



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 PM UTC

PDB ID : 3EFF / pdb_00003eff
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 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
Xtrriage (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

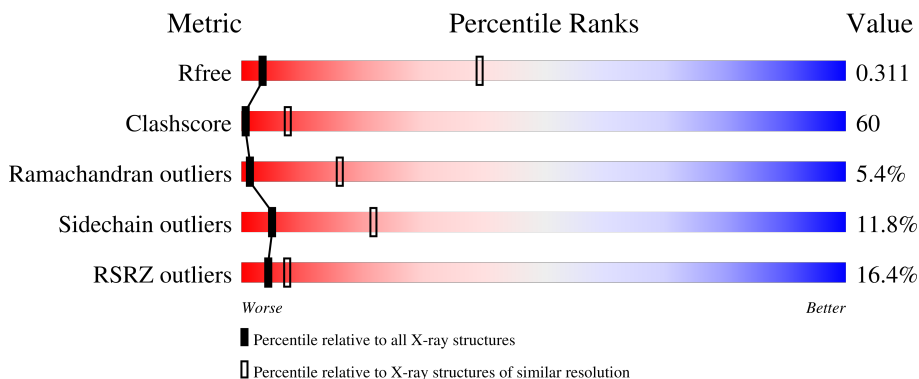
1 Overall quality at a glance

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.



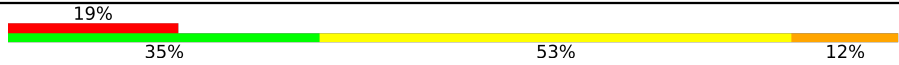


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	
1	C	215	
2	B	224	
2	D	224	
3	K	139	

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Mol	Chain	Length	Quality of chain
3	L	139	
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
			Total	C	N	O	S			
1	A	215	1653	1035	275	338	5	0	0	0
1	C	215	1653	1035	275	338	5	0	0	0

- Molecule 2 is a protein called FAB.

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

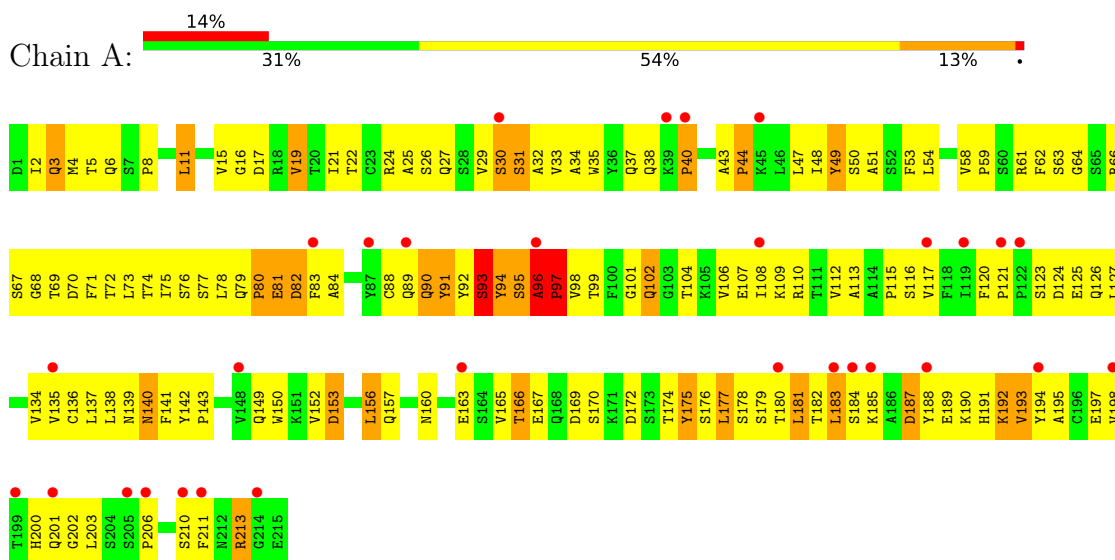
- Molecule 3 is a protein called Voltage-gated potassium channel.

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

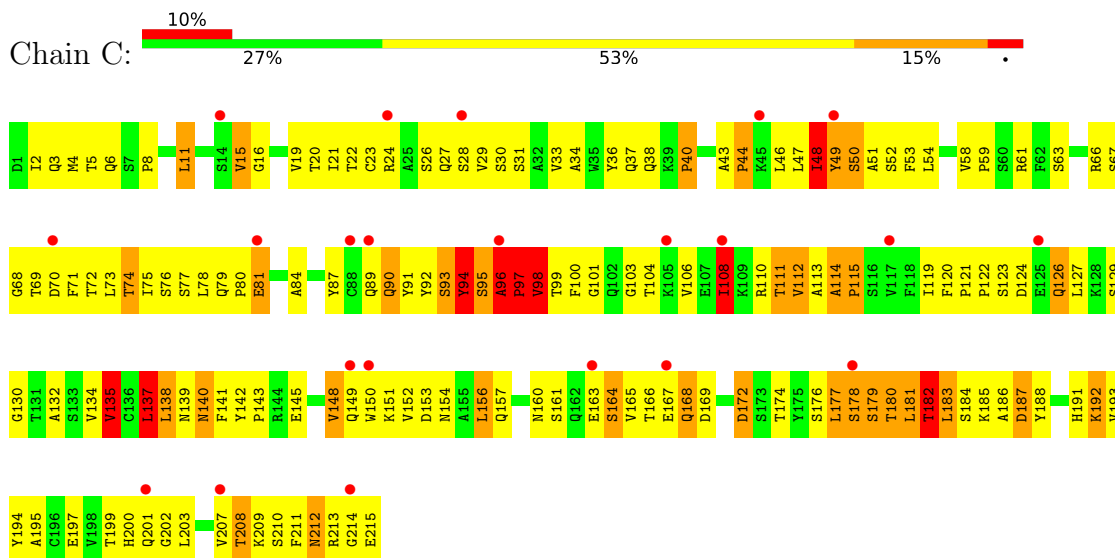
3 Residue-property plots

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

- Molecule 1: FAB

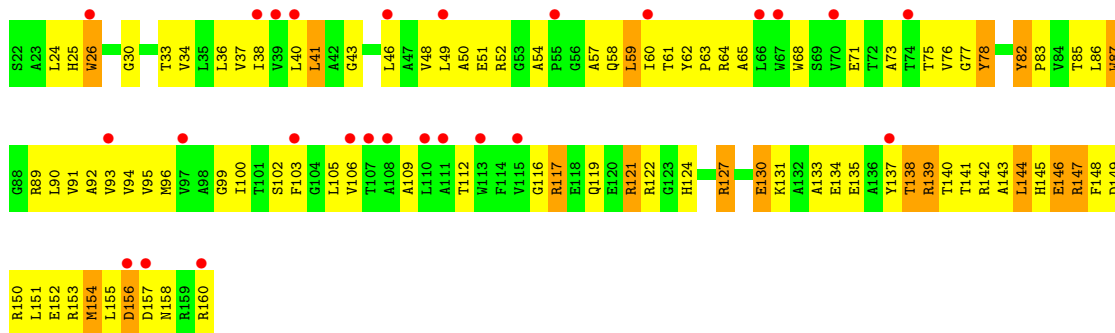


- Molecule 1: FAB

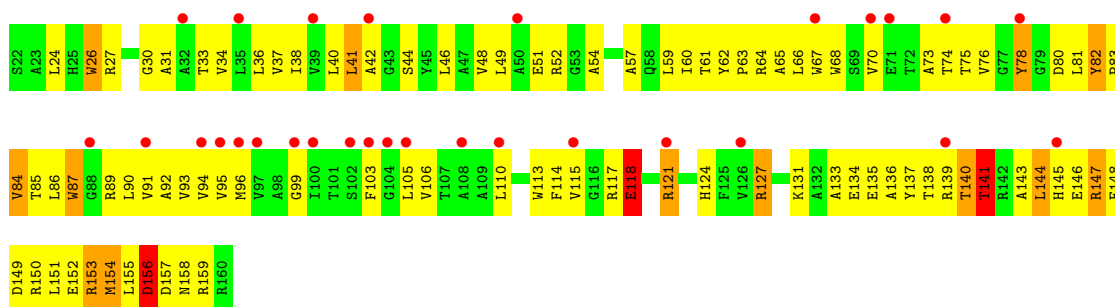


- Molecule 2: FAB

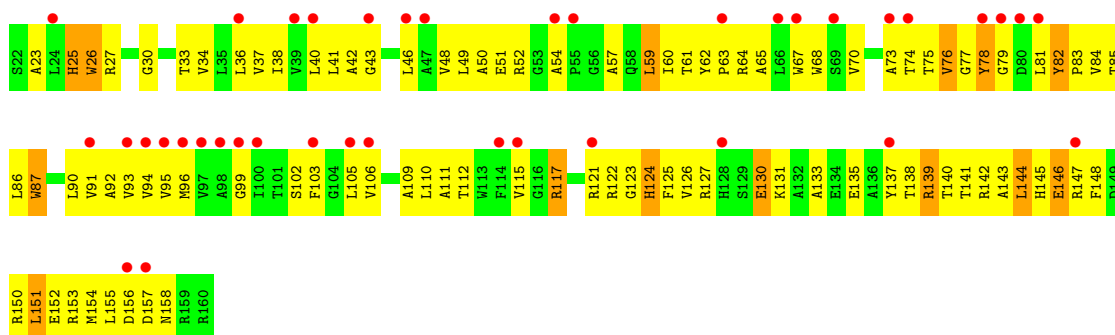




- Molecule 3: Voltage-gated potassium channel



- 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	115.80Å 173.91Å 339.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.80 40.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (40.00-3.80) 94.7 (40.00-3.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.48Å)	Xtrriage
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	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 213.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10912	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtrriage'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.*

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	0.41	0/1689	1.13	10/2292 (0.4%)
1	C	0.58	1/1689 (0.1%)	1.07	12/2292 (0.5%)
2	B	0.51	0/1698	1.01	9/2319 (0.4%)
2	D	0.63	1/1698 (0.1%)	1.09	8/2319 (0.3%)
3	K	0.41	0/1100	1.00	7/1501 (0.5%)
3	L	0.40	0/1100	0.99	4/1501 (0.3%)
3	M	0.42	0/1100	1.01	6/1501 (0.4%)
3	N	0.38	0/1100	0.99	5/1501 (0.3%)
All	All	0.49	2/11174 (0.0%)	1.04	61/15226 (0.4%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	109	VAL	CA-CB	-6.87	1.45	1.54
1	C	48	ILE	CA-CB	-5.44	1.47	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	SER	N-CA-C	-20.91	84.47	110.61
1	A	96	ALA	C-N-CD	-15.37	86.79	120.60
1	C	95	SER	N-CA-C	-9.82	89.64	107.60
2	D	131	SER	N-CA-C	-8.59	95.41	109.40
2	B	75	SER	N-CA-C	-8.24	102.25	111.07
2	D	5	VAL	N-CA-C	7.59	117.24	106.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	139	ARG	N-CA-C	-7.27	104.54	113.41
3	K	82	TYR	N-CA-C	7.13	114.55	108.13
1	A	166	THR	N-CA-C	-7.04	101.75	110.41
3	M	82	TYR	N-CA-C	6.91	114.34	108.13
3	L	82	TYR	N-CA-C	6.78	114.24	108.13
1	A	96	ALA	CA-C-N	6.71	143.12	127.00
1	A	96	ALA	C-N-CA	6.71	143.12	127.00
3	N	139	ARG	N-CA-C	-6.66	105.30	113.50
3	M	141	THR	N-CA-C	-6.64	104.05	111.28
2	D	165	TRP	N-CA-C	6.40	118.94	108.52
3	N	82	TYR	N-CA-C	6.38	113.87	108.13
2	B	124	SER	N-CA-C	-6.37	105.51	113.28
3	M	118	GLU	N-CA-C	-6.36	104.57	112.90
1	C	138	LEU	N-CA-C	-6.31	98.23	108.52
1	C	169	ASP	N-CA-C	6.20	119.25	110.50
1	A	93	SER	N-CA-C	6.19	123.98	110.80
2	B	112	ASP	N-CA-C	6.07	119.79	112.38
3	M	124	HIS	N-CA-C	-5.99	105.95	113.20
3	K	141	THR	N-CA-C	-5.87	104.06	111.11
3	K	117	ARG	N-CA-C	-5.84	106.11	113.18
1	C	108	ILE	N-CA-C	5.82	117.16	108.54
2	D	76	LYS	N-CA-C	-5.82	98.41	110.80
3	N	125	PHE	N-CA-C	-5.80	105.46	112.54
3	K	151	LEU	N-CA-C	-5.77	104.68	110.97
2	B	177	PHE	N-CA-C	5.72	117.97	110.08
3	K	154	MET	N-CA-C	-5.70	105.43	112.38
3	N	76	VAL	N-CA-C	-5.68	107.30	111.90
3	N	124	HIS	N-CA-C	-5.58	105.20	112.23
3	K	118	GLU	N-CA-C	-5.56	104.85	111.69
2	B	2	VAL	N-CA-C	5.54	116.72	109.58
2	B	126	SER	N-CA-C	5.53	118.70	110.52
2	D	177	PHE	N-CA-C	5.53	118.16	110.20
1	A	99	THR	N-CA-C	-5.39	98.86	108.13
1	A	213	ARG	N-CA-C	5.37	117.23	108.63
1	C	74	THR	N-CA-C	5.37	117.84	108.76
1	C	96	ALA	CA-C-N	5.34	126.52	119.84
1	C	96	ALA	C-N-CA	5.34	126.52	119.84
1	C	114	ALA	N-CA-C	-5.33	103.42	110.40
1	C	69	THR	N-CA-C	-5.31	107.47	114.31
3	K	58	GLN	N-CA-C	-5.29	106.96	113.41
2	B	61	ALA	N-CA-C	-5.28	103.71	110.53
3	M	117	ARG	N-CA-C	-5.26	106.63	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	155	ASP	N-CA-C	5.23	117.03	110.91
3	L	122	ARG	N-CA-C	-5.23	107.07	113.50
1	C	98	VAL	N-CA-C	5.19	120.14	109.34
1	A	193	VAL	N-CA-C	5.14	113.78	106.53
1	A	19	VAL	N-CA-C	5.13	115.69	108.36
1	C	94	TYR	N-CA-C	-5.12	102.74	110.06
2	D	61	ALA	N-CA-C	-5.12	103.92	110.53
2	B	82	GLN	N-CA-C	5.11	118.65	112.93
2	B	76	LYS	N-CA-C	-5.11	99.93	110.80
1	C	208	THR	N-CA-C	5.06	116.84	108.49
2	D	150	GLY	N-CA-C	5.04	117.39	110.69
3	M	41	LEU	N-CA-C	-5.02	107.84	114.31
3	L	41	LEU	N-CA-C	-5.00	107.86	114.31

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	226	0
1	C	1653	0	1604	226	0
2	B	1653	0	1597	232	0
2	D	1653	0	1597	236	0
3	K	1075	0	1066	160	0
3	L	1075	0	1066	126	0
3	M	1075	0	1066	131	0
3	N	1075	0	1066	112	0
All	All	10912	0	10666	1305	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 60.

All (1305) 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:C:4:MET:HE2	1:C:90:GLN:HB3	1.16	1.09
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
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.43	1.00
3:L:61:THR:HG22	3:L:63:PRO:HD2	1.43	1.00
2:B:83:MET:HE1	2:B:120:VAL:HG21	1.38	1.00
1:A:38:GLN:HE22	2:B:39:GLN:HE22	1.09	0.99
2:B:212:LYS:H	2:B:212:LYS:HD3	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:182:THR:C	1:C:183:LEU:HD12	1.90	0.95
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
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: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:HD23	1:C:11:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:C:54:LEU:O	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
3:L:76:VAL:HG21	3:M:96:MET:HE2	1.59	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:A:54:LEU:HD12	1:A:54:LEU:O	1.80	0.82
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:49:TYR:CD2	2:D:109:VAL:HA	2.19	0.77
1:C:90:GLN:HE22	1:C:93:SER:HB3	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:4:MET:CE	1:C:90:GLN:HB3	2.09	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
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
2:D:55:TYR:CE2	2:D:102:TYR:HB2	2.22	0.74
3:K:153:ARG:NH1	3:K:153:ARG:HB2	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:81:LEU:HD22	2:B:83:MET:CG	2.17	0.73
2:B:206:ILE:HG12	2:B:221:LYS:HA	1.70	0.73
3:N:106:VAL:O	3:N:110:LEU:HG	1.88	0.73
1:C:22:THR:HG22	1:C:72:THR:OG1	1.87	0.73
1:C:46:LEU:HD12	1:C:47:LEU:H	1.54	0.73
3:M:44:SER:OG	3:M:66:LEU:HA	1.88	0.73
2:D:83:MET:HE1	2:D:94:TYR:CZ	2.24	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:C	1:A:11:LEU:HD23	2.15	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:97:PRO:CD	1:A:98:VAL:N	2.46	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
2:B:6:GLU:CD	2:B:117:GLY:H	1.99	0.70
1:C:134:VAL:HG12	1:C:135:VAL:H	1.56	0.70
2:D:62:ASP:O	2:D:64:VAL:N	2.24	0.70
2:D:217:LYS:HD3	2:D:218:VAL:N	2.06	0.70
3:K:48:VAL:HG21	3:K:62:TYR:HA	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
3:L:151:LEU:HA	3:L:154:MET:HG3	1.73	0.70
3:M:127:ARG:HE	3:M:127:ARG:HA	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:9:GLY:H	2:B:118:THR:HG21	1.58	0.69
2:B:150:GLY:HA2	2:B:165:TRP:CH2	2.27	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:HD22	1:C:212:ASN:N	1.91	0.68
2:B:165:TRP:HZ3	2:B:222:VAL:HG21	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD2	2:B:80:TYR:N	2.62	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
3:K:153:ARG:HE	3:K:157:ASP:CG	2.03	0.67
1:A:2:ILE:HB	1:A:90:GLN:NE2	2.08	0.67
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:HD2	1:A:91:TYR:O	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
2:D:62:ASP:C	2:D:64:VAL:H	2.03	0.66
3:L:90:LEU:O	3:L:94:VAL:HG23	1.95	0.66
3:M:151:LEU:HD23	3:M:151:LEU:C	2.19	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:104:MET:HA	2:B:104:MET:HE2	1.77	0.66
1:C:214:GLY:O	1:C:215:GLU:HG3	1.94	0.66
1:A:137:LEU:HD23	1:A:137:LEU:C	2.20	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:54:ALA:HB3	3:M:57:ALA:HB2	1.78	0.66
3:M:137:TYR:O	3:M:140:THR:HB	1.96	0.66
2:B:91:THR:HG22	2:B:121:THR:CA	2.24	0.66
2:B:206:ILE:HG23	2:B:220:LYS:C	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:181:LEU:O	1:C:182:THR:HG23	1.96	0.65
2:D:145:GLY:N	2:D:197:SER:HG	1.95	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:K:93:VAL:HG22	3:N:70:VAL:HG11	1.80	0.64
3:L:62:TYR:HB2	3:L:63:PRO:HD3	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
2:B:51:ILE:HG23	2:B:51:ILE:O	1.96	0.64
2:B:82:GLN:O	2:B:82:GLN:HG3	1.97	0.64
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:23:ALA:CA	2:B:78:THR:HG23	2.28	0.64
2:B:109:VAL:O	2:B:110:ALA:O	2.16	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:D:207:CYS:C	2:D:208:ASN:HD22	2.06	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
1:A:25:ALA:C	1:A:27:GLN:H	2.05	0.63
2:D:211:HIS:HE1	2:D:213:PRO:HB2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:49:TYR:HD1	1.82	0.62
2:B:91:THR:O	2:B:92:ALA:HB2	1.98	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:3:GLN:HG3	2:B:25:SER:OG	2.00	0.61
2:B:165:TRP:CH2	2:B:207:CYS:HB3	2.35	0.61
3:K:59:LEU:HA	3:K:64:ARG:HD2	1.81	0.61
1:A:4:MET:HE2	1:A:90:GLN:HB3	1.81	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:HG23	2:D:51:ILE:O	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:30:GLY:O	3:K:34:VAL:HG23	2.00	0.61
3:K:100:ILE:HG21	3:N:103:PHE:CD2	2.35	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
1:C:95:SER:O	1:C:96:ALA:C	2.44	0.61
3:K:37:VAL:O	3:K:41:LEU:HG	2.00	0.61
1:A:83:PHE:CD1	1:A:107:GLU:HA	2.35	0.61
2:B:127:THR:HG22	2:B:158:PRO:HD3	1.81	0.61
2:B:132:VAL:HG21	2:B:218:VAL:HG11	1.81	0.61
2:D:173:GLY:O	2:D:193:VAL:HG23	2.00	0.61
2:B:18:LEU:HD12	2:B:120:VAL:HG13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TYR:HH	2:D:111:LEU:H	1.49	0.61
1:C:38:GLN:O	1:C:84:ALA:HB1	2.00	0.61
1:C:122:PRO:HG3	1:C:188:TYR:CZ	2.36	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
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
1:C:184:SER:O	1:C:185:LYS:C	2.44	0.61
3:K:43:GLY:HA3	3:K:68:TRP:HZ3	1.65	0.61
2:B:6:GLU:HG3	2:B:96:CYS:SG	2.40	0.60
2:B:161:VAL:HG12	2:B:211:HIS:CD2	2.36	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
1:A:49:TYR:O	1:A:50:SER:HB3	2.01	0.60
2:B:91:THR:CG2	2:B:122:VAL:H	2.14	0.60
2:D:58:THR:C	2:D:59:TYR:CD1	2.79	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
2:D:80:TYR:HD2	2:D:80:TYR:N	1.98	0.60
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:185:GLY:C	2:D:186:LEU:HD12	2.26	0.60
3:L:147:ARG:HH11	3:M:148:PHE:HB3	1.66	0.60
3:M:41:LEU:HD23	3:M:66:LEU:HD11	1.82	0.60
3:M:153:ARG:NH1	3:M:153:ARG:HB2	2.16	0.60
1:C:192:LYS:O	1:C:192:LYS:HG2	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:24:LEU:HD12	3:M:27:ARG:HB2	1.83	0.60
3:M:153:ARG:HA	3:M:157:ASP:OD2	2.02	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
2:D:181:LEU:C	2:D:181:LEU:HD23	2.25	0.60
3:L:59:LEU:HD11	3:L:65:ALA:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PRO:HB3	1:A:61:ARG:CZ	2.32	0.60
1:A:172:ASP:O	1:A:174:THR:HG23	2.02	0.60
3:L:43:GLY:HA2	3:L:91:VAL:CG1	2.32	0.60
2:D:13:GLN:N	2:D:13:GLN:OE1	2.34	0.60
2:D:67:ARG:NH1	2:D:90:ASP:OD2	2.34	0.60
2:D:147:ALA:O	2:D:194:THR:HA	2.02	0.60
3:L:54:ALA:HB3	3:L:57:ALA:HB2	1.84	0.60
1:A:4:MET:HE3	1:A:88:CYS:SG	2.42	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
3:K:151:LEU:C	3:K:151:LEU:HD23	2.27	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:20:LEU:HG	2:B:83:MET:HE2	1.83	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
1:A:91:TYR:O	1:A:91:TYR:CD2	2.55	0.59
2:B:116:GLN:OE1	2:B:116:GLN:HA	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
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:67:SER:HB3	1:A:70:ASP:HB2	1.84	0.58
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:C:37:GLN:HB2	1:C:47:LEU:HD11	1.85	0.58
1:C:165:VAL:HG12	1:C:177:LEU:CD2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:C	1:A:183:LEU:HD12	2.28	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
1:A:35:TRP:CD1	1:A:48:ILE:HB	2.37	0.58
1:C:89:GLN:HE22	2:D:111:LEU:HD21	1.67	0.58
3:K:153:ARG:NE	3:K:153:ARG:HA	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:HD12	1:C:127:LEU:N	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:NH1	1:C:61:ARG:HG2	2.17	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: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
1:A:195:ALA:HA	1:A:210:SER:HB3	1.84	0.58
1:A:183:LEU:HD12	1:A:183:LEU:N	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:36:TRP:CZ3	2:B:96:CYS:HB3	2.39	0.57
2:B:104:MET:O	2:B:106:SER:N	2.37	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
3:L:148:PHE:O	3:L:149:ASP:C	2.47	0.57
1:A:38:GLN:NE2	2:B:39:GLN:HE22	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:50:SER:C	1:C:52:SER:H	2.12	0.57
3:L:151:LEU:O	3:L:155:LEU:HD12	2.04	0.57
3:M:78:TYR:HH	3:N:68:TRP:CD1	2.22	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
1:A:93:SER:O	1:A:94:TYR:CB	2.54	0.56
1:A:191:HIS:O	1:A:213:ARG:NH1	2.30	0.56
2:B:111:LEU:CD2	2:B:111:LEU:N	2.67	0.56
2:B:166:ASN:HB2	2:B:169:ALA:HB3	1.87	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
2:D:29:ILE:O	2:D:30:SER:C	2.48	0.56
3:K:147:ARG:HG3	3:K:147:ARG:HH11	1.70	0.56
3:K:155:LEU:O	3:K:156:ASP:C	2.48	0.56
3:M:153:ARG:NE	3:M:153:ARG:HA	2.20	0.56
3:N:147:ARG:HB3	3:N:147:ARG:HH11	1.70	0.56
2:B:212:LYS:CG	2:B:213:PRO:HD3	2.28	0.56
1:C:211:PHE:C	1:C:212:ASN:HD22	2.12	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:2:VAL:HG11	2:B:98:ARG:HH11	1.71	0.56
2:B:109:VAL:O	2:B:109:VAL:CG2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:TYR:O	2:B:222:VAL:HG23	2.06	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
3:L:105:LEU:C	3:L:105:LEU:HD23	2.31	0.56
2:B:2:VAL:HG11	2:B:98:ARG:NH1	2.21	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
2:B:14:PRO:HD3	2:B:123:SER:C	2.30	0.56
1:C:95:SER:O	1:C:95:SER:OG	2.19	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: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:K:154:MET:HE2	3:K:154:MET:N	2.21	0.56
2:D:54:TYR:C	2:D:54:TYR:HD1	2.14	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:152:LEU:O	2:D:153:VAL:C	2.47	0.55
2:B:64:VAL:HG21	2:B:68:PHE:CB	2.35	0.55
3:N:49:LEU:HD12	3:N:52:ARG:HD2	1.87	0.55
3:N:99:GLY:O	3:N:103:PHE:HD1	1.88	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:13:GLN:H	2:D:13:GLN:CD	2.15	0.55
2:D:80:TYR:N	2:D:80:TYR:CD2	2.68	0.55
3:K:135:GLU:O	3:K:136:ALA:C	2.50	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
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
2:D:54:TYR:C	2:D:54:TYR:CD1	2.83	0.55
3:L:138:THR:C	3:L:141:THR:HG22	2.31	0.55
3:N:121:ARG:HA	3:N:121:ARG:NE	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:PRO:HB3	1:A:61:ARG:NH1	2.20	0.55
1:A:189:GLU:HA	1:A:213:ARG:CZ	2.37	0.55
2:B:127:THR:HG22	2:B:158:PRO:CD	2.36	0.55
2:B:147:ALA:O	2:B:194:THR:HA	2.07	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:HG23	1:C:152:VAL:O	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
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
1:C:200:HIS:C	1:C:202:GLY:H	2.15	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:2:VAL:HA	2:D:25:SER:O	2.07	0.54
2:D:149:LEU:HD23	2:D:193:VAL: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
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
2:D:81:LEU:HD23	2:D:81:LEU:C	2.33	0.54
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
3:N:138:THR:C	3:N:141:THR:HG22	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:11:LEU:HD23	1:A:11:LEU:O	2.08	0.54
1:A:112:VAL:HG12	1:A:113:ALA:N	2.23	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
3:L:150:ARG:HD3	3:M:152:GLU:CD	2.32	0.54
1:A:49:TYR:O	1:A:49:TYR:CD1	2.61	0.53
2:B:54:TYR:CD1	2:B:54:TYR:C	2.85	0.53
2:B:98:ARG:O	2:B:111:LEU:HA	2.08	0.53
2:B:60:TYR:HE2	2:B:70:ILE:HB	1.73	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
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:65:ALA:HA	3:M:68:TRP:HB3	1.90	0.53
3:M:151:LEU:HD23	3:M:151:LEU:O	2.07	0.53
1:A:79:GLN:HB3	1:A:81:GLU:OE1	2.08	0.53
3:K:157:ASP:N	3:K:157:ASP:OD1	2.38	0.53
1:A:163:GLU:HA	1:A:178:SER:O	2.08	0.53
2:B:27:PHE:CD2	2:B:98:ARG:HD2	2.43	0.53
2:B:62:ASP:C	2:B:64:VAL:H	2.17	0.53
2:B:163:VAL:HA	2:B:208:ASN:O	2.08	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
2:D:205:TYR:C	2:D:206:ILE:HG13	2.33	0.53
3:K:96:MET:HE2	3:N:76:VAL:HG21	1.90	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:54:LEU:HD12	1:C:54:LEU:C	2.33	0.53
1:C:61:ARG:O	1:C:75:ILE:HA	2.07	0.53
3:M:65:ALA:O	3:M:68:TRP:HB3	2.09	0.53
3:N:150:ARG:HG2	3:N:151:LEU:N	2.22	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:105:LEU:C	3:K:105:LEU:HD23	2.33	0.53
3:K:138:THR:HG23	3:K:139:ARG:N	2.23	0.53
3:K:152:GLU:CD	3:N:150:ARG:HD3	2.34	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:32:TYR:OH	2:B:98:ARG:NH2	2.42	0.53
2:B:111:LEU:HD23	2:B:111:LEU:H	1.73	0.53
1:C:96:ALA:O	1:C:97:PRO:C	2.51	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
1:A:81:GLU:C	1:A:83:PHE:H	2.17	0.53
2:B:91:THR:CG2	2:B:121:THR:HA	2.33	0.53
2:B:185:GLY:C	2:B:186:LEU:HD12	2.34	0.53
3:K:140:THR:O	3:K:141:THR:C	2.52	0.53
3:M:80:ASP:HB3	3:N:82:TYR:OH	2.08	0.53
3:M:147:ARG:HG3	3:M:147:ARG:NH1	2.23	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:M:149:ASP:O	3:M:150:ARG:C	2.52	0.53
2:B:2:VAL:HA	2:B:26:GLY:CA	2.33	0.52
3:L:26:TRP:HE3	3:L:26:TRP:HA	1.75	0.52
3:N:117:ARG:HG2	3:N:117:ARG:HH11	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:13:GLN:O	2:D:14:PRO:C	2.50	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
2:D:78:THR:HB	2:D:80:TYR:CE2	2.44	0.52
3:L:145:HIS:O	3:L:146:GLU:C	2.52	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:135:LEU:HB2	2:D:150:GLY:C	2.33	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:67:ARG:NH1	2:B:90:ASP:OD2	2.41	0.52
2:B:157:PHE:CD1	2:B:158:PRO:HA	2.43	0.52
1:C:137:LEU:HD23	1:C:138:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	3:M:26:TRP:CE3	2.45	0.52
1:A:3:GLN:HE21	1:A:4:MET:H	1.58	0.52
1:A:35:TRP:N	1:A:48:ILE:O	2.41	0.52
1:C:148:VAL:O	1:C:148:VAL:CG2	2.57	0.52
1:C:195:ALA:HA	1:C:210:SER:HB3	1.91	0.52
2:D:83:MET:HE1	2:D:94:TYR:CE1	2.45	0.52
3:L:26:TRP:HA	3:L:26:TRP:CE3	2.44	0.52
3:M:145:HIS:O	3:M:146:GLU:C	2.52	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
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
1:C:92:TYR:C	1:C:93:SER:O	2.53	0.51
1:C:191:HIS:O	1:C:213:ARG:CD	2.58	0.51
2:D:195:VAL:HG21	2:D:205:TYR:CE2	2.45	0.51
3:K:59:LEU:HD12	3:K:64:ARG:HG3	1.92	0.51
3:K:102:SER:O	3:K:106:VAL:HG23	2.10	0.51
3:L:147:ARG:NH1	3:L:147:ARG:CG	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
2:D:50:SER:C	2:D:70:ILE:HD13	2.35	0.51
3:K:92:ALA:HB3	3:N:67:TRP:CZ3	2.45	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:H	2:B:76:LYS:HD2	1.76	0.51
3:M:26:TRP:HA	3:M:26:TRP:HE3	1.75	0.51
3:M:105:LEU:HD23	3:M:105:LEU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:SER:O	2:D:107:TRP:HB2	2.10	0.51
2:D:145:GLY:C	2:D:196:PRO:HA	2.35	0.51
3:K:153:ARG:HB2	3:K:153:ARG:CZ	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:62:ASP:C	2:B:64:VAL:N	2.66	0.51
2:B:156:TYR:C	2:B:156:TYR:CD2	2.88	0.51
2:B:211:HIS:HE1	2:B:213:PRO:HB2	1.73	0.51
1:C:31:SER:N	1:C:66:ARG:CZ	2.74	0.51
3:K:58:GLN:O	3:K:60:ILE:N	2.40	0.51
3:K:143:ALA:HB1	3:L:145:HIS:HE1	1.76	0.51
1:C:31:SER:HB3	1:C:66:ARG:NH1	2.26	0.51
1:C:195:ALA:HA	1:C:210:SER:CB	2.41	0.51
2:D:137:PRO:HB3	2:D:149:LEU:CB	2.36	0.51
3:K:153:ARG:C	3:K:155:LEU:N	2.67	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
1:C:167:GLU:O	1:C:168:GLN:C	2.55	0.50
2:D:18:LEU:CD1	2:D:120:VAL:HG13	2.40	0.50
3:K:133:ALA:O	3:K:134:GLU:C	2.54	0.50
3:L:158:ASN:HD21	3:M:159:ARG:CB	2.24	0.50
3:N:26:TRP:HA	3:N:26:TRP:HE3	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
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:145:GLU:CD	1:C:145:GLU:H	2.20	0.50
1:C:148:VAL:O	1:C:148:VAL:HG23	2.10	0.50
3:K:151:LEU:HD13	3:N:151:LEU:HD13	1.94	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: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:K:152:GLU:HG3	3:N:154:MET:SD	2.51	0.50
3:L:144:LEU:HD21	3:L:148:PHE:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:C	1:A:27:GLN:N	2.67	0.50
2:D:103:HIS:O	3:K:153:ARG:CZ	2.59	0.50
3:M:151:LEU:C	3:M:151:LEU:CD2	2.84	0.50
3:N:145:HIS:O	3:N:146:GLU:C	2.54	0.50
1:A:30:SER:O	1:A:31:SER:C	2.54	0.50
2:B:60:TYR:OH	2:B:70:ILE:N	2.45	0.50
2:B:91:THR:HG22	2:B:121:THR:C	2.35	0.50
1:C:195:ALA:CB	1:C:210:SER:HB3	2.42	0.50
3:K:26:TRP:CE3	3:K:26:TRP:HA	2.47	0.50
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
1:A:49:TYR:CD1	1:A:49:TYR:C	2.89	0.50
2:B:4:LEU:HD21	2:B:27:PHE:HZ	1.76	0.50
2:B:35:HIS:O	2:B:96:CYS:HA	2.12	0.50
2:B:82:GLN:HA	2:B:82:GLN:HE21	1.76	0.50
1:C:90:GLN:OE1	1:C:90:GLN:C	2.55	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:N:105:LEU:C	3:N:105:LEU:HD23	2.36	0.50
2:B:54:TYR:C	2:B:54:TYR:HD1	2.20	0.49
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:HB2	3:M:153:ARG:CZ	2.42	0.49
3:M:155:LEU:O	3:M:156:ASP:C	2.55	0.49
1:A:33:VAL:HG12	1:A:34:ALA:N	2.26	0.49
1:A:90:GLN:C	1:A:90:GLN:OE1	2.56	0.49
1:A:110:ARG:HH11	1:A:110:ARG:CB	2.25	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:NH1	3:L:147:ARG:HG3	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
3:K:61:THR:CG2	3:K:63:PRO:HD2	2.27	0.49
3:K:100:ILE:HG21	3:N:103:PHE:HD2	1.77	0.49
3:K:130:GLU:O	3:K:134:GLU:HG3	2.11	0.49
3:M:49:LEU:HD12	3:M:52:ARG:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:138:THR:HG23	3:M:139:ARG:N	2.26	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:64:VAL:HG21	2:D:68:PHE:CD2	2.46	0.49
2:D:137:PRO:HG2	2:D:224:PRO:HG3	1.94	0.49
3:M:61:THR:HB	3:M:64:ARG:CG	2.40	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:K:145:HIS:O	3:K:146:GLU:C	2.55	0.49
3:M:42:ALA:O	3:M:46:LEU:HG	2.12	0.49
3:N:50:ALA:O	3:N:85:THR:HG21	2.12	0.49
1:A:49:TYR:HD1	1:A:49:TYR:C	2.21	0.49
1:A:61:ARG:O	1:A:75:ILE:HA	2.11	0.49
3:K:39:VAL:HG12	3:K:95:VAL:HG22	1.95	0.49
3:M:144:LEU:O	3:M:145:HIS:C	2.56	0.49
3:N:65:ALA:O	3:N:68:TRP:HB3	2.13	0.49
3:N:109:ALA:HA	3:N:112:THR:HG22	1.94	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:107:TRP:CZ3	3:K:154:MET:HE1	2.47	0.49
2:D:174:VAL:HG13	2:D:193:VAL:HB	1.95	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
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:62:ASP:C	2:D:64:VAL:N	2.68	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:143:ALA:O	3:L:144:LEU:C	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:78:TYR:O	3:N:79:GLY:HA3	2.13	0.48
1:A:94:TYR:CE2	3:M:147:ARG:NE	2.81	0.48
1:A:134:VAL:O	1:A:180:THR:HG23	2.13	0.48
2:B:79:ALA:C	2:B:80:TYR:HD2	2.20	0.48
1:C:92:TYR:OH	3:L:156:ASP:OD2	2.31	0.48
1:C:98:VAL:HG21	2:D:47:TRP:CD1	2.49	0.48
1:C:172:ASP:OD2	1:C:172:ASP:N	2.45	0.48
2:D:167:SER:HA	2:D:208:ASN:OD1	2.13	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
1:C:21:ILE:O	1:C:72:THR:HA	2.13	0.48
3:L:156:ASP:O	3:L:160:ARG:OXT	2.31	0.48
3:M:86:LEU:HG	3:M:87:TRP:CZ3	2.48	0.48
1:A:63:SER:O	1:A:73:LEU:HD12	2.14	0.48
2:D:119:LEU:HD23	2:D:119:LEU:C	2.39	0.48
2:D:159:GLU:OE1	2:D:159:GLU:HA	2.12	0.48
2:B:13:GLN:OE1	2:B:13:GLN:N	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:14:PRO:HD3	2:D:123:SER:C	2.39	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: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
2:B:13:GLN:O	2:B:14:PRO:C	2.57	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
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:55:TYR:O	2:D:56:SER:C	2.54	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:76:VAL:HG21	3:M:96:MET:CE	2.39	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
1:C:185:LYS:O	1:C:186:ALA:C	2.56	0.47
2:D:64:VAL:HG21	2:D:68:PHE:HB2	1.95	0.47
1:A:15:VAL:CG2	1:A:16:GLY:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:GLN:O	2:B:83:MET:C	2.55	0.47
2:B:109:VAL:O	2:B:109:VAL:HG23	2.14	0.47
2:B:154:LYS:O	2:B:155:ASP:HB2	2.14	0.47
1:C:134:VAL:C	1:C:135:VAL:HG12	2.38	0.47
1:C:182:THR:N	1:C:183:LEU:HD12	2.29	0.47
3:K:45:TYR:CD1	3:K:62:TYR:HE2	2.32	0.47
3:K:89:ARG:HB3	3:N:67:TRP:CE3	2.49	0.47
3:N:123:GLY:O	3:N:126:VAL:HB	2.14	0.47
3:N:143:ALA:O	3:N:144:LEU:C	2.57	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:K:151:LEU:C	3:K:151:LEU:CD2	2.86	0.47
3:L:124:HIS:O	3:L:124:HIS:ND1	2.47	0.47
1:C:34:ALA:HA	1:C:48:ILE:O	2.15	0.47
1:C:208:THR:HG22	1:C:208:THR:O	2.13	0.47
2:D:215:ASN:CG	2:D:215:ASN:O	2.57	0.47
3:M:149:ASP:O	3:M:152:GLU:HB3	2.14	0.47
1:A:137:LEU:C	1:A:138:LEU:HD12	2.40	0.47
2:B:49:ALA:CB	2:B:70:ILE:HD12	2.44	0.47
3:K:26:TRP:HA	3:K:26:TRP:HE3	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:24:ARG:HD3	1:A:70:ASP:OD1	2.14	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
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:N:143:ALA:O	3:N:146:GLU:N	2.48	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
2:B:211:HIS:C	2:B:213:PRO:HD2	2.40	0.47
1:C:119:ILE:HG22	1:C:209:LYS:HB3	1.97	0.47
1:C:137:LEU:HD23	1:C:137:LEU:C	2.40	0.47
2:D:96:CYS:SG	2:D:96:CYS:O	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:51:GLU:O	3:M:60:ILE:HG22	2.15	0.47
3:M:144:LEU:O	3:M:148:PHE:N	2.47	0.47
3:N:33:THR:O	3:N:37:VAL:HG23	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:137:LEU:HD23	1:C:138:LEU:C	2.40	0.47
1:C:183:LEU:HD12	1:C:183:LEU:N	2.27	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:22:CYS:C	2:D:78:THR:HG23	2.40	0.47
2:D:181:LEU:HD12	2:D:187:TYR:CE1	2.50	0.47
3:K:50:ALA:O	3:K:85:THR:HG21	2.15	0.47
2:B:36:TRP:CE3	2:B:96:CYS:HB3	2.50	0.47
2:B:107:TRP:CG	2:B:107:TRP:O	2.68	0.47
2:B:208:ASN:N	2:B:208:ASN:HD22	2.12	0.47
2:B:211:HIS:O	2:B:211:HIS:ND1	2.48	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:77:ASN:C	2:D:78:THR:OG1	2.59	0.46
2:D:91:THR:O	2:D:92:ALA:HB2	2.14	0.46
2:D:195:VAL:HG11	2:D:205:TYR:CE1	2.50	0.46
3:K:156:ASP:CG	3:N:154:MET:HE2	2.40	0.46
3:L:117:ARG:NH1	3:L:117:ARG:HG3	2.30	0.46
3:M:151:LEU:O	3:M:154:MET:HB2	2.15	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
1:A:44:PRO:CG	2:B:45:LEU:HD11	2.45	0.46
1:A:138:LEU:HD12	1:A:138:LEU:N	2.30	0.46
2:B:159:GLU:HG2	2:B:187:TYR:CE2	2.50	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
2:D:127:THR:C	2:D:128:LYS:HG3	2.40	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:36:TRP:CE2	2:B:81:LEU:HB2	2.49	0.46
3:K:58:GLN:O	3:K:64:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:36:LEU:HD13	3:N:102:SER:OG	2.15	0.46
3:N:51:GLU:CD	3:N:83:PRO:HA	2.40	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
2:D:166:ASN:C	2:D:168:GLY:H	2.24	0.46
3:K:144:LEU:O	3:K:145:HIS:C	2.58	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:78:THR:HG22	2:D:79:ALA:N	2.31	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
3:K:51:GLU:O	3:K:60:ILE:HG22	2.15	0.46
3:K:138:THR:HA	3:K:141:THR:HG23	1.98	0.46
3:L:68:TRP:O	3:L:71:GLU:HG2	2.16	0.46
1:A:49:TYR:O	1:A:50:SER:CB	2.63	0.46
1:A:127:LEU:HD12	1:A:127:LEU:N	2.30	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:HG12	1:C:193:VAL:O	2.16	0.46
2:D:2:VAL:HG22	2:D:26:GLY:C	2.41	0.46
2:D:39:GLN:C	2:D:92:ALA:HB1	2.41	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:58:THR:HB	2:D:70:ILE:CG2	2.47	0.45
2:D:152:LEU:O	2:D:154:LYS:N	2.50	0.45
3:K:36:LEU:O	3:K:40:LEU:HG	2.16	0.45
3:K:115:VAL:O	3:K:118:GLU:HB3	2.16	0.45
3:K:155:LEU:HD22	3:N:151:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:MET:HE1	2:B:120:VAL:CG2	2.27	0.45
2:B:156:TYR:CE2	2:B:187:TYR:HB2	2.51	0.45
2:B:207:CYS:O	2:B:207:CYS:SG	2.73	0.45
3:K:70:VAL:CG1	3:L:93:VAL:HG13	2.41	0.45
3:L:138:THR:O	3:L:141:THR:HG22	2.15	0.45
1:A:49:TYR:C	1:A:51:ALA:H	2.23	0.45
2:D:6:GLU:CG	2:D:96:CYS:SG	2.97	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
3:K:64:ARG:O	3:K:81:LEU:HD13	2.17	0.45
3:K:80:ASP:HB3	3:L:82:TYR:OH	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
1:A:49:TYR:HB2	2:B:109:VAL:HA	1.98	0.45
1:A:92:TYR:O	3:M:150:ARG:NH2	2.49	0.45
1:C:30:SER:O	1:C:31:SER:C	2.58	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
2:B:181:LEU:HD23	2:B:181:LEU:C	2.42	0.45
1:C:38:GLN:HE22	2:D:39:GLN:HE22	1.64	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:A:49:TYR:CB	2:B:109:VAL:HA	2.47	0.45
1:A:78:LEU:HD12	1:A:78:LEU:C	2.40	0.45
1:A:169:ASP:OD2	1:A:170:SER:N	2.46	0.45
3:M:138:THR:C	3:M:140:THR:H	2.24	0.45
2:B:149:LEU:CD2	2:B:193:VAL:HG13	2.47	0.45
1:C:200:HIS:C	1:C:202:GLY:N	2.75	0.45
3:K:86:LEU:HG	3:K:87:TRP:CZ3	2.52	0.45
3:K:96:MET:HE2	3:N:74:THR:OG1	2.17	0.45
3:K:149:ASP:O	3:K:150:ARG:C	2.59	0.45
3:N:82:TYR:HB2	3:N:83:PRO:HD2	1.99	0.45
1:A:91:TYR:OH	2:B:108:TRP:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TYR:CE1	1:A:143:PRO:HB3	2.52	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:138:THR:C	3:M:140:THR:N	2.73	0.45
1:A:29:VAL:O	1:A:31:SER:N	2.50	0.44
1:C:101:GLY:C	1:C:103:GLY:N	2.75	0.44
2:D:206:ILE:HG23	2:D:220:LYS:C	2.41	0.44
3:K:68:TRP:HZ2	3:K:92:ALA:HB2	1.82	0.44
3:K:148:PHE:HZ	3:N:148:PHE:CE1	2.35	0.44
3:K:153:ARG:CZ	3:K:153:ARG:CB	2.94	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: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: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
3:M:73:ALA:C	3:M:75:THR:H	2.25	0.44
3:N:86:LEU:HG	3:N:87:TRP:CZ3	2.52	0.44
1:A:54:LEU:HD12	1:A:54:LEU:C	2.39	0.44
1:C:27:GLN:O	1:C:28:SER:C	2.60	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:87:TRP:HA	3:K:87:TRP:CE3	2.52	0.44
3:K:151:LEU:HD13	3:N:151:LEU:CD1	2.47	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
2:B:37:VAL:HG11	2:B:114:TRP:CZ3	2.53	0.44
2:B:82:GLN:HA	2:B:82:GLN:NE2	2.32	0.44
1:C:50:SER:O	1:C:51:ALA:CB	2.65	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
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:HA	3:M:139:ARG:HD3	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
3:L:25:HIS:H	3:L:25:HIS:CD2	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:43:GLY:C	3:L:68:TRP:HZ3	2.25	0.44
3:L:87:TRP:HA	3:L:87:TRP:HE3	1.81	0.44
3:L:139:ARG:HA	3:L:142:ARG:CD	2.47	0.44
1:A:81:GLU:O	1:A:83:PHE:N	2.51	0.44
1:A:126:GLN:HG3	2:B:133:PHE:CD2	2.52	0.44
2:B:43:LYS:HB3	2:B:44:GLY:H	1.64	0.44
2:B:186:LEU:HD12	2:B:186:LEU:N	2.32	0.44
3:N:51:GLU:O	3:N:57:ALA:HB1	2.18	0.44
3:N:73:ALA:C	3:N:75:THR:H	2.26	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
3:K:76:VAL:HG21	3:L:96:MET:HE2	2.00	0.44
1:A:184:SER:O	1:A:185:LYS:C	2.60	0.44
1:C:134:VAL:O	1:C:180:THR:HG22	2.17	0.44
1:C:137:LEU:C	1:C:137:LEU:CD2	2.91	0.44
3:K:156:ASP:OD1	3:N:154:MET:HE2	2.18	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
2:B:154:LYS:HG2	2:B:155:ASP:OD2	2.18	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:82:TYR:HB2	3:L:83:PRO:HD2	2.00	0.43
3:L:155:LEU:O	3:L:157:ASP:N	2.51	0.43
3:M:51:GLU:CD	3:M:83:PRO:HA	2.43	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:79:ALA:C	2:B:80:TYR:CD2	2.95	0.43
2:B:212:LYS:N	2:B:213:PRO:CD	2.81	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
1:C:123:SER:O	1:C:126:GLN:HB2	2.18	0.43
1:C:177:LEU:O	2:D:177:PHE:CZ	2.71	0.43
2:D:91:THR:HA	2:D:120:VAL:O	2.18	0.43
1:A:141:PHE:CD1	1:A:141:PHE:C	2.96	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
3:M:135:GLU:O	3:M:136:ALA:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:142:ARG:C	3:K:144:LEU:N	2.76	0.43
3:N:43:GLY:HA2	3:N:91:VAL:CG1	2.48	0.43
1:A:189:GLU:C	1:A:213:ARG:HH12	2.26	0.43
2:B:27:PHE:CD2	2:B:27:PHE:N	2.86	0.43
2:B:39:GLN:O	2:B:40:ALA:C	2.62	0.43
1:C:81:GLU:H	1:C:81:GLU:CD	2.25	0.43
1:C:92:TYR:O	1:C:93:SER:C	2.59	0.43
2:D:64:VAL:HG21	2:D:68:PHE:CB	2.48	0.43
2:D:130:PRO:CA	2:D:156:TYR:HB3	2.49	0.43
2:D:217:LYS:HD3	2:D:217:LYS:C	2.44	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:D:52:SER:C	2:D:54:TYR:H	2.26	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:98:VAL:HB	2:D:47:TRP:CG	2.54	0.43
1:C:127:LEU:HG	1:C:132:ALA:HB2	2.01	0.43
3:K:74:THR:OG1	3:K:76:VAL:HG23	2.19	0.43
1:A:15:VAL:C	1:A:17:ASP:H	2.27	0.43
1:A:79:GLN:CB	1:A:80:PRO:HD2	2.45	0.43
1:A:137:LEU:CD2	1:A:137:LEU:C	2.91	0.43
2:D:166:ASN:C	2:D:168:GLY:N	2.77	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:29:ILE:O	2:B:30:SER:C	2.62	0.43
2:B:82:GLN:HE21	2:B:82:GLN:CA	2.32	0.43
2:D:197:SER:C	2:D:199:SER:H	2.26	0.43
2:D:210:ASN:HD22	2:D:210:ASN:C	2.27	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:HH11	3:L:147:ARG:HG3	1.84	0.43
3:N:65:ALA:HA	3:N:68:TRP:HB3	2.00	0.43
1:A:64:GLY:HA2	1:A:72:THR:O	2.19	0.42
1:A:139:ASN:ND2	1:A:140:ASN:OD1	2.52	0.42
1:C:150:TRP:C	1:C:151:LYS:HG3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:76:VAL:HG22	3:L:75:THR:CB	2.49	0.42
1:A:110:ARG:HB2	1:A:110:ARG:CZ	2.49	0.42
2:B:84:ASN:O	2:B:85:SER:C	2.62	0.42
1:C:139:ASN:ND2	1:C:140:ASN:OD1	2.51	0.42
3:L:78:TYR:OH	3:M:68:TRP:NE1	2.52	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:A:125:GLU:O	1:A:126:GLN:C	2.62	0.42
1:C:108:ILE:HG23	1:C:168:GLN:CD	2.45	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:22:CYS:C	2:B:78:THR:HG23	2.44	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:116:GLY:HA2	3:L:119:GLN:CD	2.44	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:47:TRP:CE2	2:D:49:ALA:O	2.71	0.42
2:D:149:LEU:HD23	2:D:149:LEU:H	1.84	0.42
2:D:186:LEU:N	2:D:186:LEU:CD1	2.83	0.42
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
3:K:78:TYR:HD2	3:K:78:TYR:HA	1.74	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:M:87:TRP:HA	3:M:87:TRP:HE3	1.85	0.42
3:N:86:LEU:O	3:N:90:LEU:HG	2.19	0.42
1:A:11:LEU:C	1:A:11:LEU:CD2	2.86	0.42
1:A:38:GLN:HE22	2:B:39:GLN:NE2	1.93	0.42
1:C:179:SER:C	1:C:180:THR:OG1	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:27:ARG:O	3:M:31:ALA:HB2	2.20	0.42
3:M:127:ARG:O	3:M:131:LYS:HG3	2.19	0.42
1:C:49:TYR:O	1:C:49:TYR:CD1	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:91:TYR:CD2	1:A:91:TYR:C	2.98	0.42
1:A:152:VAL:HG12	1:A:194:TYR:CE2	2.54	0.42
2:B:65:LYS:C	2:B:67:ARG:H	2.28	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
1:C:36:TYR:HH	2:D:111:LEU:N	2.18	0.42
2:D:6:GLU:OE1	2:D:117:GLY:N	2.52	0.42
2:D:9:GLY:HA3	2:D:118:THR:HG21	2.02	0.42
2:D:40:ALA:HB1	2:D:41:PRO:HD2	2.02	0.42
2:D:116:GLN:O	2:D:117:GLY:O	2.38	0.42
3:K:138:THR:C	3:K:140:THR:N	2.78	0.42
3:K:141:THR:OG1	3:K:142:ARG:N	2.53	0.42
3:M:150:ARG:O	3:M:151:LEU:C	2.63	0.42
1:A:11:LEU:HD22	1:A:106:VAL:CG1	2.47	0.42
1:C:43:ALA:O	1:C:44:PRO:C	2.62	0.42
1:C:120:PHE:CE1	2:D:135:LEU:HB3	2.55	0.42
2:D:105:TYR:O	2:D:106:SER:C	2.63	0.42
3:K:96:MET:CE	3:N:76:VAL:HG21	2.49	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:87:TRP:HA	3:M:87:TRP:CE3	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:31:SER:HB3	1:C:66:ARG:CD	2.50	0.41
1:C:50:SER:C	1:C:52:SER:N	2.78	0.41
3:N:61:THR:CG2	3:N:63:PRO:HD2	2.36	0.41
1:A:135:VAL:HA	1:A:180:THR:HA	2.02	0.41
2:B:119:LEU:HD23	2:B:119:LEU:C	2.45	0.41
2:D:18:LEU:HD23	2:D:18:LEU:HA	1.74	0.41
2:D:168:GLY:O	2:D:171:THR:CG2	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:TYR:HE2	2:D:114:TRP:HE1	1.68	0.41
1:C:129:SER:OG	1:C:130:GLY:N	2.54	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:87:TRP:CE3	3:N:87:TRP:HA	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: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:OE2	2:B:89:GLU:N	2.50	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
1:C:110:ARG:O	1:C:111:THR:C	2.62	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:67:ARG:HG2	2:D:85:SER:HB2	2.02	0.41
2:D:125:ALA:HB3	2:D:157:PHE:CE2	2.56	0.41
2:D:165:TRP:CZ3	2:D:207:CYS:HB3	2.54	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
1:A:94:TYR:HE2	3:N:145:HIS:HD2	1.69	0.41
2:B:68:PHE:CD1	2:B:83:MET:HA	2.55	0.41
2:B:181:LEU:HD23	2:B:182:GLN:O	2.21	0.41
1:C:36:TYR:OH	2:D:110:ALA:CB	2.69	0.41
1:C:142:TYR:CD1	1:C:142:TYR:C	2.98	0.41
1:C:195:ALA:CA	1:C:210:SER:HB3	2.51	0.41
3:M:133:ALA:O	3:M:134:GLU:C	2.63	0.41
1:A:94:TYR:C	1:A:96:ALA:H	2.23	0.41
1:A:101:GLY:O	1:A:102:GLN:C	2.63	0.41
1:C:11:LEU:HD23	1:C:106:VAL:HG13	1.99	0.41
2:D:149:LEU:HD23	2:D:149:LEU:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:76:VAL:HG22	3:L:75:THR:HG22	2.02	0.41
3:K:134:GLU:O	3:K:138:THR:HG22	2.20	0.41
3:L:121:ARG:HA	3:L:121:ARG:NE	2.36	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:2:VAL:CG2	2:B:26:GLY:HA3	2.49	0.41
2:B:170:LEU:CD2	2:B:174:VAL:HG22	2.51	0.41
1:C:89:GLN:HB2	1:C:100:PHE:CD1	2.56	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
2:D:18:LEU:O	2:D:83:MET:N	2.54	0.41
2:D:68:PHE:CD1	2:D:83:MET:HA	2.55	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:24:ARG:HB2	1:A:70:ASP:OD1	2.21	0.41
1:A:81:GLU:C	1:A:83:PHE:N	2.78	0.41
1:A:137:LEU:HD11	2:B:192:VAL:HG21	2.02	0.41
1:A:150:TRP:CE3	1:A:181:LEU:HG	2.56	0.41
2:B:103:HIS:O	2:B:104:MET:C	2.63	0.41
1:C:115:PRO:HD3	1:C:200:HIS:CD2	2.56	0.41
2:D:48:VAL:HG11	2:D:68:PHE:CD2	2.55	0.41
2:D:98:ARG:O	2:D:111:LEU:HA	2.20	0.41
2:D:104:MET:HB3	2:D:105:TYR:H	1.62	0.41
2:D:165:TRP:CZ2	2:D:207:CYS:HB3	2.54	0.41
3:K:44:SER:HA	3:K:65:ALA:HB1	2.02	0.41
3:K:67:TRP:CD1	3:K:67:TRP:C	2.99	0.41
3:K:82:TYR:HB2	3:K:83:PRO:HD2	2.03	0.41
3:L:87:TRP:CE3	3:L:90:LEU:CD1	3.04	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
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
2:D:212:LYS:H	2:D:212:LYS:CD	2.34	0.41
3:K:136:ALA:HB2	3:L:134:GLU:OE2	2.21	0.41
3:M:48:VAL:HG13	3:M:60:ILE:C	2.46	0.41
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:HG3	1:A:90:GLN:O	2.21	0.40
2:B:16:GLY:O	2:B:86:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:153:ARG:CZ	3:M:153:ARG:CB	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:O	1:A:29:VAL:HG12	2.21	0.40
1:A:95:SER:O	1:A:96:ALA:C	2.64	0.40
2:B:155:ASP:C	2:B:186:LEU:HD23	2.46	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:K:22:SER:C	3:K:24:LEU:H	2.30	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
2:B:2:VAL:HG22	2:B:26:GLY:C	2.46	0.40
2:B:37:VAL:HA	2:B:47:TRP:HA	2.03	0.40
2:B:55:TYR:O	2:B:56:SER:C	2.65	0.40
2:D:50:SER:O	2:D:70:ILE:HG21	2.22	0.40
2:D:102:TYR:CE1	3:K:150:ARG:HB2	2.56	0.40
2:D:170:LEU:HD23	2:D:171:THR:N	2.36	0.40
3:K:151:LEU:O	3:K:154:MET:N	2.54	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: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
2:B:177:PHE:HA	2:B:178:PRO:HD3	1.76	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:M:78:TYR:CD2	3:N:77:GLY:HA2	2.56	0.40
3:M:155:LEU:C	3:M:157:ASP:N	2.79	0.40
3:N:150:ARG:CG	3:N:151:LEU:N	2.83	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	10
1	C	213/215 (99%)	147 (69%)	46 (22%)	20 (9%)	0	8
2	B	215/224 (96%)	154 (72%)	49 (23%)	12 (6%)	1	15
2	D	215/224 (96%)	164 (76%)	33 (15%)	18 (8%)	0	9
3	K	137/139 (99%)	121 (88%)	13 (10%)	3 (2%)	5	30
3	L	137/139 (99%)	122 (89%)	13 (10%)	2 (2%)	8	36
3	M	137/139 (99%)	121 (88%)	14 (10%)	2 (2%)	8	36
3	N	137/139 (99%)	122 (89%)	13 (10%)	2 (2%)	8	36
All	All	1404/1434 (98%)	1112 (79%)	216 (15%)	76 (5%)	1	16

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%)	172 (91%)	17 (9%)	9	32
1	C	189/189 (100%)	159 (84%)	30 (16%)	2	14
2	B	184/188 (98%)	166 (90%)	18 (10%)	7	29
2	D	184/188 (98%)	161 (88%)	23 (12%)	4	21
3	K	104/107 (97%)	92 (88%)	12 (12%)	5	23
3	L	104/107 (97%)	91 (88%)	13 (12%)	4	21
3	M	104/107 (97%)	90 (86%)	14 (14%)	4	19
3	N	104/107 (97%)	94 (90%)	10 (10%)	8	29
All	All	1162/1182 (98%)	1025 (88%)	137 (12%)	5	22

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	THR
1	A	11	LEU
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	124	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
1	A	192	LYS
2	B	12	VAL
2	B	37	VAL
2	B	58	THR
2	B	64	VAL
2	B	80	TYR
2	B	104	MET
2	B	105	TYR
2	B	106	SER
2	B	109	VAL
2	B	111	LEU
2	B	112	ASP
2	B	121	THR
2	B	123	SER
2	B	153	VAL
2	B	160	PRO
2	B	174	VAL
2	B	212	LYS
2	B	217	LYS
1	C	5	THR
1	C	8	PRO
1	C	11	LEU
1	C	15	VAL
1	C	29	VAL
1	C	40	PRO
1	C	48	ILE
1	C	49	TYR

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Mol	Chain	Res	Type
1	C	81	GLU
1	C	90	GLN
1	C	97	PRO
1	C	98	VAL
1	C	108	ILE
1	C	124	ASP
1	C	126	GLN
1	C	135	VAL
1	C	137	LEU
1	C	148	VAL
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	192	LYS
1	C	199	THR
1	C	212	ASN
2	D	3	GLN
2	D	4	LEU
2	D	12	VAL
2	D	54	TYR
2	D	56	SER
2	D	58	THR
2	D	64	VAL
2	D	78	THR
2	D	80	TYR
2	D	82	GLN
2	D	83	MET
2	D	93	VAL
2	D	98	ARG
2	D	112	ASP
2	D	120	VAL
2	D	130	PRO
2	D	132	VAL
2	D	160	PRO
2	D	171	THR
2	D	174	VAL

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Mol	Chain	Res	Type
2	D	208	ASN
2	D	212	LYS
2	D	216	THR
3	K	26	TRP
3	K	78	TYR
3	K	87	TRP
3	K	113	TRP
3	K	118	GLU
3	K	121	ARG
3	K	140	THR
3	K	144	LEU
3	K	147	ARG
3	K	150	ARG
3	K	153	ARG
3	K	157	ASP
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	138	THR
3	L	140	THR
3	L	144	LEU
3	L	146	GLU
3	L	147	ARG
3	L	154	MET
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	127	ARG
3	M	140	THR
3	M	141	THR
3	M	144	LEU
3	M	147	ARG
3	M	153	ARG
3	M	154	MET
3	M	156	ASP

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Mol	Chain	Res	Type
3	N	25	HIS
3	N	26	TRP
3	N	78	TYR
3	N	87	TRP
3	N	117	ARG
3	N	130	GLU
3	N	140	THR
3	N	144	LEU
3	N	146	GLU
3	N	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	6	GLN
1	A	139	ASN
1	A	154	ASN
1	A	157	GLN
1	A	160	ASN
1	A	162	GLN
1	A	168	GLN
1	A	191	HIS
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	37	GLN
1	C	89	GLN
1	C	149	GLN
1	C	154	ASN
1	C	157	GLN
1	C	212	ASN
2	D	3	GLN
2	D	39	GLN
2	D	77	ASN
2	D	82	GLN
2	D	208	ASN

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Mol	Chain	Res	Type
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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%)	1.05	30 (13%) 6 9	68, 175, 254, 259	0
1	C	215/215 (100%)	0.59	22 (10%) 12 14	43, 105, 196, 259	0
2	B	219/224 (97%)	0.80	31 (14%) 6 9	49, 124, 239, 259	0
2	D	219/224 (97%)	0.47	18 (8%) 17 17	35, 92, 192, 259	0
3	K	139/139 (100%)	1.37	38 (27%) 1 3	65, 255, 259, 259	0
3	L	139/139 (100%)	1.27	26 (18%) 3 6	52, 251, 259, 259	0
3	M	139/139 (100%)	1.23	29 (20%) 2 4	61, 249, 259, 259	0
3	N	139/139 (100%)	1.42	39 (28%) 1 2	57, 255, 259, 259	0
All	All	1424/1434 (99%)	0.96	233 (16%) 4 7	35, 169, 259, 259	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	SER	8.8
1	A	206	PRO	6.9
3	M	145	HIS	6.4
3	K	145	HIS	6.2
3	N	80	ASP	5.9
3	L	74	THR	5.8
2	B	171	THR	5.6
2	B	132	VAL	5.5
1	C	96	ALA	5.1
3	M	100	ILE	4.8
3	M	67	TRP	4.8
3	N	137	TYR	4.7
1	C	167	GLU	4.7
1	A	122	PRO	4.4
3	M	96	MET	4.4
3	L	107	THR	4.2

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Mol	Chain	Res	Type	RSRZ
3	L	97	VAL	4.2
3	N	95	VAL	4.2
3	L	103	PHE	4.1
1	A	148	VAL	4.1
2	B	9	GLY	4.1
3	M	70	VAL	4.1
3	L	137	TYR	4.1
3	L	38	ILE	4.1
3	K	109	ALA	4.0
3	N	78	TYR	4.0
1	C	201	GLN	4.0
3	L	157	ASP	3.9
3	M	39	VAL	3.9
1	C	28	SER	3.9
3	M	97	VAL	3.8
2	B	44	GLY	3.8
2	B	45	LEU	3.7
3	K	67	TRP	3.7
1	C	14	SER	3.6
2	D	13	GLN	3.6
3	N	67	TRP	3.6
3	K	105	LEU	3.6
3	N	91	VAL	3.6
3	N	55	PRO	3.5
3	N	96	MET	3.5
3	K	158	ASN	3.5
3	M	103	PHE	3.5
3	K	73	ALA	3.5
3	L	156	ASP	3.4
2	D	104	MET	3.4
3	L	113	TRP	3.4
3	K	96	MET	3.4
3	N	157	ASP	3.4
3	L	110	LEU	3.4
3	K	47	ALA	3.3
2	D	161	VAL	3.3
3	N	39	VAL	3.3
3	K	112	THR	3.3
1	A	163	GLU	3.3
3	K	103	PHE	3.2
3	M	105	LEU	3.2
2	B	175	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
3	K	127	ARG	3.2
2	B	177	PHE	3.2
2	D	105	TYR	3.2
1	A	188	TYR	3.1
1	A	211	PHE	3.1
1	A	201	GLN	3.1
3	N	93	VAL	3.1
3	K	74	THR	3.1
3	N	97	VAL	3.1
1	A	108	ILE	3.1
1	C	214	GLY	3.1
3	L	39	VAL	3.0
1	A	87	TYR	3.0
1	C	150	TRP	3.0
3	N	36	LEU	3.0
3	L	26	TRP	3.0
3	N	79	GLY	3.0
1	C	45	LYS	2.9
2	D	212	LYS	2.9
3	N	100	ILE	2.9
3	N	46	LEU	2.9
3	N	74	THR	2.9
3	L	66	LEU	2.9
3	K	36	LEU	2.9
1	C	125	GLU	2.9
1	A	119	ILE	2.9
1	A	45	LYS	2.9
3	K	106	VAL	2.9
3	N	98	ALA	2.9
1	A	30	SER	2.8
3	M	99	GLY	2.8
2	D	106	SER	2.8
2	B	35	HIS	2.8
1	A	180	THR	2.8
1	A	117	VAL	2.8
3	K	88	GLY	2.8
3	M	32	ALA	2.8
2	B	56	SER	2.8
3	K	95	VAL	2.8
2	D	59	TYR	2.8
1	A	96	ALA	2.8
3	K	63	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	K	86	LEU	2.7
1	C	207	VAL	2.7
3	K	43	GLY	2.7
3	M	35	LEU	2.7
2	B	138	SER	2.7
3	N	81	LEU	2.7
3	N	105	LEU	2.7
2	D	200	LEU	2.7
2	B	134	PRO	2.7
3	N	156	ASP	2.6
3	M	115	VAL	2.6
3	L	67	TRP	2.6
3	M	104	GLY	2.6
1	C	24	ARG	2.6
3	K	83	PRO	2.6
2	B	110	ALA	2.6
1	A	194	TYR	2.6
3	L	49	LEU	2.6
2	B	131	SER	2.6
1	A	198	VAL	2.6
2	B	124	SER	2.6
3	N	128	HIS	2.6
2	B	104	MET	2.6
1	C	149	GLN	2.6
3	K	28	ALA	2.5
3	N	47	ALA	2.5
1	A	83	PHE	2.5
3	L	111	ALA	2.5
3	M	50	ALA	2.5
3	N	40	LEU	2.5
3	N	24	LEU	2.5
3	K	128	HIS	2.5
2	D	136	ALA	2.5
3	L	160	ARG	2.5
3	N	94	VAL	2.5
3	N	73	ALA	2.4
3	L	115	VAL	2.4
3	L	46	LEU	2.4
3	N	63	PRO	2.4
1	A	214	GLY	2.4
3	K	39	VAL	2.4
1	C	108	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	185	GLY	2.4
2	D	85	SER	2.4
3	K	72	THR	2.4
2	B	174	VAL	2.4
2	B	89	GLU	2.4
3	M	102	SER	2.4
2	B	27	PHE	2.4
3	M	94	VAL	2.4
1	A	39	LYS	2.4
1	A	185	LYS	2.4
2	B	93	VAL	2.4
3	L	70	VAL	2.4
3	M	95	VAL	2.4
1	C	89	GLN	2.3
3	M	88	GLY	2.3
3	M	91	VAL	2.3
3	K	147	ARG	2.3
2	B	113	TYR	2.3
3	K	97	VAL	2.3
3	M	121	ARG	2.3
3	L	108	ALA	2.3
3	M	42	ALA	2.3
2	D	133	PHE	2.3
2	D	147	ALA	2.3
3	M	108	ALA	2.3
3	L	55	PRO	2.3
1	A	199	THR	2.2
1	C	49	TYR	2.2
3	M	139	ARG	2.2
3	N	115	VAL	2.2
3	K	81	LEU	2.2
3	M	74	THR	2.2
3	K	111	ALA	2.2
1	C	105	LYS	2.2
2	D	220	LYS	2.2
3	M	78	TYR	2.2
3	K	24	LEU	2.2
3	L	60	ILE	2.2
2	D	169	ALA	2.2
3	L	40	LEU	2.2
1	C	81	GLU	2.2
3	N	103	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	88	ALA	2.2
1	A	184	SER	2.2
3	M	110	LEU	2.2
2	D	209	VAL	2.2
3	M	126	VAL	2.2
3	N	43	GLY	2.2
1	C	70	ASP	2.2
3	K	113	TRP	2.2
1	A	121	PRO	2.1
3	K	71	GLU	2.1
3	K	40	LEU	2.1
1	C	178	SER	2.1
2	B	167	SER	2.1
3	N	69	SER	2.1
3	N	106	VAL	2.1
3	N	114	PHE	2.1
1	A	40	PRO	2.1
2	B	170	LEU	2.1
1	A	183	LEU	2.1
3	N	121	ARG	2.1
1	C	88	CYS	2.1
2	B	176	THR	2.1
3	N	147	ARG	2.1
2	B	169	ALA	2.1
3	N	54	ALA	2.1
1	C	117	VAL	2.1
2	B	216	THR	2.1
1	A	210	SER	2.1
3	K	32	ALA	2.1
3	K	125	PHE	2.1
3	K	49	LEU	2.1
3	K	66	LEU	2.1
2	B	73	ASP	2.0
3	K	68	TRP	2.0
1	C	163	GLU	2.0
2	B	85	SER	2.0
2	D	138	SER	2.0
2	B	39	GLN	2.0
3	L	93	VAL	2.0
3	L	106	VAL	2.0
2	B	137	PRO	2.0
3	K	25	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
3	M	71	GLU	2.0
2	B	24	ALA	2.0
3	N	66	LEU	2.0
1	A	89	GLN	2.0
1	A	135	VAL	2.0
2	D	37	VAL	2.0
3	N	99	GLY	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.