Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:26 am BST

PDB ID	:	3EFF
Title	:	The Crystal Structure of Full-Length KcsA in its Closed Conformation
Authors	:	Uysal, S.; Vasquez, V.; Tereshko, T.; Esaki, K.; Fellouse, F.A.; Sidhu, S.S.; Koide, S.; Perozo, E.; Kossiakoff, A.
Deposited on	:	2008-09-08
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 following versions of software and data (see references ⓘ) were used in the production of this report:

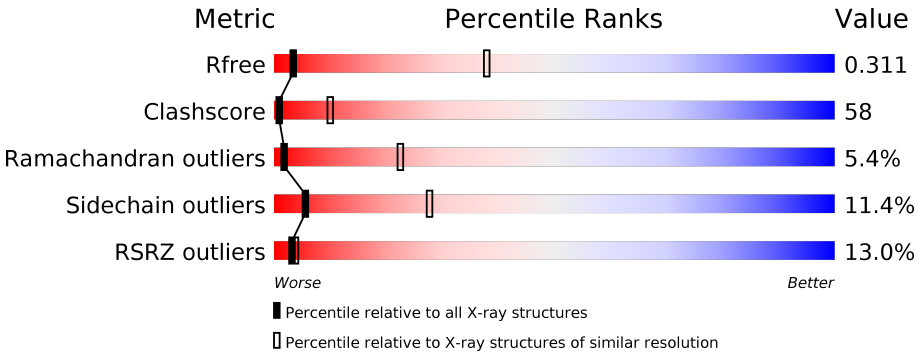
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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% 33% 55% 10%
1	C	215	2% 30% 54% 13%
2	B	224	5% 35% 54% 8%
2	D	224	29% 55% 13%
3	K	139	27% 28% 64% 7%
3	L	139	25% 35% 56% 9%

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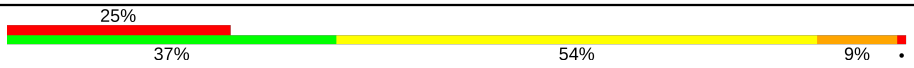
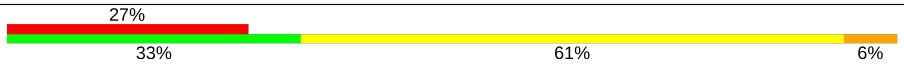
Mol	Chain	Length	Quality of chain
3	M	139	
3	N	139	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10912 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1653	1035	275	338	5			
1	C	215	Total	C	N	O	S	0	0	0
			1653	1035	275	338	5			

- Molecule 2 is a protein called FAB.

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.

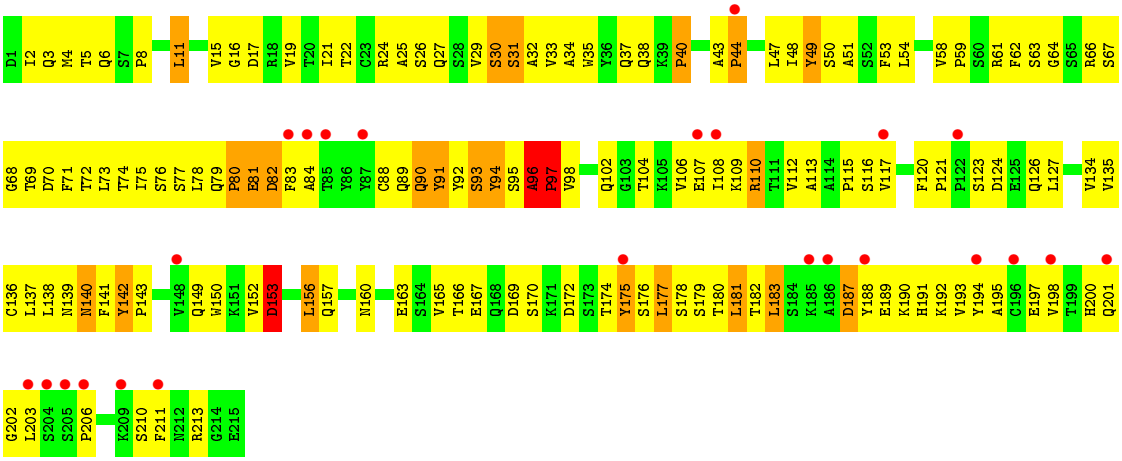
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	139	Total	C	N	O	S	0	0	0
			1075	690	192	191	2			
3	L	139	Total	C	N	O	S	0	0	0
			1075	690	192	191	2			
3	M	139	Total	C	N	O	S	0	0	0
			1075	690	192	191	2			
3	N	139	Total	C	N	O	S	0	0	0
			1075	690	192	191	2			

3 Residue-property plots (i)

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

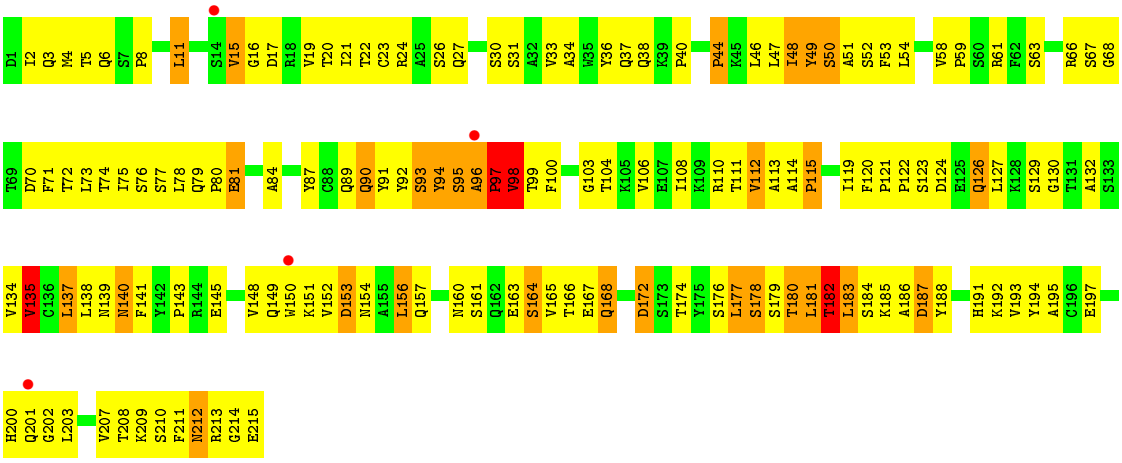
- Molecule 1: FAB

Chain A:



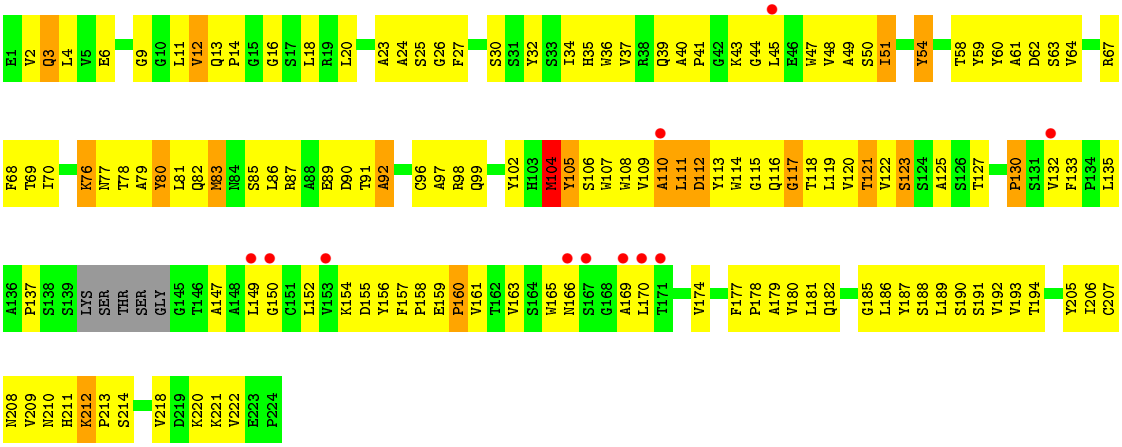
- Molecule 1: FAB

Chain C:



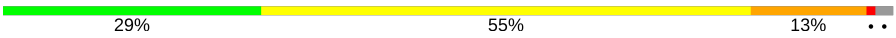
- Molecule 2: FAB

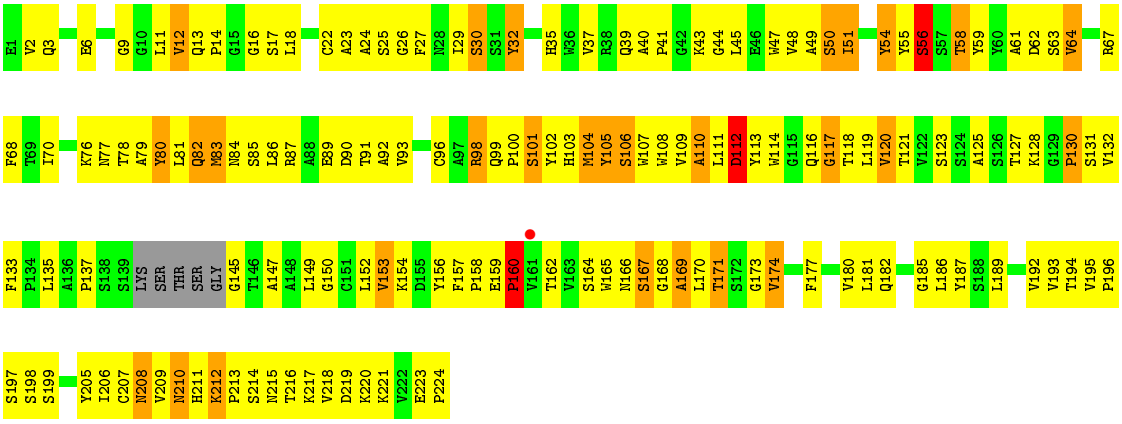
Chain B:



• Molecule 2: FAB

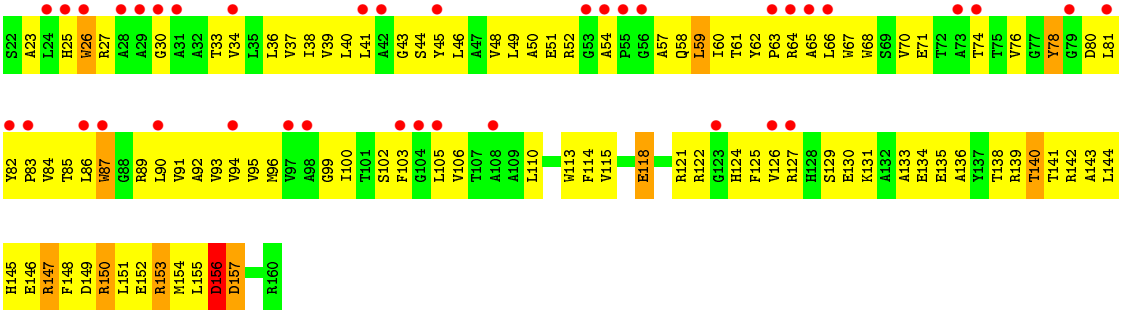
Chain D:





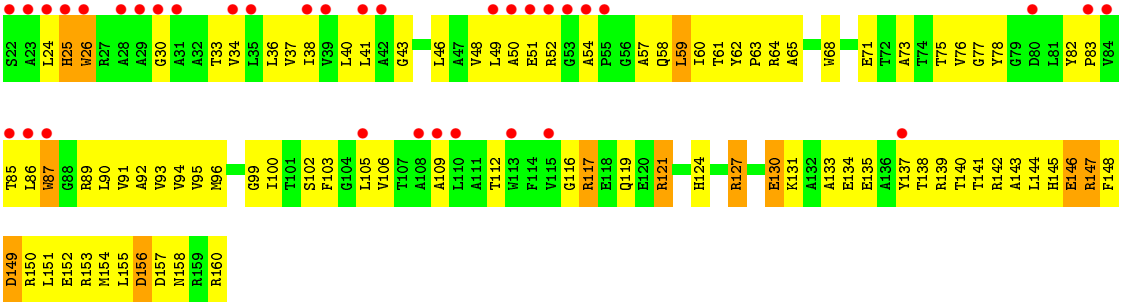
• Molecule 3: Voltage-gated potassium channel

Chain K:

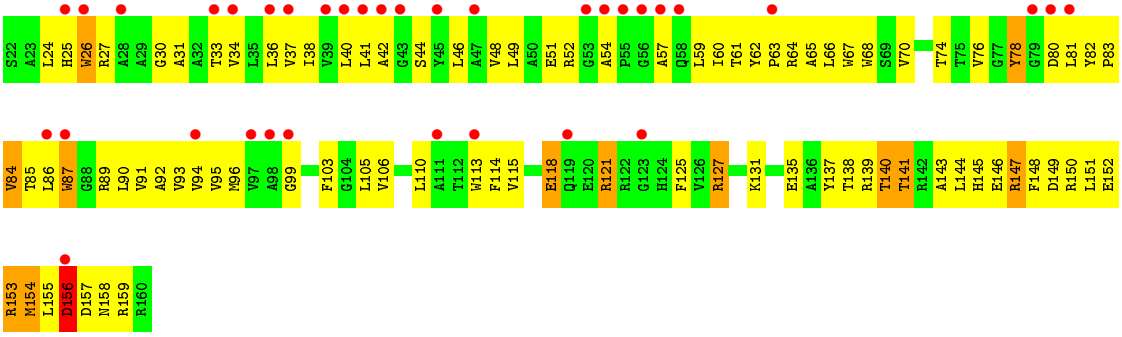


• Molecule 3: Voltage-gated potassium channel

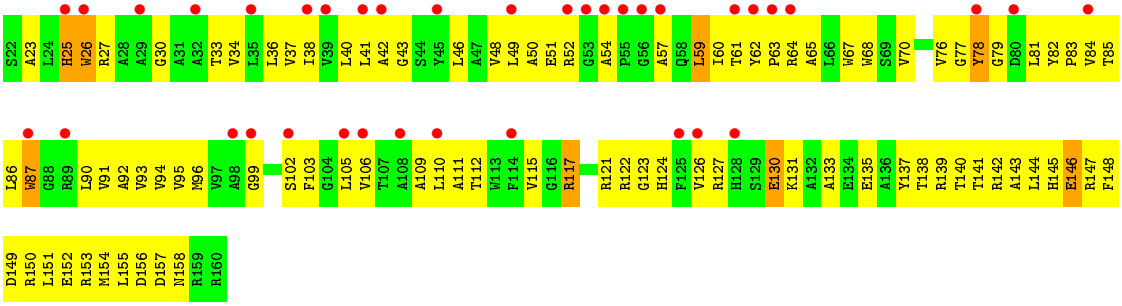
Chain L:



• Molecule 3: Voltage-gated potassium channel



• Molecule 3: Voltage-gated potassium channel



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	115.80Å 173.91Å 339.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.80 49.42 – 3.49	Depositor EDS
% Data completeness (in resolution range)	94.8 (40.00-3.80) 93.0 (49.42-3.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.270 , 0.331 0.262 , 0.311	Depositor DCC
R_{free} test set	2048 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	140.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 204.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	10912	wwPDB-VP
Average B, all atoms (Å^2)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.35	0/1689	0.76	3/2292 (0.1%)
1	C	0.45	0/1689	0.72	1/2292 (0.0%)
2	B	0.39	0/1698	0.69	0/2319
2	D	0.47	0/1698	0.74	1/2319 (0.0%)
3	K	0.31	0/1100	0.54	0/1501
3	L	0.31	0/1100	0.52	0/1501
3	M	0.33	0/1100	0.54	0/1501
3	N	0.30	0/1100	0.52	0/1501
All	All	0.38	0/11174	0.66	5/15226 (0.0%)

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	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	ALA	C-N-CD	-15.37	86.79	120.60
1	A	95	SER	N-CA-C	-9.82	84.47	111.00
1	C	95	SER	N-CA-C	-7.91	89.64	111.00
2	D	131	SER	N-CA-C	-5.78	95.41	111.00
1	A	96	ALA	C-N-CA	5.03	143.12	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	94	TYR	Sidechain

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	1653	0	1604	213	0
1	C	1653	0	1604	213	0
2	B	1653	0	1597	223	0
2	D	1653	0	1597	227	0
3	K	1075	0	1066	150	0
3	L	1075	0	1066	122	0
3	M	1075	0	1066	123	0
3	N	1075	0	1066	108	0
All	All	10912	0	10666	1241	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 58.

All (1241) 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)
3:L:116:GLY:O	3:L:119:GLN:HG2	1.45	1.16
1:A:94:TYR:HB2	3:M:150:ARG:HH21	1.16	1.08
1:C:165:VAL:HG12	1:C:177:LEU:HD22	1.37	1.05
3:K:61:THR:HG22	3:K:63:PRO:HD2	1.39	1.04
3:L:61:THR:HG22	3:L:63:PRO:HD2	1.43	1.00
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.43	1.00
1:A:38:GLN:HE22	2:B:39:GLN:HE22	1.09	0.99
2:B:212:LYS:HD3	2:B:212:LYS:H	1.23	0.99
2:D:40:ALA:HB3	2:D:43:LYS:HB2	1.44	0.99
1:A:177:LEU:HD12	1:A:178:SER:H	1.28	0.98
3:M:61:THR:HG22	3:M:63:PRO:HD2	1.45	0.98
2:B:212:LYS:HG2	2:B:213:PRO:HD3	1.45	0.96
1:C:59:PRO:HB3	1:C:61:ARG:NH1	1.82	0.95
2:B:24:ALA:HB3	2:B:77:ASN:ND2	1.82	0.94
2:D:119:LEU:HD21	2:D:121:THR:HG23	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HD2	1:A:98:VAL:H	1.32	0.93
1:A:98:VAL:HG21	2:B:47:TRP:CD1	2.05	0.92
3:N:61:THR:HG22	3:N:63:PRO:HD2	1.49	0.92
1:A:165:VAL:HG12	1:A:177:LEU:HD22	1.51	0.91
2:B:91:THR:HG22	2:B:121:THR:HA	1.52	0.91
1:C:182:THR:C	1:C:183:LEU:HD12	1.90	0.91
1:C:91:TYR:CA	1:C:97:PRO:HB3	2.01	0.90
1:C:49:TYR:HD2	2:D:109:VAL:HA	1.35	0.90
2:D:6:GLU:HG3	2:D:96:CYS:SG	2.12	0.90
1:A:97:PRO:CD	1:A:98:VAL:H	1.83	0.90
1:C:91:TYR:HA	1:C:97:PRO:HB3	1.54	0.89
1:A:189:GLU:HA	1:A:213:ARG:HH12	1.36	0.89
1:A:137:LEU:HD21	1:A:139:ASN:HB2	1.50	0.89
1:A:177:LEU:CD1	1:A:178:SER:H	1.85	0.89
1:C:11:LEU:O	1:C:11:LEU:HD23	1.70	0.89
1:A:189:GLU:HA	1:A:213:ARG:NH1	1.88	0.89
1:A:89:GLN:NE2	1:A:98:VAL:HG12	1.88	0.88
2:D:50:SER:O	2:D:70:ILE:HD13	1.72	0.88
1:A:97:PRO:HD2	1:A:98:VAL:HG22	1.52	0.88
1:C:177:LEU:HD12	1:C:178:SER:H	1.38	0.88
1:A:160:ASN:HD21	1:A:181:LEU:HD13	1.38	0.88
1:A:153:ASP:HA	1:A:193:VAL:HB	1.56	0.88
2:B:130:PRO:HB3	2:B:156:TYR:HB3	1.54	0.88
1:C:135:VAL:HB	1:C:180:THR:HG23	1.53	0.87
1:A:11:LEU:HD22	1:A:106:VAL:HG22	1.57	0.87
1:A:113:ALA:O	1:A:115:PRO:HD3	1.75	0.86
2:B:111:LEU:HB2	2:B:114:TRP:HE1	1.37	0.86
1:A:83:PHE:HB2	1:A:108:ILE:HG12	1.55	0.86
3:M:144:LEU:HD23	3:M:148:PHE:HE1	1.39	0.86
1:A:137:LEU:HD23	1:A:139:ASN:H	1.41	0.85
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.56	0.85
3:L:147:ARG:NH1	3:M:148:PHE:HB3	1.89	0.85
3:L:46:LEU:HB2	3:L:91:VAL:HG11	1.57	0.85
1:C:54:LEU:O	1:C:54:LEU:HD12	1.76	0.85
1:C:94:TYR:HB2	3:K:150:ARG:HH21	1.39	0.85
2:D:137:PRO:HB3	2:D:149:LEU:HB3	1.57	0.84
1:C:96:ALA:HB3	2:D:47:TRP:CZ2	2.14	0.83
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.61	0.82
3:M:48:VAL:HG21	3:M:62:TYR:HA	1.60	0.82
1:C:4:MET:CE	1:C:90:GLN:HB3	2.09	0.82
1:A:54:LEU:O	1:A:54:LEU:HD12	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:ALA:HB3	2:D:77:ASN:ND2	1.95	0.82
1:A:34:ALA:HA	1:A:48:ILE:O	1.81	0.81
2:B:91:THR:HG22	2:B:122:VAL:N	1.96	0.81
2:D:18:LEU:HD12	2:D:120:VAL:CG1	2.10	0.81
1:A:110:ARG:HB2	1:A:110:ARG:NH1	1.95	0.81
2:D:132:VAL:HG21	2:D:218:VAL:HG11	1.61	0.81
3:M:155:LEU:O	3:M:157:ASP:N	2.14	0.80
3:L:61:THR:HB	3:L:64:ARG:HG2	1.63	0.80
3:N:61:THR:HB	3:N:64:ARG:HG2	1.62	0.80
2:D:166:ASN:HB2	2:D:169:ALA:HB3	1.61	0.80
3:N:124:HIS:HA	3:N:127:ARG:HG2	1.63	0.80
1:C:137:LEU:HD11	2:D:192:VAL:HG21	1.63	0.79
3:N:126:VAL:O	3:N:130:GLU:HB2	1.82	0.79
2:B:91:THR:HG23	2:B:122:VAL:HG12	1.63	0.78
1:A:89:GLN:HE21	1:A:98:VAL:HG12	1.47	0.78
1:C:11:LEU:HD11	1:C:19:VAL:HG13	1.66	0.78
1:C:33:VAL:HG12	1:C:34:ALA:H	1.47	0.78
1:C:90:GLN:HE22	1:C:93:SER:HB3	1.49	0.77
1:C:49:TYR:CD2	2:D:109:VAL:HA	2.19	0.77
1:A:33:VAL:HG13	1:A:89:GLN:O	1.83	0.77
2:D:55:TYR:HE2	2:D:102:TYR:HB2	1.49	0.77
3:M:61:THR:HB	3:M:64:ARG:HG2	1.67	0.77
1:C:54:LEU:HD13	1:C:58:VAL:HB	1.64	0.77
1:C:44:PRO:HG2	2:D:45:LEU:HD11	1.65	0.77
2:B:91:THR:HG22	2:B:122:VAL:H	1.48	0.77
1:A:83:PHE:HD1	1:A:106:VAL:O	1.67	0.77
2:B:81:LEU:HD22	2:B:83:MET:HG2	1.67	0.76
2:D:118:THR:HG22	2:D:119:LEU:H	1.49	0.76
1:C:33:VAL:HG12	1:C:34:ALA:N	2.01	0.76
1:C:191:HIS:O	1:C:213:ARG:HD3	1.85	0.76
1:A:97:PRO:CD	1:A:98:VAL:N	2.46	0.76
2:B:27:PHE:CE2	2:B:98:ARG:HD2	2.21	0.76
1:A:153:ASP:OD1	1:A:191:HIS:HB3	1.86	0.76
3:K:70:VAL:HG11	3:L:93:VAL:HG13	1.66	0.75
3:K:155:LEU:O	3:K:157:ASP:N	2.18	0.75
1:A:115:PRO:HG3	1:A:141:PHE:HB2	1.69	0.75
2:B:23:ALA:N	2:B:78:THR:HG23	2.02	0.75
3:N:23:ALA:O	3:N:27:ARG:HD3	1.87	0.75
1:C:4:MET:HE2	1:C:90:GLN:HB3	1.68	0.74
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.68	0.74
1:C:46:LEU:HD12	1:C:47:LEU:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:TYR:CE2	2:D:102:TYR:HB2	2.22	0.74
3:K:153:ARG:HB2	3:K:153:ARG:NH1	2.02	0.74
2:B:211:HIS:CE1	2:B:213:PRO:HB2	2.22	0.74
1:C:92:TYR:O	1:C:93:SER:O	2.05	0.74
3:K:67:TRP:HZ3	3:L:92:ALA:HB3	1.49	0.74
3:K:129:SER:HA	3:L:130:GLU:OE2	1.87	0.74
1:C:91:TYR:CB	1:C:97:PRO:HB3	2.18	0.73
3:K:148:PHE:HB3	3:N:147:ARG:NH1	2.03	0.73
2:B:48:VAL:HG13	2:B:64:VAL:HG11	1.70	0.73
2:B:206:ILE:HG12	2:B:221:LYS:HA	1.70	0.73
2:B:81:LEU:HD22	2:B:83:MET:CG	2.17	0.73
3:N:106:VAL:O	3:N:110:LEU:HG	1.88	0.73
1:C:46:LEU:HD12	1:C:47:LEU:H	1.54	0.73
1:C:22:THR:HG22	1:C:72:THR:OG1	1.87	0.73
3:M:44:SER:OG	3:M:66:LEU:HA	1.88	0.73
3:K:127:ARG:HG3	3:K:131:LYS:HE3	1.68	0.73
1:C:89:GLN:HE22	2:D:111:LEU:CD2	2.01	0.72
1:C:67:SER:HB3	1:C:70:ASP:HB2	1.72	0.72
1:A:149:GLN:HB2	1:A:197:GLU:HB3	1.70	0.72
1:C:11:LEU:HD21	1:C:106:VAL:HG13	1.71	0.72
1:A:11:LEU:CD2	1:A:106:VAL:HG13	2.20	0.71
3:L:116:GLY:O	3:L:119:GLN:CG	2.33	0.71
2:B:64:VAL:HG21	2:B:68:PHE:HB2	1.72	0.71
2:D:107:TRP:CE3	3:K:153:ARG:HG2	2.25	0.71
2:D:2:VAL:HA	2:D:26:GLY:HA3	1.72	0.71
3:L:135:GLU:O	3:L:139:ARG:HG3	1.90	0.71
3:N:135:GLU:O	3:N:139:ARG:HG3	1.90	0.71
1:C:11:LEU:CD2	1:C:106:VAL:HG13	2.21	0.71
1:A:94:TYR:HB2	3:M:150:ARG:NH2	2.00	0.70
1:C:61:ARG:HG2	1:C:61:ARG:HH11	1.56	0.70
3:K:147:ARG:HE	3:L:145:HIS:CD2	2.09	0.70
1:C:134:VAL:HG12	1:C:135:VAL:H	1.56	0.70
2:D:217:LYS:HD3	2:D:218:VAL:N	2.06	0.70
2:D:62:ASP:O	2:D:64:VAL:N	2.24	0.70
3:K:48:VAL:HG21	3:K:62:TYR:HA	1.74	0.70
3:K:96:MET:HE2	3:N:76:VAL:HG21	1.74	0.70
3:K:106:VAL:O	3:K:110:LEU:HG	1.91	0.70
3:K:67:TRP:CZ3	3:L:92:ALA:HB3	2.26	0.70
3:K:93:VAL:HA	3:K:96:MET:SD	2.31	0.70
1:C:49:TYR:O	1:C:50:SER:HB2	1.92	0.70
1:A:109:LYS:HG3	1:A:142:TYR:OH	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:151:LEU:HA	3:L:154:MET:HG3	1.73	0.70
3:M:127:ARG:HA	3:M:127:ARG:HE	1.56	0.70
3:M:62:TYR:HB2	3:M:63:PRO:HD3	1.74	0.69
2:D:119:LEU:CD2	2:D:121:THR:HG23	2.20	0.69
2:D:195:VAL:HG11	2:D:205:TYR:CZ	2.27	0.69
1:A:163:GLU:HB3	1:A:177:LEU:HD11	1.74	0.69
1:C:165:VAL:CG1	1:C:177:LEU:HD22	2.19	0.69
2:B:150:GLY:HA2	2:B:165:TRP:CH2	2.27	0.69
2:B:9:GLY:H	2:B:118:THR:HG21	1.58	0.69
3:N:62:TYR:HB2	3:N:63:PRO:HD3	1.75	0.69
1:C:6:GLN:NE2	1:C:104:THR:N	2.41	0.69
2:D:11:LEU:HD23	2:D:12:VAL:N	2.08	0.69
3:K:61:THR:HB	3:K:64:ARG:HG2	1.74	0.69
3:K:103:PHE:CD2	3:L:100:ILE:HG21	2.27	0.69
1:A:189:GLU:CA	1:A:213:ARG:HH12	2.06	0.69
2:B:91:THR:HG23	2:B:122:VAL:CG1	2.22	0.69
1:A:149:GLN:HB3	1:A:156:LEU:HD21	1.75	0.68
1:C:112:VAL:HG12	1:C:113:ALA:H	1.59	0.68
2:D:64:VAL:HG21	2:D:68:PHE:CG	2.29	0.68
2:B:39:GLN:HG3	2:B:44:GLY:O	1.93	0.68
1:C:212:ASN:N	1:C:212:ASN:HD22	1.91	0.68
2:B:165:TRP:HZ3	2:B:222:VAL:HG21	1.59	0.68
3:K:144:LEU:HG	3:L:144:LEU:HD21	1.74	0.68
3:L:151:LEU:O	3:L:154:MET:HB2	1.92	0.68
3:L:92:ALA:O	3:L:96:MET:HG3	1.94	0.68
2:B:80:TYR:N	2:B:80:TYR:CD2	2.62	0.68
2:B:83:MET:HE1	2:B:120:VAL:HG21	1.76	0.68
1:C:134:VAL:HG12	1:C:135:VAL:N	2.09	0.68
2:D:165:TRP:CH2	2:D:207:CYS:HB3	2.29	0.68
2:B:80:TYR:N	2:B:80:TYR:HD2	1.92	0.67
1:C:6:GLN:NE2	1:C:103:GLY:HA2	2.09	0.67
3:M:151:LEU:HD23	3:M:155:LEU:HD13	1.76	0.67
1:C:15:VAL:HG23	1:C:78:LEU:O	1.93	0.67
1:A:97:PRO:HD2	1:A:98:VAL:N	2.08	0.67
3:M:44:SER:CB	3:M:66:LEU:HA	2.24	0.67
1:A:2:ILE:HB	1:A:90:GLN:HE21	1.59	0.67
2:B:111:LEU:HB2	2:B:114:TRP:NE1	2.10	0.67
1:C:137:LEU:HD12	2:D:192:VAL:HG11	1.77	0.67
1:A:98:VAL:CG2	2:B:47:TRP:CD1	2.77	0.67
1:A:11:LEU:HD23	1:A:11:LEU:C	2.15	0.67
1:A:2:ILE:HB	1:A:90:GLN:NE2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:30:GLY:O	3:N:34:VAL:HG23	1.95	0.67
1:C:115:PRO:HB3	1:C:141:PHE:HB3	1.77	0.67
3:N:59:LEU:HD11	3:N:65:ALA:HA	1.77	0.67
1:A:91:TYR:O	1:A:91:TYR:HD2	1.77	0.66
2:D:41:PRO:HD3	2:D:91:THR:O	1.94	0.66
3:N:54:ALA:HB3	3:N:57:ALA:HB2	1.77	0.66
3:L:90:LEU:O	3:L:94:VAL:HG23	1.95	0.66
3:L:58:GLN:HB3	3:L:64:ARG:NH1	2.10	0.66
1:A:137:LEU:CD2	1:A:139:ASN:H	2.07	0.66
2:B:51:ILE:O	2:B:51:ILE:HG23	1.96	0.66
2:B:6:GLU:CD	2:B:117:GLY:H	1.99	0.66
1:C:214:GLY:O	1:C:215:GLU:HG3	1.94	0.66
2:D:145:GLY:N	2:D:197:SER:HG	1.94	0.66
2:D:195:VAL:HB	2:D:205:TYR:OH	1.95	0.66
1:A:96:ALA:HB3	2:B:59:TYR:CG	2.30	0.66
2:D:211:HIS:HB3	2:D:214:SER:OG	1.95	0.66
3:M:137:TYR:O	3:M:140:THR:HB	1.96	0.66
3:M:54:ALA:HB3	3:M:57:ALA:HB2	1.78	0.66
2:B:91:THR:HG22	2:B:121:THR:CA	2.24	0.66
2:B:137:PRO:HB3	2:B:149:LEU:HB3	1.77	0.65
2:D:39:GLN:O	2:D:92:ALA:HB1	1.96	0.65
3:M:93:VAL:HA	3:M:96:MET:SD	2.35	0.65
2:D:208:ASN:N	2:D:208:ASN:HD22	1.93	0.65
1:A:198:VAL:O	1:A:206:PRO:HB3	1.97	0.65
2:B:179:ALA:HA	2:B:189:LEU:HB3	1.78	0.65
3:M:144:LEU:CD1	3:N:144:LEU:HG	2.26	0.65
1:A:22:THR:HG22	1:A:72:THR:OG1	1.96	0.65
2:B:82:GLN:O	2:B:82:GLN:HG3	1.97	0.65
1:C:181:LEU:O	1:C:182:THR:HG23	1.96	0.65
3:M:147:ARG:HE	3:N:145:HIS:CD2	2.15	0.65
1:A:110:ARG:HB2	1:A:110:ARG:HH11	1.61	0.65
2:B:64:VAL:HG21	2:B:68:PHE:CG	2.31	0.65
2:B:23:ALA:HA	2:B:78:THR:HG23	1.79	0.64
1:C:2:ILE:O	1:C:99:THR:HG21	1.98	0.64
2:B:152:LEU:HD21	2:B:154:LYS:HD2	1.80	0.64
1:C:79:GLN:HB3	1:C:80:PRO:HD2	1.78	0.64
1:C:203:LEU:HD13	1:C:207:VAL:HG23	1.80	0.64
3:L:62:TYR:HB2	3:L:63:PRO:HD3	1.80	0.64
3:K:93:VAL:HG22	3:N:70:VAL:HG11	1.80	0.64
2:B:177:PHE:O	2:B:189:LEU:HD12	1.98	0.64
2:B:36:TRP:CG	2:B:81:LEU:HD12	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:91:VAL:O	3:K:95:VAL:HG23	1.98	0.64
3:K:92:ALA:O	3:K:96:MET:HG3	1.98	0.64
2:B:109:VAL:O	2:B:110:ALA:O	2.16	0.64
2:B:23:ALA:CA	2:B:78:THR:HG23	2.28	0.64
2:D:108:TRP:HE1	3:K:153:ARG:HD3	1.63	0.64
2:D:159:GLU:OE1	2:D:160:PRO:HA	1.98	0.64
1:A:137:LEU:HD23	1:A:139:ASN:N	2.13	0.63
2:B:47:TRP:CE3	2:B:61:ALA:HB2	2.33	0.63
1:C:31:SER:H	1:C:66:ARG:CZ	2.11	0.63
2:B:24:ALA:HB3	2:B:77:ASN:HD22	1.62	0.63
2:B:130:PRO:HA	2:B:155:ASP:O	1.98	0.63
1:C:11:LEU:HD22	1:C:106:VAL:HG22	1.79	0.63
2:D:166:ASN:CB	2:D:169:ALA:HB3	2.28	0.63
3:L:147:ARG:O	3:L:150:ARG:HB3	1.99	0.63
1:A:79:GLN:HB3	1:A:80:PRO:HD2	1.79	0.63
1:C:127:LEU:H	1:C:127:LEU:HD12	1.63	0.63
2:D:211:HIS:HE1	2:D:213:PRO:HB2	1.64	0.63
3:L:30:GLY:O	3:L:34:VAL:HG23	1.98	0.63
1:A:160:ASN:ND2	1:A:181:LEU:HD13	2.12	0.63
2:D:40:ALA:HA	2:D:92:ALA:HB2	1.79	0.63
1:A:11:LEU:HD22	1:A:106:VAL:HG13	1.80	0.62
1:A:49:TYR:HD1	1:A:49:TYR:O	1.82	0.62
2:B:91:THR:O	2:B:92:ALA:HB2	1.98	0.62
3:K:153:ARG:HE	3:K:157:ASP:CG	2.03	0.62
3:K:62:TYR:HB2	3:K:63:PRO:HD3	1.80	0.62
1:A:141:PHE:HE2	1:A:177:LEU:HB2	1.64	0.62
1:A:120:PHE:HB2	1:A:135:VAL:HG13	1.80	0.62
1:C:59:PRO:HB3	1:C:61:ARG:HH12	1.64	0.62
3:N:122:ARG:O	3:N:126:VAL:HG23	2.00	0.62
1:A:89:GLN:HE22	2:B:111:LEU:HD21	1.65	0.62
1:A:89:GLN:HE22	2:B:111:LEU:CD2	2.12	0.62
2:B:119:LEU:HD23	2:B:119:LEU:O	2.00	0.62
2:B:109:VAL:HG23	2:B:112:ASP:HB3	1.80	0.62
1:C:33:VAL:CG1	1:C:34:ALA:H	2.13	0.62
3:M:153:ARG:NE	3:M:157:ASP:OD2	2.33	0.62
3:N:90:LEU:O	3:N:94:VAL:HG23	1.99	0.62
3:N:92:ALA:O	3:N:96:MET:HG3	1.98	0.62
2:B:165:TRP:CH2	2:B:207:CYS:HB3	2.35	0.61
2:B:3:GLN:HG3	2:B:25:SER:OG	2.00	0.61
2:D:62:ASP:C	2:D:64:VAL:H	2.03	0.61
3:K:59:LEU:HA	3:K:64:ARG:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:151:LEU:HD23	3:M:151:LEU:C	2.19	0.61
2:B:2:VAL:HG22	2:B:26:GLY:HA3	1.82	0.61
2:B:91:THR:CG2	2:B:122:VAL:N	2.62	0.61
2:D:108:TRP:NE1	3:K:153:ARG:HD3	2.14	0.61
1:A:112:VAL:HG13	1:A:142:TYR:O	1.99	0.61
2:D:51:ILE:O	2:D:51:ILE:HG23	2.00	0.61
3:M:91:VAL:O	3:M:95:VAL:HG23	1.99	0.61
3:N:121:ARG:HA	3:N:121:ARG:HE	1.65	0.61
3:K:100:ILE:HG21	3:N:103:PHE:CD2	2.35	0.61
3:K:30:GLY:O	3:K:34:VAL:HG23	2.00	0.61
2:B:212:LYS:HD3	2:B:212:LYS:N	2.06	0.61
1:C:6:GLN:NE2	1:C:104:THR:H	1.99	0.61
3:K:37:VAL:O	3:K:41:LEU:HG	2.00	0.61
1:A:137:LEU:C	1:A:137:LEU:HD23	2.20	0.61
1:A:83:PHE:CD1	1:A:107:GLU:HA	2.35	0.61
2:B:132:VAL:HG21	2:B:218:VAL:HG11	1.81	0.61
2:B:127:THR:HG22	2:B:158:PRO:HD3	1.81	0.61
2:D:173:GLY:O	2:D:193:VAL:HG23	2.00	0.61
1:A:49:TYR:O	1:A:50:SER:HB3	2.01	0.61
2:B:18:LEU:HD12	2:B:120:VAL:HG13	1.81	0.61
1:C:122:PRO:HG3	1:C:188:TYR:CZ	2.36	0.61
1:C:38:GLN:O	1:C:84:ALA:HB1	2.00	0.61
3:L:91:VAL:O	3:L:95:VAL:HG23	2.01	0.61
3:M:144:LEU:HD11	3:N:144:LEU:HG	1.83	0.61
2:B:149:LEU:HD12	2:B:222:VAL:HG11	1.82	0.61
2:B:206:ILE:HG23	2:B:220:LYS:C	2.21	0.61
1:C:166:THR:HG22	1:C:176:SER:H	1.66	0.61
1:C:177:LEU:CD1	1:C:178:SER:H	2.10	0.61
1:C:192:LYS:HA	1:C:213:ARG:HG2	1.82	0.61
2:D:98:ARG:NH1	2:D:112:ASP:HB3	2.16	0.61
3:K:151:LEU:HD22	3:N:151:LEU:HD21	1.83	0.61
2:B:36:TRP:NE1	2:B:81:LEU:HB2	2.16	0.61
1:C:112:VAL:HG12	1:C:113:ALA:N	2.16	0.61
3:K:43:GLY:HA3	3:K:68:TRP:HZ3	1.65	0.61
2:B:161:VAL:HG12	2:B:211:HIS:CD2	2.36	0.60
2:B:6:GLU:HG3	2:B:96:CYS:SG	2.40	0.60
2:D:18:LEU:HD12	2:D:120:VAL:HG13	1.82	0.60
3:L:147:ARG:CG	3:L:147:ARG:HH11	2.13	0.60
2:B:91:THR:CG2	2:B:122:VAL:H	2.14	0.60
1:A:156:LEU:HD13	1:A:157:GLN:N	2.16	0.60
1:C:90:GLN:OE1	1:C:92:TYR:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:LEU:O	2:D:152:LEU:HG	2.00	0.60
2:D:157:PHE:CD1	2:D:158:PRO:HA	2.35	0.60
2:D:80:TYR:N	2:D:80:TYR:HD2	1.98	0.60
3:L:147:ARG:HH11	3:M:148:PHE:HB3	1.66	0.60
3:M:153:ARG:NH1	3:M:153:ARG:HB2	2.16	0.60
3:M:41:LEU:HD23	3:M:66:LEU:HD11	1.82	0.60
1:C:192:LYS:HG2	1:C:192:LYS:O	2.01	0.60
2:D:206:ILE:HG23	2:D:220:LYS:O	2.01	0.60
2:B:159:GLU:HA	2:B:159:GLU:OE1	2.01	0.60
3:M:153:ARG:HA	3:M:157:ASP:OD2	2.02	0.60
3:M:24:LEU:HD12	3:M:27:ARG:HB2	1.83	0.60
1:A:66:ARG:HG3	1:A:71:PHE:CE2	2.36	0.60
1:C:94:TYR:HB2	3:K:150:ARG:NH2	2.14	0.60
2:D:132:VAL:HG21	2:D:218:VAL:CG1	2.29	0.60
3:L:59:LEU:HD11	3:L:65:ALA:HA	1.84	0.60
1:A:172:ASP:O	1:A:174:THR:HG23	2.02	0.60
1:A:59:PRO:HB3	1:A:61:ARG:CZ	2.32	0.60
3:L:43:GLY:HA2	3:L:91:VAL:CG1	2.32	0.60
1:C:36:TYR:HH	2:D:111:LEU:H	1.50	0.60
2:D:13:GLN:OE1	2:D:13:GLN:N	2.34	0.60
2:D:147:ALA:O	2:D:194:THR:HA	2.02	0.60
2:D:67:ARG:NH1	2:D:90:ASP:OD2	2.34	0.60
3:L:54:ALA:HB3	3:L:57:ALA:HB2	1.84	0.60
2:B:111:LEU:N	2:B:111:LEU:HD23	2.17	0.60
2:D:103:HIS:O	3:K:153:ARG:NH1	2.34	0.60
1:C:4:MET:HE1	1:C:90:GLN:HB3	1.84	0.60
1:A:35:TRP:HB2	1:A:48:ILE:HB	1.84	0.59
2:B:149:LEU:HD12	2:B:222:VAL:CG1	2.32	0.59
2:B:11:LEU:HD23	2:B:12:VAL:N	2.16	0.59
2:D:35:HIS:O	2:D:96:CYS:HA	2.02	0.59
1:A:11:LEU:HD22	1:A:106:VAL:CG2	2.32	0.59
2:D:207:CYS:C	2:D:208:ASN:HD22	2.06	0.59
1:A:91:TYR:CD2	1:A:91:TYR:O	2.55	0.59
2:B:116:GLN:HA	2:B:116:GLN:OE1	2.03	0.59
2:B:47:TRP:CZ3	2:B:61:ALA:HB2	2.37	0.59
2:D:135:LEU:HB2	2:D:150:GLY:O	2.03	0.59
2:D:168:GLY:O	2:D:171:THR:HG22	2.02	0.59
3:M:144:LEU:HD23	3:M:148:PHE:CE1	2.30	0.59
1:C:89:GLN:HE22	2:D:111:LEU:HD23	1.67	0.59
3:K:153:ARG:NE	3:K:157:ASP:OD2	2.36	0.59
3:N:147:ARG:NH1	3:N:147:ARG:HB3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ILE:HG23	2:B:220:LYS:O	2.03	0.59
3:M:30:GLY:O	3:M:34:VAL:HG23	2.02	0.59
2:B:87:ARG:HG2	2:B:89:GLU:OE2	2.03	0.59
1:C:30:SER:HA	1:C:66:ARG:NH2	2.18	0.59
1:C:49:TYR:O	1:C:49:TYR:CG	2.55	0.59
3:N:138:THR:O	3:N:142:ARG:HG3	2.02	0.59
1:A:152:VAL:O	1:A:153:ASP:HB2	2.03	0.58
1:A:177:LEU:HD12	1:A:178:SER:N	2.09	0.58
1:A:192:LYS:HA	1:A:213:ARG:CD	2.32	0.58
1:A:67:SER:HB3	1:A:70:ASP:HB2	1.84	0.58
1:C:165:VAL:HG12	1:C:177:LEU:CD2	2.25	0.58
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.85	0.58
2:D:50:SER:O	2:D:51:ILE:HB	2.01	0.58
3:K:54:ALA:HB3	3:K:57:ALA:HB2	1.85	0.58
3:N:93:VAL:HA	3:N:96:MET:SD	2.42	0.58
1:C:161:SER:HA	1:C:180:THR:O	2.02	0.58
2:D:2:VAL:HG13	2:D:27:PHE:HD2	1.68	0.58
3:L:93:VAL:HA	3:L:96:MET:SD	2.42	0.58
3:M:76:VAL:HG21	3:N:96:MET:HE2	1.85	0.58
1:A:35:TRP:CD1	1:A:48:ILE:HB	2.37	0.58
1:C:95:SER:O	1:C:95:SER:OG	2.19	0.58
1:C:89:GLN:HE22	2:D:111:LEU:HD21	1.67	0.58
3:K:153:ARG:HA	3:K:153:ARG:NE	2.18	0.58
3:L:37:VAL:O	3:L:41:LEU:HG	2.02	0.58
2:B:62:ASP:O	2:B:64:VAL:N	2.37	0.58
1:C:127:LEU:N	1:C:127:LEU:HD12	2.17	0.58
2:D:125:ALA:HB3	2:D:157:PHE:CZ	2.38	0.58
2:D:210:ASN:HD22	2:D:211:HIS:N	2.02	0.58
1:A:112:VAL:HG11	1:A:202:GLY:HA3	1.85	0.58
3:L:138:THR:O	3:L:142:ARG:HG3	2.03	0.58
2:B:205:TYR:O	2:B:222:VAL:N	2.36	0.58
1:C:61:ARG:HG2	1:C:61:ARG:NH1	2.17	0.58
1:A:25:ALA:C	1:A:27:GLN:H	2.05	0.58
1:C:91:TYR:HB2	1:C:97:PRO:HB3	1.85	0.58
2:D:181:LEU:HD23	2:D:182:GLN:O	2.04	0.58
3:L:51:GLU:O	3:L:60:ILE:HG22	2.03	0.58
1:A:117:VAL:HG21	1:A:198:VAL:HG21	1.85	0.58
2:D:39:GLN:HG3	2:D:44:GLY:O	2.04	0.58
1:A:195:ALA:HA	1:A:210:SER:HB3	1.84	0.58
1:A:11:LEU:HD11	1:A:19:VAL:HG13	1.84	0.58
1:A:78:LEU:HD12	1:A:79:GLN:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:N	1:A:183:LEU:HD12	2.19	0.58
2:B:170:LEU:HD11	2:B:193:VAL:HG21	1.86	0.58
1:C:20:THR:HG22	1:C:74:THR:OG1	2.03	0.58
3:K:89:ARG:HH22	3:N:81:LEU:HD11	1.68	0.58
3:L:99:GLY:O	3:L:103:PHE:HD1	1.86	0.58
3:N:151:LEU:O	3:N:155:LEU:HD12	2.04	0.58
2:B:104:MET:O	2:B:106:SER:N	2.37	0.57
2:B:36:TRP:CZ3	2:B:96:CYS:HB3	2.39	0.57
3:L:36:LEU:O	3:L:40:LEU:HG	2.03	0.57
2:B:2:VAL:CA	2:B:26:GLY:HA3	2.31	0.57
1:C:6:GLN:HE22	1:C:103:GLY:HA2	1.69	0.57
3:K:44:SER:OG	3:K:66:LEU:HA	2.03	0.57
3:M:92:ALA:O	3:M:96:MET:HG3	2.04	0.57
1:A:38:GLN:NE2	2:B:39:GLN:HE22	1.90	0.57
2:D:83:MET:HE2	2:D:120:VAL:HG11	1.86	0.57
3:M:24:LEU:HA	3:M:27:ARG:HD3	1.86	0.57
3:M:37:VAL:O	3:M:41:LEU:HG	2.04	0.57
3:K:81:LEU:HD11	3:L:89:ARG:NH2	2.19	0.57
3:N:117:ARG:NH1	3:N:117:ARG:HG2	2.20	0.57
1:A:8:PRO:HD2	1:A:21:ILE:HG23	1.85	0.57
2:D:212:LYS:HG2	2:D:213:PRO:HD3	1.87	0.57
1:C:30:SER:HA	1:C:66:ARG:HH22	1.70	0.57
1:C:31:SER:HB3	1:C:66:ARG:HD2	1.86	0.57
3:L:151:LEU:O	3:L:155:LEU:HD12	2.04	0.57
2:D:87:ARG:HG2	2:D:89:GLU:OE2	2.04	0.57
3:K:155:LEU:HD21	3:N:155:LEU:HG	1.85	0.57
3:N:25:HIS:CD2	3:N:25:HIS:H	2.23	0.57
1:A:166:THR:HG22	1:A:176:SER:H	1.69	0.56
2:B:82:GLN:O	2:B:82:GLN:CG	2.52	0.56
1:C:66:ARG:HG3	1:C:71:PHE:CE2	2.40	0.56
3:K:122:ARG:O	3:K:126:VAL:HG13	2.04	0.56
3:L:43:GLY:HA2	3:L:91:VAL:HG12	1.87	0.56
3:N:36:LEU:O	3:N:40:LEU:HG	2.05	0.56
2:B:2:VAL:HG13	2:B:27:PHE:HD2	1.70	0.56
2:D:218:VAL:HG22	2:D:219:ASP:N	2.20	0.56
3:K:81:LEU:HD11	3:L:89:ARG:HH22	1.69	0.56
3:M:147:ARG:HH11	3:M:147:ARG:HG3	1.70	0.56
2:B:83:MET:CE	2:B:120:VAL:HG21	2.35	0.56
2:B:166:ASN:HB2	2:B:169:ALA:HB3	1.87	0.56
1:C:95:SER:O	1:C:96:ALA:C	2.44	0.56
3:K:147:ARG:HG3	3:K:147:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:HIS:O	1:A:213:ARG:NH1	2.30	0.56
1:A:93:SER:O	1:A:94:TYR:CB	2.54	0.56
2:B:111:LEU:N	2:B:111:LEU:CD2	2.67	0.56
1:C:143:PRO:HB2	1:C:145:GLU:OE1	2.04	0.56
1:C:156:LEU:HD13	1:C:157:GLN:N	2.20	0.56
3:M:153:ARG:NE	3:M:153:ARG:HA	2.20	0.56
3:N:147:ARG:HH11	3:N:147:ARG:HB3	1.70	0.56
2:B:212:LYS:CG	2:B:213:PRO:HD3	2.28	0.56
2:D:98:ARG:HG3	2:D:99:GLN:N	2.20	0.56
3:K:99:GLY:O	3:K:103:PHE:HD1	1.89	0.56
3:N:48:VAL:HG11	3:N:62:TYR:CD1	2.40	0.56
1:A:67:SER:O	1:A:69:THR:N	2.38	0.56
2:B:109:VAL:O	2:B:109:VAL:CG2	2.53	0.56
2:B:205:TYR:O	2:B:222:VAL:HG23	2.06	0.56
2:B:2:VAL:HG11	2:B:98:ARG:HH11	1.71	0.56
2:D:24:ALA:HB3	2:D:77:ASN:HD21	1.70	0.56
3:K:155:LEU:HD11	3:L:155:LEU:CD2	2.36	0.56
2:B:2:VAL:HG11	2:B:98:ARG:NH1	2.21	0.56
1:C:184:SER:O	1:C:185:LYS:C	2.44	0.56
1:C:59:PRO:HB3	1:C:61:ARG:CZ	2.35	0.56
3:M:48:VAL:HG11	3:M:62:TYR:CD1	2.40	0.56
3:N:37:VAL:O	3:N:41:LEU:HG	2.05	0.56
1:C:120:PHE:CD1	2:D:135:LEU:HB3	2.41	0.56
3:L:147:ARG:HH12	3:M:148:PHE:HB3	1.67	0.56
2:B:159:GLU:HG2	2:B:187:TYR:CD2	2.40	0.56
2:D:58:THR:C	2:D:59:TYR:CD1	2.79	0.56
2:B:112:ASP:O	2:B:113:TYR:HD1	1.89	0.56
2:D:214:SER:O	2:D:215:ASN:HB3	2.06	0.56
3:M:150:ARG:HD3	3:N:152:GLU:OE2	2.06	0.56
1:C:192:LYS:HG3	1:C:213:ARG:HG2	1.86	0.55
2:D:181:LEU:HD23	2:D:181:LEU:C	2.25	0.55
2:B:64:VAL:HG21	2:B:68:PHE:CB	2.35	0.55
3:N:99:GLY:O	3:N:103:PHE:HD1	1.88	0.55
3:N:49:LEU:HD12	3:N:52:ARG:HD2	1.87	0.55
1:A:35:TRP:HD1	1:A:48:ILE:HB	1.71	0.55
1:C:24:ARG:HG3	1:C:70:ASP:OD1	2.06	0.55
1:A:50:SER:O	1:A:51:ALA:HB3	2.07	0.55
2:B:37:VAL:HG11	2:B:114:TRP:CH2	2.40	0.55
2:D:80:TYR:N	2:D:80:TYR:CD2	2.68	0.55
3:N:91:VAL:O	3:N:95:VAL:HG23	2.07	0.55
2:B:4:LEU:HD21	2:B:27:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PRO:HG3	1:C:188:TYR:CE2	2.41	0.55
3:M:33:THR:O	3:M:37:VAL:HG23	2.05	0.55
3:M:90:LEU:O	3:M:94:VAL:HG23	2.07	0.55
3:M:99:GLY:O	3:M:103:PHE:HD1	1.89	0.55
1:C:202:GLY:O	1:C:203:LEU:HD23	2.07	0.55
2:D:37:VAL:HG22	2:D:47:TRP:HA	1.89	0.55
3:K:151:LEU:HD23	3:K:151:LEU:C	2.27	0.55
3:N:121:ARG:NE	3:N:121:ARG:HA	2.22	0.55
1:A:34:ALA:CA	1:A:48:ILE:O	2.53	0.55
2:B:9:GLY:N	2:B:118:THR:HG21	2.21	0.55
1:C:50:SER:O	1:C:51:ALA:HB3	2.05	0.55
3:K:80:ASP:HB3	3:L:82:TYR:CZ	2.42	0.55
3:L:87:TRP:CE3	3:L:90:LEU:HD12	2.41	0.55
1:A:189:GLU:HA	1:A:213:ARG:CZ	2.37	0.55
1:A:59:PRO:HB3	1:A:61:ARG:NH1	2.20	0.55
2:B:147:ALA:O	2:B:194:THR:HA	2.07	0.55
2:B:127:THR:HG22	2:B:158:PRO:CD	2.36	0.55
1:C:181:LEU:HD12	1:C:183:LEU:HD11	1.87	0.55
2:D:132:VAL:CG2	2:D:218:VAL:HG11	2.33	0.55
3:K:90:LEU:O	3:K:94:VAL:HG23	2.07	0.55
1:C:152:VAL:O	1:C:152:VAL:HG23	2.07	0.55
2:D:35:HIS:CD2	2:D:111:LEU:HD11	2.41	0.55
3:K:140:THR:HG22	3:K:141:THR:N	2.22	0.55
3:M:138:THR:HA	3:M:141:THR:HG23	1.87	0.55
2:D:185:GLY:C	2:D:186:LEU:HD12	2.26	0.55
3:L:68:TRP:HZ2	3:L:92:ALA:HB2	1.71	0.55
3:M:127:ARG:HD3	3:M:131:LYS:HE3	1.89	0.55
1:A:152:VAL:O	1:A:152:VAL:HG23	2.07	0.54
1:A:187:ASP:HA	1:A:190:LYS:HE2	1.89	0.54
1:C:33:VAL:CG1	1:C:34:ALA:N	2.69	0.54
3:K:127:ARG:O	3:K:131:LYS:HG3	2.07	0.54
1:A:11:LEU:CD1	1:A:19:VAL:HG13	2.37	0.54
1:A:47:LEU:O	1:A:48:ILE:HD13	2.07	0.54
2:B:181:LEU:HD12	2:B:187:TYR:CE1	2.42	0.54
2:D:149:LEU:HD23	2:D:193:VAL:O	2.07	0.54
2:D:2:VAL:HA	2:D:25:SER:O	2.07	0.54
3:K:46:LEU:HB2	3:K:91:VAL:HG11	1.90	0.54
3:M:143:ALA:O	3:M:147:ARG:HB2	2.07	0.54
3:N:150:ARG:HG2	3:N:151:LEU:N	2.22	0.54
1:A:137:LEU:CD2	1:A:139:ASN:HB2	2.29	0.54
2:B:64:VAL:CG2	2:B:68:PHE:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:135:GLU:O	3:K:138:THR:HG22	2.08	0.54
3:M:34:VAL:O	3:M:38:ILE:HG13	2.07	0.54
3:N:102:SER:O	3:N:106:VAL:HG23	2.08	0.54
1:C:115:PRO:HB3	1:C:141:PHE:CB	2.38	0.54
2:D:11:LEU:HD11	2:D:157:PHE:CE2	2.42	0.54
1:A:182:THR:C	1:A:183:LEU:HD12	2.28	0.54
1:A:121:PRO:HB3	1:A:211:PHE:CE1	2.43	0.54
2:B:67:ARG:HD2	2:B:85:SER:O	2.08	0.54
1:C:34:ALA:HB2	2:D:110:ALA:HB2	1.89	0.54
3:K:144:LEU:CD1	3:L:144:LEU:HG	2.38	0.54
1:A:112:VAL:HG12	1:A:113:ALA:N	2.23	0.54
1:A:11:LEU:O	1:A:11:LEU:HD23	2.08	0.54
1:A:138:LEU:O	1:A:141:PHE:HD2	1.91	0.54
2:D:2:VAL:HG13	2:D:27:PHE:CD2	2.42	0.54
1:A:16:GLY:O	1:A:77:SER:HA	2.08	0.54
1:A:49:TYR:CD1	1:A:49:TYR:O	2.61	0.53
2:B:98:ARG:O	2:B:111:LEU:HA	2.08	0.53
2:B:125:ALA:O	2:B:157:PHE:HE2	1.91	0.53
2:B:181:LEU:HD12	2:B:187:TYR:HE1	1.73	0.53
2:B:60:TYR:HE2	2:B:70:ILE:HB	1.73	0.53
3:K:144:LEU:HD11	3:L:144:LEU:HG	1.90	0.53
3:L:124:HIS:O	3:L:127:ARG:HB2	2.08	0.53
3:M:151:LEU:HD23	3:M:151:LEU:O	2.07	0.53
3:M:65:ALA:HA	3:M:68:TRP:HB3	1.90	0.53
1:A:79:GLN:HB3	1:A:81:GLU:OE1	2.08	0.53
3:K:157:ASP:OD1	3:K:157:ASP:N	2.38	0.53
1:A:163:GLU:HA	1:A:178:SER:O	2.08	0.53
2:B:163:VAL:HA	2:B:208:ASN:O	2.08	0.53
2:B:27:PHE:CD2	2:B:98:ARG:HD2	2.43	0.53
1:C:123:SER:OG	1:C:126:GLN:HB2	2.07	0.53
2:B:81:LEU:HD22	2:B:83:MET:HG3	1.91	0.53
3:L:65:ALA:HA	3:L:68:TRP:HB3	1.90	0.53
1:A:58:VAL:HG13	1:A:59:PRO:HD2	1.89	0.53
1:C:11:LEU:CD2	1:C:106:VAL:HG22	2.38	0.53
1:C:49:TYR:HD2	2:D:109:VAL:CA	2.15	0.53
1:C:61:ARG:O	1:C:75:ILE:HA	2.07	0.53
3:L:76:VAL:HG21	3:M:96:MET:CE	2.39	0.53
3:M:65:ALA:O	3:M:68:TRP:HB3	2.09	0.53
1:A:115:PRO:HG2	1:A:200:HIS:CD2	2.44	0.53
1:A:201:GLN:O	1:A:201:GLN:HG3	2.07	0.53
3:K:138:THR:HG23	3:K:139:ARG:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HA	1:A:213:ARG:HD3	1.89	0.53
2:B:111:LEU:H	2:B:111:LEU:HD23	1.73	0.53
2:B:32:TYR:OH	2:B:98:ARG:NH2	2.42	0.53
2:D:208:ASN:N	2:D:208:ASN:ND2	2.54	0.53
3:K:33:THR:O	3:K:37:VAL:HG23	2.08	0.53
1:A:59:PRO:HB2	1:A:62:PHE:CD1	2.43	0.53
2:B:91:THR:CG2	2:B:121:THR:HA	2.33	0.53
3:M:147:ARG:HG3	3:M:147:ARG:NH1	2.23	0.53
3:M:80:ASP:HB3	3:N:82:TYR:OH	2.08	0.53
1:C:79:GLN:HB3	1:C:80:PRO:CD	2.39	0.53
2:D:116:GLN:OE1	2:D:116:GLN:HA	2.07	0.53
2:D:195:VAL:HB	2:D:196:PRO:HD2	1.91	0.53
3:K:147:ARG:HG3	3:K:147:ARG:NH1	2.23	0.53
3:L:148:PHE:O	3:L:149:ASP:C	2.47	0.53
2:B:2:VAL:HA	2:B:26:GLY:CA	2.33	0.52
3:L:26:TRP:HA	3:L:26:TRP:HE3	1.75	0.52
3:N:117:ARG:HH11	3:N:117:ARG:HG2	1.73	0.52
2:B:212:LYS:H	2:B:212:LYS:CD	2.05	0.52
1:C:33:VAL:HG13	1:C:89:GLN:O	2.09	0.52
2:D:82:GLN:O	2:D:82:GLN:HG3	2.07	0.52
3:K:48:VAL:HG11	3:K:62:TYR:CD1	2.45	0.52
3:L:48:VAL:HG11	3:L:62:TYR:CD1	2.43	0.52
1:C:50:SER:C	1:C:52:SER:H	2.12	0.52
2:D:78:THR:HB	2:D:80:TYR:CE2	2.44	0.52
3:M:46:LEU:HB2	3:M:91:VAL:HG11	1.90	0.52
1:A:93:SER:O	1:A:94:TYR:HB3	2.09	0.52
2:B:150:GLY:HA2	2:B:165:TRP:HH2	1.73	0.52
2:D:153:VAL:HB	2:D:189:LEU:HD23	1.92	0.52
3:N:26:TRP:HA	3:N:26:TRP:CE3	2.45	0.52
2:D:67:ARG:O	2:D:84:ASN:HB2	2.10	0.52
3:M:89:ARG:O	3:M:93:VAL:HG23	2.09	0.52
1:A:188:TYR:HA	1:A:194:TYR:OH	2.09	0.52
2:B:157:PHE:CD1	2:B:158:PRO:HA	2.43	0.52
2:B:67:ARG:NH1	2:B:90:ASP:OD2	2.41	0.52
1:C:137:LEU:HD23	1:C:138:LEU:N	2.25	0.52
2:D:102:TYR:O	3:K:149:ASP:HB3	2.09	0.52
3:L:50:ALA:O	3:L:85:THR:HG21	2.09	0.52
3:M:26:TRP:CE3	3:M:26:TRP:HA	2.45	0.52
1:A:35:TRP:N	1:A:48:ILE:O	2.41	0.52
1:A:3:GLN:HE21	1:A:4:MET:H	1.58	0.52
1:C:148:VAL:O	1:C:148:VAL:CG2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ALA:HA	1:C:210:SER:HB3	1.91	0.52
3:L:26:TRP:CE3	3:L:26:TRP:HA	2.44	0.52
3:N:154:MET:O	3:N:158:ASN:HB3	2.09	0.52
1:A:177:LEU:CD1	1:A:178:SER:N	2.65	0.52
2:D:29:ILE:O	2:D:30:SER:C	2.48	0.52
3:N:54:ALA:HB1	3:N:84:VAL:HG23	1.92	0.52
2:B:3:GLN:CG	2:B:25:SER:OG	2.58	0.52
3:K:155:LEU:HD22	3:N:151:LEU:CD2	2.40	0.52
3:K:155:LEU:O	3:K:156:ASP:C	2.48	0.52
2:B:14:PRO:HD3	2:B:123:SER:C	2.30	0.51
1:C:191:HIS:O	1:C:213:ARG:CD	2.58	0.51
1:C:211:PHE:C	1:C:212:ASN:HD22	2.12	0.51
2:D:195:VAL:HG21	2:D:205:TYR:CE2	2.45	0.51
3:K:102:SER:O	3:K:106:VAL:HG23	2.10	0.51
3:K:59:LEU:HD12	3:K:64:ARG:HG3	1.92	0.51
3:L:147:ARG:CG	3:L:147:ARG:NH1	2.73	0.51
3:N:34:VAL:O	3:N:38:ILE:HG13	2.10	0.51
3:N:87:TRP:CE3	3:N:90:LEU:HD12	2.44	0.51
1:A:96:ALA:HB3	2:B:59:TYR:CD2	2.45	0.51
2:B:6:GLU:OE2	2:B:115:GLY:HA3	2.10	0.51
3:K:92:ALA:HB3	3:N:67:TRP:CZ3	2.45	0.51
1:A:91:TYR:OH	2:B:108:TRP:O	2.25	0.51
2:B:2:VAL:HG13	2:B:27:PHE:CD2	2.45	0.51
1:C:181:LEU:CD1	1:C:183:LEU:HD11	2.40	0.51
3:K:127:ARG:HE	3:K:127:ARG:HA	1.75	0.51
3:L:40:LEU:HD21	3:L:73:ALA:HB2	1.92	0.51
1:C:94:TYR:CE2	3:K:147:ARG:NE	2.79	0.51
2:D:11:LEU:HD11	2:D:157:PHE:HE2	1.75	0.51
2:D:81:LEU:HD23	2:D:82:GLN:N	2.25	0.51
3:K:155:LEU:HD11	3:L:155:LEU:HD21	1.91	0.51
1:A:135:VAL:HG23	1:A:179:SER:O	2.11	0.51
2:B:76:LYS:HD2	2:B:76:LYS:H	1.76	0.51
3:M:26:TRP:HE3	3:M:26:TRP:HA	1.75	0.51
1:A:149:GLN:O	1:A:197:GLU:HB3	2.11	0.51
2:B:109:VAL:CG2	2:B:112:ASP:HB3	2.41	0.51
2:D:101:SER:O	2:D:107:TRP:HB2	2.10	0.51
2:D:54:TYR:HD1	2:D:54:TYR:C	2.14	0.51
3:K:153:ARG:CZ	3:K:153:ARG:HB2	2.41	0.51
3:L:150:ARG:HD3	3:M:152:GLU:OE2	2.10	0.51
1:A:15:VAL:HG22	1:A:16:GLY:N	2.25	0.51
2:B:211:HIS:HE1	2:B:213:PRO:HB2	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:SER:N	1:C:66:ARG:CZ	2.74	0.51
2:D:152:LEU:O	2:D:153:VAL:C	2.47	0.51
3:K:143:ALA:HB1	3:L:145:HIS:HE1	1.76	0.51
3:K:58:GLN:O	3:K:60:ILE:N	2.40	0.51
1:C:195:ALA:HA	1:C:210:SER:CB	2.41	0.51
1:C:31:SER:HB3	1:C:66:ARG:NH1	2.26	0.51
2:D:137:PRO:HB3	2:D:149:LEU:CB	2.36	0.51
3:L:105:LEU:HD23	3:L:105:LEU:C	2.31	0.51
3:L:139:ARG:HA	3:L:142:ARG:HD2	1.93	0.51
3:L:141:THR:HG23	3:L:142:ARG:N	2.26	0.51
3:M:138:THR:CG2	3:M:139:ARG:N	2.74	0.51
1:A:192:LYS:HB2	1:A:192:LYS:NZ	2.27	0.50
1:C:58:VAL:HG13	1:C:59:PRO:HD2	1.93	0.50
2:D:13:GLN:H	2:D:13:GLN:CD	2.15	0.50
2:D:18:LEU:CD1	2:D:120:VAL:HG13	2.40	0.50
3:K:135:GLU:O	3:K:136:ALA:C	2.50	0.50
3:L:158:ASN:HD21	3:M:159:ARG:CB	2.24	0.50
3:N:26:TRP:HE3	3:N:26:TRP:HA	1.75	0.50
3:N:51:GLU:O	3:N:60:ILE:HG22	2.11	0.50
1:C:81:GLU:OE1	1:C:81:GLU:N	2.44	0.50
2:D:54:TYR:CD1	2:D:54:TYR:C	2.83	0.50
3:M:59:LEU:HD13	3:M:81:LEU:HB3	1.92	0.50
1:A:44:PRO:HG2	2:B:45:LEU:HD11	1.93	0.50
1:A:79:GLN:HB2	1:A:82:ASP:OD2	2.11	0.50
1:C:148:VAL:O	1:C:148:VAL:HG23	2.10	0.50
3:L:138:THR:C	3:L:141:THR:HG22	2.31	0.50
3:M:140:THR:HG22	3:M:141:THR:N	2.26	0.50
3:M:147:ARG:HE	3:N:145:HIS:HD2	1.58	0.50
3:L:76:VAL:HG21	3:M:96:MET:HE2	1.93	0.50
3:K:151:LEU:HD13	3:N:151:LEU:HD13	1.94	0.50
3:L:24:LEU:HD12	3:L:24:LEU:N	2.26	0.50
2:B:9:GLY:HA3	2:B:118:THR:CG2	2.42	0.50
1:C:44:PRO:CG	2:D:45:LEU:HD11	2.40	0.50
2:D:50:SER:HB3	2:D:59:TYR:HB2	1.93	0.50
3:L:144:LEU:HD21	3:L:148:PHE:HE1	1.76	0.50
3:K:152:GLU:HG3	3:N:154:MET:SD	2.51	0.50
1:C:200:HIS:C	1:C:202:GLY:H	2.15	0.50
2:D:103:HIS:O	3:K:153:ARG:CZ	2.59	0.50
2:B:60:TYR:OH	2:B:70:ILE:N	2.45	0.50
1:C:195:ALA:CB	1:C:210:SER:HB3	2.42	0.50
3:K:26:TRP:HA	3:K:26:TRP:CE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:33:THR:O	3:L:37:VAL:HG23	2.12	0.50
3:M:144:LEU:HD12	3:N:144:LEU:HG	1.93	0.50
1:A:25:ALA:O	1:A:27:GLN:N	2.45	0.50
2:B:4:LEU:HD21	2:B:27:PHE:HZ	1.76	0.50
2:B:82:GLN:HE21	2:B:82:GLN:HA	1.76	0.50
2:B:35:HIS:O	2:B:96:CYS:HA	2.12	0.50
1:C:126:GLN:HG3	2:D:133:PHE:CD2	2.47	0.50
3:L:65:ALA:O	3:L:68:TRP:HB3	2.12	0.50
3:K:23:ALA:O	3:K:27:ARG:HG3	2.12	0.49
3:L:133:ALA:O	3:L:137:TYR:CD1	2.64	0.49
3:M:153:ARG:CZ	3:M:153:ARG:HB2	2.42	0.49
1:A:110:ARG:HH11	1:A:110:ARG:CB	2.25	0.49
1:A:33:VAL:HG12	1:A:34:ALA:N	2.26	0.49
2:B:165:TRP:HZ2	2:B:191:SER:O	1.95	0.49
1:C:182:THR:H	1:C:183:LEU:HD12	1.77	0.49
1:C:184:SER:O	1:C:187:ASP:N	2.44	0.49
2:D:93:VAL:HA	2:D:118:THR:O	2.13	0.49
3:L:147:ARG:HG3	3:L:147:ARG:NH1	2.27	0.49
2:B:189:LEU:N	2:B:189:LEU:HD23	2.26	0.49
1:C:31:SER:HB3	1:C:66:ARG:HH11	1.77	0.49
2:D:149:LEU:HD21	2:D:193:VAL:HG13	1.93	0.49
2:D:221:LYS:HG2	2:D:223:GLU:HG2	1.94	0.49
2:D:81:LEU:C	2:D:81:LEU:HD23	2.33	0.49
3:K:130:GLU:O	3:K:134:GLU:HG3	2.11	0.49
3:K:61:THR:CG2	3:K:63:PRO:HD2	2.27	0.49
3:M:138:THR:HG23	3:M:139:ARG:N	2.26	0.49
3:M:49:LEU:HD12	3:M:52:ARG:HD2	1.93	0.49
3:K:100:ILE:HG21	3:N:103:PHE:HD2	1.77	0.49
3:N:133:ALA:O	3:N:137:TYR:CD1	2.64	0.49
1:A:163:GLU:OE1	1:A:177:LEU:HD11	2.12	0.49
1:C:49:TYR:CD2	2:D:109:VAL:HG22	2.47	0.49
2:D:137:PRO:HG2	2:D:224:PRO:HG3	1.94	0.49
2:D:64:VAL:HG21	2:D:68:PHE:CD2	2.46	0.49
3:M:61:THR:HB	3:M:64:ARG:CG	2.40	0.49
1:C:183:LEU:N	1:C:183:LEU:HD12	2.27	0.49
1:C:48:ILE:HG23	1:C:53:PHE:O	2.12	0.49
2:D:2:VAL:HG12	2:D:113:TYR:CD2	2.47	0.49
3:M:42:ALA:O	3:M:46:LEU:HG	2.12	0.49
3:N:138:THR:C	3:N:141:THR:HG22	2.33	0.49
3:N:50:ALA:O	3:N:85:THR:HG21	2.12	0.49
1:A:61:ARG:O	1:A:75:ILE:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:39:VAL:HG12	3:K:95:VAL:HG22	1.95	0.49
3:N:109:ALA:HA	3:N:112:THR:HG22	1.94	0.49
3:N:65:ALA:O	3:N:68:TRP:HB3	2.13	0.49
1:A:136:CYS:HB2	1:A:150:TRP:CZ2	2.48	0.49
1:A:163:GLU:CB	1:A:177:LEU:HD11	2.43	0.49
2:D:174:VAL:HG13	2:D:193:VAL:HB	1.95	0.49
3:L:150:ARG:HD3	3:M:152:GLU:CD	2.32	0.49
3:N:61:THR:HB	3:N:64:ARG:CG	2.40	0.49
2:D:218:VAL:HG22	2:D:219:ASP:H	1.77	0.49
3:N:141:THR:HG23	3:N:142:ARG:N	2.28	0.49
2:B:159:GLU:OE1	2:B:160:PRO:HA	2.11	0.49
2:B:54:TYR:CD1	2:B:54:TYR:C	2.85	0.49
1:C:134:VAL:HG11	1:C:150:TRP:HZ3	1.77	0.49
2:B:135:LEU:HB2	2:B:150:GLY:O	2.13	0.49
2:B:170:LEU:CD1	2:B:193:VAL:HG21	2.42	0.49
2:D:152:LEU:HD21	2:D:154:LYS:HD2	1.95	0.49
2:D:180:VAL:O	2:D:180:VAL:HG13	2.12	0.49
3:L:155:LEU:O	3:L:158:ASN:N	2.43	0.49
3:M:36:LEU:O	3:M:40:LEU:HG	2.13	0.49
3:M:78:TYR:CE2	3:N:77:GLY:HA2	2.48	0.49
1:A:175:TYR:CD1	1:A:175:TYR:N	2.80	0.48
1:C:141:PHE:O	1:C:174:THR:HB	2.13	0.48
3:M:59:LEU:HD11	3:M:65:ALA:HA	1.95	0.48
2:B:62:ASP:C	2:B:64:VAL:H	2.17	0.48
3:K:92:ALA:HB3	3:N:67:TRP:HZ3	1.78	0.48
1:A:137:LEU:HD21	1:A:139:ASN:CB	2.34	0.48
1:A:81:GLU:C	1:A:83:PHE:H	2.17	0.48
2:D:205:TYR:C	2:D:206:ILE:HG13	2.33	0.48
3:M:78:TYR:O	3:N:79:GLY:HA3	2.13	0.48
1:A:134:VAL:O	1:A:180:THR:HG23	2.13	0.48
1:A:94:TYR:CE2	3:M:147:ARG:NE	2.81	0.48
1:C:172:ASP:OD2	1:C:172:ASP:N	2.45	0.48
1:C:98:VAL:HG21	2:D:47:TRP:CD1	2.49	0.48
2:D:167:SER:HA	2:D:208:ASN:OD1	2.13	0.48
1:C:92:TYR:OH	3:L:156:ASP:OD2	2.31	0.48
3:L:86:LEU:HG	3:L:87:TRP:CZ3	2.48	0.48
1:A:194:TYR:O	1:A:210:SER:HB2	2.14	0.48
2:B:185:GLY:C	2:B:186:LEU:HD12	2.34	0.48
1:C:21:ILE:O	1:C:72:THR:HA	2.13	0.48
3:K:105:LEU:C	3:K:105:LEU:HD23	2.33	0.48
3:L:156:ASP:O	3:L:160:ARG:OXT	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:86:LEU:HG	3:M:87:TRP:CZ3	2.48	0.48
3:K:152:GLU:CD	3:N:150:ARG:HD3	2.34	0.48
1:A:63:SER:O	1:A:73:LEU:HD12	2.14	0.48
1:C:96:ALA:O	1:C:97:PRO:C	2.51	0.48
2:D:159:GLU:HA	2:D:159:GLU:OE1	2.12	0.48
2:B:13:GLN:N	2:B:13:GLN:OE1	2.39	0.48
2:B:39:GLN:O	2:B:92:ALA:HB1	2.14	0.48
1:C:26:SER:O	1:C:27:GLN:HB3	2.13	0.48
2:D:12:VAL:HG11	2:D:18:LEU:HG	1.96	0.48
2:D:130:PRO:HB3	2:D:156:TYR:HB3	1.95	0.48
2:D:196:PRO:HG2	2:D:199:SER:OG	2.14	0.48
3:K:140:THR:O	3:K:141:THR:C	2.52	0.48
3:K:76:VAL:HG22	3:L:75:THR:HA	1.96	0.48
1:A:176:SER:O	2:B:177:PHE:HE2	1.97	0.48
1:C:49:TYR:HD1	1:C:49:TYR:H	1.61	0.48
3:L:102:SER:O	3:L:106:VAL:HG23	2.14	0.48
2:D:212:LYS:HD3	2:D:212:LYS:N	2.29	0.48
3:M:149:ASP:O	3:M:150:ARG:C	2.52	0.48
1:C:6:GLN:HE21	1:C:104:THR:N	2.11	0.48
1:C:89:GLN:HE21	1:C:98:VAL:HG13	1.78	0.48
2:D:13:GLN:O	2:D:14:PRO:C	2.50	0.48
2:D:164:SER:OG	2:D:208:ASN:HB2	2.13	0.48
3:K:65:ALA:HA	3:K:68:TRP:HB3	1.95	0.48
3:L:89:ARG:O	3:L:93:VAL:HG23	2.14	0.48
3:M:54:ALA:HB3	3:M:57:ALA:CB	2.44	0.48
1:C:49:TYR:O	1:C:50:SER:CB	2.61	0.47
2:D:64:VAL:HG21	2:D:68:PHE:HB2	1.95	0.47
3:L:145:HIS:O	3:L:146:GLU:C	2.52	0.47
1:A:15:VAL:CG2	1:A:16:GLY:N	2.77	0.47
2:B:109:VAL:HG23	2:B:109:VAL:O	2.14	0.47
2:B:154:LYS:O	2:B:155:ASP:HB2	2.14	0.47
1:C:182:THR:N	1:C:183:LEU:HD12	2.29	0.47
2:D:135:LEU:HB2	2:D:150:GLY:C	2.33	0.47
3:K:45:TYR:CD1	3:K:62:TYR:HE2	2.32	0.47
3:N:123:GLY:O	3:N:126:VAL:HB	2.14	0.47
3:K:89:ARG:HB3	3:N:67:TRP:CE3	2.49	0.47
1:A:25:ALA:C	1:A:27:GLN:N	2.67	0.47
2:B:40:ALA:HB1	2:B:41:PRO:HD2	1.94	0.47
1:C:135:VAL:HG22	1:C:135:VAL:O	2.15	0.47
3:K:144:LEU:HD23	3:K:148:PHE:HE2	1.79	0.47
3:L:124:HIS:O	3:L:124:HIS:ND1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:THR:O	1:C:208:THR:HG22	2.13	0.47
1:C:34:ALA:HA	1:C:48:ILE:O	2.15	0.47
3:M:149:ASP:O	3:M:152:GLU:HB3	2.14	0.47
2:B:49:ALA:CB	2:B:70:ILE:HD12	2.44	0.47
3:K:26:TRP:HE3	3:K:26:TRP:HA	1.78	0.47
3:M:106:VAL:O	3:M:110:LEU:HG	2.14	0.47
3:M:151:LEU:HD23	3:M:155:LEU:CD1	2.44	0.47
1:A:149:GLN:HB2	1:A:197:GLU:CB	2.43	0.47
1:A:166:THR:HG22	1:A:176:SER:N	2.29	0.47
1:A:24:ARG:HD3	1:A:70:ASP:OD1	2.14	0.47
2:D:212:LYS:HD3	2:D:212:LYS:H	1.79	0.47
3:K:34:VAL:O	3:K:38:ILE:HG13	2.14	0.47
3:K:49:LEU:HD12	3:K:52:ARG:HD2	1.95	0.47
3:K:78:TYR:CD2	3:L:77:GLY:HA2	2.48	0.47
3:M:121:ARG:O	3:M:121:ARG:HG3	2.14	0.47
3:M:145:HIS:O	3:M:146:GLU:C	2.52	0.47
3:N:143:ALA:O	3:N:146:GLU:N	2.48	0.47
2:B:62:ASP:C	2:B:64:VAL:N	2.66	0.47
1:C:119:ILE:HG22	1:C:209:LYS:HB3	1.97	0.47
2:D:96:CYS:SG	2:D:96:CYS:O	2.73	0.47
3:N:33:THR:O	3:N:37:VAL:HG23	2.15	0.47
1:A:120:PHE:HA	1:A:121:PRO:HD3	1.75	0.47
1:A:123:SER:OG	2:B:133:PHE:HB3	2.15	0.47
1:A:137:LEU:CD2	1:A:139:ASN:N	2.75	0.47
3:K:115:VAL:HG13	3:K:118:GLU:OE2	2.14	0.47
3:K:155:LEU:CD1	3:L:155:LEU:HD22	2.45	0.47
3:M:144:LEU:O	3:M:148:PHE:N	2.47	0.47
3:M:51:GLU:O	3:M:60:ILE:HG22	2.15	0.47
1:A:98:VAL:HG21	2:B:47:TRP:NE1	2.29	0.47
2:B:50:SER:HB3	2:B:59:TYR:HB2	1.96	0.47
1:C:3:GLN:HA	1:C:3:GLN:NE2	2.30	0.47
1:C:92:TYR:C	1:C:93:SER:O	2.53	0.47
3:K:149:ASP:O	3:K:152:GLU:HB3	2.15	0.47
3:M:82:TYR:HB2	3:M:83:PRO:HD2	1.97	0.47
2:B:165:TRP:CZ3	2:B:207:CYS:HB3	2.49	0.47
2:D:181:LEU:HD12	2:D:187:TYR:CE1	2.50	0.47
2:D:50:SER:C	2:D:70:ILE:HD13	2.35	0.47
3:K:50:ALA:O	3:K:85:THR:HG21	2.15	0.47
2:B:107:TRP:O	2:B:107:TRP:CG	2.68	0.47
2:B:208:ASN:HD22	2:B:208:ASN:N	2.12	0.47
2:B:211:HIS:O	2:B:211:HIS:ND1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TRP:CE3	2:B:96:CYS:HB3	2.50	0.47
1:C:212:ASN:N	1:C:212:ASN:ND2	2.62	0.47
2:B:209:VAL:HB	2:B:218:VAL:HB	1.98	0.46
1:C:90:GLN:OE1	1:C:91:TYR:N	2.48	0.46
1:C:91:TYR:O	1:C:97:PRO:HG3	2.14	0.46
2:D:195:VAL:HG11	2:D:205:TYR:CE1	2.50	0.46
2:D:91:THR:O	2:D:92:ALA:HB2	2.14	0.46
3:L:117:ARG:HG3	3:L:117:ARG:NH1	2.30	0.46
3:M:151:LEU:O	3:M:154:MET:HB2	2.15	0.46
1:C:54:LEU:C	1:C:54:LEU:HD12	2.33	0.46
1:C:66:ARG:HG2	1:C:68:GLY:H	1.80	0.46
2:D:11:LEU:HD23	2:D:12:VAL:H	1.79	0.46
3:M:105:LEU:C	3:M:105:LEU:HD23	2.36	0.46
1:A:138:LEU:HD12	1:A:138:LEU:N	2.30	0.46
1:A:44:PRO:CG	2:B:45:LEU:HD11	2.45	0.46
2:B:159:GLU:HG2	2:B:187:TYR:CE2	2.50	0.46
2:D:145:GLY:C	2:D:196:PRO:HA	2.35	0.46
3:K:150:ARG:HD3	3:L:152:GLU:OE2	2.14	0.46
3:M:48:VAL:HG22	3:M:65:ALA:CB	2.46	0.46
1:A:53:PHE:HD1	1:A:53:PHE:H	1.62	0.46
1:A:31:SER:H	1:A:66:ARG:CZ	2.28	0.46
1:A:81:GLU:OE1	1:A:81:GLU:N	2.48	0.46
2:B:156:TYR:C	2:B:156:TYR:CD2	2.88	0.46
2:B:36:TRP:CE2	2:B:81:LEU:HB2	2.49	0.46
3:K:153:ARG:C	3:K:155:LEU:N	2.67	0.46
3:K:58:GLN:O	3:K:64:ARG:NH1	2.49	0.46
3:N:36:LEU:HD13	3:N:102:SER:OG	2.15	0.46
3:N:135:GLU:HA	3:N:138:THR:HG22	1.98	0.46
1:A:2:ILE:HG12	1:A:27:GLN:HB3	1.97	0.46
1:A:6:GLN:NE2	1:A:104:THR:N	2.64	0.46
1:A:137:LEU:HD12	2:B:192:VAL:HG11	1.98	0.46
1:C:6:GLN:NE2	1:C:103:GLY:CA	2.78	0.46
3:K:96:MET:HE2	3:N:76:VAL:CG2	2.42	0.46
3:L:87:TRP:CZ3	3:L:90:LEU:HD11	2.51	0.46
3:M:155:LEU:O	3:M:158:ASN:N	2.49	0.46
1:C:212:ASN:HB2	1:C:215:GLU:OE1	2.16	0.46
2:D:153:VAL:HB	2:D:189:LEU:CD2	2.45	0.46
2:D:162:THR:HG23	2:D:212:LYS:HE2	1.97	0.46
2:D:165:TRP:CD1	2:D:174:VAL:HG11	2.51	0.46
2:D:78:THR:HG22	2:D:79:ALA:N	2.31	0.46
3:K:133:ALA:O	3:K:134:GLU:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:138:THR:HA	3:K:141:THR:HG23	1.98	0.46
3:K:51:GLU:O	3:K:60:ILE:HG22	2.15	0.46
3:L:68:TRP:O	3:L:71:GLU:HG2	2.16	0.46
1:A:127:LEU:HD12	1:A:127:LEU:N	2.30	0.46
1:A:49:TYR:O	1:A:50:SER:CB	2.63	0.46
1:C:167:GLU:O	1:C:168:GLN:C	2.55	0.46
2:D:118:THR:HG22	2:D:119:LEU:N	2.23	0.46
3:L:87:TRP:CE3	3:L:87:TRP:HA	2.51	0.46
1:A:79:GLN:HB3	1:A:80:PRO:CD	2.44	0.46
2:B:180:VAL:O	2:B:180:VAL:HG13	2.16	0.46
1:C:193:VAL:O	1:C:193:VAL:HG12	2.16	0.46
1:A:49:TYR:CE2	2:B:109:VAL:HG12	2.50	0.45
2:B:118:THR:HG22	2:B:119:LEU:H	1.81	0.45
1:C:98:VAL:CG1	2:D:47:TRP:HB2	2.46	0.45
2:D:17:SER:OG	2:D:84:ASN:HA	2.16	0.45
3:L:46:LEU:HD12	3:L:91:VAL:HG13	1.99	0.45
3:M:61:THR:CG2	3:M:63:PRO:HD2	2.31	0.45
1:A:67:SER:HB3	1:A:70:ASP:O	2.16	0.45
1:C:89:GLN:HG2	1:C:90:GLN:N	2.32	0.45
2:D:152:LEU:O	2:D:154:LYS:N	2.50	0.45
2:D:58:THR:HB	2:D:70:ILE:CG2	2.47	0.45
3:K:115:VAL:O	3:K:118:GLU:HB3	2.16	0.45
3:K:36:LEU:O	3:K:40:LEU:HG	2.16	0.45
3:K:155:LEU:HD22	3:N:151:LEU:HD23	1.97	0.45
1:A:112:VAL:HG12	1:A:113:ALA:H	1.81	0.45
2:B:91:THR:O	2:B:92:ALA:CB	2.64	0.45
2:D:29:ILE:O	2:D:32:TYR:N	2.50	0.45
3:K:68:TRP:O	3:K:71:GLU:HG2	2.15	0.45
3:K:85:THR:O	3:K:89:ARG:HG3	2.17	0.45
3:L:34:VAL:O	3:L:38:ILE:HG13	2.17	0.45
1:A:127:LEU:HD12	1:A:127:LEU:H	1.81	0.45
2:B:156:TYR:CE2	2:B:187:TYR:HB2	2.51	0.45
2:B:207:CYS:SG	2:B:207:CYS:O	2.73	0.45
3:L:138:THR:O	3:L:141:THR:HG22	2.15	0.45
3:K:70:VAL:CG1	3:L:93:VAL:HG13	2.41	0.45
1:A:30:SER:O	1:A:31:SER:C	2.54	0.45
2:B:91:THR:HG22	2:B:121:THR:C	2.35	0.45
2:D:109:VAL:HG11	2:D:112:ASP:OD1	2.16	0.45
2:D:223:GLU:HA	2:D:224:PRO:HD3	1.77	0.45
2:D:6:GLU:CG	2:D:96:CYS:SG	2.97	0.45
3:K:80:ASP:HB3	3:L:82:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:64:ARG:O	3:K:81:LEU:HD13	2.17	0.45
3:L:135:GLU:O	3:L:138:THR:HG22	2.16	0.45
3:M:54:ALA:HB1	3:M:84:VAL:HG23	1.99	0.45
3:N:145:HIS:O	3:N:146:GLU:C	2.54	0.45
1:A:49:TYR:HB2	2:B:109:VAL:HA	1.98	0.45
1:C:90:GLN:C	1:C:90:GLN:OE1	2.55	0.45
1:C:91:TYR:HA	1:C:97:PRO:CB	2.35	0.45
2:D:107:TRP:O	2:D:107:TRP:CG	2.70	0.45
1:A:92:TYR:O	3:M:150:ARG:NH2	2.49	0.45
2:B:54:TYR:HD1	2:B:54:TYR:C	2.20	0.45
1:C:121:PRO:HG3	1:C:211:PHE:CE2	2.51	0.45
1:C:178:SER:HB2	2:D:177:PHE:CE1	2.51	0.45
1:C:192:LYS:NZ	1:C:192:LYS:HB2	2.31	0.45
1:C:38:GLN:HE22	2:D:39:GLN:HE22	1.64	0.45
3:M:155:LEU:O	3:M:156:ASP:C	2.55	0.45
1:A:169:ASP:OD2	1:A:170:SER:N	2.46	0.45
1:A:49:TYR:CB	2:B:109:VAL:HA	2.47	0.45
2:B:20:LEU:HD11	2:B:83:MET:HE1	1.99	0.45
3:N:105:LEU:HD23	3:N:105:LEU:C	2.36	0.45
2:B:149:LEU:CD2	2:B:193:VAL:HG13	2.47	0.45
3:K:86:LEU:HG	3:K:87:TRP:CZ3	2.52	0.45
3:N:82:TYR:HB2	3:N:83:PRO:HD2	1.99	0.45
1:A:142:TYR:CE1	1:A:143:PRO:HB3	2.52	0.45
1:A:91:TYR:OH	2:B:108:TRP:HE3	1.99	0.45
1:C:121:PRO:HG3	1:C:211:PHE:CD2	2.52	0.45
1:C:150:TRP:O	1:C:151:LYS:HG3	2.16	0.45
3:M:151:LEU:CD2	3:M:151:LEU:C	2.84	0.45
1:A:29:VAL:O	1:A:31:SER:N	2.50	0.44
1:A:49:TYR:CD1	1:A:49:TYR:C	2.89	0.44
1:C:145:GLU:H	1:C:145:GLU:CD	2.20	0.44
3:K:148:PHE:HZ	3:N:148:PHE:CE1	2.35	0.44
3:K:153:ARG:CB	3:K:153:ARG:CZ	2.94	0.44
3:K:68:TRP:HZ2	3:K:92:ALA:HB2	1.82	0.44
3:L:36:LEU:HD13	3:L:102:SER:OG	2.16	0.44
3:N:111:ALA:O	3:N:115:VAL:HG23	2.17	0.44
1:A:49:TYR:HD1	1:A:49:TYR:C	2.21	0.44
1:C:177:LEU:O	1:C:178:SER:HB2	2.17	0.44
1:C:201:GLN:O	1:C:201:GLN:HG3	2.17	0.44
3:K:145:HIS:O	3:K:146:GLU:C	2.55	0.44
3:K:155:LEU:HB3	3:K:156:ASP:H	1.58	0.44
3:L:58:GLN:HB3	3:L:64:ARG:HH12	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:144:LEU:O	3:M:145:HIS:C	2.56	0.44
3:N:86:LEU:HG	3:N:87:TRP:CZ3	2.52	0.44
1:C:49:TYR:CE2	2:D:109:VAL:HG22	2.51	0.44
2:D:211:HIS:CE1	2:D:213:PRO:HB2	2.49	0.44
3:K:151:LEU:HD13	3:N:151:LEU:CD1	2.47	0.44
3:K:87:TRP:HA	3:K:87:TRP:CE3	2.52	0.44
3:L:68:TRP:HZ2	3:L:92:ALA:CB	2.30	0.44
1:A:32:ALA:HB1	1:A:91:TYR:CD2	2.52	0.44
2:D:174:VAL:HA	2:D:193:VAL:HG23	2.00	0.44
3:M:74:THR:OG1	3:M:76:VAL:HG23	2.18	0.44
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.99	0.44
1:A:90:GLN:C	1:A:90:GLN:OE1	2.56	0.44
2:B:37:VAL:HG11	2:B:114:TRP:CZ3	2.53	0.44
2:B:82:GLN:NE2	2:B:82:GLN:HA	2.32	0.44
1:C:114:ALA:HB1	1:C:203:LEU:HD21	1.98	0.44
1:C:127:LEU:H	1:C:127:LEU:CD1	2.30	0.44
1:C:152:VAL:HG12	1:C:194:TYR:CD2	2.52	0.44
1:C:50:SER:O	1:C:51:ALA:CB	2.65	0.44
2:D:127:THR:HG23	2:D:158:PRO:CD	2.48	0.44
3:K:141:THR:O	3:K:144:LEU:HB2	2.18	0.44
3:M:139:ARG:HD3	3:M:139:ARG:HA	1.83	0.44
1:C:79:GLN:HA	1:C:79:GLN:OE1	2.18	0.44
2:D:145:GLY:O	2:D:196:PRO:HA	2.18	0.44
2:D:62:ASP:C	2:D:64:VAL:N	2.68	0.44
3:L:139:ARG:HA	3:L:142:ARG:CD	2.47	0.44
3:L:143:ALA:O	3:L:144:LEU:C	2.56	0.44
3:L:25:HIS:CD2	3:L:25:HIS:H	2.34	0.44
3:L:87:TRP:HE3	3:L:87:TRP:HA	1.81	0.44
1:A:126:GLN:HG3	2:B:133:PHE:CD2	2.52	0.44
1:A:81:GLU:O	1:A:83:PHE:N	2.51	0.44
2:B:186:LEU:HD12	2:B:186:LEU:N	2.32	0.44
2:B:43:LYS:HB3	2:B:44:GLY:H	1.64	0.44
2:D:83:MET:HE1	2:D:120:VAL:HG21	2.00	0.44
3:N:51:GLU:O	3:N:57:ALA:HB1	2.18	0.44
1:A:4:MET:HE1	1:A:90:GLN:HB3	1.99	0.44
1:C:94:TYR:HE2	3:K:147:ARG:NE	2.16	0.44
2:D:100:PRO:HB3	2:D:106:SER:HB3	1.99	0.44
1:C:134:VAL:O	1:C:180:THR:HG22	2.17	0.44
2:D:55:TYR:O	2:D:56:SER:C	2.54	0.44
3:N:127:ARG:HH21	3:N:131:LYS:CE	2.31	0.44
1:A:19:VAL:O	1:A:74:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:LYS:HG2	2:B:155:ASP:OD2	2.18	0.43
2:B:79:ALA:C	2:B:80:TYR:HD2	2.20	0.43
1:C:134:VAL:C	1:C:135:VAL:HG12	2.38	0.43
2:D:23:ALA:N	2:D:78:THR:HG23	2.32	0.43
2:D:47:TRP:HZ3	2:D:61:ALA:HA	1.83	0.43
3:K:151:LEU:HD23	3:K:151:LEU:O	2.18	0.43
3:L:155:LEU:O	3:L:157:ASP:N	2.51	0.43
3:L:82:TYR:HB2	3:L:83:PRO:HD2	2.00	0.43
1:A:200:HIS:HB3	1:A:203:LEU:HG	1.98	0.43
2:B:14:PRO:HA	2:B:122:VAL:CG2	2.48	0.43
2:B:212:LYS:N	2:B:213:PRO:CD	2.81	0.43
2:B:82:GLN:O	2:B:83:MET:C	2.55	0.43
1:C:123:SER:O	1:C:126:GLN:HB2	2.18	0.43
1:C:16:GLY:HA2	1:C:77:SER:OG	2.19	0.43
1:C:89:GLN:OE1	2:D:110:ALA:HB1	2.17	0.43
2:D:91:THR:HA	2:D:120:VAL:O	2.18	0.43
1:C:177:LEU:O	2:D:177:PHE:CZ	2.71	0.43
2:B:125:ALA:O	2:B:157:PHE:CE2	2.71	0.43
1:C:134:VAL:HB	1:C:181:LEU:HB2	2.00	0.43
1:C:154:ASN:N	1:C:154:ASN:HD22	2.15	0.43
2:D:119:LEU:HD23	2:D:119:LEU:C	2.39	0.43
1:A:141:PHE:HE1	1:A:143:PRO:O	2.01	0.43
1:A:195:ALA:CA	1:A:210:SER:HB3	2.49	0.43
2:B:111:LEU:CB	2:B:114:TRP:NE1	2.80	0.43
1:C:87:TYR:CD2	2:D:45:LEU:HD12	2.54	0.43
3:N:43:GLY:HA2	3:N:91:VAL:CG1	2.48	0.43
2:B:27:PHE:N	2:B:27:PHE:CD2	2.86	0.43
2:D:14:PRO:HD3	2:D:123:SER:C	2.39	0.43
2:D:130:PRO:CA	2:D:156:TYR:HB3	2.49	0.43
2:D:64:VAL:HG21	2:D:68:PHE:CB	2.48	0.43
3:K:138:THR:CG2	3:K:139:ARG:N	2.80	0.43
3:M:44:SER:HB3	3:M:66:LEU:HA	1.97	0.43
1:A:40:PRO:HG2	1:A:167:GLU:OE2	2.18	0.43
2:B:13:GLN:O	2:B:14:PRO:C	2.57	0.43
3:L:109:ALA:HA	3:L:112:THR:HG22	2.01	0.43
3:M:151:LEU:O	3:M:155:LEU:HD13	2.18	0.43
1:A:35:TRP:HB2	1:A:48:ILE:CB	2.48	0.43
2:B:91:THR:CG2	2:B:122:VAL:HG12	2.41	0.43
1:C:127:LEU:HG	1:C:132:ALA:HB2	2.01	0.43
1:C:98:VAL:HB	2:D:47:TRP:CG	2.54	0.43
3:K:151:LEU:CD2	3:K:151:LEU:C	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:74:THR:OG1	3:K:76:VAL:HG23	2.19	0.43
1:A:79:GLN:CB	1:A:80:PRO:HD2	2.45	0.43
1:C:185:LYS:O	1:C:186:ALA:C	2.56	0.43
3:N:154:MET:O	3:N:158:ASN:CB	2.66	0.43
2:B:9:GLY:HA3	2:B:118:THR:HG22	2.00	0.43
2:B:82:GLN:HE21	2:B:82:GLN:CA	2.32	0.43
3:K:87:TRP:HA	3:K:87:TRP:HE3	1.82	0.43
1:A:79:GLN:OE1	1:A:79:GLN:HA	2.18	0.43
2:B:81:LEU:CD2	2:B:83:MET:HG2	2.45	0.43
3:L:147:ARG:HG3	3:L:147:ARG:HH11	1.84	0.43
3:N:143:ALA:O	3:N:144:LEU:C	2.57	0.43
3:N:65:ALA:HA	3:N:68:TRP:HB3	2.00	0.43
1:A:139:ASN:ND2	1:A:140:ASN:OD1	2.52	0.42
1:A:64:GLY:HA2	1:A:72:THR:O	2.19	0.42
2:D:103:HIS:O	2:D:104:MET:O	2.37	0.42
2:D:212:LYS:CG	2:D:213:PRO:HD3	2.48	0.42
2:D:215:ASN:CG	2:D:215:ASN:O	2.57	0.42
3:K:76:VAL:HG22	3:L:75:THR:CB	2.49	0.42
1:A:110:ARG:CZ	1:A:110:ARG:HB2	2.49	0.42
1:A:137:LEU:C	1:A:138:LEU:HD12	2.40	0.42
2:B:104:MET:HA	2:B:104:MET:HE2	1.99	0.42
1:C:139:ASN:ND2	1:C:140:ASN:OD1	2.51	0.42
3:M:115:VAL:HG13	3:M:118:GLU:OE2	2.18	0.42
3:N:87:TRP:HE3	3:N:87:TRP:HA	1.84	0.42
1:C:150:TRP:O	1:C:151:LYS:CG	2.68	0.42
2:D:159:GLU:HG2	2:D:187:TYR:CE2	2.54	0.42
3:M:135:GLU:O	3:M:138:THR:HG22	2.18	0.42
1:A:177:LEU:HD13	1:A:178:SER:H	1.80	0.42
1:A:192:LYS:O	1:A:192:LYS:HG2	2.19	0.42
2:B:36:TRP:CD1	2:B:81:LEU:HD12	2.54	0.42
2:B:60:TYR:OH	2:B:69:THR:HA	2.18	0.42
3:K:139:ARG:HA	3:K:139:ARG:HD3	1.85	0.42
3:L:127:ARG:NE	3:L:131:LYS:HE3	2.34	0.42
3:M:149:ASP:O	3:M:153:ARG:N	2.52	0.42
1:A:163:GLU:CG	1:A:177:LEU:HD11	2.50	0.42
1:A:195:ALA:CB	1:A:210:SER:HB3	2.50	0.42
2:B:206:ILE:HA	2:B:222:VAL:HG23	2.00	0.42
1:C:34:ALA:CB	2:D:110:ALA:HB2	2.49	0.42
2:D:149:LEU:H	2:D:149:LEU:HD23	1.84	0.42
2:D:186:LEU:N	2:D:186:LEU:CD1	2.83	0.42
2:D:47:TRP:CE2	2:D:49:ALA:O	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:O	1:A:72:THR:HA	2.20	0.42
1:A:33:VAL:CG1	1:A:34:ALA:N	2.82	0.42
1:C:163:GLU:O	1:C:164:SER:HB2	2.20	0.42
2:D:127:THR:C	2:D:128:LYS:HG3	2.40	0.42
2:D:22:CYS:C	2:D:78:THR:HG23	2.40	0.42
3:K:114:PHE:HB3	3:L:112:THR:HB	2.01	0.42
3:K:124:HIS:O	3:K:127:ARG:HB3	2.19	0.42
3:K:78:TYR:HA	3:K:78:TYR:HD2	1.74	0.42
3:M:87:TRP:HE3	3:M:87:TRP:HA	1.85	0.42
3:N:86:LEU:O	3:N:90:LEU:HG	2.19	0.42
1:A:38:GLN:HE22	2:B:39:GLN:NE2	1.93	0.42
2:D:9:GLY:HA3	2:D:118:THR:CG2	2.49	0.42
2:D:212:LYS:O	2:D:215:ASN:N	2.48	0.42
3:M:127:ARG:O	3:M:131:LYS:HG3	2.19	0.42
3:M:27:ARG:O	3:M:31:ALA:HB2	2.20	0.42
1:C:49:TYR:CD1	1:C:49:TYR:O	2.72	0.42
2:D:209:VAL:HB	2:D:218:VAL:HG12	2.01	0.42
3:L:154:MET:SD	3:M:152:GLU:HG3	2.59	0.42
3:M:85:THR:O	3:M:89:ARG:HG3	2.20	0.42
3:M:144:LEU:HG	3:N:144:LEU:HD21	2.02	0.42
1:A:152:VAL:HG12	1:A:194:TYR:CE2	2.54	0.42
2:B:212:LYS:O	2:B:214:SER:N	2.52	0.42
1:C:2:ILE:HB	1:C:90:GLN:HE21	1.84	0.42
2:D:116:GLN:O	2:D:117:GLY:O	2.38	0.42
2:D:40:ALA:HB1	2:D:41:PRO:HD2	2.02	0.42
2:D:6:GLU:OE1	2:D:117:GLY:N	2.52	0.42
2:D:77:ASN:C	2:D:78:THR:OG1	2.59	0.42
2:D:9:GLY:HA3	2:D:118:THR:HG21	2.02	0.42
3:K:141:THR:OG1	3:K:142:ARG:N	2.53	0.42
1:A:11:LEU:HD22	1:A:106:VAL:CG1	2.47	0.42
1:C:120:PHE:CE1	2:D:135:LEU:HB3	2.55	0.42
1:C:137:LEU:C	1:C:137:LEU:HD23	2.40	0.42
3:L:49:LEU:HD12	3:L:52:ARG:HD2	2.02	0.42
3:L:86:LEU:O	3:L:90:LEU:HG	2.20	0.42
3:M:138:THR:C	3:M:140:THR:N	2.73	0.42
3:M:87:TRP:CE3	3:M:87:TRP:HA	2.54	0.42
2:B:102:TYR:HE2	2:B:107:TRP:CE2	2.37	0.41
2:B:149:LEU:HD23	2:B:193:VAL:HG13	2.02	0.41
1:C:137:LEU:HD23	1:C:138:LEU:C	2.40	0.41
1:C:31:SER:HB3	1:C:66:ARG:CD	2.50	0.41
3:N:61:THR:CG2	3:N:63:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HA	1:A:180:THR:HA	2.02	0.41
2:D:168:GLY:O	2:D:171:THR:CG2	2.67	0.41
2:D:18:LEU:HD23	2:D:18:LEU:HA	1.74	0.41
3:K:59:LEU:HD13	3:K:81:LEU:HB3	2.03	0.41
3:L:143:ALA:O	3:L:146:GLU:N	2.53	0.41
3:N:135:GLU:O	3:N:138:THR:HG22	2.19	0.41
2:B:18:LEU:CD1	2:B:120:VAL:HG13	2.50	0.41
1:C:129:SER:OG	1:C:130:GLY:N	2.54	0.41
1:C:36:TYR:HE2	2:D:114:TRP:HE1	1.68	0.41
2:D:112:ASP:HB3	2:D:113:TYR:H	1.69	0.41
3:K:43:GLY:CA	3:K:68:TRP:HZ3	2.31	0.41
3:N:51:GLU:CD	3:N:83:PRO:HA	2.40	0.41
3:N:87:TRP:HA	3:N:87:TRP:CE3	2.54	0.41
2:B:34:ILE:O	2:B:50:SER:HA	2.20	0.41
2:D:24:ALA:HB3	2:D:77:ASN:HD22	1.81	0.41
2:D:27:PHE:CE2	2:D:98:ARG:HD3	2.55	0.41
3:K:127:ARG:CG	3:K:131:LYS:HE3	2.44	0.41
3:K:143:ALA:O	3:K:147:ARG:HB2	2.20	0.41
3:L:151:LEU:HD21	3:M:152:GLU:HA	2.03	0.41
1:A:141:PHE:CE2	1:A:177:LEU:HB2	2.49	0.41
2:B:104:MET:HA	2:B:104:MET:CE	2.51	0.41
2:B:152:LEU:HD12	2:B:190:SER:HB3	2.01	0.41
2:B:161:VAL:CG1	2:B:211:HIS:HD2	2.33	0.41
2:B:211:HIS:C	2:B:213:PRO:HD2	2.40	0.41
2:B:24:ALA:HB3	2:B:77:ASN:HD21	1.78	0.41
2:B:47:TRP:HZ3	2:B:61:ALA:CA	2.33	0.41
2:B:89:GLU:N	2:B:89:GLU:OE2	2.50	0.41
1:C:149:GLN:HB2	1:C:197:GLU:HB3	2.01	0.41
2:D:54:TYR:CE2	2:D:103:HIS:NE2	2.88	0.41
2:D:125:ALA:HB3	2:D:157:PHE:CE2	2.56	0.41
2:D:166:ASN:C	2:D:168:GLY:H	2.24	0.41
2:D:165:TRP:CZ3	2:D:207:CYS:HB3	2.54	0.41
2:D:67:ARG:HG2	2:D:85:SER:HB2	2.02	0.41
3:K:144:LEU:O	3:K:145:HIS:C	2.58	0.41
3:L:36:LEU:HD13	3:L:102:SER:CB	2.51	0.41
3:M:64:ARG:O	3:M:81:LEU:HD13	2.20	0.41
1:A:53:PHE:CD1	1:A:53:PHE:N	2.88	0.41
2:B:181:LEU:HD23	2:B:182:GLN:O	2.21	0.41
2:B:68:PHE:CD1	2:B:83:MET:HA	2.55	0.41
1:C:195:ALA:CA	1:C:210:SER:HB3	2.51	0.41
1:C:36:TYR:OH	2:D:110:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:HE2	3:N:145:HIS:HD2	1.69	0.41
1:C:11:LEU:HD23	1:C:106:VAL:HG13	1.99	0.41
2:D:149:LEU:N	2:D:149:LEU:HD23	2.36	0.41
2:D:2:VAL:HG22	2:D:26:GLY:C	2.41	0.41
3:K:134:GLU:O	3:K:138:THR:HG22	2.20	0.41
3:K:51:GLU:HB2	3:K:59:LEU:O	2.21	0.41
3:K:70:VAL:HG12	3:L:96:MET:SD	2.60	0.41
3:L:121:ARG:NE	3:L:121:ARG:HA	2.36	0.41
3:K:76:VAL:HG22	3:L:75:THR:HG22	2.02	0.41
3:M:67:TRP:HZ2	3:M:78:TYR:CD1	2.39	0.41
3:N:155:LEU:O	3:N:157:ASP:N	2.54	0.41
1:A:50:SER:O	1:A:51:ALA:CB	2.69	0.41
2:B:170:LEU:CD2	2:B:174:VAL:HG22	2.51	0.41
2:B:2:VAL:CG2	2:B:26:GLY:HA3	2.49	0.41
1:C:152:VAL:O	1:C:153:ASP:HB2	2.21	0.41
1:C:182:THR:CA	1:C:183:LEU:HD12	2.48	0.41
1:C:89:GLN:HB2	1:C:100:PHE:CD1	2.56	0.41
2:D:68:PHE:CD1	2:D:83:MET:HA	2.55	0.41
2:D:18:LEU:O	2:D:83:MET:N	2.54	0.41
3:L:153:ARG:O	3:L:157:ASP:HB3	2.21	0.41
3:N:150:ARG:O	3:N:153:ARG:N	2.53	0.41
1:A:137:LEU:HD11	2:B:192:VAL:HG21	2.02	0.41
1:C:115:PRO:HD3	1:C:200:HIS:CD2	2.56	0.41
2:D:165:TRP:CZ2	2:D:207:CYS:HB3	2.54	0.41
2:D:48:VAL:HG11	2:D:68:PHE:CD2	2.55	0.41
2:D:39:GLN:C	2:D:92:ALA:HB1	2.41	0.41
3:L:87:TRP:CE3	3:L:90:LEU:CD1	3.04	0.41
3:M:137:TYR:O	3:M:140:THR:N	2.43	0.41
3:M:153:ARG:CD	3:M:157:ASP:OD2	2.69	0.41
3:N:138:THR:HA	3:N:141:THR:HG22	2.03	0.41
1:A:150:TRP:CE3	1:A:181:LEU:HG	2.56	0.41
1:A:24:ARG:HB2	1:A:70:ASP:OD1	2.21	0.41
2:D:104:MET:HB3	2:D:105:TYR:H	1.62	0.41
2:D:98:ARG:O	2:D:111:LEU:HA	2.20	0.41
3:K:44:SER:HA	3:K:65:ALA:HB1	2.02	0.41
3:K:82:TYR:HB2	3:K:83:PRO:HD2	2.03	0.41
3:L:151:LEU:CD2	3:M:151:LEU:HD22	2.51	0.41
3:M:114:PHE:HB3	3:N:112:THR:HB	2.02	0.41
1:A:49:TYR:C	1:A:51:ALA:H	2.23	0.41
2:D:212:LYS:CD	2:D:212:LYS:H	2.34	0.41
3:K:136:ALA:HB2	3:L:134:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:66:LEU:O	3:M:70:VAL:HG23	2.21	0.41
3:M:76:VAL:HG12	3:N:77:GLY:HA3	2.03	0.41
1:A:90:GLN:O	1:A:90:GLN:HG3	2.21	0.40
2:B:16:GLY:O	2:B:86:LEU:HD12	2.21	0.40
1:C:30:SER:O	1:C:31:SER:C	2.58	0.40
3:M:153:ARG:CB	3:M:153:ARG:CZ	2.98	0.40
3:N:42:ALA:O	3:N:46:LEU:HG	2.21	0.40
3:N:78:TYR:HD2	3:N:78:TYR:HA	1.80	0.40
1:A:29:VAL:HG12	1:A:29:VAL:O	2.21	0.40
2:D:135:LEU:HD23	2:D:135:LEU:HA	1.85	0.40
2:D:186:LEU:HD12	2:D:186:LEU:N	2.37	0.40
3:L:61:THR:CG2	3:L:63:PRO:HD2	2.30	0.40
1:A:189:GLU:CB	1:A:213:ARG:HH22	2.34	0.40
1:A:78:LEU:HD12	1:A:78:LEU:C	2.40	0.40
2:B:37:VAL:HA	2:B:47:TRP:HA	2.03	0.40
2:D:170:LEU:HD23	2:D:171:THR:N	2.36	0.40
2:D:50:SER:O	2:D:70:ILE:HG21	2.22	0.40
3:K:149:ASP:O	3:K:150:ARG:C	2.59	0.40
2:D:102:TYR:CE1	3:K:150:ARG:HB2	2.56	0.40
3:K:151:LEU:O	3:K:154:MET:N	2.54	0.40
3:M:138:THR:C	3:M:140:THR:H	2.24	0.40
3:M:44:SER:HB3	3:M:66:LEU:CA	2.51	0.40
1:A:61:ARG:NE	1:A:82:ASP:OD2	2.45	0.40
2:B:177:PHE:HA	2:B:178:PRO:HD3	1.76	0.40
2:B:181:LEU:HD23	2:B:181:LEU:C	2.42	0.40
2:B:54:TYR:HD1	2:B:54:TYR:O	2.05	0.40
2:B:97:ALA:CB	2:B:114:TRP:HA	2.51	0.40
1:C:6:GLN:HE22	1:C:104:THR:H	1.64	0.40
3:L:61:THR:HB	3:L:64:ARG:CG	2.43	0.40
3:N:150:ARG:CG	3:N:151:LEU:N	2.83	0.40
3:M:78:TYR:CD2	3:N:77:GLY:HA2	2.56	0.40
1:A:6:GLN:OE1	1:A:88:CYS:HB3	2.21	0.40
2:B:188:SER:O	2:B:189:LEU:HB3	2.22	0.40
1:C:15:VAL:CG2	1:C:16:GLY:N	2.84	0.40
1:C:31:SER:CB	1:C:66:ARG:HD2	2.51	0.40
1:C:63:SER:O	1:C:73:LEU:HD12	2.21	0.40
2:D:149:LEU:CD2	2:D:193:VAL:HG13	2.51	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%)	161 (76%)	35 (16%)	17 (8%)	1 14
1	C	213/215 (99%)	147 (69%)	46 (22%)	20 (9%)	0 11
2	B	215/224 (96%)	154 (72%)	49 (23%)	12 (6%)	2 21
2	D	215/224 (96%)	164 (76%)	33 (15%)	18 (8%)	1 13
3	K	137/139 (99%)	121 (88%)	13 (10%)	3 (2%)	6 39
3	L	137/139 (99%)	122 (89%)	13 (10%)	2 (2%)	10 46
3	M	137/139 (99%)	121 (88%)	14 (10%)	2 (2%)	10 46
3	N	137/139 (99%)	122 (89%)	13 (10%)	2 (2%)	10 46
All	All	1404/1434 (98%)	1112 (79%)	216 (15%)	76 (5%)	2 22

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	93	SER
1	A	94	TYR
1	A	97	PRO
2	B	105	TYR
2	B	110	ALA
1	C	50	SER
1	C	93	SER
1	C	97	PRO
1	C	98	VAL
1	C	160	ASN
1	C	178	SER
2	D	51	ILE
2	D	63	SER
2	D	104	MET
2	D	110	ALA
2	D	112	ASP

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Mol	Chain	Res	Type
3	K	156	ASP
3	M	156	ASP
1	A	26	SER
1	A	68	GLY
1	A	82	ASP
1	A	116	SER
2	B	63	SER
2	B	92	ALA
2	B	104	MET
2	B	117	GLY
2	B	130	PRO
1	C	76	SER
1	C	140	ASN
1	C	164	SER
2	D	16	GLY
2	D	101	SER
2	D	106	SER
2	D	117	GLY
3	L	156	ASP
3	N	156	ASP
1	A	31	SER
1	A	44	PRO
1	A	140	ASN
2	B	83	MET
1	C	44	PRO
1	C	168	GLN
2	D	198	SER
3	K	59	LEU
1	A	84	ALA
2	B	51	ILE
2	B	99	GLN
1	C	40	PRO
1	C	96	ALA
1	C	135	VAL
1	C	137	LEU
2	D	50	SER
2	D	153	VAL
2	D	167	SER
1	A	96	ALA
1	A	102	GLN
2	B	30	SER
2	B	76	LYS

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Mol	Chain	Res	Type
1	C	111	THR
1	C	182	THR
2	D	30	SER
2	D	56	SER
2	D	76	LYS
3	N	59	LEU
1	A	153	ASP
1	C	23	CYS
1	C	115	PRO
2	D	160	PRO
2	D	169	ALA
3	L	59	LEU
1	A	40	PRO
1	C	112	VAL
1	A	80	PRO
3	K	84	VAL
3	M	84	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	189/189 (100%)	170 (90%)	19 (10%)	7 32
1	C	189/189 (100%)	162 (86%)	27 (14%)	3 20
2	B	184/188 (98%)	170 (92%)	14 (8%)	13 43
2	D	184/188 (98%)	162 (88%)	22 (12%)	5 25
3	K	104/107 (97%)	90 (86%)	14 (14%)	4 22
3	L	104/107 (97%)	92 (88%)	12 (12%)	5 27
3	M	104/107 (97%)	89 (86%)	15 (14%)	3 20
3	N	104/107 (97%)	95 (91%)	9 (9%)	10 38
All	All	1162/1182 (98%)	1030 (89%)	132 (11%)	5 28

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	11	LEU
1	A	17	ASP
1	A	49	TYR
1	A	76	SER
1	A	81	GLU
1	A	90	GLN
1	A	91	TYR
1	A	97	PRO
1	A	110	ARG
1	A	124	ASP
1	A	142	TYR
1	A	153	ASP
1	A	156	LEU
1	A	175	TYR
1	A	177	LEU
1	A	181	LEU
1	A	183	LEU
1	A	187	ASP
2	B	3	GLN
2	B	12	VAL
2	B	54	TYR
2	B	58	THR
2	B	80	TYR
2	B	104	MET
2	B	105	TYR
2	B	111	LEU
2	B	112	ASP
2	B	121	THR
2	B	123	SER
2	B	160	PRO
2	B	210	ASN
2	B	212	LYS
1	C	5	THR
1	C	8	PRO
1	C	11	LEU
1	C	15	VAL
1	C	17	ASP
1	C	48	ILE
1	C	49	TYR
1	C	81	GLU
1	C	90	GLN
1	C	97	PRO

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Mol	Chain	Res	Type
1	C	98	VAL
1	C	108	ILE
1	C	110	ARG
1	C	124	ASP
1	C	126	GLN
1	C	135	VAL
1	C	153	ASP
1	C	156	LEU
1	C	172	ASP
1	C	177	LEU
1	C	179	SER
1	C	180	THR
1	C	181	LEU
1	C	182	THR
1	C	183	LEU
1	C	187	ASP
1	C	212	ASN
2	D	3	GLN
2	D	12	VAL
2	D	32	TYR
2	D	54	TYR
2	D	56	SER
2	D	58	THR
2	D	64	VAL
2	D	80	TYR
2	D	82	GLN
2	D	83	MET
2	D	98	ARG
2	D	105	TYR
2	D	112	ASP
2	D	120	VAL
2	D	130	PRO
2	D	160	PRO
2	D	171	THR
2	D	174	VAL
2	D	208	ASN
2	D	210	ASN
2	D	212	LYS
2	D	216	THR
3	K	25	HIS
3	K	26	TRP
3	K	78	TYR

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Mol	Chain	Res	Type
3	K	87	TRP
3	K	113	TRP
3	K	118	GLU
3	K	121	ARG
3	K	125	PHE
3	K	140	THR
3	K	147	ARG
3	K	150	ARG
3	K	153	ARG
3	K	156	ASP
3	K	157	ASP
3	L	25	HIS
3	L	26	TRP
3	L	78	TYR
3	L	87	TRP
3	L	117	ARG
3	L	121	ARG
3	L	127	ARG
3	L	130	GLU
3	L	140	THR
3	L	146	GLU
3	L	147	ARG
3	L	149	ASP
3	M	25	HIS
3	M	26	TRP
3	M	78	TYR
3	M	87	TRP
3	M	113	TRP
3	M	118	GLU
3	M	121	ARG
3	M	125	PHE
3	M	127	ARG
3	M	140	THR
3	M	141	THR
3	M	147	ARG
3	M	153	ARG
3	M	154	MET
3	M	156	ASP
3	N	25	HIS
3	N	26	TRP
3	N	78	TYR
3	N	87	TRP

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Mol	Chain	Res	Type
3	N	117	ARG
3	N	130	GLU
3	N	140	THR
3	N	146	GLU
3	N	149	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	139	ASN
1	A	154	ASN
1	A	157	GLN
1	A	160	ASN
1	A	168	GLN
2	B	3	GLN
2	B	39	GLN
2	B	77	ASN
2	B	82	GLN
2	B	175	HIS
2	B	208	ASN
2	B	210	ASN
1	C	3	GLN
1	C	6	GLN
1	C	37	GLN
1	C	89	GLN
1	C	154	ASN
1	C	212	ASN
2	D	3	GLN
2	D	39	GLN
2	D	77	ASN
2	D	82	GLN
2	D	210	ASN
3	K	25	HIS
3	L	145	HIS
3	L	158	ASN
3	N	25	HIS
3	N	145	HIS
3	N	158	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	215/215 (100%)	0.45	24 (11%) 5 5	68, 175, 254, 259	0
1	C	215/215 (100%)	0.11	4 (1%) 66 59	43, 105, 196, 259	0
2	B	219/224 (97%)	0.20	11 (5%) 28 25	49, 124, 239, 259	0
2	D	219/224 (97%)	0.02	1 (0%) 91 87	35, 92, 192, 259	0
3	K	139/139 (100%)	1.25	38 (27%) 0 0	65, 255, 259, 259	0
3	L	139/139 (100%)	1.16	35 (25%) 0 0	52, 251, 259, 259	0
3	M	139/139 (100%)	0.93	35 (25%) 0 0	61, 249, 259, 259	0
3	N	139/139 (100%)	1.18	37 (26%) 0 0	57, 255, 259, 259	0
All	All	1424/1434 (99%)	0.56	185 (12%) 3 4	35, 169, 259, 259	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	54	ALA	17.3
3	L	54	ALA	13.7
3	L	38	ILE	7.9
3	K	81	LEU	7.5
3	N	52	ARG	7.4
3	L	50	ALA	7.4
3	N	55	PRO	7.2
1	A	206	PRO	6.7
3	K	25	HIS	6.6
3	N	63	PRO	6.5
3	K	87	TRP	6.3
3	K	105	LEU	6.2
3	L	26	TRP	6.0
1	A	185	LYS	5.6
1	A	205	SER	5.6
3	L	108	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	132	VAL	5.5
3	K	86	LEU	5.5
3	N	53	GLY	5.5
3	N	125	PHE	5.3
3	M	54	ALA	5.3
3	K	28	ALA	5.3
3	N	128	HIS	5.3
3	K	26	TRP	5.2
3	L	35	LEU	5.2
1	A	148	VAL	5.2
3	K	42	ALA	5.0
3	K	56	GLY	4.9
3	K	98	ALA	4.8
3	L	53	GLY	4.8
3	K	54	ALA	4.8
3	N	57	ALA	4.5
3	L	22	SER	4.5
3	N	78	TYR	4.3
3	M	56	GLY	4.3
3	N	25	HIS	4.3
3	L	25	HIS	4.2
3	K	55	PRO	4.1
3	L	109	ALA	4.1
3	K	90	LEU	4.1
3	K	97	VAL	4.0
3	L	85	THR	4.0
3	L	55	PRO	4.0
3	M	43	GLY	3.9
3	M	55	PRO	3.9
3	L	41	LEU	3.9
3	L	86	LEU	3.9
3	N	49	LEU	3.9
3	N	56	GLY	3.8
3	K	66	LEU	3.8
3	K	34	VAL	3.8
3	N	29	ALA	3.8
3	L	83	PRO	3.8
3	M	37	VAL	3.7
1	A	188	TYR	3.7
3	N	35	LEU	3.7
3	N	87	TRP	3.7
3	M	33	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	201	GLN	3.7
3	L	23	ALA	3.7
3	N	64	ARG	3.7
3	K	24	LEU	3.7
3	M	36	LEU	3.7
3	K	63	PRO	3.6
1	A	198	VAL	3.6
3	M	41	LEU	3.6
2	B	166	ASN	3.6
3	L	87	TRP	3.6
1	A	108	ILE	3.5
3	K	73	ALA	3.5
2	B	153	VAL	3.5
3	L	84	VAL	3.5
3	N	61	THR	3.5
3	N	102	SER	3.5
1	A	186	ALA	3.4
3	K	41	LEU	3.4
3	L	105	LEU	3.4
3	K	94	VAL	3.4
3	M	45	TYR	3.4
3	L	52	ARG	3.4
3	K	127	ARG	3.3
3	L	110	LEU	3.2
3	L	29	ALA	3.2
3	K	64	ARG	3.2
3	M	57	ALA	3.2
2	B	171	THR	3.2
3	K	123	GLY	3.1
3	K	104	GLY	3.1
2	B	170	LEU	3.1
3	M	42	ALA	3.1
3	M	34	VAL	3.1
3	N	126	VAL	3.1
3	L	49	LEU	3.1
3	N	26	TRP	3.0
3	L	42	ALA	3.0
3	L	113	TRP	3.0
3	K	53	GLY	3.0
2	B	149	LEU	3.0
3	L	137	TYR	3.0
1	A	194	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	85	THR	3.0
3	M	119	GLN	2.9
3	N	41	LEU	2.9
3	N	89	ARG	2.8
2	B	45	LEU	2.8
3	K	45	TYR	2.8
3	N	98	ALA	2.8
3	N	42	ALA	2.8
3	L	31	ALA	2.8
1	C	201	GLN	2.8
3	N	105	LEU	2.8
2	B	169	ALA	2.8
1	A	122	PRO	2.8
3	M	53	GLY	2.8
3	L	51	GLU	2.8
3	N	106	VAL	2.8
3	M	80	ASP	2.7
3	N	110	LEU	2.7
3	M	40	LEU	2.7
3	K	82	TYR	2.7
3	M	63	PRO	2.7
3	M	87	TRP	2.7
3	L	30	GLY	2.7
3	N	38	ILE	2.7
1	C	14	SER	2.6
3	K	103	PHE	2.6
1	A	107	GLU	2.5
1	A	203	LEU	2.5
3	M	97	VAL	2.5
2	B	150	GLY	2.5
2	B	167	SER	2.5
3	K	30	GLY	2.5
3	M	123	GLY	2.5
1	A	196	CYS	2.5
3	N	80	ASP	2.5
3	M	99	GLY	2.5
1	A	87	TYR	2.5
3	N	99	GLY	2.5
3	L	39	VAL	2.5
3	M	86	LEU	2.5
2	B	110	ALA	2.4
3	M	98	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	N	32	ALA	2.4
1	A	175	TYR	2.4
3	K	29	ALA	2.4
3	N	84	VAL	2.4
2	D	161	VAL	2.4
3	N	39	VAL	2.4
1	A	204	SER	2.4
3	K	31	ALA	2.4
3	M	25	HIS	2.4
3	M	81	LEU	2.4
3	M	47	ALA	2.4
3	L	28	ALA	2.4
3	K	79	GLY	2.3
3	K	108	ALA	2.3
1	A	83	PHE	2.3
1	A	211	PHE	2.3
3	L	34	VAL	2.3
3	M	28	ALA	2.3
3	N	45	TYR	2.3
3	N	108	ALA	2.3
3	L	24	LEU	2.3
3	K	126	VAL	2.2
3	K	74	THR	2.2
3	M	111	ALA	2.2
3	M	79	GLY	2.2
3	K	65	ALA	2.2
3	L	80	ASP	2.2
3	M	39	VAL	2.2
1	A	209	LYS	2.2
3	M	156	ASP	2.2
3	N	62	TYR	2.2
3	M	58	GLN	2.2
1	A	84	ALA	2.1
3	M	26	TRP	2.1
1	C	96	ALA	2.1
3	N	114	PHE	2.1
3	M	94	VAL	2.1
1	A	117	VAL	2.1
3	M	113	TRP	2.0
3	L	115	VAL	2.0
1	C	150	TRP	2.0
1	A	44	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
3	K	83	PRO	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.