:C:4:MET:HE1	1:C:90:GLN:HB3	1.69	0.71
2:D:211:HIS:HE1	2:D:213:PRO:HB2	1.56	0.71
2:B:91:THR:HG22	2:B:122:VAL:H	1.52	0.71
2:D:99:GLN:HG3	2:D:110:ALA:O	1.89	0.71
3:K:153:ARG:HH11	3:K:153:ARG:HG2	1.55	0.71
3:M:74:THR:OG1	3:M:76:VAL:HG23	1.91	0.71
1:A:119:ILE:CG2	1:A:211:PHE:HD2	2.04	0.71
2:B:173:GLY:O	2:B:193:VAL:HA	1.91	0.71
3:N:52:ARG:NE	3:N:60:ILE:O	2.24	0.71
3:N:61:THR:CG2	3:N:63:PRO:HD2	2.11	0.71
1:A:113:ALA:HB3	1:A:142:TYR:N	1.99	0.71
3:L:158:ASN:HD22	3:M:159:ARG:HD2	1.56	0.71
2:B:212:LYS:HD3	2:B:212:LYS:N	2.05	0.71
1:C:98:VAL:HG21	2:D:47:TRP:NE1	2.06	0.71
1:C:115:PRO:HB3	1:C:141:PHE:CA	2.20	0.70
1:C:137:LEU:HD11	2:D:192:VAL:CG2	2.21	0.70
3:M:58:GLN:O	3:M:64:ARG:HD2	1.92	0.70
3:N:48:VAL:HG11	3:N:62:TYR:HA	1.73	0.70
3:K:126:VAL:O	3:K:130:GLU:HB3	1.91	0.70
3:L:153:ARG:O	3:L:157:ASP:HB3	1.91	0.70
3:L:62:TYR:HB2	3:L:63:PRO:HD3	1.72	0.70
3:L:59:LEU:HD12	3:L:65:ALA:HB1	1.73	0.70
2:B:91:THR:CG2	2:B:122:VAL:N	2.50	0.70
1:C:2:ILE:HD11	1:C:29:VAL:HG22	1.70	0.70
2:B:149:LEU:HD11	2:B:205:TYR:CD2	2.26	0.70
3:K:46:LEU:HB2	3:K:91:VAL:HG11	1.73	0.70
3:L:93:VAL:O	3:L:97:VAL:HG23	1.90	0.70
1:A:192:LYS:HA	1:A:213:ARG:HD2	1.72	0.70
2:D:166:ASN:HB2	2:D:169:ALA:HB3	1.73	0.70
2:D:217:LYS:HD3	2:D:218:VAL:N	2.06	0.70
3:N:155:LEU:HD22	3:N:159:ARG:NH2	2.07	0.70
1:A:30:ASN:O	1:A:66:ARG:NE	2.24	0.69
2:B:130:PRO:HB3	2:B:155:ASP:N	2.07	0.69
3:N:122:GLN:O	3:N:126:VAL:HG13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:59:LEU:HD12	3:N:65:ALA:CB	2.21	0.69
2:B:64:VAL:HG21	2:B:68:PHE:CG	2.27	0.69
3:M:76:VAL:O	3:N:77:GLY:HA3	1.91	0.69
2:B:152:LEU:HD23	2:B:154:LYS:HB2	1.73	0.69
1:C:38:GLN:O	1:C:84:ALA:HB1	1.92	0.69
3:L:115:VAL:HA	3:L:118:GLU:HB2	1.74	0.69
3:M:25:GLN:NE2	3:M:113:TRP:NE1	2.39	0.69
2:D:54:TYR:HD1	2:D:54:TYR:O	1.74	0.69
3:K:122:GLN:O	3:K:126:VAL:HG12	1.91	0.69
3:K:140:THR:O	3:K:143:ALA:HB3	1.92	0.69
3:K:43:GLY:O	3:K:68:TRP:CE3	2.45	0.69
3:K:51:GLU:O	3:K:57:ALA:HB1	1.93	0.69
2:D:157:PHE:CD2	2:D:158:PRO:HB3	2.28	0.69
3:K:141:THR:O	3:K:144:LEU:HB2	1.93	0.69
2:B:130:PRO:CB	2:B:155:ASP:C	2.37	0.69
1:C:120:PHE:HB2	1:C:135:VAL:HG13	1.75	0.69
2:D:130:PRO:HB2	2:D:153:VAL:CG1	2.22	0.69
3:L:67:TRP:HB3	3:L:81:LEU:HD12	1.75	0.69
3:K:64:ARG:HA	3:L:89:ARG:HH12	1.57	0.69
1:A:191:HIS:O	1:A:213:ARG:NH1	2.25	0.69
1:A:20:THR:HG22	1:A:74:THR:OG1	1.93	0.68
2:D:99:GLN:HG3	2:D:110:ALA:CA	2.22	0.68
3:K:64:ARG:O	3:K:81:LEU:HD11	1.93	0.68
3:L:51:GLU:HG3	3:L:59:LEU:HD23	1.75	0.68
1:A:98:VAL:CG2	2:B:47:TRP:CG	2.75	0.68
2:D:98:ARG:NH1	2:D:112:ASP:OD1	2.25	0.68
3:L:35:LEU:HD12	3:L:38:ILE:HD12	1.75	0.68
3:N:138:THR:O	3:N:141:THR:HG22	1.94	0.68
1:A:123:SER:O	1:A:127:LEU:CD1	2.41	0.68
2:D:212:LYS:N	2:D:213:PRO:CD	2.57	0.68
3:K:39:VAL:HG12	3:K:95:VAL:HA	1.76	0.68
1:A:30:ASN:HD22	1:A:66:ARG:HH21	1.40	0.68
1:A:2:ILE:HD13	1:A:29:VAL:HG22	1.75	0.68
2:B:130:PRO:HB3	2:B:155:ASP:CA	2.23	0.68
2:B:56:SER:HB2	3:M:142:ARG:HD3	1.76	0.68
1:C:6:GLN:OE1	1:C:88:CYS:HB3	1.94	0.68
3:K:135:GLU:HA	3:K:138:THR:HB	1.75	0.68
3:K:137:TYR:HA	3:L:137:TYR:OH	1.93	0.68
3:K:118:GLU:O	3:K:122:GLN:HG3	1.95	0.67
3:K:32:ALA:HB3	3:K:105:LEU:HD22	1.75	0.67
3:L:153:ARG:O	3:L:157:ASP:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:158:ASN:HB3	3:L:159:ARG:HH12	1.59	0.67
3:L:37:VAL:O	3:L:41:LEU:HG	1.93	0.67
1:A:109:LYS:HA	1:A:142:TYR:OH	1.94	0.67
1:C:89:GLN:HB2	1:C:100:PHE:CD1	2.30	0.67
3:M:74:THR:HB	3:N:75:THR:CG2	2.24	0.67
1:C:138:LEU:HD22	1:C:177:LEU:CB	2.24	0.67
3:K:159:ARG:NH1	3:N:159:ARG:HB2	2.08	0.67
3:L:115:VAL:O	3:L:119:GLN:HG3	1.95	0.67
2:D:208:ASN:N	2:D:208:ASN:HD22	1.89	0.67
3:K:48:VAL:HG13	3:K:59:LEU:O	1.94	0.67
3:N:115:VAL:O	3:N:119:GLN:HG3	1.94	0.67
2:D:156:TYR:HE1	2:D:189:LEU:HD22	1.59	0.67
3:N:39:VAL:HG11	3:N:98:ALA:HB2	1.76	0.67
2:B:176:THR:HG23	2:B:191:SER:HB2	1.76	0.67
1:A:49:TYR:HD2	2:B:109:VAL:HG12	1.58	0.67
2:D:165:TRP:HE1	2:D:174:VAL:HG22	1.59	0.67
2:D:185:GLY:C	2:D:186:LEU:HD12	2.15	0.67
1:C:165:VAL:CG1	1:C:177:LEU:HD22	2.24	0.67
1:C:144:ARG:HB3	1:C:144:ARG:NH1	2.09	0.67
2:D:13:GLN:OE1	2:D:13:GLN:N	2.28	0.67
3:K:93:VAL:O	3:K:97:VAL:HG23	1.94	0.67
3:K:70:VAL:HG11	3:L:93:VAL:HG22	1.76	0.67
1:C:83:PHE:CE1	1:C:108:ILE:HG13	2.30	0.66
3:K:61:THR:CG2	3:K:63:PRO:HD2	2.21	0.66
1:A:144:ARG:HB3	1:A:144:ARG:NH1	2.09	0.66
2:D:152:LEU:HD21	2:D:154:LYS:HD2	1.77	0.66
3:K:138:THR:O	3:K:141:THR:HG23	1.96	0.66
1:A:165:VAL:CG1	1:A:177:LEU:HD22	2.24	0.66
2:B:185:GLY:C	2:B:186:LEU:HD12	2.16	0.66
2:D:149:LEU:HD11	2:D:205:TYR:CD2	2.31	0.66
2:D:211:HIS:CE1	2:D:213:PRO:HB2	2.30	0.66
1:A:2:ILE:HD13	1:A:29:VAL:CG2	2.26	0.66
1:A:83:PHE:CE1	1:A:108:ILE:HG13	2.31	0.66
2:B:130:PRO:HD3	2:B:156:TYR:CA	2.24	0.66
2:D:157:PHE:C	2:D:157:PHE:CD2	2.68	0.66
3:K:61:THR:HB	3:K:64:ARG:HG2	1.76	0.66
3:K:155:LEU:CD1	3:N:154:MET:HB3	2.25	0.66
2:D:157:PHE:CD2	2:D:158:PRO:CA	2.78	0.66
1:C:31:THR:HG22	1:C:66:ARG:HE	1.61	0.66
2:D:97:ALA:HB3	2:D:111:LEU:HD12	1.78	0.66
1:A:115:PRO:CD	1:A:200:HIS:CG	2.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:CD	1:A:200:HIS:CB	2.74	0.65
1:C:137:LEU:HD21	1:C:139:ASN:OD1	1.96	0.65
1:C:2:ILE:CD1	1:C:29:VAL:CG2	2.73	0.65
3:K:153:ARG:NH1	3:K:153:ARG:HG2	2.11	0.65
3:M:118:GLU:HA	3:M:121:GLN:NE2	2.11	0.65
2:B:40:ALA:HB1	2:B:41:PRO:HD2	1.79	0.65
1:C:91:TYR:HB2	1:C:97:PRO:HB2	1.78	0.65
1:C:98:VAL:CG2	2:D:47:TRP:CG	2.79	0.65
1:A:50:SER:C	1:A:52:SER:H	1.99	0.65
2:B:130:PRO:CB	2:B:155:ASP:N	2.60	0.65
3:M:102:SER:O	3:M:106:VAL:HG23	1.97	0.65
3:M:43:GLY:O	3:M:68:TRP:CE3	2.50	0.65
1:A:137:LEU:HD21	1:A:139:ASN:OD1	1.97	0.65
2:D:157:PHE:CZ	2:D:158:PRO:HB3	2.30	0.65
3:K:25:GLN:HE21	3:K:112:THR:HG23	1.61	0.65
3:K:147:ARG:HG3	3:K:147:ARG:NH1	2.11	0.65
3:K:58:GLN:O	3:K:64:ARG:HD2	1.97	0.65
1:C:11:LEU:O	1:C:11:LEU:HD23	1.97	0.64
3:K:76:VAL:HG22	3:L:75:THR:HA	1.79	0.64
3:N:61:THR:HG22	3:N:63:PRO:CD	2.13	0.64
1:A:2:ILE:HD11	1:A:29:VAL:HG22	1.78	0.64
2:B:32:TYR:CZ	2:B:98:ARG:NH2	2.66	0.64
2:B:36:TRP:CE2	2:B:81:LEU:HB2	2.33	0.64
3:K:152:GLU:OE2	3:N:150:ARG:HD3	1.97	0.64
3:M:51:GLU:O	3:M:57:ALA:HB1	1.97	0.64
3:M:93:VAL:O	3:M:97:VAL:HG23	1.98	0.64
1:A:31:THR:HG22	1:A:66:ARG:NE	2.13	0.64
1:A:49:TYR:CD1	1:A:50:SER:N	2.53	0.64
3:K:118:GLU:HA	3:K:121:GLN:NE2	2.12	0.64
3:M:158:ASN:ND2	3:N:160:ARG:HD2	2.12	0.64
2:B:166:ASN:ND2	2:B:169:ALA:HB3	2.11	0.64
2:B:212:LYS:N	2:B:213:PRO:CD	2.61	0.64
1:C:79:GLN:HA	1:C:79:GLN:OE1	1.97	0.64
3:K:120:GLN:O	3:K:124:GLN:HG3	1.97	0.64
1:A:73:LEU:HD12	1:A:74:THR:H	1.62	0.64
2:D:165:TRP:NE1	2:D:174:VAL:HG22	2.12	0.64
2:D:195:VAL:HG21	2:D:205:TYR:CE2	2.33	0.64
3:L:155:LEU:HD22	3:L:159:ARG:HH21	1.63	0.64
2:B:166:ASN:HB2	2:B:169:ALA:HB2	1.78	0.64
1:C:50:SER:C	1:C:52:SER:H	2.01	0.64
2:D:157:PHE:CE2	2:D:158:PRO:CB	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:TYR:CZ	2:D:98:ARG:NH2	2.66	0.64
3:N:48:VAL:HG22	3:N:65:ALA:HB1	1.77	0.64
1:C:27:GLN:HG3	1:C:28:ASP:H	1.62	0.64
2:D:9:GLY:H	2:D:118:THR:HG21	1.63	0.64
1:A:156:LEU:HD13	1:A:157:GLN:N	2.12	0.64
1:C:148:VAL:O	1:C:148:VAL:HG23	1.97	0.64
1:C:152:VAL:O	1:C:152:VAL:HG23	1.98	0.64
2:D:64:VAL:HG21	2:D:68:PHE:CD2	2.32	0.64
3:K:78:TYR:CE2	3:L:77:GLY:HA2	2.33	0.64
1:A:166:THR:HG22	1:A:176:SER:N	2.13	0.63
2:B:11:LEU:HD23	2:B:12:VAL:N	2.12	0.63
2:D:24:ALA:HB3	2:D:77:ASN:ND2	2.13	0.63
3:K:76:VAL:HA	3:L:75:THR:HB	1.79	0.63
3:K:75:THR:HG21	3:N:74:THR:HB	1.79	0.63
1:A:95:SER:O	1:A:95:SER:OG	2.16	0.63
1:C:156:LEU:HD13	1:C:157:GLN:N	2.13	0.63
2:B:181:LEU:HG	2:B:182:GLN:N	2.13	0.63
3:K:159:ARG:HD2	3:N:158:ASN:ND2	2.14	0.63
1:A:27:GLN:HG3	1:A:28:ASP:H	1.62	0.63
2:B:130:PRO:HG3	2:B:156:TYR:CA	2.28	0.63
1:C:138:LEU:HD22	1:C:177:LEU:HB3	1.81	0.63
2:D:11:LEU:HD23	2:D:12:VAL:N	2.13	0.63
3:L:76:VAL:CA	3:M:75:THR:HB	2.28	0.63
2:D:176:THR:HG23	2:D:191:SER:HB2	1.81	0.63
3:L:51:GLU:O	3:L:57:ALA:HB1	1.98	0.63
3:L:39:VAL:CG1	3:L:95:VAL:HA	2.26	0.63
1:A:137:LEU:CD1	2:B:192:VAL:HG11	2.29	0.63
1:C:123:SER:O	1:C:127:LEU:CD1	2.46	0.63
3:K:67:TRP:HE1	3:K:78:TYR:HD1	1.47	0.63
1:C:137:LEU:HD23	1:C:138:LEU:O	1.99	0.63
2:B:13:GLN:N	2:B:13:GLN:OE1	2.31	0.63
2:B:208:ASN:ND2	2:B:208:ASN:N	2.46	0.63
2:D:40:ALA:HB1	2:D:41:PRO:HD2	1.80	0.63
3:K:74:THR:HB	3:L:75:THR:HG21	1.80	0.63
2:B:28:ASN:C	2:B:30:SER:H	2.00	0.62
1:C:24:ARG:HG3	1:C:70:ASP:OD1	1.98	0.62
3:K:67:TRP:HZ3	3:L:89:ARG:HA	1.63	0.62
1:C:96:ALA:HB1	1:C:97:PRO:HD2	1.80	0.62
3:L:32:ALA:HB3	3:L:105:LEU:CD2	2.28	0.62
2:B:130:PRO:HB3	2:B:155:ASP:H	1.61	0.62
2:D:91:THR:HG22	2:D:122:VAL:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:O	1:A:84:ALA:HB1	1.99	0.62
2:B:24:ALA:HB3	2:B:77:ASN:ND2	2.14	0.62
1:C:169:ASP:OD2	1:C:170:SER:N	2.31	0.62
1:C:30:ASN:HD22	1:C:66:ARG:NH2	1.97	0.62
2:D:88:ALA:HA	2:D:122:VAL:HG12	1.81	0.62
3:L:122:GLN:O	3:L:126:VAL:HG13	2.00	0.62
3:M:44:SER:OG	3:M:66:LEU:HA	1.99	0.62
1:C:166:THR:HG22	1:C:176:SER:N	2.11	0.62
2:D:100:PRO:CB	2:D:106:SER:HB2	2.30	0.62
2:D:156:TYR:C	2:D:156:TYR:CD2	2.73	0.62
3:L:114:PHE:O	3:L:117:GLN:HG2	2.00	0.62
2:B:9:GLY:H	2:B:118:THR:HG21	1.65	0.62
1:A:108:ILE:CG2	1:A:168:GLN:HE22	2.11	0.62
1:C:142:TYR:C	1:C:142:TYR:CD1	2.73	0.62
2:D:102:TYR:CE2	3:K:150:ARG:HG3	2.35	0.62
2:D:2:VAL:HG11	2:D:113:TYR:CD2	2.34	0.61
2:B:91:THR:HG22	2:B:121:THR:CA	2.27	0.61
3:N:64:ARG:O	3:N:81:LEU:HD11	1.99	0.61
1:C:90:GLN:HG3	1:C:99:THR:OG1	2.01	0.61
1:A:55:GLU:HB3	1:A:58:VAL:CG2	2.31	0.61
2:B:78:THR:HG22	2:B:79:ALA:N	2.14	0.61
1:C:30:ASN:HD22	1:C:66:ARG:HH21	1.47	0.61
2:D:157:PHE:CG	2:D:158:PRO:HA	2.35	0.61
2:D:165:TRP:HE3	2:D:206:ILE:O	1.83	0.61
3:L:102:SER:O	3:L:106:VAL:HG23	2.00	0.61
1:A:152:VAL:O	1:A:152:VAL:HG23	2.00	0.61
1:C:211:PHE:C	1:C:212:ASN:HD22	2.04	0.61
2:D:173:GLY:C	2:D:193:VAL:HG23	2.21	0.61
3:L:48:VAL:HG13	3:L:59:LEU:O	2.00	0.61
3:M:49:LEU:HB2	3:M:62:TYR:OH	2.01	0.61
3:N:67:TRP:HB3	3:N:81:LEU:CD1	2.29	0.61
2:B:101:SER:O	2:B:107:TRP:HB2	2.00	0.61
3:L:137:TYR:O	3:L:140:THR:HG22	2.00	0.61
2:B:64:VAL:HG21	2:B:68:PHE:HB2	1.82	0.61
3:K:67:TRP:HZ2	3:K:78:TYR:HE1	1.48	0.61
3:M:65:ALA:HA	3:M:81:LEU:HD13	1.83	0.61
3:N:51:GLU:O	3:N:57:ALA:HB1	2.00	0.61
1:A:169:ASP:OD2	1:A:170:SER:N	2.33	0.61
1:A:27:GLN:CG	1:A:28:ASP:N	2.64	0.61
1:A:98:VAL:HG21	2:B:47:TRP:NE1	2.16	0.61
2:D:83:MET:HE1	2:D:120:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:36:LEU:O	3:K:40:LEU:HG	2.01	0.60
3:N:109:ALA:O	3:N:113:TRP:NE1	2.33	0.60
1:A:119:ILE:CG2	1:A:211:PHE:CD2	2.83	0.60
1:C:32:ALA:O	1:C:91:TYR:CD1	2.54	0.60
1:C:83:PHE:CE1	1:C:108:ILE:HB	2.36	0.60
1:A:110:ARG:HE	1:A:142:TYR:CB	2.13	0.60
3:M:64:ARG:O	3:M:81:LEU:HD11	2.00	0.60
2:B:78:THR:HG22	2:B:79:ALA:O	2.01	0.60
3:M:130:GLU:HG3	3:M:131:LYS:N	2.16	0.60
3:M:138:THR:HA	3:M:141:THR:HG23	1.84	0.60
3:N:130:GLU:O	3:N:134:GLU:HG3	2.00	0.60
2:B:105:TYR:O	2:B:105:TYR:CD1	2.51	0.60
2:D:181:LEU:HG	2:D:182:GLN:N	2.16	0.60
3:L:76:VAL:HA	3:M:75:THR:CA	2.32	0.60
3:L:67:TRP:CZ3	3:M:89:ARG:HA	2.35	0.60
2:D:212:LYS:H	2:D:213:PRO:CD	2.13	0.60
3:K:76:VAL:HG13	3:L:71:GLU:O	2.00	0.60
2:D:176:THR:HG23	2:D:191:SER:CB	2.31	0.60
3:N:39:VAL:HG11	3:N:98:ALA:CB	2.31	0.60
2:B:98:ARG:NH1	2:B:112:ASP:OD1	2.34	0.60
2:D:208:ASN:N	2:D:208:ASN:ND2	2.50	0.60
2:D:97:ALA:CB	2:D:111:LEU:HD12	2.32	0.60
3:L:39:VAL:HG21	3:L:98:ALA:HB2	1.84	0.60
3:M:67:TRP:CE3	3:N:89:ARG:HG2	2.37	0.60
3:K:82:TYR:CE1	3:N:80:ASP:HB3	2.35	0.60
3:K:124:GLN:O	3:K:128:HIS:HB2	2.02	0.59
3:K:123:GLN:O	3:K:127:ARG:HB2	2.02	0.59
2:B:116:GLN:HA	2:B:116:GLN:OE1	2.01	0.59
2:B:22:CYS:C	2:B:78:THR:HG23	2.23	0.59
3:K:127:ARG:CZ	3:K:131:LYS:HB2	2.32	0.59
1:A:90:GLN:OE1	1:A:91:TYR:N	2.35	0.59
2:D:209:VAL:O	2:D:217:LYS:HG2	2.01	0.59
3:L:80:ASP:HB3	3:M:82:TYR:CE1	2.37	0.59
2:D:86:LEU:HB3	2:D:122:VAL:CG2	2.30	0.59
1:C:115:PRO:HB3	1:C:140:ASN:C	2.22	0.59
2:D:2:VAL:HG11	2:D:113:TYR:HD2	1.66	0.59
2:B:106:SER:O	2:B:109:VAL:HG23	2.03	0.59
2:B:2:VAL:HG11	2:B:113:TYR:CD2	2.38	0.59
2:B:2:VAL:HG11	2:B:113:TYR:HD2	1.67	0.59
1:A:115:PRO:CG	1:A:200:HIS:CB	2.81	0.59
1:C:212:ASN:HB2	1:C:215:GLU:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:PHE:CD2	2:D:158:PRO:CB	2.86	0.59
1:C:137:LEU:CD1	2:D:192:VAL:HG21	2.29	0.59
2:D:212:LYS:HG2	2:D:213:PRO:HD3	1.84	0.59
3:K:49:LEU:HB2	3:K:62:TYR:OH	2.02	0.59
3:L:36:LEU:HD22	3:L:102:SER:OG	2.03	0.59
2:B:176:THR:HG23	2:B:191:SER:CB	2.32	0.59
3:K:67:TRP:CE3	3:L:89:ARG:HG2	2.38	0.59
3:L:139:ARG:HA	3:L:142:ARG:NE	2.18	0.59
1:A:137:LEU:HD23	1:A:138:LEU:C	2.23	0.59
1:A:143:PRO:O	1:A:143:PRO:CD	2.49	0.59
1:C:156:LEU:HD13	1:C:157:GLN:O	2.03	0.58
3:K:89:ARG:HA	3:N:67:TRP:HZ3	1.67	0.58
1:A:50:SER:C	1:A:52:SER:N	2.56	0.58
2:B:195:VAL:HG21	2:B:205:TYR:CE2	2.38	0.58
1:A:115:PRO:HG3	1:A:200:HIS:HB2	1.84	0.58
1:A:199:THR:HG22	1:A:200:HIS:N	2.19	0.58
3:K:138:THR:HA	3:K:141:THR:HG23	1.85	0.58
3:M:127:ARG:NH1	3:M:131:LYS:HB2	2.19	0.58
3:N:147:ARG:NH1	3:N:147:ARG:HB3	2.09	0.58
1:A:189:GLU:HA	1:A:213:ARG:NH1	2.18	0.58
1:A:79:GLN:OE1	1:A:79:GLN:HA	2.03	0.58
1:A:98:VAL:HG21	2:B:47:TRP:CD2	2.38	0.58
1:C:137:LEU:HD23	1:C:138:LEU:C	2.24	0.58
3:M:64:ARG:HG3	3:M:65:ALA:N	2.18	0.58
1:A:24:ARG:HG3	1:A:70:ASP:OD1	2.04	0.58
2:D:79:ALA:C	2:D:80:TYR:HD2	2.07	0.58
3:L:78:TYR:HE2	3:M:71:GLU:HG3	1.68	0.58
1:A:90:GLN:HG3	1:A:99:THR:OG1	2.03	0.58
3:K:131:LYS:O	3:K:135:GLU:HG3	2.03	0.58
3:M:67:TRP:HB3	3:M:81:LEU:HD12	1.86	0.58
1:A:115:PRO:HD2	1:A:203:LEU:CD1	2.34	0.58
3:L:64:ARG:O	3:L:81:LEU:HD11	2.04	0.58
3:L:76:VAL:HG22	3:M:75:THR:HG22	1.84	0.58
1:C:29:VAL:HG13	1:C:92:TYR:HB3	1.85	0.58
2:D:101:SER:O	2:D:107:TRP:HB2	2.03	0.58
3:K:67:TRP:HZ2	3:K:78:TYR:CE1	2.22	0.58
3:N:151:LEU:HA	3:N:154:MET:HB2	1.85	0.58
2:B:12:VAL:HG23	2:B:122:VAL:HG23	1.85	0.58
2:B:51:ILE:HB	2:B:70:ILE:HD13	1.85	0.58
1:C:50:SER:C	1:C:52:SER:N	2.56	0.58
2:D:165:TRP:NE1	2:D:174:VAL:CG2	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:72:THR:HG23	3:K:96:MET:CE	2.34	0.58
1:A:114:ALA:HB1	1:A:203:LEU:HD21	1.86	0.57
2:D:91:THR:HG22	2:D:121:THR:CA	2.29	0.57
1:A:73:LEU:HD12	1:A:74:THR:N	2.18	0.57
2:B:54:TYR:CD1	2:B:54:TYR:C	2.76	0.57
2:D:156:TYR:CE1	2:D:189:LEU:HD22	2.39	0.57
2:D:165:TRP:CZ2	2:D:193:VAL:CG1	2.86	0.57
2:D:91:THR:CG2	2:D:122:VAL:N	2.62	0.57
3:K:76:VAL:CA	3:L:75:THR:HB	2.34	0.57
1:A:33:VAL:HG13	1:A:89:GLN:O	2.05	0.57
2:D:202:THR:HG22	2:D:203:GLN:OE1	2.05	0.57
2:D:212:LYS:H	2:D:213:PRO:HD3	1.68	0.57
3:M:127:ARG:HD3	3:M:127:ARG:C	2.23	0.57
3:N:43:GLY:O	3:N:68:TRP:CZ3	2.57	0.57
1:A:183:LEU:N	1:A:183:LEU:HD12	2.19	0.57
1:C:89:GLN:NE2	2:D:111:LEU:CD2	2.47	0.57
3:K:153:ARG:HA	3:K:153:ARG:NE	2.19	0.57
3:M:141:THR:O	3:M:144:LEU:N	2.37	0.57
1:A:125:GLU:HG2	1:A:128:LYS:HD2	1.85	0.57
2:B:98:ARG:O	2:B:111:LEU:HA	2.05	0.57
1:C:141:PHE:HE2	1:C:177:LEU:H	1.50	0.57
1:C:90:GLN:C	1:C:90:GLN:OE1	2.43	0.57
1:C:90:GLN:OE1	1:C:91:TYR:N	2.37	0.57
3:K:158:ASN:O	3:L:160:ARG:NH2	2.38	0.57
1:C:199:THR:HG22	1:C:200:HIS:N	2.20	0.57
1:C:30:ASN:ND2	1:C:66:ARG:HH21	2.02	0.57
3:M:37:VAL:O	3:M:41:LEU:HG	2.05	0.57
2:B:130:PRO:CD	2:B:155:ASP:O	2.52	0.57
2:D:108:TRP:HE1	3:K:157:ASP:HB2	1.68	0.57
2:D:54:TYR:HD1	2:D:54:TYR:C	2.08	0.57
1:A:79:GLN:HB3	1:A:80:PRO:CD	2.35	0.57
3:N:61:THR:HB	3:N:64:ARG:HG2	1.85	0.57
1:A:138:LEU:HD22	1:A:177:LEU:CB	2.35	0.57
2:B:79:ALA:C	2:B:80:TYR:HD2	2.07	0.57
2:D:166:ASN:HB2	2:D:169:ALA:CB	2.34	0.57
3:K:59:LEU:HD12	3:K:65:ALA:HB1	1.85	0.57
3:L:76:VAL:HA	3:M:75:THR:CB	2.34	0.57
3:M:39:VAL:HG11	3:M:98:ALA:HB3	1.87	0.57
1:A:126:GLN:HG3	2:B:133:PHE:CD2	2.39	0.56
2:B:28:ASN:C	2:B:30:SER:N	2.56	0.56
2:B:67:ARG:NH1	2:B:85:SER:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:VAL:HG21	2:B:86:LEU:CD1	2.35	0.56
2:D:211:HIS:ND1	2:D:213:PRO:HD2	2.20	0.56
1:A:189:GLU:HA	1:A:213:ARG:NH2	2.20	0.56
2:B:206:ILE:HG23	2:B:220:LYS:C	2.25	0.56
1:C:79:GLN:HB3	1:C:80:PRO:CD	2.36	0.56
2:D:28:ASN:C	2:D:30:SER:H	2.07	0.56
2:D:78:THR:HG22	2:D:79:ALA:N	2.18	0.56
3:M:118:GLU:HA	3:M:121:GLN:CD	2.25	0.56
1:A:2:ILE:CD1	1:A:29:VAL:CG2	2.80	0.56
2:D:116:GLN:OE1	2:D:116:GLN:HA	2.05	0.56
2:B:165:TRP:HD1	2:B:170:LEU:O	1.86	0.56
2:B:64:VAL:HG21	2:B:68:PHE:CB	2.36	0.56
3:K:43:GLY:O	3:K:68:TRP:HZ3	1.88	0.56
2:B:149:LEU:HD11	2:B:205:TYR:HD2	1.69	0.56
1:C:144:ARG:O	1:C:144:ARG:CG	2.47	0.56
3:K:25:GLN:NE2	3:K:112:THR:HG23	2.21	0.56
3:K:76:VAL:HA	3:L:75:THR:CA	2.36	0.56
3:L:116:GLY:O	3:L:120:GLN:HG2	2.05	0.56
3:M:76:VAL:HG13	3:N:71:GLU:O	2.06	0.56
3:N:123:GLN:O	3:N:127:ARG:HG2	2.06	0.56
1:A:114:ALA:HB2	1:A:202:GLY:O	2.06	0.56
1:A:107:GLU:HB2	1:A:168:GLN:OE1	2.06	0.56
1:A:35:TRP:CH2	1:A:88:CYS:HB2	2.39	0.56
2:B:2:VAL:CG2	2:B:26:GLY:HA3	2.36	0.56
1:C:115:PRO:HB3	1:C:141:PHE:N	2.21	0.56
1:C:122:PRO:HG3	1:C:188:TYR:CZ	2.40	0.56
1:A:138:LEU:HD21	1:A:148:VAL:CG1	2.36	0.56
2:B:202:THR:HG22	2:B:203:GLN:OE1	2.05	0.56
1:A:98:VAL:CG2	2:B:47:TRP:CD2	2.89	0.56
2:B:83:MET:HE3	2:B:120:VAL:HG11	1.88	0.56
1:C:33:VAL:HA	1:C:90:GLN:HA	1.87	0.56
1:C:71:PHE:CD1	1:C:71:PHE:N	2.74	0.56
3:K:127:ARG:NH1	3:K:131:LYS:HB2	2.21	0.56
3:M:50:ALA:O	3:M:85:THR:HG21	2.06	0.56
3:N:127:ARG:O	3:N:131:LYS:HG3	2.06	0.56
1:A:141:PHE:HE2	1:A:177:LEU:H	1.52	0.56
1:A:50:SER:O	1:A:52:SER:N	2.39	0.56
2:D:156:TYR:CE2	2:D:187:TYR:HB2	2.40	0.56
2:D:54:TYR:CD1	2:D:54:TYR:C	2.78	0.56
3:L:139:ARG:HA	3:L:142:ARG:CD	2.36	0.56
3:L:78:TYR:OH	3:M:72:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:NE2	1:A:103:GLY:HA2	2.20	0.56
2:D:105:TYR:O	2:D:105:TYR:HD1	1.89	0.56
3:M:39:VAL:HG11	3:M:98:ALA:CB	2.36	0.56
1:A:110:ARG:HB2	1:A:110:ARG:HH11	1.71	0.56
1:A:27:GLN:HG3	1:A:28:ASP:N	2.21	0.56
1:C:66:ARG:HH11	1:C:68:GLY:CA	2.18	0.56
2:B:32:TYR:CD2	2:B:100:PRO:HA	2.41	0.55
2:B:79:ALA:C	2:B:80:TYR:CD2	2.80	0.55
2:D:217:LYS:HE2	2:D:219:ASP:OD2	2.06	0.55
3:L:59:LEU:HD12	3:L:65:ALA:CB	2.36	0.55
3:L:61:THR:CG2	3:L:63:PRO:HD2	2.30	0.55
3:M:141:THR:OG1	3:M:142:ARG:N	2.36	0.55
1:A:33:VAL:HA	1:A:90:GLN:HA	1.87	0.55
3:M:87:TRP:CZ3	3:M:90:LEU:HD12	2.40	0.55
3:N:124:GLN:CA	3:N:127:ARG:HG2	2.37	0.55
1:A:90:GLN:OE1	1:A:90:GLN:C	2.44	0.55
2:B:100:PRO:CB	2:B:106:SER:HB2	2.36	0.55
2:D:67:ARG:NH1	2:D:85:SER:O	2.39	0.55
2:D:94:TYR:O	2:D:117:GLY:HA2	2.07	0.55
3:K:72:THR:HG21	3:K:95:VAL:HB	1.87	0.55
3:K:76:VAL:HG22	3:L:75:THR:HG22	1.89	0.55
2:B:130:PRO:HD3	2:B:156:TYR:CB	2.36	0.55
3:K:144:LEU:O	3:K:145:HIS:C	2.43	0.55
1:A:148:VAL:HG21	1:A:179:SER:HB2	1.88	0.55
3:K:29:ALA:HA	3:K:105:LEU:CD2	2.33	0.55
1:A:199:THR:O	1:A:200:HIS:HB2	2.06	0.55
2:B:106:SER:O	2:B:109:VAL:CG2	2.55	0.55
2:B:80:TYR:N	2:B:80:TYR:CD2	2.75	0.55
3:K:65:ALA:HA	3:K:81:LEU:HD13	1.88	0.55
3:M:147:ARG:HH11	3:M:147:ARG:HG3	1.72	0.55
2:D:159:GLU:OE1	2:D:160:PRO:HA	2.07	0.55
3:K:60:ILE:HG13	3:K:61:THR:N	2.21	0.55
3:K:86:LEU:HG	3:K:87:TRP:CE3	2.42	0.55
3:L:133:ALA:O	3:L:137:TYR:HB3	2.07	0.55
3:N:71:GLU:CD	3:N:76:VAL:HB	2.25	0.55
2:D:165:TRP:CD1	2:D:174:VAL:HG21	2.42	0.55
2:D:51:ILE:O	2:D:51:ILE:HG23	2.06	0.55
3:K:110:LEU:O	3:K:114:PHE:HB2	2.06	0.55
3:K:68:TRP:HD1	3:K:81:LEU:O	1.90	0.55
2:B:32:TYR:OH	2:B:98:ARG:NH2	2.40	0.55
1:C:161:SER:HA	1:C:180:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:TRP:HE1	2:D:174:VAL:CG2	2.20	0.55
2:D:79:ALA:C	2:D:80:TYR:CD2	2.80	0.55
3:M:109:ALA:HA	3:M:112:THR:HB	1.89	0.55
2:B:54:TYR:HD1	2:B:54:TYR:C	2.10	0.55
3:L:139:ARG:HG2	3:L:142:ARG:HE	1.72	0.55
1:A:156:LEU:HD13	1:A:157:GLN:O	2.07	0.54
1:A:192:LYS:HA	1:A:213:ARG:HD3	1.86	0.54
2:B:38:ARG:NE	2:B:46:GLU:OE1	2.35	0.54
2:D:51:ILE:HB	2:D:70:ILE:HD13	1.88	0.54
1:A:143:PRO:C	1:A:145:GLU:H	2.11	0.54
2:B:88:ALA:HA	2:B:122:VAL:HG12	1.86	0.54
3:M:115:VAL:O	3:M:115:VAL:HG12	2.07	0.54
3:M:67:TRP:HE1	3:M:78:TYR:HD1	1.54	0.54
3:N:59:LEU:CD1	3:N:68:TRP:HB2	2.38	0.54
3:M:54:ALA:HB2	3:M:85:THR:CG2	2.37	0.54
2:B:51:ILE:O	2:B:51:ILE:HG23	2.07	0.54
2:D:132:VAL:HG22	2:D:153:VAL:HG13	1.90	0.54
3:K:80:ASP:HB3	3:L:82:TYR:CE1	2.42	0.54
3:M:118:GLU:O	3:M:122:GLN:HG3	2.08	0.54
1:A:119:ILE:HG21	1:A:211:PHE:CD2	2.42	0.54
1:C:125:GLU:HG2	1:C:128:LYS:HD2	1.89	0.54
1:C:114:ALA:O	1:C:140:ASN:O	2.24	0.54
1:C:156:LEU:CD1	1:C:157:GLN:O	2.55	0.54
1:C:73:LEU:HD12	1:C:74:THR:H	1.73	0.54
2:D:214:SER:C	2:D:216:THR:H	2.11	0.54
2:D:99:GLN:HG3	2:D:110:ALA:C	2.26	0.54
3:K:150:ARG:HD3	3:L:152:GLU:OE2	2.07	0.54
3:K:32:ALA:HB3	3:K:105:LEU:HD21	1.89	0.54
1:A:143:PRO:HG2	1:A:201:GLN:HB3	1.90	0.54
2:D:162:THR:HG23	2:D:212:LYS:CE	2.34	0.54
2:D:12:VAL:HG21	2:D:86:LEU:CD1	2.38	0.54
3:M:43:GLY:O	3:M:68:TRP:CZ3	2.60	0.54
2:B:156:TYR:HE1	2:B:189:LEU:HD22	1.73	0.54
2:B:205:TYR:O	2:B:222:VAL:N	2.40	0.54
1:C:110:ARG:HB2	1:C:110:ARG:HH11	1.71	0.54
1:C:11:LEU:HD23	1:C:11:LEU:C	2.28	0.54
1:C:144:ARG:CB	1:C:144:ARG:NH1	2.70	0.54
3:L:59:LEU:CD1	3:L:65:ALA:HB1	2.37	0.54
1:A:200:HIS:CG	1:A:201:GLN:N	2.76	0.54
1:C:212:ASN:N	1:C:212:ASN:ND2	2.54	0.54
2:D:32:TYR:OH	2:D:98:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ALA:HB3	1:A:92:TYR:HB2	1.89	0.54
1:A:31:THR:HG22	1:A:66:ARG:HE	1.71	0.54
2:B:29:ILE:O	2:B:29:ILE:HG22	2.07	0.54
2:B:3:GLN:O	2:B:4:LEU:HD23	2.08	0.54
2:D:78:THR:HG22	2:D:79:ALA:O	2.07	0.54
1:A:89:GLN:NE2	2:B:111:LEU:HD23	2.20	0.53
2:B:173:GLY:C	2:B:193:VAL:HG23	2.27	0.53
2:D:165:TRP:CE3	2:D:206:ILE:O	2.61	0.53
1:A:115:PRO:HD3	1:A:200:HIS:HB3	1.88	0.53
1:C:18:ARG:HH12	1:C:76:SER:HB3	1.74	0.53
2:D:70:ILE:O	2:D:70:ILE:CG2	2.57	0.53
3:M:59:LEU:HD12	3:M:65:ALA:HB1	1.88	0.53
1:A:22:THR:OG1	1:A:22:THR:O	2.12	0.53
3:K:127:ARG:NE	3:K:127:ARG:O	2.39	0.53
3:K:155:LEU:HD13	3:N:154:MET:CB	2.34	0.53
3:M:142:ARG:O	3:M:143:ALA:C	2.46	0.53
3:N:46:LEU:HB2	3:N:91:VAL:HG11	1.90	0.53
1:A:200:HIS:CD2	1:A:202:GLY:H	2.27	0.53
1:A:35:TRP:HB2	1:A:48:ILE:HG12	1.89	0.53
1:C:123:SER:OG	1:C:126:GLN:HB2	2.09	0.53
1:C:191:HIS:O	1:C:213:ARG:CD	2.55	0.53
2:D:186:LEU:N	2:D:186:LEU:CD1	2.71	0.53
3:K:155:LEU:HD12	3:N:154:MET:SD	2.49	0.53
3:K:39:VAL:CG1	3:K:95:VAL:HA	2.37	0.53
1:A:144:ARG:CB	1:A:144:ARG:NH1	2.72	0.53
1:A:36:TYR:CE2	1:A:46:LEU:HD13	2.43	0.53
2:B:206:ILE:CG2	2:B:220:LYS:H	2.21	0.53
2:B:206:ILE:HG12	2:B:221:LYS:HA	1.91	0.53
2:D:12:VAL:HG23	2:D:122:VAL:HG23	1.91	0.53
3:K:155:LEU:CD1	3:N:154:MET:CB	2.86	0.53
3:K:64:ARG:HG3	3:K:65:ALA:N	2.23	0.53
3:M:148:PHE:CE1	3:N:148:PHE:HZ	2.27	0.53
3:K:89:ARG:HG2	3:N:67:TRP:CE3	2.44	0.53
3:N:71:GLU:HB3	3:N:77:GLY:H	1.72	0.53
1:A:122:PRO:HG3	1:A:188:TYR:CZ	2.44	0.53
1:A:137:LEU:HD23	1:A:138:LEU:O	2.09	0.53
2:B:206:ILE:HA	2:B:220:LYS:O	2.08	0.53
1:C:199:THR:O	1:C:200:HIS:HB2	2.08	0.53
2:D:165:TRP:HZ2	2:D:193:VAL:CG1	2.21	0.53
3:K:130:GLU:HG3	3:K:131:LYS:N	2.24	0.53
2:B:132:VAL:HA	2:B:152:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:36:LEU:O	3:L:40:LEU:HG	2.08	0.53
3:M:59:LEU:CD1	3:M:65:ALA:HB1	2.39	0.53
2:B:64:VAL:HG21	2:B:68:PHE:CD2	2.43	0.53
2:D:186:LEU:HD12	2:D:186:LEU:N	2.24	0.53
2:D:212:LYS:HD3	2:D:212:LYS:N	2.23	0.53
2:D:22:CYS:C	2:D:78:THR:HG23	2.28	0.53
2:D:2:VAL:HG13	2:D:3:GLN:N	2.24	0.53
2:D:36:TRP:CE2	2:D:81:LEU:HB2	2.43	0.53
1:C:50:SER:O	1:C:52:SER:N	2.42	0.53
1:C:91:TYR:CB	1:C:97:PRO:HB2	2.39	0.53
3:K:141:THR:O	3:K:144:LEU:N	2.40	0.53
3:L:109:ALA:O	3:L:112:THR:HB	2.09	0.53
3:L:154:MET:CB	3:M:156:ASP:OD2	2.56	0.53
1:A:66:ARG:HG2	1:A:68:GLY:H	1.74	0.52
2:B:12:VAL:HG11	2:B:18:LEU:HG	1.91	0.52
2:D:157:PHE:C	2:D:157:PHE:HD2	2.11	0.52
2:D:19:ARG:HG3	2:D:19:ARG:NH1	2.25	0.52
2:D:2:VAL:CG1	2:D:3:GLN:N	2.72	0.52
3:L:68:TRP:HD1	3:L:81:LEU:O	1.92	0.52
3:L:143:ALA:CA	3:L:146:GLU:HB2	2.39	0.52
3:L:67:TRP:HB3	3:L:81:LEU:CD1	2.38	0.52
1:C:32:ALA:CB	1:C:92:TYR:HB2	2.38	0.52
2:D:210:ASN:ND2	2:D:211:HIS:O	2.42	0.52
3:N:23:ALA:C	3:N:25:GLN:H	2.12	0.52
1:C:30:ASN:OD1	3:K:158:ASN:OD1	2.26	0.52
3:K:50:ALA:O	3:K:85:THR:HG21	2.09	0.52
3:M:87:TRP:CZ3	3:M:90:LEU:CD1	2.92	0.52
1:C:126:GLN:HG3	2:D:133:PHE:CD2	2.45	0.52
3:L:147:ARG:CB	3:L:147:ARG:HH11	2.06	0.52
3:M:158:ASN:HD22	3:N:159:ARG:NH1	2.07	0.52
1:A:110:ARG:CG	1:A:142:TYR:CG	2.92	0.52
1:C:61:ARG:HG2	1:C:61:ARG:HH11	1.75	0.52
3:K:91:VAL:O	3:K:91:VAL:HG12	2.08	0.52
1:A:120:PHE:HB3	2:B:135:LEU:HD22	1.92	0.52
1:A:71:PHE:CD1	1:A:71:PHE:N	2.76	0.52
2:B:152:LEU:CD2	2:B:154:LYS:HB2	2.39	0.52
2:D:210:ASN:HA	2:D:217:LYS:HA	1.90	0.52
3:K:109:ALA:HA	3:K:112:THR:HB	1.91	0.52
3:K:79:GLY:HA2	3:K:82:TYR:CE2	2.45	0.52
3:K:80:ASP:HB3	3:L:82:TYR:CZ	2.44	0.52
1:A:148:VAL:HA	1:A:197:GLU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:HG3	1:A:200:HIS:CG	2.44	0.52
1:C:181:LEU:HD13	1:C:181:LEU:C	2.30	0.52
1:C:55:GLU:HB3	1:C:58:VAL:CG2	2.40	0.52
3:K:147:ARG:NH1	3:L:152:GLU:OE2	2.43	0.52
3:M:135:GLU:HA	3:M:138:THR:HB	1.91	0.52
3:M:51:GLU:OE2	3:M:85:THR:HG23	2.09	0.52
1:C:110:ARG:HH21	1:C:113:ALA:HB2	1.75	0.52
2:D:208:ASN:HA	2:D:219:ASP:OD1	2.10	0.52
1:C:92:TYR:HE1	3:K:154:MET:SD	2.33	0.52
1:A:137:LEU:HD23	1:A:138:LEU:N	2.25	0.52
1:A:119:ILE:HG23	1:A:211:PHE:HD2	1.74	0.52
1:A:192:LYS:HG3	1:A:213:ARG:CG	2.39	0.52
1:A:3:GLN:HB2	1:A:26:SER:HB3	1.92	0.52
1:A:6:GLN:NE2	1:A:86:TYR:O	2.37	0.52
2:B:80:TYR:N	2:B:80:TYR:HD2	2.08	0.52
2:B:86:LEU:HB3	2:B:122:VAL:CG2	2.33	0.52
1:C:148:VAL:HG21	1:C:179:SER:HB2	1.92	0.52
1:C:27:GLN:HG3	1:C:28:ASP:N	2.25	0.52
1:A:83:PHE:HE1	1:A:108:ILE:HG13	1.73	0.51
3:K:72:THR:HG23	3:K:96:MET:HE3	1.91	0.51
3:L:58:GLN:C	3:L:60:ILE:H	2.11	0.51
1:C:183:LEU:N	1:C:183:LEU:HD12	2.25	0.51
3:M:71:GLU:HB2	3:M:77:GLY:H	1.76	0.51
1:C:94:TYR:HE1	2:D:59:TYR:OH	1.93	0.51
3:K:118:GLU:HA	3:K:121:GLN:CD	2.31	0.51
3:N:115:VAL:O	3:N:115:VAL:HG12	2.10	0.51
1:A:11:LEU:O	1:A:11:LEU:HD23	2.10	0.51
1:A:61:ARG:O	1:A:75:ILE:HA	2.11	0.51
2:D:12:VAL:HG23	2:D:12:VAL:O	2.09	0.51
3:L:73:ALA:O	3:L:75:THR:HG23	2.09	0.51
3:L:87:TRP:CZ3	3:L:90:LEU:CD1	2.93	0.51
1:A:83:PHE:CE1	1:A:108:ILE:CB	2.92	0.51
2:B:111:LEU:HD22	2:B:111:LEU:H	1.76	0.51
2:D:165:TRP:HZ2	2:D:193:VAL:HG12	1.75	0.51
3:L:130:GLU:O	3:L:134:GLU:HG3	2.11	0.51
1:A:134:VAL:HB	1:A:181:LEU:HB3	1.93	0.51
2:B:94:TYR:O	2:B:117:GLY:HA2	2.10	0.51
2:B:166:ASN:CB	2:B:169:ALA:HB3	2.38	0.51
2:B:152:LEU:HD12	2:B:190:SER:HB3	1.92	0.51
2:B:215:ASN:ND2	2:B:215:ASN:O	2.44	0.51
1:C:83:PHE:CZ	1:C:108:ILE:HG13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:VAL:HG13	2:D:193:VAL:O	2.11	0.51
3:K:138:THR:HG22	3:K:139:ARG:N	2.25	0.51
1:C:28:ASP:OD2	3:L:156:ASP:O	2.29	0.51
2:D:28:ASN:C	2:D:30:SER:N	2.63	0.51
3:L:52:ARG:CZ	3:L:62:TYR:HE1	2.24	0.51
3:K:82:TYR:CZ	3:N:80:ASP:HB3	2.46	0.51
1:A:32:ALA:C	1:A:91:TYR:CE1	2.84	0.51
2:B:193:VAL:O	2:B:193:VAL:CG1	2.56	0.51
1:C:110:ARG:HD3	1:C:173:SER:CB	2.27	0.51
1:C:61:ARG:O	1:C:75:ILE:HA	2.10	0.51
3:K:103:PHE:CE2	3:L:100:ILE:HG12	2.45	0.51
3:K:144:LEU:HD11	3:L:144:LEU:HG	1.93	0.51
2:B:186:LEU:HD12	2:B:186:LEU:N	2.26	0.51
2:B:39:GLN:HB3	2:B:93:VAL:HG23	1.93	0.51
1:C:138:LEU:HD21	1:C:148:VAL:CG1	2.41	0.51
1:C:29:VAL:HG13	1:C:92:TYR:CB	2.40	0.51
2:D:70:ILE:O	2:D:70:ILE:HG23	2.11	0.51
3:M:91:VAL:HG12	3:M:91:VAL:O	2.11	0.51
1:A:110:ARG:HH21	1:A:113:ALA:HB2	1.76	0.50
1:A:119:ILE:HG23	1:A:211:PHE:CD2	2.46	0.50
1:A:6:GLN:OE1	1:A:88:CYS:HB3	2.11	0.50
1:A:80:PRO:HA	1:A:83:PHE:HE2	1.76	0.50
2:B:220:LYS:HA	2:B:220:LYS:HE3	1.92	0.50
2:D:173:GLY:O	2:D:193:VAL:HG23	2.11	0.50
2:D:50:SER:C	2:D:70:ILE:HD13	2.31	0.50
3:K:67:TRP:HB3	3:K:81:LEU:CD1	2.40	0.50
1:A:49:TYR:CD2	2:B:109:VAL:CG1	2.90	0.50
1:A:98:VAL:HG21	2:B:47:TRP:CE2	2.45	0.50
1:C:137:LEU:C	1:C:138:LEU:HD12	2.32	0.50
1:C:143:PRO:HD2	1:C:200:HIS:CE1	2.46	0.50
1:C:134:VAL:HB	1:C:181:LEU:HB3	1.92	0.50
2:D:3:GLN:O	2:D:4:LEU:HD23	2.10	0.50
3:M:135:GLU:O	3:M:139:ARG:HG2	2.10	0.50
1:A:138:LEU:HD22	1:A:177:LEU:HB3	1.94	0.50
1:A:2:ILE:HG21	1:A:90:GLN:HE21	1.75	0.50
2:B:186:LEU:CD1	2:B:186:LEU:N	2.74	0.50
3:K:78:TYR:CD2	3:L:77:GLY:HA2	2.46	0.50
3:K:46:LEU:CB	3:K:91:VAL:HG11	2.40	0.50
1:A:138:LEU:N	1:A:138:LEU:HD12	2.27	0.50
1:A:189:GLU:HA	1:A:213:ARG:CZ	2.41	0.50
2:B:2:VAL:HG22	2:B:27:PHE:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLN:OE1	1:C:92:TYR:N	2.43	0.50
2:D:106:SER:O	2:D:109:VAL:CG2	2.59	0.50
3:K:70:VAL:CG1	3:L:93:VAL:HG22	2.40	0.50
3:L:143:ALA:O	3:L:146:GLU:HB2	2.12	0.50
3:L:38:ILE:O	3:L:38:ILE:HG22	2.12	0.50
3:L:48:VAL:HG22	3:L:59:LEU:HG	1.93	0.50
1:A:148:VAL:HG23	1:A:148:VAL:O	2.10	0.50
1:A:168:GLN:HG3	1:A:175:TYR:CE1	2.47	0.50
1:A:115:PRO:CD	1:A:200:HIS:CD2	2.85	0.50
2:B:111:LEU:CD2	2:B:111:LEU:H	2.23	0.50
2:D:135:LEU:HB2	2:D:150:GLY:O	2.11	0.50
3:M:80:ASP:HB3	3:N:82:TYR:CE1	2.47	0.50
1:A:144:ARG:CB	1:A:144:ARG:HH11	2.18	0.50
1:A:144:ARG:CG	1:A:144:ARG:O	2.46	0.50
1:A:117:VAL:CG2	1:A:198:VAL:HG21	2.41	0.50
1:A:94:TYR:HE2	3:N:145:HIS:CD2	2.29	0.50
3:K:158:ASN:HD21	3:L:160:ARG:HD2	1.75	0.50
3:K:63:PRO:O	3:L:89:ARG:NH1	2.45	0.50
3:L:77:GLY:O	3:M:77:GLY:O	2.29	0.50
3:N:62:TYR:HB2	3:N:63:PRO:HD3	1.92	0.50
1:A:123:SER:OG	2:B:133:PHE:HB3	2.11	0.50
2:B:2:VAL:CG1	2:B:3:GLN:N	2.75	0.50
1:C:14:SER:O	1:C:17:ASP:OD1	2.28	0.50
1:C:148:VAL:HA	1:C:197:GLU:O	2.11	0.50
2:D:149:LEU:H	2:D:149:LEU:HD23	1.76	0.50
3:K:115:VAL:O	3:K:115:VAL:HG12	2.12	0.50
1:A:160:ASN:HD21	1:A:181:LEU:HD21	1.76	0.50
1:A:189:GLU:HA	1:A:213:ARG:HH12	1.75	0.50
2:B:19:ARG:NH1	2:B:19:ARG:HG3	2.25	0.50
2:D:80:TYR:N	2:D:80:TYR:CD2	2.77	0.50
3:K:48:VAL:HG22	3:K:65:ALA:HB1	1.93	0.50
1:C:94:TYR:HE2	3:L:145:HIS:CD2	2.30	0.50
3:M:24:LEU:HA	3:M:27:ARG:HB2	1.94	0.50
3:M:24:LEU:HD12	3:M:27:ARG:HB2	1.94	0.50
3:K:77:GLY:HA3	3:N:76:VAL:O	2.11	0.50
1:C:200:HIS:CD2	1:C:202:GLY:H	2.30	0.50
2:D:2:VAL:CG2	2:D:26:GLY:HA3	2.42	0.50
3:M:127:ARG:NH1	3:M:130:GLU:HG3	2.26	0.50
3:M:48:VAL:HG13	3:M:59:LEU:O	2.12	0.50
1:A:123:SER:OG	1:A:126:GLN:HB2	2.11	0.49
1:A:14:SER:O	1:A:17:ASP:OD1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HD21	2:B:27:PHE:CZ	2.46	0.49
2:D:9:GLY:N	2:D:118:THR:HG21	2.27	0.49
3:K:59:LEU:HD22	3:K:83:PRO:HD3	1.94	0.49
3:K:67:TRP:CZ3	3:L:89:ARG:HA	2.45	0.49
3:N:147:ARG:HH11	3:N:147:ARG:CB	2.14	0.49
1:A:161:SER:HA	1:A:180:THR:O	2.12	0.49
1:C:117:VAL:CG2	1:C:198:VAL:HG21	2.42	0.49
1:C:27:GLN:CG	1:C:28:ASP:N	2.75	0.49
3:K:59:LEU:CD1	3:K:65:ALA:HB1	2.42	0.49
1:A:152:VAL:O	1:A:153:ASP:HB2	2.12	0.49
1:A:168:GLN:NE2	1:A:173:SER:HB3	2.16	0.49
2:B:38:ARG:O	2:B:38:ARG:HG3	2.13	0.49
2:B:50:SER:C	2:B:70:ILE:HD13	2.33	0.49
3:M:48:VAL:HG22	3:M:65:ALA:HB1	1.94	0.49
3:N:57:ALA:O	3:N:60:ILE:HG23	2.12	0.49
1:C:55:GLU:HG3	1:C:56:SER:N	2.27	0.49
2:D:165:TRP:HD1	2:D:170:LEU:O	1.95	0.49
2:D:211:HIS:CE1	2:D:213:PRO:HD2	2.47	0.49
3:K:76:VAL:HA	3:L:75:THR:C	2.33	0.49
3:L:76:VAL:N	3:M:75:THR:HB	2.28	0.49
3:L:91:VAL:O	3:L:91:VAL:HG12	2.12	0.49
3:N:102:SER:O	3:N:106:VAL:HG23	2.11	0.49
1:A:42:LYS:HD2	2:B:116:GLN:NE2	2.26	0.49
2:B:91:THR:HG22	2:B:122:VAL:N	2.20	0.49
1:C:121:PRO:HB3	1:C:211:PHE:CE1	2.47	0.49
3:L:32:ALA:CB	3:L:105:LEU:HD11	2.43	0.49
1:A:120:PHE:CD1	2:B:135:LEU:HB3	2.47	0.49
1:A:21:ILE:O	1:A:72:THR:HG23	2.12	0.49
2:B:122:VAL:HG12	2:B:122:VAL:O	2.11	0.49
1:C:152:VAL:HG22	1:C:157:GLN:HE21	1.78	0.49
1:C:98:VAL:HG21	2:D:47:TRP:CE2	2.47	0.49
3:M:141:THR:O	3:M:144:LEU:HB2	2.13	0.49
3:M:80:ASP:HB3	3:N:82:TYR:CZ	2.48	0.49
1:A:35:TRP:CD1	1:A:48:ILE:HG13	2.48	0.49
1:C:6:GLN:NE2	1:C:86:TYR:O	2.39	0.49
2:D:152:LEU:HD23	2:D:154:LYS:HB2	1.95	0.49
2:B:159:GLU:OE1	2:B:160:PRO:HA	2.12	0.49
2:B:23:ALA:N	2:B:78:THR:HG23	2.28	0.49
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.95	0.49
2:D:80:TYR:N	2:D:80:TYR:HD2	2.11	0.49
3:K:76:VAL:HA	3:L:75:THR:CB	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:78:TYR:HE2	3:L:77:GLY:HA2	1.76	0.49
3:L:25:GLN:NE2	3:L:112:THR:HG23	2.27	0.49
2:B:180:VAL:O	2:B:180:VAL:HG13	2.13	0.49
1:C:138:LEU:N	1:C:138:LEU:CD1	2.76	0.49
1:C:3:GLN:HB2	1:C:26:SER:HB3	1.95	0.49
2:D:12:VAL:HG11	2:D:18:LEU:HG	1.95	0.49
3:K:147:ARG:HE	3:L:145:HIS:CD2	2.31	0.49
3:L:78:TYR:CE2	3:M:71:GLU:HG3	2.47	0.49
1:A:189:GLU:HA	1:A:213:ARG:HH22	1.77	0.48
1:A:114:ALA:CA	1:A:200:HIS:CD2	2.88	0.48
3:M:147:ARG:HG3	3:M:147:ARG:NH1	2.27	0.48
1:A:7:SER:HB3	1:A:22:THR:HG1	1.77	0.48
1:A:117:VAL:HG21	1:A:198:VAL:HG21	1.95	0.48
2:B:212:LYS:HG2	2:B:213:PRO:HD3	1.94	0.48
2:D:4:LEU:HD21	2:D:27:PHE:CZ	2.49	0.48
2:D:68:PHE:HE1	2:D:83:MET:HB3	1.78	0.48
3:L:104:GLY:O	3:L:107:THR:HB	2.13	0.48
3:L:72:THR:HG23	3:L:96:MET:CE	2.42	0.48
3:M:77:GLY:O	3:N:77:GLY:O	2.31	0.48
3:N:48:VAL:HG22	3:N:59:LEU:HG	1.95	0.48
2:B:165:TRP:CZ2	2:B:193:VAL:CG2	2.93	0.48
1:C:9:SER:O	1:C:104:THR:HA	2.13	0.48
2:D:165:TRP:CD1	2:D:174:VAL:CG2	2.97	0.48
2:D:68:PHE:HA	2:D:82:GLN:O	2.14	0.48
3:L:79:GLY:HA2	3:L:82:TYR:CE2	2.48	0.48
3:M:125:PHE:CD1	3:M:125:PHE:C	2.85	0.48
3:M:76:VAL:HG12	3:N:77:GLY:HA3	1.96	0.48
1:A:6:GLN:HB3	1:A:102:GLN:O	2.13	0.48
2:B:206:ILE:HG23	2:B:220:LYS:N	2.29	0.48
2:B:9:GLY:N	2:B:118:THR:HG21	2.28	0.48
1:C:4:MET:HE2	1:C:90:GLN:CB	2.24	0.48
2:D:157:PHE:CG	2:D:158:PRO:CA	2.95	0.48
3:M:44:SER:CB	3:M:66:LEU:HA	2.43	0.48
1:A:96:ALA:HB3	2:B:59:TYR:CE1	2.49	0.48
1:C:73:LEU:HD12	1:C:74:THR:N	2.28	0.48
2:D:27:PHE:CZ	2:D:98:ARG:HD2	2.48	0.48
3:N:59:LEU:HD22	3:N:83:PRO:HD3	1.95	0.48
1:A:153:ASP:HA	1:A:193:VAL:HB	1.96	0.48
2:B:130:PRO:CD	2:B:156:TYR:HA	2.33	0.48
2:B:19:ARG:HH11	2:B:19:ARG:CG	2.27	0.48
2:B:2:VAL:HG13	2:B:3:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LYS:O	1:C:40:PRO:C	2.52	0.48
1:C:18:ARG:NH1	1:C:76:SER:HB3	2.27	0.48
2:D:218:VAL:HG22	2:D:219:ASP:N	2.29	0.48
2:D:68:PHE:CD1	2:D:83:MET:HA	2.49	0.48
3:K:51:GLU:CD	3:K:83:PRO:HA	2.33	0.48
3:M:112:THR:HG22	3:M:113:TRP:HD1	1.78	0.48
3:N:24:LEU:O	3:N:28:ALA:HB2	2.13	0.48
1:A:55:GLU:HG3	1:A:56:SER:N	2.29	0.48
2:B:206:ILE:HG23	2:B:220:LYS:H	1.79	0.48
2:B:54:TYR:CD1	2:B:54:TYR:O	2.57	0.48
2:D:49:ALA:HB2	2:D:60:TYR:HD2	1.78	0.48
3:K:37:VAL:HA	3:K:40:LEU:HD12	1.96	0.48
3:L:136:ALA:HA	3:L:139:ARG:HD2	1.95	0.48
3:M:67:TRP:HZ2	3:M:78:TYR:HE1	1.61	0.48
1:A:96:ALA:HA	1:A:97:PRO:HA	1.74	0.48
1:A:89:GLN:NE2	1:A:98:VAL:HG12	2.26	0.48
2:B:102:TYR:CE2	3:M:150:ARG:HG3	2.48	0.48
2:B:12:VAL:HG23	2:B:12:VAL:O	2.13	0.48
2:B:135:LEU:HB2	2:B:150:GLY:O	2.13	0.48
1:C:168:GLN:NE2	1:C:173:SER:HB3	2.14	0.48
1:C:87:TYR:CD2	2:D:45:LEU:HD12	2.49	0.48
3:L:47:ALA:HB3	3:L:68:TRP:CZ3	2.48	0.48
1:A:18:ARG:HH12	1:A:76:SER:HB3	1.79	0.48
2:B:91:THR:O	2:B:92:ALA:HB2	2.13	0.48
1:A:126:GLN:O	1:A:131:THR:O	2.32	0.47
1:C:169:ASP:HB3	1:C:173:SER:H	1.79	0.47
2:D:130:PRO:CB	2:D:153:VAL:HG12	2.41	0.47
2:D:38:ARG:O	2:D:38:ARG:HG3	2.14	0.47
3:N:93:VAL:O	3:N:93:VAL:HG12	2.13	0.47
2:B:149:LEU:HD23	2:B:193:VAL:O	2.13	0.47
2:D:212:LYS:N	2:D:213:PRO:HD3	2.28	0.47
3:K:158:ASN:HD22	3:L:159:ARG:HH11	1.55	0.47
3:N:127:ARG:CZ	3:N:127:ARG:CB	2.92	0.47
1:A:156:LEU:CD1	1:A:157:GLN:O	2.62	0.47
1:A:115:PRO:HG2	1:A:200:HIS:HB2	1.94	0.47
2:B:49:ALA:CB	2:B:60:TYR:HD2	2.27	0.47
1:C:137:LEU:HD23	1:C:138:LEU:N	2.30	0.47
1:C:33:VAL:CG2	1:C:71:PHE:CE2	2.97	0.47
1:C:30:ASN:OD1	3:K:158:ASN:CG	2.53	0.47
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.97	0.47
2:B:68:PHE:CD1	2:B:83:MET:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:144:LEU:O	3:K:147:ARG:N	2.43	0.47
2:B:49:ALA:HB2	2:B:60:TYR:HD2	1.80	0.47
1:C:200:HIS:CG	1:C:201:GLN:N	2.82	0.47
2:D:165:TRP:CZ3	2:D:207:CYS:CB	2.97	0.47
3:M:159:ARG:HA	3:N:160:ARG:NH2	2.29	0.47
3:M:71:GLU:HB2	3:M:77:GLY:N	2.30	0.47
3:M:79:GLY:HA2	3:M:82:TYR:CE2	2.49	0.47
3:K:151:LEU:CD2	3:N:151:LEU:HD13	2.37	0.47
1:A:138:LEU:N	1:A:138:LEU:CD1	2.77	0.47
1:A:30:ASN:HD21	1:A:31:THR:HG23	1.73	0.47
1:C:66:ARG:HG2	1:C:68:GLY:H	1.79	0.47
3:K:138:THR:CA	3:K:141:THR:HG23	2.43	0.47
3:L:71:GLU:HB2	3:L:77:GLY:H	1.80	0.47
3:M:59:LEU:HD12	3:M:65:ALA:CB	2.44	0.47
1:A:108:ILE:HG22	1:A:173:SER:HB3	1.97	0.47
2:B:215:ASN:CG	2:B:215:ASN:O	2.53	0.47
1:C:192:LYS:HA	1:C:213:ARG:HG2	1.96	0.47
2:D:2:VAL:HG22	2:D:27:PHE:HD2	1.79	0.47
2:D:49:ALA:CB	2:D:60:TYR:HD2	2.28	0.47
2:B:165:TRP:CE2	2:B:170:LEU:HD13	2.49	0.47
2:B:12:VAL:HG21	2:B:86:LEU:HD13	1.96	0.47
2:D:29:ILE:O	2:D:29:ILE:HG22	2.14	0.47
1:C:98:VAL:CG2	2:D:47:TRP:CD2	2.97	0.47
3:L:32:ALA:HB3	3:L:105:LEU:HD11	1.96	0.47
3:M:72:THR:HG23	3:M:96:MET:HE2	1.97	0.47
1:A:181:LEU:C	1:A:181:LEU:HD13	2.34	0.47
1:C:7:SER:HB3	1:C:22:THR:OG1	2.15	0.47
2:D:206:ILE:HG22	2:D:207:CYS:N	2.29	0.47
3:L:124:GLN:HA	3:L:127:ARG:HG2	1.96	0.47
3:N:99:GLY:O	3:N:103:PHE:CD1	2.68	0.47
1:A:110:ARG:CG	1:A:142:TYR:CD2	2.97	0.47
2:B:18:LEU:HD12	2:B:86:LEU:HD11	1.97	0.47
1:C:135:VAL:HG22	1:C:135:VAL:O	2.14	0.47
1:C:185:LYS:HE2	1:C:189:GLU:CD	2.35	0.47
2:D:105:TYR:O	2:D:105:TYR:CD1	2.68	0.47
2:D:98:ARG:NH1	2:D:112:ASP:CG	2.68	0.47
2:D:149:LEU:HD11	2:D:205:TYR:HD2	1.79	0.47
1:A:125:GLU:CG	1:A:128:LYS:HD2	2.45	0.47
1:A:34:ALA:HA	1:A:48:ILE:O	2.15	0.47
2:B:68:PHE:HE1	2:B:83:MET:HB3	1.79	0.47
2:D:176:THR:HG23	2:D:191:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:131:LYS:O	3:M:135:GLU:HG3	2.14	0.47
3:N:52:ARG:CG	3:N:60:ILE:O	2.57	0.47
3:N:68:TRP:HD1	3:N:81:LEU:O	1.98	0.47
1:A:83:PHE:CZ	1:A:108:ILE:HG13	2.51	0.46
2:B:3:GLN:HG3	2:B:25:SER:OG	2.14	0.46
1:C:36:TYR:HA	1:C:45:LYS:O	2.15	0.46
3:K:147:ARG:CG	3:K:147:ARG:NH1	2.75	0.46
3:L:67:TRP:O	3:L:67:TRP:CD1	2.68	0.46
3:L:72:THR:HG23	3:L:96:MET:HE2	1.96	0.46
3:M:72:THR:HG23	3:M:96:MET:CE	2.45	0.46
1:A:168:GLN:HE21	1:A:173:SER:CB	2.20	0.46
3:L:99:GLY:O	3:L:103:PHE:CD1	2.68	0.46
3:L:123:GLN:O	3:L:127:ARG:HG2	2.15	0.46
3:L:43:GLY:O	3:L:68:TRP:HE3	1.97	0.46
3:M:106:VAL:O	3:M:110:LEU:HG	2.16	0.46
2:B:56:SER:HB2	3:M:142:ARG:CD	2.43	0.46
3:N:72:THR:HG21	3:N:95:VAL:HB	1.96	0.46
1:A:137:LEU:C	1:A:137:LEU:HD23	2.36	0.46
1:A:110:ARG:HG2	1:A:142:TYR:CE2	2.50	0.46
1:A:7:SER:HA	1:A:8:PRO:HA	1.62	0.46
1:C:195:ALA:CA	1:C:210:SER:HB2	2.42	0.46
3:K:38:ILE:HG22	3:K:38:ILE:O	2.15	0.46
3:M:153:ARG:HA	3:M:157:ASP:CG	2.36	0.46
1:A:11:LEU:HD23	1:A:11:LEU:C	2.35	0.46
1:A:21:ILE:O	1:A:72:THR:HA	2.16	0.46
1:C:144:ARG:HH11	1:C:144:ARG:CB	2.17	0.46
3:L:48:VAL:HG22	3:L:65:ALA:HB1	1.98	0.46
1:A:30:ASN:HD22	1:A:30:ASN:C	2.18	0.46
1:C:138:LEU:N	1:C:138:LEU:HD12	2.30	0.46
1:C:18:ARG:NH1	1:C:18:ARG:HG3	2.31	0.46
1:C:139:ASN:ND2	2:D:194:THR:HG21	2.31	0.46
3:K:89:ARG:O	3:K:93:VAL:HG23	2.15	0.46
1:A:39:LYS:O	1:A:40:PRO:C	2.54	0.46
1:A:36:TYR:HA	1:A:45:LYS:O	2.15	0.46
1:C:6:GLN:NE2	1:C:103:GLY:HA2	2.29	0.46
2:D:32:TYR:CD2	2:D:100:PRO:HA	2.49	0.46
1:C:137:LEU:CD1	2:D:192:VAL:HG11	2.41	0.46
3:L:70:VAL:HG12	3:M:96:MET:SD	2.56	0.46
3:N:67:TRP:HE1	3:N:78:TYR:HD1	1.62	0.46
3:N:87:TRP:CE3	3:N:87:TRP:HA	2.51	0.46
3:N:87:TRP:HE3	3:N:87:TRP:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:NH1	1:A:76:SER:HB3	2.31	0.46
2:B:2:VAL:HG22	2:B:26:GLY:HA3	1.97	0.46
2:B:70:ILE:CG2	2:B:70:ILE:O	2.62	0.46
1:C:89:GLN:NE2	1:C:98:VAL:HG12	2.26	0.46
3:M:86:LEU:HG	3:M:87:TRP:CE3	2.50	0.46
3:N:127:ARG:HB3	3:N:127:ARG:CZ	2.46	0.46
1:A:110:ARG:NE	1:A:142:TYR:CB	2.74	0.46
1:A:7:SER:HB3	1:A:22:THR:OG1	2.16	0.46
1:A:9:SER:O	1:A:104:THR:HA	2.16	0.46
2:B:155:ASP:HB3	2:B:186:LEU:HD23	1.97	0.46
2:D:106:SER:O	2:D:109:VAL:HG23	2.16	0.46
3:K:73:ALA:C	3:K:75:THR:H	2.20	0.46
3:K:75:THR:HB	3:N:76:VAL:HA	1.96	0.46
2:D:112:ASP:OD1	2:D:113:TYR:N	2.49	0.46
2:D:163:VAL:HB	2:D:176:THR:HG21	1.98	0.46
3:M:117:GLN:O	3:M:121:GLN:HG3	2.16	0.46
3:N:91:VAL:O	3:N:91:VAL:HG12	2.16	0.46
1:A:199:THR:HG22	1:A:200:HIS:H	1.80	0.46
1:A:87:TYR:CD2	2:B:45:LEU:HD12	2.51	0.46
2:D:165:TRP:CZ2	2:D:193:VAL:HG11	2.51	0.46
2:D:18:LEU:HD12	2:D:86:LEU:HD11	1.98	0.46
2:D:165:TRP:CZ2	2:D:193:VAL:HG12	2.50	0.46
1:C:139:ASN:ND2	2:D:194:THR:CG2	2.78	0.46
3:M:58:GLN:C	3:M:60:ILE:H	2.18	0.46
3:N:139:ARG:HA	3:N:142:ARG:CD	2.45	0.46
1:A:195:ALA:CA	1:A:210:SER:HB2	2.44	0.45
2:B:70:ILE:HG23	2:B:70:ILE:O	2.16	0.45
1:C:98:VAL:HG21	2:D:47:TRP:CD2	2.50	0.45
2:D:19:ARG:CG	2:D:19:ARG:HH11	2.28	0.45
3:M:60:ILE:HG13	3:M:61:THR:H	1.80	0.45
3:N:159:ARG:CD	3:N:160:ARG:HG3	2.39	0.45
3:N:48:VAL:CG1	3:N:61:THR:O	2.64	0.45
2:B:156:TYR:CE1	2:B:189:LEU:HD22	2.50	0.45
2:B:211:HIS:O	2:B:214:SER:O	2.34	0.45
3:L:67:TRP:CE3	3:M:89:ARG:HG2	2.50	0.45
3:M:151:LEU:CD2	3:M:151:LEU:C	2.79	0.45
3:K:148:PHE:HB3	3:N:147:ARG:NH1	2.31	0.45
1:A:152:VAL:HG22	1:A:157:GLN:HE21	1.80	0.45
1:A:192:LYS:O	1:A:213:ARG:HG2	2.16	0.45
2:B:112:ASP:OD1	2:B:112:ASP:C	2.55	0.45
2:B:122:VAL:O	2:B:122:VAL:CG1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:THR:HG22	1:C:200:HIS:H	1.80	0.45
1:C:2:ILE:HG21	1:C:90:GLN:HE21	1.82	0.45
3:L:73:ALA:HA	3:L:96:MET:HA	1.99	0.45
3:N:43:GLY:O	3:N:68:TRP:HZ3	1.98	0.45
1:A:110:ARG:HG2	1:A:142:TYR:CG	2.52	0.45
2:B:107:TRP:CH2	3:M:154:MET:CE	2.99	0.45
2:B:149:LEU:H	2:B:149:LEU:HD23	1.81	0.45
2:B:130:PRO:CG	2:B:155:ASP:C	2.82	0.45
1:C:33:VAL:HG21	1:C:71:PHE:CE2	2.52	0.45
1:C:96:ALA:CB	1:C:97:PRO:CD	2.94	0.45
2:D:41:PRO:HD3	2:D:91:THR:O	2.17	0.45
3:M:52:ARG:HH21	3:M:61:THR:HA	1.81	0.45
1:A:108:ILE:O	1:A:142:TYR:HE2	1.98	0.45
1:C:114:ALA:HA	1:C:115:PRO:HD2	1.79	0.45
1:C:141:PHE:O	1:C:175:TYR:N	2.49	0.45
3:L:151:LEU:C	3:L:153:ARG:N	2.68	0.45
3:L:76:VAL:HG13	3:M:71:GLU:O	2.15	0.45
3:N:87:TRP:CZ3	3:N:90:LEU:HD12	2.52	0.45
2:B:38:ARG:O	2:B:38:ARG:CG	2.64	0.45
2:D:157:PHE:HD2	2:D:158:PRO:N	2.11	0.45
2:D:91:THR:O	2:D:92:ALA:HB2	2.16	0.45
3:M:122:GLN:O	3:M:126:VAL:HG12	2.15	0.45
3:N:123:GLN:HA	3:N:126:VAL:HG22	1.99	0.45
3:N:37:VAL:O	3:N:37:VAL:HG12	2.16	0.45
1:A:115:PRO:HG2	1:A:198:VAL:HG12	1.99	0.45
1:A:200:HIS:CG	1:A:201:GLN:H	2.35	0.45
1:A:2:ILE:CG2	1:A:90:GLN:HE21	2.30	0.45
2:B:35:HIS:O	2:B:96:CYS:HA	2.16	0.45
1:C:203:LEU:HA	1:C:203:LEU:HD23	1.83	0.45
3:K:135:GLU:O	3:K:139:ARG:HG2	2.16	0.45
3:M:144:LEU:HD12	3:M:144:LEU:N	2.32	0.45
3:M:153:ARG:HA	3:M:157:ASP:OD1	2.17	0.45
3:M:76:VAL:HG22	3:N:75:THR:CA	2.43	0.45
1:A:11:LEU:HD21	1:A:106:VAL:CG1	2.36	0.45
2:B:130:PRO:CG	2:B:156:TYR:CA	2.93	0.45
1:C:59:PRO:HB3	1:C:61:ARG:CZ	2.45	0.45
3:N:23:ALA:HB3	3:N:26:TRP:HB2	1.99	0.45
3:N:36:LEU:O	3:N:40:LEU:HG	2.17	0.45
1:A:42:LYS:HD2	2:B:116:GLN:HE22	1.80	0.45
2:B:119:LEU:HD21	2:B:121:THR:CG2	2.31	0.45
1:C:11:LEU:HD21	1:C:106:VAL:CG1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:TRP:CG	2:D:170:LEU:HB3	2.49	0.45
3:K:48:VAL:HG12	3:K:60:ILE:O	2.17	0.45
3:L:39:VAL:HG11	3:L:94:VAL:O	2.16	0.45
3:M:150:ARG:HH11	3:M:150:ARG:HG2	1.81	0.45
1:A:137:LEU:C	1:A:138:LEU:HD12	2.37	0.45
1:A:63:SER:OG	1:A:74:THR:HB	2.17	0.45
2:B:125:ALA:HB3	2:B:157:PHE:CZ	2.52	0.45
2:B:166:ASN:HD22	2:B:169:ALA:CB	2.18	0.45
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.99	0.45
1:C:90:GLN:HE22	1:C:93:SER:HB3	1.82	0.45
3:K:25:GLN:NE2	3:K:112:THR:CG2	2.80	0.45
2:B:54:TYR:CE2	2:B:103:HIS:CD2	3.04	0.44
1:C:152:VAL:O	1:C:153:ASP:HB2	2.17	0.44
1:C:30:ASN:ND2	1:C:66:ARG:NH2	2.63	0.44
1:C:87:TYR:CG	2:D:45:LEU:HD12	2.52	0.44
2:D:64:VAL:HG21	2:D:68:PHE:CB	2.47	0.44
3:L:59:LEU:HD22	3:L:83:PRO:HD3	1.99	0.44
3:M:61:THR:CG2	3:M:63:PRO:HD2	2.33	0.44
3:L:74:THR:HB	3:M:75:THR:HG21	1.99	0.44
2:B:155:ASP:HB3	2:B:186:LEU:CD2	2.48	0.44
1:C:7:SER:HA	1:C:8:PRO:HA	1.59	0.44
1:C:90:GLN:HE22	1:C:93:SER:H	1.65	0.44
3:K:103:PHE:CZ	3:L:100:ILE:HG12	2.52	0.44
3:N:73:ALA:C	3:N:75:THR:H	2.19	0.44
1:A:152:VAL:HG12	1:A:194:TYR:CE2	2.53	0.44
1:A:96:ALA:HB3	2:B:59:TYR:CZ	2.52	0.44
2:B:68:PHE:CE1	2:B:83:MET:HB3	2.53	0.44
2:D:38:ARG:HD2	2:D:94:TYR:CZ	2.53	0.44
3:K:150:ARG:HG2	3:K:150:ARG:HH11	1.81	0.44
3:L:127:ARG:O	3:L:131:LYS:HG3	2.17	0.44
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.82	0.44
1:A:83:PHE:CE1	1:A:108:ILE:CG1	3.00	0.44
2:B:173:GLY:O	2:B:193:VAL:HG23	2.17	0.44
2:B:40:ALA:HB1	2:B:41:PRO:CD	2.47	0.44
1:C:125:GLU:CG	1:C:128:LYS:HD2	2.48	0.44
1:C:18:ARG:HG3	1:C:18:ARG:HH11	1.81	0.44
1:C:30:ASN:ND2	1:C:31:THR:CG2	2.68	0.44
2:D:207:CYS:O	2:D:219:ASP:HA	2.18	0.44
2:D:210:ASN:ND2	2:D:217:LYS:HB2	2.32	0.44
3:K:58:GLN:C	3:K:60:ILE:H	2.20	0.44
3:L:87:TRP:HZ3	3:L:90:LEU:CD1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ASN:O	1:A:66:ARG:NH2	2.51	0.44
2:B:212:LYS:N	2:B:213:PRO:HD3	2.32	0.44
1:C:36:TYR:CE2	1:C:46:LEU:HD13	2.52	0.44
2:D:38:ARG:HD3	2:D:48:VAL:HG21	1.99	0.44
2:D:54:TYR:CE2	2:D:103:HIS:CD2	3.05	0.44
3:L:87:TRP:CE3	3:L:87:TRP:HA	2.53	0.44
3:M:99:GLY:O	3:M:103:PHE:CD1	2.71	0.44
3:M:138:THR:CA	3:M:141:THR:HG23	2.48	0.44
2:B:107:TRP:CH2	3:M:154:MET:HE3	2.53	0.44
2:D:12:VAL:HG21	2:D:86:LEU:HD12	2.00	0.44
3:K:119:GLN:NE2	3:K:122:GLN:OE1	2.51	0.44
3:M:87:TRP:HE3	3:M:87:TRP:HA	1.83	0.44
1:A:30:ASN:O	1:A:31:THR:HG22	2.18	0.44
2:B:11:LEU:HD23	2:B:11:LEU:C	2.38	0.44
2:B:19:ARG:NH1	2:B:19:ARG:CG	2.80	0.44
1:C:143:PRO:O	1:C:143:PRO:HD2	2.17	0.44
3:K:59:LEU:HD12	3:K:65:ALA:CB	2.48	0.44
1:A:36:TYR:HE1	1:A:89:GLN:HB3	1.82	0.44
1:C:140:ASN:HB3	1:C:174:THR:OG1	2.17	0.44
3:L:58:GLN:HB3	3:L:64:ARG:HH11	1.83	0.44
3:N:67:TRP:O	3:N:67:TRP:CD1	2.71	0.44
3:M:67:TRP:HZ3	3:N:89:ARG:HA	1.83	0.44
1:A:115:PRO:CG	1:A:200:HIS:CG	3.00	0.44
1:A:6:GLN:NE2	1:A:104:THR:N	2.66	0.44
2:B:166:ASN:O	2:B:167:SER:C	2.53	0.44
2:D:38:ARG:O	2:D:38:ARG:CG	2.66	0.44
3:K:76:VAL:HG22	3:L:75:THR:CA	2.47	0.44
3:L:153:ARG:HG2	3:L:153:ARG:O	2.18	0.44
3:L:87:TRP:HE3	3:L:87:TRP:HA	1.83	0.44
3:L:72:THR:O	3:L:96:MET:HB3	2.18	0.44
3:L:154:MET:CB	3:M:155:LEU:HD13	2.48	0.44
3:M:67:TRP:HZ2	3:M:78:TYR:CE1	2.36	0.44
3:M:87:TRP:CE3	3:M:87:TRP:HA	2.53	0.44
1:A:143:PRO:C	1:A:145:GLU:N	2.70	0.43
1:A:194:TYR:HB2	1:A:211:PHE:CE1	2.53	0.43
1:C:112:VAL:HG12	1:C:113:ALA:N	2.32	0.43
2:D:64:VAL:HG21	2:D:68:PHE:HB2	1.99	0.43
3:K:100:ILE:HA	3:K:100:ILE:HD13	1.84	0.43
3:L:52:ARG:NH2	3:L:62:TYR:CE1	2.86	0.43
3:L:39:VAL:CG1	3:L:94:VAL:O	2.66	0.43
3:M:116:GLY:HA2	3:M:119:GLN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:59:LEU:HD11	3:N:68:TRP:CB	2.48	0.43
2:D:119:LEU:HD21	2:D:121:THR:CG2	2.35	0.43
2:D:180:VAL:O	2:D:180:VAL:HG13	2.18	0.43
2:D:130:PRO:HG3	2:D:211:HIS:HB2	2.00	0.43
3:L:74:THR:O	3:M:75:THR:HG21	2.18	0.43
3:M:74:THR:O	3:N:75:THR:CB	2.66	0.43
1:A:110:ARG:O	1:A:142:TYR:CE1	2.71	0.43
1:A:6:GLN:NE2	1:A:104:THR:H	2.17	0.43
1:C:83:PHE:HE1	1:C:108:ILE:HG13	1.78	0.43
1:C:36:TYR:HE1	1:C:89:GLN:HB3	1.82	0.43
3:K:76:VAL:HA	3:L:75:THR:O	2.18	0.43
3:M:127:ARG:HH12	3:M:130:GLU:HG3	1.83	0.43
3:N:23:ALA:O	3:N:27:ARG:N	2.51	0.43
3:M:78:TYR:CE1	3:N:82:TYR:HB3	2.52	0.43
2:D:166:ASN:OD1	2:D:206:ILE:HB	2.18	0.43
2:D:210:ASN:HD22	2:D:211:HIS:N	2.17	0.43
3:L:110:LEU:HA	3:L:113:TRP:CD1	2.53	0.43
3:N:47:ALA:HB3	3:N:68:TRP:CZ3	2.54	0.43
3:N:59:LEU:HA	3:N:65:ALA:HB2	2.00	0.43
2:B:156:TYR:HE1	2:B:189:LEU:CD2	2.31	0.43
2:D:12:VAL:CG2	2:D:122:VAL:HG23	2.48	0.43
2:D:12:VAL:O	2:D:122:VAL:HA	2.19	0.43
3:L:133:ALA:O	3:L:137:TYR:CB	2.66	0.43
3:M:138:THR:O	3:M:141:THR:HG23	2.19	0.43
3:N:153:ARG:O	3:N:154:MET:C	2.57	0.43
3:N:50:ALA:O	3:N:85:THR:HG21	2.18	0.43
2:B:112:ASP:OD1	2:B:113:TYR:N	2.52	0.43
2:B:49:ALA:HB1	2:B:60:TYR:CD2	2.53	0.43
1:C:142:TYR:CD1	1:C:143:PRO:N	2.86	0.43
2:D:13:GLN:H	2:D:13:GLN:CD	2.20	0.43
2:D:157:PHE:CD2	2:D:158:PRO:CD	3.02	0.43
2:D:19:ARG:CG	2:D:19:ARG:NH1	2.81	0.43
2:D:165:TRP:HE3	2:D:207:CYS:HA	1.83	0.43
2:D:214:SER:O	2:D:214:SER:OG	2.37	0.43
3:M:153:ARG:NH1	3:M:153:ARG:CG	2.42	0.43
3:N:48:VAL:HG22	3:N:65:ALA:CB	2.46	0.43
3:N:67:TRP:HZ2	3:N:78:TYR:CE1	2.35	0.43
1:A:120:PHE:HA	1:A:121:PRO:HD3	1.88	0.43
1:A:150:TRP:O	1:A:156:LEU:HD22	2.18	0.43
1:A:55:GLU:HB3	1:A:58:VAL:HG23	2.00	0.43
2:D:165:TRP:NE1	2:D:170:LEU:HD13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:GLN:HG3	2:D:25:SER:OG	2.19	0.43
1:A:115:PRO:HD2	1:A:203:LEU:HG	2.00	0.43
2:B:200:LEU:HB3	2:B:224:PRO:CG	2.49	0.43
2:B:156:TYR:HB2	2:B:211:HIS:CD2	2.53	0.43
2:B:41:PRO:HD3	2:B:91:THR:O	2.18	0.43
1:C:96:ALA:CB	1:C:97:PRO:HD2	2.48	0.43
2:D:149:LEU:HD12	2:D:222:VAL:CG1	2.39	0.43
2:D:149:LEU:HD23	2:D:193:VAL:O	2.19	0.43
3:K:147:ARG:NH1	3:L:148:PHE:HB3	2.34	0.43
3:K:52:ARG:HH21	3:K:61:THR:HA	1.83	0.43
3:L:67:TRP:HH2	3:M:92:ALA:CB	2.32	0.43
3:L:89:ARG:O	3:L:93:VAL:HG23	2.18	0.43
3:L:39:VAL:HG11	3:L:98:ALA:HB2	2.01	0.43
3:N:124:GLN:HA	3:N:127:ARG:CG	2.43	0.43
1:A:49:TYR:HB2	2:B:109:VAL:HA	2.01	0.43
2:B:13:GLN:HB2	2:B:14:PRO:HD2	2.01	0.43
2:B:210:ASN:HD22	2:B:211:HIS:N	2.16	0.43
1:C:148:VAL:O	1:C:148:VAL:CG2	2.66	0.43
1:C:80:PRO:HA	1:C:83:PHE:HE2	1.84	0.43
3:K:134:GLU:O	3:K:137:TYR:HD2	2.02	0.43
3:L:90:LEU:O	3:L:94:VAL:HG23	2.19	0.43
3:M:49:LEU:HD13	3:M:62:TYR:OH	2.19	0.43
3:M:43:GLY:O	3:M:68:TRP:HE3	1.98	0.43
1:A:18:ARG:HG3	1:A:18:ARG:NH1	2.34	0.43
1:C:160:ASN:HD21	1:C:181:LEU:HD21	1.84	0.43
1:C:91:TYR:CA	1:C:97:PRO:O	2.50	0.43
3:L:48:VAL:HG11	3:L:62:TYR:HA	2.01	0.43
2:B:88:ALA:HA	2:B:122:VAL:HG11	1.92	0.42
1:C:203:LEU:HD13	1:C:207:VAL:H	1.83	0.42
3:K:87:TRP:CZ3	3:K:90:LEU:HD12	2.53	0.42
3:M:87:TRP:CE3	3:M:90:LEU:HD12	2.53	0.42
3:M:89:ARG:O	3:M:93:VAL:HG23	2.19	0.42
3:N:127:ARG:O	3:N:131:LYS:CG	2.67	0.42
2:B:32:TYR:CE2	2:B:100:PRO:HA	2.54	0.42
1:C:190:LYS:HG2	1:C:190:LYS:O	2.19	0.42
3:L:100:ILE:HD12	3:L:100:ILE:HA	1.80	0.42
1:A:108:ILE:CB	1:A:168:GLN:HE22	2.32	0.42
2:B:165:TRP:CG	2:B:170:LEU:HB3	2.54	0.42
2:D:149:LEU:HD23	2:D:149:LEU:N	2.34	0.42
2:D:165:TRP:HA	2:D:165:TRP:CE3	2.53	0.42
2:D:68:PHE:CE1	2:D:83:MET:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:48:VAL:HG11	3:K:62:TYR:HA	2.00	0.42
3:K:67:TRP:CH2	3:L:68:TRP:HZ2	2.24	0.42
3:M:100:ILE:HA	3:M:100:ILE:HD13	1.91	0.42
3:M:48:VAL:HG22	3:M:65:ALA:CB	2.50	0.42
3:N:118:GLU:OE2	3:N:118:GLU:HA	2.19	0.42
1:A:30:ASN:ND2	1:A:31:THR:CG2	2.61	0.42
2:D:87:ARG:C	2:D:122:VAL:HG11	2.38	0.42
2:D:12:VAL:HG21	2:D:86:LEU:HD13	2.02	0.42
2:D:152:LEU:HD12	2:D:190:SER:HB3	2.02	0.42
2:D:91:THR:HG22	2:D:122:VAL:N	2.31	0.42
3:M:45:TYR:HA	3:M:62:TYR:CD2	2.54	0.42
3:N:51:GLU:CG	3:N:83:PRO:HB3	2.49	0.42
1:A:59:PRO:HB3	1:A:61:ARG:CZ	2.47	0.42
2:B:200:LEU:HB3	2:B:224:PRO:HG3	2.02	0.42
2:B:78:THR:CG2	2:B:79:ALA:N	2.81	0.42
1:C:61:ARG:HG2	1:C:61:ARG:NH1	2.35	0.42
2:D:217:LYS:HE2	2:D:219:ASP:CG	2.40	0.42
3:M:76:VAL:HG12	3:N:77:GLY:CA	2.49	0.42
1:A:190:LYS:O	1:A:190:LYS:HG2	2.19	0.42
2:B:69:THR:HB	2:B:82:GLN:HB3	2.01	0.42
1:C:58:VAL:CG1	1:C:59:PRO:HD2	2.50	0.42
3:M:118:GLU:O	3:M:121:GLN:HB2	2.19	0.42
2:B:161:VAL:HG21	2:B:189:LEU:HD21	2.01	0.42
1:C:167:GLU:OE1	1:C:167:GLU:HA	2.20	0.42
2:D:49:ALA:HB1	2:D:60:TYR:CD2	2.54	0.42
3:K:115:VAL:HA	3:K:118:GLU:HB2	2.00	0.42
3:K:54:ALA:HB2	3:K:85:THR:CG2	2.49	0.42
3:M:38:ILE:O	3:M:38:ILE:HG22	2.19	0.42
3:N:127:ARG:HB3	3:N:127:ARG:NH1	2.35	0.42
3:N:64:ARG:HG3	3:N:65:ALA:N	2.35	0.42
1:A:135:VAL:HG22	1:A:135:VAL:O	2.20	0.42
1:A:185:LYS:HE2	1:A:189:GLU:CD	2.40	0.42
1:A:30:ASN:ND2	1:A:30:ASN:C	2.72	0.42
2:B:12:VAL:CG2	2:B:122:VAL:HG23	2.50	0.42
2:B:51:ILE:O	2:B:51:ILE:CG2	2.67	0.42
2:D:165:TRP:HD1	2:D:170:LEU:HB3	1.74	0.42
1:A:89:GLN:HA	1:A:99:THR:O	2.19	0.42
2:D:195:VAL:HG21	2:D:205:TYR:HE2	1.81	0.42
2:D:69:THR:HB	2:D:82:GLN:HB3	2.00	0.42
3:K:76:VAL:HG22	3:L:75:THR:CB	2.49	0.42
3:M:134:GLU:O	3:M:137:TYR:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:139:ARG:HG2	3:N:142:ARG:HE	1.84	0.42
2:B:74:THR:O	2:B:76:LYS:O	2.38	0.42
1:C:192:LYS:HB2	1:C:192:LYS:NZ	2.34	0.42
2:D:51:ILE:O	2:D:51:ILE:CG2	2.67	0.42
3:K:73:ALA:O	3:K:75:THR:HG23	2.20	0.42
3:L:126:VAL:HG23	3:L:127:ARG:N	2.34	0.42
1:A:11:LEU:HD23	1:A:106:VAL:HA	1.97	0.41
1:A:152:VAL:CG2	1:A:157:GLN:HE21	2.33	0.41
1:A:189:GLU:CA	1:A:213:ARG:HH12	2.33	0.41
2:B:105:TYR:CE1	2:B:108:TRP:HB2	2.55	0.41
2:B:68:PHE:HA	2:B:82:GLN:O	2.20	0.41
3:K:137:TYR:O	3:K:140:THR:HB	2.20	0.41
3:K:67:TRP:HE3	3:L:89:ARG:HG2	1.81	0.41
3:K:67:TRP:CZ3	3:L:92:ALA:CB	3.02	0.41
3:M:36:LEU:O	3:M:40:LEU:HG	2.20	0.41
3:M:78:TYR:HB3	3:N:82:TYR:CE2	2.55	0.41
3:N:64:ARG:O	3:N:81:LEU:CD1	2.68	0.41
2:B:154:LYS:HG3	2:B:188:SER:OG	2.20	0.41
2:B:4:LEU:HD21	2:B:27:PHE:HZ	1.83	0.41
1:C:149:GLN:OE1	1:C:197:GLU:HG2	2.19	0.41
2:D:105:TYR:CE1	2:D:108:TRP:HB2	2.55	0.41
2:D:92:ALA:HB3	2:D:94:TYR:HE1	1.84	0.41
3:K:138:THR:O	3:K:141:THR:N	2.53	0.41
1:A:199:THR:CG2	1:A:200:HIS:N	2.83	0.41
1:A:30:ASN:C	1:A:31:THR:CG2	2.88	0.41
1:A:96:ALA:HB1	1:A:97:PRO:HD3	1.55	0.41
2:B:97:ALA:CB	2:B:111:LEU:HD12	2.44	0.41
2:B:98:ARG:NH1	2:B:112:ASP:CG	2.73	0.41
2:B:15:GLY:N	2:B:86:LEU:O	2.28	0.41
1:C:143:PRO:HG2	1:C:201:GLN:CB	2.50	0.41
3:L:67:TRP:HZ2	3:L:78:TYR:CE1	2.39	0.41
3:L:80:ASP:HB3	3:M:82:TYR:CZ	2.55	0.41
3:N:71:GLU:HA	3:N:76:VAL:HB	2.02	0.41
3:N:86:LEU:HG	3:N:87:TRP:CE3	2.56	0.41
3:N:87:TRP:CZ3	3:N:90:LEU:CD1	3.03	0.41
2:B:12:VAL:HG21	2:B:86:LEU:HD12	2.01	0.41
1:C:143:PRO:HD2	1:C:200:HIS:HE1	1.85	0.41
1:C:35:TRP:CH2	1:C:88:CYS:HB2	2.52	0.41
1:C:93:SER:O	1:C:96:ALA:O	2.38	0.41
2:D:209:VAL:O	2:D:218:VAL:N	2.41	0.41
2:D:217:LYS:CE	2:D:219:ASP:OD1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:144:LEU:HD11	3:N:144:LEU:HG	2.03	0.41
1:A:3:GLN:HB2	1:A:26:SER:CB	2.51	0.41
1:A:49:TYR:CB	2:B:109:VAL:HA	2.50	0.41
1:A:98:VAL:HG23	2:B:47:TRP:CD2	2.56	0.41
1:A:192:LYS:HB2	1:A:192:LYS:NZ	2.36	0.41
1:C:15:VAL:CG2	1:C:16:GLY:N	2.83	0.41
1:C:89:GLN:HA	1:C:99:THR:O	2.20	0.41
2:B:156:TYR:CD2	2:B:156:TYR:C	2.93	0.41
1:C:3:GLN:HB2	1:C:26:SER:CB	2.51	0.41
2:D:145:GLY:N	2:D:197:SER:HG	2.18	0.41
2:D:81:LEU:HA	2:D:81:LEU:HD23	1.71	0.41
3:K:135:GLU:O	3:K:138:THR:HB	2.20	0.41
3:K:47:ALA:O	3:K:59:LEU:HD23	2.20	0.41
3:K:71:GLU:HB2	3:K:77:GLY:H	1.86	0.41
3:K:70:VAL:CG1	3:L:96:MET:SD	3.05	0.41
3:L:75:THR:O	3:M:75:THR:O	2.38	0.41
2:B:195:VAL:HG21	2:B:205:TYR:HE2	1.82	0.41
1:C:95:SER:O	2:D:59:TYR:CD2	2.73	0.41
3:L:103:PHE:CE2	3:M:100:ILE:HG13	2.56	0.41
3:L:67:TRP:CH2	3:M:92:ALA:CB	3.04	0.41
3:L:76:VAL:O	3:M:77:GLY:HA3	2.21	0.41
1:A:94:TYR:HE2	3:N:145:HIS:HD2	1.66	0.41
1:A:90:GLN:HE22	1:A:93:SER:HB3	1.86	0.41
2:B:2:VAL:CG2	2:B:27:PHE:HD2	2.33	0.41
3:L:71:GLU:HB2	3:L:77:GLY:N	2.36	0.41
3:M:62:TYR:CB	3:M:63:PRO:HD3	2.40	0.41
3:M:68:TRP:HD1	3:M:81:LEU:O	2.03	0.41
3:N:117:GLN:O	3:N:121:GLN:HG3	2.20	0.41
3:N:62:TYR:N	3:N:63:PRO:CD	2.83	0.41
3:N:67:TRP:HZ2	3:N:78:TYR:HE1	1.67	0.41
1:C:150:TRP:CE2	1:C:181:LEU:HB2	2.56	0.41
3:K:48:VAL:HG22	3:K:59:LEU:HG	2.03	0.41
3:K:72:THR:HG23	3:K:96:MET:HE2	2.01	0.41
3:N:24:LEU:O	3:N:24:LEU:HG	2.21	0.41
1:A:115:PRO:HD2	1:A:203:LEU:HD11	2.03	0.41
2:B:212:LYS:H	2:B:213:PRO:HD3	1.85	0.41
1:C:152:VAL:CG2	1:C:152:VAL:O	2.69	0.41
2:D:13:GLN:HB2	2:D:14:PRO:HD2	2.02	0.41
2:D:159:GLU:HA	2:D:159:GLU:OE1	2.21	0.41
3:N:38:ILE:HG22	3:N:38:ILE:O	2.21	0.41
1:A:87:TYR:CG	2:B:45:LEU:HD12	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:SER:O	2:D:109:VAL:HG22	2.20	0.40
2:D:49:ALA:CB	2:D:60:TYR:CD2	3.04	0.40
3:K:119:GLN:HA	3:K:122:GLN:OE1	2.21	0.40
3:L:64:ARG:HG3	3:L:65:ALA:N	2.36	0.40
1:A:165:VAL:HG12	1:A:177:LEU:HA	2.03	0.40
1:A:18:ARG:HG3	1:A:18:ARG:HH11	1.86	0.40
1:A:58:VAL:CG1	1:A:59:PRO:HD2	2.51	0.40
2:B:130:PRO:CD	2:B:156:TYR:CA	2.93	0.40
2:B:163:VAL:HB	2:B:176:THR:HG21	2.02	0.40
2:D:40:ALA:HB1	2:D:41:PRO:CD	2.50	0.40
3:K:96:MET:HE1	3:N:71:GLU:OE2	2.22	0.40
3:N:49:LEU:C	3:N:51:GLU:H	2.24	0.40
2:D:221:LYS:HE3	2:D:223:GLU:OE2	2.21	0.40
3:L:159:ARG:HD2	3:L:160:ARG:CG	2.46	0.40
3:L:39:VAL:HG11	3:L:98:ALA:CB	2.51	0.40
3:N:46:LEU:CB	3:N:91:VAL:HG11	2.51	0.40
1:A:167:GLU:O	1:A:168:GLN:C	2.60	0.40
1:A:160:ASN:ND2	1:A:181:LEU:CD2	2.84	0.40
2:B:149:LEU:HD12	2:B:222:VAL:CG1	2.51	0.40
1:C:79:GLN:HB3	1:C:81:GLU:OE1	2.21	0.40
2:D:211:HIS:HB3	2:D:214:SER:OG	2.21	0.40
2:D:74:THR:O	2:D:76:LYS:O	2.39	0.40
2:D:68:PHE:HD1	2:D:83:MET:HA	1.86	0.40
3:N:51:GLU:CB	3:N:59:LEU:O	2.64	0.40
1:A:150:TRP:CE2	1:A:181:LEU:HB2	2.57	0.40
2:B:18:LEU:HD12	2:B:86:LEU:CD1	2.51	0.40
2:B:36:TRP:NE1	2:B:81:LEU:HB2	2.37	0.40
2:D:11:LEU:CD1	2:D:157:PHE:CE2	2.86	0.40
3:L:137:TYR:C	3:L:139:ARG:N	2.73	0.40
3:M:78:TYR:CE2	3:N:77:GLY:HA2	2.57	0.40
3:M:72:THR:HG21	3:M:95:VAL:HB	2.03	0.40
3:N:43:GLY:O	3:N:68:TRP:CE3	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/215 (99%)	173 (81%)	34 (16%)	6 (3%)	6	42
1	C	213/215 (99%)	177 (83%)	30 (14%)	6 (3%)	6	42
2	B	215/224 (96%)	185 (86%)	28 (13%)	2 (1%)	20	62
2	D	215/224 (96%)	188 (87%)	25 (12%)	2 (1%)	20	62
3	K	137/166 (82%)	116 (85%)	18 (13%)	3 (2%)	8	46
3	L	137/166 (82%)	125 (91%)	10 (7%)	2 (2%)	12	53
3	M	137/166 (82%)	119 (87%)	17 (12%)	1 (1%)	25	68
3	N	137/166 (82%)	116 (85%)	19 (14%)	2 (2%)	12	53
All	All	1404/1542 (91%)	1199 (85%)	181 (13%)	24 (2%)	11	51

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	PRO
1	A	143	PRO
1	C	115	PRO
1	A	40	PRO
1	C	96	ALA
2	B	26	GLY
1	C	40	PRO
2	D	26	GLY
2	B	160	PRO
2	D	160	PRO
3	K	55	PRO
3	K	73	ALA
1	A	51	ALA
1	A	206	PRO
1	C	97	PRO
1	C	206	PRO
3	M	55	PRO
3	N	73	ALA
3	K	53	GLY
3	L	53	GLY
3	L	55	PRO
3	N	55	PRO
1	C	57	GLY

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Mol	Chain	Res	Type
1	A	57	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/189 (100%)	155 (82%)	34 (18%)	2	15
1	C	189/189 (100%)	155 (82%)	34 (18%)	2	15
2	B	184/188 (98%)	150 (82%)	34 (18%)	2	14
2	D	184/188 (98%)	149 (81%)	35 (19%)	2	13
3	K	108/131 (82%)	94 (87%)	14 (13%)	5	28
3	L	108/131 (82%)	94 (87%)	14 (13%)	5	28
3	M	108/131 (82%)	95 (88%)	13 (12%)	6	31
3	N	108/131 (82%)	95 (88%)	13 (12%)	6	31
All	All	1178/1278 (92%)	987 (84%)	191 (16%)	3	20

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	9	SER
1	A	11	LEU
1	A	15	VAL
1	A	17	ASP
1	A	24	ARG
1	A	30	ASN
1	A	40	PRO
1	A	48	ILE
1	A	49	TYR
1	A	71	PHE
1	A	76	SER
1	A	88	CYS
1	A	90	GLN

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Mol	Chain	Res	Type
1	A	94	TYR
1	A	98	VAL
1	A	99	THR
1	A	107	GLU
1	A	108	ILE
1	A	110	ARG
1	A	116	SER
1	A	123	SER
1	A	126	GLN
1	A	135	VAL
1	A	142	TYR
1	A	144	ARG
1	A	153	ASP
1	A	156	LEU
1	A	158	SER
1	A	170	SER
1	A	177	LEU
1	A	183	LEU
1	A	187	ASP
1	A	210	SER
2	B	13	GLN
2	B	19	ARG
2	B	54	TYR
2	B	56	SER
2	B	58	THR
2	B	64	VAL
2	B	67	ARG
2	B	75	SER
2	B	80	TYR
2	B	81	LEU
2	B	91	THR
2	B	93	VAL
2	B	101	SER
2	B	105	TYR
2	B	106	SER
2	B	109	VAL
2	B	112	ASP
2	B	121	THR
2	B	122	VAL
2	B	126	SER
2	B	127	THR
2	B	131	SER

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Mol	Chain	Res	Type
2	B	152	LEU
2	B	158	PRO
2	B	160	PRO
2	B	167	SER
2	B	170	LEU
2	B	208	ASN
2	B	210	ASN
2	B	211	HIS
2	B	212	LYS
2	B	215	ASN
2	B	216	THR
2	B	220	LYS
1	C	5	THR
1	C	9	SER
1	C	11	LEU
1	C	15	VAL
1	C	17	ASP
1	C	24	ARG
1	C	30	ASN
1	C	40	PRO
1	C	48	ILE
1	C	49	TYR
1	C	70	ASP
1	C	71	PHE
1	C	76	SER
1	C	88	CYS
1	C	90	GLN
1	C	94	TYR
1	C	99	THR
1	C	108	ILE
1	C	110	ARG
1	C	116	SER
1	C	123	SER
1	C	133	SER
1	C	135	VAL
1	C	142	TYR
1	C	144	ARG
1	C	153	ASP
1	C	156	LEU
1	C	158	SER
1	C	170	SER
1	C	177	LEU

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Mol	Chain	Res	Type
1	C	183	LEU
1	C	187	ASP
1	C	210	SER
1	C	212	ASN
2	D	13	GLN
2	D	19	ARG
2	D	54	TYR
2	D	56	SER
2	D	58	THR
2	D	64	VAL
2	D	67	ARG
2	D	75	SER
2	D	80	TYR
2	D	81	LEU
2	D	82	GLN
2	D	91	THR
2	D	93	VAL
2	D	101	SER
2	D	103	HIS
2	D	105	TYR
2	D	106	SER
2	D	109	VAL
2	D	111	LEU
2	D	112	ASP
2	D	121	THR
2	D	122	VAL
2	D	126	SER
2	D	127	THR
2	D	131	SER
2	D	152	LEU
2	D	156	TYR
2	D	157	PHE
2	D	160	PRO
2	D	181	LEU
2	D	208	ASN
2	D	210	ASN
2	D	212	LYS
2	D	215	ASN
2	D	216	THR
3	K	64	ARG
3	K	82	TYR
3	K	87	TRP

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Mol	Chain	Res	Type
3	K	96	MET
3	K	105	LEU
3	K	112	THR
3	K	113	TRP
3	K	127	ARG
3	K	128	HIS
3	K	130	GLU
3	K	137	TYR
3	K	141	THR
3	K	147	ARG
3	K	157	ASP
3	L	26	TRP
3	L	64	ARG
3	L	82	TYR
3	L	87	TRP
3	L	96	MET
3	L	100	ILE
3	L	105	LEU
3	L	112	THR
3	L	117	GLN
3	L	123	GLN
3	L	127	ARG
3	L	146	GLU
3	L	147	ARG
3	L	159	ARG
3	M	87	TRP
3	M	96	MET
3	M	105	LEU
3	M	112	THR
3	M	114	PHE
3	M	119	GLN
3	M	127	ARG
3	M	128	HIS
3	M	130	GLU
3	M	137	TYR
3	M	147	ARG
3	M	153	ARG
3	M	157	ASP
3	N	64	ARG
3	N	82	TYR
3	N	87	TRP
3	N	96	MET

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Mol	Chain	Res	Type
3	N	105	LEU
3	N	112	THR
3	N	117	GLN
3	N	127	ARG
3	N	144	LEU
3	N	146	GLU
3	N	147	ARG
3	N	148	PHE
3	N	151	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	30	ASN
1	A	89	GLN
1	A	154	ASN
1	A	157	GLN
2	B	3	GLN
2	B	39	GLN
2	B	82	GLN
2	B	166	ASN
2	B	208	ASN
2	B	210	ASN
2	B	215	ASN
1	C	3	GLN
1	C	30	ASN
1	C	89	GLN
1	C	154	ASN
1	C	157	GLN
1	C	162	GLN
1	C	168	GLN
1	C	200	HIS
1	C	212	ASN
2	D	3	GLN
2	D	39	GLN
2	D	82	GLN
2	D	208	ASN
2	D	210	ASN
3	K	25	GLN
3	K	119	GLN
3	K	121	GLN

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Mol	Chain	Res	Type
3	K	158	ASN
3	L	25	GLN
3	L	117	GLN
3	L	145	HIS
3	L	158	ASN
3	M	25	GLN
3	M	158	ASN
3	N	117	GLN
3	N	120	GLN
3	N	145	HIS
3	N	158	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/215 (100%)	0.28	9 (4%) 37 29	98, 197, 222, 222	0
1	C	215/215 (100%)	-0.04	2 (0%) 84 77	80, 143, 198, 222	0
2	B	219/224 (97%)	0.14	10 (4%) 33 26	78, 153, 222, 222	0
2	D	219/224 (97%)	-0.09	1 (0%) 90 86	73, 134, 211, 222	0
3	K	139/166 (83%)	0.77	25 (17%) 2 2	78, 222, 222, 222	0
3	L	139/166 (83%)	0.60	14 (10%) 8 7	91, 222, 222, 222	0
3	M	139/166 (83%)	1.09	32 (23%) 1 1	90, 222, 222, 222	0
3	N	139/166 (83%)	0.85	24 (17%) 2 2	106, 222, 222, 222	0
All	All	1424/1542 (92%)	0.37	117 (8%) 12 10	73, 190, 222, 222	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	54	ALA	5.9
3	N	85	THR	5.8
3	L	38	ILE	5.8
3	M	73	ALA	5.7
3	M	79	GLY	5.2
3	K	79	GLY	5.1
3	K	55	PRO	5.0
3	M	22	SER	5.0
3	M	43	GLY	4.7
1	A	148	VAL	4.5
3	M	42	ALA	4.5
3	N	88	GLY	4.3
3	M	72	THR	4.3
3	N	116	GLY	4.3
3	K	54	ALA	4.1
3	L	108	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
3	L	86	LEU	4.1
3	L	116	GLY	4.0
3	M	33	THR	3.9
3	M	86	LEU	3.9
3	K	90	LEU	3.8
3	M	98	ALA	3.8
3	K	127	ARG	3.7
3	K	45	TYR	3.6
3	N	120	GLN	3.6
3	M	87	TRP	3.5
3	M	88	GLY	3.5
1	A	179	SER	3.4
1	A	211	PHE	3.4
3	N	49	LEU	3.3
3	K	130	GLU	3.3
3	M	99	GLY	3.3
3	M	55	PRO	3.2
3	M	95	VAL	3.1
3	N	83	PRO	3.1
3	N	47	ALA	3.1
3	N	50	ALA	3.1
3	L	53	GLY	3.1
3	K	80	ASP	3.0
3	K	32	ALA	3.0
2	B	190	SER	3.0
3	M	47	ALA	3.0
3	L	117	GLN	3.0
3	M	54	ALA	2.9
3	N	86	LEU	2.9
2	B	132	VAL	2.9
3	M	91	VAL	2.9
3	N	26	TRP	2.9
3	L	87	TRP	2.9
3	N	25	GLN	2.9
3	L	114	PHE	2.8
3	K	53	GLY	2.8
3	M	23	ALA	2.8
3	K	87	TRP	2.8
1	C	201	GLN	2.7
3	L	105	LEU	2.7
3	N	110	LEU	2.7
3	N	22	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	196	PRO	2.7
3	L	109	ALA	2.7
3	K	126	VAL	2.7
1	A	149	GLN	2.6
3	M	127	ARG	2.6
2	B	171	THR	2.6
3	N	38	ILE	2.5
3	K	82	TYR	2.5
3	M	31	ALA	2.5
2	B	170	LEU	2.5
3	N	87	TRP	2.5
3	M	41	LEU	2.5
3	K	22	SER	2.5
3	N	128	HIS	2.5
3	L	115	VAL	2.5
3	N	23	ALA	2.5
3	M	28	ALA	2.5
3	N	84	VAL	2.5
3	L	35	LEU	2.4
3	K	28	ALA	2.4
3	M	78	TYR	2.4
3	M	130	GLU	2.4
3	N	107	THR	2.4
3	N	53	GLY	2.4
1	C	113	ALA	2.4
3	K	31	ALA	2.4
3	K	86	LEU	2.4
3	M	92	ALA	2.4
2	B	137	PRO	2.4
3	L	23	ALA	2.3
3	K	128	HIS	2.3
3	M	69	SER	2.3
3	M	113	TRP	2.3
1	A	158	SER	2.3
3	K	135	GLU	2.3
3	K	134	GLU	2.2
3	M	56	GLY	2.2
3	L	85	THR	2.2
1	A	157	GLN	2.2
3	M	34	VAL	2.2
2	B	133	PHE	2.2
2	D	151	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	K	123	GLN	2.2
1	A	194	TYR	2.2
3	M	30	GLY	2.2
1	A	115	PRO	2.2
3	K	131	LYS	2.2
2	B	42	GLY	2.1
2	B	138	SER	2.1
3	N	39	VAL	2.1
3	N	46	LEU	2.1
3	K	85	THR	2.1
3	M	128	HIS	2.1
3	K	56	GLY	2.1
3	K	113	TRP	2.1
1	A	96	ALA	2.0
3	M	37	VAL	2.0
2	B	167	SER	2.0
3	N	55	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.