



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:10 PM GMT

PDB ID : 1E9S
Title : BACTERIAL CONJUGATIVE COUPLING PROTEIN TRWBDELTAN70.
UNBOUND MONOCLINIC FORM.
Authors : Gomis-Rueth, F.X.; Moncalian, G.; Cabezon, E.; De La Cruz, F.; Coll, M.
Deposited on : 2000-10-26
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

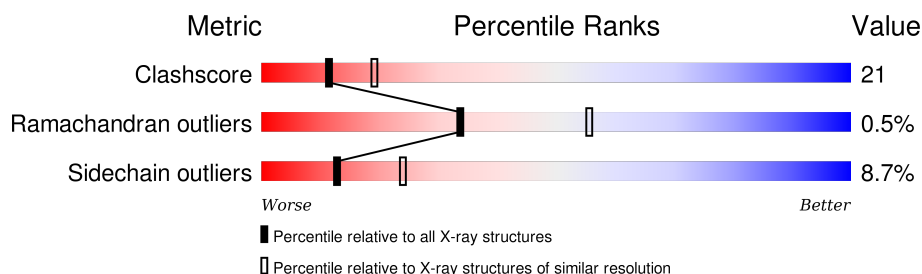
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)


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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	437	
1	B	437	
1	D	437	
1	E	437	
1	F	437	
1	G	437	
1	H	437	

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Mol	Chain	Length	Quality of chain
1	I	437	 60% 33% . .
1	J	437	 60% 33% . .
1	K	437	 56% 36% . .
1	L	437	 55% 38% 5% .
1	M	437	 59% 33% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41513 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 CONJUGAL TRANSFER PROTEIN TRWB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3353	2118	602	623	10			
1	B	422	Total	C	N	O	S	0	0	0
			3318	2097	596	615	10			
1	D	417	Total	C	N	O	S	0	0	0
			3279	2075	586	608	10			
1	E	425	Total	C	N	O	S	0	0	0
			3340	2110	600	620	10			
1	F	427	Total	C	N	O	S	0	0	0
			3348	2114	602	622	10			
1	G	427	Total	C	N	O	S	0	0	0
			3352	2116	603	623	10			
1	H	424	Total	C	N	O	S	0	0	0
			3329	2103	598	618	10			
1	I	424	Total	C	N	O	S	0	0	0
			3328	2102	598	618	10			
1	J	424	Total	C	N	O	S	0	0	0
			3328	2102	598	618	10			
1	K	422	Total	C	N	O	S	0	0	0
			3316	2096	595	615	10			
1	L	426	Total	C	N	O	S	0	0	0
			3344	2112	601	621	10			
1	M	425	Total	C	N	O	S	0	0	0
			3332	2104	599	619	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	157	Total	O	0	0
			157	157		
2	B	135	Total	O	0	0
			135	135		

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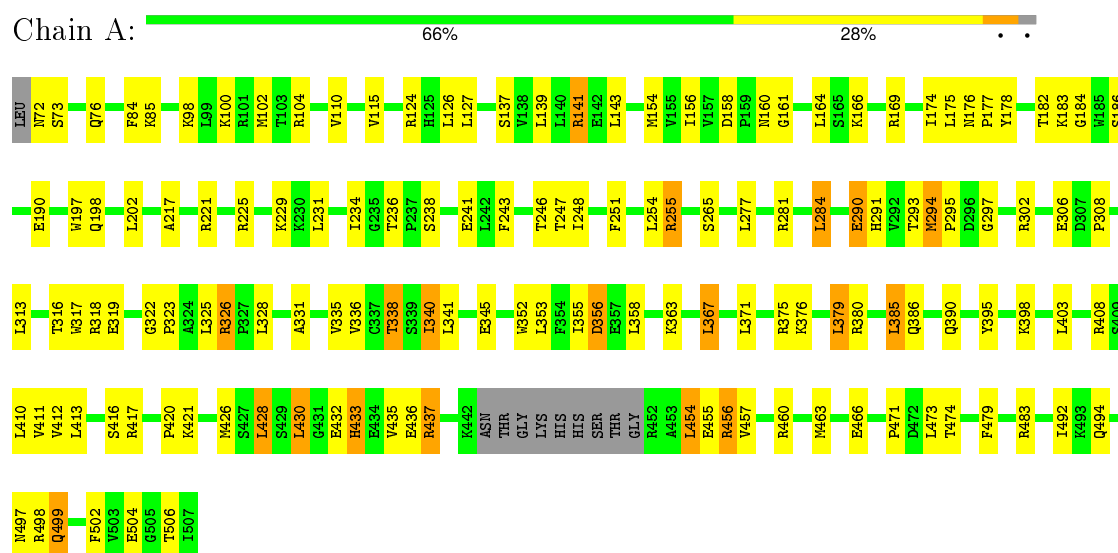
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	139	Total 139	O 139	0	0
2	E	133	Total 133	O 133	0	0
2	F	193	Total 193	O 193	0	0
2	G	167	Total 167	O 167	0	0
2	H	124	Total 124	O 124	0	0
2	I	113	Total 113	O 113	0	0
2	J	102	Total 102	O 102	0	0
2	K	84	Total 84	O 84	0	0
2	L	86	Total 86	O 86	0	0
2	M	113	Total 113	O 113	0	0

3 Residue-property plots

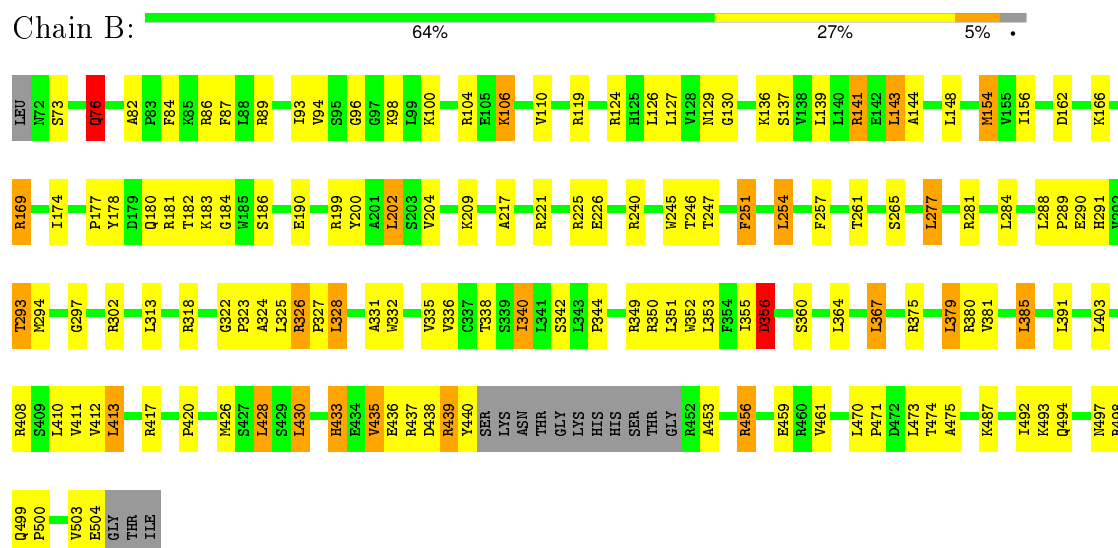
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB



• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB



Chain D: 61% 30% 5% 5%

Position	Amino Acid	Information Content (bits)
1	LEU	0.8
2	ASN	0.8
3	SER	0.8
4	VAL	0.8
5	GLY	0.8
6	GLN	0.8
7	G77	1.4
8	E78	1.4
9	A82	1.4
10	K85	1.4
11	T91	1.4
12	R92	1.4
13	K98	1.4
14	L99	1.4
15	K100	1.4
16	R101	1.4
17	M102	1.4
18	T103	1.4
19	R104	1.4
20	E105	1.4
21	Q109	1.4
22	V110	1.4
23	V115	1.4
24	L126	1.4
25	L127	1.4
26	S137	1.4
27	V138	1.4
28	L139	1.4
29	L140	1.4
30	R141	1.4
31	E142	1.4
32	L143	1.4
33	A144	1.4
34	L148	1.4
35	R153	1.4
36	M154	1.4
37	V155	1.4
38	I156	1.4
39	V157	1.4
40	D158	1.4
41	P159	1.4
42	N160	1.4
43	G161	1.4
44	L164	1.4
45	S165	1.4
46	K166	1.4
47	R169	1.4
48	I173	1.4
49	L174	1.4
50	N175	1.4
51	P177	1.4
52	T182	1.4
53	K183	1.4
54	G184	1.4
55	G185	1.4
56	S186	1.4
57	E190	1.4
58	D196	1.4
59	V197	1.4
60	O198	1.4
61	R199	1.4
62	L202	1.4
63	E215	1.4
64	V216	1.4
65	A217	1.4
66	S218	1.4
67	R221	1.4
68	K229	1.4
69	V230	1.4
70	A232	1.4
71	L233	1.4
72	T234	1.4
73	G235	1.4
74	T236	1.4
75	P237	1.4
76	S238	1.4
77	E241	1.4
78	T246	1.4
79	F251	1.4
80	L254	1.4
81	R255	1.4
82	L277	1.4
83	R281	1.4
84	L284	1.4
85	S285	1.4
86	P289	1.4
87	E290	1.4
88	H291	1.4
89	V292	1.4
90	T293	1.4
91	M294	1.4
92	P295	1.4
93	D296	1.4
94	G297	1.4
95	R302	1.4
96	S303	1.4
97	V304	1.4
98	L305	1.4
99	E306	1.4
100	D307	1.4
101	P308	1.4
102	L313	1.4
103	F314	1.4
104	K317	1.4
105	R318	1.4
106	E319	1.4
107	D320	1.4
108	M321	1.4
109	G322	1.4
110	P323	1.4
111	A324	1.4
112	L325	1.4
113	R326	1.4
114	P327	1.4
115	L328	1.4
116	A331	1.4
117	W332	1.4
118	G337	1.4
119	V336	1.4
120	H337	1.4
121	HIS	1.4
122	SER	1.4
123	S339	1.4
124	L340	1.4
125	ARG	1.4
126	A453	1.4
127	L454	1.4
128	E455	1.4
129	R456	1.4
130	V457	1.4
131	R460	1.4
132	V461	1.4
133	V462	1.4
134	M463	1.4
135	E466	1.4
136	P471	1.4
137	D472	1.4

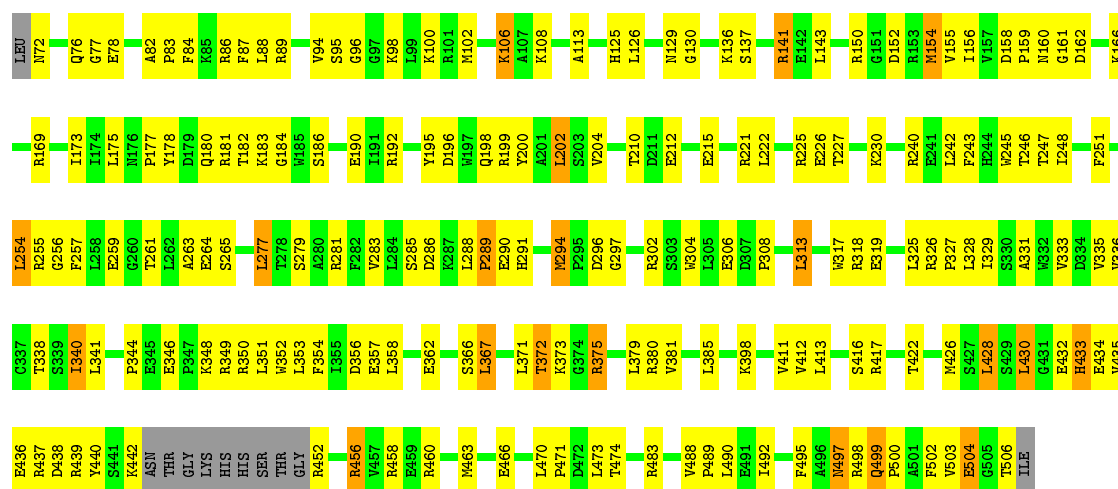
Chain E:

Position	Conserved Amino Acids
1	L490, L403, C297, Q180
2	E491, L403, C297, R181
3	I492, R408, I301, T182
4	Q493, R408, I301, K183
5	Q494, R408, R302, G184
6	F495, L410, S303, W185
7	R498, V411, W304, S186
8	Q499, L413, F314, E190
9	E504, S416, F314, R86
10	E504, R417, T315, F87
11	GLY, W317, T316, L88
12	THR, M426, W317, R89
13	ILE, L430, L325, V94
14	L430, R326, E12, S95
15	L431, G431, R327, K98
16	L432, E432, L328, L99
17	L433, E433, L329, W216
18	E434, E434, L329, A217
19	E435, W332, R221, R101
20	E436, V333, V333, E105
21	R437, D334, V335, K106
22	D438, V335, E226, A107
23	S441, C337, R230, V110
24	K442, C337, R230, V110
25	N443, S339, L233, A113
26	T444, L340, L234, A113
27	GLY, L344, G235, M117
28	LYS, L351, R240, R124
29	HIS, L351, R240, R124
30	HIS, L351, R240, R124
31	SER, R350, F243, L127
32	THR, L351, F243, V128
33	GLY, W352, T246, M129
34	R452, L353, T247, G130
35	A453, F354, T247, G130
36	L454, L355, T250, L143
37	E455, D356, F251, A144
38	R456, E357, T254, L148
39	E459, S360, R255, L148
40	R460, L361, G256, M154
41	E466, E362, F257, V155
42	E466, L367, T258, V157
43	L470, L367, T261, D158
44	P471, L371, L277, P159
45	D472, L371, L277, P159
46	L473, R375, R281, K166
47	T474, R375, R281, K166
48	A475, K376, R281, K166
49	F479, L379, L284, D170
50	THR, R380, L284, D170
51	R483, L385, R287, L175
52	R483, L385, R287, L175
53	R486, Q386, E290, M176
54	A486, E290, E290, P177
55	A486, E290, E290, Y178
56	A486, E290, E290, D170

Chain F:

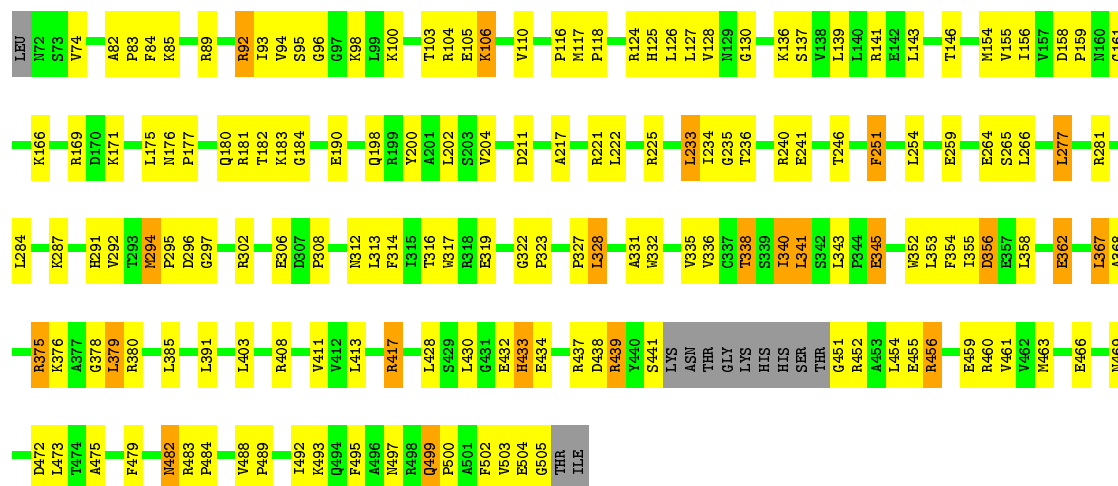
Label	Category
Q180	Yellow
R181	Yellow
T182	Orange
K183	Yellow
K184	Yellow
Y200	Yellow
A201	Yellow
L202	Yellow
P206	Yellow
A217	Yellow
R221	Yellow
L224	Yellow
R225	Yellow
E226	Yellow
K229	Yellow
L233	Yellow
R234	Orange
G235	Yellow
S239	Yellow
K240	Orange
T236	Yellow
L237	Yellow
L242	Yellow
P243	Yellow
E244	Green
W245	Yellow
K246	Yellow
T247	Yellow
P251	Orange
D252	Yellow
G253	Green
L254	Yellow
R255	Orange
T261	Yellow
S265	Yellow
A268	Yellow
L277	Orange
T278	Green
S279	Yellow
A280	Yellow
R281	Yellow
P282	Yellow
V283	Yellow
L284	Yellow
K287	Yellow
E291	Yellow
Q294	Orange
G297	Yellow
L313	Yellow
F314	Yellow
L315	Yellow
T316	Yellow
K317	Yellow
K318	Yellow
E319	Yellow
A324	Yellow
L325	Yellow
R326	Yellow
P327	Yellow
L328	Yellow
A331	Yellow
V335	Yellow
V336	Yellow
G337	Green
T338	Orange
S339	Yellow
L340	Orange
L341	Yellow
P344	Yellow
E345	Green
E346	Yellow
P347	Yellow
K348	Yellow
R349	Yellow
W352	Orange
L353	Yellow
F354	Green
L355	Yellow
R356	Orange
E357	Yellow
L358	Yellow
E362	Yellow
L367	Yellow
A368	Yellow
T372	Orange
K373	Yellow
R375	Yellow
K376	Yellow
L379	Yellow
R380	Yellow
G384	Yellow
L385	Orange
R386	Yellow

Chain L:  55% 38% 5% .



• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain M:  59% 33% 5% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.40 Å 153.40 Å 162.50 Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.2 (50.00-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	41513	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

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	0.42	0/3418	0.67	1/4617 (0.0%)
1	B	0.42	0/3383	0.66	0/4572
1	D	0.41	0/3344	0.69	1/4520 (0.0%)
1	E	0.41	0/3405	0.66	1/4601 (0.0%)
1	F	0.42	0/3413	0.69	1/4611 (0.0%)
1	G	0.41	0/3417	0.66	0/4617
1	H	0.40	0/3394	0.65	1/4587 (0.0%)
1	I	0.39	0/3393	0.66	0/4585
1	J	0.40	0/3393	0.64	0/4585
1	K	0.40	0/3381	0.63	0/4569
1	L	0.40	0/3409	0.65	0/4606
1	M	0.41	0/3397	0.64	0/4590
All	All	0.41	0/40747	0.66	5/55060 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	F	157	VAL	N-CA-C	-5.22	96.91	111.00
1	D	104	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	E	157	VAL	N-CA-C	-5.10	97.22	111.00
1	H	157	VAL	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	200	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	3353	0	3385	109	0
1	B	3318	0	3346	140	0
1	D	3279	0	3307	111	0
1	E	3340	0	3371	141	0
1	F	3348	0	3377	123	0
1	G	3352	0	3380	150	0
1	H	3329	0	3356	145	0
1	I	3328	0	3354	137	0
1	J	3328	0	3354	142	0
1	K	3316	0	3345	191	0
1	L	3344	0	3374	173	0
1	M	3332	0	3357	161	0
2	A	157	0	0	9	0
2	B	135	0	0	7	0
2	D	139	0	0	10	0
2	E	133	0	0	8	0
2	F	193	0	0	9	0
2	G	167	0	0	10	0
2	H	124	0	0	8	0
2	I	113	0	0	8	0
2	J	102	0	0	6	0
2	K	84	0	0	5	0
2	L	86	0	0	4	0
2	M	113	0	0	4	0
All	All	41513	0	40306	1647	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 21.

All (1647) 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:J:76:GLN:HG2	1:J:77:GLY:H	1.07	1.16
1:I:106:LYS:HD3	1:I:106:LYS:H	1.04	1.15
1:E:127:LEU:HD11	1:E:385:LEU:HD22	1.27	1.09
1:J:492:ILE:HD13	1:J:492:ILE:H	1.14	1.08
1:F:372:THR:HG22	1:F:373:LYS:HG3	1.40	1.03
1:G:127:LEU:HD11	1:G:385:LEU:HD22	1.36	1.03
1:M:106:LYS:HD3	1:M:106:LYS:H	1.17	1.01
1:J:127:LEU:HD11	1:J:385:LEU:HD22	1.39	1.01
1:K:436:GLU:HG2	1:K:454:LEU:HD22	1.41	1.00
1:E:106:LYS:HD3	1:E:106:LYS:H	1.23	0.99
1:L:412:VAL:HG22	1:L:426:MET:HE3	1.44	0.99
1:J:226:GLU:HG3	1:J:261:THR:HB	1.45	0.99
1:H:367:LEU:HD13	1:H:403:LEU:HD11	1.49	0.94
1:F:173:ILE:HD12	1:F:183:LYS:HE3	1.49	0.94
1:B:226:GLU:HG3	1:B:261:THR:HB	1.51	0.93
1:F:235:GLY:HA2	2:I:2009:HOH:O	1.67	0.93
1:K:173:ILE:HD12	1:K:183:LYS:HE3	1.51	0.92
1:B:124:ARG:HH21	1:B:408:ARG:HH12	1.17	0.91
1:M:169:ARG:HH21	1:M:171:LYS:HD3	1.33	0.91
1:K:154:MET:HE3	1:K:156:ILE:HD11	1.53	0.91
1:I:134:THR:HG21	1:I:413:LEU:O	1.72	0.90
1:B:141:ARG:HH11	1:B:141:ARG:HG2	1.36	0.90
1:F:176:ASN:H	1:F:182:THR:HG23	1.35	0.90
1:K:412:VAL:HG22	1:K:426:MET:HE3	1.53	0.89
1:A:290:GLU:HG2	1:A:325:LEU:HD23	1.54	0.89
1:L:442:LYS:HD2	1:M:452:ARG:HH21	1.37	0.89
1:L:497:ASN:N	1:L:497:ASN:HD22	1.69	0.89
1:B:290:GLU:HG2	1:B:325:LEU:HD23	1.52	0.88
1:I:246:THR:O	1:I:281:ARG:HD2	1.73	0.88
1:E:226:GLU:HG3	1:E:261:THR:HB	1.56	0.88
1:E:180:GLN:HB2	1:E:504:GLU:HB2	1.54	0.88
1:I:154:MET:CE	1:I:156:ILE:HD11	2.04	0.88
1:I:106:LYS:HD3	1:I:106:LYS:N	1.89	0.88
1:E:412:VAL:HG22	1:E:426:MET:CE	2.01	0.88
1:J:76:GLN:HG2	1:J:77:GLY:N	1.87	0.87
1:K:226:GLU:HG3	1:K:261:THR:HB	1.54	0.87
1:H:294:MET:HE2	1:H:295:PRO:HD2	1.57	0.87
1:K:357:GLU:HG3	2:K:2066:HOH:O	1.75	0.86
1:G:357:GLU:HG3	2:G:2122:HOH:O	1.75	0.86
1:E:246:THR:O	1:E:281:ARG:HD2	1.73	0.86
1:G:72:ASN:HD21	1:G:438:ASP:HB2	1.39	0.86
1:K:169:ARG:HD3	1:K:498:ARG:HH22	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:O	1:A:281:ARG:HD2	1.75	0.85
1:L:226:GLU:HG3	1:L:261:THR:HB	1.56	0.85
1:E:154:MET:HE3	1:E:156:ILE:HD11	1.59	0.85
1:K:182:THR:HG22	1:K:183:LYS:O	1.77	0.85
1:G:372:THR:HG22	1:G:373:LYS:HG3	1.58	0.85
1:M:259:GLU:HA	1:M:264:GLU:HG3	1.59	0.85
1:J:290:GLU:HG2	1:J:325:LEU:HD23	1.59	0.85
1:B:124:ARG:NH2	1:B:408:ARG:HH12	1.74	0.84
1:B:412:VAL:HG22	1:B:426:MET:HE3	1.59	0.84
1:L:106:LYS:HD3	1:L:106:LYS:H	1.43	0.84
1:B:96:GLY:O	1:B:100:LYS:HG3	1.78	0.84
1:M:432:GLU:HG2	1:M:460:ARG:HD3	1.61	0.83
1:K:169:ARG:HH11	1:K:169:ARG:HG3	1.42	0.83
1:L:290:GLU:HG2	1:L:325:LEU:HD23	1.59	0.83
1:G:340:ILE:HD13	1:G:379:LEU:HG	1.61	0.83
1:L:240:ARG:HB2	1:L:240:ARG:NH1	1.93	0.83
1:D:290:GLU:HG2	1:D:325:LEU:HD23	1.61	0.82
1:J:246:THR:O	1:J:281:ARG:HD2	1.78	0.82
1:D:367:LEU:HD13	1:D:403:LEU:HD11	1.60	0.82
1:M:106:LYS:CD	1:M:106:LYS:H	1.88	0.82
1:E:177:PRO:HB3	1:E:294:MET:HG2	1.61	0.81
1:F:499:GLN:HG3	1:F:500:PRO:HD2	1.62	0.81
1:I:94:VAL:HG13	1:I:98:LYS:HB3	1.61	0.81
1:H:246:THR:O	1:H:281:ARG:HD2	1.79	0.81
1:B:240:ARG:HB2	1:B:240:ARG:HH11	1.46	0.81
1:J:336:VAL:O	1:J:340:ILE:HG23	1.80	0.80
1:L:108:LYS:HE3	1:L:150:ARG:HG3	1.63	0.80
1:G:94:VAL:CG1	1:G:98:LYS:HB3	2.12	0.80
1:D:127:LEU:HD11	1:D:385:LEU:HD22	1.63	0.80
1:E:240:ARG:HB2	1:E:240:ARG:NH1	1.97	0.80
1:K:169:ARG:HD3	1:K:498:ARG:NH2	1.96	0.80
1:G:327:PRO:HG2	2:G:2115:HOH:O	1.82	0.80
1:K:246:THR:O	1:K:281:ARG:HD2	1.82	0.80
1:F:237:PRO:HG3	1:I:104:ARG:NH2	1.97	0.80
1:J:160:ASN:HD21	1:J:319:GLU:CD	1.85	0.80
1:L:259:GLU:HA	1:L:264:GLU:HG3	1.64	0.79
1:D:498:ARG:O	1:D:499:GLN:HG2	1.82	0.79
1:H:463:MET:HB2	1:H:466:GLU:HG3	1.64	0.79
1:B:154:MET:HB3	1:B:352:TRP:HB2	1.65	0.79
1:A:154:MET:CE	1:A:156:ILE:HD11	2.13	0.79
1:F:237:PRO:HG3	1:I:104:ARG:HH21	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:255:ARG:HH11	1:L:277:LEU:HD12	1.48	0.79
1:G:259:GLU:HA	1:G:264:GLU:HG3	1.65	0.78
1:A:127:LEU:HD11	1:A:385:LEU:HD22	1.64	0.78
1:F:176:ASN:H	1:F:182:THR:CG2	1.96	0.78
1:E:154:MET:CE	1:E:156:ILE:HD11	2.14	0.78
1:F:225:ARG:O	1:F:229:LYS:HG3	1.82	0.78
1:B:336:VAL:O	1:B:340:ILE:HG23	1.83	0.78
1:H:177:PRO:HB3	1:H:294:MET:HG2	1.65	0.78
1:B:412:VAL:HG22	1:B:426:MET:CE	2.14	0.78
1:L:182:THR:HG22	1:L:183:LYS:O	1.84	0.78
1:H:375:ARG:HB2	1:H:375:ARG:HH11	1.48	0.78
1:L:240:ARG:HB2	1:L:240:ARG:HH11	1.50	0.77
1:M:175:LEU:HD12	1:M:313:LEU:HD21	1.65	0.77
1:K:127:LEU:HD11	1:K:385:LEU:HD13	1.65	0.77
1:I:124:ARG:NH2	1:I:408:ARG:HH12	1.82	0.77
1:M:110:VAL:HG11	1:M:143:LEU:HD23	1.65	0.77
1:F:234:ILE:O	1:F:234:ILE:HG22	1.83	0.77
1:J:84:PHE:HB3	1:J:437:ARG:NH1	2.00	0.77
1:B:437:ARG:HD2	1:D:456:ARG:NH1	1.99	0.77
1:A:198:GLN:HG2	2:G:2012:HOH:O	1.85	0.77
1:F:127:LEU:HD11	1:F:385:LEU:HD22	1.67	0.77
1:A:291:HIS:HD2	2:A:2040:HOH:O	1.68	0.77
1:K:497:ASN:HD22	1:K:497:ASN:N	1.83	0.76
1:G:290:GLU:HG2	1:G:325:LEU:HD23	1.67	0.76
1:I:127:LEU:HD11	1:I:385:LEU:CD2	2.15	0.76
1:M:502:PHE:CE2	1:M:504:GLU:HB2	2.21	0.76
1:I:502:PHE:CE2	1:I:504:GLU:HB3	2.20	0.76
1:G:499:GLN:HG3	1:G:500:PRO:HD2	1.67	0.76
1:K:473:LEU:HD11	1:K:492:ILE:HD11	1.67	0.76
1:K:73:SER:HB3	1:K:85:LYS:HA	1.68	0.75
1:G:154:MET:CE	1:G:156:ILE:HD11	2.16	0.75
1:D:246:THR:O	1:D:281:ARG:HD2	1.86	0.75
1:E:412:VAL:HG22	1:E:426:MET:HE2	1.68	0.75
1:G:182:THR:HG22	1:G:183:LYS:O	1.87	0.75
1:H:127:LEU:HD11	1:H:385:LEU:HD22	1.67	0.75
1:D:154:MET:CE	1:D:156:ILE:HD11	2.17	0.75
1:K:230:LYS:HD3	1:K:257:PHE:CE2	2.22	0.75
1:G:154:MET:HE2	1:G:156:ILE:HD11	1.69	0.75
1:L:336:VAL:O	1:L:340:ILE:HG23	1.85	0.75
1:K:166:LYS:HE2	1:K:497:ASN:ND2	2.02	0.75
1:I:473:LEU:HD11	1:I:492:ILE:HD11	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:PRO:HG2	2:B:2088:HOH:O	1.86	0.75
1:I:182:THR:HG22	1:I:183:LYS:O	1.86	0.75
1:G:226:GLU:HG3	1:G:261:THR:HB	1.69	0.75
1:M:126:LEU:HD11	1:M:411:VAL:HG23	1.69	0.74
1:M:154:MET:HB3	1:M:352:TRP:HB2	1.68	0.74
1:A:367:LEU:HD13	1:A:403:LEU:HD11	1.69	0.74
1:L:412:VAL:HG22	1:L:426:MET:CE	2.16	0.74
1:M:92:ARG:HB2	1:M:484:PRO:HB3	1.70	0.74
1:M:156:ILE:HG22	1:M:158:ASP:HB2	1.69	0.74
1:I:318:ARG:HD3	1:I:502:PHE:CE2	2.22	0.74
1:I:372:THR:HG23	1:I:373:LYS:HG3	1.70	0.74
1:K:412:VAL:HG22	1:K:426:MET:CE	2.16	0.74
1:K:84:PHE:CG	1:K:435:VAL:HG21	2.23	0.74
1:M:177:PRO:HA	1:M:294:MET:HE2	1.69	0.74
1:D:473:LEU:HD11	1:D:492:ILE:HD11	1.68	0.73
1:K:452:ARG:HB3	1:K:452:ARG:NH1	2.03	0.73
1:A:169:ARG:HG3	1:A:498:ARG:HH22	1.52	0.73
1:M:327:PRO:HG2	2:M:2073:HOH:O	1.87	0.73
1:A:410:LEU:HD11	1:A:426:MET:HE1	1.71	0.73
1:I:154:MET:HE3	1:I:156:ILE:HD11	1.70	0.73
1:M:336:VAL:O	1:M:340:ILE:HG23	1.88	0.73
1:K:134:THR:HG21	1:K:413:LEU:HB3	1.70	0.73
1:G:246:THR:O	1:G:281:ARG:HD2	1.89	0.73
1:I:225:ARG:O	1:I:229:LYS:HG3	1.89	0.73
1:H:440:TYR:HA	1:H:452:ARG:HB2	1.71	0.73
1:H:177:PRO:HA	1:H:294:MET:HE2	1.71	0.73
1:A:154:MET:HE3	1:A:156:ILE:HD11	1.71	0.72
1:J:190:GLU:OE1	1:J:302:ARG:HG3	1.87	0.72
1:J:200:TYR:HE1	1:J:335:VAL:HG13	1.54	0.72
1:A:225:ARG:HD2	2:A:2067:HOH:O	1.88	0.72
1:I:124:ARG:HH11	1:I:124:ARG:HG3	1.54	0.72
1:K:74:VAL:HG12	1:K:75:GLY:H	1.54	0.72
1:K:134:THR:HG21	1:K:413:LEU:O	1.89	0.72
1:D:190:GLU:OE1	1:D:302:ARG:HG3	1.90	0.72
1:F:234:ILE:CG2	1:F:234:ILE:O	2.38	0.72
1:M:413:LEU:HD23	1:M:475:ALA:HB2	1.72	0.72
1:L:246:THR:O	1:L:281:ARG:HD2	1.90	0.72
1:M:124:ARG:HH21	1:M:375:ARG:HG3	1.54	0.72
1:H:294:MET:CE	1:H:295:PRO:HD2	2.19	0.72
1:K:78:GLU:OE1	1:K:78:GLU:HA	1.89	0.72
1:M:352:TRP:CE2	1:M:380:ARG:HD3	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:LEU:HD11	1:J:411:VAL:HG23	1.71	0.72
1:I:255:ARG:HG3	1:I:255:ARG:HH11	1.54	0.72
1:G:126:LEU:HD11	1:G:411:VAL:HG23	1.71	0.71
1:B:246:THR:O	1:B:281:ARG:HD2	1.90	0.71
1:G:94:VAL:HG12	1:G:95:SER:N	2.05	0.71
1:K:78:GLU:HG3	1:K:95:SER:CA	2.20	0.71
1:I:158:ASP:OD2	1:I:161:GLY:HA2	1.91	0.71
1:B:106:LYS:HE3	1:B:106:LYS:H	1.54	0.71
1:I:154:MET:HE2	1:I:156:ILE:HD11	1.71	0.71
1:K:129:ASN:HB3	1:K:426:MET:HE1	1.73	0.71
1:D:154:MET:HE3	1:D:156:ILE:HD11	1.72	0.71
1:A:473:LEU:HD11	1:A:492:ILE:HD11	1.73	0.70
1:F:160:ASN:HD21	1:F:319:GLU:HG3	1.56	0.70
1:E:412:VAL:HG22	1:E:426:MET:HE3	1.73	0.70
1:D:432:GLU:HG2	1:D:460:ARG:HD3	1.72	0.70
1:G:410:LEU:HD11	1:G:426:MET:HE1	1.73	0.70
1:J:154:MET:HE3	1:J:156:ILE:HD11	1.71	0.70
1:I:259:GLU:HA	1:I:264:GLU:HG3	1.73	0.70
1:K:75:GLY:HA3	1:K:84:PHE:H	1.55	0.70
1:A:412:VAL:HG22	1:A:426:MET:CE	2.21	0.70
1:G:72:ASN:ND2	1:G:438:ASP:HB2	2.04	0.70
1:B:240:ARG:HB2	1:B:240:ARG:NH1	2.05	0.70
1:A:432:GLU:HG2	1:A:460:ARG:HD3	1.72	0.70
1:F:420:PRO:HB2	1:G:428:LEU:HD22	1.74	0.70
1:J:76:GLN:CG	1:J:77:GLY:H	1.92	0.69
1:A:498:ARG:O	1:A:499:GLN:HG2	1.92	0.69
1:M:379:LEU:HD22	1:M:380:ARG:N	2.07	0.69
1:F:226:GLU:HG3	1:F:261:THR:HB	1.72	0.69
1:E:240:ARG:HB2	1:E:240:ARG:HH11	1.55	0.69
1:E:230:LYS:HD3	1:E:257:PHE:CZ	2.27	0.69
1:M:294:MET:CE	1:M:295:PRO:HD2	2.22	0.69
1:A:318:ARG:HD2	1:A:502:PHE:CE2	2.28	0.69
1:F:336:VAL:O	1:F:340:ILE:HG23	1.91	0.69
1:J:154:MET:HB3	1:J:352:TRP:HB2	1.73	0.69
1:B:190:GLU:OE1	1:B:302:ARG:HG3	1.93	0.69
1:A:190:GLU:OE1	1:A:302:ARG:HG3	1.92	0.69
1:M:190:GLU:OE1	1:M:302:ARG:HG3	1.92	0.69
1:K:85:LYS:HD2	1:K:454:LEU:HD21	1.75	0.69
1:J:436:GLU:HB3	1:J:454:LEU:HD21	1.73	0.69
1:I:173:ILE:HD12	1:I:183:LYS:HE3	1.73	0.69
1:I:106:LYS:H	1:I:106:LYS:CD	1.84	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:ARG:HD3	2:G:2116:HOH:O	1.93	0.69
1:B:225:ARG:HD2	2:B:2058:HOH:O	1.92	0.69
1:I:367:LEU:HD13	1:I:403:LEU:HD11	1.75	0.69
1:G:372:THR:HG22	1:G:373:LYS:CG	2.23	0.68
1:L:255:ARG:NH1	1:L:277:LEU:HD12	2.07	0.68
1:J:331:ALA:O	1:J:335:VAL:HG23	1.93	0.68
1:H:336:VAL:O	1:H:340:ILE:HG23	1.94	0.68
1:H:279:SER:O	1:H:283:VAL:HG23	1.93	0.68
1:H:155:VAL:HG13	1:H:313:LEU:HD12	1.75	0.68
1:M:502:PHE:HE2	1:M:504:GLU:HB2	1.59	0.68
1:K:78:GLU:HG3	1:K:95:SER:HA	1.75	0.68
1:L:190:GLU:OE1	1:L:302:ARG:HG3	1.94	0.68
1:J:492:ILE:CD1	1:J:492:ILE:H	1.92	0.68
1:K:313:LEU:HD23	1:K:314:PHE:N	2.08	0.68
1:B:126:LEU:HD11	1:B:411:VAL:HG23	1.76	0.68
1:E:443:ASN:OD1	1:F:451:GLY:HA3	1.92	0.68
1:I:124:ARG:HG3	1:I:124:ARG:NH1	2.09	0.68
1:J:412:VAL:HG22	1:J:426:MET:CE	2.24	0.68
1:F:246:THR:O	1:F:281:ARG:HD2	1.92	0.68
1:E:432:GLU:HG2	1:E:460:ARG:HD3	1.76	0.68
1:J:94:VAL:HG13	1:J:98:LYS:HB3	1.76	0.68
1:D:412:VAL:HG22	1:D:426:MET:CE	2.23	0.68
1:M:504:GLU:HG3	1:M:505:GLY:N	2.09	0.67
1:A:412:VAL:HG22	1:A:426:MET:HE3	1.77	0.67
1:K:413:LEU:HD12	1:K:475:ALA:HB2	1.77	0.67
1:E:110:VAL:HG11	1:E:143:LEU:HD23	1.76	0.67
1:L:473:LEU:HD11	1:L:492:ILE:HD11	1.74	0.67
1:B:169:ARG:HH11	1:B:169:ARG:HG3	1.59	0.67
1:K:173:ILE:HG23	1:K:183:LYS:HG3	1.75	0.67
1:D:169:ARG:HG3	1:D:498:ARG:NH2	2.10	0.67
1:J:327:PRO:HG2	2:J:2070:HOH:O	1.94	0.67
1:J:230:LYS:HD3	1:J:257:PHE:CE1	2.30	0.67
1:B:124:ARG:NH2	1:B:408:ARG:NH1	2.43	0.67
1:A:293:THR:HG21	2:A:2091:HOH:O	1.94	0.67
1:L:432:GLU:HG2	1:L:460:ARG:HD3	1.76	0.67
1:B:180:GLN:HE21	1:B:504:GLU:HG3	1.59	0.67
1:I:145:TYR:CZ	1:I:149:LEU:HD21	2.30	0.67
1:J:184:GLY:HA3	1:J:297:GLY:HA3	1.76	0.67
1:L:497:ASN:N	1:L:497:ASN:ND2	2.42	0.66
1:I:94:VAL:CG1	1:I:98:LYS:HB3	2.25	0.66
1:E:106:LYS:H	1:E:106:LYS:CD	2.01	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ARG:HH11	1:F:141:ARG:HG2	1.60	0.66
1:A:169:ARG:HG3	1:A:498:ARG:NH2	2.09	0.66
1:H:290:GLU:HG2	1:H:325:LEU:HD23	1.76	0.66
1:B:87:PHE:HA	1:B:435:VAL:HG23	1.77	0.66
1:H:439:ARG:HD3	1:H:453:ALA:O	1.96	0.66
1:F:173:ILE:HG23	1:F:183:LYS:HG3	1.75	0.66
1:A:410:LEU:HD11	1:A:426:MET:CE	2.26	0.66
1:A:502:PHE:CE2	1:A:504:GLU:HB2	2.31	0.66
1:F:82:ALA:HB2	1:G:456:ARG:HD2	1.77	0.66
1:L:160:ASN:HD21	1:L:319:GLU:CD	1.99	0.66
1:K:74:VAL:HG12	1:K:75:GLY:N	2.10	0.66
1:J:372:THR:HG22	1:J:373:LYS:HG3	1.78	0.66
1:B:94:VAL:CG2	1:B:98:LYS:HD3	2.25	0.66
1:H:158:ASP:HB3	1:H:316:THR:HG22	1.76	0.66
1:F:134:THR:HA	1:F:472:ASP:OD1	1.96	0.66
1:D:176:ASN:H	1:D:182:THR:HG23	1.60	0.66
1:H:294:MET:HG3	1:H:328:LEU:HD11	1.78	0.65
1:F:346:GLU:OE2	1:F:348:LYS:HB2	1.96	0.65
1:L:503:VAL:O	1:L:504:GLU:HB2	1.96	0.65
1:E:255:ARG:HH11	1:E:255:ARG:HG3	1.61	0.65
1:L:180:GLN:HB2	1:L:504:GLU:HB2	1.76	0.65
1:G:367:LEU:HD13	1:G:403:LEU:HD11	1.78	0.65
1:M:251:PHE:CE1	1:M:277:LEU:HD13	2.30	0.65
1:J:200:TYR:CE1	1:J:335:VAL:HG13	2.32	0.65
1:J:432:GLU:HG2	1:J:460:ARG:HD3	1.79	0.65
1:B:184:GLY:HA3	1:B:297:GLY:HA3	1.79	0.65
1:B:182:THR:HG22	1:B:183:LYS:O	1.97	0.65
1:M:106:LYS:N	1:M:106:LYS:HD3	2.02	0.65
1:K:452:ARG:HB3	1:K:452:ARG:HH11	1.60	0.64
1:H:94:VAL:HG13	1:H:98:LYS:HB3	1.79	0.64
1:A:398:LYS:HG3	2:G:2134:HOH:O	1.97	0.64
1:A:436:GLU:HB3	1:A:454:LEU:HD21	1.79	0.64
1:H:138:VAL:HG21	1:H:492:ILE:HG12	1.79	0.64
1:L:184:GLY:HA3	1:L:297:GLY:HA3	1.79	0.64
1:L:463:MET:HB2	1:L:466:GLU:HG3	1.79	0.64
1:I:101:ARG:O	1:I:104:ARG:HG2	1.97	0.64
1:I:139:LEU:HD11	1:I:411:VAL:HG11	1.80	0.64
1:K:251:PHE:CE2	1:K:277:LEU:HD12	2.33	0.64
1:L:96:GLY:O	1:L:100:LYS:HG3	1.97	0.64
1:G:473:LEU:HD11	1:G:492:ILE:HD11	1.79	0.64
1:M:222:LEU:HA	1:M:225:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:200:TYR:O	1:H:204:VAL:HG23	1.98	0.64
1:K:433:HIS:O	1:K:433:HIS:HD2	1.80	0.64
1:E:379:LEU:HD22	1:E:380:ARG:N	2.12	0.63
1:H:302:ARG:O	1:H:306:GLU:HG3	1.98	0.63
1:I:255:ARG:HG3	1:I:255:ARG:NH1	2.12	0.63
1:E:357:GLU:OE2	1:E:386:GLN:HG3	1.98	0.63
1:E:106:LYS:HD3	1:E:106:LYS:N	2.06	0.63
1:F:154:MET:HE3	1:F:156:ILE:HD11	1.80	0.63
1:L:338:THR:HG23	1:L:366:SER:OG	1.97	0.63
1:A:98:LYS:O	1:A:102:MET:HG3	1.98	0.63
1:B:413:LEU:HD12	1:B:475:ALA:HB2	1.78	0.63
1:D:318:ARG:HD2	1:D:502:PHE:CE2	2.34	0.63
1:L:442:LYS:HD2	1:M:452:ARG:NH2	2.11	0.63
1:J:154:MET:CE	1:J:156:ILE:HD11	2.28	0.63
1:G:413:LEU:HD12	1:G:475:ALA:HB2	1.79	0.63
1:G:166:LYS:HD3	1:G:495:PHE:HB2	1.80	0.63
1:H:281:ARG:NH2	1:I:265:SER:HB3	2.14	0.63
1:J:199:ARG:HE	1:J:338:THR:CG2	2.12	0.63
1:G:110:VAL:CG1	1:G:143:LEU:HD23	2.29	0.63
1:D:336:VAL:O	1:D:340:ILE:HG23	1.99	0.63
1:G:412:VAL:HG22	1:G:426:MET:CE	2.29	0.63
1:L:88:LEU:HD21	1:L:436:GLU:HG3	1.81	0.63
1:B:124:ARG:HH21	1:B:408:ARG:NH1	1.92	0.62
1:M:294:MET:HE2	1:M:295:PRO:HD2	1.79	0.62
1:G:329:ILE:O	1:G:333:VAL:HG23	1.99	0.62
1:E:113:ALA:HA	1:E:490:LEU:HD23	1.81	0.62
1:M:124:ARG:HH22	1:M:375:ARG:NH1	1.95	0.62
1:L:195:TYR:HE1	1:L:199:ARG:HH11	1.47	0.62
1:E:94:VAL:HG13	1:E:98:LYS:HB3	1.82	0.62
1:I:412:VAL:HG22	1:I:426:MET:HE3	1.80	0.62
1:H:176:ASN:H	1:H:182:THR:CG2	2.12	0.62
1:D:436:GLU:HG2	1:D:454:LEU:HD22	1.81	0.62
1:E:350:ARG:HG2	1:E:380:ARG:NH2	2.15	0.62
1:M:94:VAL:CG2	1:M:98:LYS:HD3	2.29	0.62
1:L:247:THR:HG22	1:L:248:ILE:HD13	1.80	0.62
1:K:177:PRO:HG3	1:K:325:LEU:HD21	1.81	0.62
1:H:432:GLU:OE1	1:H:458:ARG:HD2	1.99	0.62
1:M:118:PRO:HG2	1:M:483:ARG:NH1	2.14	0.62
1:B:326:ARG:HD3	2:B:2086:HOH:O	1.98	0.62
1:B:106:LYS:H	1:B:106:LYS:CE	2.11	0.62
1:B:180:GLN:HE21	1:B:504:GLU:HB2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:MET:HB3	1:E:352:TRP:HB2	1.81	0.62
1:I:124:ARG:NH2	1:I:408:ARG:NH1	2.46	0.62
1:F:137:SER:O	1:F:141:ARG:HB2	2.00	0.62
1:I:126:LEU:HD11	1:I:411:VAL:HG23	1.82	0.62
1:I:221:ARG:O	1:I:225:ARG:HG2	1.99	0.62
1:F:245:TRP:O	1:F:254:LEU:HG	2.00	0.62
1:H:327:PRO:HG2	2:H:2085:HOH:O	1.99	0.62
1:L:372:THR:HG22	1:L:373:LYS:CG	2.30	0.62
1:H:181:ARG:NH1	1:H:500:PRO:HG2	2.15	0.62
1:M:438:ASP:OD1	1:M:454:LEU:HD23	1.99	0.62
1:B:180:GLN:HE21	1:B:504:GLU:CG	2.13	0.62
1:G:432:GLU:HG2	1:G:460:ARG:HD3	1.80	0.62
1:K:289:PRO:O	1:K:293:THR:HG23	2.00	0.62
1:H:84:PHE:CG	1:H:435:VAL:HG11	2.35	0.62
1:D:326:ARG:HD3	2:D:2083:HOH:O	2.00	0.62
1:B:433:HIS:NE2	1:B:459:GLU:HG3	2.15	0.62
1:F:176:ASN:N	1:F:182:THR:HG23	2.11	0.61
1:G:154:MET:HB3	1:G:352:TRP:HB2	1.82	0.61
1:J:177:PRO:HG2	1:J:178:TYR:CD1	2.35	0.61
1:I:173:ILE:CD1	1:I:183:LYS:HE3	2.30	0.61
1:D:182:THR:HG21	1:D:294:MET:HE1	1.80	0.61
1:L:372:THR:HG22	1:L:373:LYS:HG3	1.83	0.61
1:D:255:ARG:HH11	1:D:255:ARG:HG3	1.65	0.61
1:H:177:PRO:HA	1:H:294:MET:CE	2.29	0.61
1:H:436:GLU:OE2	1:H:456:ARG:NH1	2.32	0.61
1:K:139:LEU:HD11	1:K:411:VAL:HG11	1.81	0.61
1:L:154:MET:HB3	1:L:352:TRP:HB2	1.83	0.61
1:D:169:ARG:HG3	1:D:498:ARG:HH22	1.65	0.61
1:A:154:MET:HE2	1:A:156:ILE:HD11	1.81	0.61
1:A:158:ASP:OD2	1:A:161:GLY:HA2	2.01	0.61
1:F:436:GLU:HG2	1:F:456:ARG:HD3	1.81	0.61
1:M:104:ARG:NH1	1:M:105:GLU:O	2.34	0.61
1:J:437:ARG:HH11	1:J:437:ARG:HG3	1.64	0.61
1:E:254:LEU:HD22	1:E:258:LEU:HG	1.83	0.61
1:D:290:GLU:HG2	1:D:325:LEU:CD2	2.29	0.61
1:G:243:PHE:O	1:G:247:THR:HB	2.01	0.61
1:I:154:MET:HB3	1:I:352:TRP:HB2	1.82	0.61
1:D:184:GLY:HA3	1:D:297:GLY:HA3	1.83	0.61
1:D:141:ARG:HG2	1:D:141:ARG:HH11	1.66	0.61
1:L:126:LEU:HD11	1:L:411:VAL:HG23	1.83	0.61
1:B:124:ARG:NH1	1:B:124:ARG:HG3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:GLY:O	1:G:101:ARG:HG3	1.99	0.60
1:B:202:LEU:HD12	1:B:221:ARG:CD	2.31	0.60
1:J:169:ARG:NH2	1:J:171:LYS:NZ	2.49	0.60
1:K:182:THR:HG21	1:K:294:MET:CE	2.31	0.60
1:B:137:SER:O	1:B:141:ARG:HB2	2.00	0.60
1:K:357:GLU:OE2	1:K:386:GLN:HG3	2.00	0.60
1:L:497:ASN:HD22	1:L:497:ASN:H	1.50	0.60
1:H:254:LEU:HD12	1:H:281:ARG:HD3	1.82	0.60
1:F:357:GLU:HG3	2:F:2143:HOH:O	2.01	0.60
1:B:344:PRO:O	1:B:349:ARG:NH2	2.33	0.60
1:I:336:VAL:O	1:I:340:ILE:HG23	2.00	0.60
1:A:85:LYS:HE2	1:A:454:LEU:HG	1.83	0.60
1:F:463:MET:HB2	1:F:466:GLU:HG3	1.84	0.60
1:E:124:ARG:HH11	1:E:124:ARG:HG3	1.66	0.60
1:I:456:ARG:N	1:I:456:ARG:HD2	2.17	0.60
1:L:154:MET:CE	1:L:156:ILE:HD11	2.32	0.60
1:F:175:LEU:HD12	1:F:313:LEU:HD21	1.84	0.60
1:E:380:ARG:HG3	1:E:380:ARG:HH11	1.66	0.60
1:G:110:VAL:HG11	1:G:143:LEU:HD23	1.82	0.60
1:E:438:ASP:OD1	1:E:454:LEU:HD12	2.02	0.60
1:G:190:GLU:OE1	1:G:302:ARG:HG3	2.01	0.60
2:A:2130:HOH:O	1:G:417:ARG:HG2	2.00	0.60
1:F:124:ARG:HB3	1:F:408:ARG:HG3	1.83	0.60
1:E:426:MET:O	1:E:430:LEU:HD22	2.02	0.60
1:M:251:PHE:CZ	1:M:277:LEU:HD13	2.37	0.60
1:I:412:VAL:HG22	1:I:426:MET:CE	2.31	0.60
1:M:338:THR:O	1:M:341:LEU:HB2	2.02	0.60
1:J:410:LEU:HD11	1:J:426:MET:HE1	1.84	0.60
1:B:324:ALA:HB2	2:D:2045:HOH:O	2.02	0.60
1:D:411:VAL:HG12	1:D:413:LEU:CD1	2.32	0.60
1:J:291:HIS:HE1	2:J:2074:HOH:O	1.85	0.59
1:H:154:MET:HB3	1:H:352:TRP:HB2	1.82	0.59
1:K:169:ARG:NH1	1:K:169:ARG:HG3	2.12	0.59
1:M:83:PRO:O	1:M:437:ARG:HD3	2.02	0.59
1:A:421:LYS:HB3	2:A:2136:HOH:O	2.01	0.59
1:J:139:LEU:HD11	1:J:411:VAL:HG11	1.84	0.59
1:I:169:ARG:HH12	1:I:171:LYS:CG	2.15	0.59
1:M:417:ARG:NH2	1:M:469:ASN:OD1	2.36	0.59
1:G:225:ARG:O	1:G:229:LYS:HB2	2.02	0.59
1:K:85:LYS:CD	1:K:454:LEU:HD21	2.32	0.59
1:K:154:MET:CE	1:K:156:ILE:HD11	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:230:LYS:HE2	1:K:257:PHE:O	2.02	0.59
1:K:134:THR:O	1:K:134:THR:HG22	2.03	0.59
1:H:94:VAL:CG1	1:H:95:SER:N	2.66	0.59
1:K:86:ARG:HG2	1:K:86:ARG:HH11	1.67	0.59
1:D:498:ARG:C	1:D:499:GLN:HG2	2.23	0.59
1:B:202:LEU:HD12	1:B:221:ARG:HD3	1.84	0.59
1:H:243:PHE:O	1:H:247:THR:HB	2.03	0.59
1:E:106:LYS:HG2	1:E:107:ALA:H	1.67	0.59
1:D:410:LEU:HD11	1:D:426:MET:HE1	1.84	0.59
1:F:82:ALA:O	1:F:437:ARG:NH1	2.36	0.59
1:B:440:TYR:O	1:D:453:ALA:HB1	2.03	0.59
1:G:375:ARG:NH2	1:G:376:LYS:NZ	2.51	0.59
1:B:351:LEU:HD12	1:B:379:LEU:HD23	1.84	0.59
1:M:246:THR:O	1:M:281:ARG:HD2	2.02	0.59
1:I:432:GLU:HG2	1:I:460:ARG:HD3	1.83	0.59
1:H:94:VAL:HG12	1:H:95:SER:O	2.03	0.59
1:D:197:TRP:CE2	1:D:229:LYS:HG2	2.37	0.59
1:D:98:LYS:O	1:D:102:MET:HG3	2.03	0.59
1:B:124:ARG:HH11	1:B:124:ARG:HG3	1.66	0.59
1:M:110:VAL:CG1	1:M:143:LEU:HD23	2.33	0.59
1:H:426:MET:O	1:H:430:LEU:HD22	2.03	0.59
1:G:137:SER:O	1:G:141:ARG:HB2	2.02	0.59
1:A:160:ASN:HD21	1:A:319:GLU:CD	2.05	0.59
1:K:182:THR:HG21	1:K:294:MET:HE2	1.84	0.58
1:E:180:GLN:HB2	1:E:504:GLU:CB	2.30	0.58
1:I:177:PRO:HG2	1:I:178:TYR:CD1	2.38	0.58
1:F:162:ASP:HB3	2:F:2041:HOH:O	2.02	0.58
1:F:439:ARG:NH1	1:F:439:ARG:HB2	2.18	0.58
1:L:173:ILE:HD12	1:L:183:LYS:NZ	2.18	0.58
1:G:413:LEU:HD12	1:G:475:ALA:CB	2.33	0.58
1:H:76:GLN:C	1:H:78:GLU:H	2.07	0.58
1:B:104:ARG:HD2	2:B:2009:HOH:O	2.01	0.58
1:K:200:TYR:O	1:K:204:VAL:HG23	2.03	0.58
1:M:182:THR:HG21	1:M:294:MET:CE	2.33	0.58
1:D:255:ARG:NH1	1:D:255:ARG:HG3	2.17	0.58
1:H:331:ALA:O	1:H:335:VAL:HG23	2.02	0.58
1:H:251:PHE:HE2	1:H:255:ARG:HH12	1.51	0.58
1:A:463:MET:HB2	1:A:466:GLU:HG3	1.85	0.58
1:G:104:ARG:HH11	1:G:104:ARG:HG2	1.68	0.58
1:F:420:PRO:CB	1:G:428:LEU:HD22	2.33	0.58
1:E:124:ARG:HB3	1:E:408:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD11	1:A:411:VAL:HG23	1.85	0.58
1:K:329:ILE:O	1:K:333:VAL:HG23	2.02	0.58
1:M:504:GLU:HG3	1:M:505:GLY:H	1.69	0.58
1:F:357:GLU:OE2	1:F:386:GLN:HG3	2.04	0.58
1:L:357:GLU:HG3	2:L:2059:HOH:O	2.03	0.58
1:G:223:LEU:HD23	1:G:284:LEU:HD22	1.85	0.58
1:K:134:THR:CG2	1:K:413:LEU:HB3	2.34	0.58
1:M:493:LYS:HD3	1:M:495:PHE:CZ	2.39	0.58
1:F:338:THR:O	1:F:341:LEU:HB2	2.03	0.58
1:J:186:SER:H	1:J:189:ASN:ND2	2.02	0.58
1:L:84:PHE:CG	1:L:435:VAL:HG11	2.38	0.58
1:I:410:LEU:HD11	1:I:426:MET:HE1	1.85	0.58
1:H:479:PHE:O	1:M:417:ARG:NH1	2.36	0.58
1:F:96:GLY:O	1:F:100:LYS:HG3	2.04	0.58
1:K:169:ARG:CD	1:K:498:ARG:HH22	2.15	0.57
1:L:226:GLU:CG	1:L:261:THR:HB	2.33	0.57
1:H:436:GLU:HG2	1:H:456:ARG:HD3	1.85	0.57
1:K:499:GLN:HG3	1:K:500:PRO:HD2	1.86	0.57
1:G:159:PRO:HG3	1:G:317:TRP:CH2	2.39	0.57
1:A:455:GLU:HG2	1:A:457:VAL:HG23	1.86	0.57
1:E:367:LEU:HD22	1:E:371:LEU:HG	1.86	0.57
1:B:318:ARG:HH11	1:B:318:ARG:HG2	1.70	0.57
1:A:494:GLN:OE1	1:A:494:GLN:HA	2.02	0.57
1:B:410:LEU:HD11	1:B:426:MET:HE1	1.86	0.57
1:J:169:ARG:NH2	1:J:171:LYS:HZ3	2.02	0.57
1:M:182:THR:HG22	1:M:183:LYS:O	2.05	0.57
1:B:106:LYS:N	1:B:106:LYS:HE3	2.19	0.57
1:L:466:GLU:OE2	1:M:89:ARG:HD2	2.05	0.57
1:K:104:ARG:HG2	1:K:104:ARG:HH11	1.69	0.57
1:I:281:ARG:NH2	1:J:265:SER:HB3	2.20	0.57
1:M:322:GLY:N	1:M:323:PRO:HD2	2.19	0.57
1:F:473:LEU:HD11	1:F:492:ILE:HD11	1.86	0.57
1:A:408:ARG:HD2	1:G:416:SER:HB2	1.86	0.57
1:M:156:ILE:HG13	1:M:354:PHE:HB2	1.87	0.57
1:J:169:ARG:NH1	1:J:172:ASP:OD2	2.38	0.57
1:L:94:VAL:HG22	1:L:95:SER:H	1.69	0.57
1:A:306:GLU:O	1:A:308:PRO:HD3	2.05	0.57
1:I:338:THR:O	1:I:341:LEU:HB2	2.04	0.57
1:B:154:MET:HE2	1:B:156:ILE:HD11	1.87	0.57
1:M:331:ALA:O	1:M:335:VAL:HG23	2.05	0.57
1:E:313:LEU:HD23	1:E:314:PHE:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:SER:HB2	1:F:408:ARG:HD2	1.87	0.56
1:G:94:VAL:CG1	1:G:95:SER:N	2.68	0.56
1:E:255:ARG:HG3	1:E:255:ARG:NH1	2.20	0.56
1:L:466:GLU:CD	1:M:89:ARG:HD2	2.25	0.56
1:L:488:VAL:HG13	1:L:489:PRO:HD2	1.86	0.56
1:E:184:GLY:HA3	1:E:297:GLY:HA3	1.87	0.56
1:E:399:GLU:HG3	2:E:2105:HOH:O	2.04	0.56
1:M:287:LYS:HE3	1:M:362:GLU:OE2	2.05	0.56
1:A:255:ARG:HG3	1:A:255:ARG:HH11	1.69	0.56
2:B:2087:HOH:O	1:D:198:GLN:HG2	2.04	0.56
1:A:176:ASN:H	1:A:182:THR:HG23	1.69	0.56
1:D:345:GLU:OE2	1:D:376:LYS:HD2	2.04	0.56
1:I:184:GLY:HA3	1:I:297:GLY:HA3	1.87	0.56
1:J:375:ARG:NH2	1:J:376:LYS:HE2	2.19	0.56
1:D:463:MET:HB2	1:D:466:GLU:HG3	1.87	0.56
1:K:414:GLY:HA2	1:K:467:ILE:CG2	2.36	0.56
1:G:200:TYR:O	1:G:204:VAL:HG23	2.05	0.56
1:G:85:LYS:HE3	1:G:86:ARG:NH2	2.20	0.56
1:L:499:GLN:HG3	1:L:500:PRO:HD2	1.86	0.56
1:J:413:LEU:HD12	1:J:475:ALA:HB2	1.87	0.56
1:L:329:ILE:O	1:L:333:VAL:HG23	2.05	0.56
1:A:336:VAL:O	1:A:340:ILE:HG23	2.04	0.56
1:L:255:ARG:HH11	1:L:277:LEU:CD1	2.17	0.56
1:I:96:GLY:O	1:I:100:LYS:HG3	2.05	0.56
1:M:141:ARG:HH11	1:M:141:ARG:HG2	1.70	0.56
1:A:326:ARG:HD3	2:A:2101:HOH:O	2.06	0.56
1:F:372:THR:CG2	1:F:373:LYS:HG3	2.25	0.56
1:D:182:THR:HG22	1:D:183:LYS:N	2.21	0.56
1:A:85:LYS:CE	1:A:454:LEU:HG	2.36	0.56
1:B:470:LEU:HD21	1:B:487:LYS:HE3	1.87	0.56
1:B:290:GLU:HG2	1:B:325:LEU:CD2	2.30	0.56
1:B:94:VAL:HG22	1:B:98:LYS:HB3	1.88	0.56
1:H:432:GLU:HG2	1:H:460:ARG:HD3	1.87	0.56
1:D:126:LEU:HD11	1:D:411:VAL:HG23	1.86	0.56
1:K:326:ARG:N	1:K:327:PRO:HD2	2.20	0.56
1:L:221:ARG:O	1:L:225:ARG:HG2	2.06	0.56
1:H:254:LEU:CD1	1:H:281:ARG:HD3	2.36	0.56
1:G:177:PRO:HB3	1:G:294:MET:HG2	1.88	0.56
1:M:124:ARG:NH2	1:M:375:ARG:NH1	2.54	0.56
1:F:94:VAL:HG22	1:F:98:LYS:HD3	1.88	0.56
1:J:97:GLY:O	1:J:101:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLU:OE2	1:E:89:ARG:HD2	2.06	0.55
1:J:413:LEU:HD12	1:J:475:ALA:CB	2.35	0.55
1:E:233:LEU:C	1:E:235:GLY:H	2.08	0.55
1:G:94:VAL:HG12	1:G:98:LYS:HB3	1.88	0.55
1:K:77:GLY:O	1:K:78:GLU:HB2	2.06	0.55
1:G:410:LEU:HD21	1:G:426:MET:HE3	1.89	0.55
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.21	0.55
1:K:318:ARG:HB2	1:K:321:MET:HE2	1.87	0.55
1:J:243:PHE:O	1:J:247:THR:HB	2.07	0.55
1:K:177:PRO:HG2	1:K:178:TYR:CD1	2.42	0.55
1:J:254:LEU:HD12	1:J:281:ARG:HH11	1.72	0.55
1:G:436:GLU:OE2	1:G:456:ARG:NH1	2.39	0.55
1:F:346:GLU:OE1	1:F:346:GLU:HA	2.06	0.55
1:L:82:ALA:O	1:L:437:ARG:NH1	2.39	0.55
1:J:177:PRO:CA	1:J:294:MET:HE2	2.36	0.55
1:F:217:ALA:O	1:F:221:ARG:HG3	2.06	0.55
1:K:304:TRP:CZ2	1:K:313:LEU:HB2	2.41	0.55
1:H:190:GLU:OE1	1:H:302:ARG:HG3	2.07	0.55
1:M:463:MET:HB2	1:M:466:GLU:HG3	1.87	0.55
1:I:177:PRO:HB3	1:I:294:MET:HG2	1.89	0.55
1:A:176:ASN:H	1:A:182:THR:CG2	2.19	0.55
1:H:224:LEU:HD12	1:H:242:LEU:HD21	1.89	0.55
1:H:160:ASN:HD21	1:H:319:GLU:CD	2.09	0.55
1:L:173:ILE:HG23	1:L:183:LYS:CG	2.36	0.55
1:M:177:PRO:HB3	1:M:294:MET:HG2	1.88	0.55
1:K:463:MET:HB2	1:K:466:GLU:HG3	1.89	0.55
1:B:331:ALA:O	1:B:335:VAL:HG23	2.07	0.55
1:I:240:ARG:HG3	1:I:240:ARG:HH11	1.72	0.55
1:L:83:PRO:O	1:L:437:ARG:HD3	2.07	0.55
1:A:236:THR:CG2	1:A:241:GLU:HG3	2.36	0.55
1:F:324:ALA:HB2	2:G:2049:HOH:O	2.06	0.55
1:H:176:ASN:H	1:H:182:THR:HG23	1.72	0.55
1:I:182:THR:HG22	1:I:183:LYS:N	2.22	0.55
1:K:413:LEU:HD12	1:K:475:ALA:CB	2.36	0.55
1:M:124:ARG:NH2	1:M:375:ARG:HG3	2.20	0.55
1:F:83:PRO:O	1:F:437:ARG:HD3	2.07	0.55
1:L:177:PRO:HB3	1:L:294:MET:HG2	1.88	0.55
1:L:198:GLN:HE21	1:L:202:LEU:HD22	1.72	0.55
1:A:217:ALA:O	1:A:221:ARG:HG3	2.07	0.55
1:K:226:GLU:CG	1:K:261:THR:HB	2.33	0.55
1:K:384:GLY:O	1:K:385:LEU:HD12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:MET:CE	1:F:156:ILE:HD11	2.36	0.55
1:H:166:LYS:HE2	1:H:497:ASN:HD21	1.72	0.55
1:K:222:LEU:HA	1:K:225:ARG:NH1	2.22	0.55
1:G:105:GLU:HB2	1:G:109:GLN:NE2	2.22	0.55
1:B:84:PHE:CD2	1:B:435:VAL:HG21	2.42	0.55
1:B:217:ALA:O	1:B:221:ARG:HG3	2.07	0.55
1:H:83:PRO:O	1:H:437:ARG:HD3	2.07	0.55
1:I:157:VAL:HG12	1:I:317:TRP:CH2	2.41	0.55
1:I:291:HIS:HE1	2:I:2041:HOH:O	1.89	0.55
1:J:254:LEU:HD12	1:J:281:ARG:NH1	2.23	0.54
1:B:180:GLN:NE2	1:B:504:GLU:HB2	2.22	0.54
1:B:291:HIS:HE1	2:B:2046:HOH:O	1.90	0.54
1:F:156:ILE:HG22	1:F:158:ASP:HB2	1.90	0.54
1:J:254:LEU:CD1	1:J:281:ARG:HD3	2.37	0.54
1:K:78:GLU:HG3	1:K:95:SER:N	2.22	0.54
1:B:254:LEU:HD12	1:B:281:ARG:NH1	2.22	0.54
1:D:412:VAL:HG22	1:D:426:MET:HE2	1.88	0.54
1:L:154:MET:HE3	1:L:156:ILE:HD11	1.88	0.54
1:L:177:PRO:HG2	1:L:178:TYR:HD1	1.73	0.54
1:J:492:ILE:HD13	1:J:492:ILE:N	2.00	0.54
1:F:233:LEU:C	1:F:235:GLY:H	2.10	0.54
1:B:154:MET:CE	1:B:156:ILE:HD11	2.37	0.54
1:J:454:LEU:HD23	1:J:455:GLU:N	2.23	0.54
1:G:412:VAL:HG22	1:G:426:MET:HE3	1.89	0.54
1:H:84:PHE:CB	1:H:435:VAL:HG11	2.37	0.54
1:J:247:THR:HG22	1:J:248:ILE:HD13	1.88	0.54
1:G:72:ASN:N	2:G:2001:HOH:O	2.41	0.54
1:A:139:LEU:C	1:A:139:LEU:HD23	2.28	0.54
1:H:281:ARG:HH22	1:I:265:SER:HB3	1.72	0.54
1:L:180:GLN:HB2	1:L:504:GLU:CG	2.36	0.54
1:E:350:ARG:HG2	1:E:380:ARG:CZ	2.38	0.54
1:B:73:SER:O	1:B:76:GLN:NE2	2.40	0.54
1:H:411:VAL:HG12	1:H:413:LEU:CD1	2.37	0.54
1:L:470:LEU:HD23	1:L:471:PRO:HD2	1.88	0.54
1:D:355:ILE:O	1:D:356:ASP:C	2.46	0.54
1:H:454:LEU:O	1:M:439:ARG:HD2	2.08	0.54
1:F:252:ASP:HB2	2:F:2106:HOH:O	2.08	0.54
1:D:231:LEU:HD23	1:D:234:ILE:HD11	1.90	0.54
1:D:236:THR:CG2	1:D:241:GLU:HG3	2.38	0.54
1:H:368:ALA:HB3	2:H:2091:HOH:O	2.08	0.54
1:B:200:TYR:O	1:B:204:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:290:GLU:HG2	1:L:325:LEU:CD2	2.37	0.54
1:G:126:LEU:HD11	1:G:411:VAL:CG2	2.37	0.54
1:B:106:LYS:CD	1:B:106:LYS:H	2.20	0.54
1:B:180:GLN:HE21	1:B:504:GLU:CB	2.19	0.54
1:L:338:THR:O	1:L:341:LEU:HB2	2.08	0.54
1:K:184:GLY:HA3	1:K:297:GLY:HA3	1.90	0.54
1:G:96:GLY:O	1:G:100:LYS:HG3	2.08	0.54
1:A:291:HIS:HE1	2:A:2105:HOH:O	1.90	0.54
1:H:94:VAL:CG1	1:H:98:LYS:HB3	2.37	0.54
1:F:327:PRO:HG2	2:F:2136:HOH:O	2.08	0.54
1:J:440:TYR:HE2	1:K:454:LEU:HD12	1.72	0.54
1:E:410:LEU:HD11	1:E:426:MET:HE1	1.90	0.54
1:A:331:ALA:O	1:A:335:VAL:HG23	2.07	0.54
1:G:291:HIS:HE1	2:G:2117:HOH:O	1.91	0.54
1:E:417:ARG:NH1	1:F:479:PHE:O	2.41	0.54
1:E:281:ARG:NH2	1:F:265:SER:HB3	2.23	0.53
1:J:145:TYR:CE2	1:J:149:LEU:HD11	2.44	0.53
1:E:177:PRO:CA	1:E:294:MET:HE2	2.39	0.53
1:G:226:GLU:HG3	1:G:261:THR:CB	2.38	0.53
1:E:86:ARG:O	1:E:435:VAL:HG22	2.08	0.53
1:M:177:PRO:HA	1:M:294:MET:CE	2.39	0.53
1:J:177:PRO:HA	1:J:294:MET:HE2	1.90	0.53
1:G:463:MET:HB2	1:G:466:GLU:HG3	1.89	0.53
1:L:173:ILE:HD12	1:L:183:LYS:HZ2	1.73	0.53
1:J:166:LYS:HD3	1:J:495:PHE:HB2	1.90	0.53
1:I:230:LYS:O	1:I:234:ILE:HG23	2.08	0.53
1:D:177:PRO:HB3	1:D:294:MET:HG2	1.90	0.53
1:E:94:VAL:HG22	1:E:98:LYS:HD3	1.90	0.53
1:B:127:LEU:HD11	1:B:385:LEU:HD22	1.91	0.53
1:G:331:ALA:O	1:G:335:VAL:HG23	2.09	0.53
1:B:328:LEU:HD13	1:B:332:TRP:CH2	2.44	0.53
1:D:503:VAL:O	1:D:504:GLU:HB3	2.09	0.53
1:K:173:ILE:HG12	1:K:304:TRP:HE1	1.74	0.53
1:F:384:GLY:O	1:F:385:LEU:HD13	2.08	0.53
1:F:154:MET:HB3	1:F:352:TRP:HB2	1.91	0.53
1:G:142:GLU:O	1:G:146:THR:HG23	2.08	0.53
1:L:198:GLN:HE21	1:L:202:LEU:CD2	2.21	0.53
1:J:177:PRO:HG2	1:J:178:TYR:HD1	1.71	0.53
1:J:145:TYR:CZ	1:J:149:LEU:HD11	2.43	0.53
1:E:170:ASP:HB3	2:E:2029:HOH:O	2.07	0.53
1:D:291:HIS:HD2	2:D:2037:HOH:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:338:THR:O	1:G:341:LEU:HB2	2.09	0.53
1:M:181:ARG:NH1	1:M:500:PRO:HG2	2.24	0.53
1:A:141:ARG:HG2	1:A:141:ARG:HH11	1.74	0.53
1:K:173:ILE:CG2	1:K:183:LYS:HG3	2.39	0.53
1:H:466:GLU:OE2	1:I:89:ARG:HD2	2.09	0.53
1:F:113:ALA:HA	1:F:490:LEU:HD23	1.91	0.53
1:D:196:ASP:HA	1:D:199:ARG:HB3	1.91	0.53
1:H:96:GLY:O	1:H:100:LYS:HG3	2.08	0.53
1:K:336:VAL:O	1:K:340:ILE:HG23	2.08	0.53
1:I:466:GLU:CD	1:J:89:ARG:HD2	2.30	0.53
1:K:158:ASP:OD2	1:K:161:GLY:HA2	2.09	0.53
1:D:233:LEU:C	1:D:235:GLY:H	2.12	0.53
1:D:154:MET:HE2	1:D:156:ILE:HD11	1.89	0.53
1:I:259:GLU:HA	1:I:264:GLU:CG	2.39	0.53
1:K:358:LEU:HD11	1:K:367:LEU:HD11	1.90	0.53
1:F:224:LEU:HD12	1:F:242:LEU:HD21	1.91	0.53
1:L:129:ASN:HB3	1:L:426:MET:CE	2.40	0.52
1:E:281:ARG:HH21	1:F:265:SER:HB3	1.73	0.52
1:K:379:LEU:HD23	1:K:380:ARG:H	1.74	0.52
1:K:173:ILE:HG13	1:K:304:TRP:NE1	2.24	0.52
1:D:173:ILE:HD12	1:D:183:LYS:HE2	1.90	0.52
1:L:243:PHE:O	1:L:247:THR:HB	2.08	0.52
1:M:236:THR:HG21	1:M:241:GLU:HG3	1.91	0.52
1:I:88:LEU:HD21	1:I:436:GLU:HG3	1.91	0.52
1:K:202:LEU:HD12	1:K:221:ARG:HD3	1.90	0.52
1:K:152:ASP:OD1	1:K:350:ARG:NE	2.40	0.52
1:M:155:VAL:C	1:M:156:ILE:HD12	2.30	0.52
1:M:200:TYR:O	1:M:204:VAL:HG23	2.10	0.52
1:G:367:LEU:CD1	1:G:403:LEU:HD11	2.39	0.52
1:F:291:HIS:HD2	2:F:2061:HOH:O	1.91	0.52
1:I:437:ARG:HD3	1:J:456:ARG:CZ	2.40	0.52
1:B:110:VAL:CG1	1:B:143:LEU:HD23	2.39	0.52
1:K:85:LYS:HG3	1:K:436:GLU:O	2.10	0.52
1:G:159:PRO:HG3	1:G:317:TRP:CZ2	2.45	0.52
1:K:414:GLY:HA2	1:K:467:ILE:HG22	1.91	0.52
1:I:498:ARG:O	1:I:499:GLN:HG3	2.09	0.52
1:L:452:ARG:HG2	1:L:452:ARG:HH11	1.73	0.52
1:J:281:ARG:NH2	1:K:265:SER:HB3	2.24	0.52
1:M:176:ASN:H	1:M:182:THR:HG23	1.74	0.52
1:G:247:THR:HG22	1:G:248:ILE:HD13	1.92	0.52
1:A:345:GLU:OE2	1:A:376:LYS:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:93:ILE:HB	1:M:461:VAL:HG11	1.90	0.52
1:K:145:TYR:CE1	1:K:149:LEU:HD21	2.45	0.52
1:H:410:LEU:HD21	1:H:426:MET:HE3	1.90	0.52
1:J:466:GLU:OE2	1:K:89:ARG:HD2	2.09	0.52
1:G:145:TYR:CZ	1:G:149:LEU:HD11	2.44	0.52
1:G:160:ASN:HD21	1:G:319:GLU:HG3	1.75	0.52
1:D:78:GLU:HA	2:D:2001:HOH:O	2.08	0.52
1:G:94:VAL:HG12	1:G:95:SER:H	1.75	0.52
1:D:358:LEU:HB3	1:D:385:LEU:CD1	2.40	0.52
1:K:190:GLU:OE1	1:K:302:ARG:HG3	2.09	0.52
1:H:318:ARG:HE	1:H:321:MET:HE3	1.74	0.52
1:F:413:LEU:HD12	1:F:413:LEU:N	2.25	0.52
1:G:92:ARG:HB2	1:G:484:PRO:HB3	1.91	0.52
1:K:353:LEU:HD22	1:K:355:ILE:HG13	1.91	0.52
1:K:226:GLU:OE2	1:K:262:LEU:HB2	2.10	0.52
1:K:466:GLU:OE2	1:L:89:ARG:HD2	2.10	0.52
1:A:85:LYS:NZ	1:A:454:LEU:HG	2.24	0.52
1:F:463:MET:HE3	1:G:458:ARG:HD3	1.92	0.52
1:F:94:VAL:CG2	1:F:98:LYS:HD3	2.40	0.52
1:A:236:THR:HG22	1:A:241:GLU:HG3	1.92	0.52
1:A:386:GLN:HB2	1:A:390:GLN:OE1	2.10	0.52
1:I:352:TRP:CE2	1:I:380:ARG:HD3	2.45	0.52
1:L:471:PRO:HG2	1:L:474:THR:OG1	2.10	0.52
1:K:247:THR:HG22	1:K:248:ILE:HD13	1.91	0.52
1:A:281:ARG:NH2	1:B:265:SER:HB3	2.25	0.52
1:G:94:VAL:HG13	1:G:98:LYS:HD3	1.92	0.52
1:B:433:HIS:HD2	1:B:433:HIS:O	1.93	0.52
1:K:196:ASP:O	1:K:200:TYR:HD2	1.93	0.52
1:K:331:ALA:O	1:K:335:VAL:HG23	2.10	0.52
1:K:173:ILE:CG1	1:K:304:TRP:HE1	2.23	0.51
1:M:126:LEU:HD11	1:M:411:VAL:CG2	2.39	0.51
1:D:412:VAL:HG22	1:D:426:MET:HE3	1.90	0.51
1:A:177:PRO:HB3	1:A:294:MET:HG2	1.91	0.51
1:A:175:LEU:HA	1:A:182:THR:HG23	1.91	0.51
1:G:340:ILE:HD13	1:G:379:LEU:CG	2.38	0.51
1:M:177:PRO:CA	1:M:294:MET:HE2	2.40	0.51
1:M:182:THR:HG21	1:M:294:MET:HE1	1.91	0.51
1:H:440:TYR:HA	1:H:452:ARG:CB	2.39	0.51
1:H:283:VAL:O	1:H:287:LYS:HG2	2.10	0.51
1:M:246:THR:HB	1:M:284:LEU:HD23	1.92	0.51
1:F:439:ARG:HB2	1:F:439:ARG:CZ	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:PRO:O	1:F:349:ARG:NH2	2.43	0.51
1:A:243:PHE:O	1:A:247:THR:HB	2.10	0.51
1:M:367:LEU:HD13	1:M:403:LEU:HD11	1.92	0.51
1:K:133:GLY:O	1:K:472:ASP:OD2	2.28	0.51
1:L:212:GLU:O	1:L:215:GLU:HB3	2.10	0.51
1:J:254:LEU:HD12	1:J:281:ARG:HD3	1.93	0.51
1:J:156:ILE:HG22	1:J:158:ASP:HB2	1.92	0.51
1:L:96:GLY:HA3	1:L:488:VAL:HG22	1.92	0.51
1:A:411:VAL:HG12	1:A:413:LEU:CD1	2.41	0.51
1:H:82:ALA:O	1:H:437:ARG:NH1	2.44	0.51
1:K:184:GLY:HA2	1:K:295:PRO:O	2.10	0.51
1:F:411:VAL:HG12	1:F:413:LEU:CD1	2.40	0.51
1:M:385:LEU:HD21	1:M:391:LEU:HD22	1.91	0.51
1:J:126:LEU:HD11	1:J:411:VAL:CG2	2.38	0.51
1:E:87:PHE:HA	1:E:435:VAL:CG2	2.41	0.51
1:M:358:LEU:HD11	1:M:367:LEU:HD11	1.91	0.51
1:L:380:ARG:HG3	1:L:380:ARG:HH11	1.74	0.51
1:J:84:PHE:HB3	1:J:437:ARG:HH12	1.76	0.51
1:I:222:LEU:HA	1:I:225:ARG:NH1	2.26	0.51
1:H:439:ARG:HG2	1:H:453:ALA:HB3	1.93	0.51
1:L:437:ARG:HD2	1:M:456:ARG:NH2	2.26	0.51
1:I:491:GLU:OE2	1:I:493:LYS:HD3	2.11	0.51
1:K:159:PRO:HG3	1:K:317:TRP:CH2	2.46	0.51
1:J:440:TYR:CE2	1:K:454:LEU:HD12	2.45	0.51
1:J:158:ASP:OD2	1:J:161:GLY:HA2	2.10	0.51
1:J:412:VAL:HG22	1:J:426:MET:HE3	1.90	0.51
1:H:126:LEU:HD11	1:H:411:VAL:HG23	1.92	0.51
1:E:503:VAL:O	1:E:504:GLU:CB	2.58	0.51
1:A:412:VAL:HG22	1:A:426:MET:HE2	1.91	0.51
1:K:433:HIS:CD2	1:K:433:HIS:C	2.84	0.51
1:L:129:ASN:HB3	1:L:426:MET:HE1	1.92	0.51
1:K:433:HIS:O	1:K:433:HIS:CD2	2.62	0.51
1:I:294:MET:SD	1:I:295:PRO:HD2	2.51	0.51
1:K:455:GLU:HG3	1:K:455:GLU:O	2.10	0.51
1:D:494:GLN:HA	1:D:494:GLN:OE1	2.11	0.51
1:L:159:PRO:HG3	1:L:317:TRP:CH2	2.45	0.51
1:L:256:GLY:O	1:L:259:GLU:HB2	2.11	0.51
1:K:497:ASN:N	1:K:497:ASN:ND2	2.55	0.51
1:K:84:PHE:HA	1:K:437:ARG:HG3	1.93	0.51
1:D:302:ARG:O	1:D:306:GLU:HG3	2.11	0.51
1:B:433:HIS:C	1:B:433:HIS:CD2	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:HIS:HE1	2:D:2049:HOH:O	1.94	0.51
1:E:186:SER:HB3	2:E:2075:HOH:O	2.10	0.51
1:D:100:LYS:HG2	1:D:115:VAL:HA	1.93	0.51
1:D:277:LEU:HD22	1:D:277:LEU:O	2.10	0.51
1:I:86:ARG:CZ	1:I:86:ARG:HB2	2.40	0.51
1:M:313:LEU:HD23	1:M:314:PHE:N	2.26	0.51
1:H:139:LEU:HD23	1:H:139:LEU:C	2.30	0.51
1:J:241:GLU:HA	1:J:241:GLU:OE1	2.10	0.51
1:M:482:ASN:C	1:M:482:ASN:HD22	2.14	0.51
1:M:158:ASP:OD2	1:M:161:GLY:HA2	2.11	0.50
1:F:466:GLU:OE2	1:G:89:ARG:HD2	2.11	0.50
1:G:432:GLU:OE1	1:G:458:ARG:HD2	2.11	0.50
1:J:87:PHE:HA	1:J:435:VAL:HG22	1.93	0.50
1:D:154:MET:HB3	1:D:352:TRP:HB2	1.93	0.50
1:E:124:ARG:HB3	1:E:408:ARG:CG	2.41	0.50
1:J:345:GLU:OE2	1:J:376:LYS:HD2	2.12	0.50
1:L:177:PRO:HG2	1:L:178:TYR:CD1	2.46	0.50
1:A:84:PHE:HA	1:A:437:ARG:HG3	1.93	0.50
1:F:184:GLY:HA3	1:F:297:GLY:HA3	1.92	0.50
1:B:247:THR:HG21	2:D:2064:HOH:O	2.11	0.50
1:J:175:LEU:HD12	1:J:313:LEU:HD21	1.93	0.50
1:I:134:THR:CG2	1:I:413:LEU:O	2.55	0.50
1:L:226:GLU:HG3	1:L:261:THR:CB	2.35	0.50
1:I:483:ARG:NH1	2:I:2111:HOH:O	2.44	0.50
1:D:328:LEU:HD13	1:D:332:TRP:CH2	2.46	0.50
1:M:110:VAL:HG11	1:M:143:LEU:CD2	2.39	0.50
1:B:413:LEU:CD1	1:B:475:ALA:HB2	2.40	0.50
1:L:439:ARG:NH2	1:M:456:ARG:H	2.09	0.50
1:F:473:LEU:HA	1:F:490:LEU:HD12	1.93	0.50
1:L:318:ARG:HD2	1:L:502:PHE:CE2	2.46	0.50
1:H:118:PRO:HB3	1:H:483:ARG:NH1	2.26	0.50
1:F:182:THR:HG22	1:F:183:LYS:H	1.77	0.50
1:A:504:GLU:HG3	1:A:506:THR:H	1.76	0.50
1:J:291:HIS:HD2	2:J:2027:HOH:O	1.93	0.50
1:M:127:LEU:HD11	1:M:385:LEU:HD22	1.93	0.50
1:K:255:ARG:NH1	1:K:267:PHE:O	2.34	0.50
1:H:221:ARG:HD2	2:H:2057:HOH:O	2.11	0.50
1:I:313:LEU:HD23	1:I:314:PHE:N	2.27	0.50
1:I:414:GLY:HA2	1:I:467:ILE:HG22	1.93	0.50
1:L:173:ILE:HG23	1:L:183:LYS:HG2	1.93	0.50
1:I:145:TYR:CE2	1:I:149:LEU:HD11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:503:VAL:O	1:L:504:GLU:CB	2.60	0.50
1:A:184:GLY:HA3	1:A:297:GLY:HA3	1.92	0.50
1:G:160:ASN:ND2	1:G:319:GLU:HG3	2.27	0.50
1:I:488:VAL:HG13	1:I:489:PRO:HD2	1.94	0.50
1:B:322:GLY:N	1:B:323:PRO:HD2	2.27	0.50
1:M:217:ALA:O	1:M:221:ARG:HG3	2.12	0.50
1:D:352:TRP:CE2	1:D:380:ARG:HD3	2.46	0.50
1:D:164:LEU:HD11	1:D:174:ILE:HD11	1.93	0.50
1:L:84:PHE:CB	1:L:435:VAL:HG11	2.41	0.50
1:K:318:ARG:HD2	1:K:502:PHE:CE2	2.46	0.50
1:F:441:SER:O	1:F:450:THR:HG23	2.12	0.50
1:J:112:VAL:HA	2:J:2009:HOH:O	2.12	0.50
1:M:488:VAL:HG13	1:M:489:PRO:HD2	1.93	0.50
1:K:436:GLU:HG2	1:K:454:LEU:CD2	2.28	0.50
1:G:182:THR:HG22	1:G:183:LYS:N	2.26	0.50
1:L:196:ASP:O	1:L:200:TYR:HD2	1.95	0.50
1:I:291:HIS:HD2	2:I:2031:HOH:O	1.93	0.50
1:L:362:GLU:OE2	2:L:2061:HOH:O	2.19	0.50
1:D:144:ALA:O	1:D:148:LEU:HG	2.12	0.50
1:E:411:VAL:HG12	1:E:413:LEU:HD13	1.92	0.50
1:K:456:ARG:N	1:K:456:ARG:HD2	2.26	0.50
1:H:367:LEU:HD22	1:H:371:LEU:HG	1.94	0.50
1:I:134:THR:O	1:I:134:THR:HG22	2.11	0.50
1:H:254:LEU:O	1:H:258:LEU:HG	2.12	0.50
1:D:182:THR:HG22	1:D:183:LYS:H	1.75	0.50
1:F:224:LEU:CD1	1:F:242:LEU:HD21	2.42	0.50
1:J:399:GLU:HG3	2:J:2085:HOH:O	2.11	0.50
1:J:113:ALA:O	1:J:488:VAL:HG11	2.12	0.50
1:E:498:ARG:O	1:E:499:GLN:HG2	2.11	0.50
1:J:350:ARG:HG2	1:J:380:ARG:CZ	2.41	0.50
1:F:177:PRO:HB3	1:F:294:MET:HG2	1.94	0.49
1:B:326:ARG:HD2	1:B:360:SER:O	2.11	0.49
1:A:247:THR:HG22	1:A:248:ILE:HD13	1.93	0.49
1:L:137:SER:O	1:L:141:ARG:HB2	2.12	0.49
1:F:160:ASN:ND2	1:F:319:GLU:HG3	2.24	0.49
1:L:87:PHE:HA	1:L:435:VAL:HG22	1.93	0.49
1:I:119:ARG:HD3	1:I:122:GLU:OE2	2.13	0.49
1:J:483:ARG:HH11	1:J:483:ARG:HG2	1.76	0.49
1:K:488:VAL:HG13	1:K:489:PRO:HD2	1.94	0.49
1:I:329:ILE:O	1:I:333:VAL:HG23	2.12	0.49
1:I:452:ARG:HG3	1:I:452:ARG:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:230:LYS:HD3	1:K:257:PHE:CZ	2.47	0.49
1:E:357:GLU:HG3	2:E:2093:HOH:O	2.12	0.49
1:D:159:PRO:HG3	1:D:317:TRP:CH2	2.47	0.49
1:H:414:GLY:HA2	1:H:467:ILE:HG23	1.94	0.49
1:B:141:ARG:CG	1:B:141:ARG:HH11	2.15	0.49
1:H:175:LEU:HG	1:H:313:LEU:HD21	1.93	0.49
1:L:198:GLN:NE2	1:L:202:LEU:HD22	2.28	0.49
1:L:279:SER:O	1:L:283:VAL:HG23	2.12	0.49
1:G:94:VAL:CG1	1:G:95:SER:H	2.26	0.49
1:D:436:GLU:HG2	1:D:454:LEU:CD2	2.42	0.49
1:M:504:GLU:CG	1:M:505:GLY:N	2.73	0.49
1:J:98:LYS:O	1:J:102:MET:HG3	2.12	0.49
1:L:306:GLU:O	1:L:308:PRO:HD3	2.12	0.49
1:K:294:MET:HG3	1:K:328:LEU:HD11	1.95	0.49
1:D:85:LYS:HE2	1:D:454:LEU:HD21	1.95	0.49
1:D:379:LEU:HD22	1:D:380:ARG:N	2.28	0.49
1:M:93:ILE:HB	1:M:461:VAL:CG1	2.42	0.49
1:A:290:GLU:HG2	1:A:325:LEU:CD2	2.34	0.49
1:H:182:THR:HG22	1:H:183:LYS:N	2.26	0.49
1:M:184:GLY:HA2	1:M:295:PRO:O	2.13	0.49
1:G:85:LYS:HD3	1:G:454:LEU:HD21	1.95	0.49
1:J:322:GLY:N	1:J:323:PRO:HD2	2.27	0.49
1:E:325:LEU:HA	2:E:2086:HOH:O	2.13	0.49
1:I:433:HIS:O	1:I:433:HIS:HD2	1.95	0.49
1:H:493:LYS:HD3	1:H:495:PHE:CZ	2.47	0.49
1:K:304:TRP:CH2	1:K:313:LEU:HB2	2.46	0.49
1:D:246:THR:HB	1:D:284:LEU:HD23	1.95	0.49
1:M:176:ASN:O	1:M:182:THR:OG1	2.23	0.49
1:K:379:LEU:HD23	1:K:380:ARG:N	2.26	0.49
1:E:413:LEU:HD12	1:E:475:ALA:HB2	1.94	0.49
1:G:224:LEU:CD1	1:G:242:LEU:HD21	2.43	0.49
1:E:287:LYS:HE3	1:E:362:GLU:OE2	2.13	0.49
1:B:226:GLU:CG	1:B:261:THR:HB	2.34	0.49
1:K:129:ASN:HB3	1:K:426:MET:CE	2.42	0.49
1:K:129:ASN:CB	1:K:426:MET:HE1	2.40	0.49
1:I:249:ALA:O	1:I:281:ARG:NH2	2.35	0.49
1:A:436:GLU:CB	1:A:454:LEU:HD21	2.43	0.49
1:E:470:LEU:HD23	1:E:471:PRO:HD2	1.95	0.49
1:I:233:LEU:C	1:I:235:GLY:H	2.16	0.49
1:D:324:ALA:HB2	2:E:2039:HOH:O	2.13	0.49
1:G:357:GLU:HG2	1:G:386:GLN:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:294:MET:HE1	1:M:295:PRO:HD2	1.93	0.49
1:H:453:ALA:HA	1:M:441:SER:HA	1.95	0.49
1:J:177:PRO:N	1:J:294:MET:HE2	2.28	0.49
1:B:438:ASP:HB3	1:B:440:TYR:CE1	2.48	0.49
1:H:224:LEU:CD1	1:H:242:LEU:HD21	2.43	0.49
1:M:236:THR:HG22	1:M:236:THR:O	2.13	0.49
1:K:417:ARG:NH2	1:K:469:ASN:HD21	2.10	0.49
1:K:169:ARG:NH1	1:K:169:ARG:CG	2.76	0.48
1:E:353:LEU:HB2	1:E:379:LEU:HD21	1.95	0.48
1:L:200:TYR:O	1:L:204:VAL:HG23	2.13	0.48
1:K:246:THR:HB	1:K:284:LEU:HD23	1.94	0.48
1:L:227:THR:CG2	1:L:242:LEU:HD12	2.43	0.48
1:J:94:VAL:HG13	1:J:95:SER:N	2.28	0.48
1:L:180:GLN:HB2	1:L:504:GLU:CB	2.41	0.48
1:K:364:LEU:HB2	1:K:367:LEU:HB2	1.95	0.48
1:E:433:HIS:O	1:E:433:HIS:HD2	1.96	0.48
1:L:113:ALA:HA	1:L:490:LEU:HD23	1.93	0.48
1:K:173:ILE:HD12	1:K:183:LYS:CE	2.35	0.48
1:I:104:ARG:HB2	1:I:104:ARG:CZ	2.43	0.48
1:K:84:PHE:CG	1:K:435:VAL:CG2	2.94	0.48
1:F:124:ARG:HB3	1:F:408:ARG:CG	2.43	0.48
1:L:452:ARG:HG2	1:L:452:ARG:NH1	2.28	0.48
1:A:420:PRO:HB2	1:B:428:LEU:HD13	1.95	0.48
1:D:331:ALA:O	1:D:335:VAL:HG23	2.12	0.48
1:J:492:ILE:CD1	1:J:492:ILE:N	2.70	0.48
1:K:177:PRO:HB3	1:K:294:MET:HG2	1.96	0.48
1:H:246:THR:HB	1:H:284:LEU:HD23	1.95	0.48
1:H:439:ARG:NE	1:H:455:GLU:HB3	2.29	0.48
1:M:328:LEU:O	1:M:331:ALA:HB3	2.14	0.48
1:L:470:LEU:HD22	1:L:474:THR:HB	1.96	0.48
1:A:322:GLY:N	1:A:323:PRO:HD2	2.28	0.48
1:D:338:THR:O	1:D:341:LEU:HB2	2.13	0.48
1:L:222:LEU:HD11	1:L:263:ALA:HB2	1.95	0.48
1:D:306:GLU:O	1:D:308:PRO:HD3	2.13	0.48
1:E:443:ASN:HA	1:F:451:GLY:HA2	1.95	0.48
1:E:110:VAL:CG1	1:E:143:LEU:HD23	2.41	0.48
1:G:192:ARG:NH2	1:G:306:GLU:OE1	2.47	0.48
1:F:166:LYS:HD2	1:F:495:PHE:HB2	1.96	0.48
1:L:433:HIS:HD2	1:L:433:HIS:O	1.97	0.48
1:K:85:LYS:CE	1:K:454:LEU:HD21	2.44	0.48
1:E:110:VAL:HG11	1:E:143:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:439:ARG:NH2	1:M:455:GLU:HA	2.29	0.48
1:E:76:GLN:HG3	1:E:77:GLY:H	1.78	0.48
1:A:479:PHE:O	1:G:417:ARG:NH1	2.46	0.48
1:K:358:LEU:HD11	1:K:367:LEU:CD1	2.43	0.48
1:A:73:SER:C	1:A:76:GLN:HE22	2.16	0.48
1:E:212:GLU:O	1:E:215:GLU:HB3	2.14	0.48
1:G:397:VAL:HG23	2:G:2138:HOH:O	2.12	0.48
1:H:175:LEU:HA	1:H:182:THR:HG23	1.96	0.48
1:E:367:LEU:HD13	1:E:403:LEU:HD11	1.96	0.48
1:K:202:LEU:HD12	1:K:221:ARG:CD	2.44	0.48
1:L:344:PRO:O	1:L:349:ARG:NH2	2.46	0.48
1:H:225:ARG:HD2	2:H:2059:HOH:O	2.12	0.48
1:A:471:PRO:HG2	1:A:474:THR:OG1	2.13	0.48
1:G:461:VAL:HG11	1:G:485:ILE:HD11	1.96	0.48
1:L:158:ASP:OD2	1:L:161:GLY:HA2	2.14	0.48
1:I:182:THR:CG2	1:I:183:LYS:N	2.77	0.48
1:D:326:ARG:HB3	1:D:327:PRO:HD3	1.96	0.48
1:E:437:ARG:HD2	1:F:456:ARG:NH2	2.29	0.48
1:J:169:ARG:HH21	1:J:171:LYS:NZ	2.10	0.48
1:A:137:SER:O	1:A:141:ARG:HB2	2.14	0.48
1:B:247:THR:CG2	2:D:2064:HOH:O	2.61	0.48
1:E:177:PRO:N	1:E:294:MET:HE2	2.29	0.48
1:K:246:THR:CB	1:K:284:LEU:HD23	2.44	0.48
1:E:76:GLN:HG3	1:E:78:GLU:HG2	1.95	0.48
1:A:182:THR:HG22	1:A:183:LYS:N	2.29	0.48
1:K:318:ARG:HD3	1:K:321:MET:HE2	1.96	0.48
1:K:301:ILE:O	1:K:305:LEU:HG	2.14	0.48
1:G:488:VAL:HG13	1:G:489:PRO:HD2	1.96	0.48
1:D:236:THR:HG21	1:D:241:GLU:HG3	1.95	0.47
1:I:73:SER:O	1:I:76:GLN:HG2	2.14	0.47
1:K:420:PRO:HB2	1:L:428:LEU:HD13	1.96	0.47
1:E:105:GLU:HG2	1:E:106:LYS:HD3	1.96	0.47
1:F:182:THR:HG21	1:F:294:MET:HE1	1.95	0.47
1:L:175:LEU:HD12	1:L:313:LEU:HD21	1.95	0.47
1:G:175:LEU:HD12	1:G:313:LEU:HD21	1.94	0.47
1:K:212:GLU:HG2	1:K:216:TRP:CZ2	2.48	0.47
1:J:233:LEU:HA	1:J:233:LEU:HD23	1.70	0.47
1:M:438:ASP:OD2	1:M:452:ARG:HD2	2.14	0.47
1:B:503:VAL:O	1:B:504:GLU:HB3	2.14	0.47
1:G:236:THR:CG2	1:G:241:GLU:HG3	2.44	0.47
1:F:173:ILE:HG23	1:F:183:LYS:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:352:TRP:HB3	1:J:354:PHE:CE1	2.49	0.47
1:B:169:ARG:NH1	1:B:169:ARG:HG3	2.27	0.47
1:H:251:PHE:CD2	1:H:255:ARG:NH1	2.82	0.47
1:E:327:PRO:HG2	2:E:2086:HOH:O	2.15	0.47
1:H:301:ILE:O	1:H:305:LEU:HG	2.14	0.47
1:F:375:ARG:O	1:F:375:ARG:HD2	2.13	0.47
1:I:243:PHE:O	1:I:247:THR:HB	2.14	0.47
1:B:355:ILE:O	1:B:356:ASP:C	2.53	0.47
1:H:502:PHE:HE2	1:H:504:GLU:HB2	1.79	0.47
1:B:141:ARG:CG	1:B:141:ARG:NH1	2.77	0.47
1:B:119:ARG:HH12	1:B:350:ARG:HH11	1.61	0.47
1:H:439:ARG:CZ	1:H:455:GLU:HB3	2.44	0.47
1:J:199:ARG:HE	1:J:338:THR:HG22	1.78	0.47
1:L:411:VAL:HG12	1:L:413:LEU:CD1	2.45	0.47
1:L:94:VAL:CG2	1:L:98:LYS:HD3	2.45	0.47
1:B:470:LEU:CD2	1:B:487:LYS:HE3	2.45	0.47
1:E:355:ILE:O	1:E:356:ASP:C	2.52	0.47
1:F:251:PHE:CZ	1:F:277:LEU:HD13	2.49	0.47
1:A:231:LEU:HD23	1:A:234:ILE:HD11	1.96	0.47
1:L:285:SER:HB2	1:M:266:LEU:HD11	1.96	0.47
1:B:251:PHE:CZ	1:B:277:LEU:HD12	2.50	0.47
1:B:141:ARG:NH1	1:B:141:ARG:HG2	2.13	0.47
1:L:182:THR:CG2	1:L:183:LYS:N	2.78	0.47
1:M:92:ARG:HH11	1:M:92:ARG:HG3	1.80	0.47
1:B:139:LEU:HD11	1:B:411:VAL:HG11	1.95	0.47
1:E:124:ARG:HG3	1:E:124:ARG:NH1	2.29	0.47
1:B:291:HIS:CE1	2:B:2046:HOH:O	2.68	0.47
1:E:166:LYS:HD2	1:E:495:PHE:HB2	1.97	0.47
1:H:326:ARG:HD2	1:H:360:SER:O	2.14	0.47
1:M:117:MET:HG3	1:M:479:PHE:CE1	2.49	0.47
1:G:346:GLU:HA	1:G:346:GLU:OE1	2.14	0.47
1:A:72:ASN:N	2:A:2001:HOH:O	2.47	0.47
1:G:165:SER:OG	1:G:501:ALA:HB2	2.15	0.47
1:E:101:ARG:HD2	2:E:2006:HOH:O	2.14	0.47
1:I:327:PRO:HG2	2:I:2078:HOH:O	2.14	0.47
1:F:110:VAL:HG13	1:F:143:LEU:HD23	1.97	0.47
1:H:351:LEU:HD13	1:H:352:TRP:N	2.28	0.47
1:B:144:ALA:O	1:B:148:LEU:HG	2.15	0.47
1:F:283:VAL:O	1:F:287:LYS:HG2	2.15	0.47
1:B:166:LYS:HE2	1:B:497:ASN:HD21	1.80	0.47
1:M:103:THR:OG1	1:M:116:PRO:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:ARG:HG2	1:G:498:ARG:NH2	2.30	0.47
1:G:490:LEU:N	1:G:490:LEU:HD12	2.29	0.47
1:D:499:GLN:HE21	1:D:499:GLN:HB3	1.52	0.47
1:L:173:ILE:HG23	1:L:183:LYS:HG3	1.97	0.47
1:H:127:LEU:O	1:H:410:LEU:HD12	2.15	0.47
1:J:410:LEU:HD21	1:J:426:MET:HE3	1.96	0.47
1:M:358:LEU:HD11	1:M:367:LEU:CD1	2.44	0.47
1:H:217:ALA:O	1:H:221:ARG:HG3	2.15	0.47
1:H:110:VAL:HG12	2:H:2008:HOH:O	2.13	0.47
1:G:98:LYS:O	1:G:102:MET:HG3	2.15	0.47
1:D:176:ASN:H	1:D:182:THR:CG2	2.26	0.47
1:H:478:GLY:C	1:M:417:ARG:HH11	2.19	0.47
1:I:439:ARG:NH1	1:J:439:ARG:HH22	2.13	0.47
1:I:94:VAL:CG1	1:I:95:SER:N	2.77	0.46
1:L:196:ASP:HA	1:L:199:ARG:HB3	1.97	0.46
1:F:313:LEU:HD23	1:F:314:PHE:N	2.30	0.46
1:G:236:THR:HG22	1:G:236:THR:O	2.14	0.46
1:L:72:ASN:ND2	1:L:440:TYR:HE1	2.13	0.46
1:F:355:ILE:O	1:F:356:ASP:C	2.52	0.46
1:I:227:THR:O	1:I:231:LEU:HG	2.15	0.46
1:B:289:PRO:O	1:B:293:THR:HG23	2.15	0.46
1:G:430:LEU:HD12	1:G:430:LEU:HA	1.84	0.46
1:K:304:TRP:HZ2	1:K:312:ASN:C	2.19	0.46
1:B:129:ASN:HB3	1:B:426:MET:CE	2.45	0.46
1:L:175:LEU:HA	1:L:182:THR:HG23	1.97	0.46
1:E:94:VAL:HG13	1:E:95:SER:N	2.29	0.46
1:M:137:SER:O	1:M:141:ARG:HB2	2.15	0.46
1:G:315:ILE:HG23	1:G:332:TRP:CE3	2.50	0.46
1:A:338:THR:O	1:A:341:LEU:HB2	2.14	0.46
1:D:82:ALA:N	1:E:88:LEU:HD13	2.29	0.46
1:J:437:ARG:HG3	1:J:437:ARG:NH1	2.30	0.46
1:G:182:THR:HG21	1:G:294:MET:HE1	1.96	0.46
1:I:358:LEU:HD11	1:I:367:LEU:HD11	1.97	0.46
1:A:85:LYS:HZ3	1:A:454:LEU:HG	1.80	0.46
1:G:199:ARG:HE	1:G:338:THR:HB	1.81	0.46
1:I:414:GLY:HA2	1:I:467:ILE:CG2	2.45	0.46
1:E:179:ASP:O	1:E:182:THR:HG22	2.16	0.46
1:D:386:GLN:HB2	1:D:390:GLN:OE1	2.16	0.46
1:G:344:PRO:O	1:G:349:ARG:NH2	2.42	0.46
1:I:331:ALA:O	1:I:335:VAL:HG23	2.15	0.46
1:B:177:PRO:HG2	1:B:178:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:ARG:HG2	1:L:498:ARG:HH22	1.80	0.46
1:I:94:VAL:HG22	1:I:98:LYS:HD3	1.96	0.46
1:K:78:GLU:CA	1:K:78:GLU:OE1	2.57	0.46
1:H:192:ARG:HG2	1:H:302:ARG:NH1	2.30	0.46
1:M:385:LEU:HD12	2:M:2080:HOH:O	2.15	0.46
1:H:118:PRO:HB3	1:H:483:ARG:HH12	1.79	0.46
1:G:414:GLY:HA2	1:G:467:ILE:HG23	1.98	0.46
1:H:226:GLU:OE1	1:H:261:THR:HB	2.14	0.46
1:K:182:THR:CG2	1:K:183:LYS:N	2.78	0.46
1:G:94:VAL:HG11	1:G:98:LYS:HB3	1.91	0.46
1:D:85:LYS:HD3	1:D:438:ASP:OD1	2.16	0.46
1:M:182:THR:HG21	1:M:294:MET:HE3	1.98	0.46
1:L:439:ARG:HH22	1:M:456:ARG:H	1.62	0.46
1:L:372:THR:HG22	1:L:373:LYS:HG2	1.97	0.46
1:G:159:PRO:HG2	1:G:356:ASP:OD2	2.16	0.46
1:K:104:ARG:HG2	1:K:104:ARG:NH1	2.31	0.46
1:F:94:VAL:HG13	1:F:95:SER:N	2.30	0.46
1:E:355:ILE:O	1:E:356:ASP:O	2.34	0.46
1:I:289:PRO:O	1:I:293:THR:HG23	2.16	0.46
1:G:124:ARG:HB3	1:G:408:ARG:HG3	1.98	0.46
1:D:166:LYS:HD2	1:D:495:PHE:HB2	1.97	0.46
1:J:503:VAL:O	1:J:504:GLU:CB	2.62	0.46
1:K:413:LEU:CD1	1:K:475:ALA:HB2	2.44	0.46
1:B:379:LEU:HD13	1:B:381:VAL:HG23	1.97	0.46
1:K:380:ARG:HG3	1:K:380:ARG:HH11	1.81	0.46
1:L:291:HIS:HD2	2:L:2024:HOH:O	1.97	0.46
1:M:345:GLU:CD	1:M:376:LYS:HD2	2.35	0.46
1:D:92:ARG:HB2	1:D:484:PRO:HB3	1.97	0.46
1:K:136:LYS:O	1:K:140:LEU:HD13	2.15	0.46
1:J:75:GLY:O	1:J:76:GLN:C	2.54	0.46
1:E:503:VAL:O	1:E:504:GLU:HB2	2.15	0.46
1:L:304:TRP:CZ2	1:L:313:LEU:HB2	2.51	0.46
1:I:127:LEU:HD11	1:I:385:LEU:HD23	1.93	0.46
1:L:338:THR:HG23	1:L:366:SER:CB	2.45	0.46
1:B:110:VAL:HG12	1:B:143:LEU:HD23	1.96	0.46
1:F:279:SER:O	1:F:283:VAL:HG23	2.15	0.46
1:G:322:GLY:N	1:G:323:PRO:HD2	2.30	0.46
1:H:322:GLY:N	1:H:323:PRO:HD2	2.30	0.46
1:E:117:MET:HG3	1:E:479:PHE:CE1	2.50	0.46
1:B:420:PRO:HB2	1:D:428:LEU:HD13	1.97	0.46
1:H:439:ARG:O	1:H:452:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:126:LEU:HD11	1:K:411:VAL:HG23	1.98	0.46
1:D:139:LEU:HD22	1:D:140:LEU:HD12	1.97	0.46
1:D:236:THR:HG22	1:D:236:THR:O	2.16	0.46
1:L:227:THR:HG22	1:L:242:LEU:HD12	1.98	0.46
1:E:157:VAL:HG12	1:E:317:TRP:HH2	1.80	0.46
1:H:113:ALA:O	1:H:488:VAL:HG11	2.16	0.46
1:G:86:ARG:NE	1:G:436:GLU:OE1	2.46	0.46
1:K:86:ARG:CG	1:K:86:ARG:HH11	2.27	0.46
1:G:157:VAL:HG12	1:G:317:TRP:CH2	2.51	0.46
1:B:318:ARG:HG2	1:B:318:ARG:NH1	2.31	0.46
1:K:221:ARG:HD2	2:K:2037:HOH:O	2.16	0.46
1:E:493:LYS:HD3	1:E:495:PHE:CZ	2.51	0.46
1:E:326:ARG:HD2	1:E:360:SER:O	2.16	0.46
1:K:182:THR:HG22	1:K:183:LYS:N	2.31	0.46
1:G:357:GLU:CG	1:G:386:GLN:HE21	2.29	0.46
1:G:110:VAL:HG11	1:G:143:LEU:CD2	2.46	0.46
1:M:437:ARG:O	1:M:455:GLU:HG2	2.16	0.46
1:J:177:PRO:HB3	1:J:294:MET:HG2	1.98	0.46
1:M:233:LEU:C	1:M:235:GLY:H	2.20	0.46
1:E:301:ILE:HD12	1:E:335:VAL:HG11	1.98	0.46
1:A:416:SER:HB2	1:B:408:ARG:HD2	1.98	0.45
1:L:497:ASN:ND2	1:L:497:ASN:H	2.10	0.45
1:L:154:MET:HE2	1:L:156:ILE:HD11	1.98	0.45
1:K:98:LYS:O	1:K:102:MET:HG3	2.17	0.45
1:D:160:ASN:HD21	1:D:319:GLU:CD	2.18	0.45
1:F:99:LEU:HD22	1:F:486:ALA:HB3	1.97	0.45
1:I:181:ARG:CZ	1:I:503:VAL:HG23	2.45	0.45
1:E:452:ARG:HH11	1:E:452:ARG:HB3	1.81	0.45
1:H:433:HIS:HD2	1:H:433:HIS:O	1.99	0.45
1:H:473:LEU:C	1:H:490:LEU:HD13	2.36	0.45
1:H:184:GLY:HA3	1:H:297:GLY:HA3	1.98	0.45
1:E:177:PRO:HA	1:E:294:MET:HE2	1.99	0.45
1:G:94:VAL:CG1	1:G:98:LYS:HD3	2.46	0.45
1:L:259:GLU:HA	1:L:264:GLU:CG	2.41	0.45
1:F:234:ILE:HG13	2:I:2011:HOH:O	2.16	0.45
1:I:372:THR:CG2	1:I:373:LYS:HG3	2.41	0.45
1:H:439:ARG:NH2	1:M:439:ARG:CZ	2.79	0.45
1:J:94:VAL:HG22	1:J:98:LYS:HD3	1.97	0.45
1:M:455:GLU:O	1:M:455:GLU:HG3	2.15	0.45
1:K:243:PHE:O	1:K:247:THR:HB	2.17	0.45
1:K:247:THR:HG22	1:K:248:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:THR:HB	1:D:461:VAL:HG21	1.98	0.45
1:F:457:VAL:HG12	1:F:459:GLU:CG	2.45	0.45
1:D:158:ASP:OD2	1:D:161:GLY:HA2	2.17	0.45
1:D:455:GLU:HG2	1:D:457:VAL:HG23	1.99	0.45
1:E:199:ARG:HE	1:E:338:THR:HB	1.81	0.45
1:F:179:ASP:O	1:F:182:THR:OG1	2.35	0.45
1:I:466:GLU:OE2	1:J:89:ARG:HD2	2.17	0.45
1:G:240:ARG:HG2	1:G:292:VAL:HG13	1.97	0.45
1:F:180:GLN:NE2	1:F:505:GLY:HA3	2.31	0.45
1:K:124:ARG:HB3	1:K:408:ARG:HG3	1.98	0.45
1:G:289:PRO:O	1:G:293:THR:HG23	2.16	0.45
1:E:148:LEU:HD11	1:E:154:MET:HE1	1.97	0.45
1:K:74:VAL:CG1	1:K:75:GLY:H	2.21	0.45
1:G:412:VAL:HG22	1:G:426:MET:HE2	1.98	0.45
1:H:354:PHE:CE1	1:H:382:VAL:HG21	2.52	0.45
1:I:159:PRO:HG3	1:I:317:TRP:CZ2	2.51	0.45
1:E:498:ARG:C	1:E:499:GLN:HG2	2.37	0.45
1:I:379:LEU:HD22	1:I:380:ARG:N	2.32	0.45
1:A:246:THR:HB	1:A:284:LEU:HD23	1.98	0.45
1:L:152:ASP:OD1	1:L:350:ARG:CZ	2.64	0.45
1:M:200:TYR:OH	1:M:302:ARG:HD2	2.16	0.45
1:L:195:TYR:C	1:L:195:TYR:CD1	2.89	0.45
1:B:433:HIS:CD2	1:B:459:GLU:HG3	2.52	0.45
1:D:471:PRO:HG2	1:D:474:THR:OG1	2.17	0.45
1:J:440:TYR:C	1:J:440:TYR:CD1	2.89	0.45
1:B:352:TRP:CE2	1:B:380:ARG:HD3	2.52	0.45
1:L:182:THR:HG22	1:L:183:LYS:N	2.31	0.45
1:I:176:ASN:O	1:I:182:THR:OG1	2.19	0.45
1:M:198:GLN:CD	1:M:225:ARG:HH21	2.20	0.45
1:F:411:VAL:HG12	1:F:413:LEU:HD12	1.97	0.45
1:L:155:VAL:HG23	1:L:351:LEU:HD11	1.99	0.45
1:M:240:ARG:HG2	1:M:292:VAL:HG13	1.98	0.45
1:A:358:LEU:HB3	1:A:385:LEU:CD1	2.47	0.45
1:M:180:GLN:NE2	1:M:504:GLU:O	2.50	0.45
1:D:176:ASN:O	1:D:182:THR:OG1	2.28	0.45
1:M:236:THR:CG2	1:M:241:GLU:HG3	2.46	0.45
1:H:318:ARG:HE	1:H:321:MET:CE	2.28	0.45
1:J:358:LEU:HD21	1:J:403:LEU:HD21	1.98	0.45
1:E:329:ILE:O	1:E:333:VAL:HG23	2.17	0.45
1:H:176:ASN:H	1:H:182:THR:HG21	1.79	0.45
1:I:316:THR:O	1:I:317:TRP:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:247:THR:HG22	1:I:248:ILE:HD13	1.97	0.45
1:F:379:LEU:HD22	1:F:380:ARG:N	2.32	0.45
1:D:217:ALA:O	1:D:221:ARG:HG3	2.16	0.45
1:J:240:ARG:HH11	1:J:240:ARG:HG3	1.82	0.45
1:B:84:PHE:HA	1:B:437:ARG:HG3	1.98	0.45
1:E:438:ASP:OD1	1:E:454:LEU:CD1	2.65	0.45
1:E:433:HIS:NE2	1:E:459:GLU:HG3	2.32	0.45
1:E:99:LEU:HD22	1:E:486:ALA:HB3	1.98	0.45
1:H:338:THR:HG23	1:H:366:SER:OG	2.17	0.45
1:K:322:GLY:N	1:K:323:PRO:HD2	2.32	0.45
1:M:124:ARG:HA	1:M:124:ARG:HD3	1.74	0.45
1:D:182:THR:HG21	1:D:294:MET:CE	2.47	0.45
1:D:137:SER:O	1:D:141:ARG:HB2	2.16	0.45
1:A:236:THR:O	1:A:236:THR:HG22	2.17	0.45
1:B:76:GLN:HB2	1:B:76:GLN:HE21	1.58	0.45
1:K:352:TRP:HB3	1:K:354:PHE:CE1	2.52	0.45
1:G:93:ILE:HG13	1:G:485:ILE:HG13	1.98	0.45
1:M:316:THR:O	1:M:317:TRP:HB3	2.16	0.45
1:K:290:GLU:HG3	1:K:325:LEU:HD23	1.99	0.44
1:G:379:LEU:HD13	1:G:381:VAL:HG23	1.98	0.44
1:G:104:ARG:NH1	1:G:104:ARG:HG2	2.32	0.44
1:F:180:GLN:NE2	1:F:505:GLY:O	2.49	0.44
1:K:112:VAL:HA	2:K:2012:HOH:O	2.16	0.44
1:G:474:THR:HG21	1:G:487:LYS:NZ	2.32	0.44
1:A:433:HIS:HD2	1:A:433:HIS:O	2.00	0.44
1:L:240:ARG:CB	1:L:240:ARG:HH11	2.27	0.44
1:A:141:ARG:NH1	2:A:2025:HOH:O	2.49	0.44
1:A:379:LEU:HD22	1:A:380:ARG:N	2.33	0.44
1:L:460:ARG:HG3	1:L:460:ARG:HH11	1.82	0.44
1:F:82:ALA:HB3	1:F:437:ARG:NH1	2.32	0.44
1:E:379:LEU:CD2	1:E:380:ARG:N	2.78	0.44
1:H:458:ARG:HD3	1:M:463:MET:HE3	2.00	0.44
1:H:436:GLU:CD	1:H:456:ARG:HH11	2.20	0.44
1:H:502:PHE:CE2	1:H:504:GLU:HB2	2.53	0.44
1:H:229:LYS:O	1:H:233:LEU:HG	2.17	0.44
1:D:215:GLU:O	1:D:218:SER:HB2	2.16	0.44
1:E:73:SER:O	1:E:74:VAL:HG23	2.17	0.44
1:B:93:ILE:HB	1:B:461:VAL:HG11	1.98	0.44
1:E:243:PHE:O	1:E:247:THR:HB	2.18	0.44
1:I:226:GLU:OE1	1:I:226:GLU:HA	2.17	0.44
1:L:150:ARG:NE	1:L:350:ARG:NH1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:92:ARG:NH1	1:M:92:ARG:HG3	2.32	0.44
1:J:302:ARG:O	1:J:306:GLU:HG3	2.16	0.44
1:I:234:ILE:O	1:I:234:ILE:HG13	2.17	0.44
1:K:186:SER:HB3	2:K:2053:HOH:O	2.16	0.44
1:A:430:LEU:HA	1:A:430:LEU:HD12	1.80	0.44
1:E:154:MET:HE2	1:E:156:ILE:HD11	1.95	0.44
1:F:499:GLN:HG3	1:F:500:PRO:CD	2.41	0.44
1:A:302:ARG:O	1:A:306:GLU:HG3	2.17	0.44
1:M:302:ARG:O	1:M:306:GLU:HG3	2.18	0.44
1:B:130:GLY:HA3	1:B:413:LEU:HB2	1.98	0.44
1:M:82:ALA:O	1:M:437:ARG:NH1	2.50	0.44
1:K:181:ARG:NH2	1:K:500:PRO:O	2.42	0.44
1:A:182:THR:HG21	1:A:294:MET:HE1	1.98	0.44
1:B:473:LEU:HD11	1:B:492:ILE:HD11	1.98	0.44
1:G:184:GLY:HA3	1:G:297:GLY:HA3	1.99	0.44
1:K:137:SER:O	1:K:141:ARG:HB2	2.17	0.44
1:J:368:ALA:HB3	2:J:2077:HOH:O	2.16	0.44
1:G:139:LEU:C	1:G:139:LEU:HD23	2.38	0.44
1:G:433:HIS:HD2	1:G:433:HIS:O	2.01	0.44
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.87	0.44
1:M:169:ARG:NH1	1:M:312:ASN:HD21	2.16	0.44
1:E:226:GLU:HG3	1:E:261:THR:CB	2.38	0.44
1:E:76:GLN:CG	1:E:77:GLY:H	2.31	0.44
1:K:139:LEU:CD1	1:K:411:VAL:HG11	2.46	0.44
1:I:113:ALA:O	1:I:488:VAL:HG11	2.18	0.44
1:I:137:SER:O	1:I:141:ARG:HB2	2.18	0.44
1:F:106:LYS:HE3	2:F:2013:HOH:O	2.17	0.44
1:L:210:THR:HG21	1:M:211:ASP:OD2	2.17	0.44
1:H:155:VAL:HG13	1:H:313:LEU:CD1	2.44	0.44
1:F:141:ARG:NH1	1:F:141:ARG:HG2	2.31	0.44
1:J:338:THR:O	1:J:341:LEU:HB2	2.18	0.44
1:F:159:PRO:HG2	1:F:356:ASP:OD2	2.18	0.44
1:L:371:LEU:HD23	1:L:381:VAL:HG21	2.00	0.44
1:M:74:VAL:HB	1:M:84:PHE:O	2.18	0.44
1:E:106:LYS:HG2	1:E:107:ALA:N	2.30	0.44
1:G:158:ASP:OD2	1:G:161:GLY:HA2	2.17	0.44
1:B:503:VAL:O	1:B:504:GLU:CB	2.65	0.44
1:M:499:GLN:HG3	1:M:500:PRO:HD2	2.00	0.44
1:M:159:PRO:HG3	1:M:317:TRP:CH2	2.53	0.44
1:F:87:PHE:CE2	1:F:92:ARG:HG2	2.53	0.44
1:E:441:SER:OG	1:E:442:LYS:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:GLU:HB3	1:H:380:ARG:HE	1.82	0.44
1:E:190:GLU:OE1	1:E:302:ARG:HG3	2.18	0.44
1:H:227:THR:HG23	1:H:257:PHE:CE2	2.53	0.44
1:H:439:ARG:NH2	1:M:439:ARG:NH2	2.66	0.44
1:E:78:GLU:OE1	1:E:95:SER:HB3	2.18	0.44
1:I:159:PRO:HG3	1:I:317:TRP:CH2	2.53	0.44
1:I:313:LEU:HD22	1:I:315:ILE:HG13	2.00	0.44
1:G:236:THR:HG22	1:G:241:GLU:HG3	2.00	0.44
1:F:255:ARG:NH2	1:F:268:ALA:HB1	2.33	0.44
1:E:198:GLN:NE2	1:E:202:LEU:HD22	2.32	0.44
1:F:368:ALA:HB3	2:F:2149:HOH:O	2.16	0.44
1:B:471:PRO:HG2	1:B:474:THR:OG1	2.18	0.44
1:K:173:ILE:CG1	1:K:304:TRP:NE1	2.79	0.43
1:A:380:ARG:HG3	1:A:380:ARG:HH11	1.82	0.43
1:M:156:ILE:CG2	1:M:158:ASP:HB2	2.43	0.43
1:L:94:VAL:HG22	1:L:98:LYS:HB3	2.00	0.43
1:E:304:TRP:CZ2	1:E:313:LEU:HB2	2.52	0.43
1:H:417:ARG:NH1	1:I:479:PHE:O	2.51	0.43
1:M:368:ALA:HB3	2:M:2088:HOH:O	2.17	0.43
1:K:173:ILE:HG23	1:K:183:LYS:CG	2.44	0.43
1:H:159:PRO:O	1:H:160:ASN:HB2	2.18	0.43
1:H:338:THR:O	1:H:341:LEU:HB2	2.19	0.43
1:L:483:ARG:NH1	2:L:2082:HOH:O	2.50	0.43
1:F:177:PRO:HG2	1:F:178:TYR:CD2	2.53	0.43
1:I:94:VAL:CG2	1:I:98:LYS:HD3	2.48	0.43
1:H:410:LEU:HD11	1:H:426:MET:HE1	1.99	0.43
1:M:176:ASN:H	1:M:182:THR:CG2	2.31	0.43
1:B:254:LEU:CD1	1:B:281:ARG:HD3	2.48	0.43
1:M:482:ASN:C	1:M:482:ASN:ND2	2.71	0.43
1:B:288:LEU:N	1:B:289:PRO:CD	2.81	0.43
1:H:137:SER:O	1:H:141:ARG:HB2	2.18	0.43
1:D:289:PRO:O	1:D:293:THR:HG23	2.17	0.43
1:H:250:THR:HG23	2:H:2066:HOH:O	2.18	0.43
1:E:217:ALA:O	1:E:221:ARG:HG3	2.18	0.43
1:K:236:THR:O	1:K:236:THR:HG22	2.19	0.43
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.83	0.43
1:B:86:ARG:O	1:B:435:VAL:HG22	2.18	0.43
1:B:326:ARG:N	1:B:327:PRO:HD2	2.33	0.43
1:H:94:VAL:HG12	1:H:95:SER:N	2.33	0.43
1:L:141:ARG:HH11	1:L:141:ARG:HG2	1.83	0.43
1:G:461:VAL:CG1	1:G:485:ILE:HD11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:ILE:HG12	1:H:485:ILE:CG1	2.49	0.43
1:H:105:GLU:OE2	1:H:119:ARG:HG3	2.18	0.43
1:F:331:ALA:O	1:F:335:VAL:HG23	2.18	0.43
1:J:76:GLN:CG	1:J:77:GLY:N	2.63	0.43
1:L:412:VAL:CG2	1:L:426:MET:HE3	2.32	0.43
1:M:379:LEU:HD22	1:M:380:ARG:H	1.81	0.43
1:A:265:SER:HB3	1:G:281:ARG:NH2	2.34	0.43
1:L:84:PHE:CB	1:L:435:VAL:CG1	2.97	0.43
1:G:355:ILE:O	1:G:356:ASP:C	2.56	0.43
1:I:159:PRO:HG2	1:I:356:ASP:OD2	2.19	0.43
1:H:139:LEU:HD11	1:H:411:VAL:HG11	2.00	0.43
1:I:175:LEU:HD12	1:I:313:LEU:HD21	1.99	0.43
1:I:245:TRP:O	1:I:254:LEU:HG	2.18	0.43
1:M:473:LEU:HD11	1:M:492:ILE:HD11	2.00	0.43
1:D:358:LEU:HB3	1:D:385:LEU:HD11	2.00	0.43
1:M:433:HIS:CD2	1:M:459:GLU:HG3	2.53	0.43
1:D:322:GLY:N	1:D:323:PRO:HD2	2.33	0.43
1:F:316:THR:O	1:F:317:TRP:HB3	2.19	0.43
1:J:226:GLU:CG	1:J:261:THR:HB	2.32	0.43
1:D:436:GLU:HG3	1:D:456:ARG:HG3	2.00	0.43
1:H:185:TRP:NE1	1:H:190:GLU:OE2	2.43	0.43
1:L:88:LEU:HD11	1:L:436:GLU:HG3	2.01	0.43
1:G:247:THR:HG22	1:G:248:ILE:CD1	2.48	0.43
1:M:328:LEU:HD22	1:M:332:TRP:CE2	2.54	0.43
1:I:326:ARG:HB3	1:I:327:PRO:CD	2.49	0.43
1:F:99:LEU:CD2	1:F:486:ALA:HB3	2.49	0.43
1:L:367:LEU:HD22	1:L:371:LEU:HD11	2.01	0.43
1:J:93:ILE:HB	1:J:461:VAL:HG11	2.01	0.43
1:F:398:LYS:HD3	1:F:398:LYS:HA	1.77	0.43
1:H:182:THR:HG21	1:H:294:MET:HE3	2.01	0.43
1:K:281:ARG:NH2	1:L:265:SER:HB3	2.33	0.43
1:J:158:ASP:O	1:J:316:THR:HA	2.18	0.43
1:L:143:LEU:HD22	1:L:354:PHE:HZ	1.83	0.43
1:J:110:VAL:HG12	1:J:117:MET:HB3	2.00	0.43
1:I:210:THR:HG21	1:J:211:ASP:OD2	2.19	0.43
1:J:440:TYR:CE2	1:K:454:LEU:HB2	2.54	0.43
1:K:254:LEU:CD1	1:K:281:ARG:HD3	2.49	0.43
1:B:380:ARG:HH11	1:B:380:ARG:CG	2.32	0.43
1:L:175:LEU:CD1	1:L:313:LEU:HD21	2.48	0.43
1:M:413:LEU:CD2	1:M:475:ALA:HB2	2.46	0.43
1:M:124:ARG:HB3	1:M:408:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ILE:HG22	1:D:174:ILE:N	2.33	0.43
1:I:169:ARG:NH1	1:I:171:LYS:CG	2.81	0.43
1:I:417:ARG:NH1	1:J:479:PHE:O	2.51	0.43
1:E:159:PRO:HG2	1:E:356:ASP:OD2	2.19	0.43
1:L:367:LEU:HD22	1:L:371:LEU:HG	2.00	0.43
1:L:358:LEU:HB3	1:L:385:LEU:CD1	2.48	0.43
1:F:367:LEU:HD13	1:F:403:LEU:HD11	2.01	0.43
1:E:473:LEU:CD1	1:E:492:ILE:HD11	2.48	0.43
2:I:2107:HOH:O	1:J:124:ARG:HG3	2.19	0.43
1:B:439:ARG:HG3	1:B:453:ALA:O	2.19	0.43
1:L:166:LYS:HD2	1:L:495:PHE:HB2	2.00	0.43
1:E:315:ILE:HG23	1:E:332:TRP:CE3	2.53	0.43
1:L:430:LEU:HA	1:L:430:LEU:HD12	1.85	0.43
1:M:85:LYS:NZ	1:M:454:LEU:HD21	2.34	0.43
1:B:245:TRP:CZ3	1:B:257:PHE:HB2	2.54	0.43
1:B:385:LEU:HD21	1:B:391:LEU:HD22	2.01	0.43
1:J:367:LEU:HD22	1:J:371:LEU:HG	2.00	0.43
1:E:466:GLU:OE2	1:F:89:ARG:HD2	2.19	0.43
1:I:87:PHE:CZ	1:I:92:ARG:HG3	2.53	0.43
1:J:153:ARG:NH2	1:J:304:TRP:CE2	2.87	0.43
1:H:193:ASN:HB2	1:H:195:TYR:CE1	2.54	0.43
1:L:130:GLY:O	1:L:136:LYS:HE2	2.19	0.43
1:A:499:GLN:HB3	1:A:499:GLN:HE21	1.55	0.42
1:M:130:GLY:HA3	1:M:413:LEU:HB2	2.01	0.42
1:B:139:LEU:O	1:B:139:LEU:HD23	2.18	0.42
1:L:492:ILE:HG22	1:L:492:ILE:O	2.18	0.42
1:H:84:PHE:CB	1:H:435:VAL:CG1	2.97	0.42
1:D:139:LEU:HD11	1:D:411:VAL:HG11	2.01	0.42
1:E:233:LEU:C	1:E:235:GLY:N	2.72	0.42
1:L:159:PRO:HG3	1:L:317:TRP:CZ2	2.54	0.42
1:I:439:ARG:CZ	1:J:439:ARG:HH22	2.31	0.42
1:K:359:ALA:HB1	1:K:390:GLN:HG2	2.00	0.42
1:H:329:ILE:O	1:H:333:VAL:HG23	2.19	0.42
1:H:134:THR:HA	1:H:472:ASP:OD1	2.19	0.42
1:M:139:LEU:C	1:M:139:LEU:HD23	2.40	0.42
1:E:290:GLU:HB3	1:E:328:LEU:HD12	2.00	0.42
1:B:174:ILE:O	1:B:182:THR:HA	2.19	0.42
1:B:351:LEU:HD13	1:B:351:LEU:C	2.40	0.42
1:L:98:LYS:O	1:L:102:MET:HG3	2.19	0.42
1:I:157:VAL:HG12	1:I:317:TRP:HH2	1.80	0.42
1:M:181:ARG:CZ	1:M:503:VAL:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:479:PHE:HB2	1:J:483:ARG:HD2	2.01	0.42
1:H:494:GLN:HA	1:H:494:GLN:NE2	2.35	0.42
1:G:272:GLU:HA	1:G:272:GLU:OE1	2.19	0.42
1:F:243:PHE:O	1:F:247:THR:HB	2.18	0.42
1:B:119:ARG:HH12	1:B:350:ARG:NH1	2.17	0.42
1:H:251:PHE:CE2	1:H:255:ARG:NH1	2.83	0.42
1:D:199:ARG:NH2	1:D:342:SER:OG	2.51	0.42
1:J:103:THR:OG1	1:J:116:PRO:HG2	2.18	0.42
1:D:142:GLU:HB2	2:D:2136:HOH:O	2.19	0.42
1:K:114:GLY:N	1:K:142:GLU:OE2	2.46	0.42
1:G:76:GLN:HE21	1:G:76:GLN:HB2	1.60	0.42
1:K:223:LEU:HD23	1:K:284:LEU:HD22	2.02	0.42
1:I:367:LEU:HD22	1:I:371:LEU:CD1	2.49	0.42
1:B:182:THR:CG2	1:B:183:LYS:N	2.82	0.42
1:G:238:SER:OG	1:G:241:GLU:HG2	2.20	0.42
1:B:162:ASP:O	1:B:166:LYS:HG2	2.19	0.42
1:F:180:GLN:HB2	1:F:503:VAL:HG12	2.01	0.42
1:B:498:ARG:HG2	1:B:499:GLN:HG3	2.02	0.42
1:B:199:ARG:NH2	1:B:342:SER:OG	2.37	0.42
1:J:130:GLY:O	1:J:136:LYS:HE3	2.20	0.42
1:D:320:ASP:OD1	1:D:321:MET:HG3	2.19	0.42
1:B:181:ARG:NH1	1:B:500:PRO:HG2	2.35	0.42
1:M:340:ILE:HA	1:M:343:LEU:HG	2.01	0.42
1:J:94:VAL:CG1	1:J:95:SER:N	2.81	0.42
1:J:245:TRP:CZ3	1:J:257:PHE:HB2	2.54	0.42
1:G:355:ILE:O	1:G:356:ASP:O	2.38	0.42
1:F:473:LEU:CD1	1:F:492:ILE:HD11	2.50	0.42
1:L:198:GLN:O	1:L:202:LEU:HD22	2.19	0.42
1:E:413:LEU:HD12	1:E:475:ALA:CB	2.50	0.42
1:L:326:ARG:N	1:L:327:PRO:HD2	2.35	0.42
1:D:313:LEU:HD23	1:D:314:PHE:N	2.34	0.42
1:J:131:ALA:HB2	1:J:415:GLY:HA2	2.00	0.42
1:H:373:LYS:HD3	1:M:319:GLU:CD	2.40	0.42
1:E:294:MET:HG3	1:E:328:LEU:HD11	2.02	0.42
1:M:352:TRP:CZ2	1:M:380:ARG:HD3	2.54	0.42
1:H:435:VAL:CG1	1:H:436:GLU:N	2.82	0.42
1:L:113:ALA:HA	1:L:490:LEU:CD2	2.49	0.42
1:E:375:ARG:NH2	1:E:376:LYS:NZ	2.67	0.42
1:K:439:ARG:HA	1:L:456:ARG:HH22	1.83	0.42
1:M:355:ILE:O	1:M:356:ASP:C	2.57	0.42
1:K:100:LYS:HG2	1:K:115:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ARG:NH1	1:G:437:ARG:HD2	2.35	0.42
1:J:417:ARG:NH1	1:K:479:PHE:O	2.52	0.42
1:B:364:LEU:HD12	1:B:367:LEU:HG	2.01	0.42
1:L:77:GLY:C	1:L:78:GLU:HG3	2.39	0.42
1:H:288:LEU:N	1:H:289:PRO:CD	2.83	0.42
1:K:143:LEU:O	1:K:143:LEU:HD23	2.20	0.42
1:D:364:LEU:HB2	1:D:367:LEU:HB2	2.02	0.42
1:B:350:ARG:HG2	1:B:380:ARG:CZ	2.49	0.42
1:K:74:VAL:CG1	1:K:75:GLY:N	2.77	0.42
1:M:184:GLY:HA3	1:M:297:GLY:HA3	2.02	0.42
1:M:306:GLU:O	1:M:308:PRO:HD3	2.20	0.42
1:K:463:MET:HE3	1:L:458:ARG:HD3	2.01	0.42
1:I:456:ARG:H	1:I:456:ARG:HD2	1.85	0.42
1:G:157:VAL:HG12	1:G:317:TRP:HH2	1.85	0.42
1:F:375:ARG:NH2	1:F:376:LYS:HE2	2.34	0.42
1:A:197:TRP:CE2	1:A:229:LYS:HG2	2.54	0.42
1:M:96:GLY:O	1:M:100:LYS:HG3	2.19	0.42
1:G:103:THR:OG1	1:G:116:PRO:HG2	2.20	0.42
1:M:460:ARG:HH11	1:M:460:ARG:HG3	1.85	0.42
1:B:87:PHE:C	1:B:87:PHE:CD1	2.93	0.42
1:G:182:THR:CG2	1:G:183:LYS:N	2.83	0.42
1:E:175:LEU:HD12	1:E:313:LEU:HD21	2.02	0.42
1:E:87:PHE:HA	1:E:435:VAL:HG23	2.02	0.42
1:I:399:GLU:HG3	2:I:2096:HOH:O	2.18	0.42
1:K:279:SER:O	1:K:283:VAL:HG23	2.19	0.42
1:F:206:PRO:HG2	1:F:362:GLU:OE2	2.19	0.42
1:E:336:VAL:O	1:E:340:ILE:HG23	2.19	0.42
1:E:344:PRO:O	1:E:349:ARG:NH2	2.52	0.42
1:L:435:VAL:CG1	1:L:436:GLU:N	2.83	0.42
1:H:499:GLN:HG2	1:H:500:PRO:HD2	2.01	0.42
1:K:86:ARG:CG	1:K:86:ARG:NH1	2.83	0.42
1:H:159:PRO:HG3	1:H:317:TRP:CZ2	2.54	0.42
1:E:130:GLY:HA3	1:E:413:LEU:HB2	2.02	0.42
1:E:433:HIS:CD2	1:E:433:HIS:C	2.92	0.42
2:H:2097:HOH:O	1:I:398:LYS:HD2	2.20	0.42
1:A:363:LYS:HG3	1:A:395:TYR:CD2	2.55	0.42
1:I:223:LEU:HD23	1:I:284:LEU:CD2	2.50	0.42
1:K:412:VAL:HG13	1:K:426:MET:HE2	2.02	0.42
1:K:75:GLY:C	1:K:77:GLY:H	2.23	0.42
1:J:316:THR:O	1:J:317:TRP:HB3	2.20	0.42
1:E:113:ALA:HA	1:E:490:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:PRO:HG3	1:H:317:TRP:CH2	2.55	0.42
1:L:178:TYR:N	1:L:178:TYR:CD1	2.88	0.42
1:I:254:LEU:HD22	1:I:258:LEU:HG	2.01	0.42
1:F:358:LEU:HD11	1:F:367:LEU:HD11	2.02	0.42
1:B:367:LEU:HD13	1:B:403:LEU:HD11	2.02	0.42
1:I:192:ARG:HG2	1:I:302:ARG:NH1	2.34	0.42
1:D:105:GLU:HB2	1:D:109:GLN:NE2	2.35	0.42
1:F:474:THR:HG21	1:F:487:LYS:CE	2.50	0.42
1:J:326:ARG:NH1	1:J:361:LEU:O	2.53	0.42
1:J:346:GLU:OE2	1:J:348:LYS:HB2	2.20	0.42
1:J:408:ARG:HG3	1:J:408:ARG:HH11	1.84	0.42
1:F:173:ILE:CG2	1:F:183:LYS:HG3	2.47	0.41
1:H:184:GLY:HA2	1:H:295:PRO:O	2.20	0.41
1:I:124:ARG:HH11	1:I:124:ARG:CG	2.27	0.41
1:I:358:LEU:HD11	1:I:367:LEU:CD1	2.50	0.41
1:L:432:GLU:OE1	1:L:458:ARG:HD2	2.20	0.41
1:L:181:ARG:CZ	1:L:503:VAL:HG23	2.49	0.41
1:L:344:PRO:O	1:L:346:GLU:HG2	2.20	0.41
1:A:164:LEU:HD11	1:A:174:ILE:HD11	2.01	0.41
1:K:157:VAL:HB	1:K:356:ASP:H	1.85	0.41
1:G:318:ARG:HH11	1:G:318:ARG:HG2	1.85	0.41
1:E:410:LEU:HD11	1:E:426:MET:CE	2.50	0.41
1:J:160:ASN:ND2	1:J:319:GLU:CD	2.65	0.41
1:A:294:MET:SD	1:A:295:PRO:HD2	2.60	0.41
1:D:503:VAL:O	1:D:504:GLU:CB	2.67	0.41
1:E:433:HIS:CD2	1:E:459:GLU:HG3	2.56	0.41
1:K:430:LEU:HA	1:K:430:LEU:HD12	1.83	0.41
1:F:173:ILE:HG22	1:F:174:ILE:N	2.36	0.41
1:K:410:LEU:HD21	1:K:426:MET:HE3	2.02	0.41
1:E:180:GLN:HB2	1:E:504:GLU:CG	2.50	0.41
1:B:245:TRP:O	1:B:254:LEU:HG	2.20	0.41
1:D:326:ARG:CD	2:D:2083:HOH:O	2.65	0.41
1:J:169:ARG:NH1	1:J:169:ARG:HB2	2.35	0.41
1:A:182:THR:HG22	1:A:183:LYS:O	2.21	0.41
1:J:105:GLU:HG2	1:J:106:LYS:N	2.35	0.41
1:A:355:ILE:O	1:A:356:ASP:C	2.58	0.41
1:H:259:GLU:HA	1:H:264:GLU:CD	2.40	0.41
1:G:455:GLU:HG3	1:G:455:GLU:O	2.19	0.41
1:H:376:LYS:HD3	1:H:376:LYS:HA	1.90	0.41
1:J:433:HIS:O	1:J:433:HIS:HD2	2.03	0.41
1:A:316:THR:O	1:A:317:TRP:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:VAL:O	1:G:340:ILE:HG23	2.19	0.41
1:K:254:LEU:C	1:K:254:LEU:HD23	2.41	0.41
1:I:127:LEU:HD13	1:I:407:PHE:CG	2.56	0.41
1:L:473:LEU:CD1	1:L:492:ILE:HD11	2.47	0.41
1:J:207:ARG:HB2	1:J:363:LYS:HG2	2.02	0.41
1:M:128:VAL:O	1:M:136:LYS:HE2	2.21	0.41
1:L:422:THR:O	1:L:426:MET:HG2	2.20	0.41
1:K:182:THR:HG21	1:K:294:MET:HE1	2.02	0.41
1:G:156:ILE:HG22	1:G:158:ASP:HB2	2.02	0.41
1:B:180:GLN:HG3	1:B:504:GLU:OE1	2.21	0.41
1:L:84:PHE:HB3	1:L:437:ARG:HG3	2.02	0.41
1:K:414:GLY:HA2	1:K:467:ILE:HG23	2.02	0.41
1:K:352:TRP:CE2	1:K:380:ARG:HD3	2.55	0.41
1:G:433:HIS:CD2	1:G:433:HIS:C	2.94	0.41
1:K:87:PHE:CD1	1:K:87:PHE:C	2.94	0.41
1:K:230:LYS:CE	1:K:257:PHE:O	2.68	0.41
1:B:413:LEU:HD12	1:B:475:ALA:CB	2.48	0.41
1:E:473:LEU:HD11	1:E:492:ILE:HD11	2.02	0.41
1:L:230:LYS:HD3	1:L:257:PHE:CE2	2.55	0.41
1:E:250:THR:HA	2:F:2110:HOH:O	2.20	0.41
1:E:251:PHE:CZ	1:E:277:LEU:HD13	2.56	0.41
1:B:436:GLU:OE2	1:B:456:ARG:HD2	2.21	0.41
1:J:430:LEU:HD12	1:J:430:LEU:HA	1.86	0.41
1:B:84:PHE:CG	1:B:435:VAL:HG21	2.55	0.41
1:G:175:LEU:CD1	1:G:313:LEU:HD21	2.51	0.41
1:A:367:LEU:HD22	1:A:371:LEU:CD1	2.51	0.41
1:B:136:LYS:HG2	1:B:413:LEU:CD2	2.51	0.41
1:K:318:ARG:HG2	1:K:318:ARG:HH11	1.85	0.41
1:E:452:ARG:HH11	1:E:452:ARG:CB	2.34	0.41
1:A:433:HIS:CD2	1:A:433:HIS:C	2.94	0.41
1:H:259:GLU:HG2	1:H:264:GLU:OE2	2.21	0.41
1:M:291:HIS:CE1	2:M:2041:HOH:O	2.73	0.41
1:L:375:ARG:NH1	1:L:375:ARG:HG3	2.35	0.41
1:A:178:TYR:OH	1:A:290:GLU:OE2	2.31	0.41
1:H:375:ARG:HB2	1:H:375:ARG:NH1	2.25	0.41
1:B:180:GLN:HG3	1:B:504:GLU:CB	2.50	0.41
1:M:94:VAL:HG13	1:M:95:SER:O	2.20	0.41
1:D:184:GLY:HA2	1:D:295:PRO:O	2.20	0.41
1:K:379:LEU:CD2	1:K:380:ARG:N	2.83	0.41
1:H:234:ILE:HD11	1:H:236:THR:OG1	2.21	0.41
1:K:199:ARG:NH2	1:K:342:SER:OG	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:493:LYS:HB3	1:K:495:PHE:CE1	2.56	0.41
1:I:72:ASN:OD1	1:I:438:ASP:HB2	2.20	0.41
1:L:106:LYS:CD	1:L:106:LYS:H	2.23	0.41
1:A:154:MET:HB3	1:A:352:TRP:HB2	2.03	0.41
1:A:352:TRP:CE2	1:A:380:ARG:HD3	2.56	0.41
1:J:84:PHE:CG	1:J:435:VAL:HG11	2.56	0.41
1:B:84:PHE:CD2	1:B:435:VAL:CG2	3.04	0.41
1:G:175:LEU:HA	1:G:182:THR:HG23	2.03	0.41
1:M:380:ARG:HH11	1:M:380:ARG:HG3	1.85	0.41
1:L:281:ARG:NH2	1:M:265:SER:HB3	2.36	0.41
1:L:416:SER:HB2	1:M:408:ARG:HD2	2.03	0.41
1:E:75:GLY:O	1:E:76:GLN:C	2.59	0.41
1:E:76:GLN:HG3	1:E:77:GLY:N	2.35	0.41
1:M:166:LYS:HG3	1:M:495:PHE:HB3	2.02	0.41
1:A:124:ARG:HB3	1:A:408:ARG:HG3	2.02	0.41
1:A:139:LEU:O	1:A:139:LEU:HD23	2.21	0.41
1:L:452:ARG:HG2	1:L:452:ARG:O	2.21	0.41
1:G:125:HIS:HB2	1:G:407:PHE:HA	2.03	0.41
1:L:245:TRP:O	1:L:254:LEU:HG	2.21	0.41
1:J:279:SER:O	1:J:283:VAL:HG23	2.21	0.41
1:A:428:LEU:HD13	1:G:420:PRO:HB2	2.03	0.41
1:K:122:GLU:N	1:K:123:PRO:HD2	2.35	0.41
1:F:84:PHE:CD1	1:F:84:PHE:N	2.89	0.41
1:K:454:LEU:HD23	1:K:454:LEU:HA	1.89	0.41
1:K:328:LEU:HD13	1:K:332:TRP:CH2	2.56	0.41
1:E:144:ALA:O	1:E:148:LEU:HG	2.21	0.41
1:M:259:GLU:HA	1:M:264:GLU:CG	2.41	0.41
1:M:378:GLY:O	1:M:380:ARG:NH1	2.54	0.41
1:B:180:GLN:HG3	1:B:504:GLU:HB2	2.03	0.41
1:I:145:TYR:CE1	1:I:149:LEU:HD21	2.54	0.41
1:G:110:VAL:HG13	1:G:146:THR:OG1	2.21	0.41
1:H:88:LEU:HD13	1:M:82:ALA:HB2	2.02	0.41
1:K:340:ILE:HG13	1:K:379:LEU:HD12	2.02	0.41
1:J:180:GLN:NE2	1:J:504:GLU:OE1	2.54	0.41
1:I:236:THR:HB	1:I:241:GLU:OE2	2.21	0.41
1:G:483:ARG:NH1	2:G:2163:HOH:O	2.53	0.41
1:J:183:LYS:HA	1:J:183:LYS:HD3	1.98	0.41
1:J:437:ARG:O	1:J:455:GLU:HG2	2.20	0.40
1:B:82:ALA:O	1:B:437:ARG:NH1	2.54	0.40
1:G:326:ARG:HD2	1:G:360:SER:O	2.22	0.40
1:M:277:LEU:HD22	1:M:277:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:199:ARG:HE	1:J:338:THR:HG21	1.83	0.40
1:H:88:LEU:CD1	1:M:82:ALA:HB2	2.51	0.40
1:H:352:TRP:HB3	1:H:354:PHE:CE2	2.55	0.40
1:E:86:ARG:HH11	1:E:86:ARG:HG3	1.86	0.40
1:I:433:HIS:C	1:I:433:HIS:CD2	2.94	0.40
1:H:104:ARG:NH1	2:H:2006:HOH:O	2.54	0.40
1:F:404:ARG:NH1	2:F:2165:HOH:O	2.48	0.40
1:J:226:GLU:HG3	1:J:261:THR:CB	2.33	0.40
1:G:153:ARG:C	1:G:154:MET:HG2	2.41	0.40
1:K:134:THR:O	1:K:134:THR:CG2	2.66	0.40
1:M:94:VAL:HG22	1:M:98:LYS:HB3	2.04	0.40
1:A:184:GLY:HA2	1:A:295:PRO:O	2.21	0.40
1:D:78:GLU:HG2	2:D:2001:HOH:O	2.20	0.40
1:K:186:SER:H	1:K:189:ASN:ND2	2.19	0.40
1:L:166:LYS:HD2	1:L:495:PHE:CB	2.52	0.40
1:J:144:ALA:O	1:J:148:LEU:HG	2.21	0.40
1:K:244:HIS:HD2	2:K:2043:HOH:O	2.03	0.40
1:E:183:LYS:HD3	1:E:183:LYS:HA	1.90	0.40
1:L:398:LYS:HD3	1:L:398:LYS:HA	1.83	0.40
1:M:106:LYS:CD	1:M:106:LYS:N	2.67	0.40
1:I:413:LEU:HD12	1:I:475:ALA:CB	2.51	0.40
1:E:129:ASN:HB3	1:E:426:MET:HE1	2.03	0.40
1:M:110:VAL:HG13	1:M:146:THR:OG1	2.21	0.40
1:G:199:ARG:NH2	1:G:342:SER:OG	2.47	0.40
1:A:166:LYS:HD3	1:A:497:ASN:HD22	1.85	0.40
1:L:331:ALA:O	1:L:335:VAL:HG23	2.22	0.40
1:H:439:ARG:HH22	1:M:439:ARG:NH2	2.19	0.40
1:M:441:SER:HB2	1:M:451:GLY:HA3	2.02	0.40
1:K:463:MET:SD	1:L:434:GLU:HG3	2.62	0.40
1:A:466:GLU:OE2	1:B:89:ARG:HD2	2.21	0.40
1:D:238:SER:HB3	1:D:241:GLU:HB2	2.03	0.40
1:J:350:ARG:HG2	1:J:380:ARG:NH2	2.37	0.40
1:J:483:ARG:HH11	1:J:483:ARG:CG	2.34	0.40
1:E:471:PRO:HG2	1:E:474:THR:OG1	2.22	0.40
1:K:119:ARG:HD3	1:K:122:GLU:OE2	2.21	0.40
1:L:288:LEU:N	1:L:289:PRO:CD	2.85	0.40
1:J:318:ARG:HD2	1:J:502:PHE:CZ	2.57	0.40
1:D:153:ARG:NH2	1:D:304:TRP:CE2	2.89	0.40
1:A:100:LYS:HG2	1:A:115:VAL:HA	2.04	0.40
1:G:357:GLU:CG	1:G:386:GLN:NE2	2.85	0.40
1:I:97:GLY:O	1:I:101:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:MET:HE3	1:G:156:ILE:HD11	1.99	0.40
1:J:154:MET:HA	1:J:351:LEU:HD22	2.03	0.40
1:L:192:ARG:HG2	1:L:302:ARG:NH1	2.35	0.40
1:B:385:LEU:HA	1:B:385:LEU:HD12	1.90	0.40
1:K:352:TRP:CZ2	1:K:380:ARG:HD3	2.57	0.40
1:F:474:THR:HG21	1:F:487:LYS:HE3	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	423/437 (97%)	407 (96%)	15 (4%)	1 (0%)	52	75
1	B	418/437 (96%)	397 (95%)	19 (4%)	2 (0%)	34	55
1	D	413/437 (94%)	395 (96%)	15 (4%)	3 (1%)	26	46
1	E	421/437 (96%)	401 (95%)	16 (4%)	4 (1%)	19	34
1	F	423/437 (97%)	401 (95%)	20 (5%)	2 (0%)	34	55
1	G	423/437 (97%)	410 (97%)	12 (3%)	1 (0%)	52	75
1	H	420/437 (96%)	398 (95%)	20 (5%)	2 (0%)	34	55
1	I	420/437 (96%)	398 (95%)	20 (5%)	2 (0%)	34	55
1	J	420/437 (96%)	402 (96%)	16 (4%)	2 (0%)	34	55
1	K	418/437 (96%)	401 (96%)	15 (4%)	2 (0%)	34	55
1	L	422/437 (97%)	405 (96%)	14 (3%)	3 (1%)	26	46
1	M	421/437 (96%)	403 (96%)	15 (4%)	3 (1%)	26	46
All	All	5042/5244 (96%)	4818 (96%)	197 (4%)	27 (0%)	34	55

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	356	ASP
1	E	76	GLN
1	E	356	ASP
1	G	356	ASP
1	H	76	GLN
1	J	76	GLN
1	K	74	VAL
1	A	356	ASP
1	B	356	ASP
1	E	442	LYS
1	F	234	ILE
1	F	356	ASP
1	H	356	ASP
1	I	356	ASP
1	J	356	ASP
1	K	356	ASP
1	L	356	ASP
1	L	504	GLU
1	M	125	HIS
1	M	356	ASP
1	D	182	THR
1	D	234	ILE
1	I	504	GLU
1	L	125	HIS
1	B	76	GLN
1	E	234	ILE
1	M	234	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	356/364 (98%)	323 (91%)	33 (9%)	11	21
1	B	352/364 (97%)	316 (90%)	36 (10%)	9	17
1	D	348/364 (96%)	317 (91%)	31 (9%)	12	23
1	E	355/364 (98%)	327 (92%)	28 (8%)	15	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	355/364 (98%)	324 (91%)	31 (9%)	13	24
1	G	356/364 (98%)	324 (91%)	32 (9%)	12	22
1	H	353/364 (97%)	325 (92%)	28 (8%)	15	28
1	I	353/364 (97%)	326 (92%)	27 (8%)	16	30
1	J	353/364 (97%)	318 (90%)	35 (10%)	10	18
1	K	352/364 (97%)	329 (94%)	23 (6%)	21	39
1	L	355/364 (98%)	322 (91%)	33 (9%)	11	21
1	M	353/364 (97%)	323 (92%)	30 (8%)	13	25
All	All	4241/4368 (97%)	3874 (91%)	367 (9%)	13	24

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	110	VAL
1	A	141	ARG
1	A	143	LEU
1	A	186	SER
1	A	202	LEU
1	A	238	SER
1	A	251	PHE
1	A	254	LEU
1	A	255	ARG
1	A	277	LEU
1	A	284	LEU
1	A	290	GLU
1	A	294	MET
1	A	313	LEU
1	A	326	ARG
1	A	328	LEU
1	A	338	THR
1	A	340	ILE
1	A	353	LEU
1	A	367	LEU
1	A	375	ARG
1	A	379	LEU
1	A	385	LEU
1	A	417	ARG
1	A	428	LEU

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	433	HIS
1	A	435	VAL
1	A	454	LEU
1	A	456	ARG
1	A	483	ARG
1	A	499	GLN
1	B	76	GLN
1	B	106	LYS
1	B	141	ARG
1	B	143	LEU
1	B	154	MET
1	B	169	ARG
1	B	186	SER
1	B	202	LEU
1	B	209	LYS
1	B	251	PHE
1	B	254	LEU
1	B	277	LEU
1	B	284	LEU
1	B	293	THR
1	B	294	MET
1	B	313	LEU
1	B	326	ARG
1	B	328	LEU
1	B	338	THR
1	B	340	ILE
1	B	353	LEU
1	B	356	ASP
1	B	367	LEU
1	B	375	ARG
1	B	379	LEU
1	B	385	LEU
1	B	413	LEU
1	B	417	ARG
1	B	428	LEU
1	B	430	LEU
1	B	433	HIS
1	B	435	VAL
1	B	439	ARG
1	B	456	ARG
1	B	493	LYS

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Mol	Chain	Res	Type
1	B	494	GLN
1	D	104	ARG
1	D	110	VAL
1	D	141	ARG
1	D	143	LEU
1	D	154	MET
1	D	186	SER
1	D	202	LEU
1	D	251	PHE
1	D	254	LEU
1	D	277	LEU
1	D	284	LEU
1	D	285	SER
1	D	294	MET
1	D	313	LEU
1	D	326	ARG
1	D	328	LEU
1	D	338	THR
1	D	340	ILE
1	D	353	LEU
1	D	367	LEU
1	D	375	ARG
1	D	379	LEU
1	D	385	LEU
1	D	428	LEU
1	D	430	LEU
1	D	433	HIS
1	D	435	VAL
1	D	454	LEU
1	D	456	ARG
1	D	483	ARG
1	D	499	GLN
1	E	78	GLU
1	E	94	VAL
1	E	106	LYS
1	E	129	ASN
1	E	143	LEU
1	E	154	MET
1	E	186	SER
1	E	202	LEU
1	E	233	LEU
1	E	251	PHE

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Mol	Chain	Res	Type
1	E	254	LEU
1	E	277	LEU
1	E	284	LEU
1	E	294	MET
1	E	328	LEU
1	E	338	THR
1	E	353	LEU
1	E	367	LEU
1	E	379	LEU
1	E	385	LEU
1	E	413	LEU
1	E	417	ARG
1	E	430	LEU
1	E	433	HIS
1	E	435	VAL
1	E	454	LEU
1	E	456	ARG
1	E	483	ARG
1	F	76	GLN
1	F	94	VAL
1	F	110	VAL
1	F	141	ARG
1	F	143	LEU
1	F	182	THR
1	F	202	LEU
1	F	251	PHE
1	F	254	LEU
1	F	277	LEU
1	F	284	LEU
1	F	294	MET
1	F	326	ARG
1	F	328	LEU
1	F	338	THR
1	F	340	ILE
1	F	353	LEU
1	F	362	GLU
1	F	367	LEU
1	F	372	THR
1	F	379	LEU
1	F	385	LEU
1	F	417	ARG
1	F	430	LEU

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Mol	Chain	Res	Type
1	F	433	HIS
1	F	435	VAL
1	F	439	ARG
1	F	454	LEU
1	F	456	ARG
1	F	483	ARG
1	F	499	GLN
1	G	143	LEU
1	G	154	MET
1	G	186	SER
1	G	202	LEU
1	G	251	PHE
1	G	254	LEU
1	G	255	ARG
1	G	277	LEU
1	G	289	PRO
1	G	290	GLU
1	G	294	MET
1	G	296	ASP
1	G	313	LEU
1	G	318	ARG
1	G	328	LEU
1	G	338	THR
1	G	341	LEU
1	G	345	GLU
1	G	353	LEU
1	G	360	SER
1	G	362	GLU
1	G	367	LEU
1	G	372	THR
1	G	375	ARG
1	G	379	LEU
1	G	385	LEU
1	G	417	ARG
1	G	430	LEU
1	G	433	HIS
1	G	434	GLU
1	G	435	VAL
1	G	499	GLN
1	H	76	GLN
1	H	93	ILE
1	H	140	LEU

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Mol	Chain	Res	Type
1	H	141	ARG
1	H	194	ASP
1	H	202	LEU
1	H	237	PRO
1	H	240	ARG
1	H	241	GLU
1	H	251	PHE
1	H	254	LEU
1	H	277	LEU
1	H	284	LEU
1	H	294	MET
1	H	296	ASP
1	H	328	LEU
1	H	338	THR
1	H	340	ILE
1	H	353	LEU
1	H	362	GLU
1	H	367	LEU
1	H	375	ARG
1	H	417	ARG
1	H	428	LEU
1	H	430	LEU
1	H	433	HIS
1	H	439	ARG
1	H	506	THR
1	I	104	ARG
1	I	106	LYS
1	I	143	LEU
1	I	170	ASP
1	I	186	SER
1	I	194	ASP
1	I	202	LEU
1	I	240	ARG
1	I	251	PHE
1	I	254	LEU
1	I	277	LEU
1	I	284	LEU
1	I	294	MET
1	I	298	ASP
1	I	328	LEU
1	I	338	THR
1	I	340	ILE

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Mol	Chain	Res	Type
1	I	341	LEU
1	I	353	LEU
1	I	360	SER
1	I	367	LEU
1	I	375	ARG
1	I	379	LEU
1	I	385	LEU
1	I	430	LEU
1	I	433	HIS
1	I	435	VAL
1	J	76	GLN
1	J	104	ARG
1	J	110	VAL
1	J	137	SER
1	J	143	LEU
1	J	154	MET
1	J	169	ARG
1	J	180	GLN
1	J	194	ASP
1	J	202	LEU
1	J	225	ARG
1	J	254	LEU
1	J	277	LEU
1	J	290	GLU
1	J	294	MET
1	J	296	ASP
1	J	313	LEU
1	J	328	LEU
1	J	338	THR
1	J	340	ILE
1	J	341	LEU
1	J	351	LEU
1	J	353	LEU
1	J	362	GLU
1	J	366	SER
1	J	367	LEU
1	J	379	LEU
1	J	385	LEU
1	J	428	LEU
1	J	430	LEU
1	J	433	HIS
1	J	434	GLU

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Mol	Chain	Res	Type
1	J	435	VAL
1	J	440	TYR
1	J	492	ILE
1	K	76	GLN
1	K	85	LYS
1	K	104	ARG
1	K	194	ASP
1	K	202	LEU
1	K	226	GLU
1	K	251	PHE
1	K	294	MET
1	K	298	ASP
1	K	328	LEU
1	K	338	THR
1	K	340	ILE
1	K	353	LEU
1	K	367	LEU
1	K	375	ARG
1	K	379	LEU
1	K	417	ARG
1	K	428	LEU
1	K	430	LEU
1	K	433	HIS
1	K	454	LEU
1	K	472	ASP
1	K	497	ASN
1	L	76	GLN
1	L	86	ARG
1	L	106	LYS
1	L	141	ARG
1	L	154	MET
1	L	162	ASP
1	L	186	SER
1	L	202	LEU
1	L	251	PHE
1	L	254	LEU
1	L	277	LEU
1	L	286	ASP
1	L	289	PRO
1	L	294	MET
1	L	296	ASP
1	L	313	LEU

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Mol	Chain	Res	Type
1	L	328	LEU
1	L	340	ILE
1	L	348	LYS
1	L	353	LEU
1	L	367	LEU
1	L	372	THR
1	L	375	ARG
1	L	379	LEU
1	L	417	ARG
1	L	428	LEU
1	L	430	LEU
1	L	433	HIS
1	L	438	ASP
1	L	456	ARG
1	L	497	ASN
1	L	499	GLN
1	L	506	THR
1	M	92	ARG
1	M	106	LYS
1	M	202	LEU
1	M	233	LEU
1	M	251	PHE
1	M	254	LEU
1	M	277	LEU
1	M	294	MET
1	M	296	ASP
1	M	328	LEU
1	M	338	THR
1	M	340	ILE
1	M	341	LEU
1	M	345	GLU
1	M	353	LEU
1	M	362	GLU
1	M	367	LEU
1	M	375	ARG
1	M	379	LEU
1	M	417	ARG
1	M	428	LEU
1	M	430	LEU
1	M	433	HIS
1	M	434	GLU
1	M	439	ARG

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Mol	Chain	Res	Type
1	M	456	ARG
1	M	472	ASP
1	M	482	ASN
1	M	497	ASN
1	M	499	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	160	ASN
1	A	291	HIS
1	A	497	ASN
1	A	499	GLN
1	B	76	GLN
1	B	180	GLN
1	B	291	HIS
1	B	497	ASN
1	D	160	ASN
1	D	291	HIS
1	D	497	ASN
1	D	499	GLN
1	E	160	ASN
1	E	244	HIS
1	E	291	HIS
1	E	497	ASN
1	F	76	GLN
1	F	160	ASN
1	F	180	GLN
1	F	291	HIS
1	F	433	HIS
1	F	499	GLN
1	G	76	GLN
1	G	244	HIS
1	G	291	HIS
1	G	309	ASN
1	G	386	GLN
1	G	497	ASN
1	G	499	GLN
1	H	160	ASN
1	H	180	GLN
1	H	291	HIS

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Mol	Chain	Res	Type
1	H	433	HIS
1	H	494	GLN
1	H	497	ASN
1	H	499	GLN
1	I	76	GLN
1	I	189	ASN
1	I	291	HIS
1	I	433	HIS
1	I	497	ASN
1	I	499	GLN
1	J	76	GLN
1	J	129	ASN
1	J	160	ASN
1	J	180	GLN
1	J	189	ASN
1	J	291	HIS
1	K	76	GLN
1	K	129	ASN
1	K	189	ASN
1	K	291	HIS
1	K	433	HIS
1	K	469	ASN
1	K	497	ASN
1	L	76	GLN
1	L	160	ASN
1	L	291	HIS
1	L	386	GLN
1	L	433	HIS
1	L	494	GLN
1	L	497	ASN
1	L	499	GLN
1	M	180	GLN
1	M	291	HIS
1	M	312	ASN
1	M	482	ASN
1	M	494	GLN
1	M	499	GLN

5.3.3 RNA ⓘ

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.