



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:08 PM UTC

PDB ID : 3PJS / pdb_00003pjs
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

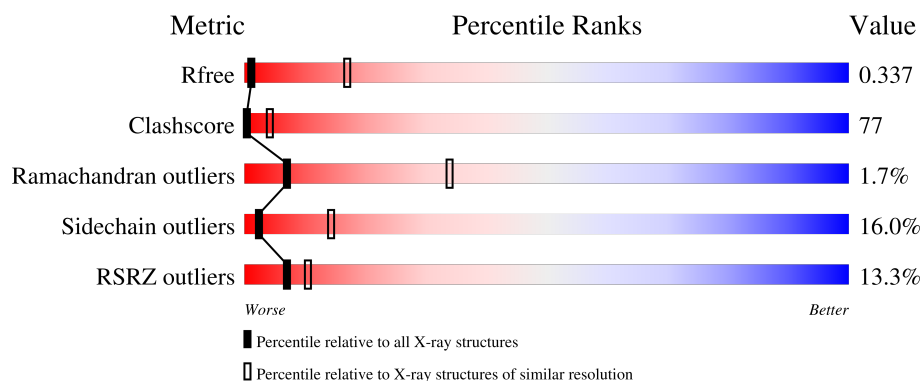
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	215	 11% 25% 52% 18% 5%
1	C	215	 11% 26% 51% 19% .
2	B	224	 8% 27% 50% 17% . .
2	D	224	 8% 29% 49% 16% 5% .
3	K	166	 13% 16% 52% 13% . 16%

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Mol	Chain	Length	Quality of chain
3	L	166	15%13%56%14%16%
3	M	166	17%20%47%14%•16%
3	N	166	17%19%50%14%•16%

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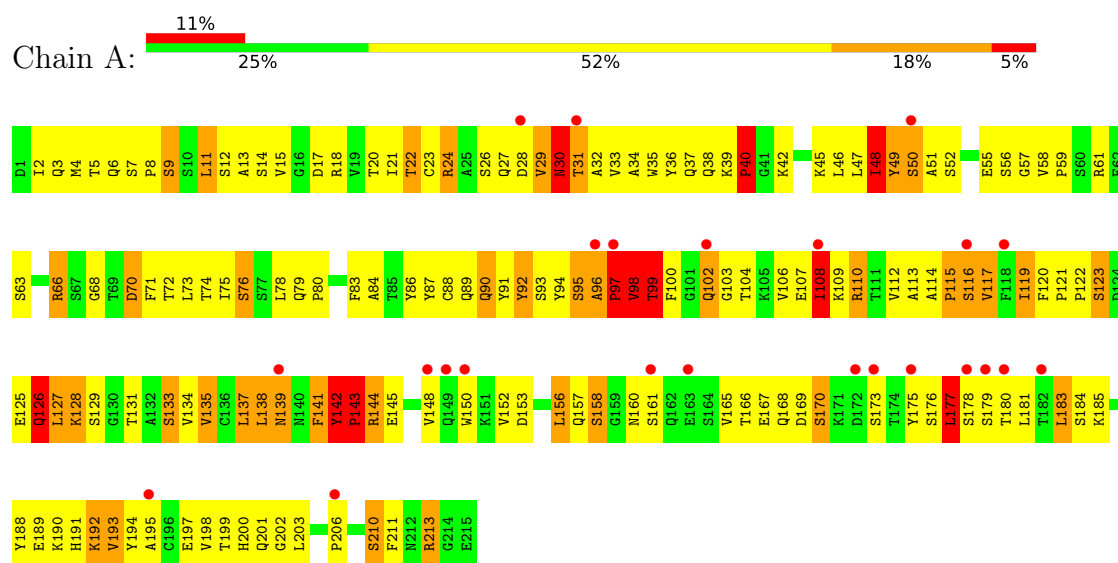
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Chain	Residue	Modelled	Actual	Comment	Reference
N	117	GLN	ARG	engineered mutation	UNP P0A334
N	120	GLN	GLU	engineered mutation	UNP P0A334
N	121	GLN	ARG	engineered mutation	UNP P0A334
N	122	GLN	ARG	engineered mutation	UNP P0A334
N	123	GLN	GLY	engineered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

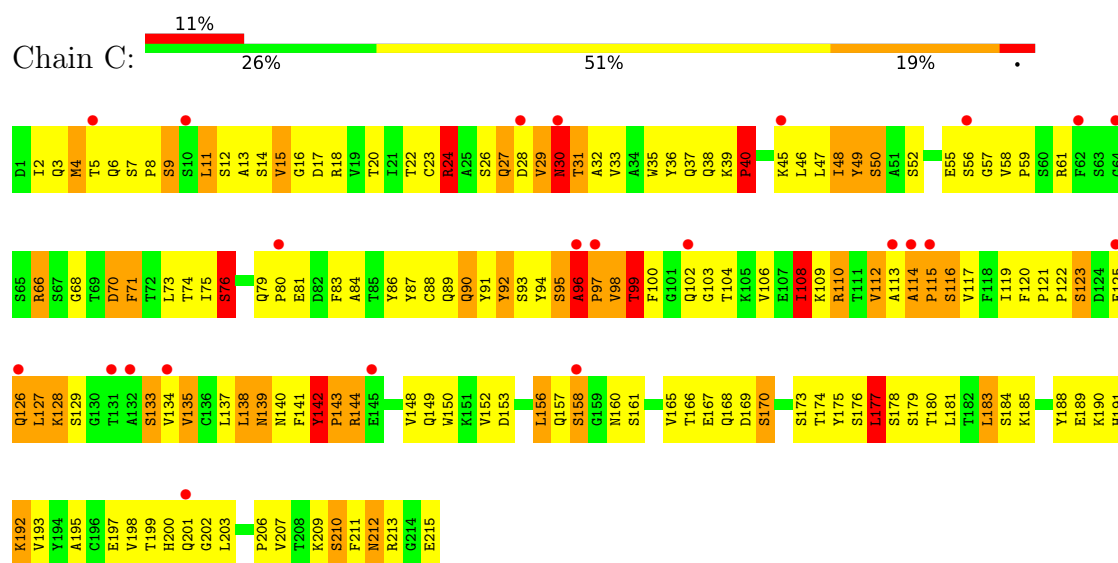
3 Residue-property plots [i](#)

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

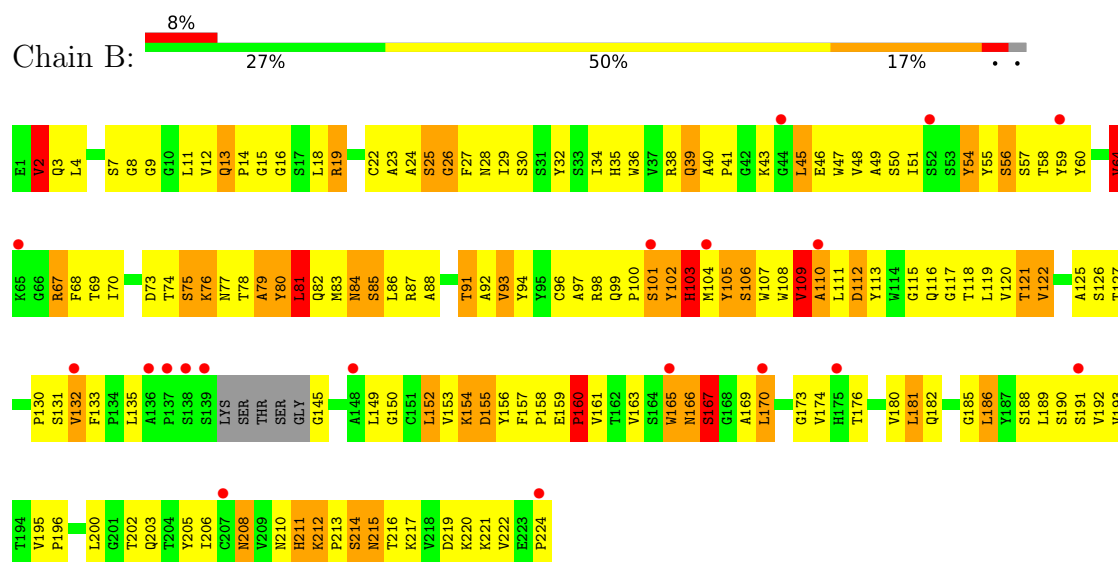
• Molecule 1: FAB light chain



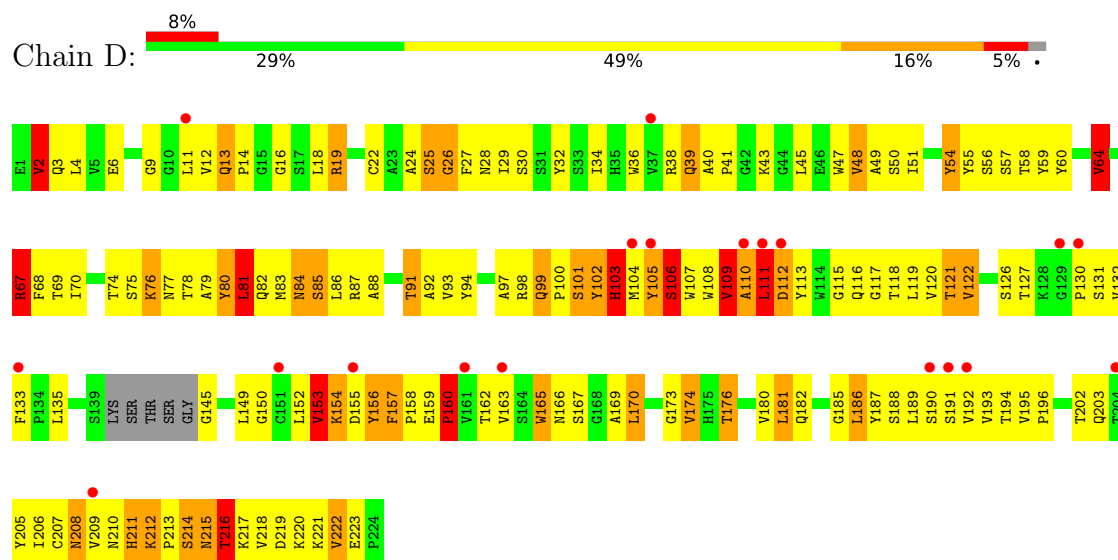
• Molecule 1: FAB light chain



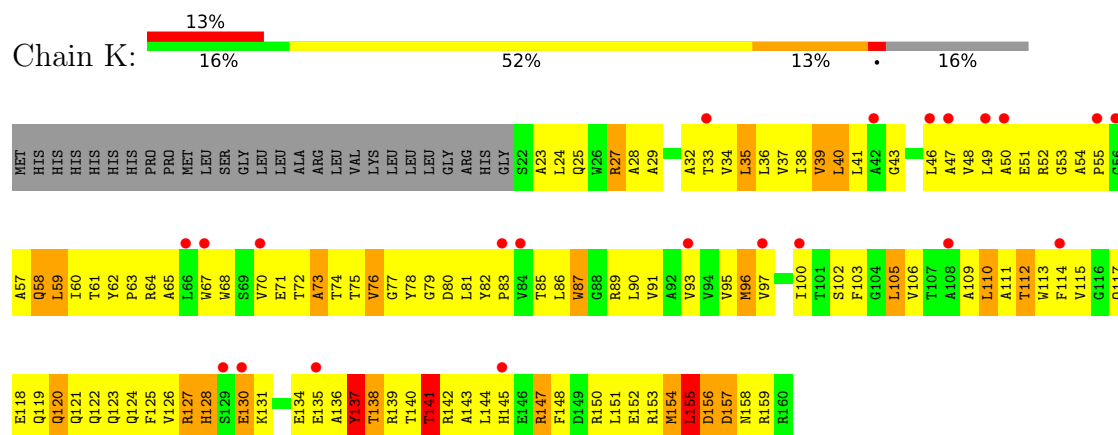
• Molecule 2: FAB heavy chain



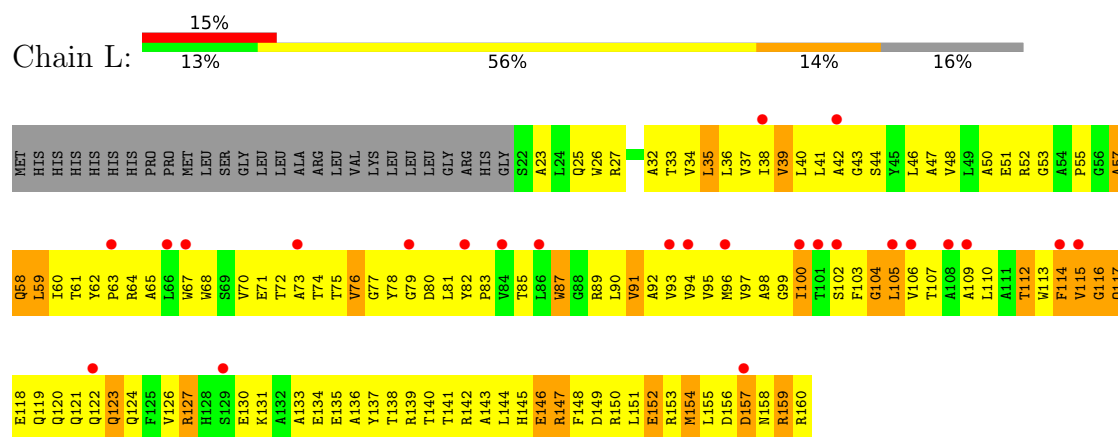
• Molecule 2: FAB heavy chain



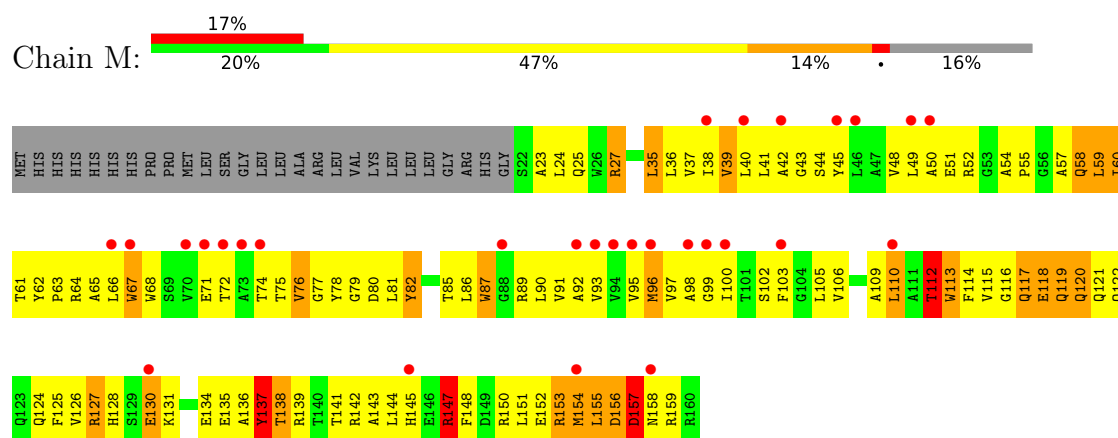
• Molecule 3: Voltage-gated potassium channel



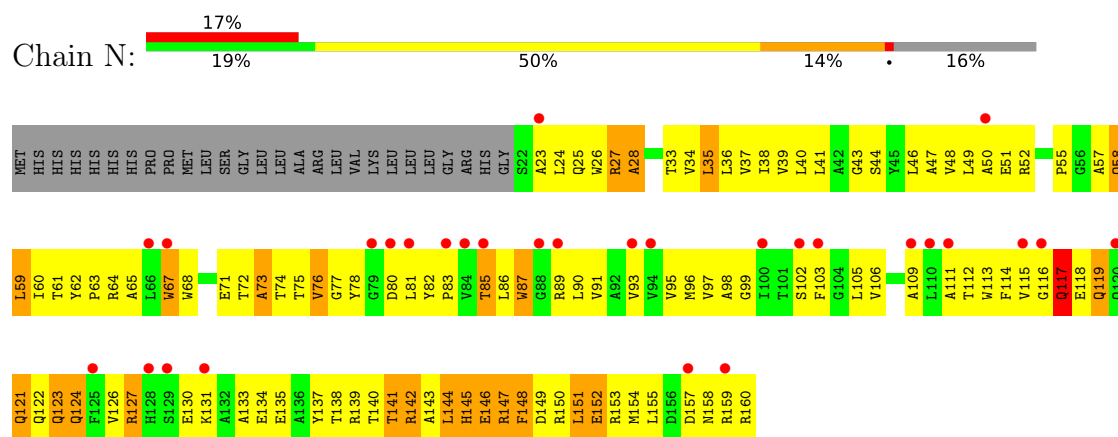
• Molecule 3: Voltage-gated potassium channel



• 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 40.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	82.4 (40.00-3.80) 82.3 (40.00-3.80)	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	1513 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	135.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 197.5	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	0.87	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 i

5.1 Standard geometry i

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	0.92	8/1694 (0.5%)	2.07	42/2300 (1.8%)
1	C	0.90	5/1694 (0.3%)	1.69	36/2300 (1.6%)
2	B	1.06	6/1698 (0.4%)	1.63	42/2319 (1.8%)
2	D	1.04	4/1698 (0.2%)	1.77	45/2319 (1.9%)
3	K	0.79	1/1113 (0.1%)	1.39	20/1517 (1.3%)
3	L	0.86	0/1113	1.37	22/1517 (1.5%)
3	M	0.79	1/1113 (0.1%)	1.37	22/1517 (1.5%)
3	N	0.84	2/1113 (0.2%)	1.36	23/1517 (1.5%)
All	All	0.92	27/11236 (0.2%)	1.64	252/15306 (1.6%)

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 (27) 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
2	D	103	HIS	CA-C	-10.53	1.45	1.52
2	B	154	LYS	C-O	-9.79	1.11	1.24
1	A	115	PRO	CA-C	9.72	1.66	1.52
2	B	166	ASN	C-O	-9.09	1.10	1.23
1	A	116	SER	N-CA	8.76	1.57	1.46
1	A	115	PRO	C-N	8.49	1.45	1.33
1	C	48	ILE	CA-CB	-7.69	1.44	1.54
2	B	103	HIS	CA-C	-7.05	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	CA-CB	-6.80	1.45	1.54
2	D	104	MET	CA-C	-6.49	1.48	1.52
3	M	60	ILE	CA-CB	6.13	1.61	1.54
1	C	142	TYR	CA-C	-6.09	1.45	1.52
2	B	110	ALA	CA-C	-5.98	1.45	1.53
1	C	98	VAL	CA-CB	-5.97	1.46	1.54
2	B	85	SER	CA-C	-5.67	1.46	1.53
2	B	48	VAL	CA-CB	-5.58	1.49	1.55
1	C	4	MET	SD-CE	-5.55	1.65	1.79
1	A	142	TYR	C-O	-5.54	1.17	1.24
1	A	98	VAL	CA-CB	-5.48	1.47	1.54
2	D	48	VAL	CA-CB	-5.26	1.50	1.55
3	K	141	THR	CA-CB	5.25	1.61	1.53
3	N	85	THR	CA-CB	5.24	1.60	1.53
1	C	112	VAL	CA-CB	-5.12	1.49	1.54
1	A	142	TYR	CA-CB	-5.12	1.45	1.53
3	N	76	VAL	CA-CB	5.02	1.60	1.54
2	D	85	SER	CA-C	-5.01	1.47	1.53

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	TYR	CA-C-N	36.10	164.97	119.84
1	A	142	TYR	C-N-CA	36.10	164.97	119.84
2	D	154	LYS	N-CA-C	24.15	144.04	112.88
1	C	29	VAL	N-CA-C	-22.77	75.55	108.80
1	A	96	ALA	CB-CA-C	-22.09	81.62	110.34
1	A	96	ALA	N-CA-C	20.72	154.93	108.93
2	D	109	VAL	N-CA-C	-18.94	79.62	108.97
1	A	29	VAL	N-CA-C	-18.84	80.00	109.20
1	A	96	ALA	C-N-CD	-17.89	81.25	120.60
1	C	50	SER	N-CA-C	-17.43	84.69	110.48
1	A	95	SER	N-CA-C	-16.82	79.43	108.20
1	A	50	SER	N-CA-C	-16.57	84.02	110.20
2	D	154	LYS	CB-CA-C	-15.47	84.58	110.72
1	A	142	TYR	C-N-CD	-15.22	62.58	125.00
1	C	116	SER	N-CA-CB	-14.90	86.13	110.41
2	B	109	VAL	N-CA-C	-14.59	94.14	110.05
2	D	214	SER	N-CA-C	-14.37	85.81	109.24
3	K	156	ASP	N-CA-CB	14.29	134.64	110.49
3	M	156	ASP	N-CA-C	-14.14	96.49	113.88
1	C	142	TYR	CA-C-N	13.76	160.01	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	TYR	C-N-CA	13.76	160.01	127.00
1	C	142	TYR	C-N-CD	-13.56	90.77	120.60
1	A	29	VAL	CB-CA-C	13.39	130.34	111.19
2	B	103	HIS	N-CA-C	13.32	130.74	111.96
2	D	55	TYR	N-CA-C	-13.11	91.57	110.59
2	D	155	ASP	N-CA-C	-13.00	84.87	107.49
2	B	55	TYR	N-CA-C	-12.98	91.76	110.59
1	A	22	THR	CB-CA-C	-12.55	89.32	110.16
1	A	102	GLN	N-CA-C	-12.10	91.81	109.96
2	B	154	LYS	N-CA-C	12.08	128.15	113.41
1	C	23	CYS	N-CA-C	-11.86	90.64	108.79
3	L	157	ASP	N-CA-C	-11.83	99.05	114.31
2	B	57	SER	N-CA-C	11.82	128.01	110.52
2	B	214	SER	N-CA-C	-11.79	91.21	109.95
2	D	109	VAL	CB-CA-C	11.72	129.00	111.31
1	C	177	LEU	CB-CA-C	-11.65	90.31	109.53
2	B	166	ASN	CB-CA-C	-11.63	94.03	111.70
2	B	165	TRP	N-CA-C	11.47	123.77	111.03
1	C	102	GLN	N-CA-C	-11.31	92.99	109.96
1	C	96	ALA	N-CA-C	-10.96	85.59	109.81
2	B	153	VAL	N-CA-C	-10.93	91.19	107.37
2	D	211	HIS	N-CA-C	-10.71	92.20	109.76
2	D	57	SER	N-CA-C	10.69	126.99	110.42
1	C	29	VAL	CB-CA-C	10.65	126.58	110.82
1	C	95	SER	CB-CA-C	10.47	131.25	110.42
2	D	102	TYR	CA-C-N	-10.42	110.04	122.44
2	D	102	TYR	C-N-CA	-10.42	110.04	122.44
1	C	23	CYS	CB-CA-C	10.04	129.30	110.62
2	D	103	HIS	N-CA-C	9.88	126.04	111.02
2	D	76	LYS	N-CA-C	-9.49	95.16	109.86
3	N	157	ASP	N-CA-C	-9.47	100.25	114.64
1	A	23	CYS	N-CA-CB	-9.46	95.71	110.65
2	B	76	LYS	N-CA-C	-9.44	95.22	109.86
1	C	139	ASN	N-CA-C	9.34	125.10	112.68
2	B	105	TYR	N-CA-C	-9.26	98.56	113.19
3	N	59	LEU	N-CA-C	-9.25	98.88	111.55
1	A	139	ASN	N-CA-C	9.19	124.90	112.68
2	D	110	ALA	N-CA-C	9.09	124.89	113.43
3	N	76	VAL	N-CA-C	-9.07	101.89	110.42
1	A	98	VAL	N-CA-C	-8.79	95.53	108.89
1	A	138	LEU	N-CA-C	-8.76	95.49	109.59
3	M	76	VAL	N-CA-C	-8.73	102.80	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	59	LEU	N-CA-C	-8.72	103.18	113.21
1	A	66	ARG	CG-CD-NE	8.65	131.03	112.00
1	C	66	ARG	CG-CD-NE	8.65	131.03	112.00
1	C	138	LEU	N-CA-C	-8.56	95.81	109.59
1	A	97	PRO	CA-N-CD	8.46	123.34	111.50
3	K	156	ASP	N-CA-C	-8.37	92.98	110.80
2	D	165	TRP	N-CA-C	8.33	121.98	111.24
2	D	111	LEU	N-CA-C	-8.28	90.23	107.37
2	B	211	HIS	N-CA-C	-8.18	94.21	108.20
2	D	103	HIS	CA-C-N	-8.13	112.77	122.44
2	D	103	HIS	C-N-CA	-8.13	112.77	122.44
2	B	155	ASP	N-CA-C	-8.06	93.67	108.02
1	A	177	LEU	CB-CA-C	-8.02	95.79	109.83
3	M	59	LEU	N-CA-C	-7.98	103.99	112.93
2	D	105	TYR	N-CA-CB	7.97	123.96	110.49
1	C	30	ASN	N-CA-C	-7.89	94.00	110.80
3	K	76	VAL	N-CA-C	-7.87	103.02	110.42
2	B	110	ALA	N-CA-C	-7.82	97.98	109.63
1	A	143	PRO	N-CA-C	-7.80	96.41	112.47
2	D	105	TYR	N-CA-C	-7.80	94.19	110.80
3	K	137	TYR	N-CA-C	-7.78	102.75	111.07
2	D	216	THR	N-CA-C	7.66	121.72	109.24
2	D	106	SER	N-CA-C	7.65	121.71	112.38
3	K	120	GLN	N-CA-C	-7.57	103.11	111.36
2	B	102	TYR	CA-C-N	-7.54	110.74	122.42
2	B	102	TYR	C-N-CA	-7.54	110.74	122.42
2	D	170	LEU	N-CA-C	-7.48	94.83	107.99
1	C	114	ALA	C-N-CD	-7.46	94.42	125.00
3	M	156	ASP	CB-CA-C	7.36	120.94	109.03
3	K	154	MET	N-CA-C	-7.35	103.58	112.54
3	L	44	SER	N-CA-C	-7.29	102.66	112.94
1	C	30	ASN	N-CA-CB	-7.29	98.17	110.49
3	L	116	GLY	N-CA-C	-7.27	105.65	114.66
3	K	59	LEU	N-CA-C	-7.23	104.84	112.93
2	D	222	VAL	N-CA-C	7.18	113.89	106.21
1	C	178	SER	N-CA-CB	-7.14	98.45	110.80
1	C	126	GLN	N-CA-C	-7.14	104.57	113.28
3	L	23	ALA	N-CA-C	-7.13	98.39	108.23
3	L	35	LEU	N-CA-C	-7.11	104.60	113.28
1	C	129	SER	N-CA-C	-7.11	97.71	109.80
3	N	111	ALA	N-CA-C	-7.08	104.53	113.02
1	A	30	ASN	N-CA-C	-6.99	95.90	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	ALA	CB-CA-C	6.98	119.30	108.61
3	L	33	THR	N-CA-C	-6.96	104.94	113.50
3	L	76	VAL	N-CA-C	-6.94	104.01	110.53
1	A	126	GLN	N-CA-C	-6.93	104.83	113.28
1	A	117	VAL	N-CA-C	6.84	118.98	109.55
1	C	95	SER	N-CA-C	-6.80	96.32	110.80
2	B	167	SER	N-CA-CB	6.79	121.75	111.70
3	K	155	LEU	N-CA-C	6.77	125.22	110.80
3	N	58	GLN	N-CA-C	-6.77	104.23	113.30
2	D	2	VAL	N-CA-C	6.71	120.38	109.78
3	K	24	LEU	N-CA-C	-6.68	103.52	112.94
1	C	108	ILE	N-CA-C	6.65	118.62	108.71
1	A	129	SER	N-CA-C	-6.64	98.52	109.80
3	L	58	GLN	N-CA-C	-6.63	104.91	114.12
2	D	170	LEU	N-CA-CB	6.61	120.20	110.35
2	B	152	LEU	CB-CA-C	6.58	119.55	110.34
1	A	22	THR	N-CA-C	6.57	119.12	108.41
2	D	81	LEU	N-CA-C	-6.54	98.58	109.24
3	M	157	ASP	N-CA-C	-6.50	104.11	111.07
3	L	42	ALA	N-CA-C	-6.47	103.81	112.94
1	A	97	PRO	N-CA-CB	-6.46	95.49	102.60
3	L	115	VAL	N-CA-C	-6.46	105.27	113.22
3	M	155	LEU	N-CA-C	6.42	124.47	110.80
1	A	127	LEU	N-CA-C	-6.39	104.63	112.88
1	C	127	LEU	N-CA-C	-6.35	104.68	112.88
3	M	120	GLN	N-CA-C	-6.34	104.46	111.82
1	A	116	SER	CB-CA-C	-6.32	100.38	111.05
2	D	99	GLN	CA-C-N	-6.32	114.15	120.21
2	D	99	GLN	C-N-CA	-6.32	114.15	120.21
3	L	27	ARG	N-CA-C	-6.32	105.21	113.17
3	M	147	ARG	N-CA-C	6.29	118.14	111.28
2	D	110	ALA	N-CA-CB	6.28	121.19	110.51
2	B	2	VAL	N-CA-C	6.27	119.69	109.78
1	C	143	PRO	CA-N-CD	-6.25	102.75	111.50
2	D	25	SER	N-CA-C	6.25	119.52	109.83
2	D	84	ASN	N-CA-C	6.24	121.23	112.93
2	B	39	GLN	N-CA-C	-6.24	100.12	110.17
3	M	136	ALA	N-CA-C	-6.24	104.02	111.69
2	B	154	LYS	O-C-N	-6.22	113.52	122.36
2	B	81	LEU	N-CA-C	-6.22	99.11	109.24
1	A	213	ARG	N-CA-C	6.18	119.45	110.42
3	K	40	LEU	N-CA-C	-6.18	106.06	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	39	GLN	N-CA-C	-6.17	99.64	109.76
1	C	128	LYS	N-CA-C	-6.13	105.84	113.38
3	N	27	ARG	N-CA-C	-6.12	104.98	112.88
1	A	141	PHE	N-CA-C	6.11	118.69	109.41
1	A	30	ASN	N-CA-CB	-6.10	100.19	110.49
2	B	84	ASN	N-CA-C	6.08	120.51	112.72
2	B	25	SER	N-CA-C	6.07	119.24	109.83
3	N	35	LEU	N-CA-C	-6.07	105.83	113.18
2	B	64	VAL	CA-C-N	-6.05	114.27	121.90
2	B	64	VAL	C-N-CA	-6.05	114.27	121.90
3	M	137	TYR	N-CA-C	-6.04	104.39	110.97
3	N	67	TRP	N-CA-C	-6.03	105.97	113.15
3	L	121	GLN	N-CA-C	-6.02	105.20	112.54
3	M	82	TYR	N-CA-C	6.01	113.53	108.13
3	M	35	LEU	N-CA-C	-5.99	105.97	113.28
1	C	193	VAL	N-CA-C	5.97	114.95	106.53
1	A	108	ILE	N-CA-C	5.95	117.57	108.71
3	K	33	THR	N-CA-C	-5.94	106.08	113.38
3	K	35	LEU	N-CA-C	-5.92	106.06	113.28
3	N	121	GLN	N-CA-C	-5.92	105.55	112.89
1	A	66	ARG	CB-CG-CD	-5.90	97.72	111.30
3	N	149	ASP	N-CA-C	-5.90	105.93	113.01
2	B	219	ASP	N-CA-C	-5.88	101.31	110.42
3	N	133	ALA	N-CA-C	-5.87	105.43	113.30
3	N	44	SER	N-CA-C	-5.85	105.73	112.92
3	M	27	ARG	N-CA-C	-5.84	105.73	112.92
3	K	27	ARG	N-CA-C	-5.81	105.38	112.88
1	A	23	CYS	N-CA-C	5.77	118.12	108.02
3	L	154	MET	N-CA-C	-5.76	104.97	112.23
3	K	117	GLN	N-CA-C	-5.76	104.45	112.45
2	B	76	LYS	CA-C-N	-5.72	115.36	123.03
2	B	76	LYS	C-N-CA	-5.72	115.36	123.03
1	A	178	SER	N-CA-CB	-5.71	101.22	110.81
1	A	193	VAL	N-CA-C	5.69	114.56	106.53
2	B	48	VAL	CB-CA-C	-5.68	106.88	111.71
2	B	99	GLN	CA-C-N	-5.67	113.75	120.11
2	B	99	GLN	C-N-CA	-5.67	113.75	120.11
2	D	76	LYS	CA-C-N	-5.67	115.43	123.03
2	D	76	LYS	C-N-CA	-5.67	115.43	123.03
1	A	128	LYS	N-CA-C	-5.64	106.06	113.17
1	C	24	ARG	N-CA-C	-5.63	99.12	108.75
2	D	67	ARG	N-CA-C	5.60	120.12	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	115	GLY	N-CA-C	-5.60	104.90	112.57
3	M	118	GLU	N-CA-C	-5.59	105.72	112.54
3	K	136	ALA	N-CA-C	-5.57	105.29	111.36
3	L	149	ASP	N-CA-C	-5.57	106.33	113.01
2	B	34	ILE	N-CA-C	5.56	115.86	107.80
2	D	174	VAL	N-CA-C	5.56	115.79	107.51
3	K	110	LEU	N-CA-C	-5.56	105.85	113.30
2	B	115	GLY	N-CA-C	-5.55	104.97	112.57
3	K	34	VAL	N-CA-C	-5.54	105.24	113.39
2	B	48	VAL	N-CA-C	5.53	116.68	111.48
2	B	132	VAL	CB-CA-C	-5.53	103.96	111.15
3	M	154	MET	N-CA-C	-5.52	105.21	112.72
3	M	110	LEU	N-CA-C	-5.52	105.76	112.88
1	C	98	VAL	N-CA-C	5.49	117.22	108.87
1	A	158	SER	N-CA-C	5.48	118.39	109.24
3	K	58	GLN	N-CA-C	-5.48	105.39	113.61
1	A	66	ARG	N-CA-C	5.47	117.42	108.55
3	N	117	GLN	N-CA-C	-5.40	106.86	113.50
3	M	58	GLN	N-CA-C	-5.39	106.63	114.12
3	N	28	ALA	N-CA-C	-5.39	106.64	113.43
1	C	133	SER	N-CA-C	5.37	117.59	108.02
2	D	64	VAL	CA-C-N	-5.36	115.15	121.90
2	D	64	VAL	C-N-CA	-5.36	115.15	121.90
3	L	57	ALA	N-CA-C	5.35	117.39	108.02
3	L	152	GLU	N-CA-C	-5.34	105.86	112.38
3	M	117	GLN	N-CA-C	-5.34	105.03	112.45
3	N	145	HIS	N-CA-C	-5.32	105.53	112.23
2	D	48	VAL	N-CA-C	5.32	116.48	111.48
3	N	124	GLN	N-CA-C	-5.30	105.58	111.36
2	B	79	ALA	N-CA-C	-5.30	101.92	110.14
2	B	45	LEU	N-CA-C	5.30	117.86	109.96
3	L	34	VAL	N-CA-C	-5.30	105.26	113.16
2	D	110	ALA	CB-CA-C	-5.30	100.75	109.65
1	C	24	ARG	N-CA-CB	5.29	120.70	111.13
3	N	152	GLU	N-CA-C	-5.28	106.34	112.89
3	K	111	ALA	N-CA-C	-5.27	105.50	112.94
2	B	154	LYS	CA-C-N	-5.24	115.42	122.86
2	B	154	LYS	C-N-CA	-5.24	115.42	122.86
3	L	104	GLY	N-CA-C	-5.22	108.18	114.66
2	D	167	SER	N-CA-CB	-5.20	103.80	111.71
3	N	34	VAL	N-CA-C	-5.18	105.04	112.35
3	M	112	THR	N-CA-C	-5.17	107.52	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	141	THR	N-CA-C	-5.17	105.82	111.82
3	M	42	ALA	N-CA-C	-5.17	107.36	113.97
3	M	67	TRP	N-CA-C	-5.16	107.01	113.15
3	M	39	VAL	N-CA-C	-5.14	107.82	113.43
1	A	99	THR	N-CA-C	-5.13	99.86	110.80
2	B	155	ASP	N-CA-CB	5.13	118.64	110.84
1	C	158	SER	N-CA-C	5.13	117.81	109.24
3	L	39	VAL	N-CA-C	-5.12	107.85	113.43
3	N	116	GLY	N-CA-C	-5.11	107.69	115.66
2	D	153	VAL	N-CA-C	-5.11	100.11	107.37
1	C	76	SER	N-CA-C	-5.09	102.95	110.48
3	N	142	ARG	N-CA-C	-5.07	105.02	111.11
3	N	33	THR	N-CA-C	-5.06	107.28	113.50
3	N	119	GLN	N-CA-C	-5.06	107.11	113.28
1	A	115	PRO	CB-CA-C	5.05	119.89	111.56
3	L	114	PHE	N-CA-C	5.04	118.53	112.38
2	B	152	LEU	N-CA-C	-5.04	99.61	107.93
2	D	34	ILE	N-CA-C	5.04	115.57	108.36
3	L	91	VAL	N-CA-C	-5.03	107.43	111.91
1	A	133	SER	N-CA-C	5.03	116.97	108.02
3	K	39	VAL	N-CA-C	-5.00	108.10	112.90
1	C	99	THR	N-CA-C	-5.00	100.14	110.80

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

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	301	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1658	0	1606	250	0
2	B	1653	0	1597	296	0
2	D	1653	0	1597	284	0
3	K	1090	0	1093	191	0
3	L	1090	0	1093	197	0
3	M	1090	0	1093	187	0
3	N	1090	0	1093	177	0
All	All	10982	0	10778	1679	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 77.

All (1679) 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
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:HB3	2:B:155:ASP:C	1.51	1.34
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
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:A:4:MET:HE2	1:A:90:GLN:HB3	1.24	1.16
1:C:98:VAL:HG21	2:D:47:TRP:CD1	1.82	1.14
1:A:32:ALA:O	1:A:91:TYR:CD1	2.02	1.12
2:B:130:PRO:HB3	2:B:155:ASP:O	0.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:98:VAL:HG21	2:B:47:TRP:CD1	1.87	1.08
2:B:165:TRP:HE1	2:B:174:VAL:HG21	0.97	1.08
1:C:4:MET:HE2	1:C:90:GLN:HB3	1.15	1.07
1:C:115:PRO:HG3	1:C:141:PHE:HB2	1.34	1.07
2:B:91:THR:CG2	2:B:122:VAL:H	1.67	1.06
2:B:165:TRP:HH2	2:B:193:VAL:CG1	1.49	1.06
1:C:115:PRO:HB3	1:C:141:PHE:HB3	1.31	1.06
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:HH11	3:M:153:ARG:CG	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:HB3	3:L:147:ARG:HH11	1.17	1.02
2:D:39:GLN:O	2:D:92:ALA:HB1	1.60	1.01
1:C:110:ARG:HD3	1:C:173:SER:HB2	1.41	1.01
3:M:153:ARG:HG2	3:M:153:ARG:NH1	1.56	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:O	1:A:142:TYR:HD1	1.46	0.98
2:D:165:TRP:CD1	2:D:170:LEU:HB3	2.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:HE22	2:B:39:GLN:HE22	1.03	0.97
3:N:147:ARG:HB3	3:N:147:ARG:HH11	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:115:PRO:HD3	1:A:200:HIS:CD2	2.00	0.96
1:A:144:ARG:HG2	1:A:144:ARG:O	1.64	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:HH11	3:M:153:ARG:HG2	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
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:104:MET:O	3:M:153:ARG:NE	2.00	0.94
2:B:165:TRP:HZ2	2:B:193:VAL:HB	0.77	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:4:MET:HE2	1:C:90:GLN:CB	1.99	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
3:K:72:THR:HG23	3:K:96:MET:HE2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:155:LEU:HD13	3:N:154:MET:HB3	1.54	0.90
3:L:43:GLY:O	3:L:68:TRP:CZ3	2.24	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:52:ARG:HA	3:M:60:ILE:HG22	1.55	0.89
3:M:127:ARG:O	3:M:127:ARG:HD3	1.72	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
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:32:ALA:O	1:A:91:TYR:CE1	2.27	0.87
1:A:110:ARG:HE	1:A:142:TYR:HB3	1.39	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:40:ALA:HB3	2:B:43:LYS:HB2	1.57	0.86
2:B:87:ARG:O	2:B:122:VAL:HG11	1.75	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
3:L:72:THR:HG23	3:L:96:MET:HE2	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
1:A:142:TYR:CD1	1:A:142:TYR:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:58:GLN:O	3:L:64:ARG:HD2	1.76	0.85
3:M:151:LEU:O	3:M:151:LEU:HD23	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
3:L:150:ARG:HD3	3:M:152:GLU:CD	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:4:MET:HE2	1:A:90:GLN:CB	2.08	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:K:147:ARG:HH11	3:K:147:ARG:HG3	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
3:M:72:THR:HG23	3:M:96:MET:HE2	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:B:54:TYR:HD1	1.67	0.78
2:B:104:MET:O	3:M:153:ARG:CD	2.31	0.77
1:C:90:GLN:O	1:C:97:PRO:O	2.00	0.77
3:L:154:MET:HB3	3:M:156:ASP:OD2	1.84	0.77
3:M:147:ARG:HE	3:N:145:HIS:CD2	2.03	0.77
3:M:151:LEU:HD23	3:M:151:LEU:C	2.07	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:49:TYR:CE2	2:D:109:VAL:CG1	2.67	0.77
1:C:122:PRO:HB2	1:C:127:LEU:HD11	1.67	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:HD12	2:D:192:VAL:HG11	1.65	0.75
1:C:191:HIS:O	1:C:213:ARG:HD3	1.86	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:112:VAL:HG13	1:A:201:GLN:CG	2.17	0.74
1:A:113:ALA:O	1:A:200:HIS:NE2	2.20	0.74
2:D:11:LEU:HD11	2:D:157:PHE:CE2	2.21	0.74
1:A:143:PRO:HD2	1:A:143:PRO:O	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
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:K:96:MET:HE1	3:N:71:GLU:OE2	1.88	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:B:83:MET:HE1	2:B:120:VAL:HG21	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:TYR:HE2	2:B:70:ILE:H	1.34	0.73
2:B:165:TRP:CE2	2:B:174:VAL:HG22	2.23	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: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
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
2:D:185:GLY:C	2:D:186:LEU:HD12	2.15	0.72
3:K:60:ILE:HG13	3:K:61:THR:H	1.55	0.72
2:B:130:PRO:CB	2:B:155:ASP:C	2.37	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:HD22	1:C:212:ASN:N	1.85	0.71
3:N:124:GLN:HA	3:N:127:ARG:HG2	1.72	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:HG2	3:K:153:ARG:HH11	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
2:B:185:GLY:C	2:B:186:LEU:HD12	2.16	0.71
3:N:61:THR:CG2	3:N:63:PRO:HD2	2.11	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:157:PHE:CD2	2:D:157:PHE:C	2.68	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:59:LEU:HD12	3:L:65:ALA:HB1	1.73	0.70
3:L:62:TYR:HB2	3:L:63:PRO:HD3	1.72	0.70
3:L:153:ARG:O	3:L:157:ASP:HB3	1.91	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:59:LEU:HD12	3:N:65:ALA:CB	2.21	0.69
3:N:122:GLN:O	3:N:126:VAL:HG13	1.92	0.69
1:A:50:SER:C	1:A:52:SER:H	1.99	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:O	2:D:54:TYR:HD1	1.74	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
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
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
1:C:120:PHE:HB2	1:C:135:VAL:HG13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:PRO:HB2	2:D:153:VAL:CG1	2.22	0.69
3:K:64:ARG:HA	3:L:89:ARG:HH12	1.57	0.69
3:L:67:TRP:HB3	3:L:81:LEU:HD12	1.75	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
1:C:50:SER:C	1:C:52:SER:H	2.01	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:83:MET:HE1	2:D:120:VAL:HG21	1.75	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:56:SER:HB2	3:M:142:ARG:HD3	1.76	0.68
2:B:130:PRO:HB3	2:B:155:ASP:CA	2.23	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:32:ALA:HB3	3:K:105:LEU:HD22	1.75	0.67
3:K:118:GLU:O	3:K:122:GLN:HG3	1.95	0.67
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
3:L:153:ARG:O	3:L:157:ASP:HB2	1.94	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:156:ASP:OD2	3:N:154:MET:HE2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:28:ASN:C	2:B:30:SER:H	2.00	0.67
2:D:165:TRP:HE1	2:D:174:VAL:HG22	1.59	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:N	2:D:13:GLN:OE1	2.28	0.67
2:D:156:TYR:C	2:D:156:TYR:CD2	2.73	0.67
3:K:70:VAL:HG11	3:L:93:VAL:HG22	1.76	0.67
3:K:93:VAL:O	3:K:97:VAL:HG23	1.94	0.67
1:C:83:PHE:CE1	1:C:108:ILE:HG13	2.30	0.66
1:C:142:TYR:CD1	1:C:142:TYR:C	2.73	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: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
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:211:PHE:C	1:C:212:ASN:HD22	2.04	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
2:D:173:GLY:C	2:D:193:VAL:HG23	2.21	0.66
1:A:115:PRO:CD	1:A:200:HIS:CB	2.74	0.65
1:A:115:PRO:CD	1:A:200:HIS:CG	2.78	0.65
1:C:2:ILE:CD1	1:C:29:VAL:CG2	2.73	0.65
1:C:137:LEU:HD21	1:C:139:ASN:OD1	1.96	0.65
3:K:153:ARG:HG2	3:K:153:ARG:NH1	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
2:B:130:PRO:CB	2:B:155:ASP:N	2.60	0.65
3:M:43:GLY:O	3:M:68:TRP:CE3	2.50	0.65
3:M:102:SER:O	3:M:106:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:58:GLN:O	3:K:64:ARG:HD2	1.97	0.65
3:K:147:ARG:HG3	3:K:147:ARG:NH1	2.11	0.65
1:C:11:LEU:HD23	1:C:11:LEU:O	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
2:B:22:CYS:C	2:B:78:THR:HG23	2.23	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:OE1	1:C:79:GLN:HA	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:115:PRO:HB3	1:C:140:ASN:C	2.22	0.64
2:D:32:TYR:CZ	2:D:98:ARG:NH2	2.66	0.64
2:D:157:PHE:CE2	2:D:158:PRO:CB	2.75	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:HG23	1:C:148:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:ALA:HB3	2:D:77:ASN:ND2	2.13	0.63
3:K:75:THR:HG21	3:N:74:THR:HB	1.79	0.63
3:K:76:VAL:HA	3:L:75: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
1:A:137:LEU:HD23	1:A:138:LEU:C	2.23	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
1:A:50:SER:C	1:A:52:SER:N	2.56	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:39:VAL:CG1	3:L:95:VAL:HA	2.26	0.63
3:L:51:GLU:O	3:L:57:ALA:HB1	1.98	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
1:C:137:LEU:HD23	1:C:138:LEU:C	2.24	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:D:79:ALA:C	2:D:80:TYR:HD2	2.07	0.63
2:B:13:GLN:OE1	2:B:13:GLN:N	2.31	0.63
2:B:208:ASN:N	2:B:208:ASN:ND2	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
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
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
2:B:54:TYR:CD1	2:B:54:TYR:C	2.76	0.62
1:C:30:ASN:HD22	1:C:66:ARG:NH2	1.97	0.62
1:C:169:ASP:OD2	1:C:170:SER:N	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:127:ARG:HD3	3:M:127:ARG:C	2.23	0.62
1:C:166:THR:HG22	1:C:176:SER:N	2.11	0.62
1:C:50:SER:C	1:C:52:SER:N	2.56	0.62
1:C:90:GLN:C	1:C:90:GLN:OE1	2.43	0.62
2:D:100:PRO:CB	2:D:106:SER:HB2	2.30	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
2:D:54:TYR:HD1	2:D:54:TYR:C	2.08	0.62
1:A:108:ILE:CG2	1:A:168:GLN:HE22	2.11	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:D:28:ASN:C	2:D:30:SER:H	2.07	0.61
2:B:79:ALA:C	2:B:80:TYR:HD2	2.07	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
2:B:206:ILE:HG23	2:B:220:LYS:C	2.25	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:M:118:GLU:HA	3:M:121:GLN:CD	2.25	0.61
3:L:102:SER:O	3:L:106:VAL:HG23	2.00	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: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
1:A:169:ASP:OD2	1:A:170:SER:N	2.33	0.61
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:A:152:VAL:HG23	1:A:152:VAL:O	2.00	0.60
1:C:32:ALA:O	1:C:91:TYR:CD1	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:PHE:CE1	1:C:108:ILE:HB	2.36	0.60
2:D:54:TYR:C	2:D:54:TYR:CD1	2.78	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:79:ALA:C	2:B:80:TYR:CD2	2.80	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:67:TRP:CZ3	3:M:89:ARG:HA	2.35	0.60
3:L:76:VAL:HA	3:M:75:THR:CA	2.32	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
3:N:72:THR:HG23	3:N:96:MET:HE2	1.83	0.60
1:A:90:GLN:C	1:A:90:GLN:OE1	2.44	0.60
2:B:98:ARG:NH1	2:B:112:ASP:OD1	2.34	0.60
2:D:97:ALA:CB	2:D:111:LEU:HD12	2.32	0.60
3:K:82:TYR:CE1	3:N:80:ASP:HB3	2.35	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:123:GLN:O	3:K:127:ARG:HB2	2.02	0.59
3:K:124:GLN:O	3:K:128:HIS:HB2	2.02	0.59
3:N:71:GLU:CD	3:N:76:VAL:HB	2.25	0.59
2:B:116:GLN:OE1	2:B:116:GLN:HA	2.01	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:79:ALA:C	2:D:80:TYR:CD2	2.80	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:B:54:TYR:HD1	2:B:54:TYR:C	2.10	0.59
2:D:86:LEU:HB3	2:D:122:VAL:CG2	2.30	0.59
2:D:2:VAL:HG11	2:D:113:TYR:HD2	1.66	0.59
1:A:143:PRO:C	1:A:145:GLU:H	2.11	0.59
2:B:2:VAL:HG11	2:B:113:TYR:CD2	2.38	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:HD2	1.67	0.59
1:A:115:PRO:CG	1:A:200:HIS:CB	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:CD1	2:D:192:VAL:HG21	2.29	0.59
1:C:212:ASN:HB2	1:C:215:GLU:OE1	2.03	0.59
2:D:157:PHE:CD2	2:D:158:PRO:CB	2.86	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
2:D:99:GLN:HG3	2:D:110:ALA:C	2.26	0.59
2:D:214:SER:C	2:D:216:THR:H	2.11	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:143:PRO:O	1:A:143:PRO:CD	2.49	0.59
1:C:11:LEU:HD23	1:C:11:LEU:C	2.28	0.58
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
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:K:144:LEU:O	3:K:145:HIS:C	2.43	0.58
3:M:127:ARG:NH1	3:M:131:LYS:HB2	2.19	0.58
3:N:147:ARG:HB3	3:N:147:ARG:NH1	2.09	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:A:189:GLU:HA	1:A:213:ARG:NH1	2.18	0.58
2:B:173:GLY:C	2:B:193:VAL:HG23	2.27	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
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
3:M:142:ARG:O	3:M:143:ALA:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HB	2:B:70:ILE:HD13	1.85	0.58
2:D:165:TRP:NE1	2:D:174:VAL:CG2	2.67	0.58
1:A:114:ALA:HB1	1:A:203:LEU:HD21	1.86	0.57
2:B:28:ASN:C	2:B:30:SER:N	2.56	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:D:91:THR:CG2	2:D:122:VAL:N	2.62	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
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:N:43:GLY:O	3:N:68:TRP:CZ3	2.57	0.57
1:A:183:LEU:HD12	1:A:183:LEU:N	2.19	0.57
1:C:89:GLN:NE2	2:D:111:LEU:CD2	2.47	0.57
3:K:153:ARG:NE	3:K:153:ARG:HA	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:90:GLN:OE1	1:C:91:TYR:N	2.37	0.57
1:C:141:PHE:HE2	1:C:177:LEU:H	1.50	0.57
2:D:22:CYS:C	2:D:78:THR:HG23	2.28	0.57
3:K:158:ASN:O	3:L:160:ARG:NH2	2.38	0.57
1:C:30:ASN:ND2	1:C:66:ARG:HH21	2.02	0.57
1:C:199:THR:HG22	1:C:200:HIS:N	2.20	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
1:A:79:GLN:HB3	1:A:80:PRO:CD	2.35	0.57
2:D:157:PHE:C	2:D:157:PHE:HD2	2.11	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: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:12:VAL:HG21	2:B:86:LEU:CD1	2.35	0.56
2:B:67:ARG:NH1	2:B:85:SER:O	2.38	0.56
2:D:211:HIS:ND1	2:D:213:PRO:HD2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:58:GLN:C	3:L:60:ILE:H	2.11	0.56
1:A:189:GLU:HA	1:A:213:ARG:NH2	2.20	0.56
1:C:79:GLN:HB3	1:C:80:PRO:CD	2.36	0.56
2:D:78:THR:HG22	2:D:79:ALA:N	2.18	0.56
1:A:2:ILE:CD1	1:A:29:VAL:CG2	2.80	0.56
2:B:64:VAL:HG21	2:B:68:PHE:CB	2.36	0.56
2:B:165:TRP:HD1	2:B:170:LEU:O	1.86	0.56
2:D:116:GLN:OE1	2:D:116:GLN:HA	2.05	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:35:TRP:CH2	1:A:88:CYS:HB2	2.39	0.56
1:A:107:GLU:HB2	1:A:168:GLN:OE1	2.06	0.56
1:A:114:ALA:HB2	1:A:202:GLY:O	2.06	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:C:181:LEU:HD13	1:C:181:LEU:C	2.30	0.56
1:A:98:VAL:CG2	2:B:47:TRP:CD2	2.89	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:C:33:VAL:HA	1:C:90:GLN:HA	1.87	0.56
1:C:71:PHE:N	1:C:71:PHE:CD1	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:23:ALA:C	3:N:25:GLN:H	2.12	0.56
3:N:127:ARG:O	3:N:131:LYS:HG3	2.06	0.56
1:A:50:SER:O	1:A:52:SER:N	2.39	0.56
1:A:141:PHE:HE2	1:A:177:LEU:H	1.52	0.56
2:D:156:TYR:CE2	2:D:187:TYR:HB2	2.40	0.56
3:L:78:TYR:OH	3:M:72:THR:OG1	2.23	0.56
3:L:139:ARG:HA	3:L:142:ARG:CD	2.36	0.56
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:27:GLN:HG3	1:A:28:ASP:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HB2	1:A:110:ARG:HH11	1.71	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:D:28:ASN:C	2:D:30:SER:N	2.63	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:32:ALA:C	1:A:91:TYR:CE1	2.84	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
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
2:D:50:SER:C	2:D:70:ILE:HD13	2.31	0.55
1:A:148:VAL:HG21	1:A:179:SER:HB2	1.88	0.55
1:C:137:LEU:C	1:C:138:LEU:HD12	2.32	0.55
3:K:29:ALA:HA	3:K:105:LEU:CD2	2.33	0.55
2:B:80:TYR:CD2	2:B:80:TYR:N	2.75	0.55
2:B:106:SER:O	2:B:109:VAL:CG2	2.55	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
2:D:51:ILE:O	2:D:51:ILE:HG23	2.06	0.55
2:D:165:TRP:CD1	2:D:174:VAL:HG21	2.42	0.55
2:D:208:ASN:N	2:D:208:ASN:ND2	2.50	0.55
3:K:68:TRP:HD1	3:K:81:LEU:O	1.90	0.55
3:K:110:LEU:O	3:K:114:PHE:HB2	2.06	0.55
3:K:118:GLU:HA	3:K:121:GLN:CD	2.31	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
2:D:165:TRP:HE1	2:D:174:VAL:CG2	2.20	0.55
3:M:109:ALA:HA	3:M:112:THR:HB	1.89	0.55
3:L:139:ARG:HG2	3:L:142:ARG:HE	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:88:ALA:HA	2:B:122:VAL:HG12	1.86	0.54
3:M:67:TRP:HE1	3:M:78:TYR:HD1	1.54	0.54
3:M:115:VAL:O	3:M:115:VAL:HG12	2.07	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:HG23	2:B:51:ILE:O	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
2:B:50:SER:C	2:B:70:ILE:HD13	2.33	0.54
1:C:73:LEU:HD12	1:C:74:THR:H	1.73	0.54
1:C:114:ALA:O	1:C:140:ASN:O	2.24	0.54
1:C:125:GLU:HG2	1:C:128:LYS:HD2	1.89	0.54
1:C:156:LEU:CD1	1:C:157:GLN:O	2.55	0.54
3:K:32:ALA:HB3	3:K:105:LEU:HD21	1.89	0.54
3:K:150:ARG:HD3	3:L:152:GLU:OE2	2.07	0.54
1:A:143:PRO:HG2	1:A:201:GLN:HB3	1.90	0.54
2:D:12:VAL:HG21	2:D:86:LEU:CD1	2.38	0.54
2:D:162:THR:HG23	2:D:212:LYS:CE	2.34	0.54
3:K:76:VAL:HA	3:L:75:THR:C	2.33	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:HH11	1:C:110:ARG:HB2	1.71	0.54
1:C:144:ARG:NH1	1:C:144:ARG:CB	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
1:A:31:THR:HG22	1:A:66:ARG:HE	1.71	0.54
1:A:32:ALA:HB3	1:A:92:TYR:HB2	1.89	0.54
2:B:3:GLN:O	2:B:4:LEU:HD23	2.08	0.54
2:B:29:ILE:HG22	2:B:29:ILE:O	2.07	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:D:165:TRP:CE3	2:D:206:ILE:O	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:HD3	1:A:200:HIS:HB3	1.88	0.53
1:A:199:THR:O	1:A:200:HIS:HB2	2.06	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:O	1:A:22:THR:OG1	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:N:46:LEU:HB2	3:N:91:VAL:HG11	1.90	0.53
1:A:35:TRP:HB2	1:A:48:ILE:HG12	1.89	0.53
1:A:200:HIS:CD2	1:A:202:GLY:H	2.27	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:39:VAL:CG1	3:K:95:VAL:HA	2.37	0.53
3:K:155:LEU:HD12	3:N:154:MET:SD	2.49	0.53
3:M:125:PHE:C	3:M:125:PHE:CD1	2.85	0.53
1:A:36:TYR:CE2	1:A:46:LEU:HD13	2.43	0.53
1:A:144:ARG:NH1	1:A:144:ARG:CB	2.72	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
2:D:107:TRP:CH2	3:K:154:MET:HE1	2.43	0.53
3:K:51:GLU:CD	3:K:83:PRO:HA	2.33	0.53
3:K:64:ARG:HG3	3:K:65:ALA:N	2.23	0.53
3:K:89:ARG:HG2	3:N:67:TRP:CE3	2.44	0.53
3:K:155:LEU:CD1	3:N:154:MET:CB	2.86	0.53
3:M:148:PHE:CE1	3:N:148:PHE:HZ	2.27	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
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
1:C:39:LYS:O	1:C:40:PRO:C	2.52	0.53
2:D:2:VAL:HG13	2:D:3:GLN:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:TRP:CE2	2:D:81:LEU:HB2	2.43	0.53
2:D:212:LYS:N	2:D:212:LYS:HD3	2.23	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:19:ARG:HG3	2:D:19:ARG:NH1	2.25	0.52
2:D:186:LEU:HD12	2:D:186:LEU:N	2.24	0.52
3:L:68:TRP:HD1	3:L:81:LEU:O	1.92	0.52
3:L:67:TRP:HB3	3:L:81:LEU:CD1	2.38	0.52
3:L:143:ALA:CA	3:L:146:GLU:HB2	2.39	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
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:30:ASN:OD1	3:K:158:ASN:CG	2.53	0.52
1:C:126:GLN:HG3	2:D:133:PHE:CD2	2.45	0.52
3:L:147:ARG:HH11	3:L:147:ARG:CB	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:71:PHE:N	1:A:71:PHE:CD1	2.76	0.52
1:A:120:PHE:HB3	2:B:135:LEU:HD22	1.92	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: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
3:K:109:ALA:HA	3:K:112:THR:HB	1.91	0.52
1:A:115:PRO:HG3	1:A:200:HIS:CG	2.44	0.52
1:A:148:VAL:HA	1:A:197:GLU:O	2.10	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:51:GLU:OE2	3:M:85:THR:HG23	2.09	0.52
3:M:135:GLU:HA	3:M:138:THR:HB	1.91	0.52
2:B:215:ASN:CG	2:B:215:ASN:O	2.53	0.52
1:C:92:TYR:HE1	3:K:154:MET:SD	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:119:ILE:HG23	1:A:211:PHE:HD2	1.74	0.52
1:A:137:LEU:HD23	1:A:138:LEU:N	2.25	0.52
1:A:192:LYS:HG3	1:A:213:ARG:CG	2.39	0.52
2:B:80:TYR:HD2	2:B:80:TYR:N	2.08	0.52
2:B:86:LEU:HB3	2:B:122:VAL:CG2	2.33	0.52
1:C:27:GLN:HG3	1:C:28:ASP:N	2.25	0.52
1:C:148:VAL:HG21	1:C:179:SER:HB2	1.92	0.52
1:A:83:PHE:HE1	1:A:108:ILE:HG13	1.73	0.51
1:A:181:LEU:C	1:A:181:LEU:HD13	2.34	0.51
1:C:183:LEU:N	1:C:183:LEU:HD12	2.25	0.51
1:C:185:LYS:HE2	1:C:189:GLU:CD	2.35	0.51
2:D:98:ARG:NH1	2:D:112:ASP:CG	2.68	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
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:H	2:B:111:LEU:HD22	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
1:A:137:LEU:HD23	1:A:137:LEU:C	2.36	0.51
2:B:94:TYR:O	2:B:117:GLY:HA2	2.10	0.51
2:B:152:LEU:HD12	2:B:190:SER:HB3	1.92	0.51
2:B:166:ASN:CB	2:B:169:ALA:HB3	2.38	0.51
2:B:215:ASN:O	2:B:215:ASN:ND2	2.44	0.51
1:C:83:PHE:CZ	1:C:108:ILE:HG13	2.46	0.51
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
3:M:153:ARG:HA	3:M:157:ASP:CG	2.36	0.51
1:A:11:LEU:HD23	1:A:11:LEU:C	2.35	0.51
1:C:28:ASP:OD2	3:L:156:ASP:O	2.29	0.51
3:K:82:TYR:CZ	3:N:80:ASP:HB3	2.46	0.51
3:L:52:ARG:CZ	3:L:62:TYR:HE1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:O	1:A:40:PRO:C	2.54	0.51
1:C:61:ARG:O	1:C:75:ILE:HA	2.10	0.51
1:C:110:ARG:HD3	1:C:173:SER:CB	2.27	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
3:N:115:VAL:O	3:N:115:VAL:HG12	2.10	0.51
2:B:39:GLN:HB3	2:B:93:VAL:HG23	1.93	0.51
2:B:186:LEU:HD12	2:B:186:LEU:N	2.26	0.51
1:C:29:VAL:HG13	1:C:92:TYR:CB	2.40	0.51
1:C:138:LEU:HD21	1:C:148:VAL:CG1	2.41	0.51
2:D:70:ILE:O	2:D:70:ILE:HG23	2.11	0.51
3:M:91:VAL:O	3:M:91:VAL:HG12	2.11	0.51
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
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
2:B:220:LYS:HE3	2:B:220:LYS:HA	1.92	0.50
2:D:173:GLY:O	2:D:193:VAL:HG23	2.11	0.50
3:K:67:TRP:HB3	3:K:81:LEU:CD1	2.40	0.50
3:K:73:ALA:C	3:K:75:THR:H	2.20	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:134:VAL:HB	1:C:181:LEU:HB3	1.92	0.50
1:C:143:PRO:HD2	1:C:200:HIS:CE1	2.46	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:2:ILE:HG21	1:A:90:GLN:HE21	1.75	0.50
1:A:138:LEU:HD22	1:A:177:LEU:HB3	1.94	0.50
2:B:186:LEU:N	2:B:186:LEU:CD1	2.74	0.50
3:K:46:LEU:CB	3:K:91:VAL:HG11	2.40	0.50
3:K:78:TYR:CD2	3:L:77:GLY:HA2	2.46	0.50
3:M:58:GLN:C	3:M:60:ILE:H	2.18	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
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:38:ILE:HG22	3:L:38:ILE:O	2.12	0.50
3:L:48:VAL:HG22	3:L:59:LEU:HG	1.93	0.50
3:L:143:ALA:O	3:L:146:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:CD	1:A:200:HIS:CD2	2.85	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
2:B:111:LEU:CD2	2:B:111:LEU:H	2.23	0.50
2:B:193:VAL:CG1	2:B:193:VAL:O	2.56	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:30:ASN:HD22	1:A:30:ASN:C	2.18	0.50
1:A:94:TYR:HE2	3:N:145:HIS:CD2	2.29	0.50
1:A:117:VAL:CG2	1:A:198:VAL:HG21	2.41	0.50
1:A:144:ARG:O	1:A:144:ARG:CG	2.46	0.50
1:A:144:ARG:HH11	1:A:144:ARG:CB	2.18	0.50
2:B:112:ASP:OD1	2:B:112:ASP:C	2.55	0.50
2:B:130:PRO:CG	2:B:155:ASP:C	2.82	0.50
3:K:63:PRO:O	3:L:89:ARG:NH1	2.45	0.50
3:K:158:ASN:HD21	3:L:160:ARG:HD2	1.75	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
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:HD23	2:D:149:LEU:H	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
1:C:94:TYR:HE2	3:L:145:HIS:CD2	2.30	0.50
2:D:80:TYR:CD2	2:D:80:TYR:N	2.77	0.50
3:K:48:VAL:HG22	3:K:65:ALA:HB1	1.93	0.50
3:K:77:GLY:HA3	3:N:76:VAL:O	2.11	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
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:L:151:LEU:C	3:L:153:ARG:N	2.68	0.50
3:M:48:VAL:HG13	3:M:59:LEU:O	2.12	0.50
3:M:127:ARG:NH1	3:M:130:GLU:HG3	2.26	0.50
1:A:14:SER:O	1:A:17:ASP:OD1	2.29	0.49
1:A:123:SER:OG	1:A:126:GLN:HB2	2.11	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:58:GLN:C	3:K:60:ILE:H	2.20	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:49:LEU:HB2	3:N:62:TYR:HH	1.75	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:27:GLN:CG	1:C:28:ASP:N	2.75	0.49
1:C:117:VAL:CG2	1:C:198:VAL:HG21	2.42	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:HG3	2:B:38:ARG:O	2.13	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:A:137:LEU:C	1:A:138:LEU:HD12	2.37	0.49
2:B:11:LEU:HD23	2:B:11:LEU:C	2.38	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: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:21:ILE:O	1:A:72:THR:HG23	2.12	0.49
1:A:120:PHE:CD1	2:B:135:LEU:HB3	2.47	0.49
2:B:122:VAL:HG12	2:B:122:VAL:O	2.11	0.49
1:C:98:VAL:HG21	2:D:47:TRP:CE2	2.47	0.49
1:C:152:VAL:HG22	1:C:157:GLN:HE21	1.78	0.49
3:M:80:ASP:HB3	3:N:82:TYR:CZ	2.48	0.49
3:M:141:THR:O	3:M:144:LEU:HB2	2.13	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:2:VAL:CG1	2:D:3:GLN:N	2.72	0.49
2:D:152:LEU:HD23	2:D:154:LYS:HB2	1.95	0.49
3:N:73:ALA:C	3:N:75:THR:H	2.19	0.49
2:B:23:ALA:N	2:B:78:THR:HG23	2.28	0.49
2:B:159:GLU:OE1	2:B:160:PRO:HA	2.12	0.49
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:TYR:HD2	2:D:80:TYR:N	2.11	0.49
3:K:76:VAL:HA	3:L:75:THR:CB	2.40	0.49
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:3:GLN:HB2	1:C:26:SER:HB3	1.95	0.49
1:C:138:LEU:N	1:C:138:LEU:CD1	2.76	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:114:ALA:CA	1:A:200:HIS:CD2	2.88	0.48
1:A:189:GLU:HA	1:A:213:ARG:HH22	1.77	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
2:B:166:ASN:O	2:B:167:SER:C	2.53	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: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:68:PHE:HA	2:D:82:GLN:O	2.14	0.48
2:D:165:TRP:CD1	2:D:174:VAL:CG2	2.97	0.48
3:L:79:GLY:HA2	3:L:82:TYR:CE2	2.48	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:9:GLY:N	2:B:118:THR:HG21	2.28	0.48
2:B:206:ILE:HG23	2:B:220:LYS:N	2.29	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:2:VAL:HG13	2:B:3:GLN:N	2.28	0.48
2:B:19:ARG:CG	2:B:19:ARG:HH11	2.27	0.48
2:B:130:PRO:CD	2:B:156:TYR:HA	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:NH1	1:C:76:SER:HB3	2.27	0.48
2:D:68:PHE:CD1	2:D:83:MET:HA	2.49	0.48
2:D:218:VAL:HG22	2:D:219:ASP:N	2.29	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: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
3:N:153:ARG:O	3:N:154:MET:C	2.57	0.48
1:A:89:GLN:NE2	1:A:98:VAL:HG12	2.26	0.48
1:A:96:ALA:HA	1:A:97:PRO:HA	1.74	0.48
2:B:12:VAL:HG23	2:B:12:VAL:O	2.13	0.48
2:B:102:TYR:CE2	3:M:150:ARG:HG3	2.48	0.48
2:B:135:LEU:HB2	2:B:150:GLY:O	2.13	0.48
1:C:87:TYR:CD2	2:D:45:LEU:HD12	2.49	0.48
1:C:168:GLN:NE2	1:C:173:SER:HB3	2.14	0.48
2:D:13:GLN:H	2:D:13:GLN:CD	2.20	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:38:ARG:HG3	2:D:38:ARG:O	2.14	0.47
2:D:130:PRO:CB	2:D:153:VAL:HG12	2.41	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:115:PRO:HG2	1:A:200:HIS:HB2	1.94	0.47
1:A:156:LEU:CD1	1:A:157:GLN:O	2.62	0.47
2:B:49:ALA:CB	2:B:60:TYR:HD2	2.27	0.47
1:C:33:VAL:CG2	1:C:71:PHE:CE2	2.97	0.47
1:C:137:LEU:HD23	1:C:138:LEU:N	2.30	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
3:K:144:LEU:O	3:K:147:ARG:N	2.43	0.47
3:M:151:LEU:C	3:M:151:LEU:CD2	2.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:151:LEU:CD2	3:N:151:LEU:HD13	2.37	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:M:159:ARG:HA	3:N:160:ARG:NH2	2.29	0.47
1:A:30:ASN:HD21	1:A:31:THR:HG23	1.73	0.47
1:A:138:LEU:N	1:A:138:LEU:CD1	2.77	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:12:VAL:HG21	2:B:86:LEU:HD13	1.96	0.47
2:B:165:TRP:CE2	2:B:170:LEU:HD13	2.49	0.47
1:C:98:VAL:CG2	2:D:47:TRP:CD2	2.97	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:29:ILE:O	2:D:29:ILE:HG22	2.14	0.47
2:D:49:ALA:CB	2:D:60:TYR:HD2	2.28	0.47
2:D:87:ARG:C	2:D:122:VAL:HG11	2.38	0.47
2:D:217:LYS:HE2	2:D:219:ASP:CG	2.40	0.47
3:L:32:ALA:HB3	3:L:105:LEU:HD11	1.96	0.47
1:C:7:SER:HB3	1:C:22:THR:OG1	2.15	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:O	1:C:135:VAL:HG22	2.14	0.47
2:D:105:TYR:O	2:D:105:TYR:CD1	2.68	0.47
2:D:149:LEU:HD11	2:D:205:TYR:HD2	1.79	0.47
2:D:206:ILE:HG22	2:D:207:CYS:N	2.29	0.47
1:A:34:ALA:HA	1:A:48:ILE:O	2.15	0.47
1:A:125:GLU:CG	1:A:128:LYS:HD2	2.45	0.47
1:A:185:LYS:HE2	1:A:189:GLU:CD	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	3:K:147:ARG:CG	2.75	0.46
3:L:67:TRP:O	3:L:67:TRP:CD1	2.68	0.46
1:A:168:GLN:HE21	1:A:173:SER:CB	2.20	0.46
2:B:2:VAL:CG1	2:B:3:GLN:N	2.75	0.46
2:B:56:SER:HB2	3:M:142:ARG:CD	2.43	0.46
3:L:43:GLY:O	3:L:68:TRP:HE3	1.97	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:M:106:VAL:O	3:M:110:LEU:HG	2.16	0.46
3:N:72:THR:HG21	3:N:95:VAL:HB	1.96	0.46
1:A:7:SER:HA	1:A:8:PRO:HA	1.62	0.46
1:A:110:ARG:HG2	1:A:142:TYR:CE2	2.50	0.46
1:C:195:ALA:CA	1:C:210:SER:HB2	2.42	0.46
3:K:38:ILE:O	3:K:38:ILE:HG22	2.15	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
2:B:98:ARG:NH1	2:B:112:ASP:CG	2.73	0.46
1:C:18:ARG:NH1	1:C:18:ARG:HG3	2.31	0.46
1:C:138:LEU:HD12	1:C:138:LEU:N	2.30	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:30:ASN:C	1:A:31:THR:CG2	2.88	0.46
1:A:36:TYR:HA	1:A:45:LYS:O	2.15	0.46
1:C:4:MET:HE2	1:C:90:GLN:CG	2.45	0.46
1:C:6:GLN:NE2	1:C:103:GLY:HA2	2.29	0.46
1:C:137:LEU:CD1	2:D:192:VAL:HG11	2.41	0.46
2:D:32:TYR:CD2	2:D:100:PRO:HA	2.49	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:HA	3:N:87:TRP:CE3	2.51	0.46
3:N:87:TRP:HA	3:N:87:TRP:HE3	1.81	0.46
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:O	2:B:70:ILE:CG2	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:CZ	3:N:127:ARG:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:110:ARG:NE	1:A:142:TYR:CB	2.74	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:75:THR:HB	3:N:76:VAL:HA	1.96	0.46
1:A:30:ASN:ND2	1:A:30:ASN:C	2.72	0.46
2:B:156:TYR:C	2:B:156:TYR:CD2	2.93	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:87:TYR:CD2	2:B:45:LEU:HD12	2.51	0.46
1:A:199:THR:HG22	1:A:200:HIS:H	1.80	0.46
1:C:139:ASN:ND2	2:D:194:THR:CG2	2.78	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:HG11	2.51	0.46
2:D:165:TRP:CZ2	2:D:193:VAL:HG12	2.50	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:O	2:B:70:ILE:HG23	2.16	0.45
1:C:98:VAL:HG21	2:D:47:TRP:CD2	2.50	0.45
2:D:19:ARG:HH11	2:D:19:ARG:CG	2.28	0.45
3:M:60:ILE:HG13	3:M:61:THR:H	1.80	0.45
3:N:48:VAL:CG1	3:N:61:THR:O	2.64	0.45
3:N:159:ARG:CD	3:N:160:ARG:HG3	2.39	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:K:148:PHE:HB3	3:N:147:ARG:NH1	2.31	0.45
3:L:67:TRP:CE3	3:M:89:ARG:HG2	2.50	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:122:VAL:CG1	2:B:122:VAL:O	2.64	0.45
1:C:2:ILE:HG21	1:C:90:GLN:HE21	1.82	0.45
1:C:199:THR:HG22	1:C:200:HIS:H	1.80	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:HD23	2:B:149:LEU:H	1.81	0.45
1:C:33:VAL:HG21	1:C:71:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:54:TYR:O	2:B:54:TYR:CD1	2.57	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:76:VAL:HG13	3:M:71:GLU:O	2.15	0.45
3:N:23:ALA:C	3:N:25:GLN:N	2.75	0.45
3:N:87:TRP:CZ3	3:N:90:LEU:HD12	2.52	0.45
1:A:167:GLU:O	1:A:168:GLN:C	2.60	0.45
2:B:38:ARG:O	2:B:38:ARG:CG	2.64	0.45
2:D:91:THR:O	2:D:92:ALA:HB2	2.16	0.45
2:D:157:PHE:HD2	2:D:158:PRO:N	2.11	0.45
3:M:122:GLN:O	3:M:126:VAL:HG12	2.15	0.45
3:N:37:VAL:O	3:N:37:VAL:HG12	2.16	0.45
3:N:49:LEU:C	3:N:51:GLU:H	2.24	0.45
3:N:123:GLN:HA	3:N:126:VAL:HG22	1.99	0.45
1:A:2:ILE:CG2	1:A:90:GLN:HE21	2.30	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
2:B:35:HIS:O	2:B:96:CYS:HA	2.16	0.45
1:C:203:LEU:HD23	1:C:203:LEU:HA	1.83	0.45
3:K:135:GLU:O	3:K:139:ARG:HG2	2.16	0.45
3:M:76:VAL:HG22	3:N:75:THR:CA	2.43	0.45
3:M:144:LEU:N	3:M:144:LEU:HD12	2.32	0.45
3:M:153:ARG:HA	3:M:157:ASP:OD1	2.17	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
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:63:SER:OG	1:A:74:THR:HB	2.17	0.45
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:M:141:THR:O	3:M:142:ARG:C	2.59	0.45
2:B:54:TYR:CE2	2:B:103:HIS:CD2	3.04	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
1:C:152:VAL:O	1:C:153:ASP:HB2	2.17	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:L:74:THR:HB	3:M:75:THR:HG21	1.99	0.44
3:M:61:THR:CG2	3:M:63:PRO:HD2	2.33	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:L:144:LEU:HD13	3:L:144:LEU:C	2.43	0.44
1:A:96:ALA:HB3	2:B:59:TYR:CZ	2.52	0.44
1:A:152:VAL:HG12	1:A:194:TYR:CE2	2.53	0.44
2:B:68:PHE:CE1	2:B:83:MET:HB3	2.53	0.44
2:D:13:GLN:N	2:D:13:GLN:CD	2.75	0.44
2:D:38:ARG:HD2	2:D:94:TYR:CZ	2.53	0.44
2:D:210:ASN:CG	2:D:217:LYS:HB2	2.42	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:HH11	1:A:61:ARG:HG2	1.82	0.44
1:A:83:PHE:CE1	1:A:108:ILE:CG1	3.00	0.44
1:A:143:PRO:C	1:A:145:GLU:N	2.70	0.44
2:B:40:ALA:HB1	2:B:41:PRO:CD	2.47	0.44
2:B:173:GLY:O	2:B:193:VAL:HG23	2.17	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
1:C:125:GLU:CG	1:C:128:LYS:HD2	2.48	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:72:THR:HG23	3:K:96:MET:CE	2.34	0.44
3:K:125:PHE:CD1	3:K:125:PHE:C	2.95	0.44
3:L:87:TRP:HZ3	3:L:90:LEU:CD1	2.29	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	3:L:87:TRP:CE3	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:11:LEU:C	2:B:11:LEU:CD2	2.91	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:L:137:TYR:C	3:L:139:ARG:N	2.73	0.44
3:M:87:TRP:HA	3:M:87:TRP:HE3	1.83	0.44
1:A:30:ASN:O	1:A:31:THR:HG22	2.18	0.44
2:B:19:ARG:NH1	2:B:19:ARG:CG	2.80	0.44
1:C:143:PRO:HD2	1:C:143:PRO:O	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:M:67:TRP:HZ3	3:N:89:ARG:HA	1.83	0.44
3:N:67:TRP:CD1	3:N:67:TRP:O	2.71	0.44
1:A:6:GLN:NE2	1:A:104:THR:N	2.66	0.44
1:A:115:PRO:CG	1:A:200:HIS:CG	3.00	0.44
2:B:74:THR:C	2:B:76:LYS:O	2.61	0.44
2:B:157:PHE:CD2	2:B:157:PHE:C	2.96	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:72:THR:O	3:L:96:MET:HB3	2.18	0.44
3:L:87:TRP:HA	3:L:87:TRP:HE3	1.83	0.44
3:L:153:ARG:O	3:L:153:ARG:HG2	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:194:TYR:HB2	1:A:211:PHE:CE1	2.53	0.43
2:B:13:GLN:CD	2:B:13:GLN:H	2.26	0.43
2:D:64:VAL:HG21	2:D:68:PHE:HB2	1.99	0.43
3:K:100:ILE:HD13	3:K:100:ILE:HA	1.84	0.43
3:L:39:VAL:CG1	3:L:94:VAL:O	2.66	0.43
3:L:52:ARG:NH2	3:L:62:TYR:CE1	2.86	0.43
3:M:116:GLY:HA2	3:M:119:GLN:HB2	1.99	0.43
3:N:59:LEU:HD11	3:N:68:TRP:CB	2.48	0.43
1:C:112:VAL:HG12	1:C:113:ALA:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:LEU:HD21	2:D:121:THR:CG2	2.35	0.43
2:D:130:PRO:HG3	2:D:211:HIS:HB2	2.00	0.43
2:D:180:VAL:HG13	2:D:180:VAL:O	2.18	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:6:GLN:NE2	1:A:104:THR:H	2.17	0.43
1:A:110:ARG:O	1:A:142:TYR:CE1	2.71	0.43
2:B:210:ASN:HD22	2:B:210:ASN:C	2.26	0.43
1:C:36:TYR:HE1	1:C:89:GLN:HB3	1.82	0.43
1:C:83:PHE:HE1	1:C:108:ILE:HG13	1.78	0.43
3:K:76:VAL:HA	3:L:75:THR:O	2.18	0.43
3:M:78:TYR:CE1	3:N:82:TYR:HB3	2.52	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
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
2:D:215:ASN:O	2:D:215:ASN:CG	2.61	0.43
3:L:110:LEU:HA	3:L:113:TRP:CD1	2.53	0.43
3:L:143:ALA:C	3:L:146:GLU:HB2	2.44	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:O	2:D:122:VAL:HA	2.19	0.43
2:D:12:VAL:CG2	2:D:122:VAL:HG23	2.48	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:50:ALA:O	3:N:85:THR:HG21	2.18	0.43
2:B:49:ALA:HB1	2:B:60:TYR:CD2	2.53	0.43
2:B:112:ASP:OD1	2:B:113:TYR:N	2.52	0.43
1:C:142:TYR:CD1	1:C:143:PRO:N	2.86	0.43
2:D:19:ARG:NH1	2:D:19:ARG:CG	2.81	0.43
2:D:157:PHE:CD2	2:D:158:PRO:CD	3.02	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:K:138:THR:C	3:K:141:THR:HG23	2.44	0.43
3:M:153:ARG:CG	3:M:153:ARG:NH1	2.42	0.43
3:M:153:ARG:HD3	3:M:157:ASP:CG	2.44	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:55:GLU:HB3	1:A:58:VAL:HG23	2.00	0.43
1:A:120:PHE:HA	1:A:121:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:O	1:A:156:LEU:HD22	2.18	0.43
2:B:107:TRP:CH2	3:M:154:MET:HE1	2.54	0.43
2:D:3:GLN:HG3	2:D:25:SER:OG	2.19	0.43
2:D:165:TRP:NE1	2:D:170:LEU:HD13	2.33	0.43
3:L:58:GLN:C	3:L:60:ILE:N	2.77	0.43
1:A:115:PRO:HD2	1:A:203:LEU:HG	2.00	0.43
2:B:41:PRO:HD3	2:B:91:THR:O	2.18	0.43
2:B:156:TYR:HB2	2:B:211:HIS:CD2	2.53	0.43
2:B:200:LEU:HB3	2:B:224:PRO:CG	2.49	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:52:ARG:HH21	3:K:61:THR:HA	1.83	0.43
3:K:147:ARG:NH1	3:L:148:PHE:HB3	2.34	0.43
3:L:39:VAL:HG11	3:L:98:ALA:HB2	2.01	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: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:73:ASP:OD1	2:B:75:SER:OG	2.30	0.43
2:B:210:ASN:HD22	2:B:211:HIS:N	2.16	0.43
1:C:80:PRO:HA	1:C:83:PHE:HE2	1.84	0.43
1:C:148:VAL:O	1:C:148:VAL:CG2	2.66	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:43:GLY:O	3:M:68:TRP:HE3	1.98	0.43
3:M:49:LEU:C	3:M:51:GLU:H	2.26	0.43
3:M:49:LEU:HD13	3:M:62:TYR:OH	2.19	0.43
1:A:18:ARG:NH1	1:A:18:ARG:HG3	2.34	0.43
1:C:91:TYR:CA	1:C:97:PRO:O	2.50	0.43
1:C:160:ASN:HD21	1:C:181:LEU:HD21	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:100:ILE:HA	3:L:100:ILE:HD12	1.80	0.42
1:A:108:ILE:CB	1:A:168:GLN:HE22	2.32	0.42
2:B:110:ALA:O	2:B:111:LEU:C	2.62	0.42
2:B:165:TRP:CG	2:B:170:LEU:HB3	2.54	0.42
1:C:184:SER:O	1:C:185:LYS:C	2.61	0.42
2:D:11:LEU:HD23	2:D:11:LEU:C	2.44	0.42
2:D:68:PHE:CE1	2:D:83:MET:HB3	2.55	0.42
2:D:149:LEU:HD23	2:D:149:LEU:N	2.34	0.42
2:D:165:TRP:CE3	2:D:165:TRP:HA	2.53	0.42
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:K:142:ARG:O	3:K:143:ALA:C	2.61	0.42
3:M:48:VAL:HG22	3:M:65:ALA:CB	2.50	0.42
3:M:100:ILE:HD13	3:M:100:ILE:HA	1.91	0.42
3:N:118:GLU:HA	3:N:118:GLU:OE2	2.19	0.42
3:N:148:PHE:C	3:N:150:ARG:N	2.75	0.42
1:A:30:ASN:ND2	1:A:31:THR:CG2	2.61	0.42
2:D:12:VAL:HG21	2:D:86:LEU:HD13	2.02	0.42
2:D:91:THR:HG22	2:D:122:VAL:N	2.31	0.42
2:D:152:LEU:HD12	2:D:190:SER:HB3	2.02	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
1:A:184:SER:O	1:A:185:LYS:C	2.61	0.42
2:B:78:THR:CG2	2:B:79:ALA:N	2.81	0.42
2:B:200:LEU:HB3	2:B:224:PRO:HG3	2.02	0.42
1:C:61:ARG:NH1	1:C:61:ARG:HG2	2.35	0.42
3:M:76:VAL:HG12	3:N:77:GLY:CA	2.49	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
2:D:214:SER:C	2:D:216:THR:N	2.76	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:HA	1:C:167:GLU:OE1	2.20	0.42
1:C:181:LEU:C	1:C:181:LEU:CD1	2.92	0.42
2:D:49:ALA:HB1	2:D:60:TYR:CD2	2.54	0.42
3:K:54:ALA:HB2	3:K:85:THR:CG2	2.49	0.42
3:K:115:VAL:HA	3:K:118:GLU:HB2	2.00	0.42
3:N:64:ARG:HG3	3:N:65:ALA:N	2.35	0.42
3:N:127:ARG:HB3	3:N:127:ARG:NH1	2.35	0.42
1:A:135:VAL:O	1:A:135:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:N:51:GLU:CD	3:N:83:PRO:HA	2.45	0.42
1:A:89:GLN:HA	1:A:99:THR:O	2.19	0.42
2:D:69:THR:HB	2:D:82:GLN:HB3	2.00	0.42
2:D:195:VAL:HG21	2:D:205:TYR:HE2	1.81	0.42
3:K:76:VAL:HG22	3:L:75:THR:CB	2.49	0.42
3:L:73:ALA:C	3:L:75:THR:H	2.27	0.42
3:M:38:ILE:O	3:M:38:ILE:HG22	2.19	0.42
3:M:134:GLU:O	3:M:137:TYR:HB3	2.19	0.42
3:N:73:ALA:C	3:N:75:THR:N	2.78	0.42
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:K:138:THR:O	3:K:139:ARG:C	2.63	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:68:PHE:HA	2:B:82:GLN:O	2.20	0.41
2:B:105:TYR:CE1	2:B:108:TRP:HB2	2.55	0.41
3:K:67:TRP:CZ3	3:L:92:ALA:CB	3.02	0.41
3:K:67:TRP:HE3	3:L:89:ARG:HG2	1.81	0.41
3:K:137:TYR:O	3:K:140:THR:HB	2.20	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
1:A:190:LYS:HG2	1:A:190:LYS:O	2.19	0.41
2:B:4:LEU:HD21	2:B:27:PHE:HZ	1.83	0.41
2:B:154:LYS:HG3	2:B:188:SER:OG	2.20	0.41
1:C:149:GLN:OE1	1:C:197:GLU:HG2	2.19	0.41
2:D:92:ALA:HB3	2:D:94:TYR:HE1	1.84	0.41
2:D:105:TYR:CE1	2:D:108:TRP:HB2	2.55	0.41
3:K:138:THR:O	3:K:141:THR:N	2.53	0.41
3:M:25:GLN:CD	3:M:113:TRP:HE1	2.26	0.41
1:A:96:ALA:HB1	1:A:97:PRO:HD3	1.55	0.41
1:A:199:THR:CG2	1:A:200:HIS:N	2.83	0.41
2:B:15:GLY:N	2:B:86:LEU:O	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ALA:CB	2:B:111:LEU:HD12	2.44	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: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
1:C:143:PRO:HD2	1:C:200:HIS:HE1	1.85	0.41
2:D:209:VAL:O	2:D:218:VAL:N	2.41	0.41
2:D:217:LYS:HD3	2:D:217:LYS:C	2.46	0.41
2:D:217:LYS:CE	2:D:219:ASP:OD1	2.69	0.41
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
2:B:8:GLY:O	2:B:9:GLY:C	2.61	0.41
2:D:74:THR:C	2:D:76:LYS:O	2.63	0.41
3:K:152:GLU:CD	3:N:150:ARG:HD3	2.45	0.41
3:M:144:LEU:O	3:M:145:HIS:C	2.60	0.41
1:A:192:LYS:NZ	1:A:192:LYS:HB2	2.36	0.41
1:C:89:GLN:HA	1:C:99:THR:O	2.20	0.41
3:N:23:ALA:C	3:N:27:ARG:HD3	2.46	0.41
1:C:3:GLN:HB2	1:C:26:SER:CB	2.51	0.41
2:D:81:LEU:HD23	2:D:81:LEU:HA	1.71	0.41
3:K:47:ALA:O	3:K:59:LEU:HD23	2.20	0.41
3:K:70:VAL:CG1	3:L:96:MET:SD	3.05	0.41
3:K:71:GLU:HB2	3:K:77:GLY:H	1.86	0.41
3:K:135:GLU:O	3:K:138:THR:HB	2.20	0.41
3:L:75:THR:O	3:M:75:THR:O	2.38	0.41
1:A:94:TYR:HE2	3:N:145:HIS:HD2	1.66	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: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
3:L:103:PHE:CE2	3:M:100:ILE:HG13	2.56	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
1:C:150:TRP:CE2	1:C:181:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLU:CD	2:D:117:GLY:H	2.29	0.41
3:K:48:VAL:HG22	3:K:59:LEU:HG	2.03	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:24:LEU:O	3:N:24:LEU:HG	2.21	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
3:N:117:GLN:O	3:N:121:GLN:HG3	2.20	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:15:VAL:CG2	1:C:16:GLY:N	2.83	0.41
1:C:152:VAL:O	1:C:152:VAL:CG2	2.69	0.41
2:D:13:GLN:HB2	2:D:14:PRO:HD2	2.02	0.41
2:D:159:GLU:OE1	2:D:159:GLU:HA	2.21	0.41
3:N:38:ILE:O	3:N:38:ILE:HG22	2.21	0.41
1:A:87:TYR:CG	2:B:45:LEU:HD12	2.55	0.40
2:B:87:ARG:C	2:B:122:VAL:HG11	2.41	0.40
2:D:49:ALA:CB	2:D:60:TYR:CD2	3.04	0.40
2:D:106:SER:O	2:D:109:VAL:HG22	2.20	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
3:L:76:VAL:HA	3:M:75:THR:C	2.46	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
1:A:165:VAL:HG12	1:A:177:LEU:HA	2.03	0.40
2:B:13:GLN:N	2:B:13:GLN:CD	2.79	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:N:141:THR:O	3:N:142:ARG:C	2.64	0.40
2:B:210:ASN:C	2:B:210:ASN:ND2	2.79	0.40
2:D:210:ASN:ND2	2:D:210:ASN:C	2.79	0.40
2:D:210:ASN:HD22	2:D:210:ASN:C	2.29	0.40
2:D:221:LYS:HE3	2:D:223:GLU:OE2	2.21	0.40
3:L:39:VAL:HG11	3:L:98:ALA:CB	2.51	0.40
3:L:159:ARG:HD2	3:L:160:ARG:CG	2.46	0.40
3:M:23:ALA:C	3:M:25:GLN:H	2.29	0.40
3:N:46:LEU:CB	3:N:91:VAL:HG11	2.51	0.40
1:A:30:ASN:C	1:A:66:ARG:HH21	2.30	0.40
1:A:160:ASN:ND2	1:A:181:LEU:CD2	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:PHE:HD1	2:D:83:MET:HA	1.86	0.40
2:D:74:THR:O	2:D:76:LYS:O	2.39	0.40
2:D:211:HIS:HB3	2:D:214:SER:OG	2.21	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:M:72:THR:HG21	3:M:95:VAL:HB	2.03	0.40
3:M:78:TYR:CE2	3:N:77:GLY:HA2	2.57	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/215 (99%)	173 (81%)	34 (16%)	6 (3%)	4	26
1	C	213/215 (99%)	177 (83%)	30 (14%)	6 (3%)	4	26
2	B	215/224 (96%)	185 (86%)	28 (13%)	2 (1%)	14	45
2	D	215/224 (96%)	188 (87%)	25 (12%)	2 (1%)	14	45
3	K	137/166 (82%)	116 (85%)	18 (13%)	3 (2%)	5	30
3	L	137/166 (82%)	125 (91%)	10 (7%)	2 (2%)	8	36
3	M	137/166 (82%)	119 (87%)	17 (12%)	1 (1%)	18	51
3	N	137/166 (82%)	116 (85%)	19 (14%)	2 (2%)	8	36
All	All	1404/1542 (91%)	1199 (85%)	181 (13%)	24 (2%)	7	34

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
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	12
1	C	189/189 (100%)	155 (82%)	34 (18%)	2	12
2	B	184/188 (98%)	149 (81%)	35 (19%)	1	10
2	D	184/188 (98%)	149 (81%)	35 (19%)	1	10
3	K	108/131 (82%)	95 (88%)	13 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	108/131 (82%)	97 (90%)	11 (10%)	7	27
3	M	108/131 (82%)	93 (86%)	15 (14%)	3	18
3	N	108/131 (82%)	97 (90%)	11 (10%)	7	27
All	All	1178/1278 (92%)	990 (84%)	188 (16%)	2	14

All (188) 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	24	ARG
1	A	30	ASN
1	A	31	THR
1	A	40	PRO
1	A	48	ILE
1	A	49	TYR
1	A	70	ASP
1	A	76	SER
1	A	78	LEU
1	A	90	GLN
1	A	98	VAL
1	A	99	THR
1	A	108	ILE
1	A	110	ARG
1	A	116	SER
1	A	119	ILE
1	A	123	SER
1	A	126	GLN
1	A	133	SER
1	A	135	VAL
1	A	137	LEU
1	A	142	TYR
1	A	144	ARG
1	A	156	LEU
1	A	158	SER
1	A	170	SER
1	A	177	LEU
1	A	183	LEU
1	A	192	LYS

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Mol	Chain	Res	Type
1	A	210	SER
2	B	2	VAL
2	B	7	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	103	HIS
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
2	B	158	PRO
2	B	160	PRO
2	B	167	SER
2	B	170	LEU
2	B	181	LEU
2	B	186	LEU
2	B	208	ASN
2	B	212	LYS
2	B	215	ASN
2	B	216	THR
2	B	217	LYS
1	C	5	THR
1	C	9	SER
1	C	11	LEU
1	C	15	VAL
1	C	24	ARG
1	C	27	GLN

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Mol	Chain	Res	Type
1	C	30	ASN
1	C	31	THR
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	90	GLN
1	C	99	THR
1	C	108	ILE
1	C	110	ARG
1	C	116	SER
1	C	119	ILE
1	C	123	SER
1	C	133	SER
1	C	135	VAL
1	C	142	TYR
1	C	144	ARG
1	C	156	LEU
1	C	158	SER
1	C	170	SER
1	C	177	LEU
1	C	183	LEU
1	C	192	LYS
1	C	209	LYS
1	C	210	SER
1	C	212	ASN
2	D	2	VAL
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	91	THR
2	D	93	VAL
2	D	101	SER

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Mol	Chain	Res	Type
2	D	103	HIS
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	153	VAL
2	D	156	TYR
2	D	157	PHE
2	D	160	PRO
2	D	176	THR
2	D	181	LEU
2	D	186	LEU
2	D	208	ASN
2	D	212	LYS
2	D	215	ASN
2	D	216	THR
3	K	87	TRP
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	138	THR
3	K	141	THR
3	K	147	ARG
3	K	157	ASP
3	L	26	TRP
3	L	87	TRP
3	L	100	ILE
3	L	105	LEU
3	L	112	THR
3	L	117	GLN
3	L	123	GLN
3	L	127	ARG

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Mol	Chain	Res	Type
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	113	TRP
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	138	THR
3	M	147	ARG
3	M	153	ARG
3	M	157	ASP
3	N	87	TRP
3	N	105	LEU
3	N	112	THR
3	N	117	GLN
3	N	123	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) 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

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Mol	Chain	Res	Type
2	B	208	ASN
2	B	210	ASN
2	B	211	HIS
2	B	215	ASN
1	C	3	GLN
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
3	K	158	ASN
3	L	25	GLN
3	L	117	GLN
3	L	121	GLN
3	L	145	HIS
3	L	158	ASN
3	M	25	GLN
3	M	119	GLN
3	M	158	ASN
3	N	117	GLN
3	N	120	GLN
3	N	145	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	0.81	24 (11%)	10 13	98, 197, 222, 222	0
1	C	215/215 (100%)	0.61	23 (10%)	11 14	80, 142, 198, 222	0
2	B	219/224 (97%)	0.66	19 (8%)	16 16	78, 153, 222, 222	0
2	D	219/224 (97%)	0.61	19 (8%)	16 16	73, 134, 211, 222	0
3	K	139/166 (83%)	1.06	22 (15%)	5 8	78, 222, 222, 222	0
3	L	139/166 (83%)	1.22	25 (17%)	3 6	91, 222, 222, 222	0
3	M	139/166 (83%)	1.14	29 (20%)	2 4	90, 222, 222, 222	0
3	N	139/166 (83%)	1.25	29 (20%)	2 4	106, 222, 222, 222	0
All	All	1424/1542 (92%)	0.87	190 (13%)	7 10	73, 190, 222, 222	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ALA	8.0
1	C	102	GLN	6.2
3	K	93	VAL	5.4
1	C	113	ALA	5.4
3	M	70	VAL	5.3
1	A	179	SER	5.1
3	M	73	ALA	5.0
3	M	95	VAL	4.9
3	L	157	ASP	4.7
3	M	72	THR	4.4
1	A	163	GLU	4.4
1	C	28	ASP	4.3
3	L	115	VAL	4.2
3	L	108	ALA	4.2
1	A	180	THR	4.2
3	M	96	MET	4.1

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Mol	Chain	Res	Type	RSRZ
3	L	94	VAL	4.1
3	K	66	LEU	4.0
1	A	148	VAL	4.0
1	A	108	ILE	4.0
2	D	37	VAL	3.9
1	C	115	PRO	3.9
3	N	85	THR	3.8
3	L	84	VAL	3.8
3	N	80	ASP	3.8
1	C	114	ALA	3.8
3	K	46	LEU	3.7
2	B	132	VAL	3.7
2	B	224	PRO	3.7
3	M	154	MET	3.6
3	L	106	VAL	3.6
3	M	50	ALA	3.5
3	N	84	VAL	3.5
2	D	190	SER	3.5
3	N	115	VAL	3.5
3	N	128	HIS	3.5
3	L	67	TRP	3.4
2	D	133	PHE	3.4
2	D	155	ASP	3.4
1	A	150	TRP	3.3
3	K	100	ILE	3.3
3	L	101	THR	3.3
2	B	148	ALA	3.2
3	K	50	ALA	3.2
3	N	125	PHE	3.2
3	N	50	ALA	3.2
3	M	66	LEU	3.1
1	C	96	ALA	3.1
3	M	49	LEU	3.1
2	B	136	ALA	3.1
3	N	93	VAL	3.1
3	N	100	ILE	3.1
2	D	129	GLY	3.1
3	N	88	GLY	3.1
2	B	137	PRO	3.0
3	K	145	HIS	3.0
1	C	134	VAL	3.0
2	D	110	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	M	42	ALA	3.0
3	M	100	ILE	3.0
1	A	175	TYR	3.0
2	D	11	LEU	3.0
2	D	104	MET	2.9
3	N	120	GLN	2.9
2	B	52	SER	2.9
1	A	28	ASP	2.9
3	L	96	MET	2.9
1	C	131	THR	2.9
3	N	131	LYS	2.9
3	L	38	ILE	2.9
3	N	23	ALA	2.9
3	M	74	THR	2.8
3	M	67	TRP	2.8
1	C	30	ASN	2.8
3	M	46	LEU	2.8
1	A	97	PRO	2.8
2	D	161	VAL	2.8
1	A	31	THR	2.8
3	L	73	ALA	2.8
3	N	159	ARG	2.8
3	N	157	ASP	2.8
1	C	201	GLN	2.8
3	L	114	PHE	2.8
2	D	130	PRO	2.8
3	N	79	GLY	2.8
1	A	178	SER	2.7
2	B	207	CYS	2.7
2	B	104	MET	2.7
3	K	135	GLU	2.7
3	M	110	LEU	2.7
3	N	81	LEU	2.7
3	M	145	HIS	2.7
2	D	112	ASP	2.7
3	L	42	ALA	2.7
3	M	88	GLY	2.7
3	M	99	GLY	2.7
2	D	111	LEU	2.7
1	A	206	PRO	2.6
2	D	151	CYS	2.6
3	L	82	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
3	N	129	SER	2.6
1	C	80	PRO	2.6
3	N	116	GLY	2.6
3	L	102	SER	2.6
3	N	67	TRP	2.6
2	D	209	VAL	2.6
3	M	98	ALA	2.6
3	K	33	THR	2.5
1	C	158	SER	2.5
3	L	100	ILE	2.5
2	D	192	VAL	2.5
1	C	126	GLN	2.5
2	B	170	LEU	2.5
2	D	105	TYR	2.5
3	L	66	LEU	2.5
1	A	50	SER	2.5
1	C	56	SER	2.5
2	B	138	SER	2.5
2	D	204	THR	2.5
1	A	173	SER	2.5
1	C	97	PRO	2.4
2	B	139	SER	2.4
3	K	84	VAL	2.4
3	M	38	ILE	2.4
3	K	108	ALA	2.4
2	D	163	VAL	2.4
1	C	132	ALA	2.4
3	K	56	GLY	2.4
3	K	47	ALA	2.4
1	A	116	SER	2.4
3	N	103	PHE	2.4
2	B	44	GLY	2.4
3	N	83	PRO	2.4
1	A	161	SER	2.4
3	M	103	PHE	2.4
3	K	49	LEU	2.4
3	N	89	ARG	2.4
1	C	145	GLU	2.4
2	B	191	SER	2.3
3	M	158	ASN	2.3
3	M	40	LEU	2.3
3	N	94	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	109	ALA	2.3
3	M	92	ALA	2.3
3	M	130	GLU	2.3
1	C	64	GLY	2.3
3	K	55	PRO	2.3
3	L	63	PRO	2.3
3	L	122	GLN	2.3
3	L	79	GLY	2.3
1	A	102	GLN	2.3
1	A	172	ASP	2.3
1	C	5	THR	2.2
2	B	110	ALA	2.2
3	K	97	VAL	2.2
3	K	42	ALA	2.2
1	A	118	PHE	2.2
3	K	129	SER	2.2
2	B	59	TYR	2.2
3	M	45	TYR	2.2
2	B	65	LYS	2.2
2	B	101	SER	2.1
3	K	67	TRP	2.1
1	C	125	GLU	2.1
3	L	105	LEU	2.1
3	N	66	LEU	2.1
1	C	45	LYS	2.1
1	A	149	GLN	2.1
3	K	70	VAL	2.1
3	L	93	VAL	2.1
3	M	71	GLU	2.1
1	A	195	ALA	2.1
3	K	83	PRO	2.1
1	C	62	PHE	2.1
2	B	165	TRP	2.0
3	K	130	GLU	2.0
2	D	191	SER	2.0
3	L	129	SER	2.0
1	A	139	ASN	2.0
2	B	175	HIS	2.0
1	A	182	THR	2.0
3	L	86	LEU	2.0
3	N	102	SER	2.0
3	N	110	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	N	111	ALA	2.0
3	M	93	VAL	2.0
3	K	114	PHE	2.0
1	C	10	SER	2.0
3	N	109	ALA	2.0
3	M	94	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.