Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:33 am BST

PDB ID	:	2DVY
Title	:	Crystal structure of restriction endonucleases PabI
Authors	:	Miyazono, K.; Watanabe, M.; Kamo, M.; Sawasaki, T.; Nagata, K.; Endo, Y.; Tanokura, M.; Kobayashi, I.
Deposited on	:	2006-08-01
Resolution	:	3.00 Å(reported)

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

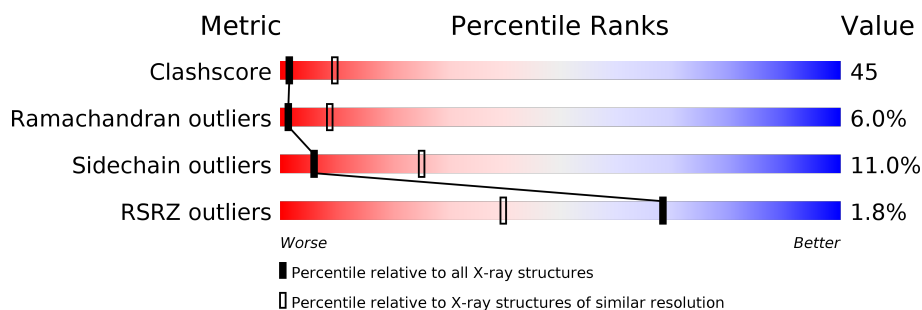|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.00 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	Percentile Ranks	Value
Clashscore		45
Ramachandran outliers		6.0%
Sidechain outliers		11.0%
RSRZ outliers		1.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	226	39% 51% 8% ••
1	B	226	% 38% 48% 8% • 5%
1	C	226	% 32% 52% 12% •
1	D	226	3% 34% 50% 8% • 5%
1	E	226	2% 36% 51% 12% •
1	F	226	3% 20% 62% 10% • 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10623 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 Restriction endonuclease PabI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total 1817	C 1167	N 310	O 335	S 5	0	0	0
1	B	215	Total 1747	C 1123	N 295	O 325	S 4	0	0	0
1	C	218	Total 1776	C 1142	N 300	O 329	S 5	0	0	0
1	D	214	Total 1747	C 1120	N 299	O 324	S 4	0	0	0
1	E	223	Total 1817	C 1167	N 310	O 335	S 5	0	0	0
1	F	211	Total 1719	C 1106	N 289	O 320	S 4	0	0	0

3 Residue-property plots ⓘ

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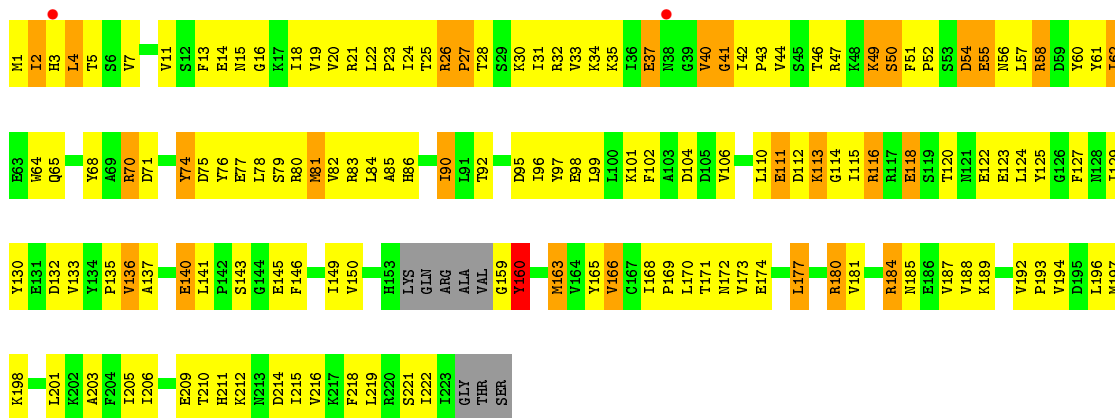
- Molecule 1: Restriction endonuclease PabI
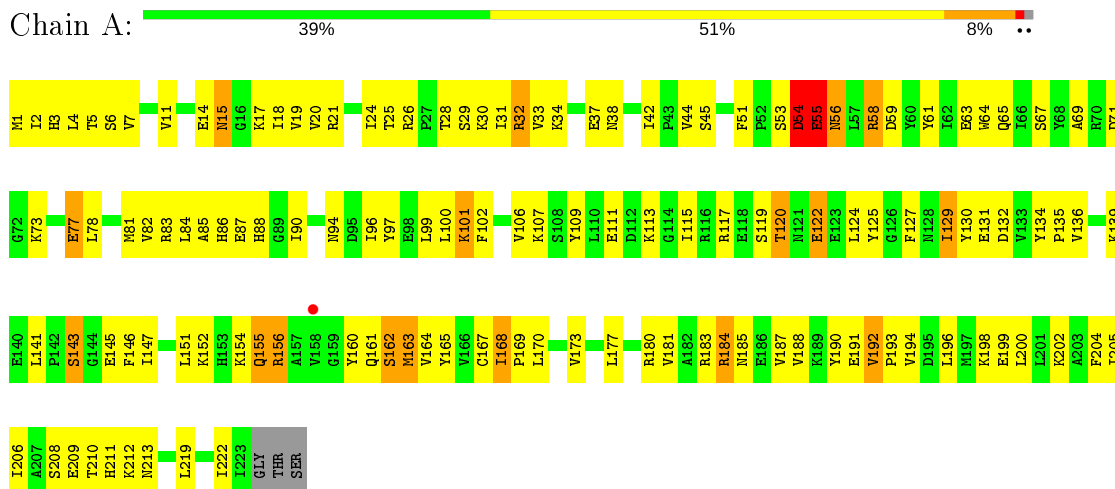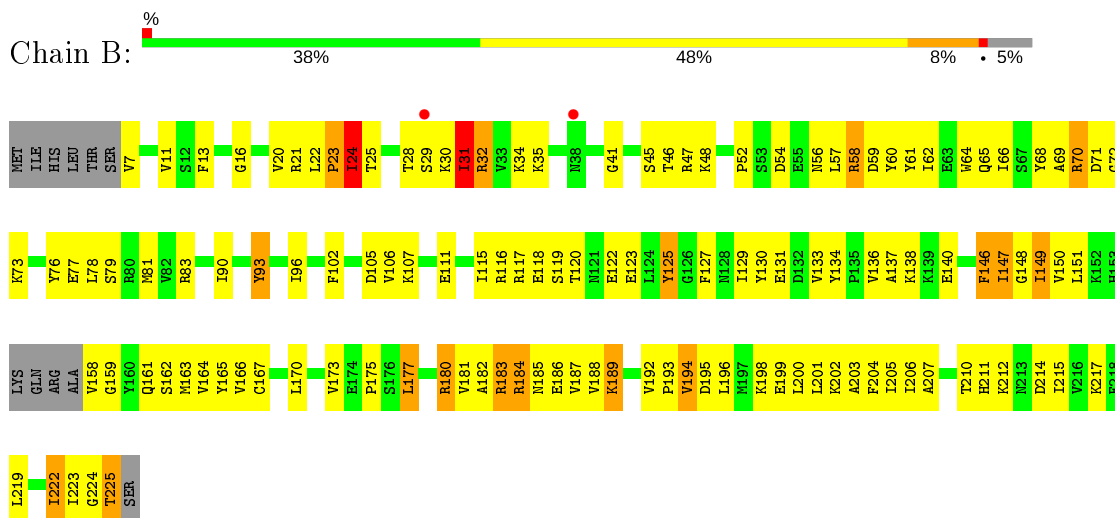
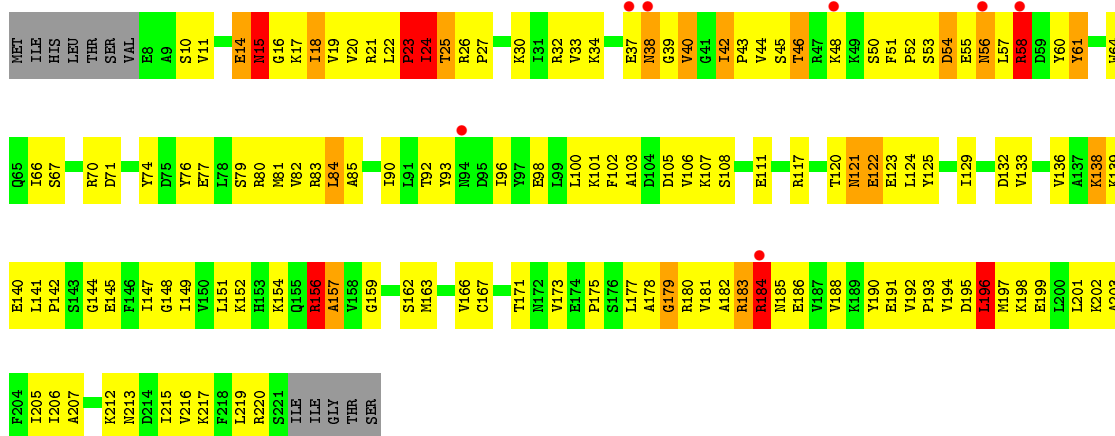- Molecule 1: Restriction endonuclease PabI

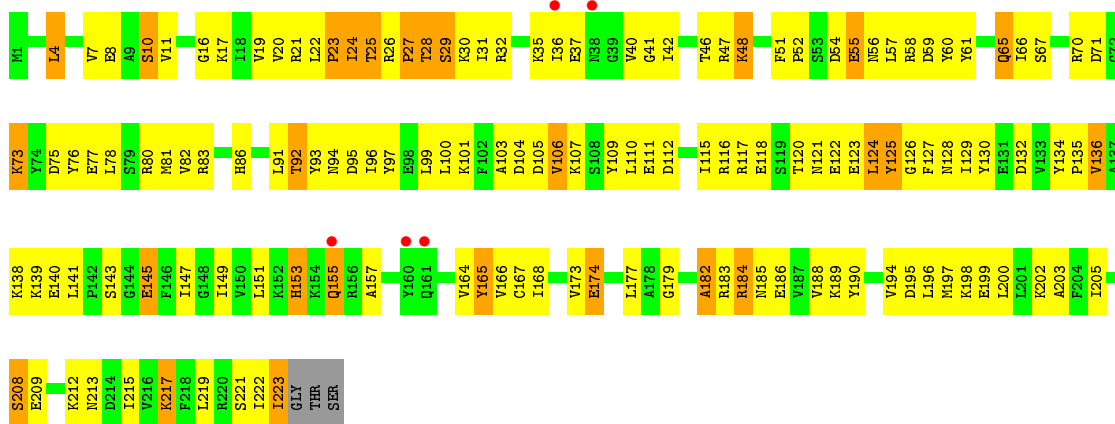
- Molecule 1: Restriction endonuclease PabI

● Molecule 1: Restriction endonuclease PabI

Chain D:

● Molecule 1: Restriction endonuclease PabI

Chain E:

● Molecule 1: Restriction endonuclease PabI

Chain F:
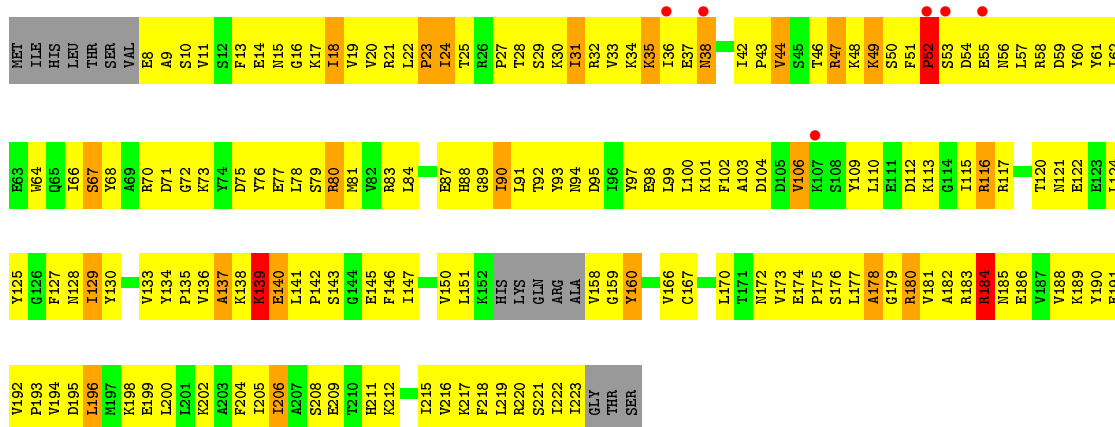
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.57Å 113.96Å 89.17Å 90.00° 116.23° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.94 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.00) 94.6 (19.94-2.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.318 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10623	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.52	0/1853	0.73	1/2501 (0.0%)
1	B	0.48	0/1781	0.68	0/2404
1	C	0.56	0/1811	0.81	1/2444 (0.0%)
1	D	0.48	1/1782 (0.1%)	0.67	0/2404
1	E	0.45	0/1853	0.67	0/2501
1	F	0.43	0/1752	0.67	0/2364
All	All	0.49	1/10832 (0.0%)	0.71	2/14618 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	58	ARG	CZ-NH2	5.62	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	TYR	N-CA-C	5.84	126.76	111.00
1	A	120	THR	N-CA-C	-5.52	96.10	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1817	0	1859	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1747	0	1776	128	0
1	C	1776	0	1810	180	0
1	D	1747	0	1775	175	0
1	E	1817	0	1859	186	0
1	F	1719	0	1750	234	0
All	All	10623	0	10829	960	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 45.

All (960) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:LEU:HB2	1:D:129:ILE:HD11	1.16	1.16
1:F:13:PHE:HB2	1:F:84:LEU:HD21	1.33	1.09
1:A:61:TYR:CD2	1:A:167:CYS:HB3	1.94	1.01
1:E:132:ASP:HB2	1:F:134:TYR:HB2	1.38	1.00
1:F:50:SER:HA	1:F:181:VAL:HB	1.42	0.99
1:F:47:ARG:NH1	1:F:49:LYS:H	1.61	0.97
1:F:30:LYS:HE2	1:F:76:TYR:OH	1.66	0.95
1:A:61:TYR:HD2	1:A:167:CYS:HB3	1.25	0.95
1:B:177:LEU:H	1:B:177:LEU:HD12	1.28	0.94
1:A:2:ILE:O	1:C:160:TYR:HB3	1.67	0.94
1:A:4:LEU:O	1:D:40:VAL:HG11	1.67	0.94
1:C:5:THR:HA	1:E:40:VAL:HG21	1.50	0.94
1:F:19:VAL:HG22	1:F:191:GLU:HA	1.48	0.93
1:F:205:ILE:HG23	1:F:212:LYS:HG3	1.49	0.93
1:C:47:ARG:HH22	1:C:184:ARG:HH21	1.19	0.90
1:D:18:ILE:HD13	1:D:19:VAL:N	1.86	0.90
1:C:180:ARG:HD2	1:C:181:VAL:O	1.71	0.89
1:F:219:LEU:HA	1:F:222:ILE:HG22	1.54	0.89
1:E:54:ASP:HA	1:E:57:LEU:HB3	1.55	0.89
1:B:170:LEU:O	1:B:173:VAL:HG22	1.73	0.89
1:F:138:LYS:HB2	1:F:138:LYS:NZ	1.86	0.89
1:F:138:LYS:HB2	1:F:138:LYS:HZ3	1.38	0.88
1:C:122:GLU:HG2	1:C:123:GLU:H	1.39	0.88
1:F:198:LYS:O	1:F:202:LYS:HG3	1.72	0.88
1:D:61:TYR:HD2	1:D:167:CYS:HB3	1.38	0.87
1:B:202:LYS:HA	1:B:205:ILE:HD12	1.57	0.87
1:E:23:PRO:O	1:E:24:ILE:HG12	1.74	0.87
1:E:110:LEU:HD11	1:E:135:PRO:HB2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:LEU:HB2	1:D:129:ILE:CD1	2.05	0.85
1:C:136:VAL:HG11	1:D:132:ASP:OD2	1.76	0.84
1:B:11:VAL:HG22	1:B:20:VAL:HG22	1.59	0.84
1:C:149:ILE:HD11	1:C:203:ALA:HB1	1.59	0.84
1:C:49:LYS:HG3	1:C:50:SER:H	1.41	0.83
1:A:29:SER:HA	1:A:32:ARG:NH2	1.94	0.83
1:B:122:GLU:HG2	1:B:123:GLU:H	1.44	0.83
1:E:70:ARG:HB2	1:E:76:TYR:CD2	2.15	0.82
1:C:160:TYR:HD2	1:C:160:TYR:H	1.27	0.81
1:A:55:GLU:O	1:A:56:ASN:HB2	1.78	0.81
1:F:49:LYS:HE2	1:F:49:LYS:N	1.95	0.81
1:D:162:SER:OG	1:D:207:ALA:HB1	1.80	0.81
1:F:25:THR:HA	1:F:46:THR:OG1	1.81	0.80
1:B:77:GLU:O	1:B:81:MET:HG3	1.82	0.80
1:D:183:ARG:HB3	1:D:184:ARG:HE	1.47	0.80
1:E:61:TYR:CD2	1:E:167:CYS:HB3	2.18	0.79
1:A:184:ARG:HG2	1:A:185:ASN:OD1	1.82	0.79
1:C:110:LEU:HD11	1:C:135:PRO:HB2	1.64	0.79
1:B:205:ILE:HG23	1:B:212:LYS:HG3	1.65	0.79
1:F:53:SER:HA	1:F:178:ALA:HB1	1.65	0.79
1:A:106:VAL:HG13	1:B:125:TYR:CE2	2.17	0.79
1:C:26:ARG:HD3	1:F:116:ARG:NH2	1.98	0.78
1:D:93:TYR:HA	1:D:96:ILE:HG22	1.66	0.78
1:D:61:TYR:CD2	1:D:167:CYS:HB3	2.19	0.78
1:F:158:VAL:HG12	1:F:159:GLY:H	1.48	0.77
1:F:219:LEU:HA	1:F:222:ILE:CG2	2.13	0.77
1:B:201:LEU:O	1:B:205:ILE:HG13	1.84	0.77
1:A:168:ILE:HD11	1:A:173:VAL:CG1	2.15	0.77
1:D:147:ILE:HD11	1:D:196:LEU:HD23	1.66	0.77
1:F:115:ILE:HD11	1:F:151:LEU:HD23	1.66	0.77
1:D:80:ARG:O	1:D:84:LEU:HB2	1.85	0.76
1:D:23:PRO:O	1:D:24:ILE:HG12	1.86	0.76
1:F:77:GLU:O	1:F:81:MET:HG3	1.86	0.76
1:C:2:ILE:HD13	1:F:160:TYR:HB3	1.67	0.76
1:B:222:ILE:HG13	1:B:222:ILE:O	1.83	0.76
1:B:163:MET:HE3	1:B:165:TYR:HB3	1.67	0.75
1:C:160:TYR:HD2	1:C:160:TYR:N	1.85	0.75
1:E:46:THR:HG22	1:E:51:PHE:HZ	1.51	0.75
1:C:62:ILE:HD13	1:C:62:ILE:O	1.87	0.75
1:C:74:TYR:HD1	1:C:74:TYR:N	1.85	0.75
1:A:168:ILE:HD11	1:A:173:VAL:HG13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LYS:HA	1:C:44:VAL:HG23	1.68	0.75
1:C:2:ILE:CD1	1:F:160:TYR:HB3	2.16	0.74
1:B:7:VAL:HG13	1:B:23:PRO:HG3	1.69	0.74
1:F:35:LYS:HB3	1:F:42:ILE:HD11	1.68	0.73
1:D:177:LEU:HA	1:D:180:ARG:HD3	1.70	0.73
1:A:199:GLU:OE1	1:A:202:LYS:HE2	1.88	0.73
1:A:29:SER:HA	1:A:32:ARG:HH21	1.53	0.73
1:F:176:SER:O	1:F:177:LEU:HD23	1.88	0.73
1:D:11:VAL:HG22	1:D:20:VAL:HG12	1.71	0.72
1:B:163:MET:CE	1:B:165:TYR:HB3	2.19	0.72
1:C:160:TYR:CD2	1:C:160:TYR:N	2.56	0.72
1:C:130:TYR:HB2	1:D:136:VAL:HG22	1.71	0.72
1:F:170:LEU:O	1:F:173:VAL:HG12	1.89	0.72
1:B:47:ARG:NH2	1:D:107:LYS:HD2	2.05	0.72
1:F:34:LYS:HG2	1:F:43:PRO:HA	1.71	0.72
1:B:122:GLU:HG2	1:B:123:GLU:N	2.04	0.72
1:C:70:ARG:HH11	1:C:70:ARG:HB3	1.53	0.72
1:C:130:TYR:HB2	1:D:136:VAL:CG2	2.20	0.71
1:C:169:PRO:HG2	1:C:172:ASN:OD1	1.90	0.71
1:E:96:ILE:O	1:E:100:LEU:HG	1.90	0.71
1:E:29:SER:HA	1:E:32:ARG:HE	1.54	0.71
1:F:61:TYR:CD2	1:F:167:CYS:HB3	2.25	0.71
1:F:204:PHE:O	1:F:211:HIS:HB3	1.90	0.71
1:D:55:GLU:O	1:D:56:ASN:HB2	1.90	0.71
1:E:202:LYS:HA	1:E:205:ILE:HD12	1.72	0.71
1:E:110:LEU:CD1	1:E:135:PRO:HB2	2.21	0.70
1:B:70:ARG:HB3	1:B:70:ARG:NH2	2.07	0.70
1:F:120:THR:HG21	1:F:122:GLU:OE2	1.91	0.70
1:E:19:VAL:HG12	1:E:20:VAL:N	2.04	0.70
1:E:198:LYS:O	1:E:202:LYS:HG3	1.92	0.70
1:F:50:SER:CA	1:F:181:VAL:HB	2.18	0.69
1:B:25:THR:HG21	1:B:185:ASN:HA	1.75	0.69
1:D:53:SER:OG	1:D:178:ALA:HB1	1.93	0.69
1:E:26:ARG:O	1:E:28:THR:N	2.24	0.69
1:A:151:LEU:O	1:A:152:LYS:HD2	1.93	0.68
1:F:216:VAL:HG13	1:F:217:LYS:H	1.58	0.68
1:B:136:VAL:HG23	1:B:137:ALA:N	2.08	0.68
1:D:124:LEU:CB	1:D:129:ILE:HD11	2.11	0.68
1:B:193:PRO:HG2	1:B:196:LEU:HB2	1.74	0.68
1:C:51:PHE:HE2	1:C:177:LEU:HD12	1.58	0.68
1:E:125:TYR:CZ	1:F:106:VAL:HA	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLU:HB3	1:C:42:ILE:HG12	1.73	0.68
1:E:109:TYR:CE2	1:E:209:GLU:HB2	2.28	0.68
1:B:105:ASP:O	1:B:107:LYS:HG2	1.94	0.68
1:B:215:ILE:O	1:B:219:LEU:HG	1.93	0.68
1:D:50:SER:HA	1:D:180:ARG:O	1.92	0.68
1:F:191:GLU:OE1	1:F:191:GLU:N	2.26	0.68
1:F:110:LEU:HD11	1:F:135:PRO:HB2	1.75	0.68
1:B:177:LEU:H	1:B:177:LEU:CD1	2.03	0.68
1:E:106:VAL:HG12	1:E:109:TYR:CE1	2.28	0.68
1:F:9:ALA:HB1	1:F:21:ARG:O	1.94	0.68
1:F:31:ILE:C	1:F:31:ILE:HD13	2.14	0.68
1:E:73:LYS:HB3	1:E:73:LYS:NZ	2.09	0.68
1:F:158:VAL:HG12	1:F:159:GLY:N	2.08	0.68
1:F:216:VAL:HG13	1:F:217:LYS:N	2.09	0.67
1:F:177:LEU:HD22	1:F:180:ARG:HD2	1.75	0.67
1:B:177:LEU:N	1:B:177:LEU:HD12	2.07	0.67
1:C:102:PHE:O	1:C:106:VAL:HG23	1.94	0.67
1:B:115:ILE:HD13	1:B:134:TYR:CE1	2.29	0.67
1:E:117:ARG:HG3	1:E:117:ARG:HH11	1.58	0.67
1:F:61:TYR:C	1:F:62:ILE:HD12	2.15	0.67
1:F:47:ARG:NH1	1:F:49:LYS:N	2.38	0.67
1:A:51:PHE:CE2	1:A:177:LEU:HD13	2.30	0.67
1:B:147:ILE:O	1:B:147:ILE:HD13	1.94	0.67
1:E:115:ILE:HD12	1:E:153:HIS:CD2	2.30	0.67
1:E:77:GLU:O	1:E:81:MET:HG3	1.94	0.66
1:D:120:THR:O	1:D:122:GLU:N	2.28	0.66
1:F:17:LYS:O	1:F:19:VAL:HG23	1.94	0.66
1:A:143:SER:HB2	1:A:145:GLU:OE1	1.96	0.66
1:D:205:ILE:HG23	1:D:212:LYS:HG3	1.77	0.66
1:C:4:LEU:HG	1:C:5:THR:N	2.11	0.66
1:D:70:ARG:HG2	1:D:71:ASP:OD1	1.96	0.66
1:E:96:ILE:H	1:E:96:ILE:HD12	1.60	0.66
1:C:77:GLU:O	1:C:81:MET:HG2	1.95	0.66
1:C:5:THR:HA	1:E:40:VAL:CG2	2.25	0.66
1:B:70:ARG:C	1:B:72:GLY:H	1.98	0.66
1:F:110:LEU:CD1	1:F:113:LYS:HD3	2.26	0.66
1:D:11:VAL:CG1	1:D:18:ILE:HD11	2.26	0.66
1:B:180:ARG:HD2	1:B:181:VAL:O	1.95	0.66
1:C:74:TYR:N	1:C:74:TYR:CD1	2.57	0.66
1:A:11:VAL:HG22	1:A:20:VAL:HG12	1.77	0.65
1:D:53:SER:HB2	1:D:179:GLY:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:ILE:HD11	1:F:170:LEU:HG	1.77	0.65
1:E:183:ARG:HB2	1:E:183:ARG:NH1	2.10	0.65
1:A:14:GLU:HG3	1:A:15:ASN:OD1	1.96	0.65
1:A:139:LYS:HB2	1:B:127:PHE:CD1	2.31	0.65
1:D:15:ASN:N	1:D:15:ASN:HD22	1.95	0.65
1:F:103:ALA:HB2	1:F:205:ILE:HD13	1.78	0.65
1:F:205:ILE:CG2	1:F:212:LYS:HG3	2.26	0.65
1:A:106:VAL:HG13	1:B:125:TYR:CZ	2.32	0.65
1:C:106:VAL:HA	1:D:125:TYR:CZ	2.32	0.65
1:D:34:LYS:HB3	1:D:43:PRO:HA	1.78	0.65
1:E:219:LEU:O	1:E:222:ILE:HG22	1.97	0.65
1:F:11:VAL:HG11	1:F:80:ARG:HG2	1.79	0.65
1:D:154:LYS:NZ	1:E:121:ASN:HD21	1.95	0.64
1:E:19:VAL:HG12	1:E:20:VAL:H	1.61	0.64
1:A:33:VAL:HG12	1:A:44:VAL:CG2	2.26	0.64
1:E:11:VAL:HB	1:E:80:ARG:HD3	1.80	0.64
1:C:95:ASP:O	1:C:99:LEU:HD12	1.98	0.64
1:D:154:LYS:HZ1	1:E:121:ASN:HD21	1.46	0.64
1:E:16:GLY:O	1:E:17:LYS:HG3	1.97	0.64
1:A:117:ARG:HE	1:B:136:VAL:HG11	1.62	0.64
1:A:90:ILE:HD12	1:A:90:ILE:H	1.63	0.64
1:E:166:VAL:HB	1:E:200:LEU:HD21	1.80	0.64
1:F:99:LEU:HD21	1:F:198:LYS:HG2	1.79	0.63
1:F:143:SER:HB2	1:F:145:GLU:OE1	1.98	0.63
1:D:120:THR:C	1:D:122:GLU:H	2.02	0.63
1:E:115:ILE:HD13	1:E:134:TYR:CE1	2.33	0.63
1:E:91:LEU:HD22	1:E:197:MET:CE	2.28	0.63
1:A:162:SER:O	1:A:211:HIS:HE1	1.82	0.63
1:E:127:PHE:CD2	1:F:139:LYS:HB2	2.33	0.63
1:A:5:THR:OG1	1:A:26:ARG:NH2	2.32	0.63
1:C:113:LYS:HE3	1:D:129:ILE:HG21	1.80	0.63
1:E:51:PHE:HB2	1:E:177:LEU:O	1.99	0.63
1:E:10:SER:O	1:E:20:VAL:HA	1.98	0.63
1:A:96:ILE:HG22	1:A:100:LEU:CD1	2.29	0.62
1:C:40:VAL:HG12	1:C:41:GLY:N	2.14	0.62
1:B:31:ILE:HG23	1:B:31:ILE:O	1.99	0.62
1:A:28:THR:HG22	1:A:29:SER:H	1.63	0.62
1:B:24:ILE:HG13	1:B:24:ILE:O	1.99	0.62
1:C:78:LEU:O	1:C:82:VAL:HG23	2.00	0.62
1:F:19:VAL:HG13	1:F:190:TYR:C	2.19	0.62
1:F:173:VAL:HG22	1:F:188:VAL:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:HG2	1:B:21:ARG:HH11	1.66	0.61
1:C:110:LEU:HD23	1:C:149:ILE:HG22	1.80	0.61
1:E:195:ASP:O	1:E:199:GLU:HG2	2.00	0.61
1:A:125:TYR:CZ	1:B:106:VAL:HA	2.35	0.61
1:E:173:VAL:HG12	1:E:190:TYR:HB2	1.80	0.61
1:C:13:PHE:CZ	1:C:16:GLY:HA2	2.36	0.61
1:B:25:THR:HG21	1:B:185:ASN:CA	2.31	0.61
1:B:21:ARG:NH1	1:B:189:LYS:HB3	2.16	0.61
1:D:100:LEU:HD22	1:D:216:VAL:HG23	1.82	0.61
1:F:92:THR:OG1	1:F:95:ASP:HB2	1.99	0.61
1:D:93:TYR:HA	1:D:96:ILE:CG2	2.31	0.61
1:A:151:LEU:C	1:A:152:LYS:HD2	2.22	0.60
1:A:4:LEU:HD12	1:D:40:VAL:HG13	1.81	0.60
1:E:91:LEU:HD22	1:E:197:MET:HE2	1.83	0.60
1:A:130:TYR:HB2	1:B:136:VAL:HG22	1.83	0.60
1:C:58:ARG:HB2	1:C:171:THR:HG21	1.82	0.60
1:E:115:ILE:HD13	1:E:134:TYR:HE1	1.67	0.60
1:E:145:GLU:H	1:E:145:GLU:CD	2.03	0.60
1:C:136:VAL:HB	1:C:150:VAL:HG12	1.83	0.60
1:D:82:VAL:HA	1:D:197:MET:CE	2.31	0.60
1:F:110:LEU:HD22	1:F:137:ALA:HB2	1.84	0.60
1:A:202:LYS:HA	1:A:205:ILE:HD12	1.84	0.60
1:E:23:PRO:O	1:E:24:ILE:HG23	2.02	0.60
1:E:46:THR:HG22	1:E:51:PHE:CZ	2.34	0.60
1:F:44:VAL:HG13	1:F:48:LYS:HD3	1.84	0.60
1:A:111:GLU:HG2	1:A:151:LEU:HD11	1.84	0.59
1:D:27:PRO:HD3	1:D:46:THR:HG21	1.83	0.59
1:C:26:ARG:HD3	1:F:116:ARG:CZ	2.32	0.59
1:F:21:ARG:HA	1:F:188:VAL:O	2.02	0.59
1:A:21:ARG:HA	1:A:188:VAL:O	2.02	0.59
1:B:136:VAL:HB	1:B:150:VAL:HG12	1.84	0.59
1:B:35:LYS:HD3	1:B:60:TYR:CZ	2.37	0.59
1:D:100:LEU:HA	1:D:103:ALA:HB3	1.83	0.59
1:D:61:TYR:CD1	1:D:61:TYR:N	2.70	0.59
1:E:83:ARG:HH11	1:E:83:ARG:HG2	1.66	0.59
1:C:124:LEU:HD11	1:D:108:SER:O	2.02	0.59
1:B:175:PRO:O	1:B:177:LEU:HD12	2.02	0.59
1:B:56:ASN:O	1:B:58:ARG:N	2.35	0.59
1:C:122:GLU:HG2	1:C:123:GLU:N	2.13	0.59
1:F:110:LEU:HD12	1:F:113:LYS:HD3	1.84	0.59
1:D:152:LYS:NZ	1:D:152:LYS:HB2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:ILE:HG12	1:F:24:ILE:O	2.01	0.59
1:C:43:PRO:HG3	1:D:157:ALA:H	1.67	0.59
1:C:106:VAL:HA	1:D:125:TYR:CE1	2.37	0.59
1:C:7:VAL:HG23	1:F:116:ARG:HG2	1.83	0.59
1:B:129:ILE:CG2	1:B:130:TYR:N	2.66	0.59
1:D:15:ASN:N	1:D:15:ASN:ND2	2.50	0.59
1:A:109:TYR:CE2	1:A:209:GLU:HB2	2.38	0.58
1:A:17:LYS:HD2	1:A:191:GLU:OE1	2.03	0.58
1:D:212:LYS:HA	1:D:215:ILE:HG22	1.82	0.58
1:D:11:VAL:HG11	1:D:81:MET:HG2	1.86	0.58
1:E:105:ASP:O	1:E:107:LYS:HG2	2.02	0.58
1:F:28:THR:O	1:F:30:LYS:N	2.32	0.58
1:A:122:GLU:CD	1:A:129:ILE:HD11	2.24	0.58
1:B:83:ARG:HH11	1:B:83:ARG:HG2	1.68	0.58
1:E:122:GLU:HG3	1:E:123:GLU:N	2.18	0.58
1:A:106:VAL:O	1:A:107:LYS:HG2	2.04	0.58
1:C:90:ILE:HD13	1:C:90:ILE:H	1.68	0.58
1:A:164:VAL:HB	1:A:204:PHE:CZ	2.38	0.58
1:C:215:ILE:O	1:C:219:LEU:HG	2.03	0.58
1:D:11:VAL:HG13	1:D:18:ILE:HD11	1.84	0.58
1:E:120:THR:C	1:E:122:GLU:H	2.07	0.58
1:E:51:PHE:CE2	1:E:177:LEU:HD23	2.39	0.58
1:A:18:ILE:O	1:A:192:VAL:HG23	2.04	0.58
1:E:130:TYR:HB2	1:F:136:VAL:CG2	2.34	0.58
1:F:183:ARG:HD2	1:F:184:ARG:NH1	2.18	0.58
1:A:88:HIS:HB2	1:A:90:ILE:CD1	2.33	0.57
1:B:61:TYR:CD2	1:B:167:CYS:HB3	2.39	0.57
1:D:18:ILE:HD13	1:D:18:ILE:C	2.24	0.57
1:F:37:GLU:O	1:F:38:ASN:C	2.42	0.57
1:A:53:SER:O	1:A:54:ASP:CB	2.52	0.57
1:A:96:ILE:HG22	1:A:100:LEU:HD11	1.86	0.57
1:E:183:ARG:HB2	1:E:183:ARG:HH11	1.69	0.57
1:A:206:ILE:HD13	1:B:127:PHE:CD2	2.39	0.57
1:F:19:VAL:HG12	1:F:20:VAL:N	2.18	0.57
1:D:190:TYR:CE2	1:D:192:VAL:HA	2.40	0.57
1:F:19:VAL:HG13	1:F:190:TYR:O	2.05	0.57
1:C:212:LYS:O	1:C:216:VAL:HG23	2.05	0.57
1:E:134:TYR:HE2	1:F:134:TYR:CD2	2.22	0.57
1:C:149:ILE:HD11	1:C:203:ALA:CB	2.33	0.57
1:E:164:VAL:C	1:E:165:TYR:HD2	2.08	0.57
1:E:134:TYR:CE2	1:F:134:TYR:CD2	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:PHE:O	1:C:14:GLU:HG3	2.04	0.57
1:E:125:TYR:CE2	1:F:106:VAL:HA	2.40	0.57
1:A:147:ILE:HD12	1:A:147:ILE:N	2.19	0.56
1:C:74:TYR:CD2	1:C:218:PHE:HB2	2.40	0.56
1:F:196:LEU:HD23	1:F:200:LEU:HG	1.86	0.56
1:B:64:TRP:CZ2	1:B:66:ILE:HG13	2.40	0.56
1:B:70:ARG:HH21	1:B:70:ARG:HB3	1.70	0.56
1:C:26:ARG:HE	1:C:26:ARG:HA	1.70	0.56
1:F:25:THR:HA	1:F:46:THR:HG1	1.68	0.56
1:C:68:TYR:OH	1:C:211:HIS:HD2	1.88	0.56
1:C:79:SER:O	1:C:83:ARG:HG2	2.05	0.56
1:E:92:THR:O	1:E:95:ASP:HB2	2.06	0.56
1:C:49:LYS:CG	1:C:50:SER:H	2.12	0.56
1:C:18:ILE:HD13	1:C:197:MET:HE2	1.88	0.56
1:D:34:LYS:HB2	1:D:42:ILE:O	2.06	0.56
1:E:106:VAL:HG12	1:E:109:TYR:HE1	1.69	0.56
1:E:165:TYR:CD2	1:E:165:TYR:N	2.73	0.56
1:E:52:PRO:HD2	1:E:60:TYR:CE2	2.41	0.56
1:F:93:TYR:CD1	1:F:94:ASN:N	2.73	0.56
1:A:29:SER:CA	1:A:32:ARG:HH21	2.18	0.56
1:A:31:ILE:O	1:A:32:ARG:HB3	2.05	0.56
1:A:129:ILE:C	1:A:130:TYR:HD2	2.10	0.55
1:D:54:ASP:O	1:D:55:GLU:HB3	2.06	0.55
1:D:140:GLU:HG2	1:D:141:LEU:N	2.22	0.55
1:D:58:ARG:HB3	1:D:171:THR:HG21	1.87	0.55
1:A:55:GLU:CD	1:A:55:GLU:H	2.10	0.55
1:B:129:ILE:HG22	1:B:130:TYR:N	2.19	0.55
1:D:74:TYR:O	1:D:79:SER:HB3	2.06	0.55
1:C:26:ARG:HD3	1:F:116:ARG:HH22	1.67	0.55
1:F:35:LYS:C	1:F:35:LYS:HD3	2.27	0.55
1:A:102:PHE:O	1:A:106:VAL:HG23	2.07	0.55
1:A:190:TYR:OH	1:A:196:LEU:CD2	2.55	0.55
1:B:138:LYS:NZ	1:B:140:GLU:HG2	2.22	0.55
1:C:49:LYS:HG3	1:C:50:SER:N	2.19	0.55
1:D:181:VAL:HG12	1:D:182:ALA:N	2.20	0.55
1:D:25:THR:HG23	1:D:26:ARG:HG3	1.89	0.55
1:B:28:THR:C	1:B:30:LYS:H	2.10	0.55
1:C:132:ASP:OD1	1:D:136:VAL:HG11	2.07	0.55
1:D:152:LYS:HZ2	1:D:152:LYS:HB2	1.72	0.55
1:E:128:ASN:ND2	1:E:130:TYR:HE2	2.05	0.55
1:A:96:ILE:O	1:A:100:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ILE:HA	1:C:99:LEU:HD12	1.89	0.55
1:E:140:GLU:HG2	1:E:141:LEU:N	2.22	0.55
1:E:47:ARG:HH21	1:E:184:ARG:HA	1.71	0.55
1:B:158:VAL:HG22	1:B:159:GLY:N	2.21	0.55
1:B:46:THR:HG22	1:B:182:ALA:HB3	1.89	0.55
1:E:121:ASN:ND2	1:E:121:ASN:O	2.40	0.55
1:E:54:ASP:O	1:E:55:GLU:HG2	2.07	0.54
1:D:147:ILE:HD11	1:D:196:LEU:CD2	2.35	0.54
1:A:155:GLN:HE21	1:A:156:ARG:CG	2.20	0.54
1:E:7:VAL:CG1	1:E:23:PRO:HG3	2.37	0.54
1:E:132:ASP:O	1:F:133:VAL:HA	2.08	0.54
1:F:158:VAL:CG1	1:F:159:GLY:H	2.18	0.54
1:C:37:GLU:HB3	1:C:42:ILE:CG1	2.37	0.54
1:D:117:ARG:HB2	1:D:132:ASP:OD1	2.06	0.54
1:D:182:ALA:HA	1:D:186:GLU:OE1	2.07	0.54
1:C:26:ARG:HH11	1:C:185:ASN:HD21	1.56	0.54
1:D:103:ALA:O	1:D:212:LYS:HD2	2.06	0.54
1:E:183:ARG:CB	1:E:183:ARG:HH11	2.21	0.54
1:B:70:ARG:C	1:B:72:GLY:N	2.61	0.54
1:C:110:LEU:CD1	1:C:135:PRO:HB2	2.37	0.54
1:C:64:TRP:CH2	1:C:81:MET:HE1	2.42	0.54
1:D:70:ARG:HB2	1:D:76:TYR:CD2	2.43	0.54
1:E:19:VAL:CG1	1:E:20:VAL:N	2.70	0.54
1:F:129:ILE:HD12	1:F:130:TYR:N	2.23	0.54
1:F:129:ILE:C	1:F:130:TYR:HD2	2.10	0.54
1:F:140:GLU:HA	1:F:146:PHE:HA	1.89	0.54
1:C:5:THR:O	1:F:116:ARG:HG3	2.07	0.54
1:D:100:LEU:CD2	1:D:216:VAL:HG23	2.38	0.54
1:F:205:ILE:HG23	1:F:212:LYS:CG	2.32	0.54
1:A:53:SER:O	1:A:54:ASP:HB3	2.07	0.54
1:D:120:THR:C	1:D:122:GLU:N	2.60	0.54
1:E:127:PHE:CE1	1:F:206:ILE:HG12	2.42	0.54
1:D:27:PRO:HD3	1:D:46:THR:CG2	2.38	0.54
1:D:52:PRO:HD2	1:D:60:TYR:CE1	2.43	0.54
1:F:175:PRO:HD2	1:F:188:VAL:HG12	1.90	0.54
1:A:97:TYR:O	1:A:101:LYS:HG2	2.07	0.53
1:A:28:THR:HG22	1:A:29:SER:N	2.23	0.53
1:D:76:TYR:H	1:D:79:SER:HB2	1.72	0.53
1:E:149:ILE:HD11	1:E:203:ALA:HB1	1.89	0.53
1:E:165:TYR:HD2	1:E:165:TYR:N	2.06	0.53
1:C:74:TYR:HD2	1:C:218:PHE:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ARG:HB3	1:D:184:ARG:HH21	1.73	0.53
1:E:66:ILE:HD11	1:E:81:MET:HE3	1.88	0.53
1:A:6:SER:H	1:D:40:VAL:HG21	1.72	0.53
1:C:2:ILE:HD11	1:F:160:TYR:HB3	1.91	0.53
1:E:136:VAL:HG11	1:F:117:ARG:NH1	2.23	0.53
1:F:181:VAL:O	1:F:181:VAL:HG13	2.07	0.53
1:F:23:PRO:O	1:F:25:THR:N	2.42	0.53
1:F:99:LEU:O	1:F:102:PHE:HB3	2.08	0.53
1:A:97:TYR:CE2	1:A:101:LYS:HD2	2.43	0.53
1:D:212:LYS:O	1:D:215:ILE:HG22	2.08	0.53
1:D:25:THR:O	1:D:46:THR:HG21	2.08	0.53
1:D:74:TYR:O	1:D:83:ARG:NH2	2.41	0.53
1:E:168:ILE:HD13	1:E:190:TYR:CD2	2.43	0.53
1:E:19:VAL:CG1	1:E:20:VAL:H	2.21	0.53
1:F:32:ARG:HD3	1:F:34:LYS:HE3	1.91	0.53
1:A:115:ILE:HD13	1:A:134:TYR:CE1	2.44	0.53
1:C:125:TYR:HB3	1:D:102:PHE:HE1	1.73	0.53
1:C:65:GLN:NE2	1:C:163:MET:HG3	2.23	0.53
1:B:223:ILE:O	1:B:225:THR:N	2.41	0.53
1:C:5:THR:O	1:F:116:ARG:HA	2.09	0.53
1:F:20:VAL:O	1:F:189:LYS:HA	2.08	0.53
1:F:23:PRO:O	1:F:24:ILE:HG22	2.07	0.53
1:E:164:VAL:C	1:E:165:TYR:CD2	2.82	0.53
1:E:23:PRO:O	1:E:24:ILE:CG1	2.52	0.53
1:E:83:ARG:NH1	1:E:83:ARG:HG2	2.23	0.53
1:E:106:VAL:HA	1:F:125:TYR:CZ	2.43	0.53
1:A:21:ARG:HB3	1:A:187:VAL:CG1	2.39	0.53
1:A:1:MET:HG3	1:C:160:TYR:CD1	2.43	0.53
1:F:36:ILE:O	1:F:36:ILE:HG23	2.08	0.53
1:A:1:MET:HG3	1:C:160:TYR:HD1	1.74	0.53
1:C:98:GLU:HA	1:C:101:LYS:HD3	1.90	0.53
1:F:90:ILE:HD12	1:F:90:ILE:H	1.72	0.53
1:D:103:ALA:HA	1:D:205:ILE:HG21	1.91	0.53
1:E:217:LYS:HE3	1:E:217:LYS:HA	1.90	0.53
1:F:70:ARG:HG2	1:F:70:ARG:HH11	1.74	0.53
1:A:6:SER:N	1:D:40:VAL:HG21	2.24	0.52
1:E:215:ILE:O	1:E:215:ILE:HG22	2.08	0.52
1:F:30:LYS:HE2	1:F:76:TYR:HH	1.68	0.52
1:C:127:PHE:CD2	1:D:206:ILE:HD13	2.43	0.52
1:E:70:ARG:HB2	1:E:76:TYR:CE2	2.45	0.52
1:B:21:ARG:HB3	1:B:187:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:ILE:HG13	1:E:25:THR:N	2.24	0.52
1:F:172:ASN:HB3	1:F:190:TYR:HE1	1.74	0.52
1:A:152:LYS:HB2	1:A:161:GLN:HB2	1.90	0.52
1:B:199:GLU:OE1	1:B:202:LYS:HE3	2.10	0.52
1:C:116:ARG:HH11	1:C:116:ARG:HG2	1.74	0.52
1:C:26:ARG:HE	1:C:26:ARG:CA	2.22	0.52
1:D:138:LYS:HZ2	1:D:138:LYS:HB2	1.74	0.52
1:D:183:ARG:HB3	1:D:184:ARG:NE	2.20	0.52
1:D:195:ASP:O	1:D:197:MET:N	2.43	0.52
1:E:120:THR:C	1:E:122:GLU:N	2.61	0.52
1:E:183:ARG:O	1:E:184:ARG:C	2.48	0.52
1:F:150:VAL:O	1:F:151:LEU:HD12	2.09	0.52
1:F:56:ASN:C	1:F:58:ARG:H	2.12	0.52
1:C:51:PHE:HD2	1:C:177:LEU:HB3	1.74	0.52
1:C:30:LYS:NZ	1:C:77:GLU:OE2	2.37	0.52
1:E:129:ILE:C	1:E:130:TYR:HD2	2.13	0.52
1:B:183:ARG:O	1:B:184:ARG:C	2.48	0.52
1:B:35:LYS:O	1:B:41:GLY:HA2	2.10	0.52
1:C:30:LYS:O	1:C:31:ILE:HG13	2.10	0.52
1:F:57:LEU:HD11	1:F:170:LEU:HB2	1.90	0.52
1:F:100:LEU:HD22	1:F:220:ARG:NH1	2.25	0.52
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.75	0.52
1:D:52:PRO:O	1:D:57:LEU:HB2	2.10	0.52
1:F:115:ILE:HG12	1:F:134:TYR:CE1	2.45	0.52
1:A:2:ILE:HD12	1:A:2:ILE:N	2.25	0.52
1:B:21:ARG:HA	1:B:188:VAL:O	2.10	0.52
1:B:205:ILE:CG2	1:B:212:LYS:HG3	2.39	0.52
1:B:61:TYR:HD2	1:B:167:CYS:HB3	1.74	0.52
1:E:57:LEU:C	1:E:59:ASP:H	2.13	0.52
1:F:139:LYS:HD3	1:F:139:LYS:C	2.30	0.52
1:B:21:ARG:HB3	1:B:187:VAL:HG11	1.93	0.51
1:B:70:ARG:O	1:B:72:GLY:N	2.43	0.51
1:B:83:ARG:NH1	1:B:83:ARG:HG2	2.25	0.51
1:C:218:PHE:O	1:C:221:SER:OG	2.25	0.51
1:D:98:GLU:HA	1:D:101:LYS:NZ	2.24	0.51
1:F:34:LYS:HA	1:F:44:VAL:HG23	1.93	0.51
1:B:60:TYR:HB3	1:B:170:LEU:CD1	2.39	0.51
1:A:106:VAL:HA	1:B:125:TYR:OH	2.11	0.51
1:D:34:LYS:HG3	1:D:61:TYR:CZ	2.45	0.51
1:F:173:VAL:HG21	1:F:188:VAL:CG2	2.40	0.51
1:A:206:ILE:HD13	1:B:127:PHE:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:HD3	1:B:34:LYS:HE3	1.93	0.51
1:C:125:TYR:CE1	1:D:106:VAL:HG22	2.46	0.51
1:C:18:ILE:HD11	1:C:85:ALA:HA	1.92	0.51
1:C:19:VAL:HG11	1:C:189:LYS:HE3	1.91	0.51
1:E:51:PHE:O	1:E:179:GLY:N	2.43	0.51
1:F:208:SER:HB3	1:F:211:HIS:HB2	1.91	0.51
1:D:33:VAL:C	1:D:44:VAL:HG22	2.30	0.51
1:E:205:ILE:HG23	1:E:212:LYS:CD	2.40	0.51
1:E:54:ASP:HA	1:E:57:LEU:CB	2.36	0.51
1:A:170:LEU:HD13	1:A:177:LEU:HD12	1.92	0.51
1:A:196:LEU:HD11	1:A:200:LEU:HD11	1.92	0.51
1:D:11:VAL:HG22	1:D:20:VAL:CG1	2.38	0.51
1:D:23:PRO:C	1:D:24:ILE:HG23	2.31	0.51
1:A:19:VAL:HG12	1:A:20:VAL:N	2.26	0.51
1:C:70:ARG:HB2	1:C:76:TYR:CG	2.46	0.51
1:D:212:LYS:CA	1:D:215:ILE:HG22	2.41	0.51
1:D:58:ARG:HH21	1:D:58:ARG:HG2	1.75	0.51
1:E:149:ILE:HG12	1:E:164:VAL:HG22	1.93	0.51
1:E:66:ILE:HD11	1:E:81:MET:CE	2.41	0.51
1:B:115:ILE:HD13	1:B:134:TYR:CD1	2.46	0.51
1:C:180:ARG:CD	1:C:181:VAL:O	2.54	0.51
1:B:147:ILE:HD11	1:B:203:ALA:HB2	1.93	0.51
1:C:116:ARG:NH1	1:C:116:ARG:HG2	2.26	0.51
1:E:36:ILE:HA	1:E:40:VAL:O	2.11	0.51
1:F:84:LEU:C	1:F:84:LEU:HD23	2.31	0.51
1:F:216:VAL:CG1	1:F:217:LYS:H	2.24	0.50
1:D:45:SER:OG	1:D:48:LYS:HD2	2.11	0.50
1:F:184:ARG:N	1:F:184:ARG:HD3	2.26	0.50
1:F:219:LEU:CA	1:F:222:ILE:HG22	2.36	0.50
1:F:8:GLU:OE1	1:F:70:ARG:NH2	2.35	0.50
1:C:52:PRO:HB2	1:C:55:GLU:HG2	1.93	0.50
1:D:14:GLU:O	1:D:16:GLY:N	2.45	0.50
1:D:156:ARG:O	1:D:157:ALA:CB	2.58	0.50
1:E:129:ILE:HG22	1:E:130:TYR:N	2.25	0.50
1:E:75:ASP:O	1:E:80:ARG:HB2	2.11	0.50
1:A:56:ASN:ND2	1:A:59:ASP:OD1	2.44	0.50
1:C:83:ARG:HG3	1:C:84:LEU:N	2.26	0.50
1:D:58:ARG:HA	1:D:171:THR:HG23	1.92	0.50
1:D:82:VAL:HA	1:D:197:MET:HE1	1.93	0.50
1:F:71:ASP:O	1:F:73:LYS:HE3	2.10	0.50
1:A:119:SER:HB2	1:A:130:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ILE:C	1:C:130:TYR:CD2	2.85	0.50
1:C:70:ARG:NH1	1:C:70:ARG:HB3	2.24	0.50
1:F:182:ALA:CB	1:F:186:GLU:HG2	2.41	0.50
1:E:130:TYR:CE2	1:F:138:LYS:NZ	2.76	0.50
1:F:90:ILE:CG2	1:F:194:VAL:HG12	2.41	0.50
1:A:106:VAL:HG22	1:B:125:TYR:CE1	2.47	0.50
1:B:136:VAL:CG2	1:B:137:ALA:N	2.75	0.50
1:E:11:VAL:HB	1:E:80:ARG:CD	2.41	0.50
1:A:199:GLU:HA	1:A:199:GLU:OE1	2.11	0.50
1:B:70:ARG:O	1:B:71:ASP:HB2	2.11	0.50
1:F:66:ILE:HD11	1:F:78:LEU:HB2	1.94	0.50
1:A:2:ILE:CD1	1:A:2:ILE:N	2.75	0.50
1:C:177:LEU:HD22	1:C:180:ARG:NH2	2.26	0.50
1:F:129:ILE:HD12	1:F:130:TYR:O	2.12	0.50
1:A:77:GLU:O	1:A:81:MET:HG3	2.12	0.49
1:C:140:GLU:HB2	1:C:146:PHE:CE1	2.47	0.49
1:F:173:VAL:CG2	1:F:188:VAL:HB	2.40	0.49
1:F:64:TRP:CD1	1:F:64:TRP:C	2.86	0.49
1:A:190:TYR:OH	1:A:196:LEU:HD22	2.12	0.49
1:A:94:ASN:O	1:A:97:TYR:HB3	2.12	0.49
1:C:49:LYS:NZ	1:C:60:TYR:CE1	2.80	0.49
1:D:64:TRP:O	1:D:166:VAL:HG12	2.12	0.49
1:F:13:PHE:CZ	1:F:16:GLY:HA2	2.47	0.49
1:A:33:VAL:O	1:A:44:VAL:HG22	2.12	0.49
1:C:35:LYS:HB3	1:C:60:TYR:CE1	2.47	0.49
1:D:37:GLU:HG2	1:D:38:ASN:ND2	2.27	0.49
1:A:206:ILE:CD1	1:B:127:PHE:CD2	2.95	0.49
1:B:96:ILE:CD1	1:B:222:ILE:HD11	2.42	0.49
1:C:58:ARG:HA	1:C:171:THR:HG23	1.94	0.49
1:F:57:LEU:HD22	1:F:178:ALA:HB2	1.94	0.49
1:C:112:ASP:O	1:C:114:GLY:N	2.45	0.49
1:C:86:HIS:ND1	1:C:222:ILE:HG22	2.26	0.49
1:D:175:PRO:O	1:D:177:LEU:HD12	2.11	0.49
1:E:125:TYR:CG	1:F:106:VAL:HG22	2.48	0.49
1:E:129:ILE:O	1:E:130:TYR:HD2	1.94	0.49
1:E:110:LEU:HD23	1:E:149:ILE:HG22	1.95	0.49
1:E:25:THR:O	1:E:27:PRO:HD3	2.12	0.49
1:F:206:ILE:HD12	1:F:206:ILE:O	2.12	0.49
1:D:205:ILE:HG23	1:D:212:LYS:CG	2.43	0.49
1:D:215:ILE:O	1:D:219:LEU:HG	2.12	0.49
1:C:43:PRO:CG	1:D:157:ALA:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:VAL:CG1	1:D:20:VAL:N	2.76	0.49
1:F:222:ILE:O	1:F:223:ILE:O	2.30	0.49
1:F:47:ARG:HH12	1:F:49:LYS:HA	1.78	0.49
1:C:26:ARG:O	1:C:28:THR:N	2.46	0.49
1:D:166:VAL:HG13	1:D:166:VAL:O	2.12	0.49
1:F:150:VAL:C	1:F:151:LEU:HD12	2.33	0.49
1:A:122:GLU:OE2	1:A:129:ILE:HD11	2.12	0.49
1:C:118:GLU:OE1	1:C:118:GLU:HA	2.13	0.49
1:F:90:ILE:CD1	1:F:90:ILE:H	2.26	0.49
1:C:125:TYR:CZ	1:D:106:VAL:HA	2.48	0.48
1:E:128:ASN:CG	1:E:128:ASN:O	2.51	0.48
1:F:141:LEU:HG	1:F:142:PRO:HD2	1.93	0.48
1:F:42:ILE:HD12	1:F:43:PRO:O	2.13	0.48
1:B:158:VAL:HG22	1:B:159:GLY:H	1.78	0.48
1:B:47:ARG:CZ	1:D:107:LYS:HD2	2.43	0.48
1:D:190:TYR:CE2	1:D:192:VAL:HG22	2.48	0.48
1:D:51:PHE:N	1:D:51:PHE:CD2	2.78	0.48
1:E:111:GLU:HA	1:E:151:LEU:HD21	1.94	0.48
1:F:196:LEU:HD22	1:F:200:LEU:HD11	1.94	0.48
1:A:147:ILE:CD1	1:A:147:ILE:N	2.76	0.48
1:C:113:LYS:CE	1:D:129:ILE:HD13	2.43	0.48
1:C:52:PRO:C	1:C:54:ASP:H	2.13	0.48
1:D:21:ARG:HA	1:D:188:VAL:O	2.13	0.48
1:F:47:ARG:HH12	1:F:49:LYS:N	2.11	0.48
1:F:72:GLY:C	1:F:73:LYS:HG3	2.34	0.48
1:A:56:ASN:O	1:A:59:ASP:HB2	2.13	0.48
1:C:47:ARG:HH11	1:C:47:ARG:HG3	1.78	0.48
1:D:85:ALA:HA	1:D:90:ILE:HD12	1.96	0.48
1:E:208:SER:OG	1:E:209:GLU:N	2.46	0.48
1:F:19:VAL:CG1	1:F:20:VAL:N	2.77	0.48
1:F:199:GLU:O	1:F:202:LYS:HB2	2.12	0.48
1:A:96:ILE:HG22	1:A:100:LEU:HD12	1.96	0.48
1:A:71:ASP:C	1:A:73:LYS:H	2.15	0.48
1:B:117:ARG:HA	1:B:131:GLU:O	2.13	0.48
1:B:60:TYR:HB3	1:B:170:LEU:HD11	1.95	0.48
1:A:24:ILE:HD12	1:A:177:LEU:HD11	1.94	0.48
1:B:111:GLU:HG3	1:B:162:SER:HB3	1.95	0.48
1:D:82:VAL:HG13	1:D:83:ARG:N	2.29	0.48
1:F:204:PHE:HD1	1:F:211:HIS:HD2	1.61	0.48
1:F:10:SER:HB2	1:F:21:ARG:HB2	1.94	0.48
1:F:64:TRP:O	1:F:166:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:GLU:HG3	1:F:88:HIS:ND1	2.28	0.48
1:A:119:SER:HB2	1:A:130:TYR:CZ	2.49	0.48
1:E:109:TYR:O	1:E:112:ASP:HB2	2.13	0.48
1:F:170:LEU:HA	1:F:173:VAL:HG12	1.95	0.48
1:F:180:ARG:HD3	1:F:182:ALA:N	2.29	0.48
1:F:47:ARG:NH2	1:F:181:VAL:HG21	2.29	0.48
1:A:184:ARG:CZ	1:A:184:ARG:HB2	2.43	0.48
1:E:26:ARG:HG3	1:E:26:ARG:HH11	1.77	0.48
1:E:7:VAL:HG21	1:E:28:THR:OG1	2.12	0.48
1:A:101:LYS:HA	1:A:101:LYS:HE3	1.96	0.48
1:A:78:LEU:HA	1:A:81:MET:HG3	1.95	0.48
1:D:81:MET:CE	1:D:192:VAL:HG11	2.44	0.48
1:E:129:ILE:CG2	1:E:130:TYR:N	2.77	0.48
1:A:21:ARG:NH1	1:A:21:ARG:HG3	2.29	0.47
1:A:37:GLU:O	1:A:38:ASN:HB2	2.14	0.47
1:C:174:GLU:O	1:C:188:VAL:HA	2.14	0.47
1:E:132:ASP:CB	1:F:134:TYR:HB2	2.26	0.47
1:F:58:ARG:C	1:F:60:TYR:H	2.18	0.47
1:E:47:ARG:O	1:E:48:LYS:HB2	2.13	0.47
1:E:82:VAL:HG13	1:E:91:LEU:CD2	2.44	0.47
1:A:90:ILE:HG22	1:A:194:VAL:CG1	2.44	0.47
1:C:92:THR:O	1:C:96:ILE:HG13	2.15	0.47
1:D:181:VAL:CG1	1:D:182:ALA:N	2.77	0.47
1:D:10:SER:O	1:D:20:VAL:HA	2.14	0.47
1:E:145:GLU:HA	1:E:167:CYS:O	2.14	0.47
1:F:28:THR:C	1:F:30:LYS:H	2.15	0.47
1:F:35:LYS:HB3	1:F:42:ILE:CD1	2.43	0.47
1:B:31:ILE:C	1:B:31:ILE:HD13	2.34	0.47
1:E:100:LEU:O	1:E:103:ALA:HB3	2.15	0.47
1:B:69:ALA:O	1:B:76:TYR:HD2	1.97	0.47
1:D:82:VAL:HA	1:D:197:MET:HE2	1.96	0.47
1:F:14:GLU:O	1:F:17:LYS:N	2.48	0.47
1:F:48:LYS:C	1:F:49:LYS:HE2	2.34	0.47
1:B:11:VAL:HG22	1:B:20:VAL:CG2	2.40	0.47
1:C:49:LYS:NZ	1:C:60:TYR:HE1	2.11	0.47
1:D:111:GLU:HA	1:D:151:LEU:HD11	1.97	0.47
1:D:213:ASN:O	1:D:216:VAL:HG12	2.15	0.47
1:D:66:ILE:HG12	1:D:67:SER:N	2.30	0.47
1:F:109:TYR:O	1:F:112:ASP:HB2	2.14	0.47
1:F:140:GLU:OE1	1:F:141:LEU:O	2.33	0.47
1:F:46:THR:HG22	1:F:46:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:HIS:O	1:A:5:THR:HG23	2.14	0.47
1:C:218:PHE:CE2	1:C:222:ILE:HD11	2.50	0.47
1:F:216:VAL:CG1	1:F:217:LYS:N	2.77	0.47
1:C:56:ASN:O	1:C:58:ARG:N	2.48	0.47
1:F:124:LEU:O	1:F:127:PHE:HB2	2.15	0.47
1:A:58:ARG:HG3	1:A:58:ARG:H	1.41	0.47
1:C:201:LEU:O	1:C:205:ILE:HG13	2.15	0.47
1:C:62:ILE:CD1	1:C:168:ILE:HD12	2.45	0.47
1:C:33:VAL:HA	1:C:61:TYR:O	2.15	0.47
1:E:23:PRO:C	1:E:24:ILE:HG23	2.34	0.47
1:F:158:VAL:CG1	1:F:159:GLY:N	2.76	0.47
1:B:146:PHE:CD1	1:B:146:PHE:C	2.88	0.47
1:C:96:ILE:O	1:C:99:LEU:HB2	2.15	0.47
1:E:96:ILE:N	1:E:96:ILE:HD12	2.30	0.47
1:F:11:VAL:HB	1:F:80:ARG:HD3	1.97	0.47
1:A:141:LEU:HD21	1:A:196:LEU:HA	1.96	0.46
1:C:180:ARG:HH11	1:C:180:ARG:HG2	1.79	0.46
1:D:194:VAL:HG13	1:D:195:ASP:N	2.30	0.46
1:E:106:VAL:HG21	1:E:205:ILE:HG22	1.97	0.46
1:A:194:VAL:O	1:A:198:LYS:N	2.41	0.46
1:D:138:LYS:NZ	1:D:138:LYS:HB2	2.30	0.46
1:D:195:ASP:O	1:D:198:LYS:HG2	2.14	0.46
1:D:82:VAL:O	1:D:85:ALA:HB3	2.14	0.46
1:E:35:LYS:HE3	1:E:37:GLU:OE1	2.15	0.46
1:E:73:LYS:HB3	1:E:73:LYS:HZ3	1.79	0.46
1:E:78:LEU:O	1:E:82:VAL:HG23	2.16	0.46
1:F:36:ILE:HG22	1:F:59:ASP:HA	1.96	0.46
1:B:28:THR:O	1:B:30:LYS:N	2.42	0.46
1:B:31:ILE:O	1:B:31:ILE:HD13	2.16	0.46
1:C:125:TYR:CD1	1:D:106:VAL:HG22	2.51	0.46
1:C:47:ARG:HH22	1:C:184:ARG:NH2	1.99	0.46
1:D:173:VAL:HB	1:D:188:VAL:HB	1.96	0.46
1:F:89:GLY:O	1:F:91:LEU:N	2.48	0.46
1:A:124:LEU:O	1:A:127:PHE:HB2	2.15	0.46
1:C:65:GLN:HG2	1:C:165:TYR:CE2	2.50	0.46
1:E:129:ILE:O	1:E:130:TYR:CD2	2.68	0.46
1:A:155:GLN:HE21	1:A:156:ARG:HG3	1.80	0.46
1:A:34:LYS:HE3	1:A:63:GLU:OE2	2.16	0.46
1:B:22:LEU:HA	1:B:23:PRO:HD3	1.79	0.46
1:C:90:ILE:H	1:C:90:ILE:CD1	2.28	0.46
1:E:122:GLU:CG	1:E:123:GLU:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:ILE:O	1:F:130:TYR:HD2	1.98	0.46
1:F:110:LEU:HD22	1:F:137:ALA:CB	2.45	0.46
1:F:62:ILE:O	1:F:62:ILE:HG22	2.14	0.46
1:F:109:TYR:CE2	1:F:209:GLU:HA	2.51	0.46
1:C:127:PHE:CD1	1:D:139:LYS:HB2	2.51	0.46
1:E:35:LYS:HA	1:E:59:ASP:O	2.16	0.46
1:E:125:TYR:CE1	1:F:106:VAL:HG13	2.51	0.46
1:F:62:ILE:HD12	1:F:62:ILE:N	2.30	0.46
1:F:76:TYR:CE1	1:F:77:GLU:HG3	2.50	0.46
1:D:17:LYS:HD3	1:D:191:GLU:OE1	2.16	0.46
1:E:122:GLU:HG3	1:E:123:GLU:H	1.79	0.46
1:F:109:TYR:CE1	1:F:212:LYS:HD3	2.50	0.46
1:F:183:ARG:HD2	1:F:184:ARG:HH11	1.80	0.46
1:F:109:TYR:HB3	1:F:208:SER:N	2.31	0.46
1:F:47:ARG:HH12	1:F:49:LYS:CA	2.29	0.46
1:F:70:ARG:HG2	1:F:70:ARG:NH1	2.30	0.46
1:A:25:THR:HG21	1:A:185:ASN:HA	1.98	0.46
1:C:2:ILE:HD11	1:F:115:ILE:CD1	2.46	0.46
1:D:154:LYS:NZ	1:E:121:ASN:ND2	2.64	0.46
1:E:120:THR:HG23	1:E:122:GLU:HB3	1.97	0.46
1:E:147:ILE:N	1:E:147:ILE:HD12	2.31	0.46
1:E:21:ARG:HA	1:E:188:VAL:O	2.16	0.46
1:E:138:LYS:HD2	1:F:130:TYR:CE1	2.50	0.46
1:C:112:ASP:O	1:C:113:LYS:C	2.53	0.45
1:C:170:LEU:HA	1:C:173:VAL:HG22	1.98	0.45
1:C:75:ASP:OD2	1:C:83:ARG:HD2	2.16	0.45
1:D:24:ILE:HG13	1:D:24:ILE:O	2.15	0.45
1:F:11:VAL:CG1	1:F:80:ARG:HG2	2.45	0.45
1:F:138:LYS:HB2	1:F:138:LYS:HZ2	1.77	0.45
1:F:177:LEU:HB3	1:F:180:ARG:O	2.17	0.45
1:A:122:GLU:HG3	1:A:122:GLU:H	1.49	0.45
1:C:34:LYS:HB2	1:C:42:ILE:O	2.16	0.45
1:C:61:TYR:CE1	1:C:169:PRO:HB3	2.51	0.45
1:D:199:GLU:OE1	1:D:202:LYS:HG3	2.16	0.45
1:F:129:ILE:C	1:F:129:ILE:HD12	2.35	0.45
1:A:130:TYR:N	1:A:130:TYR:HD2	2.15	0.45
1:B:119:SER:O	1:B:120:THR:C	2.53	0.45
1:B:150:VAL:C	1:B:151:LEU:HD12	2.37	0.45
1:B:93:TYR:C	1:B:93:TYR:CD1	2.89	0.45
1:C:30:LYS:HG2	1:C:31:ILE:HG13	1.98	0.45
1:D:37:GLU:O	1:D:39:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:ARG:NH1	1:E:186:GLU:HG2	2.32	0.45
1:A:219:LEU:O	1:A:222:ILE:HG12	2.17	0.45
1:E:117:ARG:HG3	1:E:117:ARG:NH1	2.29	0.45
1:E:130:TYR:HB2	1:F:136:VAL:HG23	1.98	0.45
1:F:138:LYS:HA	1:F:147:ILE:O	2.16	0.45
1:B:21:ARG:NH1	1:B:21:ARG:HG2	2.29	0.45
1:C:2:ILE:HD11	1:F:115:ILE:HD11	1.98	0.45
1:C:30:LYS:O	1:C:31:ILE:CG1	2.64	0.45
1:E:120:THR:O	1:E:121:ASN:HB3	2.16	0.45
1:E:125:TYR:CD1	1:F:106:VAL:HG13	2.51	0.45
1:F:18:ILE:O	1:F:192:VAL:HB	2.17	0.45
1:F:90:ILE:HD12	1:F:90:ILE:N	2.32	0.45
1:A:64:TRP:CD1	1:A:64:TRP:C	2.88	0.45
1:F:110:LEU:CD1	1:F:135:PRO:HB2	2.44	0.45
1:A:212:LYS:O	1:A:213:ASN:C	2.54	0.45
1:B:149:ILE:HD11	1:B:207:ALA:HA	1.99	0.45
1:D:149:ILE:HD11	1:D:203:ALA:HB1	1.99	0.45
1:D:45:SER:CB	1:D:48:LYS:HD2	2.46	0.45
1:E:174:GLU:HG2	1:E:189:LYS:HB3	1.97	0.45
1:E:35:LYS:O	1:E:41:GLY:HA2	2.17	0.45
1:C:26:ARG:NH2	1:F:112:ASP:O	2.50	0.45
1:D:213:ASN:HA	1:D:216:VAL:HG12	1.99	0.45
1:D:30:LYS:O	1:D:32:ARG:HG3	2.17	0.45
1:C:71:ASP:HB3	1:F:128:ASN:OD1	2.17	0.45
1:F:145:GLU:OE2	1:F:172:ASN:ND2	2.50	0.45
1:B:78:LEU:HD13	1:B:200:LEU:HD13	1.98	0.45
1:C:192:VAL:HA	1:C:193:PRO:HD3	1.78	0.45
1:E:125:TYR:CD2	1:F:106:VAL:HG22	2.52	0.45
1:E:51:PHE:CD2	1:E:177:LEU:HD23	2.52	0.45
1:A:84:LEU:O	1:A:87:GLU:HB3	2.17	0.45
1:C:30:LYS:O	1:C:30:LYS:CG	2.64	0.45
1:D:102:PHE:O	1:D:106:VAL:HG23	2.17	0.45
1:F:202:LYS:O	1:F:206:ILE:HG23	2.17	0.45
1:B:149:ILE:HD12	1:B:207:ALA:HB2	1.99	0.44
1:C:125:TYR:CE2	1:D:106:VAL:HG13	2.52	0.44
1:E:25:THR:OG1	1:E:185:ASN:HA	2.16	0.44
1:E:219:LEU:C	1:E:222:ILE:HG22	2.38	0.44
1:E:30:LYS:HG2	1:E:31:ILE:HG13	1.98	0.44
1:F:83:ARG:NH2	1:F:218:PHE:HE1	2.16	0.44
1:C:23:PRO:O	1:C:23:PRO:HG2	2.17	0.44
1:E:117:ARG:NH1	1:E:132:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:SER:C	1:F:177:LEU:HD23	2.38	0.44
1:F:98:GLU:OE1	1:F:98:GLU:HA	2.16	0.44
1:A:155:GLN:HG2	1:A:156:ARG:N	2.31	0.44
1:B:24:ILE:HG12	1:B:186:GLU:O	2.17	0.44
1:C:51:PHE:CE2	1:C:177:LEU:HD12	2.45	0.44
1:C:68:TYR:HE1	1:C:214:ASP:HB3	1.81	0.44
1:C:18:ILE:CD1	1:C:90:ILE:HG13	2.48	0.44
1:F:212:LYS:O	1:F:216:VAL:HG12	2.18	0.44
1:A:86:HIS:CE1	1:A:222:ILE:O	2.71	0.44
1:C:136:VAL:HG23	1:C:137:ALA:O	2.17	0.44
1:D:34:LYS:HA	1:D:44:VAL:HG13	1.99	0.44
1:D:76:TYR:CE1	1:D:77:GLU:HG3	2.52	0.44
1:E:136:VAL:HG21	1:F:117:ARG:NH1	2.33	0.44
1:A:82:VAL:O	1:A:83:ARG:C	2.56	0.44
1:A:85:ALA:HA	1:A:90:ILE:HD13	2.00	0.44
1:D:101:LYS:O	1:D:105:ASP:N	2.47	0.44
1:D:140:GLU:HG2	1:D:141:LEU:H	1.81	0.44
1:D:140:GLU:C	1:D:141:LEU:HD12	2.37	0.44
1:F:97:TYR:HA	1:F:100:LEU:HB2	1.99	0.44
1:F:52:PRO:HG2	1:F:56:ASN:HB2	1.99	0.44
1:F:56:ASN:C	1:F:58:ARG:N	2.71	0.44
1:A:193:PRO:HD2	1:A:196:LEU:HB3	1.98	0.44
1:B:52:PRO:HB2	1:B:56:ASN:HB2	1.99	0.44
1:C:115:ILE:HD11	1:C:159:GLY:O	2.17	0.44
1:C:129:ILE:HG22	1:C:130:TYR:N	2.33	0.44
1:F:211:HIS:O	1:F:215:ILE:HG12	2.18	0.44
1:B:163:MET:HE1	1:B:165:TYR:HB3	1.99	0.44
1:D:205:ILE:HG12	1:D:215:ILE:HG21	1.99	0.44
1:E:215:ILE:HG22	1:E:219:LEU:HD12	2.00	0.44
1:E:73:LYS:HB3	1:E:73:LYS:HZ2	1.80	0.44
1:F:14:GLU:O	1:F:15:ASN:C	2.54	0.44
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.79	0.44
1:B:102:PHE:CE2	1:B:202:LYS:HG2	2.53	0.44
1:C:65:GLN:HE21	1:C:163:MET:HG3	1.82	0.44
1:D:154:LYS:HB2	1:D:157:ALA:O	2.17	0.44
1:E:194:VAL:HG13	1:E:195:ASP:N	2.32	0.44
1:B:56:ASN:C	1:B:58:ARG:N	2.72	0.44
1:D:183:ARG:O	1:D:185:ASN:N	2.51	0.44
1:E:183:ARG:O	1:E:184:ARG:O	2.35	0.44
1:E:56:ASN:HA	1:E:59:ASP:OD2	2.17	0.44
1:E:65:GLN:OE1	1:E:66:ILE:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LYS:HA	1:D:147:ILE:O	2.17	0.43
1:D:61:TYR:HD1	1:D:61:TYR:N	2.14	0.43
1:F:84:LEU:O	1:F:84:LEU:HD23	2.18	0.43
1:A:184:ARG:NH1	1:A:184:ARG:HB2	2.32	0.43
1:A:132:ASP:OD2	1:B:136:VAL:HG11	2.18	0.43
1:B:35:LYS:HE2	1:B:35:LYS:HB3	1.77	0.43
1:B:60:TYR:C	1:B:170:LEU:HG	2.39	0.43
1:A:184:ARG:NH2	1:C:209:GLU:OE2	2.49	0.43
1:C:34:LYS:CB	1:C:42:ILE:O	2.66	0.43
1:F:54:ASP:C	1:F:56:ASN:H	2.22	0.43
1:C:21:ARG:HB3	1:C:187:VAL:CG1	2.49	0.43
1:C:78:LEU:HA	1:C:81:MET:HG3	1.99	0.43
1:D:33:VAL:O	1:D:44:VAL:HG22	2.19	0.43
1:F:9:ALA:CB	1:F:22:LEU:HD23	2.48	0.43
1:F:68:TYR:O	1:F:79:SER:HB3	2.18	0.43
1:A:19:VAL:HG12	1:A:20:VAL:H	1.82	0.43
1:B:68:TYR:OH	1:B:214:ASP:OD2	2.35	0.43
1:B:62:ILE:O	1:B:167:CYS:HA	2.17	0.43
1:E:139:LYS:HD2	1:E:140:GLU:N	2.33	0.43
1:E:82:VAL:HG13	1:E:91:LEU:HD23	2.00	0.43
1:A:120:THR:OG1	1:A:122:GLU:OE2	2.23	0.43
1:A:130:TYR:N	1:A:130:TYR:CD2	2.85	0.43
1:A:111:GLU:HG3	1:A:208:SER:HB3	2.00	0.43
1:B:13:PHE:HZ	1:B:16:GLY:HA2	1.83	0.43
1:D:64:TRP:NE1	1:D:77:GLU:OE2	2.50	0.43
1:E:149:ILE:HD11	1:E:203:ALA:CB	2.48	0.43
1:E:215:ILE:O	1:E:215:ILE:CG2	2.66	0.43
1:A:33:VAL:HG12	1:A:44:VAL:HG23	1.99	0.43
1:B:64:TRP:CD1	1:B:64:TRP:C	2.89	0.43
1:B:73:LYS:HA	1:B:73:LYS:HD2	1.69	0.43
1:C:111:GLU:HG2	1:C:112:ASP:N	2.33	0.43
1:C:11:VAL:HB	1:C:80:ARG:HG2	2.01	0.43
1:D:212:LYS:HA	1:D:215:ILE:CG2	2.48	0.43
1:E:124:LEU:O	1:E:126:GLY:N	2.52	0.43
1:E:183:ARG:N	1:E:186:GLU:HG3	2.34	0.43
1:F:54:ASP:O	1:F:56:ASN:N	2.50	0.43
1:A:115:ILE:HG13	1:A:160:TYR:CE1	2.53	0.43
1:C:18:ILE:HD13	1:C:197:MET:CE	2.49	0.43
1:C:205:ILE:O	1:C:205:ILE:HG22	2.18	0.43
1:C:40:VAL:HG12	1:C:41:GLY:H	1.81	0.43
1:C:78:LEU:HA	1:C:81:MET:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ILE:HG23	1:F:133:VAL:O	2.19	0.43
1:F:89:GLY:O	1:F:90:ILE:C	2.57	0.43
1:A:31:ILE:HG22	1:A:32:ARG:N	2.34	0.43
1:D:198:LYS:HA	1:D:201:LEU:HD12	2.00	0.43
1:F:120:THR:HG22	1:F:121:ASN:H	1.84	0.43
1:F:146:PHE:CD1	1:F:146:PHE:N	2.87	0.43
1:B:162:SER:O	1:B:211:HIS:HE1	2.01	0.43
1:F:221:SER:C	1:F:223:ILE:H	2.20	0.43
1:F:22:LEU:HD11	1:F:64:TRP:CE3	2.54	0.43
1:B:161:GLN:HB2	1:B:161:GLN:HE21	1.72	0.42
1:C:166:VAL:HG22	1:C:166:VAL:O	2.18	0.42
1:C:60:TYR:HB3	1:C:170:LEU:CD1	2.49	0.42
1:E:117:ARG:HH11	1:E:117:ARG:CG	2.29	0.42
1:E:122:GLU:CG	1:E:123:GLU:H	2.32	0.42
1:E:109:TYR:HB3	1:E:208:SER:HA	2.01	0.42
1:E:28:THR:HG22	1:E:29:SER:N	2.33	0.42
1:F:101:LYS:O	1:F:104:ASP:HB2	2.19	0.42
1:A:146:PHE:C	1:A:147:ILE:HD12	2.39	0.42
1:B:194:VAL:O	1:B:198:LYS:HG3	2.19	0.42
1:C:206:ILE:HG13	1:C:206:ILE:O	2.19	0.42
1:C:26:ARG:HH11	1:C:185:ASN:ND2	2.16	0.42
1:E:195:ASP:N	1:E:195:ASP:OD2	2.52	0.42
1:E:101:LYS:O	1:E:104:ASP:N	2.53	0.42
1:F:32:ARG:CD	1:F:34:LYS:HE3	2.49	0.42
1:A:99:LEU:O	1:A:102:PHE:HB3	2.19	0.42
1:B:120:THR:CG2	1:B:131:GLU:HG3	2.49	0.42
1:B:138:LYS:HA	1:B:148:GLY:HA2	2.00	0.42
1:A:34:LYS:HA	1:A:42:ILE:O	2.20	0.42
1:B:45:SER:OG	1:B:48:LYS:HB3	2.19	0.42
1:C:166:VAL:HG13	1:C:166:VAL:O	2.18	0.42
1:C:24:ILE:O	1:C:46:THR:HG21	2.20	0.42
1:C:84:LEU:HD23	1:C:84:LEU:HA	1.69	0.42
1:D:11:VAL:HG13	1:D:20:VAL:HG12	2.01	0.42
1:E:196:LEU:HG	1:E:200:LEU:CD1	2.49	0.42
1:E:94:ASN:O	1:E:97:TYR:HB3	2.19	0.42
1:F:145:GLU:CD	1:F:145:GLU:H	2.23	0.42
1:F:78:LEU:O	1:F:79:SER:C	2.58	0.42
1:B:192:VAL:HA	1:B:193:PRO:HD2	1.91	0.42
1:D:20:VAL:HG23	1:D:22:LEU:CD1	2.49	0.42
1:D:77:GLU:O	1:D:81:MET:HG3	2.19	0.42
1:F:174:GLU:HA	1:F:175:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASP:OD2	1:B:56:ASN:ND2	2.52	0.42
1:C:194:VAL:HG22	1:C:198:LYS:HE3	2.02	0.42
1:F:90:ILE:HG23	1:F:194:VAL:HG12	2.01	0.42
1:A:61:TYR:HA	1:A:169:PRO:HA	2.02	0.42
1:A:192:VAL:HA	1:A:193:PRO:HD3	1.65	0.42
1:C:24:ILE:HD12	1:C:24:ILE:O	2.19	0.42
1:C:31:ILE:CG2	1:C:32:ARG:N	2.83	0.42
1:E:70:ARG:HG2	1:E:71:ASP:OD2	2.20	0.42
1:A:14:GLU:HG2	1:A:19:VAL:HG21	2.01	0.42
1:D:156:ARG:O	1:D:157:ALA:HB2	2.20	0.42
1:D:61:TYR:HD2	1:D:167:CYS:CB	2.22	0.42
1:F:115:ILE:HG12	1:F:134:TYR:CD1	2.54	0.42
1:A:131:GLU:HB3	1:B:133:VAL:CG1	2.50	0.42
1:C:219:LEU:HD23	1:C:222:ILE:CD1	2.50	0.42
1:C:56:ASN:HB3	1:C:60:TYR:HE2	1.84	0.42
1:A:17:LYS:HD2	1:A:191:GLU:CD	2.40	0.41
1:B:64:TRP:NE1	1:B:66:ILE:HA	2.35	0.41
1:E:105:ASP:O	1:E:107:LYS:N	2.52	0.41
1:E:129:ILE:HG21	1:F:113:LYS:NZ	2.35	0.41
1:E:182:ALA:HA	1:E:186:GLU:OE2	2.20	0.41
1:A:163:MET:HB3	1:A:165:TYR:HE2	1.85	0.41
1:A:183:ARG:O	1:A:184:ARG:C	2.58	0.41
1:B:164:VAL:HB	1:B:204:PHE:CZ	2.54	0.41
1:C:34:LYS:HE2	1:C:34:LYS:HB3	1.85	0.41
1:C:40:VAL:CG1	1:C:41:GLY:N	2.78	0.41
1:C:85:ALA:HB1	1:C:90:ILE:HB	2.01	0.41
1:E:183:ARG:O	1:E:186:GLU:HG3	2.20	0.41
1:E:7:VAL:HG11	1:E:28:THR:OG1	2.20	0.41
1:E:8:GLU:OE1	1:E:76:TYR:OH	2.29	0.41
1:B:166:VAL:HG22	1:B:167:CYS:N	2.36	0.41
1:B:35:LYS:HA	1:B:59:ASP:O	2.20	0.41
1:C:133:VAL:HG22	1:D:133:VAL:HG22	2.02	0.41
1:D:19:VAL:HG12	1:D:20:VAL:N	2.35	0.41
1:C:20:VAL:HG12	1:C:22:LEU:HG	2.03	0.41
1:C:35:LYS:HB2	1:C:35:LYS:HE3	1.93	0.41
1:E:136:VAL:HG22	1:E:136:VAL:O	2.19	0.41
1:F:120:THR:CG2	1:F:122:GLU:HG3	2.50	0.41
1:F:191:GLU:H	1:F:191:GLU:CD	2.18	0.41
1:F:31:ILE:CD1	1:F:31:ILE:C	2.84	0.41
1:B:16:GLY:O	1:B:90:ILE:HD11	2.19	0.41
1:F:23:PRO:C	1:F:25:THR:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLN:HG2	1:B:65:GLN:O	2.18	0.41
1:E:20:VAL:HG23	1:E:190:TYR:HB3	2.01	0.41
1:E:57:LEU:HA	1:E:60:TYR:HD2	1.85	0.41
1:E:86:HIS:CE1	1:E:223:ILE:HG12	2.56	0.41
1:A:115:ILE:HG13	1:A:151:LEU:HD23	2.01	0.41
1:A:129:ILE:HA	1:B:137:ALA:HA	2.02	0.41
1:D:45:SER:O	1:D:46:THR:C	2.59	0.41
1:E:93:TYR:CD2	1:E:223:ILE:HD11	2.56	0.41
1:E:37:GLU:HG3	1:E:42:ILE:HD13	2.03	0.41
1:A:155:GLN:NE2	1:A:156:ARG:HG3	2.36	0.41
1:A:78:LEU:HD12	1:A:81:MET:HE2	2.03	0.41
1:C:219:LEU:HD23	1:C:222:ILE:HD12	2.02	0.41
1:D:154:LYS:HG3	1:D:159:GLY:O	2.20	0.41
1:D:202:LYS:O	1:D:203:ALA:C	2.58	0.41
1:D:83:ARG:C	1:D:85:ALA:H	2.23	0.41
1:E:24:ILE:CG1	1:E:25:THR:N	2.84	0.41
1:A:4:LEU:HD12	1:D:40:VAL:CG1	2.49	0.41
1:B:193:PRO:O	1:B:196:LEU:N	2.53	0.41
1:C:31:ILE:O	1:C:32:ARG:HB3	2.21	0.41
1:C:77:GLU:HB2	1:C:78:LEU:H	1.66	0.41
1:E:177:LEU:HD12	1:E:177:LEU:N	2.36	0.41
1:E:4:LEU:O	1:E:4:LEU:HD23	2.20	0.41
1:E:127:PHE:HD2	1:F:139:LYS:HB2	1.82	0.41
1:F:192:VAL:HA	1:F:193:PRO:HD3	1.75	0.41
1:F:47:ARG:HH12	1:F:49:LYS:H	1.54	0.41
1:D:53:SER:O	1:D:54:ASP:O	2.39	0.41
1:E:120:THR:O	1:E:122:GLU:N	2.53	0.41
1:E:212:LYS:O	1:E:213:ASN:C	2.59	0.41
1:F:170:LEU:CA	1:F:173:VAL:HG12	2.51	0.41
1:F:9:ALA:HB1	1:F:22:LEU:HD23	2.03	0.41
1:F:47:ARG:HA	1:F:47:ARG:HD2	1.76	0.41
1:F:61:TYR:CE2	1:F:167:CYS:SG	3.12	0.41
1:F:66:ILE:HG12	1:F:67:SER:N	2.35	0.41
1:A:61:TYR:CE2	1:A:167:CYS:HB3	2.51	0.41
1:C:2:ILE:HG12	1:C:3:HIS:N	2.33	0.41
1:D:142:PRO:C	1:D:144:GLY:H	2.25	0.41
1:D:183:ARG:HD3	1:D:186:GLU:OE1	2.21	0.41
1:E:97:TYR:O	1:E:100:LEU:HB2	2.21	0.41
1:E:25:THR:HG23	1:E:26:ARG:H	1.86	0.41
1:F:61:TYR:CD2	1:F:167:CYS:CB	3.02	0.41
1:A:30:LYS:HD2	1:A:65:GLN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ILE:HG22	1:B:90:ILE:O	2.21	0.40
1:C:174:GLU:O	1:C:189:LYS:N	2.47	0.40
1:C:31:ILE:HG22	1:C:32:ARG:N	2.35	0.40
1:F:42:ILE:HD12	1:F:42:ILE:O	2.20	0.40
1:B:203:ALA:O	1:B:206:ILE:HG12	2.22	0.40
1:F:11:VAL:CG1	1:F:81:MET:HG2	2.52	0.40
1:A:168:ILE:HA	1:A:169:PRO:HD2	1.91	0.40
1:A:131:GLU:HB3	1:B:133:VAL:HG13	2.04	0.40
1:C:25:THR:O	1:C:27:PRO:HD3	2.22	0.40
1:C:113:LYS:HE3	1:D:129:ILE:HD13	2.02	0.40
1:D:212:LYS:C	1:D:215:ILE:HG22	2.42	0.40
1:D:22:LEU:HA	1:D:23:PRO:HD3	1.95	0.40
1:F:177:LEU:CD2	1:F:180:ARG:HD2	2.49	0.40
1:F:70:ARG:O	1:F:73:LYS:HD2	2.21	0.40
1:A:210:THR:O	1:A:211:HIS:C	2.60	0.40
1:C:140:GLU:HG3	1:C:141:LEU:N	2.35	0.40
1:D:216:VAL:HG13	1:D:217:LYS:N	2.36	0.40
1:D:219:LEU:O	1:D:220:ARG:C	2.59	0.40
1:A:6:SER:H	1:D:40:VAL:CG2	2.34	0.40
1:B:28:THR:C	1:B:30:LYS:N	2.75	0.40
1:C:97:TYR:CE2	1:C:101:LYS:HD2	2.56	0.40
1:C:64:TRP:HH2	1:C:81:MET:CE	2.35	0.40
1:C:99:LEU:O	1:C:102:PHE:HB3	2.22	0.40
1:D:138:LYS:HA	1:D:148:GLY:HA2	2.04	0.40
1:D:149:ILE:HD11	1:D:203:ALA:CB	2.52	0.40
1:D:18:ILE:CD1	1:D:18:ILE:C	2.90	0.40
1:E:117:ARG:CG	1:E:117:ARG:NH1	2.85	0.40
1:E:183:ARG:HB2	1:E:186:GLU:CG	2.51	0.40
1:F:23:PRO:O	1:F:24:ILE:CG2	2.70	0.40
1:F:33:VAL:HG22	1:F:62:ILE:HG13	2.03	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	221/226 (98%)	178 (80%)	33 (15%)	10 (4%)	2	14
1	B	211/226 (93%)	165 (78%)	37 (18%)	9 (4%)	2	15
1	C	214/226 (95%)	173 (81%)	30 (14%)	11 (5%)	2	12
1	D	212/226 (94%)	150 (71%)	46 (22%)	16 (8%)	1	5
1	E	221/226 (98%)	171 (77%)	35 (16%)	15 (7%)	1	6
1	F	207/226 (92%)	141 (68%)	50 (24%)	16 (8%)	1	5
All	All	1286/1356 (95%)	978 (76%)	231 (18%)	77 (6%)	1	9

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	56	ASN
1	A	184	ARG
1	B	57	LEU
1	C	49	LYS
1	C	50	SER
1	C	54	ASP
1	C	55	GLU
1	C	57	LEU
1	C	90	ILE
1	C	184	ARG
1	D	15	ASN
1	D	38	ASN
1	D	46	THR
1	D	54	ASP
1	D	157	ALA
1	E	23	PRO
1	E	24	ILE
1	E	28	THR
1	E	48	LYS
1	E	55	GLU
1	E	106	VAL
1	E	125	TYR
1	E	155	GLN
1	E	184	ARG
1	F	24	ILE
1	F	184	ARG

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Mol	Chain	Res	Type
1	A	15	ASN
1	A	54	ASP
1	A	155	GLN
1	B	29	SER
1	B	125	TYR
1	B	224	GLY
1	C	40	VAL
1	D	24	ILE
1	D	92	THR
1	D	121	ASN
1	D	184	ARG
1	D	196	LEU
1	E	29	SER
1	F	29	SER
1	F	90	ILE
1	A	32	ARG
1	A	154	LYS
1	B	184	ARG
1	C	113	LYS
1	D	23	PRO
1	E	27	PRO
1	E	153	HIS
1	F	38	ASN
1	F	55	GLU
1	F	178	ALA
1	A	77	GLU
1	B	31	ILE
1	D	156	ARG
1	E	157	ALA
1	E	182	ALA
1	F	137	ALA
1	F	185	ASN
1	B	194	VAL
1	D	56	ASN
1	D	179	GLY
1	D	193	PRO
1	E	221	SER
1	F	52	PRO
1	F	139	LYS
1	A	69	ALA
1	B	23	PRO
1	C	27	PRO

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Mol	Chain	Res	Type
1	D	40	VAL
1	B	24	ILE
1	C	41	GLY
1	F	51	PHE
1	F	27	PRO
1	F	179	GLY
1	F	44	VAL
1	F	106	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	202/204 (99%)	182 (90%)	20 (10%)	8	30
1	B	194/204 (95%)	173 (89%)	21 (11%)	6	26
1	C	198/204 (97%)	171 (86%)	27 (14%)	3	17
1	D	193/204 (95%)	173 (90%)	20 (10%)	7	27
1	E	202/204 (99%)	180 (89%)	22 (11%)	6	25
1	F	191/204 (94%)	171 (90%)	20 (10%)	7	27
All	All	1180/1224 (96%)	1050 (89%)	130 (11%)	6	25

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	45	SER
1	A	54	ASP
1	A	55	GLU
1	A	58	ARG
1	A	67	SER
1	A	101	LYS
1	A	113	LYS
1	A	122	GLU
1	A	129	ILE

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Mol	Chain	Res	Type
1	A	135	PRO
1	A	136	VAL
1	A	143	SER
1	A	156	ARG
1	A	162	SER
1	A	163	MET
1	A	168	ILE
1	A	180	ARG
1	A	181	VAL
1	A	192	VAL
1	B	24	ILE
1	B	31	ILE
1	B	32	ARG
1	B	58	ARG
1	B	70	ARG
1	B	79	SER
1	B	93	TYR
1	B	116	ARG
1	B	118	GLU
1	B	146	PHE
1	B	147	ILE
1	B	149	ILE
1	B	177	LEU
1	B	180	ARG
1	B	183	ARG
1	B	189	LYS
1	B	195	ASP
1	B	210	THR
1	B	217	LYS
1	B	222	ILE
1	B	225	THR
1	C	1	MET
1	C	2	ILE
1	C	4	LEU
1	C	15	ASN
1	C	26	ARG
1	C	37	GLU
1	C	58	ARG
1	C	62	ILE
1	C	70	ARG
1	C	74	TYR
1	C	81	MET

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Mol	Chain	Res	Type
1	C	104	ASP
1	C	111	GLU
1	C	116	ARG
1	C	118	GLU
1	C	120	THR
1	C	136	VAL
1	C	140	GLU
1	C	143	SER
1	C	145	GLU
1	C	160	TYR
1	C	163	MET
1	C	166	VAL
1	C	177	LEU
1	C	180	ARG
1	C	196	LEU
1	C	210	THR
1	D	14	GLU
1	D	15	ASN
1	D	18	ILE
1	D	23	PRO
1	D	24	ILE
1	D	25	THR
1	D	42	ILE
1	D	58	ARG
1	D	61	TYR
1	D	84	LEU
1	D	121	ASN
1	D	122	GLU
1	D	123	GLU
1	D	138	LYS
1	D	145	GLU
1	D	156	ARG
1	D	163	MET
1	D	183	ARG
1	D	184	ARG
1	D	196	LEU
1	E	4	LEU
1	E	10	SER
1	E	22	LEU
1	E	25	THR
1	E	58	ARG
1	E	65	GLN

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Mol	Chain	Res	Type
1	E	67	SER
1	E	73	LYS
1	E	92	THR
1	E	99	LEU
1	E	116	ARG
1	E	118	GLU
1	E	124	LEU
1	E	136	VAL
1	E	143	SER
1	E	145	GLU
1	E	155	GLN
1	E	165	TYR
1	E	174	GLU
1	E	208	SER
1	E	217	LYS
1	E	223	ILE
1	F	18	ILE
1	F	23	PRO
1	F	31	ILE
1	F	35	LYS
1	F	47	ARG
1	F	49	LYS
1	F	52	PRO
1	F	67	SER
1	F	75	ASP
1	F	80	ARG
1	F	116	ARG
1	F	129	ILE
1	F	139	LYS
1	F	140	GLU
1	F	160	TYR
1	F	180	ARG
1	F	184	ARG
1	F	195	ASP
1	F	196	LEU
1	F	206	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	65	GLN

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Mol	Chain	Res	Type
1	A	86	HIS
1	A	155	GLN
1	A	211	HIS
1	B	121	ASN
1	B	161	GLN
1	B	211	HIS
1	C	15	ASN
1	C	38	ASN
1	C	56	ASN
1	C	65	GLN
1	C	94	ASN
1	C	128	ASN
1	C	185	ASN
1	C	211	HIS
1	D	15	ASN
1	D	121	ASN
1	D	128	ASN
1	D	155	GLN
1	D	161	GLN
1	D	185	ASN
1	D	213	ASN
1	E	121	ASN
1	E	153	HIS
1	E	211	HIS
1	F	65	GLN
1	F	121	ASN
1	F	128	ASN
1	F	161	GLN
1	F	211	HIS
1	F	213	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	223/226 (98%)	-0.33	1 (0%)	92	79	31, 52, 76, 91	0
1	B	215/226 (95%)	-0.20	2 (0%)	84	63	29, 59, 87, 94	0
1	C	218/226 (96%)	-0.40	2 (0%)	84	63	22, 48, 78, 95	0
1	D	214/226 (94%)	0.01	7 (3%)	46	20	25, 80, 113, 119	0
1	E	223/226 (98%)	-0.12	5 (2%)	62	33	39, 70, 101, 111	0
1	F	211/226 (93%)	0.14	6 (2%)	53	25	45, 80, 118, 134	0
All	All	1304/1356 (96%)	-0.15	23 (1%)	68	40	22, 65, 104, 134	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	SER	4.5
1	F	53	SER	3.7
1	F	55	GLU	3.6
1	B	38	ASN	3.5
1	C	3	HIS	3.0
1	D	94	ASN	3.0
1	D	38	ASN	3.0
1	A	158	VAL	2.9
1	E	161	GLN	2.9
1	D	37	GLU	2.7
1	C	38	ASN	2.5
1	E	38	ASN	2.5
1	D	184	ARG	2.5
1	E	36	ILE	2.4
1	F	38	ASN	2.4
1	D	48	LYS	2.2
1	E	160	TYR	2.2
1	F	36	ILE	2.2
1	D	58	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	107	LYS	2.1
1	F	52	PRO	2.0
1	E	155	GLN	2.0
1	D	56	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.