Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:51 PM GMT

PDB ID	:	4JK2
Title	:	X-ray crystal structure of Escherichia coli sigma70 holoenzyme in complex with guanosine pentaphosphate (pppGpp)
Authors	:	Murakami, K.S.
Deposited on	:	2013-03-09
Resolution	:	4.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

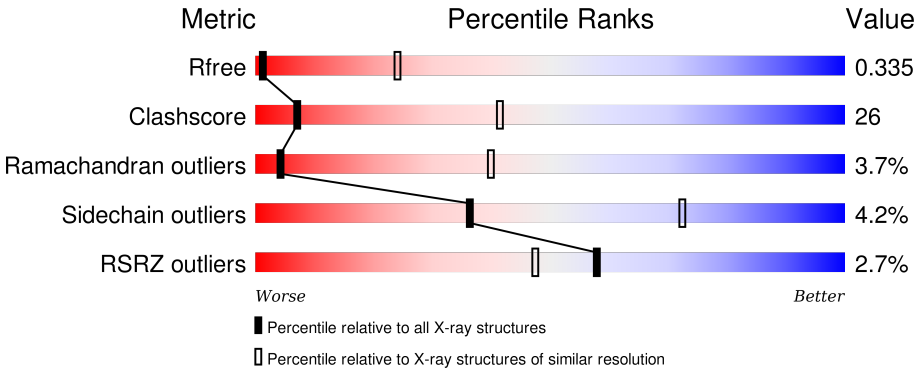
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	329	59% 36%
1	B	329	38% 27% 33%
1	F	329	4% 46% 22% 30%
1	G	329	40% 24% 34%
2	C	1342	53% 41% 5%

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Mol	Chain	Length	Quality of chain
2	H	1342	3% 53% 41% 5%
3	D	1407	% 39% 39% 5% 18%
3	I	1407	3% 41% 37% 5% 18%
4	E	91	59% 35%
4	J	91	% 53% 29% 16%
5	X	613	3% 47% 35% 16%
5	Y	613	3% 43% 30% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	0O2	D	1503	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 56129 atoms, of which 10 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 Escherichia coli RNA polymerase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

- Molecule 2 is a protein called Escherichia coli RNA polymerase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

- Molecule 3 is a protein called Escherichia coli RNA polymerase beta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

- Molecule 4 is a protein called Escherichia coli RNA polymerase omega subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

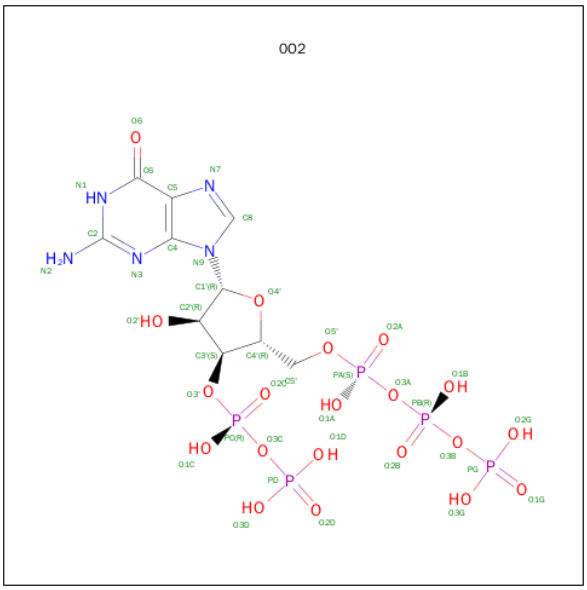
- Molecule 5 is a protein called Escherichia coli RNA polymerase sigma70 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	2	Total	Zn	0	0
			2	2		
6	D	2	Total	Zn	0	0
			2	2		

- Molecule 7 is GUANOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE) 3'-(TRIHYDROGEN DIPHOSPHATE) (three-letter code: 0O2) (formula: $C_{10}H_{18}N_5O_{20}P_5$).



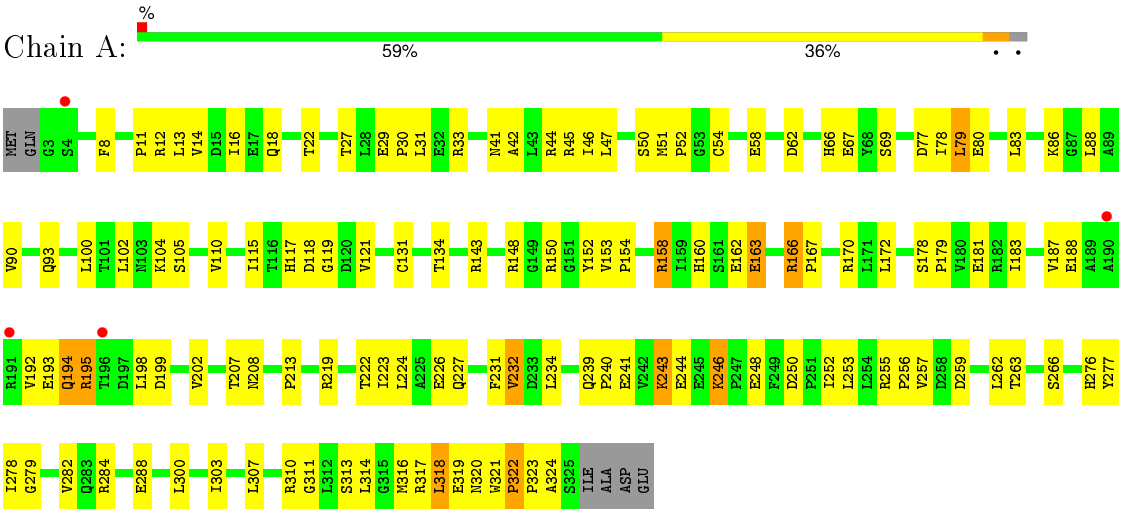
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	D	1	Total	C	H	N	O	P	0	0
			50	10	10	5	20	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

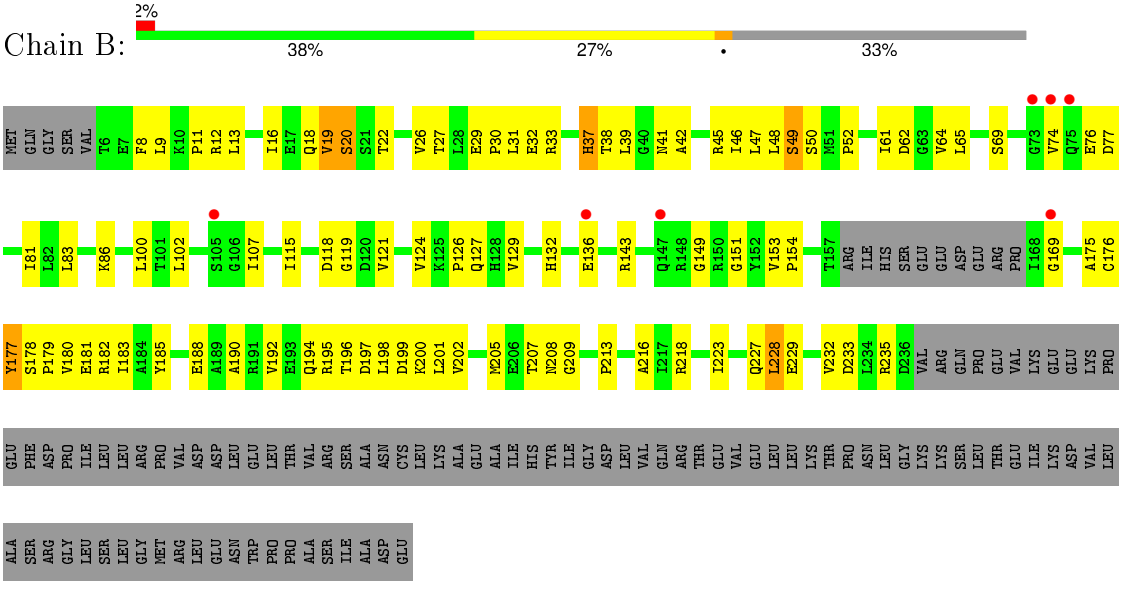
• Molecule 1: Escherichia coli RNA polymerase alpha subunit

Chain A:



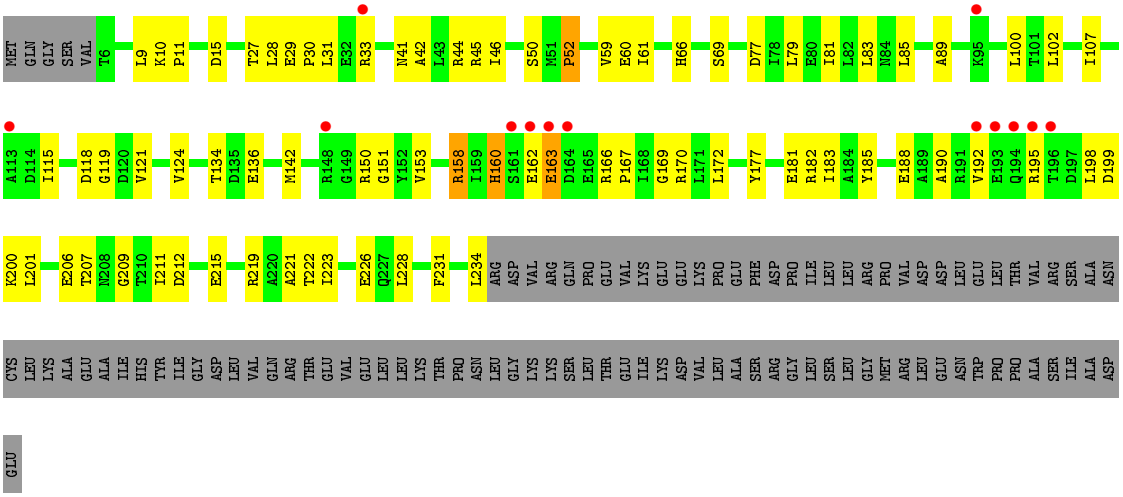
• Molecule 1: Escherichia coli RNA polymerase alpha subunit

Chain B:



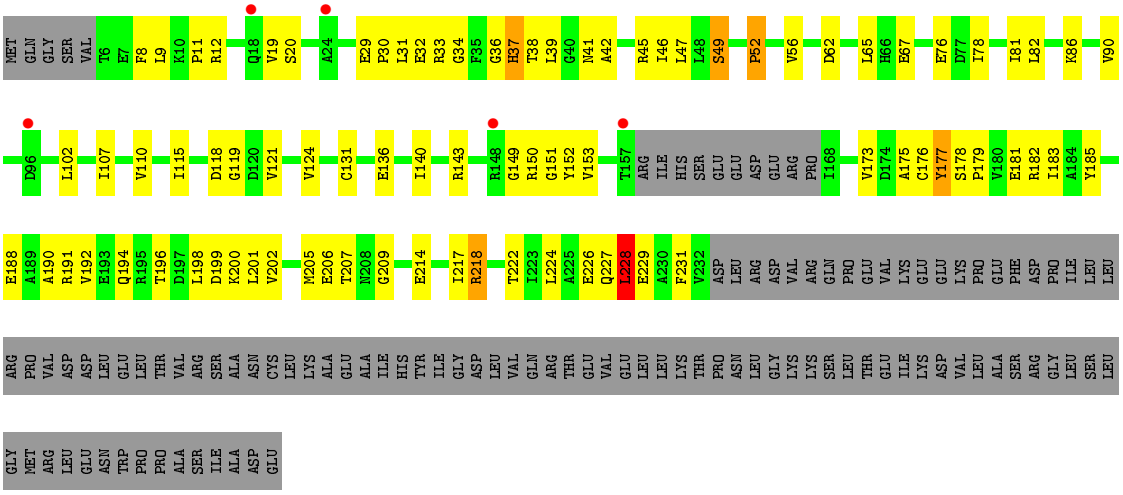
• Molecule 1: Escherichia coli RNA polymerase alpha subunit

Chain F:



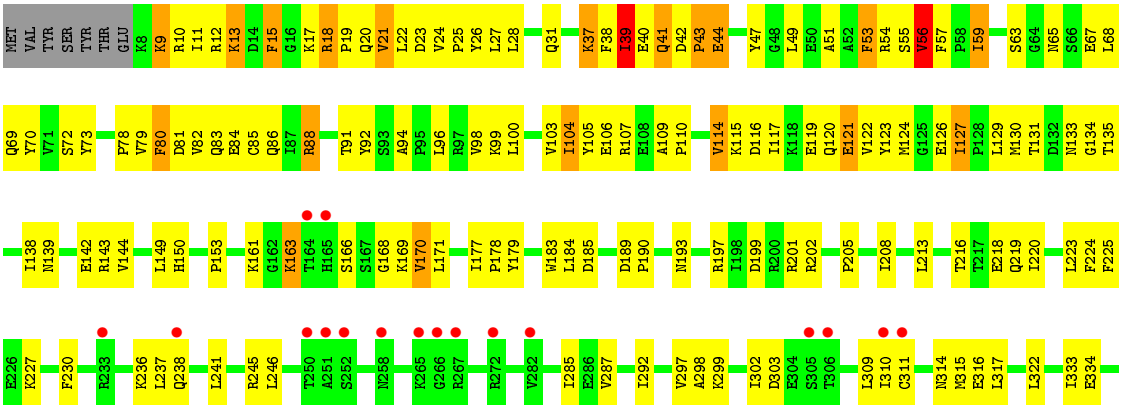
• Molecule 1: Escherichia coli RNA polymerase alpha subunit

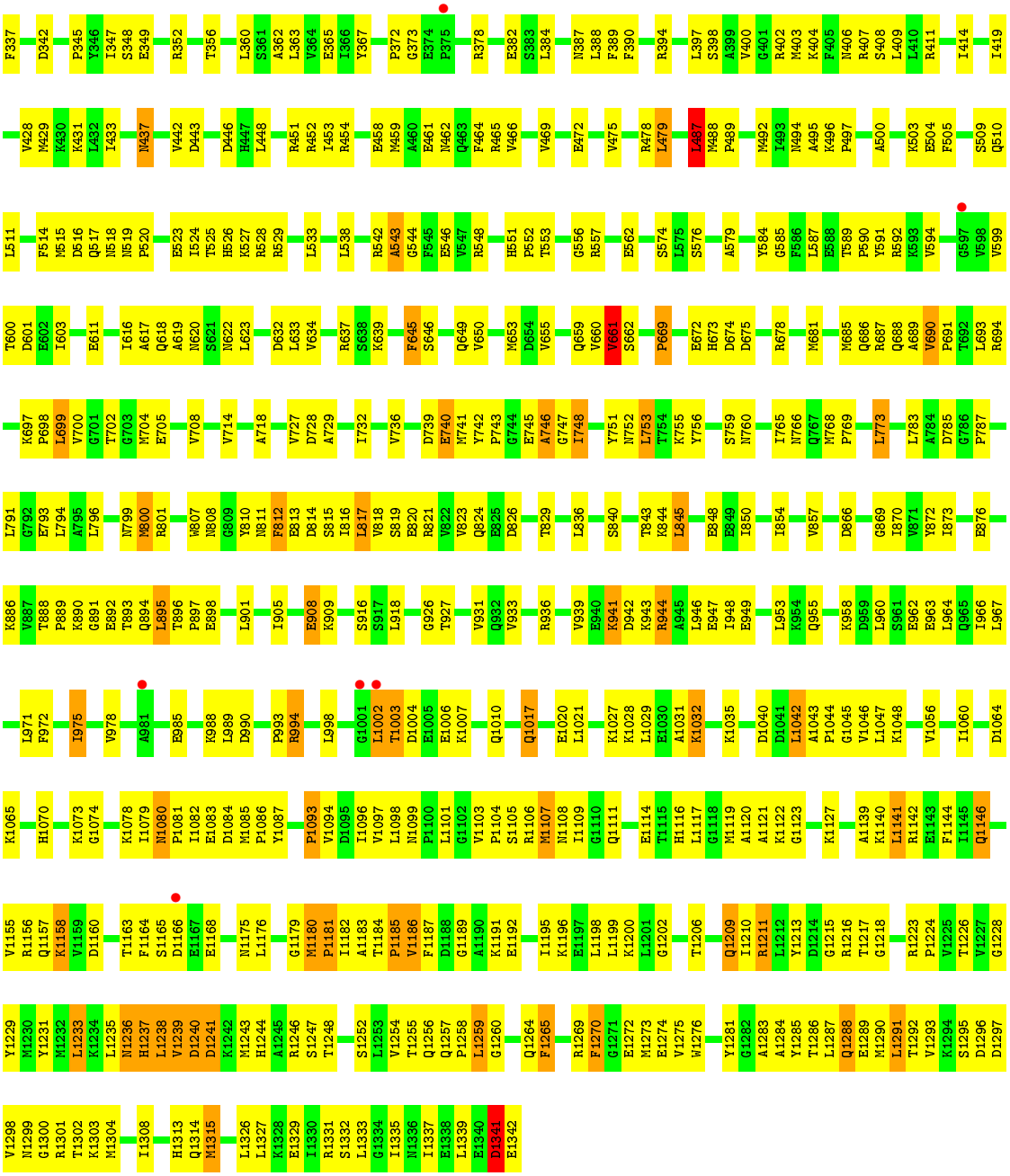
Chain G:



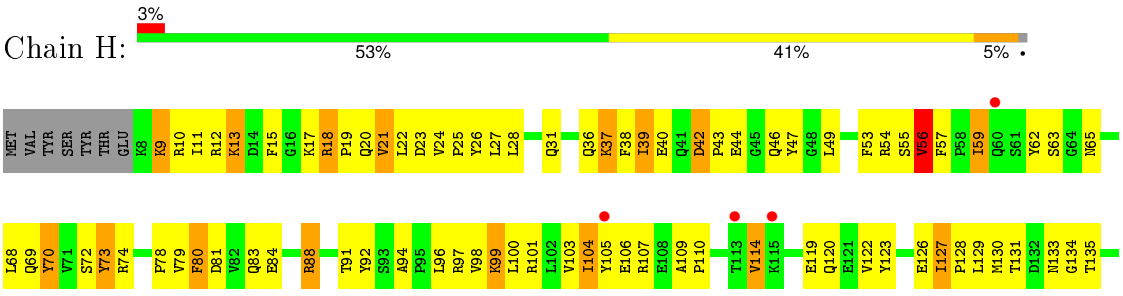
• Molecule 2: Escherichia coli RNA polymerase beta subunit

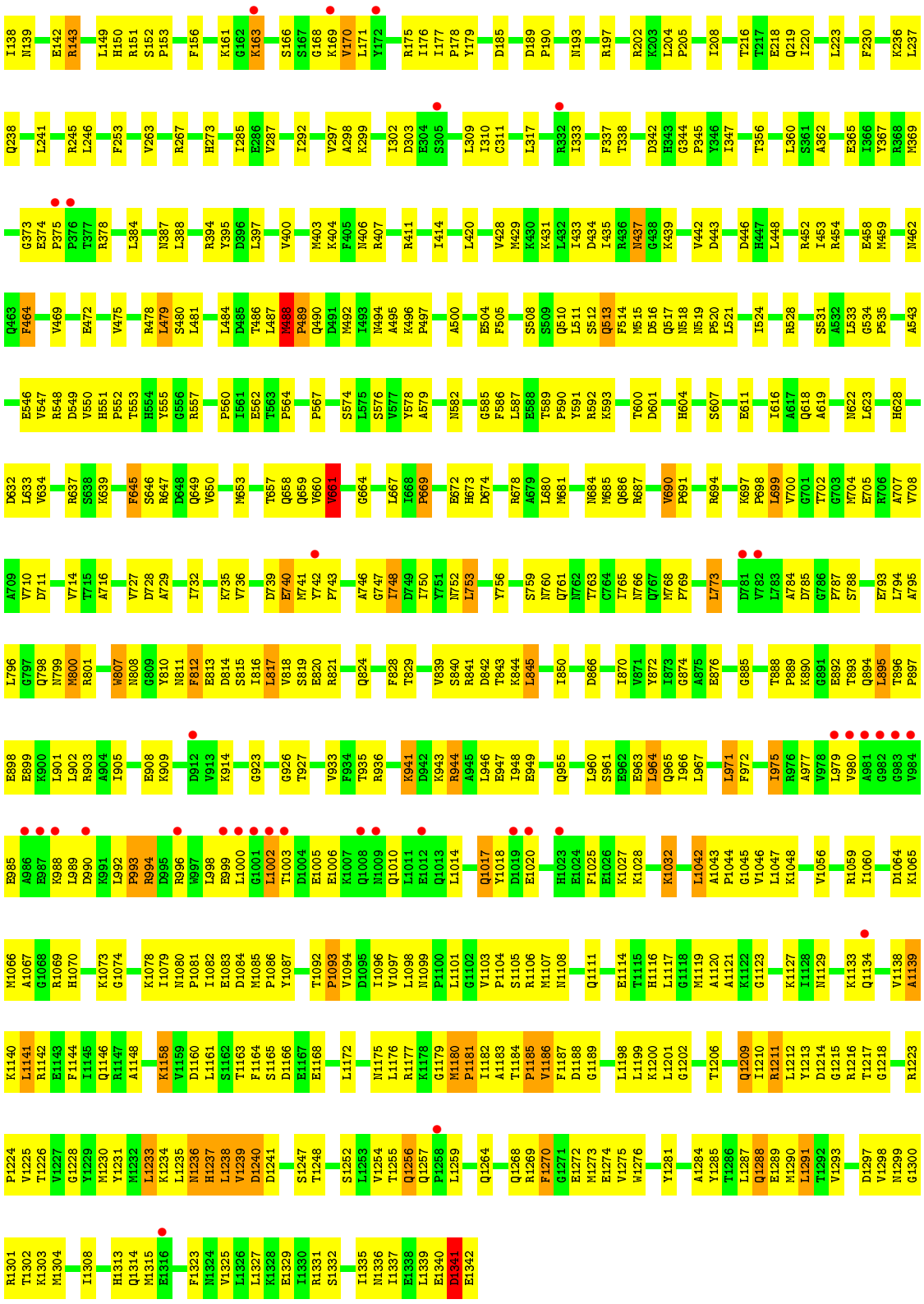
Chain C:



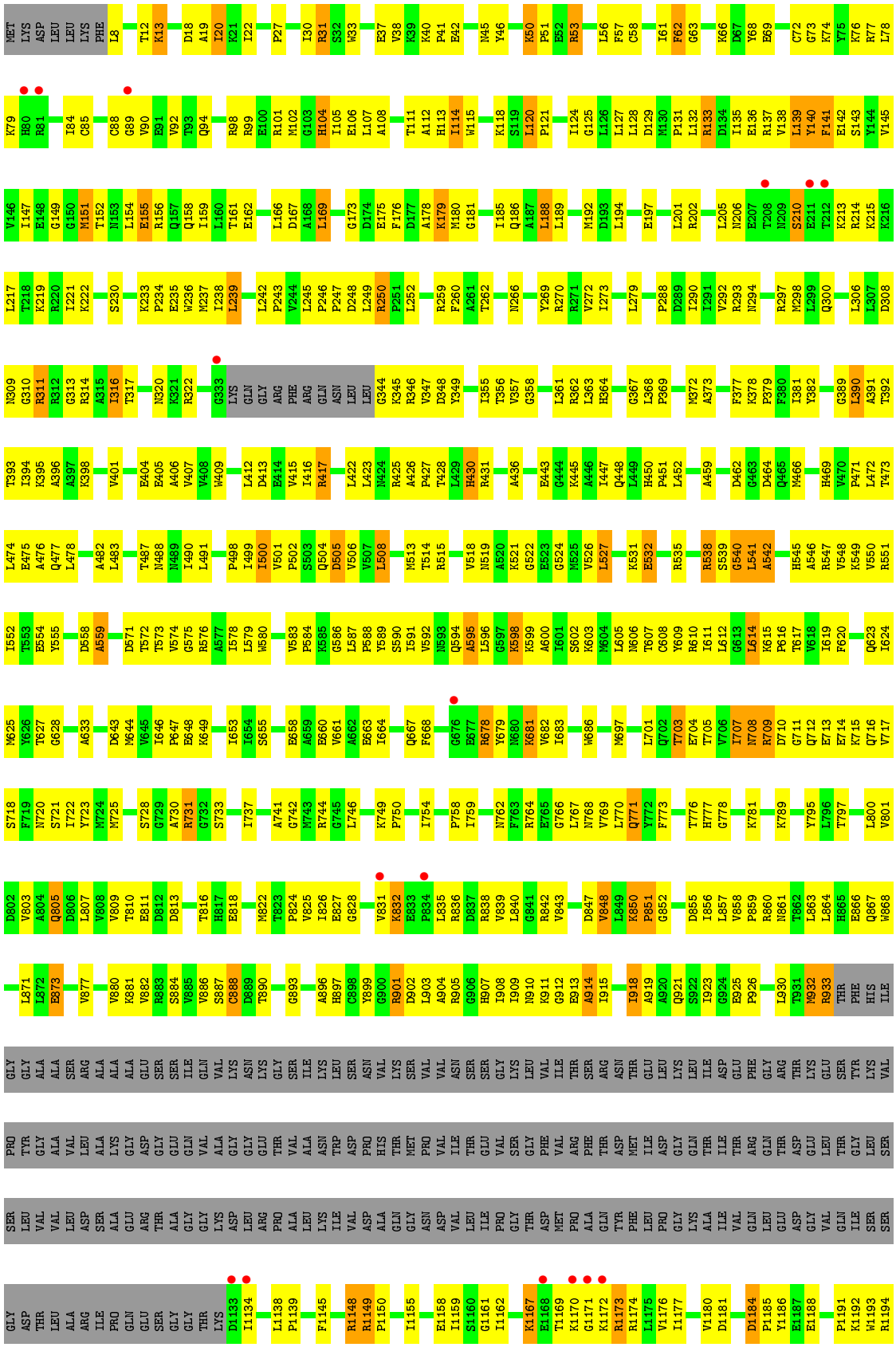


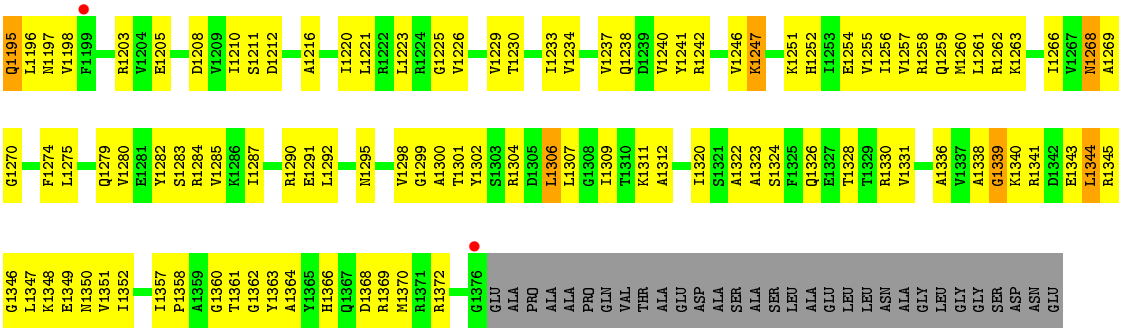
• Molecule 2: Escherichia coli RNA polymerase beta subunit





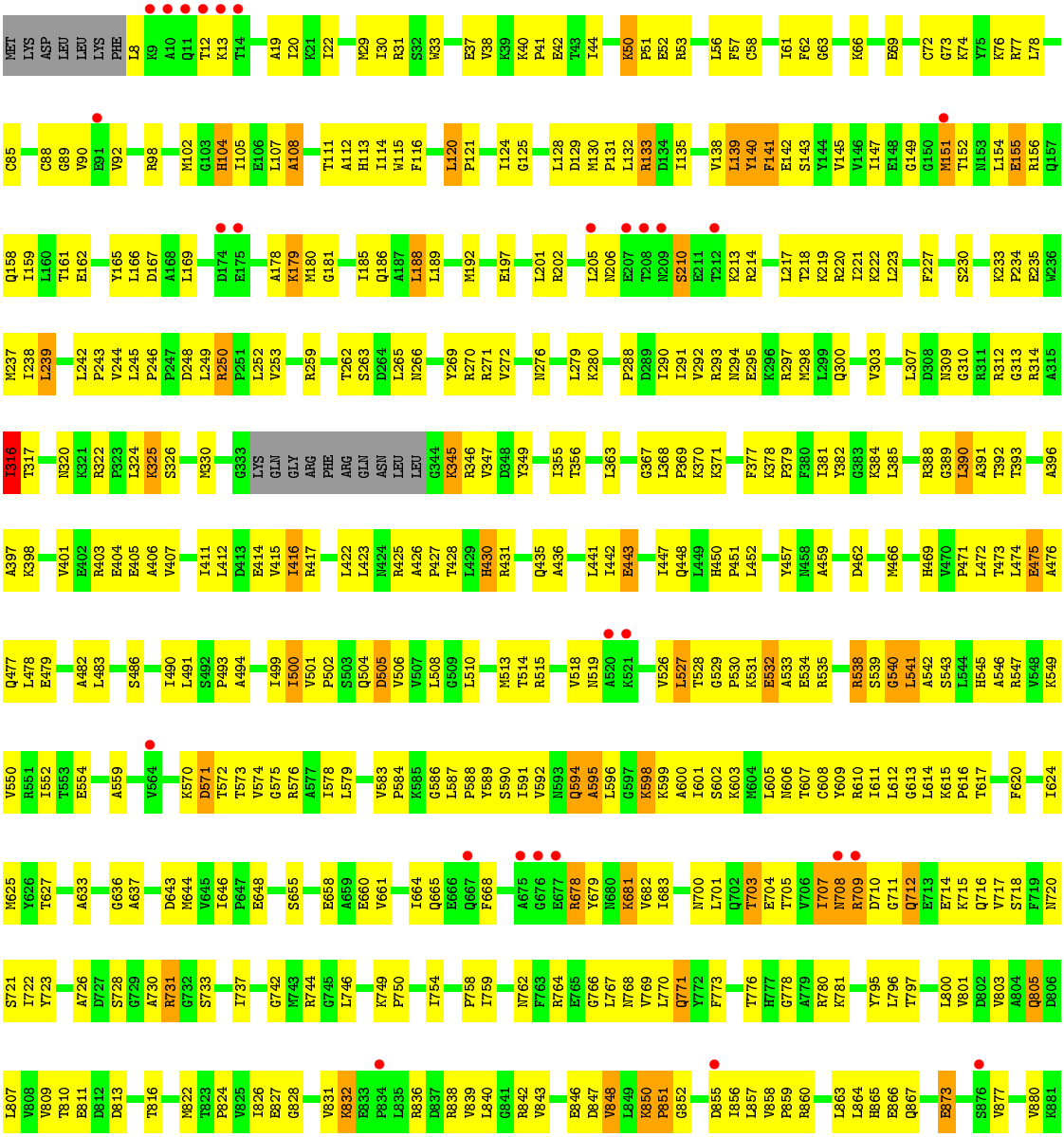
• Molecule 3: Escherichia coli RNA polymerase beta' subunit

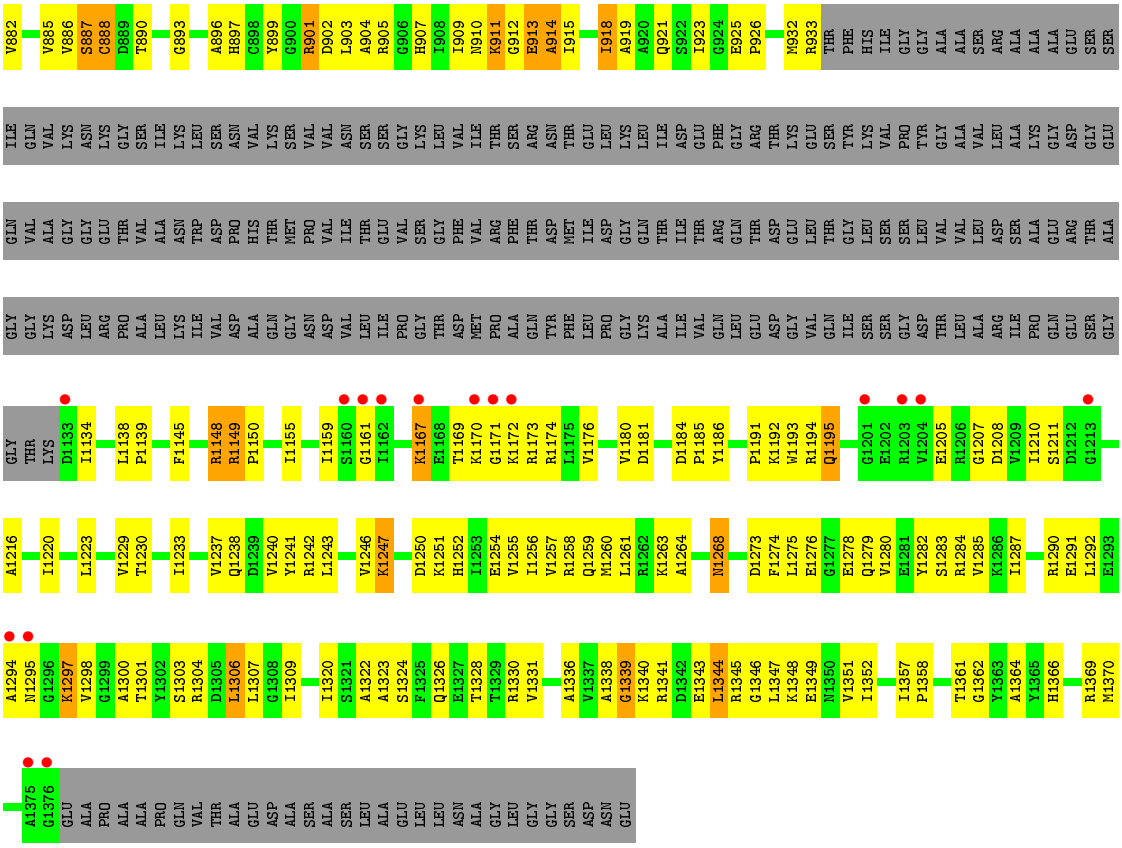




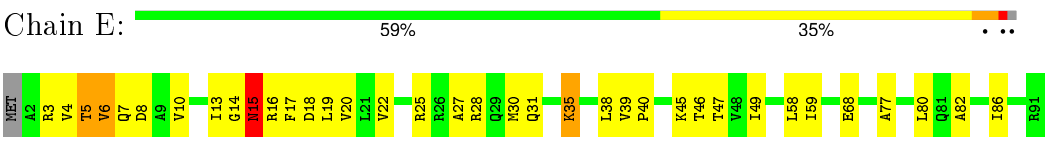
• Molecule 3: Escherichia coli RNA polymerase beta' subunit

Chain I:

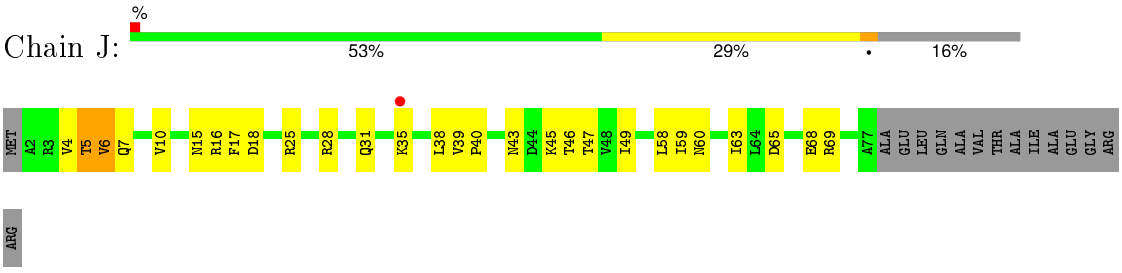




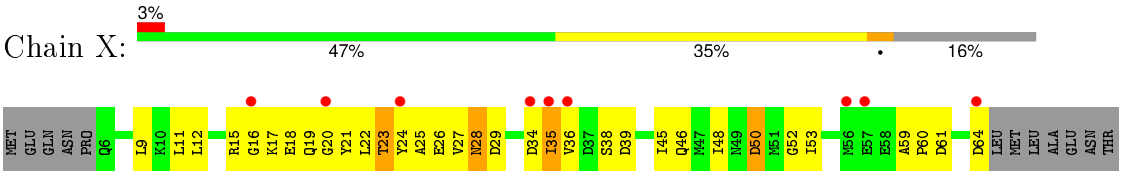
• Molecule 4: Escherichia coli RNA polymerase omega subunit

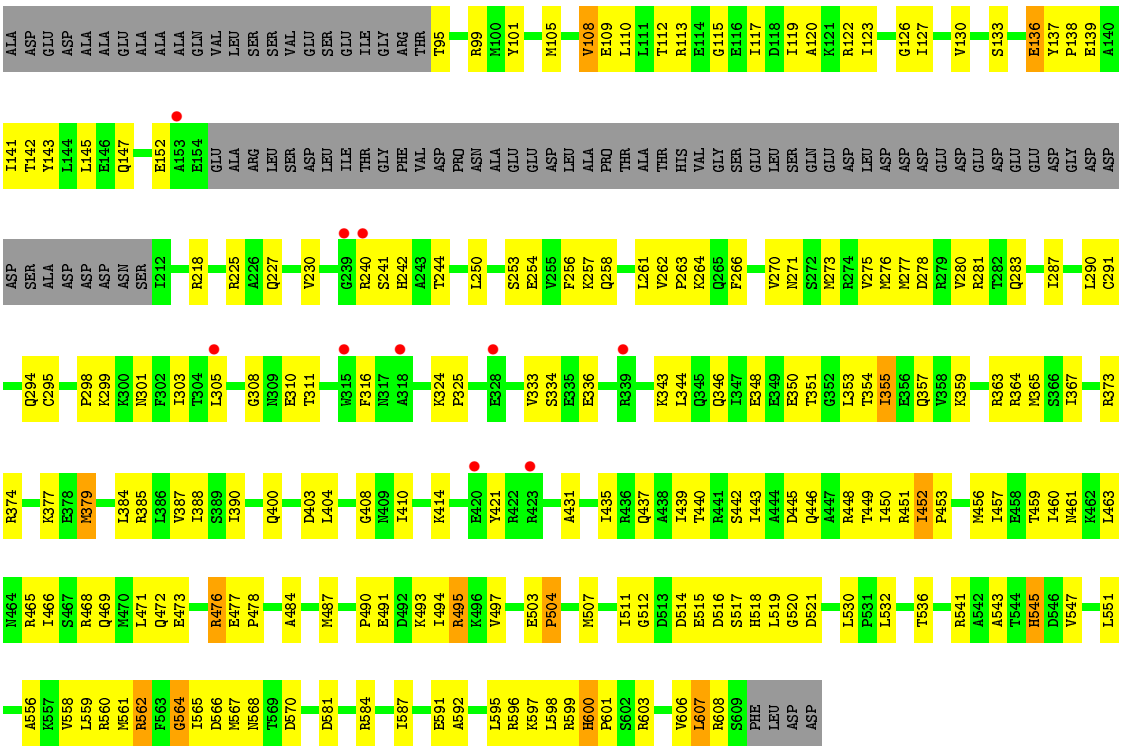


• Molecule 4: Escherichia coli RNA polymerase omega subunit



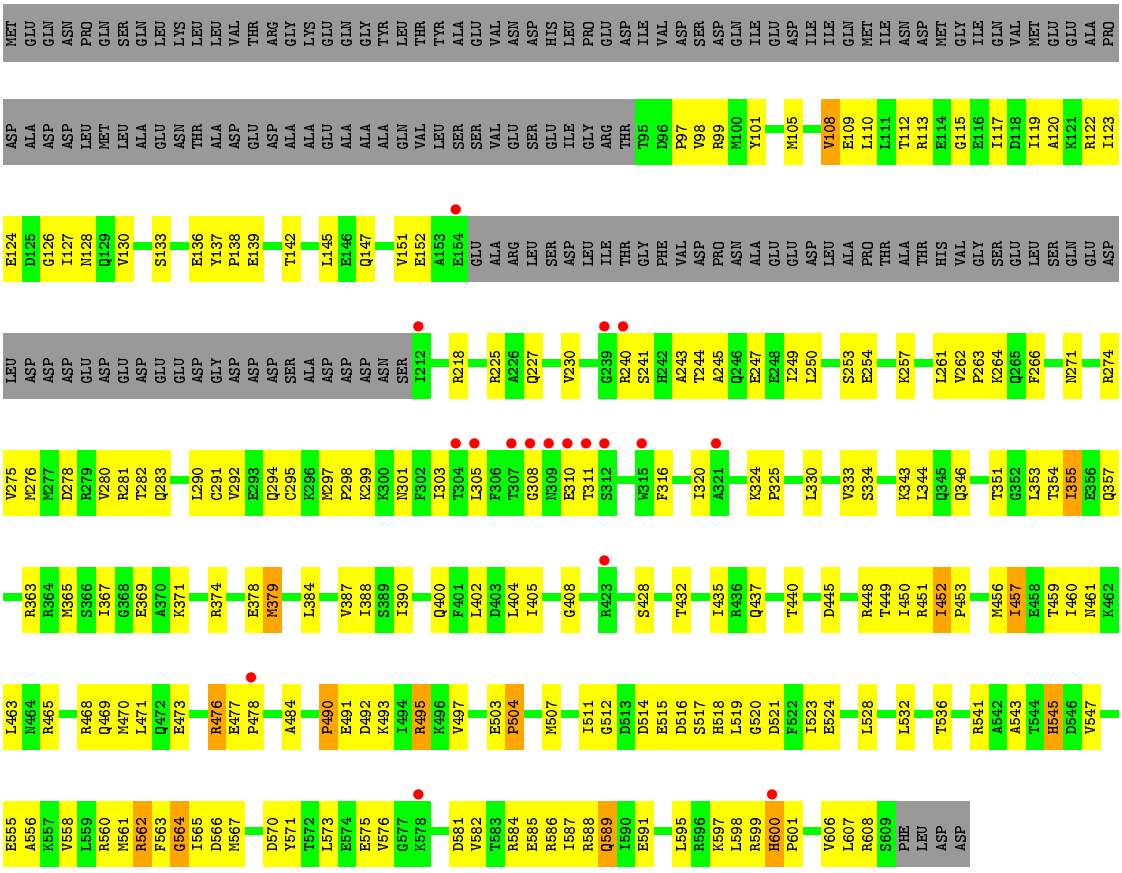
• Molecule 5: Escherichia coli RNA polymerase sigma70 subunit





- Molecule 5: Escherichia coli RNA polymerase sigma70 subunit

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	185.32Å 205.41Å 309.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 4.20 30.04 – 4.20	Depositor EDS
% Data completeness (in resolution range)	80.4 (29.94-4.20) 70.4 (30.04-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 4.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.244 , 0.322 0.264 , 0.335	Depositor DCC
R_{free} test set	3080 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	159.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 57.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 69537 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	56129	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 0O2

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	0.19	0/2548	0.36	0/3454
1	B	0.19	0/1725	0.39	0/2337
1	F	0.19	0/1797	0.38	0/2436
1	G	0.19	0/1690	0.37	0/2290
2	C	0.20	0/10690	0.38	0/14423
2	H	0.20	0/10690	0.37	0/14423
3	D	0.20	0/9198	0.38	0/12413
3	I	0.20	0/9198	0.38	0/12413
4	E	0.19	0/710	0.38	0/956
4	J	0.19	0/607	0.37	0/817
5	X	0.19	0/4253	0.36	0/5719
5	Y	0.20	0/3783	0.36	0/5083
All	All	0.20	0/56889	0.38	0/76764

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2514	0	2566	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1706	0	1738	91	0
1	F	1775	0	1800	79	0
1	G	1671	0	1706	91	0
2	C	10523	0	10546	600	0
2	H	10523	0	10546	574	0
3	D	9060	0	9257	658	0
3	I	9060	0	9257	591	0
4	E	708	0	719	52	0
4	J	605	0	612	33	0
5	X	4198	0	4250	197	0
5	Y	3732	0	3809	157	0
6	D	2	0	0	0	0
6	I	2	0	0	0	0
7	D	40	10	16	9	0
All	All	56119	10	56822	2973	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 26.

All (2973) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.23	1.20
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.24	1.18
2:H:488:MET:HB2	2:H:490:GLN:H	1.07	1.11
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.30	1.09
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.28	1.08
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.21	1.08
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.33	1.07
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.34	1.06
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.38	1.03
2:C:54:ARG:H	2:C:55:SER:HB2	1.21	1.02
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.41	1.01
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.42	1.01
2:H:54:ARG:H	2:H:55:SER:HB2	1.19	1.01
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.41	1.01
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.42	1.01
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.40	1.00
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.38	1.00
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.44	1.00
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.40	0.99
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.44	0.99
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.45	0.99
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.44	0.98
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.41	0.98
2:H:1101:LEU:HD21	3:I:508:LEU:HD12	1.46	0.98
2:H:487:LEU:HB3	2:H:488:MET:HA	1.47	0.96
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.48	0.95
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.46	0.95
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.47	0.94
1:B:12:ARG:H	1:B:30:PRO:HG2	1.30	0.94
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.47	0.94
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.47	0.94
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.50	0.93
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.50	0.93
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.48	0.93
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.49	0.93
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.50	0.92
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.50	0.92
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.49	0.92
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.51	0.91
2:C:163:LYS:H	2:C:163:LYS:HD3	1.34	0.91
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.53	0.91
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.52	0.91
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.52	0.90
2:H:488:MET:HB2	2:H:490:GLN:N	1.85	0.90
3:D:546:ALA:H	3:D:547:ARG:HA	1.34	0.90
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.54	0.90
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.54	0.89
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.54	0.89
2:C:131:THR:HG21	2:C:135:THR:HG22	1.55	0.89
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.53	0.88
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.55	0.88
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	1.53	0.88
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.03	0.88
3:I:546:ALA:H	3:I:547:ARG:HA	1.37	0.88
1:F:163:GLU:HG3	1:F:170:ARG:HH12	1.38	0.88
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.55	0.87
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.56	0.87
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.03	0.87
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.57	0.87
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.57	0.86
2:H:908:GLU:HG2	2:H:909:LYS:H	1.38	0.86
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.39	0.86
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.58	0.86
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.56	0.86
3:D:643:ASP:O	3:D:720:ASN:ND2	2.09	0.85
5:X:448:ARG:HD2	5:X:452:ILE:HD12	1.58	0.85
2:H:38:PHE:HE2	2:H:49:LEU:HD12	1.41	0.85
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.57	0.85
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.59	0.85
1:F:221:ALA:HB1	1:G:228:LEU:HD12	1.57	0.85
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.58	0.85
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.57	0.85
3:I:1247:LYS:H	3:I:1247:LYS:HD3	1.41	0.85
5:X:35:ILE:HG13	5:X:36:VAL:H	1.41	0.85
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.58	0.84
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.58	0.84
5:Y:448:ARG:HH12	5:Y:457:ILE:HD11	1.42	0.84
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.60	0.84
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.57	0.84
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.60	0.84
2:C:690:VAL:HG22	2:C:691:PRO:HD2	1.59	0.84
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.58	0.84
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.60	0.84
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.03	0.84
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.58	0.84
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.57	0.83
2:H:487:LEU:CB	2:H:488:MET:HA	2.07	0.83
3:D:1149:ARG:HD3	3:D:1149:ARG:H	1.43	0.83
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.59	0.83
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.59	0.83
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.60	0.83
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.59	0.82
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.04	0.82
2:H:513:GLN:HA	2:H:513:GLN:HE21	1.44	0.82
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.60	0.82
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.62	0.82
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.61	0.82
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.44	0.82
5:X:240:ARG:HD3	5:X:244:THR:HB	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.61	0.82
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	1.61	0.82
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.60	0.81
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.63	0.81
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.62	0.81
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.61	0.81
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.62	0.81
3:D:487:THR:HG21	4:E:4:VAL:HG12	1.60	0.81
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.63	0.81
3:D:1247:LYS:H	3:D:1247:LYS:HD3	1.45	0.81
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.44	0.81
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.46	0.81
2:H:487:LEU:HB3	2:H:488:MET:CA	2.10	0.81
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.61	0.81
4:J:5:THR:HA	4:J:6:VAL:CB	2.11	0.81
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.17	0.80
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	1.60	0.80
3:I:230:SER:HB2	3:I:1339:GLY:H	1.46	0.80
3:D:541:LEU:H	3:D:541:LEU:HD23	1.46	0.80
3:D:828:GLY:HA2	3:D:832:LYS:H	1.45	0.80
2:H:54:ARG:N	2:H:55:SER:HB2	1.96	0.80
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.64	0.80
3:I:541:LEU:H	3:I:541:LEU:HD23	1.46	0.80
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.64	0.80
4:E:5:THR:HA	4:E:6:VAL:CB	2.11	0.80
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.64	0.80
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	1.64	0.80
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.63	0.79
2:H:163:LYS:HD3	2:H:163:LYS:H	1.48	0.79
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.64	0.79
3:D:128:LEU:HD21	3:D:188:LEU:HD13	1.65	0.79
2:C:54:ARG:N	2:C:55:SER:HB2	1.98	0.78
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.65	0.78
3:D:259:ARG:HH21	5:X:504:PRO:HB2	1.49	0.78
2:C:37:LYS:HE3	2:C:37:LYS:HA	1.65	0.78
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.66	0.78
1:F:150:ARG:HH12	1:G:8:PHE:HA	1.45	0.78
3:I:610:ARG:CG	3:I:864:LEU:HD13	2.12	0.78
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.66	0.78
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.49	0.77
2:C:131:THR:CG2	2:C:135:THR:HG22	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.67	0.77
2:C:1304:MET:HE1	3:D:472:LEU:HD13	1.66	0.77
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.49	0.77
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.65	0.77
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.50	0.77
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.49	0.77
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.67	0.77
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.67	0.77
3:I:643:ASP:O	3:I:720:ASN:ND2	2.16	0.76
3:I:828:GLY:HA2	3:I:832:LYS:H	1.48	0.76
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.67	0.76
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.67	0.76
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.67	0.76
5:Y:448:ARG:HD2	5:Y:452:ILE:HD12	1.66	0.76
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.49	0.76
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.16	0.76
1:B:29:GLU:HA	1:B:200:LYS:CB	2.16	0.75
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.66	0.75
2:C:170:VAL:HG23	2:C:171:LEU:H	1.50	0.75
1:G:12:ARG:H	1:G:30:PRO:HG2	1.51	0.75
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.68	0.75
3:I:850:LYS:O	3:I:852:GLY:N	2.20	0.75
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.68	0.75
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.68	0.75
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.65	0.75
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.69	0.75
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.67	0.75
2:H:131:THR:CG2	2:H:135:THR:HG22	2.16	0.75
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.68	0.74
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	1.67	0.74
2:C:800:MET:HE2	2:C:800:MET:HA	1.67	0.74
3:I:20:ILE:HD11	3:I:1320:ILE:CD1	2.15	0.74
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.67	0.74
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.68	0.74
3:D:836:ARG:HH12	3:D:839:VAL:HB	1.53	0.74
2:C:127:ILE:HD13	2:C:127:ILE:H	1.52	0.74
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.69	0.74
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.51	0.74
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.70	0.74
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.68	0.74
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.69	0.74
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.68	0.74
3:I:422:LEU:HA	3:I:436:ALA:HA	1.69	0.74
2:H:800:MET:HE2	2:H:800:MET:HA	1.69	0.73
4:E:5:THR:HA	4:E:6:VAL:HB	1.68	0.73
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.52	0.73
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.70	0.73
4:J:5:THR:HA	4:J:6:VAL:HB	1.68	0.73
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.71	0.73
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.70	0.73
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.69	0.73
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.70	0.73
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.53	0.73
2:C:660:VAL:HG22	2:C:661:VAL:H	1.53	0.73
5:X:108:VAL:HG23	5:X:109:GLU:H	1.53	0.73
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.71	0.73
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.70	0.73
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.71	0.73
1:B:41:ASN:HD21	2:C:1217:THR:HG22	1.54	0.73
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.69	0.73
2:H:600:THR:HG22	2:H:601:ASP:H	1.53	0.73
5:X:511:ILE:HG23	5:X:512:GLY:H	1.53	0.73
2:H:660:VAL:HG22	2:H:661:VAL:H	1.53	0.73
4:E:5:THR:HB	4:E:7:GLN:HB2	1.71	0.73
3:D:546:ALA:H	3:D:547:ARG:CA	2.02	0.73
4:E:10:VAL:CG2	4:E:16:ARG:HG2	2.18	0.73
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.71	0.72
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.70	0.72
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.54	0.72
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.71	0.72
2:H:127:ILE:HD13	2:H:127:ILE:H	1.53	0.72
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.71	0.72
3:D:828:GLY:HA2	3:D:832:LYS:N	2.05	0.72
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.71	0.72
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.71	0.72
4:J:15:ASN:HD21	4:J:17:PHE:HB2	1.53	0.72
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.71	0.72
2:C:600:THR:HG22	2:C:601:ASP:H	1.53	0.72
4:J:5:THR:CA	4:J:6:VAL:HB	2.20	0.72
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.71	0.72
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.70	0.72
2:H:616:ILE:HB	2:H:637:ARG:HB2	1.71	0.72
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.71	0.72
3:D:230:SER:HB2	3:D:1339:GLY:H	1.55	0.72
3:I:1268:ASN:HB3	3:I:1300:ALA:CB	2.19	0.72
2:C:54:ARG:H	2:C:55:SER:CB	2.01	0.71
2:H:54:ARG:H	2:H:55:SER:CB	1.98	0.71
3:D:615:LYS:HD2	7:D:1503:0O2:H16	1.55	0.71
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.21	0.71
1:F:11:PRO:HG2	1:G:228:LEU:H	1.55	0.71
4:E:5:THR:HB	4:E:7:GLN:H	1.54	0.71
3:I:828:GLY:HA2	3:I:832:LYS:N	2.04	0.71
2:H:131:THR:HG23	2:H:133:ASN:H	1.54	0.71
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	1.72	0.71
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.23	0.71
2:H:21:VAL:HG13	2:H:22:LEU:H	1.56	0.71
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.25	0.71
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.73	0.71
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.19	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.71	0.71
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.56	0.71
3:D:546:ALA:N	3:D:547:ARG:HA	2.04	0.71
3:I:546:ALA:N	3:I:547:ARG:HA	2.05	0.71
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.72	0.71
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.54	0.71
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.72	0.71
5:X:112:THR:HG22	5:X:113:ARG:H	1.55	0.71
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.54	0.71
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.25	0.71
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.21	0.71
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.71	0.71
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.54	0.71
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.71	0.70
2:H:131:THR:HG21	2:H:135:THR:HG22	1.71	0.70
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.73	0.70
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.73	0.70
2:C:1042:LEU:H	2:C:1042:LEU:HD13	1.56	0.70
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.74	0.70
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.22	0.70
2:H:142:GLU:HG2	2:H:515:MET:SD	2.31	0.70
1:B:49:SER:HA	1:B:151:GLY:HA2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.56	0.70
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.72	0.70
3:I:412:LEU:O	3:I:416:ILE:HD12	1.92	0.70
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.26	0.70
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.21	0.70
2:H:309:LEU:H	2:H:309:LEU:HD23	1.55	0.70
2:H:684:ASN:HA	2:H:687:ARG:HD3	1.74	0.70
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.74	0.70
2:H:91:THR:HG22	2:H:139:ASN:H	1.57	0.70
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.56	0.70
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.74	0.70
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.21	0.70
3:I:546:ALA:H	3:I:547:ARG:CA	2.04	0.70
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.27	0.70
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.21	0.69
5:X:457:ILE:O	5:X:461:ASN:ND2	2.25	0.69
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.73	0.69
2:H:241:LEU:HD22	2:H:285:ILE:HD13	1.73	0.69
2:C:302:ILE:HA	2:C:309:LEU:HA	1.73	0.69
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.27	0.69
5:X:101:TYR:HE2	5:X:388:ILE:HD11	1.57	0.69
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.72	0.69
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.72	0.69
1:G:65:LEU:H	1:G:65:LEU:HD23	1.55	0.69
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.74	0.69
3:D:316:ILE:HG23	3:D:317:THR:H	1.57	0.69
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.72	0.69
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.73	0.69
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.92	0.69
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.57	0.69
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.28	0.69
3:D:850:LYS:O	3:D:852:GLY:N	2.25	0.69
2:C:131:THR:HG23	2:C:133:ASN:H	1.57	0.69
5:X:139:GLU:HA	5:X:142:THR:HG22	1.74	0.69
2:H:1239:VAL:O	2:H:1241:ASP:N	2.26	0.69
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.74	0.69
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.75	0.69
3:I:836:ARG:HH12	3:I:839:VAL:HB	1.56	0.69
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.74	0.69
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.74	0.69
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.56	0.69
5:X:476:ARG:H	5:X:476:ARG:HD2	1.57	0.69
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.28	0.69
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.75	0.69
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.75	0.69
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.74	0.68
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.23	0.68
2:C:309:LEU:HD23	2:C:309:LEU:H	1.56	0.68
3:D:932:MET:O	3:D:933:ARG:HG3	1.93	0.68
2:H:151:ARG:HH22	2:H:175:ARG:HH11	1.40	0.68
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.28	0.68
2:C:845:LEU:H	2:C:845:LEU:HD13	1.58	0.68
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.73	0.68
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.26	0.68
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.24	0.68
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.74	0.68
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.25	0.68
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.75	0.68
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.74	0.68
2:C:528:ARG:NH2	2:C:576:SER:O	2.27	0.68
3:D:905:ARG:HB2	4:E:16:ARG:HH12	1.59	0.68
3:D:778:GLY:HA2	3:D:781:LYS:HE3	1.75	0.68
2:H:170:VAL:HG23	2:H:171:LEU:H	1.58	0.68
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.76	0.68
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.58	0.68
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.74	0.68
3:D:142:GLU:HG2	3:D:293:ARG:HB2	1.74	0.68
1:F:192:VAL:HG21	1:F:198:LEU:HD12	1.74	0.68
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.26	0.68
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.76	0.68
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.74	0.68
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.27	0.68
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.76	0.68
3:D:609:TYR:HE2	3:D:614:LEU:HD22	1.57	0.67
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.24	0.67
2:C:488:MET:N	2:C:489:PRO:HD3	2.09	0.67
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.75	0.67
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.58	0.67
2:H:55:SER:CB	2:H:56:VAL:HG22	2.24	0.67
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.76	0.67
2:C:1239:VAL:O	2:C:1241:ASP:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:557:ARG:HB3	2:C:587:LEU:HD23	1.76	0.67
2:H:845:LEU:H	2:H:845:LEU:HD13	1.57	0.67
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.77	0.67
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.74	0.67
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.93	0.67
2:H:1042:LEU:H	2:H:1042:LEU:HD13	1.59	0.67
3:I:133:ARG:O	3:I:133:ARG:NH2	2.26	0.67
2:C:20:GLN:O	2:C:22:LEU:N	2.27	0.67
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.76	0.67
3:D:590:SER:O	3:D:594:GLN:N	2.27	0.67
1:A:90:VAL:HG13	1:A:121:VAL:HG13	1.76	0.67
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.30	0.67
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.77	0.67
1:G:45:ARG:O	3:I:538:ARG:NH2	2.27	0.67
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.76	0.67
3:D:362:ARG:HH12	7:D:1503:0O2:H7	1.58	0.67
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.27	0.67
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.77	0.67
3:D:711:GLY:O	3:D:712:GLN:HG2	1.94	0.67
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.27	0.67
2:H:99:LYS:N	2:H:99:LYS:HD3	2.09	0.67
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.74	0.67
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.77	0.67
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.28	0.67
2:C:843:THR:HG22	2:C:844:LYS:H	1.60	0.67
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.59	0.67
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.58	0.67
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.09	0.67
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.27	0.67
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.76	0.67
2:C:403:MET:HG3	2:C:414:ILE:HB	1.77	0.67
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.77	0.66
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.77	0.66
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.60	0.66
2:C:55:SER:CB	2:C:56:VAL:HG22	2.25	0.66
3:D:588:PRO:HG2	3:D:591:ILE:HD11	1.76	0.66
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.26	0.66
2:C:533:LEU:HD23	2:C:533:LEU:H	1.60	0.66
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.76	0.66
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.24	0.66
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.78	0.66
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.60	0.66
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	1.77	0.66
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.78	0.66
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.61	0.66
2:H:55:SER:CB	2:H:56:VAL:HG13	2.25	0.66
3:D:822:MET:SD	3:D:838:ARG:NH1	2.69	0.66
2:C:106:GLU:N	2:C:107:ARG:HA	2.08	0.66
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.10	0.66
2:H:528:ARG:NH2	2:H:576:SER:O	2.29	0.66
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.78	0.66
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.77	0.66
3:I:1167:LYS:HB3	3:I:1170:LYS:HD2	1.77	0.66
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.77	0.66
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.25	0.66
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.26	0.66
2:H:923:GLY:HA2	3:I:371:LYS:HE3	1.78	0.66
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.26	0.66
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.78	0.66
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.61	0.66
2:C:756:TYR:H	2:C:766:ASN:HB3	1.61	0.66
2:H:152:SER:HG	2:H:404:LYS:HZ2	1.42	0.66
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.78	0.66
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.61	0.65
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.78	0.65
3:D:139:LEU:HD21	3:D:185:ILE:HD13	1.76	0.65
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.60	0.65
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.77	0.65
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.77	0.65
2:H:488:MET:CB	2:H:490:GLN:H	1.95	0.65
3:I:527:LEU:HD13	3:I:531:LYS:HB3	1.78	0.65
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.29	0.65
2:C:202:ARG:HD3	5:X:35:ILE:HB	1.77	0.65
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.60	0.65
3:I:644:MET:O	3:I:764:ARG:NH1	2.29	0.65
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.76	0.65
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.78	0.65
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.79	0.65
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.79	0.65
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.78	0.65
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:5:THR:CA	4:E:6:VAL:HB	2.25	0.65
1:F:11:PRO:CG	1:G:228:LEU:H	2.10	0.65
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.10	0.65
3:I:827:GLU:O	3:I:831:VAL:HG12	1.96	0.65
3:I:708:ASN:OD1	3:I:712:GLN:HB2	1.97	0.65
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.78	0.65
2:H:1140:LYS:HE2	2:H:1166:ASP:HB3	1.78	0.65
2:C:1273:MET:HB3	3:D:428:THR:HB	1.79	0.65
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.62	0.65
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.79	0.65
3:D:588:PRO:CG	3:D:591:ILE:HD11	2.27	0.65
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.60	0.65
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.78	0.65
3:I:504:GLN:HA	3:I:730:ALA:HA	1.78	0.65
3:D:527:LEU:HD13	3:D:531:LYS:HB3	1.79	0.65
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.78	0.65
2:H:1288:GLN:HA	2:H:1288:GLN:HE21	1.62	0.64
2:H:106:GLU:N	2:H:107:ARG:HA	2.10	0.64
2:H:484:LEU:H	2:H:484:LEU:HD22	1.62	0.64
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.28	0.64
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.78	0.64
3:I:145:VAL:HG22	3:I:180:MET:SD	2.37	0.64
2:C:189:ASP:OD1	2:C:193:ASN:N	2.24	0.64
2:H:360:LEU:HD13	2:H:378:ARG:HH11	1.62	0.64
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.11	0.64
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.33	0.64
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.12	0.64
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.13	0.64
2:H:667:LEU:O	2:H:1069:ARG:NH2	2.31	0.64
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.78	0.64
3:I:711:GLY:O	3:I:712:GLN:HG2	1.97	0.64
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.63	0.64
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.79	0.64
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.63	0.64
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.79	0.64
2:C:897:PRO:HB3	5:X:564:GLY:O	1.97	0.64
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.32	0.64
1:B:227:GLN:O	1:B:228:LEU:HG	1.96	0.64
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.80	0.64
2:H:504:GLU:O	2:H:508:SER:HB3	1.98	0.64
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:514:THR:HG23	3:I:576:ARG:HE	1.63	0.64
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.13	0.64
3:I:590:SER:O	3:I:594:GLN:N	2.30	0.64
3:I:1297:LYS:NZ	3:I:1297:LYS:HA	2.13	0.64
3:D:405:GLU:O	3:D:407:VAL:N	2.30	0.64
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.30	0.64
2:C:55:SER:CB	2:C:56:VAL:HG13	2.26	0.64
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.62	0.64
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.79	0.64
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.63	0.64
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.77	0.63
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.80	0.63
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.79	0.63
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.80	0.63
4:J:15:ASN:HD22	4:J:18:ASP:H	1.44	0.63
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.80	0.63
3:D:614:LEU:HG	4:E:5:THR:HG21	1.79	0.63
3:I:809:VAL:HG13	3:I:912:GLY:H	1.64	0.63
3:I:1155:ILE:HG13	3:I:1210:ILE:CG2	2.28	0.63
2:H:1237:HIS:O	2:H:1238:LEU:HG	1.99	0.63
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.78	0.63
3:D:932:MET:SD	3:D:932:MET:N	2.67	0.63
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.81	0.63
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.79	0.63
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.80	0.63
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.32	0.63
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.80	0.63
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.29	0.63
3:I:598:LYS:NZ	3:I:726:ALA:O	2.32	0.63
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.81	0.63
1:A:284:ARG:NH1	1:A:288:GLU:HG3	2.13	0.63
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.29	0.63
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.30	0.63
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.81	0.63
2:H:1273:MET:HB3	3:I:428:THR:HB	1.81	0.63
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.26	0.63
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.80	0.63
3:D:27:PRO:O	3:D:31:ARG:HD3	1.98	0.63
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.30	0.63
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.63	0.63
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.81	0.63
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.32	0.62
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.29	0.62
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.63	0.62
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.33	0.62
3:I:513:MET:HE2	3:I:579:LEU:HB2	1.81	0.62
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.13	0.62
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.17	0.62
3:D:573:THR:HG22	3:D:576:ARG:CG	2.29	0.62
1:A:11:PRO:HD3	1:B:227:GLN:HG3	1.80	0.62
2:C:21:VAL:HG13	2:C:22:LEU:H	1.63	0.62
2:H:176:ILE:HD11	2:H:428:VAL:HG21	1.81	0.62
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.19	0.62
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.34	0.62
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.82	0.62
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.82	0.62
2:C:634:VAL:H	2:C:645:PHE:HE2	1.47	0.62
2:H:1252:SER:OG	2:H:1255:THR:O	2.17	0.62
2:C:714:VAL:HG23	2:C:787:PRO:HD2	1.82	0.62
2:H:678:ARG:HE	2:H:1106:ARG:HG2	1.65	0.62
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.30	0.62
2:H:20:GLN:O	2:H:22:LEU:N	2.32	0.62
2:H:91:THR:HG22	2:H:139:ASN:N	2.14	0.62
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.15	0.62
3:I:579:LEU:HD23	3:I:627:THR:HG21	1.81	0.62
3:D:107:LEU:HD12	3:D:107:LEU:H	1.64	0.62
2:H:562:GLU:HG2	2:H:574:SER:CB	2.29	0.62
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.65	0.62
4:E:5:THR:HA	4:E:6:VAL:CG1	2.30	0.62
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.14	0.62
3:D:77:ARG:HG3	3:D:78:LEU:H	1.62	0.62
2:H:660:VAL:O	2:H:661:VAL:HG22	2.00	0.62
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.32	0.62
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.82	0.62
2:C:901:LEU:O	2:C:905:ILE:HG13	2.00	0.62
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.64	0.62
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.64	0.62
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.25	0.62
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.14	0.62
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.82	0.62
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.82	0.62
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.82	0.62
4:E:5:THR:HA	4:E:6:VAL:HG12	1.82	0.61
1:B:49:SER:OG	3:D:538:ARG:NH2	2.33	0.61
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.81	0.61
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.81	0.61
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.81	0.61
2:C:1244:HIS:HB3	2:C:1265:PHE:CD2	2.34	0.61
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.29	0.61
3:I:213:LYS:O	3:I:217:LEU:HG	1.99	0.61
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.82	0.61
3:D:768:ASN:O	3:D:771:GLN:NE2	2.34	0.61
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.65	0.61
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.33	0.61
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.01	0.61
2:H:908:GLU:HG2	2:H:909:LYS:N	2.14	0.61
1:B:227:GLN:O	1:B:229:GLU:N	2.30	0.61
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.81	0.61
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.82	0.61
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.29	0.61
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.81	0.61
1:F:9:LEU:O	1:G:227:GLN:NE2	2.33	0.61
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.31	0.61
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.01	0.61
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.27	0.61
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.33	0.61
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.34	0.61
4:J:5:THR:HA	4:J:6:VAL:CG1	2.30	0.61
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.23	0.61
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.65	0.61
3:D:720:ASN:O	3:D:722:ILE:N	2.34	0.61
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.16	0.61
3:I:139:LEU:HD13	3:I:140:TYR:N	2.16	0.61
2:H:152:SER:OG	2:H:404:LYS:NZ	2.25	0.61
3:I:77:ARG:HG3	3:I:78:LEU:H	1.64	0.61
2:H:487:LEU:HB3	2:H:488:MET:CG	2.30	0.61
3:I:107:LEU:HD12	3:I:107:LEU:H	1.65	0.61
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.29	0.61
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.82	0.61
3:D:422:LEU:HA	3:D:436:ALA:HA	1.83	0.61
3:D:1362:GLY:O	3:D:1364:ALA:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.82	0.61
3:D:1191:PRO:O	3:D:1193:TRP:N	2.32	0.61
3:I:1191:PRO:O	3:I:1193:TRP:N	2.33	0.61
3:D:527:LEU:HD12	3:D:535:ARG:NE	2.15	0.61
3:D:139:LEU:HD13	3:D:140:TYR:N	2.16	0.61
3:D:827:GLU:O	3:D:831:VAL:HG12	2.00	0.61
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.83	0.61
2:H:517:GLN:HE21	2:H:760:ASN:H	1.48	0.61
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.83	0.61
2:C:91:THR:HG22	2:C:139:ASN:H	1.65	0.61
1:B:65:LEU:HD23	1:B:65:LEU:H	1.65	0.61
2:H:714:VAL:HG23	2:H:787:PRO:HD2	1.83	0.61
2:H:55:SER:HB3	2:H:56:VAL:CB	2.31	0.60
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.36	0.60
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.32	0.60
2:H:618:GLN:OE1	2:H:637:ARG:NH1	2.33	0.60
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.65	0.60
1:G:49:SER:OG	3:I:538:ARG:NH2	2.33	0.60
3:I:1297:LYS:HA	3:I:1297:LYS:HZ3	1.66	0.60
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.66	0.60
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.83	0.60
3:D:1338:ALA:O	3:D:1340:LYS:N	2.34	0.60
4:E:13:ILE:HD11	4:E:19:LEU:HD23	1.82	0.60
1:G:191:ARG:NH2	3:I:442:ILE:HA	2.17	0.60
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.67	0.60
3:I:233:LYS:HD2	3:I:234:PRO:HD2	1.83	0.60
2:H:892:GLU:O	2:H:893:THR:OG1	2.19	0.60
2:C:747:GLY:O	2:C:748:ILE:HG13	2.00	0.60
2:C:752:ASN:O	2:C:753:LEU:HG	2.01	0.60
2:H:1304:MET:HE1	3:I:472:LEU:HD13	1.83	0.60
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.82	0.60
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.36	0.60
3:I:252:LEU:HD23	3:I:252:LEU:H	1.66	0.60
2:C:517:GLN:HE21	2:C:760:ASN:H	1.49	0.60
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.83	0.60
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.84	0.60
3:D:202:ARG:O	3:D:206:ASN:ND2	2.34	0.60
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.82	0.60
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.82	0.60
5:X:584:ARG:O	5:X:587:ILE:HG22	2.01	0.60
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:595:LEU:O	5:X:599:ARG:NH1	2.35	0.60
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.34	0.60
4:J:5:THR:HB	4:J:7:GLN:HB2	1.83	0.60
1:G:181:GLU:HG2	3:I:531:LYS:HD3	1.83	0.60
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.84	0.60
1:G:191:ARG:HH22	3:I:442:ILE:HA	1.67	0.60
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.35	0.60
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.82	0.60
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.83	0.60
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.35	0.60
5:X:240:ARG:O	5:X:242:HIS:N	2.34	0.60
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.66	0.60
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.16	0.60
2:C:1252:SER:OG	2:C:1255:THR:O	2.19	0.60
2:C:963:GLU:O	2:C:966:ILE:HG22	2.02	0.60
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.84	0.60
5:X:9:LEU:HD22	5:X:60:PRO:HB3	1.82	0.60
2:C:562:GLU:HG2	2:C:574:SER:CB	2.31	0.60
3:D:500:ILE:H	3:D:500:ILE:HD13	1.65	0.60
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.02	0.60
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.35	0.60
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.65	0.60
3:D:145:VAL:HG22	3:D:180:MET:SD	2.41	0.60
3:D:85:CYS:HB3	3:D:88:CYS:O	2.02	0.60
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.32	0.60
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.17	0.60
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.37	0.60
2:H:800:MET:HA	2:H:800:MET:CE	2.32	0.60
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.17	0.60
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.35	0.60
3:D:128:LEU:CD1	3:D:192:MET:HE3	2.28	0.60
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.17	0.60
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.84	0.60
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.65	0.60
3:D:579:LEU:HD23	3:D:627:THR:HG21	1.82	0.60
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.83	0.60
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.83	0.60
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.66	0.60
3:D:252:LEU:HD23	3:D:252:LEU:H	1.67	0.60
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.67	0.60
2:H:894:GLN:HE21	3:I:77:ARG:HD3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:151:MET:N	3:D:151:MET:SD	2.74	0.60
3:I:1338:ALA:O	3:I:1340:LYS:N	2.35	0.60
2:C:660:VAL:O	2:C:661:VAL:HG22	2.01	0.59
3:D:546:ALA:HB3	3:D:547:ARG:O	2.02	0.59
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.36	0.59
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.83	0.59
3:I:681:LYS:HB2	3:I:681:LYS:NZ	2.17	0.59
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.67	0.59
2:H:646:SER:HB2	2:H:649:GLN:HG3	1.84	0.59
3:D:473:THR:HB	3:D:476:ALA:HB2	1.83	0.59
3:D:66:LYS:HG3	3:D:69:GLU:OE2	2.01	0.59
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.83	0.59
3:D:583:VAL:CG1	3:D:587:LEU:HD22	2.31	0.59
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.30	0.59
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.83	0.59
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.32	0.59
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.32	0.59
4:J:5:THR:HA	4:J:6:VAL:HG12	1.82	0.59
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.85	0.59
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.68	0.59
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.17	0.59
3:I:720:ASN:O	3:I:722:ILE:N	2.35	0.59
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.84	0.59
2:C:619:ALA:HA	2:C:653:MET:HE2	1.84	0.59
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.84	0.59
2:H:543:ALA:HB1	2:H:548:ARG:HD2	1.85	0.59
2:C:163:LYS:HD3	2:C:163:LYS:N	2.14	0.59
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.33	0.59
3:D:316:ILE:HG23	3:D:317:THR:N	2.17	0.59
2:H:130:MET:SD	2:H:134:GLY:HA2	2.42	0.59
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.18	0.59
2:C:372:PRO:CB	5:X:34:ASP:HB3	2.31	0.59
5:X:442:SER:OG	5:X:446:GLN:NE2	2.34	0.59
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.68	0.59
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.85	0.59
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.85	0.59
3:D:858:VAL:HB	3:D:859:PRO:CD	2.26	0.59
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.83	0.59
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.85	0.59
3:I:50:LYS:NZ	3:I:50:LYS:HB3	2.18	0.59
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:45:LYS:O	4:E:49:ILE:HG12	2.03	0.59
3:D:125:GLY:O	3:D:129:ASP:N	2.36	0.59
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.83	0.59
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.15	0.59
2:C:801:ARG:NH1	2:C:1093:PRO:O	2.36	0.59
2:H:94:ALA:N	2:H:126:GLU:OE2	2.27	0.59
1:G:176:CYS:O	1:G:178:SER:N	2.33	0.59
3:D:213:LYS:O	3:D:217:LEU:HG	2.01	0.59
3:D:589:TYR:O	3:D:591:ILE:N	2.34	0.59
3:I:1261:LEU:CD2	3:I:1306:LEU:HD22	2.32	0.59
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.33	0.59
2:C:91:THR:HG22	2:C:138:ILE:HA	1.85	0.59
3:D:313:GLY:H	5:X:38:SER:HB3	1.67	0.59
3:D:389:GLY:O	3:D:391:ALA:N	2.36	0.59
2:H:69:GLN:HE22	2:H:101:ARG:HH21	1.50	0.59
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.02	0.59
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.32	0.59
2:H:302:ILE:HG22	2:H:309:LEU:HB3	1.85	0.59
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.85	0.59
3:I:128:LEU:HD11	3:I:188:LEU:HD22	1.84	0.59
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.85	0.59
4:E:14:GLY:O	4:E:15:ASN:ND2	2.36	0.59
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.03	0.59
2:C:1288:GLN:HE21	2:C:1288:GLN:HA	1.68	0.59
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	1.84	0.59
5:X:515:GLU:N	5:X:516:ASP:HA	2.18	0.59
3:I:704:GLU:HB2	3:I:718:SER:HG	1.67	0.59
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.18	0.58
5:Y:119:ILE:HG21	5:Y:379:MET:HG2	1.85	0.58
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.28	0.58
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.67	0.58
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.37	0.58
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.86	0.58
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.86	0.58
3:I:85:CYS:HB3	3:I:88:CYS:O	2.02	0.58
3:I:707:ILE:HG22	3:I:708:ASN:H	1.68	0.58
2:H:99:LYS:H	2:H:99:LYS:HD3	1.68	0.58
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.39	0.58
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.39	0.58
3:D:114:ILE:HG21	3:D:308:ASP:HB3	1.83	0.58
2:C:42:ASP:O	2:C:44:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:809:VAL:HG13	3:D:912:GLY:H	1.66	0.58
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.85	0.58
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.33	0.58
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.34	0.58
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.18	0.58
3:I:768:ASN:O	3:I:771:GLN:NE2	2.37	0.58
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.36	0.58
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.84	0.58
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.18	0.58
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.84	0.58
2:C:387:ASN:HB3	2:C:394:ARG:HG3	1.86	0.58
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.04	0.58
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.03	0.58
3:I:142:GLU:HG2	3:I:293:ARG:HB2	1.84	0.58
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.02	0.58
2:H:747:GLY:O	2:H:748:ILE:HG13	2.03	0.58
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.85	0.58
3:I:550:VAL:HG23	3:I:552:ILE:HD11	1.86	0.58
5:X:517:SER:O	5:X:518:HIS:ND1	2.37	0.58
3:D:19:ALA:HA	3:D:1344:LEU:HD12	1.86	0.58
2:C:800:MET:HA	2:C:800:MET:CE	2.34	0.58
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.34	0.58
3:D:504:GLN:HA	3:D:730:ALA:HA	1.84	0.58
3:I:246:PRO:HB2	3:I:249:LEU:HD13	1.85	0.58
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.68	0.58
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.86	0.58
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.85	0.58
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.19	0.58
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.84	0.58
3:I:701:LEU:HD23	3:I:723:TYR:HB2	1.86	0.58
2:C:1200:LYS:O	2:C:1202:GLY:N	2.34	0.58
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.86	0.58
2:C:166:SER:O	2:C:168:GLY:N	2.34	0.58
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.37	0.58
1:A:104:LYS:HD3	1:A:105:SER:N	2.19	0.58
2:H:1101:LEU:CD1	3:I:504:GLN:HB2	2.28	0.58
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.39	0.58
1:G:49:SER:HA	1:G:151:GLY:HA2	1.86	0.58
3:D:709:ARG:O	3:D:711:GLY:N	2.37	0.58
3:I:478:LEU:HD12	4:J:47:THR:HG23	1.86	0.58
3:I:591:ILE:HA	3:I:594:GLN:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.68	0.58
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.39	0.58
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.85	0.58
2:H:237:LEU:HD13	2:H:292:ILE:HD12	1.85	0.58
3:I:125:GLY:O	3:I:129:ASP:N	2.37	0.58
2:C:54:ARG:HG2	2:C:55:SER:CB	2.34	0.57
3:D:610:ARG:CG	3:D:864:LEU:HD13	2.27	0.57
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.85	0.57
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.19	0.57
3:I:389:GLY:O	3:I:391:ALA:N	2.37	0.57
2:C:898:GLU:N	2:C:898:GLU:OE1	2.34	0.57
2:C:55:SER:HB3	2:C:56:VAL:CB	2.34	0.57
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.29	0.57
5:X:35:ILE:HG23	5:X:36:VAL:HG13	1.86	0.57
5:Y:457:ILE:HG23	5:Y:461:ASN:HD21	1.69	0.57
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.33	0.57
1:B:176:CYS:C	1:B:178:SER:H	2.08	0.57
2:H:189:ASP:OD1	2:H:193:ASN:N	2.31	0.57
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.86	0.57
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.69	0.57
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.86	0.57
3:D:179:LYS:H	3:D:179:LYS:HD3	1.69	0.57
5:Y:283:GLN:NE2	5:Y:343:LYS:HD2	2.19	0.57
1:B:64:VAL:HG13	1:B:69:SER:OG	2.04	0.57
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.19	0.57
3:I:1297:LYS:CE	3:I:1297:LYS:HA	2.34	0.57
3:D:393:THR:HG21	5:X:607:LEU:HD22	1.86	0.57
3:D:395:LYS:HG3	5:X:536:THR:CG2	2.34	0.57
1:F:181:GLU:OE1	1:F:181:GLU:N	2.38	0.57
2:C:94:ALA:N	2:C:126:GLU:OE2	2.25	0.57
2:C:406:ASN:HB3	2:C:411:ARG:HB2	1.85	0.57
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.04	0.57
2:H:1200:LYS:O	2:H:1202:GLY:N	2.36	0.57
3:D:120:LEU:CB	3:D:121:PRO:CD	2.81	0.57
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.86	0.57
3:D:619:ILE:HD13	7:D:1503:0O2:O3D	2.05	0.57
3:D:423:LEU:CD2	3:D:447:ILE:HD11	2.35	0.57
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.86	0.57
5:X:17:LYS:N	5:X:18:GLU:HA	2.19	0.57
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.86	0.57
1:G:19:VAL:O	1:G:20:SER:OG	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.87	0.57
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.37	0.57
2:C:24:VAL:HG11	2:C:704:MET:HE1	1.87	0.57
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.05	0.57
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.39	0.57
3:I:202:ARG:O	3:I:206:ASN:ND2	2.33	0.57
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.40	0.57
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.34	0.57
3:I:704:GLU:HB2	3:I:718:SER:OG	2.05	0.57
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.69	0.57
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.86	0.57
3:D:1343:GLU:HA	3:D:1344:LEU:CB	2.31	0.57
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.86	0.57
3:I:1280:VAL:HA	3:I:1283:SER:HB2	1.87	0.57
3:I:824:PRO:O	3:I:826:ILE:HG13	2.05	0.57
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.86	0.57
1:A:318:LEU:O	1:A:320:ASN:N	2.33	0.57
2:H:533:LEU:HD23	2:H:533:LEU:H	1.69	0.57
5:X:503:GLU:N	5:X:504:PRO:HA	2.20	0.57
3:I:905:ARG:HG2	3:I:907:HIS:H	1.70	0.57
2:C:106:GLU:H	2:C:107:ARG:HA	1.70	0.57
2:H:753:LEU:O	2:H:753:LEU:HD12	2.05	0.57
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.85	0.57
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.40	0.57
3:D:886:VAL:CG1	3:D:1230:THR:HG21	2.35	0.57
2:C:403:MET:HG2	2:C:407:ARG:HH12	1.70	0.57
4:E:15:ASN:HD21	4:E:18:ASP:HB2	1.70	0.57
3:I:88:CYS:O	3:I:90:VAL:N	2.38	0.57
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.70	0.56
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.05	0.56
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.34	0.56
3:D:417:ARG:HH12	4:E:3:ARG:HH22	1.53	0.56
1:B:42:ALA:O	1:B:46:ILE:HG12	2.04	0.56
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.85	0.56
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.87	0.56
1:A:227:GLN:HE22	1:B:11:PRO:HD3	1.71	0.56
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.05	0.56
2:H:496:LYS:N	2:H:497:PRO:HD2	2.20	0.56
1:B:65:LEU:HA	1:B:169:GLY:HA2	1.87	0.56
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.40	0.56
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:141:PHE:O	3:D:297:ARG:HD3	2.04	0.56
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.35	0.56
2:C:542:ARG:O	2:C:544:GLY:N	2.34	0.56
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.88	0.56
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.04	0.56
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.31	0.56
3:I:546:ALA:HB3	3:I:547:ARG:O	2.06	0.56
5:X:503:GLU:HB3	5:X:504:PRO:O	2.05	0.56
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.35	0.56
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.05	0.56
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.35	0.56
2:H:548:ARG:NH2	2:H:567:PRO:O	2.39	0.56
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.87	0.56
2:H:1111:GLN:HG3	2:H:1230:MET:HE2	1.87	0.56
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.70	0.56
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.38	0.56
3:I:919:ALA:O	3:I:923:ILE:HG12	2.05	0.56
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.70	0.56
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.25	0.56
5:X:390:ILE:HD11	5:X:435:ILE:CG2	2.35	0.56
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.20	0.56
3:D:316:ILE:HG13	3:D:317:THR:N	2.21	0.56
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.36	0.56
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.86	0.56
1:A:232:VAL:HA	1:B:218:ARG:HG3	1.87	0.56
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.41	0.56
3:D:850:LYS:HD2	3:D:851:PRO:CD	2.26	0.56
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.35	0.56
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.86	0.56
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.87	0.56
2:H:488:MET:H	2:H:489:PRO:HA	1.70	0.56
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.17	0.56
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.26	0.56
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.87	0.56
3:D:51:PRO:HB3	3:D:57:PHE:O	2.05	0.56
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.85	0.56
3:I:478:LEU:CD1	4:J:47:THR:HG23	2.36	0.56
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.40	0.56
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.87	0.56
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.70	0.56
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1155:ILE:HG13	3:D:1210:ILE:CG2	2.30	0.56
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.21	0.56
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.20	0.56
2:H:367:TYR:CD1	2:H:384:LEU:HD13	2.40	0.56
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.41	0.56
3:D:488:ASN:HD21	4:E:6:VAL:CG1	2.19	0.56
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.88	0.56
3:D:905:ARG:HH22	4:E:10:VAL:HG11	1.71	0.56
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.36	0.56
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.87	0.56
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.41	0.56
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.21	0.56
5:X:22:LEU:HD13	5:X:48:ILE:HD12	1.88	0.56
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.87	0.56
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.06	0.56
3:D:1369:ARG:NH1	3:D:1369:ARG:HB3	2.19	0.56
2:H:810:TYR:CE1	2:H:1078:LYS:HD2	2.41	0.56
2:C:753:LEU:O	2:C:753:LEU:HD12	2.06	0.56
5:X:363:ARG:O	5:X:367:ILE:HG12	2.05	0.56
3:I:1362:GLY:O	3:I:1364:ALA:N	2.37	0.56
3:D:166:LEU:HD12	3:D:167:ASP:N	2.21	0.56
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.19	0.56
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.36	0.56
5:Y:476:ARG:HD2	5:Y:476:ARG:H	1.71	0.56
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.87	0.56
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.88	0.55
3:I:914:ALA:O	3:I:918:ILE:HG22	2.05	0.55
2:C:487:LEU:HD13	2:C:488:MET:H	1.71	0.55
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.27	0.55
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.21	0.55
2:H:505:PHE:O	2:H:512:SER:OG	2.23	0.55
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.88	0.55
2:H:531:SER:OG	2:H:533:LEU:HD23	2.06	0.55
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.88	0.55
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.41	0.55
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.35	0.55
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.88	0.55
1:F:10:LYS:HD2	1:G:226:GLU:O	2.06	0.55
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.71	0.55
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.39	0.55
3:D:919:ALA:O	3:D:923:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.87	0.55
2:H:9:LYS:HD3	2:H:9:LYS:N	2.20	0.55
3:I:166:LEU:HD12	3:I:167:ASP:N	2.20	0.55
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.36	0.55
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.05	0.55
5:X:120:ALA:CB	5:X:421:TYR:HB3	2.36	0.55
3:I:573:THR:HG22	3:I:576:ARG:CG	2.37	0.55
2:H:639:LYS:HE2	2:H:639:LYS:HA	1.88	0.55
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.89	0.55
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.06	0.55
2:C:681:MET:O	2:C:685:MET:HG2	2.06	0.55
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.69	0.55
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.37	0.55
3:D:368:LEU:HG	3:D:373:ALA:HB2	1.88	0.55
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.37	0.55
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.89	0.55
4:J:4:VAL:O	4:J:5:THR:OG1	2.23	0.55
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.71	0.55
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.87	0.55
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.72	0.55
2:C:646:SER:HB2	2:C:649:GLN:HG3	1.89	0.55
2:H:178:PRO:HA	2:H:397:LEU:HD23	1.89	0.55
2:H:263:VAL:HG22	2:H:273:HIS:CD2	2.40	0.55
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.89	0.55
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.27	0.55
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.88	0.55
3:I:120:LEU:CB	3:I:121:PRO:CD	2.85	0.55
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.42	0.55
3:D:473:THR:HB	3:D:476:ALA:CB	2.37	0.55
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.70	0.55
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.40	0.55
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.42	0.55
2:C:817:LEU:HD21	2:C:1080:ASN:HB2	1.87	0.55
5:X:379:MET:CE	5:X:379:MET:HA	2.36	0.55
2:H:664:GLY:O	2:H:686:GLN:NE2	2.39	0.55
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.06	0.55
1:G:42:ALA:O	1:G:46:ILE:HG12	2.07	0.55
5:Y:387:VAL:HG13	5:Y:408:GLY:HA3	1.88	0.55
3:D:905:ARG:HG2	3:D:907:HIS:H	1.72	0.55
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.42	0.55
2:C:496:LYS:N	2:C:497:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.88	0.55
2:C:894:GLN:O	2:C:895:LEU:HB2	2.06	0.55
1:A:282:VAL:HG22	1:A:316:MET:HE2	1.89	0.55
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.24	0.55
2:C:142:GLU:HG2	2:C:515:MET:SD	2.47	0.55
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.88	0.55
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.35	0.55
1:A:11:PRO:HB3	1:A:31:LEU:CD2	2.35	0.55
2:H:1284:ALA:HB3	3:I:1361:THR:HB	1.88	0.55
2:H:106:GLU:HG2	2:H:109:ALA:H	1.71	0.55
3:I:500:ILE:HD13	3:I:500:ILE:H	1.72	0.55
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.89	0.55
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.07	0.55
1:G:86:LYS:NZ	3:I:526:VAL:O	2.39	0.55
3:D:609:TYR:CE2	3:D:614:LEU:HD22	2.41	0.54
2:C:163:LYS:H	2:C:163:LYS:CD	2.10	0.54
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.42	0.54
3:D:1262:ARG:HH22	3:D:1312:ALA:HB1	1.72	0.54
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.07	0.54
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.71	0.54
2:H:453:ILE:HG22	2:H:585:GLY:O	2.07	0.54
2:H:936:ARG:HH11	5:Y:495:ARG:HH11	1.53	0.54
2:H:524:ILE:HD12	2:H:708:VAL:HG13	1.88	0.54
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.42	0.54
2:H:459:MET:SD	2:H:511:LEU:HD22	2.47	0.54
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.38	0.54
3:D:514:THR:HG21	3:D:595:ALA:O	2.07	0.54
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.88	0.54
2:C:639:LYS:HE2	2:C:639:LYS:HA	1.89	0.54
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.08	0.54
2:H:38:PHE:CE2	2:H:49:LEU:HD12	2.32	0.54
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.35	0.54
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.89	0.54
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.07	0.54
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.88	0.54
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.37	0.54
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.89	0.54
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.07	0.54
2:H:740:GLU:HB2	2:H:741:MET:SD	2.47	0.54
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.88	0.54
3:I:120:LEU:HD22	3:I:1330:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:128:LEU:HD12	3:I:192:MET:CE	2.37	0.54
2:H:1255:THR:O	2:H:1257:GLN:N	2.38	0.54
3:I:589:TYR:O	3:I:591:ILE:N	2.37	0.54
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.89	0.54
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.23	0.54
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	1.90	0.54
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.88	0.54
2:C:678:ARG:HD3	2:C:681:MET:HG3	1.90	0.54
4:J:15:ASN:ND2	4:J:18:ASP:H	2.06	0.54
3:I:297:ARG:HH22	5:Y:101:TYR:HB2	1.71	0.54
3:I:253:VAL:HG11	5:Y:523:ILE:HG21	1.90	0.54
2:H:660:VAL:HG22	2:H:661:VAL:N	2.22	0.54
1:F:150:ARG:NH1	1:G:8:PHE:HA	2.20	0.54
2:C:91:THR:HG22	2:C:139:ASN:N	2.23	0.54
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.07	0.54
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.54
2:H:54:ARG:HG2	2:H:55:SER:CB	2.36	0.54
4:E:5:THR:CA	4:E:6:VAL:CB	2.85	0.54
3:I:40:LYS:HB3	3:I:42:GLU:HG2	1.90	0.54
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.73	0.54
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.34	0.54
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.08	0.54
3:I:549:LYS:HE2	3:I:571:ASP:OD2	2.07	0.54
2:H:704:MET:HA	2:H:704:MET:HE2	1.90	0.54
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.73	0.54
3:I:405:GLU:O	3:I:407:VAL:N	2.41	0.54
3:D:450:HIS:NE2	3:D:625:MET:SD	2.81	0.54
3:I:151:MET:N	3:I:151:MET:SD	2.81	0.54
1:G:118:ASP:OD1	1:G:119:GLY:N	2.41	0.54
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.90	0.54
1:F:118:ASP:OD1	1:F:119:GLY:N	2.41	0.54
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.90	0.54
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.89	0.54
5:X:556:ALA:O	5:X:560:ARG:HB2	2.08	0.54
3:D:88:CYS:O	3:D:90:VAL:N	2.41	0.54
5:X:600:HIS:H	5:X:601:PRO:HD2	1.72	0.54
1:B:176:CYS:O	1:B:178:SER:N	2.41	0.54
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.23	0.54
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.08	0.54
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.90	0.54
3:I:810:THR:HG22	3:I:893:GLY:HA3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.30	0.53
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.08	0.53
3:D:128:LEU:HA	3:D:192:MET:HE3	1.90	0.53
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.90	0.53
3:I:571:ASP:N	3:I:571:ASP:OD1	2.39	0.53
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.90	0.53
2:C:1141:LEU:H	2:C:1141:LEU:CD1	2.20	0.53
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.40	0.53
1:B:118:ASP:OD1	1:B:119:GLY:N	2.41	0.53
2:H:442:VAL:HG12	2:H:443:ASP:H	1.74	0.53
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.34	0.53
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.31	0.53
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.89	0.53
2:H:752:ASN:O	2:H:753:LEU:HG	2.08	0.53
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.89	0.53
2:C:494:ASN:OD1	2:C:495:ALA:N	2.41	0.53
2:H:728:ASP:OD2	2:H:729:ALA:N	2.41	0.53
2:C:134:GLY:O	2:C:527:LYS:NZ	2.40	0.53
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.39	0.53
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.43	0.53
2:C:1303:LYS:HA	2:C:1303:LYS:HE2	1.89	0.53
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.90	0.53
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	1.90	0.53
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.90	0.53
1:G:29:GLU:HA	1:G:200:LYS:CB	2.38	0.53
3:D:393:THR:HG23	3:D:396:ALA:H	1.73	0.53
5:X:437:GLN:HA	5:X:440:THR:HG22	1.89	0.53
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.08	0.53
2:C:31:GLN:HG3	2:C:130:MET:HE1	1.90	0.53
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.74	0.53
3:D:746:LEU:CD1	3:D:758:PRO:HG3	2.28	0.53
3:D:584:PRO:HG2	3:D:587:LEU:CD1	2.33	0.53
3:D:591:ILE:HD12	3:D:592:VAL:N	2.24	0.53
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.07	0.53
3:I:363:LEU:O	3:I:486:SER:OG	2.20	0.53
2:C:756:TYR:H	2:C:766:ASN:CB	2.22	0.53
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.90	0.53
3:I:1357:ILE:HD12	3:I:1357:ILE:H	1.73	0.53
2:H:387:ASN:HB3	2:H:394:ARG:HG3	1.89	0.53
2:H:1332:SER:O	3:I:243:PRO:HG2	2.09	0.53
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.28	0.53
2:C:1119:MET:O	2:C:1123:GLY:N	2.40	0.53
3:I:709:ARG:O	3:I:711:GLY:N	2.42	0.53
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.44	0.53
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.91	0.53
2:H:494:ASN:OD1	2:H:495:ALA:N	2.40	0.53
3:D:294:ASN:ND2	3:D:298:MET:SD	2.81	0.53
2:H:1274:GLU:N	2:H:1274:GLU:OE1	2.41	0.53
2:C:728:ASP:OD2	2:C:729:ALA:N	2.41	0.53
1:A:80:GLU:HB2	2:C:694:ARG:NH2	2.19	0.53
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.44	0.53
2:C:360:LEU:HD13	2:C:378:ARG:NH1	2.23	0.53
3:D:425:ARG:CD	3:D:459:ALA:HB2	2.39	0.53
2:C:106:GLU:HG2	2:C:109:ALA:H	1.73	0.53
3:D:41:PRO:HB3	3:D:270:ARG:HG3	1.90	0.53
3:D:490:ILE:O	3:D:499:ILE:HG22	2.09	0.53
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.91	0.53
5:X:355:ILE:O	5:X:355:ILE:HD13	2.08	0.53
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.91	0.53
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.30	0.53
2:C:122:VAL:HG22	5:X:472:GLN:HE21	1.72	0.53
1:B:19:VAL:O	1:B:20:SER:HB3	2.08	0.53
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.09	0.53
3:D:1241:TYR:HB3	3:D:1246:VAL:HG23	1.91	0.53
5:Y:576:VAL:HG12	5:Y:587:ILE:HG12	1.90	0.53
2:C:818:VAL:HG22	2:C:819:SER:H	1.74	0.53
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.43	0.53
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.43	0.53
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.44	0.53
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.39	0.53
3:I:591:ILE:HD12	3:I:592:VAL:N	2.23	0.53
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.90	0.53
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.91	0.53
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.08	0.53
1:A:42:ALA:O	1:A:46:ILE:HG12	2.08	0.53
1:F:79:LEU:O	1:F:83:LEU:HD13	2.09	0.53
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.90	0.53
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.24	0.53
5:X:301:ASN:O	5:X:305:LEU:HD13	2.09	0.53
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.74	0.53
3:I:664:ILE:HD12	3:I:681:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.90	0.53
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	1.90	0.53
3:D:1159:ILE:HD12	3:D:1186:TYR:HE2	1.74	0.53
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.90	0.53
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.90	0.53
1:G:182:ARG:CG	1:G:206:GLU:HB3	2.38	0.53
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.90	0.53
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.90	0.53
5:Y:584:ARG:O	5:Y:587:ILE:HG22	2.09	0.53
2:C:367:TYR:CD1	2:C:384:LEU:HD13	2.44	0.53
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.44	0.53
2:H:844:LYS:NZ	2:H:844:LYS:HB2	2.23	0.52
2:H:106:GLU:H	2:H:107:ARG:HA	1.74	0.52
2:C:1335:ILE:HD11	3:D:22:ILE:HG13	1.91	0.52
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.08	0.52
2:H:37:LYS:HE3	2:H:37:LYS:HA	1.91	0.52
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.45	0.52
4:J:45:LYS:O	4:J:49:ILE:HG12	2.09	0.52
2:C:205:PRO:O	2:C:208:ILE:HG22	2.10	0.52
3:I:679:TYR:CZ	3:I:683:ILE:HD11	2.44	0.52
2:C:402:ARG:NH2	2:C:419:ILE:O	2.43	0.52
3:D:152:THR:O	3:D:154:LEU:N	2.38	0.52
2:C:311:CYS:SG	2:C:315:MET:HB2	2.49	0.52
3:I:197:GLU:O	3:I:201:LEU:HD23	2.09	0.52
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.44	0.52
3:D:413:ASP:O	3:D:417:ARG:HG2	2.10	0.52
5:X:264:LYS:HD2	5:X:264:LYS:H	1.73	0.52
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.74	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.41	0.52
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.91	0.52
2:C:946:LEU:O	2:C:949:GLU:HG3	2.09	0.52
1:A:195:ARG:HH21	1:A:198:LEU:HD21	1.73	0.52
4:E:5:THR:HB	4:E:7:GLN:N	2.24	0.52
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.35	0.52
2:C:96:LEU:HD22	2:C:127:ILE:HD12	1.92	0.52
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.23	0.52
5:Y:264:LYS:H	5:Y:264:LYS:HD2	1.74	0.52
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.90	0.52
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.09	0.52
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.44	0.52
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1251:LYS:O	3:I:1255:VAL:HG23	2.10	0.52
3:I:797:THR:O	3:I:801:VAL:HG23	2.09	0.52
1:A:134:THR:HG21	2:C:727:VAL:O	2.09	0.52
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.42	0.52
2:C:1244:HIS:HB3	2:C:1265:PHE:CG	2.45	0.52
3:I:648:GLU:N	3:I:648:GLU:OE2	2.43	0.52
3:I:393:THR:HG23	3:I:396:ALA:H	1.73	0.52
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.09	0.52
2:H:992:LEU:HD23	2:H:996:ARG:HG3	1.91	0.52
5:X:484:ALA:CB	5:X:494:ILE:HD12	2.39	0.52
5:X:466:ILE:HD12	5:X:487:MET:HE2	1.91	0.52
4:E:77:ALA:O	4:E:80:LEU:HD22	2.10	0.52
5:X:493:LYS:O	5:X:497:VAL:HG23	2.09	0.52
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.39	0.52
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.75	0.52
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.39	0.52
5:X:541:ARG:O	5:X:545:HIS:HB2	2.10	0.52
3:D:118:LYS:HE3	5:X:39:ASP:OD2	2.09	0.52
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.91	0.52
2:H:131:THR:HG22	2:H:135:THR:HG22	1.91	0.52
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.92	0.52
3:D:615:LYS:HD2	7:D:1503:0O2:N2	2.23	0.52
3:D:655:SER:O	3:D:658:GLU:HG2	2.09	0.52
2:H:888:THR:O	2:H:914:LYS:N	2.36	0.52
4:E:82:ALA:O	4:E:86:ILE:HG13	2.10	0.52
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.45	0.52
2:H:699:LEU:H	2:H:799:ASN:HD21	1.56	0.52
3:D:746:LEU:HB3	3:D:754:ILE:HG21	1.91	0.52
4:E:5:THR:CB	4:E:7:GLN:H	2.20	0.52
2:C:127:ILE:HD13	2:C:127:ILE:N	2.25	0.52
2:C:302:ILE:HG22	2:C:309:LEU:CB	2.39	0.52
2:H:18:ARG:HD3	2:H:619:ALA:O	2.09	0.52
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.91	0.52
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.91	0.52
2:C:975:ILE:HD13	2:C:975:ILE:O	2.09	0.52
5:X:598:LEU:O	5:X:599:ARG:HD2	2.08	0.52
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.91	0.52
2:H:741:MET:N	2:H:741:MET:SD	2.82	0.52
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.45	0.52
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.92	0.52
2:H:694:ARG:O	2:H:798:GLN:NE2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.91	0.52
3:I:504:GLN:HG3	3:I:505:ASP:H	1.75	0.52
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.33	0.52
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.90	0.52
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.92	0.52
3:D:810:THR:OG1	3:D:811:GLU:N	2.42	0.52
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.39	0.52
3:D:646:ILE:HG22	3:D:741:ALA:O	2.09	0.52
5:X:119:ILE:O	5:X:123:ILE:HG13	2.10	0.52
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.75	0.52
3:D:63:GLY:O	3:D:98:ARG:NH2	2.42	0.52
2:C:843:THR:HG22	2:C:844:LYS:N	2.24	0.52
2:C:755:LYS:HZ1	2:C:756:TYR:HE2	1.58	0.52
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.09	0.52
2:C:891:GLY:O	2:C:893:THR:HG23	2.10	0.52
2:C:179:TYR:HE2	2:C:462:ASN:HD21	1.58	0.52
1:G:31:LEU:HB2	1:G:199:ASP:O	2.10	0.52
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.40	0.52
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.91	0.52
3:D:504:GLN:HG3	3:D:505:ASP:H	1.75	0.52
3:I:451:PRO:HG2	3:I:625:MET:SD	2.50	0.52
2:H:403:MET:HG3	2:H:414:ILE:HB	1.91	0.52
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.10	0.52
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.24	0.52
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.91	0.52
2:C:80:PHE:O	2:C:84:GLU:HB3	2.10	0.52
2:H:446:ASP:OD1	2:H:547:VAL:N	2.29	0.52
3:I:858:VAL:HB	3:I:859:PRO:CD	2.26	0.51
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.10	0.51
3:D:767:LEU:HB3	3:D:771:GLN:NE2	2.24	0.51
2:H:21:VAL:HG13	2:H:22:LEU:N	2.23	0.51
2:C:487:LEU:CD1	2:C:488:MET:H	2.23	0.51
3:D:703:THR:HA	3:D:717:VAL:HA	1.90	0.51
5:X:400:GLN:O	5:X:404:LEU:HD13	2.11	0.51
1:B:33:ARG:NE	1:B:197:ASP:HB2	2.26	0.51
1:G:192:VAL:CG1	1:G:194:GLN:HG2	2.40	0.51
2:C:699:LEU:H	2:C:799:ASN:HD21	1.56	0.51
2:H:496:LYS:HE2	5:Y:471:LEU:CD2	2.39	0.51
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.93	0.51
5:Y:379:MET:CE	5:Y:379:MET:HA	2.41	0.51
3:I:807:LEU:O	3:I:807:LEU:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.51
3:I:430:HIS:HA	3:I:921:GLN:HB3	1.92	0.51
2:H:800:MET:HG2	2:H:1096:ILE:HD13	1.91	0.51
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.44	0.51
3:D:664:ILE:CD1	3:D:681:LYS:HE3	2.40	0.51
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.10	0.51
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.93	0.51
5:X:484:ALA:HB2	5:X:494:ILE:HD12	1.92	0.51
3:D:133:ARG:NH2	3:D:133:ARG:HB2	2.25	0.51
2:C:1104:PRO:HG3	3:D:725:MET:SD	2.51	0.51
2:H:1281:TYR:CZ	3:I:431:ARG:HG2	2.45	0.51
1:B:107:ILE:HD11	1:B:136:GLU:HG2	1.91	0.51
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.09	0.51
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.92	0.51
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.45	0.51
2:C:1106:ARG:O	2:C:1108:ASN:N	2.40	0.51
2:C:21:VAL:HG13	2:C:22:LEU:N	2.26	0.51
3:D:20:ILE:CD1	3:D:1320:ILE:HD11	2.41	0.51
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.40	0.51
2:H:634:VAL:H	2:H:645:PHE:HE2	1.59	0.51
5:Y:99:ARG:HD3	5:Y:99:ARG:O	2.11	0.51
2:H:1336:ASN:HB2	3:I:33:TRP:HH2	1.75	0.51
3:D:68:TYR:OH	3:D:94:GLN:NE2	2.44	0.51
1:G:41:ASN:HD21	2:H:1217:THR:HG22	1.76	0.51
2:C:59:ILE:CG2	2:C:479:LEU:HB3	2.41	0.51
2:C:936:ARG:HD2	2:C:1047:LEU:H	1.74	0.51
2:H:153:PRO:HD2	2:H:452:ARG:HD3	1.92	0.51
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.92	0.51
2:C:9:LYS:N	2:C:9:LYS:HD3	2.25	0.51
1:B:77:ASP:O	1:B:81:ILE:HG13	2.10	0.51
3:I:482:ALA:C	3:I:483:LEU:HD12	2.31	0.51
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.92	0.51
2:H:989:LEU:HG	2:H:990:ASP:H	1.76	0.51
2:C:989:LEU:HG	2:C:990:ASP:H	1.76	0.51
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.92	0.51
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.30	0.51
4:E:5:THR:HB	4:E:7:GLN:CB	2.38	0.51
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.92	0.51
3:I:245:LEU:O	3:I:250:ARG:NH1	2.43	0.51
2:H:1335:ILE:HD11	3:I:22:ILE:CG1	2.41	0.51
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.39	0.51
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.76	0.51
1:A:248:GLU:N	1:A:248:GLU:OE1	2.42	0.51
1:A:207:THR:OG1	1:A:208:ASN:N	2.44	0.51
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.76	0.51
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.24	0.51
4:E:4:VAL:O	4:E:5:THR:OG1	2.24	0.51
1:B:41:ASN:ND2	2:C:1217:THR:HG22	2.23	0.51
1:B:45:ARG:O	3:D:538:ARG:NH2	2.44	0.51
3:D:899:TYR:CE1	3:D:915:ILE:HD12	2.46	0.51
5:X:600:HIS:H	5:X:601:PRO:CD	2.23	0.51
5:X:545:HIS:NE2	5:X:566:ASP:OD2	2.44	0.51
3:D:648:GLU:N	3:D:648:GLU:OE2	2.42	0.51
5:X:311:THR:HG21	5:X:348:GLU:CD	2.31	0.51
2:H:1247:SER:O	2:H:1248:THR:HG23	2.11	0.51
3:I:1174:ARG:HA	3:I:1192:LYS:HG3	1.92	0.51
4:J:5:THR:HB	4:J:7:GLN:H	1.75	0.51
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.75	0.51
3:D:316:ILE:O	3:D:317:THR:OG1	2.20	0.51
2:C:576:SER:HB3	2:C:579:ALA:HB2	1.93	0.51
3:I:857:LEU:HB2	3:I:860:ARG:HB2	1.91	0.51
5:X:277:MET:HE1	5:X:359:LYS:HE2	1.93	0.51
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.30	0.51
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.93	0.51
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.44	0.51
2:C:844:LYS:NZ	2:C:844:LYS:HB2	2.26	0.51
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.75	0.51
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.10	0.51
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.93	0.51
1:A:118:ASP:OD1	1:A:119:GLY:N	2.44	0.51
2:C:1105:SER:HB2	3:D:731:ARG:HD3	1.93	0.51
2:H:901:LEU:O	2:H:905:ILE:HG13	2.11	0.51
2:C:49:LEU:HD21	2:C:464:PHE:HB3	1.93	0.51
3:I:140:TYR:OH	3:I:312:ARG:NH1	2.42	0.51
3:I:473:THR:HB	3:I:476:ALA:HB2	1.93	0.51
2:H:1335:ILE:HD11	3:I:22:ILE:HG13	1.92	0.51
3:D:886:VAL:HG11	3:D:1230:THR:HG21	1.92	0.51
2:H:681:MET:O	2:H:685:MET:HG2	2.11	0.51
1:B:129:VAL:HG11	1:B:132:HIS:HE1	1.76	0.51
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.92	0.51
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ILE:O	1:A:307:LEU:HD13	2.10	0.51
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.10	0.51
3:I:822:MET:HG2	3:I:839:VAL:HG22	1.93	0.50
7:D:1503:0O2:O2'	7:D:1503:0O2:O1C	2.29	0.50
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.41	0.50
3:D:396:ALA:CB	5:X:606:VAL:HG11	2.41	0.50
1:G:179:PRO:O	1:G:207:THR:OG1	2.25	0.50
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.46	0.50
5:Y:437:GLN:HA	5:Y:440:THR:HG22	1.93	0.50
1:A:256:PRO:HA	1:A:277:TYR:HA	1.92	0.50
2:H:812:PHE:CD2	2:H:813:GLU:HG3	2.46	0.50
2:H:36:GLN:O	2:H:39:ILE:HG22	2.11	0.50
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.37	0.50
1:F:42:ALA:O	1:F:46:ILE:HG12	2.11	0.50
5:Y:449:THR:HG23	5:Y:503:GLU:OE1	2.12	0.50
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.92	0.50
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.46	0.50
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.41	0.50
3:D:701:LEU:HD23	3:D:723:TYR:HB2	1.93	0.50
3:D:262:THR:HG1	3:D:266:ASN:HD22	1.58	0.50
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.10	0.50
3:D:1174:ARG:HA	3:D:1192:LYS:HG3	1.92	0.50
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.11	0.50
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.12	0.50
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.24	0.50
5:X:384:LEU:O	5:X:384:LEU:HD13	2.10	0.50
2:C:149:LEU:HD12	2:C:452:ARG:O	2.11	0.50
3:D:910:ASN:HB3	4:E:15:ASN:HA	1.92	0.50
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.92	0.50
1:A:263:THR:HG23	1:A:266:SER:H	1.76	0.50
2:H:818:VAL:HG22	2:H:819:SER:H	1.76	0.50
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.93	0.50
3:I:1260:MET:HE2	3:I:1306:LEU:HD11	1.92	0.50
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.32	0.50
2:C:1285:TYR:HA	2:C:1288:GLN:HB3	1.92	0.50
3:D:840:LEU:O	3:D:840:LEU:HD12	2.11	0.50
3:D:478:LEU:CD1	4:E:47:THR:HG23	2.41	0.50
3:D:482:ALA:C	3:D:483:LEU:HD12	2.32	0.50
2:H:707:ALA:O	2:H:710:VAL:HG12	2.11	0.50
3:I:152:THR:O	3:I:154:LEU:N	2.42	0.50
2:C:442:VAL:HG12	2:C:443:ASP:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.93	0.50
2:H:38:PHE:O	2:H:39:ILE:HB	2.10	0.50
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.27	0.50
3:I:513:MET:CE	3:I:579:LEU:HB2	2.41	0.50
2:C:184:LEU:HB2	2:C:389:PHE:CE1	2.46	0.50
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.26	0.50
5:X:561:MET:HA	5:X:567:MET:SD	2.50	0.50
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.46	0.50
2:H:487:LEU:CB	2:H:488:MET:HG3	2.39	0.50
3:D:545:HIS:O	3:D:573:THR:OG1	2.18	0.50
1:A:80:GLU:HA	2:C:694:ARG:HH12	1.77	0.50
1:F:52:PRO:HG2	1:F:219:ARG:NH2	2.24	0.50
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.92	0.50
3:D:57:PHE:HB3	3:D:98:ARG:HH11	1.76	0.50
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.46	0.50
2:H:946:LEU:O	2:H:949:GLU:HG3	2.11	0.50
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.26	0.50
1:A:47:LEU:HD23	1:A:51:MET:SD	2.52	0.50
3:I:355:ILE:HG21	3:I:466:MET:SD	2.52	0.50
3:D:546:ALA:N	3:D:547:ARG:CA	2.69	0.50
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.40	0.50
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.77	0.50
5:X:101:TYR:OH	5:X:384:LEU:HD11	2.11	0.50
3:D:245:LEU:O	3:D:250:ARG:NH1	2.44	0.50
3:I:1171:GLY:N	3:I:1172:LYS:O	2.44	0.50
2:C:1335:ILE:HD11	3:D:22:ILE:CG1	2.41	0.50
3:I:842:ARG:HB3	3:I:882:VAL:HG21	1.94	0.50
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.93	0.50
1:F:151:GLY:O	1:F:177:TYR:HB2	2.12	0.50
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.93	0.50
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.46	0.50
2:C:131:THR:HG22	2:C:135:THR:N	2.27	0.50
2:C:697:LYS:HZ3	2:C:791:LEU:HD11	1.77	0.50
3:I:644:MET:HG3	3:I:764:ARG:HD3	1.92	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.93	0.50
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.45	0.50
3:D:478:LEU:HD12	4:E:47:THR:HG23	1.93	0.50
3:I:316:ILE:N	3:I:316:ILE:HD13	2.27	0.50
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.44	0.50
3:D:173:GLY:O	3:D:175:GLU:HG3	2.11	0.50
3:I:608:CYS:O	3:I:612:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.93	0.50
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.45	0.50
3:D:614:LEU:CD1	4:E:5:THR:HG21	2.42	0.50
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.12	0.50
3:I:370:LYS:HA	3:I:441:LEU:HD12	1.94	0.50
2:H:1335:ILE:HD12	3:I:1336:ALA:HB2	1.94	0.50
3:I:513:MET:O	3:I:575:GLY:HA3	2.12	0.50
3:I:660:GLU:O	3:I:664:ILE:HG12	2.12	0.50
5:Y:283:GLN:CD	5:Y:343:LYS:HD2	2.32	0.50
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.76	0.50
3:I:1255:VAL:O	3:I:1258:ARG:HB3	2.11	0.50
3:D:515:ARG:HH22	3:D:717:VAL:C	2.15	0.50
5:X:283:GLN:NE2	5:X:343:LYS:HD2	2.26	0.50
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.12	0.50
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.12	0.49
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.93	0.49
3:I:546:ALA:N	3:I:547:ARG:CA	2.70	0.49
2:C:38:PHE:CE2	2:C:49:LEU:HD12	2.35	0.49
2:C:813:GLU:HG2	3:D:504:GLN:NE2	2.26	0.49
3:D:899:TYR:CZ	3:D:915:ILE:HD12	2.47	0.49
5:X:290:LEU:O	5:X:294:GLN:HB3	2.12	0.49
3:I:678:ARG:O	3:I:681:LYS:HG3	2.11	0.49
2:C:1087:TYR:O	2:C:1213:TYR:N	2.28	0.49
2:H:698:PRO:HD3	2:H:795:ALA:HB2	1.94	0.49
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.26	0.49
2:H:384:LEU:O	2:H:388:LEU:HG	2.12	0.49
5:Y:519:LEU:HD13	5:Y:519:LEU:O	2.11	0.49
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.93	0.49
3:D:392:THR:HG22	5:X:603:ARG:HG2	1.94	0.49
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.94	0.49
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.95	0.49
2:H:794:LEU:HD21	2:H:796:LEU:CG	2.39	0.49
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.12	0.49
3:D:57:PHE:CD1	3:D:247:PRO:HB3	2.46	0.49
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.11	0.49
3:I:579:LEU:HD13	3:I:579:LEU:O	2.12	0.49
3:I:810:THR:OG1	3:I:811:GLU:N	2.42	0.49
1:B:9:LEU:H	1:B:9:LEU:HD23	1.77	0.49
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.12	0.49
2:H:127:ILE:N	2:H:127:ILE:HD13	2.26	0.49
2:H:138:ILE:HB	2:H:143:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1042:LEU:N	2:H:1042:LEU:HD13	2.26	0.49
2:H:735:LYS:HA	2:H:748:ILE:HA	1.94	0.49
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.92	0.49
1:A:310:ARG:HA	1:A:310:ARG:NE	2.28	0.49
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.92	0.49
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.48	0.49
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.26	0.49
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.13	0.49
2:C:475:VAL:O	2:C:479:LEU:HB2	2.12	0.49
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.42	0.49
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.93	0.49
2:C:1288:GLN:CA	2:C:1288:GLN:HE21	2.26	0.49
3:I:840:LEU:HD12	3:I:840:LEU:O	2.11	0.49
3:D:550:VAL:HG23	3:D:552:ILE:HD11	1.92	0.49
5:X:278:ASP:OD1	5:X:281:ARG:NH2	2.45	0.49
2:H:1119:MET:O	2:H:1123:GLY:N	2.45	0.49
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.78	0.49
3:D:589:TYR:O	3:D:591:ILE:HG13	2.13	0.49
5:X:108:VAL:HB	5:X:110:LEU:HG	1.94	0.49
1:A:88:LEU:HD22	1:A:90:VAL:HG23	1.95	0.49
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.42	0.49
2:H:895:LEU:HD21	2:H:903:ARG:CZ	2.41	0.49
5:X:115:GLY:O	5:X:119:ILE:HG12	2.13	0.49
2:H:998:LEU:O	2:H:998:LEU:HD13	2.12	0.49
5:X:310:GLU:O	5:X:344:LEU:HD23	2.12	0.49
2:C:12:ARG:O	2:C:13:LYS:HG2	2.11	0.49
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.47	0.49
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.28	0.49
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.77	0.49
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.33	0.49
2:C:818:VAL:HG22	2:C:819:SER:N	2.28	0.49
2:H:975:ILE:HD13	2:H:975:ILE:O	2.12	0.49
3:I:1161:GLY:HA2	3:I:1181:ASP:HB2	1.95	0.49
2:H:590:PRO:O	2:H:659:GLN:NE2	2.46	0.49
3:D:614:LEU:CG	4:E:5:THR:HG21	2.42	0.49
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.32	0.49
5:X:35:ILE:HG23	5:X:36:VAL:N	2.28	0.49
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.36	0.49
2:H:72:SER:O	2:H:98:VAL:HG23	2.12	0.49
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.94	0.49
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:998:LEU:HD13	2:C:998:LEU:O	2.13	0.49
3:D:807:LEU:O	3:D:807:LEU:HD12	2.12	0.49
2:H:395:TYR:CE2	2:H:420:LEU:HG	2.48	0.49
2:C:510:GLN:O	2:C:511:LEU:HB2	2.13	0.49
3:I:227:PHE:O	3:I:230:SER:OG	2.24	0.49
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.42	0.49
5:X:511:ILE:HG23	5:X:512:GLY:N	2.25	0.49
2:H:1252:SER:HA	5:Y:524:GLU:HA	1.95	0.49
2:C:971:LEU:HD21	2:C:1017:GLN:HE22	1.78	0.49
5:X:379:MET:HE2	5:X:379:MET:HA	1.95	0.49
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.94	0.49
2:H:1270:PHE:CE2	2:H:1274:GLU:HB3	2.48	0.49
2:H:840:SER:HB3	2:H:850:ILE:HD11	1.94	0.49
1:G:9:LEU:HD23	1:G:9:LEU:H	1.78	0.49
2:C:119:GLU:HG2	2:C:120:GLN:N	2.28	0.49
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.12	0.49
2:H:1066:MET:HG3	2:H:1234:LYS:HA	1.94	0.49
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.27	0.49
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.43	0.49
2:C:808:ASN:H	3:D:633:ALA:HB2	1.78	0.49
2:H:119:GLU:HG2	2:H:120:GLN:N	2.26	0.49
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.43	0.49
3:D:531:LYS:NZ	3:D:531:LYS:HB3	2.28	0.49
2:H:843:THR:HG22	2:H:844:LYS:H	1.78	0.49
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.39	0.49
2:C:741:MET:SD	2:C:741:MET:N	2.85	0.49
1:A:158:ARG:HB2	1:A:158:ARG:HH21	1.77	0.49
3:D:452:LEU:HG	3:D:625:MET:SD	2.53	0.49
2:C:1335:ILE:HD12	3:D:1336:ALA:HB2	1.95	0.49
2:C:751:TYR:HE1	2:C:783:LEU:HD12	1.76	0.49
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.77	0.49
1:F:60:GLU:HG3	1:F:169:GLY:O	2.12	0.49
1:A:79:LEU:O	1:A:83:LEU:HD13	2.13	0.49
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.94	0.49
2:H:12:ARG:O	2:H:13:LYS:HG2	2.12	0.49
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.93	0.49
1:B:227:GLN:C	1:B:229:GLU:H	2.16	0.49
3:D:918:ILE:HD11	3:D:1252:HIS:NE2	2.27	0.49
3:I:245:LEU:CD1	3:I:246:PRO:HD2	2.40	0.49
3:I:543:SER:O	3:I:574:VAL:HB	2.13	0.49
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:317:THR:H	3:I:324:LEU:HD21	1.77	0.49
3:D:644:MET:O	3:D:764:ARG:NH1	2.46	0.49
1:G:152:TYR:OH	3:I:535:ARG:NH1	2.38	0.48
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.13	0.48
3:D:120:LEU:HA	5:X:46:GLN:OE1	2.13	0.48
3:I:1261:LEU:HD21	3:I:1306:LEU:CD2	2.38	0.48
3:D:824:PRO:O	3:D:826:ILE:HG13	2.12	0.48
2:C:740:GLU:HB2	2:C:741:MET:SD	2.53	0.48
2:C:812:PHE:H	2:C:815:SER:HB2	1.78	0.48
3:I:519:ASN:HD21	3:I:707:ILE:HG21	1.78	0.48
3:D:914:ALA:O	3:D:918:ILE:HG22	2.13	0.48
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.28	0.48
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.94	0.48
1:A:310:ARG:HE	1:A:310:ARG:HA	1.77	0.48
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.95	0.48
2:C:866:ASP:HA	2:C:872:TYR:OH	2.12	0.48
5:X:126:GLY:O	5:X:130:VAL:HG23	2.13	0.48
2:C:660:VAL:HG22	2:C:661:VAL:N	2.23	0.48
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.95	0.48
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.26	0.48
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.48	0.48
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.12	0.48
1:F:182:ARG:HH11	2:H:1092:THR:HG22	1.78	0.48
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.43	0.48
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.26	0.48
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.43	0.48
5:X:123:ILE:O	5:X:127:ILE:HG12	2.13	0.48
2:C:99:LYS:HG2	2:C:121:GLU:HB3	1.94	0.48
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.13	0.48
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.95	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.13	0.48
3:I:531:LYS:NZ	3:I:531:LYS:HB3	2.28	0.48
3:I:221:ILE:HG13	3:I:222:LYS:N	2.28	0.48
2:C:727:VAL:CG2	2:C:773:LEU:HB3	2.40	0.48
3:I:233:LYS:CD	3:I:234:PRO:HD2	2.43	0.48
3:D:124:ILE:HA	3:D:237:MET:HE2	1.95	0.48
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.96	0.48
3:D:8:LEU:HD23	3:D:8:LEU:N	2.29	0.48
1:F:44:ARG:HG3	1:F:183:ILE:HG22	1.96	0.48
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.77	0.48
3:D:873:GLU:OE2	3:D:877:VAL:HB	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1343:GLU:CA	3:I:1344:LEU:HB2	2.39	0.48
2:C:747:GLY:C	2:C:748:ILE:HG13	2.34	0.48
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.48	0.48
2:C:529:ARG:HH22	2:C:687:ARG:NH2	2.12	0.48
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.13	0.48
5:X:143:TYR:O	5:X:147:GLN:HG2	2.13	0.48
2:H:1339:LEU:HD12	2:H:1339:LEU:N	2.28	0.48
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.95	0.48
3:I:1216:ALA:O	3:I:1220:ILE:HG13	2.13	0.48
1:B:192:VAL:HG12	1:B:194:GLN:H	1.78	0.48
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.29	0.48
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.37	0.48
3:I:746:LEU:HB3	3:I:754:ILE:HG21	1.96	0.48
5:Y:457:ILE:HG23	5:Y:461:ASN:ND2	2.28	0.48
3:D:450:HIS:HE2	3:D:625:MET:CE	2.27	0.48
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.12	0.48
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.94	0.48
3:D:398:LYS:HD2	5:X:532:LEU:HD11	1.95	0.48
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.13	0.48
5:X:519:LEU:O	5:X:519:LEU:HD13	2.12	0.48
3:I:646:ILE:HD12	3:I:646:ILE:O	2.12	0.48
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.95	0.48
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.28	0.48
3:D:128:LEU:HD11	3:D:188:LEU:CD2	2.37	0.48
3:D:221:ILE:HG13	3:D:222:LYS:N	2.29	0.48
2:C:678:ARG:NE	2:C:1106:ARG:HG2	2.24	0.48
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.95	0.48
3:D:915:ILE:HG22	3:D:1255:VAL:HG11	1.96	0.48
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.48	0.48
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.94	0.48
3:I:703:THR:O	3:I:718:SER:N	2.47	0.48
1:A:243:LYS:HD3	1:A:243:LYS:N	2.29	0.48
1:G:90:VAL:HG13	1:G:121:VAL:HG13	1.94	0.48
3:D:646:ILE:HD12	3:D:646:ILE:O	2.13	0.48
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.96	0.48
5:X:227:GLN:HA	5:X:230:VAL:HG12	1.96	0.48
5:X:11:LEU:HD22	5:X:15:ARG:NH2	2.28	0.48
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.95	0.48
2:H:898:GLU:N	2:H:898:GLU:OE1	2.37	0.48
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.14	0.48
3:D:608:CYS:O	3:D:612:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:572:THR:HG22	3:I:594:GLN:OE1	2.14	0.48
3:I:51:PRO:HB3	3:I:57:PHE:O	2.14	0.48
3:D:579:LEU:HD13	3:D:579:LEU:O	2.14	0.48
2:H:747:GLY:C	2:H:748:ILE:HG13	2.34	0.48
3:I:888:CYS:SG	3:I:890:THR:HB	2.54	0.48
1:A:192:VAL:O	1:A:194:GLN:N	2.45	0.48
2:H:808:ASN:H	3:I:633:ALA:HB2	1.79	0.48
3:I:294:ASN:ND2	3:I:298:MET:SD	2.87	0.48
3:D:918:ILE:HD13	3:D:919:ALA:N	2.29	0.48
3:I:573:THR:CG2	3:I:576:ARG:HG3	2.43	0.48
2:H:72:SER:OG	2:H:99:LYS:HE3	2.13	0.48
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.42	0.48
5:X:145:LEU:HD11	5:X:225:ARG:HH21	1.78	0.48
3:D:843:VAL:HG11	3:D:897:HIS:HB3	1.96	0.48
2:C:98:VAL:HG11	2:C:124:MET:SD	2.53	0.48
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.14	0.48
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.46	0.48
3:I:147:ILE:HD12	3:I:178:ALA:HB2	1.96	0.48
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.13	0.48
2:C:59:ILE:HD11	2:C:63:SER:OG	2.14	0.48
2:H:127:ILE:O	2:H:127:ILE:HG12	2.14	0.48
3:D:363:LEU:HD12	3:D:450:HIS:ND1	2.29	0.48
3:I:707:ILE:HD11	3:I:716:GLN:HG3	1.96	0.48
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.49	0.48
3:D:41:PRO:HG3	3:D:273:ILE:HG22	1.95	0.48
1:G:82:LEU:O	1:G:86:LYS:HG3	2.14	0.48
2:H:818:VAL:HG22	2:H:819:SER:N	2.28	0.48
2:C:225:PHE:CZ	2:C:347:ILE:HB	2.49	0.48
1:G:47:LEU:HD13	1:G:205:MET:HE2	1.96	0.48
3:I:899:TYR:CD2	3:I:909:ILE:HG12	2.49	0.48
3:D:120:LEU:HG	5:X:46:GLN:CB	2.42	0.48
1:G:196:THR:OG1	3:I:443:GLU:HG3	2.14	0.48
3:I:377:PHE:O	3:I:381:ILE:HG13	2.14	0.48
3:I:265:LEU:HD11	3:I:330:MET:SD	2.54	0.48
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.14	0.48
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.14	0.48
5:X:119:ILE:HD12	5:X:122:ARG:HH21	1.79	0.48
2:C:718:ALA:HB2	2:C:783:LEU:HG	1.96	0.48
5:Y:316:PHE:CZ	5:Y:320:ILE:HD11	2.48	0.48
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.95	0.48
5:X:271:ASN:O	5:X:275:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.29	0.48
2:H:356:THR:HG21	2:H:362:ALA:HA	1.95	0.48
3:I:714:GLU:HG2	3:I:715:LYS:H	1.79	0.48
3:D:1347:LEU:HD22	3:D:1357:ILE:CG2	2.44	0.47
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.49	0.47
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.13	0.47
3:I:910:ASN:HB3	4:J:15:ASN:OD1	2.13	0.47
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.96	0.47
2:H:759:SER:HB3	2:H:763:THR:H	1.80	0.47
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.96	0.47
1:B:195:ARG:HH21	1:B:198:LEU:HD21	1.79	0.47
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.30	0.47
2:H:618:GLN:OE1	3:I:769:VAL:HG13	2.14	0.47
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.29	0.47
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.96	0.47
1:F:182:ARG:NH1	2:H:1092:THR:HG22	2.29	0.47
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.97	0.47
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.49	0.47
3:D:269:TYR:CD2	3:D:306:LEU:HD11	2.49	0.47
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.49	0.47
2:H:750:ILE:HD13	2:H:963:GLU:OE2	2.14	0.47
3:D:487:THR:HG21	4:E:4:VAL:CG1	2.40	0.47
2:C:699:LEU:HD12	2:C:1121:ALA:HB1	1.95	0.47
1:A:58:GLU:HG2	1:A:172:LEU:HD23	1.96	0.47
2:C:812:PHE:N	2:C:815:SER:HB2	2.28	0.47
1:F:45:ARG:NE	1:G:38:THR:OG1	2.46	0.47
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.14	0.47
4:E:18:ASP:O	4:E:22:VAL:HG12	2.14	0.47
3:I:679:TYR:O	3:I:683:ILE:HG13	2.14	0.47
2:H:963:GLU:O	2:H:967:LEU:HD13	2.14	0.47
3:I:288:PRO:O	3:I:292:VAL:HG12	2.14	0.47
1:F:28:LEU:HD22	1:G:231:PHE:CZ	2.49	0.47
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.95	0.47
3:I:161:THR:HG22	3:I:162:GLU:H	1.79	0.47
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.78	0.47
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.28	0.47
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.44	0.47
3:I:591:ILE:HD12	3:I:592:VAL:HG13	1.97	0.47
3:D:179:LYS:HD3	3:D:179:LYS:N	2.29	0.47
2:C:893:THR:O	2:C:895:LEU:N	2.41	0.47
1:F:28:LEU:HD13	1:G:231:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:O	1:A:226:GLU:HG3	2.13	0.47
3:D:358:GLY:HA3	3:D:361:LEU:HD23	1.96	0.47
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.96	0.47
2:C:131:THR:HG22	2:C:135:THR:H	1.80	0.47
3:I:201:LEU:HD12	3:I:205:LEU:HD11	1.97	0.47
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.30	0.47
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	1.96	0.47
3:D:714:GLU:HG2	3:D:715:LYS:H	1.79	0.47
2:C:963:GLU:O	2:C:967:LEU:HD13	2.13	0.47
2:C:562:GLU:HG2	2:C:574:SER:HB3	1.95	0.47
1:B:33:ARG:HE	1:B:197:ASP:HB2	1.79	0.47
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.79	0.47
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.14	0.47
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.50	0.47
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.14	0.47
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.95	0.47
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.29	0.47
3:I:614:LEU:CG	4:J:7:GLN:HG3	2.43	0.47
3:D:364:HIS:HB3	3:D:487:THR:HG23	1.95	0.47
3:I:514:THR:HG21	3:I:595:ALA:O	2.15	0.47
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.79	0.47
3:I:8:LEU:N	3:I:8:LEU:HD23	2.30	0.47
5:Y:428:SER:O	5:Y:432:THR:OG1	2.28	0.47
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.15	0.47
1:A:252:ILE:HG22	1:A:278:ILE:HD11	1.96	0.47
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.55	0.47
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.76	0.47
3:D:310:GLY:O	3:D:314:ARG:HG2	2.14	0.47
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.95	0.47
2:H:908:GLU:CD	2:H:908:GLU:H	2.18	0.47
5:X:431:ALA:O	5:X:435:ILE:HG13	2.15	0.47
2:H:1304:MET:O	2:H:1308:ILE:HG13	2.14	0.47
3:I:349:TYR:CD1	3:I:472:LEU:HD11	2.49	0.47
2:C:127:ILE:HG12	2:C:127:ILE:O	2.14	0.47
1:B:151:GLY:O	1:B:177:TYR:HB2	2.14	0.47
3:I:450:HIS:CE1	3:I:452:LEU:HD12	2.49	0.47
3:I:473:THR:CG2	3:I:475:GLU:HG2	2.44	0.47
2:H:1314:GLN:O	3:I:473:THR:HG23	2.15	0.47
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.50	0.47
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.30	0.47
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1106:ARG:O	2:H:1108:ASN:N	2.38	0.47
2:C:153:PRO:HD2	2:C:452:ARG:HD3	1.96	0.47
2:H:546:GLU:O	2:H:548:ARG:N	2.43	0.47
2:C:237:LEU:HB2	2:C:287:VAL:O	2.14	0.47
3:D:474:LEU:HD11	4:E:27:ALA:HB3	1.97	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.67	0.47
3:D:797:THR:O	3:D:801:VAL:HG23	2.15	0.47
1:A:234:LEU:HD12	1:A:234:LEU:N	2.29	0.47
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.49	0.47
2:C:702:THR:HA	2:C:1184:THR:O	2.15	0.47
2:C:941:LYS:O	2:C:941:LYS:HD2	2.14	0.47
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.50	0.47
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.49	0.47
3:I:12:THR:O	3:I:13:LYS:HD2	2.14	0.47
2:H:876:GLU:N	2:H:876:GLU:OE2	2.48	0.47
5:X:457:ILE:HG23	5:X:461:ASN:HD21	1.80	0.47
2:H:59:ILE:HB	2:H:480:SER:OG	2.15	0.47
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.80	0.47
3:D:1346:GLY:O	3:D:1350:ASN:HB2	2.15	0.47
5:Y:291:CYS:O	5:Y:295:CYS:HB2	2.14	0.47
2:H:1233:LEU:O	2:H:1233:LEU:HD12	2.15	0.47
3:D:856:ILE:HG13	3:D:857:LEU:O	2.14	0.47
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.97	0.47
3:D:1343:GLU:CA	3:D:1344:LEU:HB2	2.32	0.47
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.15	0.47
3:I:720:ASN:ND2	3:I:720:ASN:O	2.48	0.47
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.96	0.47
1:A:12:ARG:HB2	1:A:30:PRO:HG2	1.96	0.47
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.77	0.47
1:B:19:VAL:O	1:B:20:SER:CB	2.63	0.47
5:Y:545:HIS:NE2	5:Y:566:ASP:OD2	2.29	0.47
3:D:154:LEU:HD22	3:D:176:PHE:CE1	2.49	0.47
2:C:538:LEU:HD12	2:C:538:LEU:N	2.29	0.47
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.15	0.47
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	1.97	0.47
2:H:845:LEU:CD2	2:H:889:PRO:HG2	2.41	0.47
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.30	0.47
3:D:356:THR:O	3:D:448:GLN:HA	2.15	0.47
2:H:966:ILE:HG23	2:H:967:LEU:HD12	1.97	0.47
3:D:539:SER:OG	3:D:540:GLY:N	2.48	0.47
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.14	0.47
2:C:41:GLN:CD	2:C:42:ASP:H	2.17	0.46
1:G:190:ALA:N	1:G:198:LEU:O	2.37	0.46
3:I:298:MET:HE3	5:Y:402:LEU:HB3	1.96	0.46
2:H:1017:GLN:HA	2:H:1020:GLU:HB3	1.97	0.46
3:D:423:LEU:HB3	3:D:466:MET:CE	2.44	0.46
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.15	0.46
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.29	0.46
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.50	0.46
2:C:28:LEU:HD22	2:C:527:LYS:HD2	1.96	0.46
5:Y:608:ARG:HB3	5:Y:608:ARG:NH1	2.31	0.46
3:D:607:THR:O	3:D:611:ILE:HG12	2.15	0.46
3:I:72:CYS:SG	3:I:73:GLY:N	2.88	0.46
3:I:210:SER:O	3:I:214:ARG:HG3	2.15	0.46
1:B:232:VAL:O	1:B:233:ASP:HB2	2.15	0.46
2:C:216:THR:O	2:C:220:ILE:HG13	2.15	0.46
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.96	0.46
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.50	0.46
3:D:545:HIS:HA	3:D:546:ALA:HA	1.80	0.46
5:X:448:ARG:NH1	5:X:452:ILE:HD12	2.31	0.46
1:F:221:ALA:CB	1:G:228:LEU:HD12	2.37	0.46
3:D:260:PHE:O	5:X:504:PRO:HG2	2.15	0.46
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.39	0.46
3:D:1301:THR:CG2	3:I:1301:THR:HG23	2.45	0.46
2:C:843:THR:HB	2:C:845:LEU:HD22	1.96	0.46
5:Y:101:TYR:HE2	5:Y:388:ILE:HD11	1.79	0.46
1:G:36:GLY:O	1:G:201:LEU:HD13	2.14	0.46
5:Y:124:GLU:HG2	5:Y:128:ASN:ND2	2.31	0.46
3:I:605:LEU:HD13	3:I:605:LEU:O	2.15	0.46
3:D:33:TRP:HB3	3:D:102:MET:HG3	1.96	0.46
1:B:179:PRO:O	1:B:207:THR:OG1	2.29	0.46
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.49	0.46
2:H:697:LYS:HE2	2:H:793:GLU:HB3	1.97	0.46
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.29	0.46
2:H:516:ASP:OD2	2:H:518:ASN:ND2	2.48	0.46
5:X:291:CYS:O	5:X:295:CYS:HB2	2.15	0.46
3:D:580:TRP:HE1	3:D:589:TYR:HB3	1.80	0.46
3:D:824:PRO:CB	3:D:836:ARG:HD3	2.45	0.46
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	1.96	0.46
1:F:45:ARG:NH1	2:H:1216:ARG:HA	2.26	0.46
3:D:394:ILE:HG21	5:X:536:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:VAL:HG22	2:C:123:TYR:N	2.29	0.46
3:I:611:ILE:HG13	3:I:612:LEU:HD23	1.97	0.46
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.96	0.46
3:D:825:VAL:CG2	3:D:835:LEU:HB2	2.45	0.46
5:Y:278:ASP:OD1	5:Y:281:ARG:NH2	2.48	0.46
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.51	0.46
5:Y:484:ALA:HB1	5:Y:490:PRO:O	2.15	0.46
2:C:356:THR:HG21	2:C:362:ALA:HA	1.97	0.46
2:C:1287:LEU:HD23	3:D:1357:ILE:HD11	1.98	0.46
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.27	0.46
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.37	0.46
2:H:59:ILE:HD11	2:H:63:SER:HB3	1.96	0.46
3:D:233:LYS:HB3	3:D:236:TRP:CE2	2.50	0.46
5:Y:379:MET:HE2	5:Y:379:MET:HA	1.97	0.46
1:G:185:TYR:HA	1:G:202:VAL:O	2.15	0.46
2:C:866:ASP:HA	2:C:872:TYR:CZ	2.50	0.46
2:H:1006:GLU:CD	2:H:1006:GLU:H	2.19	0.46
3:I:911:LYS:O	3:I:911:LYS:HD2	2.15	0.46
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.49	0.46
2:H:1297:ASP:OD1	2:H:1300:GLY:HA3	2.15	0.46
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.16	0.46
2:C:908:GLU:CG	2:C:909:LYS:H	2.27	0.46
1:A:66:HIS:CE1	1:A:69:SER:HB2	2.50	0.46
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.98	0.46
3:I:356:THR:O	3:I:448:GLN:HA	2.16	0.46
2:C:843:THR:HB	2:C:845:LEU:CD2	2.46	0.46
2:C:372:PRO:HB3	5:X:34:ASP:HB3	1.98	0.46
3:I:1180:VAL:HG22	3:I:1185:PRO:HA	1.97	0.46
3:D:33:TRP:O	3:D:102:MET:HB2	2.15	0.46
3:I:773:PHE:O	3:I:776:THR:HG22	2.15	0.46
3:I:1241:TYR:HB3	3:I:1246:VAL:HG23	1.96	0.46
3:D:868:TRP:HA	3:D:871:LEU:HD23	1.96	0.46
1:F:207:THR:HG23	1:F:209:GLY:H	1.81	0.46
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.80	0.46
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.50	0.46
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.45	0.46
5:X:139:GLU:HG3	5:X:351:THR:HA	1.97	0.46
3:I:1159:ILE:HD12	3:I:1186:TYR:CE2	2.47	0.46
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.29	0.46
3:I:138:VAL:O	3:I:143:SER:HB3	2.15	0.46
3:D:73:GLY:O	3:D:76:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:773:PHE:O	3:D:776:THR:HG22	2.16	0.46
2:C:1246:ARG:NE	3:D:348:ASP:OD2	2.34	0.46
3:D:12:THR:C	3:D:13:LYS:HD2	2.36	0.46
3:I:766:GLY:C	3:I:767:LEU:HD22	2.36	0.46
3:D:369:PRO:HB2	3:D:372:MET:CB	2.46	0.46
2:C:1255:THR:O	2:C:1257:GLN:N	2.42	0.46
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.46	0.46
2:H:1032:LYS:NZ	2:H:1032:LYS:HB2	2.30	0.46
1:F:41:ASN:CG	2:H:1218:GLY:HA3	2.36	0.46
2:H:1290:MET:SD	3:I:347:VAL:HG11	2.55	0.46
5:X:276:MET:O	5:X:280:VAL:HG23	2.16	0.46
2:C:505:PHE:HA	2:C:509:SER:CB	2.46	0.46
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.50	0.46
3:D:161:THR:HG22	3:D:162:GLU:H	1.79	0.46
3:D:586:GLY:O	3:D:587:LEU:HB2	2.16	0.46
3:I:217:LEU:O	3:I:221:ILE:HG12	2.15	0.46
3:I:899:TYR:CZ	3:I:915:ILE:HD12	2.51	0.46
5:X:264:LYS:HD2	5:X:264:LYS:N	2.30	0.46
1:B:37:HIS:CE1	2:C:1216:ARG:HD3	2.51	0.46
3:I:1194:ARG:HD2	3:I:1194:ARG:N	2.30	0.46
5:Y:585:GLU:O	5:Y:589:GLN:N	2.43	0.46
1:B:18:GLN:C	1:B:20:SER:H	2.19	0.46
3:D:72:CYS:SG	3:D:73:GLY:N	2.87	0.46
3:D:1195:GLN:N	3:D:1195:GLN:OE1	2.48	0.46
2:C:886:LYS:HD3	2:C:916:SER:O	2.16	0.46
2:C:408:SER:O	2:C:431:LYS:NZ	2.31	0.46
3:D:521:LYS:HB2	3:D:542:ALA:HB2	1.98	0.46
2:H:1269:ARG:N	2:H:1269:ARG:HD3	2.31	0.46
3:I:19:ALA:HA	3:I:1344:LEU:HD12	1.97	0.46
3:I:539:SER:O	3:I:541:LEU:N	2.49	0.46
3:D:720:ASN:ND2	3:D:720:ASN:O	2.48	0.46
2:C:59:ILE:CG2	2:C:479:LEU:HD13	2.45	0.46
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.98	0.46
2:H:895:LEU:HD21	2:H:903:ARG:NH2	2.30	0.46
3:I:129:ASP:HB2	3:I:220:ARG:CZ	2.45	0.46
2:H:453:ILE:HG23	2:H:453:ILE:O	2.16	0.46
2:H:205:PRO:O	2:H:208:ILE:HG22	2.16	0.46
2:C:944:ARG:HD3	2:C:944:ARG:O	2.15	0.46
5:X:346:GLN:O	5:X:350:GLU:HG3	2.16	0.46
3:D:1197:ASN:HD22	3:D:1212:ASP:HB3	1.81	0.46
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.16	0.46
5:X:459:THR:O	5:X:463:LEU:HD13	2.16	0.46
3:D:138:VAL:O	3:D:143:SER:HB3	2.16	0.46
3:D:573:THR:HG23	3:D:576:ARG:H	1.80	0.46
2:C:876:GLU:N	2:C:876:GLU:OE2	2.49	0.46
3:D:1287:ILE:O	3:D:1290:ARG:HG2	2.16	0.46
2:C:475:VAL:HG23	2:C:492:MET:SD	2.56	0.46
1:A:29:GLU:O	1:A:31:LEU:N	2.49	0.46
2:H:500:ALA:O	2:H:504:GLU:HB2	2.16	0.46
5:Y:562:ARG:HG3	5:Y:591:GLU:CD	2.36	0.46
2:C:1272:GLU:HG3	2:C:1276:TRP:CZ2	2.51	0.46
1:A:27:THR:HG22	1:A:202:VAL:HG13	1.98	0.46
2:H:40:GLU:O	2:H:73:TYR:OH	2.33	0.46
1:B:74:VAL:HG12	1:B:76:GLU:H	1.81	0.46
3:I:613:GLY:O	3:I:617:THR:OG1	2.22	0.46
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.97	0.45
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.98	0.45
1:G:218:ARG:HH12	1:G:222:THR:HB	1.81	0.45
2:C:515:MET:HE2	2:C:523:GLU:HB3	1.97	0.45
3:I:44:ILE:HG22	5:Y:450:ILE:HG22	1.97	0.45
3:D:832:LYS:HA	3:D:832:LYS:HZ1	1.80	0.45
2:C:800:MET:HG2	2:C:1096:ILE:HD13	1.98	0.45
2:H:600:THR:HG22	2:H:601:ASP:N	2.28	0.45
3:D:678:ARG:O	3:D:681:LYS:HG3	2.16	0.45
3:I:596:LEU:HD23	3:I:596:LEU:N	2.31	0.45
3:D:1226:VAL:HA	3:D:1229:VAL:HG12	1.98	0.45
2:H:337:PHE:O	2:H:338:THR:OG1	2.26	0.45
3:I:263:SER:HB2	5:Y:507:MET:HE2	1.98	0.45
3:I:800:LEU:O	3:I:803:VAL:HG12	2.16	0.45
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.17	0.45
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.16	0.45
3:I:390:LEU:HD12	3:I:390:LEU:N	2.31	0.45
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.31	0.45
3:D:111:THR:HG23	3:D:300:GLN:NE2	2.30	0.45
2:H:510:GLN:NE2	2:H:534:GLY:HA2	2.30	0.45
3:I:620:PHE:O	3:I:624:ILE:HG23	2.16	0.45
3:D:1347:LEU:HD23	3:D:1358:PRO:CG	2.30	0.45
3:I:238:ILE:HG13	3:I:238:ILE:O	2.16	0.45
3:D:1198:VAL:HB	3:D:1210:ILE:CD1	2.47	0.45
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.16	0.45
3:D:120:LEU:HG	5:X:46:GLN:CD	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:264:LYS:N	5:Y:264:LYS:HD2	2.31	0.45
5:X:112:THR:HG22	5:X:113:ARG:N	2.27	0.45
3:I:589:TYR:O	3:I:591:ILE:HG13	2.16	0.45
2:H:521:LEU:HD22	2:H:667:LEU:HD12	1.99	0.45
3:D:415:VAL:HG23	3:D:416:ILE:HG23	1.97	0.45
1:A:163:GLU:CB	1:A:166:ARG:HB3	2.45	0.45
1:A:318:LEU:HD13	1:A:318:LEU:N	2.32	0.45
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.51	0.45
2:H:1276:TRP:HE3	2:H:1276:TRP:HA	1.81	0.45
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.81	0.45
2:C:314:ASN:HD21	2:C:348:SER:HA	1.80	0.45
1:A:300:LEU:HD13	1:A:300:LEU:O	2.17	0.45
2:C:1006:GLU:CD	2:C:1006:GLU:H	2.19	0.45
2:H:1117:LEU:HD11	2:H:1182:ILE:CD1	2.47	0.45
5:Y:400:GLN:O	5:Y:404:LEU:HD13	2.15	0.45
3:D:127:LEU:HD11	3:D:194:LEU:HD11	1.99	0.45
3:D:818:GLU:HA	3:D:881:LYS:HE2	1.98	0.45
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.98	0.45
3:D:1269:ALA:N	3:D:1300:ALA:HB2	2.30	0.45
3:D:822:MET:HG2	3:D:839:VAL:HG22	1.97	0.45
3:D:290:ILE:O	3:D:293:ARG:HG3	2.15	0.45
3:D:909:ILE:O	3:D:909:ILE:HD12	2.16	0.45
3:I:145:VAL:HG21	3:I:165:TYR:CD2	2.52	0.45
1:A:317:ARG:C	1:A:318:LEU:HD13	2.36	0.45
3:I:214:ARG:O	3:I:218:THR:HG22	2.16	0.45
3:D:74:LYS:HB3	3:D:74:LYS:NZ	2.31	0.45
3:D:1307:LEU:HD23	3:D:1307:LEU:H	1.81	0.45
3:D:605:LEU:O	3:D:605:LEU:HD13	2.17	0.45
3:I:29:MET:HE3	3:I:29:MET:HA	1.98	0.45
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.81	0.45
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.51	0.45
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.16	0.45
2:C:518:ASN:OD1	2:C:1236:ASN:ND2	2.48	0.45
2:C:1199:LEU:HD13	2:C:1206:THR:HA	1.98	0.45
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.98	0.45
3:I:813:ASP:OD1	3:I:896:ALA:HB3	2.16	0.45
3:D:514:THR:HG23	3:D:576:ARG:HE	1.80	0.45
2:C:131:THR:HG23	2:C:133:ASN:N	2.30	0.45
3:I:586:GLY:O	3:I:587:LEU:HB2	2.17	0.45
3:D:362:ARG:HH22	7:D:1503:0O2:H7	1.82	0.45
1:F:45:ARG:HD3	1:G:34:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:101:TYR:CE2	5:X:388:ILE:HD11	2.45	0.45
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.99	0.45
4:E:15:ASN:ND2	4:E:18:ASP:HB2	2.31	0.45
2:C:1141:LEU:HD22	2:C:1141:LEU:O	2.16	0.45
1:B:129:VAL:HG11	1:B:132:HIS:CE1	2.51	0.45
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.98	0.45
2:H:1103:VAL:H	2:H:1104:PRO:HD2	1.80	0.45
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.31	0.45
3:I:501:VAL:HG21	3:I:602:SER:HB2	1.99	0.45
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.46	0.45
2:C:620:ASN:HD21	3:D:769:VAL:HG12	1.80	0.45
3:I:846:GLU:HA	3:I:858:VAL:HA	1.98	0.45
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.42	0.45
2:C:96:LEU:HB2	2:C:127:ILE:CD1	2.47	0.45
2:H:143:ARG:NH1	2:H:512:SER:O	2.50	0.45
2:C:845:LEU:N	2:C:845:LEU:HD13	2.27	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:N	2.31	0.45
2:C:22:LEU:HD13	2:C:23:ASP:O	2.17	0.45
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.16	0.45
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.81	0.45
3:I:33:TRP:O	3:I:102:MET:HB2	2.16	0.45
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	1.97	0.45
2:C:1191:LYS:O	2:C:1195:ILE:HG13	2.16	0.45
5:X:445:ASP:N	5:X:445:ASP:OD1	2.38	0.45
2:H:88:ARG:NH1	2:H:88:ARG:HB3	2.30	0.45
5:Y:445:ASP:N	5:Y:445:ASP:OD1	2.39	0.45
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.99	0.45
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.38	0.45
2:C:699:LEU:HD11	2:C:1179:GLY:CA	2.43	0.45
3:I:583:VAL:HG13	3:I:587:LEU:HD22	1.98	0.45
1:B:48:LEU:HB3	3:D:538:ARG:HD3	1.99	0.45
3:D:246:PRO:HB2	3:D:249:LEU:HD13	1.98	0.45
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.98	0.45
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.81	0.45
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.80	0.45
2:H:169:LYS:HD3	2:H:169:LYS:HA	1.76	0.45
5:X:543:ALA:O	5:X:547:VAL:HG23	2.16	0.45
3:D:513:MET:O	3:D:575:GLY:HA3	2.17	0.45
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.46	0.45
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.98	0.45
5:X:592:ALA:O	5:X:596:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:446:ASP:OD1	2:C:546:GLU:HB3	2.17	0.45
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.32	0.45
3:D:238:ILE:HG13	3:D:238:ILE:O	2.15	0.45
3:I:1345:ARG:HG2	3:I:1370:MET:HE1	1.98	0.45
5:Y:448:ARG:NH1	5:Y:452:ILE:HD12	2.32	0.45
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.46	0.45
2:C:49:LEU:CD1	2:C:461:GLU:HA	2.47	0.45
3:I:1297:LYS:HE2	3:I:1297:LYS:HA	1.97	0.45
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.82	0.45
1:A:241:GLU:OE2	1:A:243:LYS:HE3	2.17	0.45
2:C:1272:GLU:HA	2:C:1275:VAL:HG22	1.99	0.45
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.52	0.45
4:J:60:ASN:H	4:J:63:ILE:HB	1.82	0.45
2:C:958:LYS:O	2:C:962:GLU:HG2	2.17	0.45
2:H:994:ARG:N	2:H:994:ARG:HD3	2.31	0.45
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.32	0.45
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.97	0.45
5:X:451:ARG:O	5:X:452:ILE:HG13	2.17	0.45
5:X:240:ARG:HD3	5:X:244:THR:CB	2.40	0.45
5:X:449:THR:HG23	5:X:503:GLU:OE1	2.16	0.45
3:D:619:ILE:HD11	3:D:623:GLN:HE21	1.82	0.45
2:H:1238:LEU:HD12	2:H:1239:VAL:O	2.16	0.45
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.52	0.45
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.99	0.45
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.98	0.45
2:C:462:ASN:O	2:C:466:VAL:HG23	2.17	0.45
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.16	0.45
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.99	0.45
2:H:297:VAL:HB	2:H:317:LEU:HD21	1.98	0.45
3:I:113:HIS:CE1	3:I:115:TRP:HB2	2.51	0.45
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.51	0.45
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.51	0.45
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.98	0.45
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.80	0.45
5:Y:276:MET:O	5:Y:280:VAL:HG23	2.17	0.45
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.82	0.45
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.99	0.45
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.82	0.45
2:C:1017:GLN:HA	2:C:1020:GLU:HB3	1.98	0.45
2:C:453:ILE:HG23	2:C:453:ILE:O	2.17	0.45
2:H:149:LEU:HD12	2:H:452:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:704:GLU:O	3:I:705:THR:OG1	2.28	0.45
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.99	0.45
3:D:1307:LEU:HD23	3:D:1307:LEU:N	2.32	0.45
3:D:733:SER:O	3:D:737:ILE:HG12	2.17	0.45
5:Y:354:THR:HG23	5:Y:357:GLN:HB3	1.97	0.45
2:C:821:ARG:HB2	2:C:1082:ILE:CD1	2.47	0.45
3:D:210:SER:O	3:D:214:ARG:HG3	2.17	0.45
3:I:527:LEU:HD12	3:I:535:ARG:NE	2.32	0.45
2:C:1258:PRO:HG2	3:D:346:ARG:CB	2.47	0.45
3:I:1247:LYS:N	3:I:1247:LYS:HD3	2.22	0.45
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.82	0.45
3:I:120:LEU:HD22	3:I:1330:ARG:HD2	1.99	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.17	0.45
2:H:475:VAL:O	2:H:479:LEU:HB2	2.16	0.45
2:H:669:PRO:HG2	2:H:1070:HIS:CE1	2.51	0.45
2:H:756:TYR:H	2:H:766:ASN:HB3	1.82	0.45
3:D:395:LYS:HD3	5:X:607:LEU:HD13	1.99	0.45
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.99	0.45
3:I:856:ILE:HG13	3:I:857:LEU:O	2.16	0.45
1:A:181:GLU:N	1:A:181:GLU:OE2	2.50	0.45
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.17	0.45
2:H:1081:PRO:O	2:H:1085:MET:HG3	2.17	0.45
2:H:489:PRO:HB2	2:H:492:MET:CB	2.37	0.44
3:D:527:LEU:HD13	3:D:531:LYS:CB	2.45	0.44
5:X:113:ARG:O	5:X:117:ILE:HD13	2.18	0.44
3:D:915:ILE:O	3:D:918:ILE:HG23	2.16	0.44
3:D:66:LYS:HB2	3:D:69:GLU:HG2	1.99	0.44
5:Y:119:ILE:CG2	5:Y:379:MET:HG2	2.45	0.44
3:D:701:LEU:HD21	3:D:723:TYR:HB2	1.99	0.44
3:I:1357:ILE:N	3:I:1357:ILE:HD12	2.32	0.44
3:I:515:ARG:HH22	3:I:717:VAL:C	2.19	0.44
3:I:74:LYS:HB3	3:I:74:LYS:NZ	2.32	0.44
3:D:596:LEU:HD23	3:D:596:LEU:N	2.32	0.44
2:H:961:SER:O	2:H:965:GLN:HG3	2.17	0.44
3:D:663:GLU:O	3:D:667:GLN:HG3	2.17	0.44
5:Y:555:GLU:OE2	5:Y:597:LYS:NZ	2.33	0.44
2:H:1291:LEU:HD13	3:I:345:LYS:NZ	2.31	0.44
2:C:310:ILE:O	2:C:311:CYS:HB3	2.18	0.44
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.98	0.44
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.82	0.44
2:H:1027:LYS:HB2	2:H:1027:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.88	0.44
3:D:239:LEU:HD12	3:D:239:LEU:O	2.17	0.44
3:D:1161:GLY:HA2	3:D:1181:ASP:CB	2.47	0.44
1:B:126:PRO:HG2	1:B:127:GLN:OE1	2.18	0.44
4:J:65:ASP:O	4:J:69:ARG:HG3	2.16	0.44
2:H:593:LYS:HD2	2:H:604:HIS:NE2	2.32	0.44
5:Y:561:MET:HA	5:Y:567:MET:SD	2.57	0.44
1:F:61:ILE:HG12	1:F:142:MET:HB3	1.98	0.44
3:D:526:VAL:HG12	3:D:549:LYS:O	2.17	0.44
3:I:539:SER:OG	3:I:540:GLY:N	2.50	0.44
2:H:807:TRP:HH2	2:H:1216:ARG:HE	1.65	0.44
3:D:316:ILE:CG2	3:D:317:THR:H	2.25	0.44
3:D:664:ILE:HG21	3:D:681:LYS:CD	2.44	0.44
2:H:484:LEU:N	2:H:484:LEU:HD22	2.31	0.44
1:G:178:SER:HA	1:G:179:PRO:HD3	1.87	0.44
2:H:1111:GLN:CG	2:H:1230:MET:HE2	2.48	0.44
2:C:88:ARG:NH1	2:C:88:ARG:HB3	2.33	0.44
3:I:161:THR:HG22	3:I:162:GLU:N	2.33	0.44
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.98	0.44
2:C:1027:LYS:HB2	2:C:1027:LYS:NZ	2.33	0.44
2:H:1120:ALA:HB1	2:H:1198:LEU:HB3	1.99	0.44
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.17	0.44
4:E:30:MET:O	4:E:35:LYS:HG2	2.17	0.44
3:I:490:ILE:O	3:I:499:ILE:HG22	2.18	0.44
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.99	0.44
2:C:823:VAL:HG22	2:C:1060:ILE:HG13	1.99	0.44
2:H:820:GLU:O	2:H:824:GLN:HG3	2.18	0.44
3:D:217:LEU:O	3:D:221:ILE:HG12	2.16	0.44
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.53	0.44
3:I:909:ILE:O	3:I:909:ILE:HD12	2.18	0.44
3:I:378:LYS:HD2	3:I:382:TYR:OH	2.16	0.44
7:D:1503:0O2:O2G	4:E:3:ARG:NH2	2.50	0.44
2:H:1238:LEU:HD12	2:H:1239:VAL:N	2.32	0.44
3:D:703:THR:O	3:D:718:SER:N	2.50	0.44
3:D:825:VAL:HG23	3:D:835:LEU:HB2	1.99	0.44
2:H:943:LYS:O	2:H:947:GLU:HG2	2.17	0.44
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.99	0.44
1:F:185:TYR:HB2	1:F:201:LEU:HD11	1.98	0.44
2:H:429:MET:O	2:H:433:ILE:HG13	2.17	0.44
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.98	0.44
2:H:702:THR:HA	2:H:1184:THR:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.48	0.44
3:D:1344:LEU:H	3:D:1345:ARG:HG3	1.83	0.44
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.35	0.44
1:A:80:GLU:HG3	2:C:694:ARG:HH12	1.83	0.44
3:I:416:ILE:HG13	3:I:441:LEU:CD2	2.48	0.44
1:G:65:LEU:HD23	1:G:65:LEU:N	2.30	0.44
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.30	0.44
2:C:1298:VAL:HG23	2:C:1299:ASN:N	2.29	0.44
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.31	0.44
3:I:700:ASN:O	3:I:704:GLU:HG2	2.17	0.44
2:H:1276:TRP:CD2	3:I:801:VAL:HG11	2.53	0.44
2:C:985:GLU:HG2	2:C:989:LEU:HD13	2.00	0.44
2:H:161:LYS:HB3	2:H:161:LYS:NZ	2.33	0.44
3:D:1184:ASP:HA	3:D:1185:PRO:HD3	1.80	0.44
2:H:839:VAL:HG11	2:H:841:ARG:HE	1.83	0.44
5:X:61:ASP:HA	5:X:64:ASP:OD2	2.17	0.44
2:H:821:ARG:NE	2:H:1082:ILE:HD13	2.33	0.44
4:E:5:THR:CA	4:E:7:GLN:H	2.30	0.44
2:C:1108:ASN:O	2:C:1108:ASN:ND2	2.51	0.44
3:I:899:TYR:CE1	3:I:915:ILE:HG23	2.53	0.44
3:I:1284:ARG:HA	3:I:1287:ILE:CG1	2.46	0.44
2:C:68:LEU:HG	2:C:100:LEU:HD23	2.00	0.44
3:I:412:LEU:O	3:I:415:VAL:HG22	2.18	0.44
2:C:812:PHE:HB2	3:D:357:VAL:HG21	2.00	0.44
4:E:15:ASN:ND2	4:E:18:ASP:OD1	2.51	0.44
1:F:234:LEU:HD21	1:G:217:ILE:HD11	1.98	0.44
2:C:892:GLU:O	2:C:893:THR:OG1	2.22	0.44
2:H:736:VAL:HG11	2:H:740:GLU:HA	1.98	0.44
3:D:704:GLU:HB2	3:D:718:SER:OG	2.18	0.44
1:G:33:ARG:HD3	2:H:1081:PRO:HG3	1.98	0.44
3:I:1195:GLN:N	3:I:1195:GLN:OE1	2.48	0.44
1:G:67:GLU:O	1:G:78:ILE:HB	2.18	0.44
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.51	0.44
2:H:179:TYR:HE2	2:H:462:ASN:HD21	1.64	0.44
2:C:177:ILE:HD12	2:C:177:ILE:N	2.33	0.44
1:G:81:ILE:HG23	1:G:131:CYS:SG	2.58	0.44
2:H:845:LEU:N	2:H:845:LEU:HD13	2.30	0.44
1:A:88:LEU:HD22	1:A:90:VAL:CG2	2.48	0.44
4:J:10:VAL:CG2	4:J:16:ARG:HG2	2.47	0.44
3:D:233:LYS:CD	3:D:234:PRO:HD2	2.48	0.44
2:H:202:ARG:NE	2:H:369:MET:HG2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.47	0.44
3:I:664:ILE:HG21	3:I:681:LYS:HD2	2.00	0.44
3:D:382:TYR:HE1	3:D:401:VAL:CG2	2.31	0.44
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.83	0.44
3:D:161:THR:HG22	3:D:162:GLU:N	2.33	0.44
2:H:1086:PRO:HA	2:H:1213:TYR:O	2.18	0.44
2:H:1103:VAL:HB	2:H:1104:PRO:HD3	2.00	0.44
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.53	0.44
1:F:163:GLU:HG3	1:F:170:ARG:NH1	2.18	0.44
3:I:41:PRO:HB3	3:I:270:ARG:HG3	1.99	0.44
3:D:572:THR:HG22	3:D:594:GLN:OE1	2.18	0.44
1:A:45:ARG:NE	1:B:38:THR:OG1	2.46	0.44
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.26	0.44
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.21	0.44
2:C:11:ILE:HG21	2:C:697:LYS:HZ1	1.80	0.44
3:I:124:ILE:HG13	3:I:189:LEU:HD11	1.99	0.44
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.53	0.44
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.82	0.44
1:F:158:ARG:HE	1:F:172:LEU:HD13	1.82	0.44
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.32	0.44
3:I:12:THR:C	3:I:13:LYS:HD2	2.39	0.44
2:C:1233:LEU:HD12	2:C:1233:LEU:O	2.18	0.44
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.99	0.44
3:I:873:GLU:OE2	3:I:877:VAL:HB	2.18	0.44
5:X:469:GLN:O	5:X:473:GLU:HB2	2.18	0.44
3:D:888:CYS:SG	3:D:890:THR:HB	2.58	0.44
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.46	0.44
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.43	0.44
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.99	0.44
1:F:11:PRO:HD2	1:G:227:GLN:HA	1.99	0.44
3:D:766:GLY:C	3:D:767:LEU:HD22	2.37	0.44
2:C:1081:PRO:O	2:C:1085:MET:HG3	2.17	0.44
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.33	0.44
2:C:697:LYS:NZ	2:C:791:LEU:HD11	2.32	0.44
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.30	0.44
2:H:106:GLU:CG	2:H:109:ALA:H	2.31	0.44
3:D:490:ILE:HG23	3:D:500:ILE:CD1	2.48	0.44
5:X:532:LEU:O	5:X:536:THR:HG23	2.18	0.44
5:Y:123:ILE:O	5:Y:127:ILE:HG12	2.18	0.44
3:I:801:VAL:O	3:I:805:GLN:HG2	2.17	0.44
3:D:515:ARG:NH2	3:D:717:VAL:HG12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:30:ILE:HD13	3:I:33:TRP:CZ3	2.53	0.44
1:A:178:SER:HA	1:A:179:PRO:HD3	1.75	0.44
2:H:850:ILE:HG23	2:H:885:GLY:O	2.17	0.44
3:D:842:ARG:HD2	3:D:882:VAL:HG21	1.99	0.44
3:D:801:VAL:O	3:D:805:GLN:HG2	2.17	0.44
1:B:22:THR:HG22	1:B:208:ASN:O	2.18	0.44
2:H:890:LYS:NZ	2:H:890:LYS:HB3	2.32	0.44
3:I:388:ARG:NH2	3:I:414:GLU:OE2	2.51	0.44
5:X:254:GLU:O	5:X:258:GLN:HG3	2.18	0.44
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.99	0.44
2:C:297:VAL:HB	2:C:317:LEU:HD21	2.00	0.44
2:H:828:PHE:HB2	2:H:1060:ILE:HD13	2.00	0.44
2:H:632:ASP:O	2:H:633:LEU:HD23	2.18	0.44
2:C:345:PRO:O	2:C:349:GLU:HG2	2.18	0.44
1:B:190:ALA:N	1:B:198:LEU:O	2.37	0.43
5:Y:451:ARG:O	5:Y:452:ILE:HG13	2.18	0.43
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.53	0.43
3:I:832:LYS:HZ2	3:I:832:LYS:HB2	1.83	0.43
2:H:562:GLU:HG2	2:H:574:SER:HB3	1.98	0.43
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.86	0.43
5:Y:477:GLU:N	5:Y:477:GLU:OE1	2.46	0.43
2:C:384:LEU:O	2:C:388:LEU:HG	2.17	0.43
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.48	0.43
2:H:73:TYR:O	2:H:74:ARG:HB2	2.17	0.43
1:B:180:VAL:HG11	1:B:183:ILE:HG12	2.00	0.43
3:I:63:GLY:O	3:I:98:ARG:NH2	2.51	0.43
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.51	0.43
2:C:1247:SER:O	2:C:1248:THR:HG23	2.18	0.43
2:C:19:PRO:HA	2:C:1157:GLN:HE21	1.83	0.43
2:C:1185:PRO:HB2	2:C:1186:VAL:H	1.69	0.43
2:C:515:MET:HE2	2:C:523:GLU:CG	2.48	0.43
1:F:31:LEU:HB2	1:F:199:ASP:O	2.17	0.43
3:I:222:LYS:HZ2	3:I:1276:GLU:HB2	1.82	0.43
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.49	0.43
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	2.00	0.43
3:I:1257:VAL:HA	3:I:1260:MET:CB	2.49	0.43
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	2.00	0.43
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.53	0.43
5:Y:240:ARG:HD3	5:Y:244:THR:CB	2.47	0.43
1:B:46:ILE:HG23	1:B:50:SER:HB2	2.00	0.43
3:I:1307:LEU:HD23	3:I:1307:LEU:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:843:VAL:HG21	3:I:897:HIS:HA	2.00	0.43
3:D:62:PHE:O	3:D:101:ARG:HG3	2.18	0.43
5:X:465:ARG:O	5:X:468:ARG:HG2	2.17	0.43
5:X:299:LYS:O	5:X:303:ILE:HG12	2.18	0.43
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.48	0.43
1:A:33:ARG:HG2	1:A:199:ASP:OD2	2.18	0.43
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.26	0.43
3:I:508:LEU:HD23	3:I:508:LEU:O	2.19	0.43
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.44	0.43
3:I:52:GLU:OE1	5:Y:451:ARG:HD2	2.17	0.43
2:C:1166:ASP:C	2:C:1168:GLU:H	2.22	0.43
2:C:170:VAL:O	2:C:171:LEU:HB2	2.18	0.43
5:X:105:MET:O	5:X:385:ARG:NH1	2.50	0.43
3:I:905:ARG:NH2	4:J:10:VAL:HG11	2.30	0.43
2:C:11:ILE:HD13	2:C:697:LYS:HE3	1.99	0.43
5:X:456:MET:O	5:X:460:ILE:HG13	2.18	0.43
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.50	0.43
2:H:73:TYR:CD2	2:H:73:TYR:N	2.86	0.43
1:G:110:VAL:HG21	1:G:140:ILE:HD11	2.01	0.43
2:H:216:THR:O	2:H:220:ILE:HG13	2.18	0.43
2:H:1067:ALA:HB3	2:H:1235:LEU:HD11	2.00	0.43
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.48	0.43
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.99	0.43
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.48	0.43
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.47	0.43
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.33	0.43
3:D:681:LYS:HB2	3:D:681:LYS:HZ2	1.84	0.43
3:D:136:GLU:HA	3:D:139:LEU:HD12	2.00	0.43
2:C:590:PRO:O	2:C:659:GLN:NE2	2.50	0.43
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.18	0.43
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	1.99	0.43
1:A:179:PRO:O	1:A:207:THR:OG1	2.25	0.43
1:A:246:LYS:N	1:A:246:LYS:HD3	2.33	0.43
2:H:177:ILE:N	2:H:177:ILE:HD12	2.33	0.43
2:H:944:ARG:HD3	2:H:944:ARG:O	2.17	0.43
3:D:390:LEU:HD12	3:D:390:LEU:N	2.32	0.43
3:I:239:LEU:HD12	3:I:239:LEU:O	2.19	0.43
2:C:1158:LYS:O	2:C:1158:LYS:HD2	2.19	0.43
2:C:161:LYS:HB3	2:C:161:LYS:NZ	2.34	0.43
2:C:219:GLN:O	2:C:223:LEU:HG	2.17	0.43
1:F:77:ASP:O	1:F:81:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	2.00	0.43
2:H:657:THR:OG1	2:H:1187:PHE:HB2	2.18	0.43
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.51	0.43
2:C:533:LEU:N	2:C:533:LEU:HD23	2.31	0.43
3:D:500:ILE:H	3:D:500:ILE:CD1	2.31	0.43
3:D:66:LYS:HB3	3:D:66:LYS:NZ	2.33	0.43
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.18	0.43
3:D:886:VAL:HG13	3:D:1230:THR:HG21	2.00	0.43
3:D:1159:ILE:HD12	3:D:1186:TYR:CE2	2.53	0.43
1:G:183:ILE:HD11	1:G:205:MET:HE2	2.00	0.43
3:I:179:LYS:N	3:I:179:LYS:HD3	2.33	0.43
2:H:866:ASP:HA	2:H:872:TYR:OH	2.17	0.43
3:D:1162:ILE:HG12	3:D:1203:ARG:HG2	2.00	0.43
3:D:79:LYS:HE3	5:X:568:ASN:C	2.38	0.43
3:D:215:LYS:O	3:D:219:LYS:HG3	2.19	0.43
1:G:227:GLN:O	1:G:228:LEU:HD23	2.19	0.43
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.89	0.43
1:F:150:ARG:HD2	1:G:8:PHE:CZ	2.54	0.43
3:I:1284:ARG:HA	3:I:1287:ILE:CD1	2.49	0.43
1:G:191:ARG:NH2	3:I:441:LEU:O	2.52	0.43
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.83	0.43
2:H:106:GLU:CB	2:H:107:ARG:HA	2.49	0.43
3:I:532:GLU:OE2	3:I:574:VAL:HG13	2.19	0.43
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.76	0.43
2:H:748:ILE:HD12	2:H:748:ILE:C	2.39	0.43
3:I:796:LEU:HG	3:I:800:LEU:HD23	2.01	0.43
3:I:611:ILE:HG22	3:I:865:HIS:CE1	2.54	0.43
2:H:1163:THR:HG22	2:H:1164:PHE:H	1.84	0.43
2:C:363:LEU:HD13	2:C:382:GLU:HG2	2.00	0.43
2:H:816:ILE:HD13	2:H:1074:GLY:CA	2.43	0.43
1:F:11:PRO:HA	1:F:30:PRO:O	2.19	0.43
1:G:227:GLN:O	1:G:229:GLU:N	2.52	0.43
3:D:620:PHE:O	3:D:624:ILE:HG23	2.19	0.43
3:I:1287:ILE:O	3:I:1291:GLU:HG2	2.19	0.43
2:H:555:TYR:OH	2:H:637:ARG:NH2	2.52	0.43
3:D:619:ILE:HD13	7:D:1503:0O2:H2	1.83	0.43
2:C:811:ASN:HA	2:C:815:SER:HB2	2.00	0.43
3:D:355:ILE:HA	3:D:447:ILE:HG23	1.99	0.43
2:C:617:ALA:HB2	2:C:650:VAL:HG21	2.01	0.43
2:C:611:GLU:HG2	2:C:616:ILE:HD11	2.00	0.43
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:37:GLU:HB2	3:I:104:HIS:HE1	1.83	0.43
5:X:343:LYS:O	5:X:346:GLN:HB3	2.18	0.43
2:H:993:PRO:HB2	2:H:994:ARG:H	1.60	0.43
5:X:469:GLN:O	5:X:473:GLU:N	2.47	0.43
2:C:1086:PRO:HG2	2:C:1094:VAL:HG21	2.01	0.43
5:X:141:ILE:HG13	5:X:256:PHE:CD1	2.53	0.43
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.33	0.43
2:H:582:ASN:HB3	2:H:586:PHE:C	2.39	0.43
2:C:51:ALA:HB3	2:C:465:ARG:HH11	1.83	0.43
2:C:500:ALA:O	2:C:504:GLU:HB2	2.18	0.43
1:G:56:VAL:HG12	1:G:173:VAL:HG11	2.01	0.43
2:C:622:ASN:OD1	2:C:623:LEU:N	2.51	0.43
3:D:1167:LYS:HB3	3:D:1170:LYS:HD2	2.00	0.43
2:H:1185:PRO:HB2	2:H:1186:VAL:H	1.66	0.43
3:D:573:THR:HG22	3:D:576:ARG:CD	2.48	0.43
3:D:259:ARG:HH21	5:X:504:PRO:CB	2.26	0.43
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.19	0.43
1:F:66:HIS:HB3	2:H:874:GLY:HA2	2.00	0.43
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.34	0.43
3:I:885:VAL:O	3:I:1258:ARG:HD3	2.19	0.43
2:H:333:ILE:N	2:H:333:ILE:HD12	2.34	0.43
2:C:826:ASP:HA	2:C:829:THR:HG23	1.99	0.43
3:I:733:SER:O	3:I:737:ILE:HG12	2.19	0.43
3:I:159:ILE:N	3:I:159:ILE:HD12	2.33	0.43
2:H:622:ASN:OD1	2:H:623:LEU:N	2.52	0.43
3:I:276:ASN:O	3:I:280:LYS:HG3	2.19	0.43
2:C:1287:LEU:HD23	3:D:1357:ILE:CD1	2.48	0.43
1:F:219:ARG:O	1:F:223:ILE:HG13	2.18	0.43
3:D:591:ILE:HA	3:D:594:GLN:HB2	2.01	0.43
2:H:842:ASP:HB2	2:H:1046:VAL:HG11	2.01	0.43
2:H:894:GLN:O	2:H:895:LEU:HB2	2.18	0.43
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.53	0.43
3:D:393:THR:H	3:D:396:ALA:HB3	1.83	0.43
3:D:1257:VAL:HA	3:D:1260:MET:CB	2.47	0.43
3:D:491:LEU:HB2	3:D:904:ALA:HA	2.00	0.43
5:X:283:GLN:O	5:X:287:ILE:HG13	2.18	0.43
2:C:17:LYS:N	2:C:17:LYS:HD2	2.34	0.43
1:G:110:VAL:HB	1:G:131:CYS:HB2	1.99	0.43
2:H:768:MET:O	2:H:785:ASP:N	2.50	0.43
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.19	0.43
2:H:999:GLU:HG2	2:H:1000:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:901:ARG:HB3	3:D:908:ILE:HA	2.01	0.43
3:D:112:ALA:HA	3:D:238:ILE:HG22	2.00	0.43
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.49	0.43
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.34	0.43
2:H:971:LEU:HG	2:H:1018:TYR:HD1	1.84	0.43
3:I:1287:ILE:O	3:I:1290:ARG:HG2	2.18	0.43
3:I:120:LEU:HB3	3:I:121:PRO:HD3	1.97	0.43
1:A:11:PRO:HA	1:A:30:PRO:O	2.18	0.43
3:D:416:ILE:O	3:D:416:ILE:HD12	2.19	0.43
3:I:809:VAL:CG1	3:I:913:GLU:H	2.32	0.43
2:C:453:ILE:HG22	2:C:585:GLY:O	2.19	0.43
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.24	0.43
3:I:655:SER:O	3:I:658:GLU:HG2	2.19	0.43
2:H:1276:TRP:CE2	3:I:801:VAL:HG11	2.54	0.43
3:I:431:ARG:HH21	3:I:493:PRO:HG3	1.83	0.43
2:H:896:THR:HG22	2:H:898:GLU:OE1	2.18	0.43
1:F:28:LEU:HD13	1:G:231:PHE:HE2	1.82	0.43
3:I:1307:LEU:HD23	3:I:1307:LEU:N	2.34	0.43
1:B:213:PRO:HA	1:B:216:ALA:HB3	2.00	0.43
2:C:1209:GLN:O	2:C:1210:ILE:HG13	2.19	0.43
2:H:935:THR:HA	2:H:1048:LYS:HB3	2.00	0.43
1:A:257:VAL:HG13	1:A:276:HIS:O	2.19	0.43
2:C:515:MET:HA	2:C:526:HIS:CE1	2.54	0.42
5:Y:460:ILE:HG12	5:Y:497:VAL:HG13	2.01	0.42
3:D:1284:ARG:HA	3:D:1287:ILE:CD1	2.49	0.42
2:C:794:LEU:HD21	2:C:796:LEU:CG	2.46	0.42
3:D:660:GLU:O	3:D:664:ILE:HG12	2.19	0.42
2:H:170:VAL:O	2:H:171:LEU:HB2	2.19	0.42
2:H:1314:GLN:HG2	2:H:1315:MET:H	1.83	0.42
3:D:377:PHE:O	3:D:381:ILE:HG13	2.18	0.42
3:I:252:LEU:N	3:I:252:LEU:HD23	2.33	0.42
2:H:130:MET:CG	2:H:134:GLY:HA2	2.48	0.42
3:D:704:GLU:O	3:D:705:THR:OG1	2.27	0.42
3:I:149:GLY:HA2	3:I:156:ARG:HG2	2.01	0.42
5:X:250:LEU:O	5:X:254:GLU:HG2	2.18	0.42
3:D:508:LEU:HD22	3:D:508:LEU:O	2.18	0.42
2:C:1329:GLU:O	2:C:1332:SER:HB3	2.19	0.42
1:G:222:THR:O	1:G:226:GLU:HG2	2.19	0.42
1:F:167:PRO:HG2	1:F:170:ARG:HG3	2.00	0.42
2:C:49:LEU:HG	2:C:461:GLU:HB2	2.00	0.42
2:C:556:GLY:O	2:C:579:ALA:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:557:ARG:NH2	2:H:607:SER:O	2.51	0.42
3:I:595:ALA:HB1	3:I:596:LEU:HD23	2.01	0.42
3:I:124:ILE:HA	3:I:237:MET:HE2	2.00	0.42
2:C:1252:SER:HB3	2:C:1259:LEU:HD23	2.01	0.42
1:F:134:THR:HG21	2:H:727:VAL:O	2.18	0.42
2:C:966:ILE:HG23	2:C:967:LEU:HD12	2.01	0.42
2:C:542:ARG:HG2	2:C:543:ALA:N	2.33	0.42
1:A:22:THR:HB	1:A:207:THR:O	2.18	0.42
2:H:972:PHE:HA	2:H:975:ILE:HG22	2.01	0.42
3:D:506:VAL:HG23	3:D:628:GLY:HA3	2.00	0.42
3:D:800:LEU:O	3:D:803:VAL:HG12	2.18	0.42
2:H:896:THR:CG2	2:H:897:PRO:HD2	2.49	0.42
2:H:518:ASN:OD1	2:H:1236:ASN:ND2	2.52	0.42
2:H:347:ILE:HD11	2:H:433:ILE:HD11	2.01	0.42
2:C:994:ARG:N	2:C:994:ARG:HD3	2.34	0.42
3:I:1173:ARG:CZ	3:I:1176:VAL:HG21	2.50	0.42
3:D:746:LEU:HB3	3:D:754:ILE:CG2	2.49	0.42
2:H:812:PHE:N	2:H:815:SER:HB2	2.34	0.42
3:D:614:LEU:HD12	4:E:5:THR:HG21	2.01	0.42
1:A:227:GLN:NE2	1:B:11:PRO:HD3	2.32	0.42
3:D:527:LEU:HB2	3:D:535:ARG:CZ	2.50	0.42
5:X:448:ARG:HH11	5:X:452:ILE:HD12	1.85	0.42
3:D:584:PRO:HD3	3:D:620:PHE:CD1	2.54	0.42
2:C:1293:VAL:HG21	2:C:1304:MET:CB	2.49	0.42
3:D:362:ARG:NH1	7:D:1503:0O2:H7	2.32	0.42
2:C:645:PHE:CD1	2:C:650:VAL:HB	2.54	0.42
3:D:789:LYS:HD2	3:D:932:MET:SD	2.59	0.42
3:I:128:LEU:HD13	3:I:189:LEU:HD23	2.01	0.42
3:D:1221:LEU:HB2	3:D:1229:VAL:HG21	2.01	0.42
3:D:1229:VAL:O	3:D:1233:ILE:HG13	2.19	0.42
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.49	0.42
1:A:152:TYR:CE1	1:A:154:PRO:HD3	2.53	0.42
3:I:704:GLU:HB3	3:I:705:THR:H	1.72	0.42
3:I:661:VAL:O	3:I:665:GLN:HG3	2.19	0.42
1:B:19:VAL:HG12	1:B:19:VAL:O	2.20	0.42
3:I:805:GLN:HE21	3:I:805:GLN:HB2	1.65	0.42
3:D:843:VAL:HA	3:D:861:ASN:HA	2.01	0.42
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.83	0.42
2:H:941:LYS:O	2:H:941:LYS:HD2	2.19	0.42
3:D:288:PRO:O	3:D:292:VAL:HG12	2.19	0.42
1:A:250:ASP:HB3	1:A:253:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:333:ILE:HD12	2:C:333:ILE:N	2.33	0.42
2:H:699:LEU:HD13	2:H:1181:PRO:HB3	2.01	0.42
3:D:201:LEU:HD12	3:D:205:LEU:HD11	2.02	0.42
2:C:68:LEU:HA	2:C:68:LEU:HD12	1.90	0.42
2:H:96:LEU:HB2	2:H:127:ILE:CD1	2.49	0.42
3:D:355:ILE:HG12	3:D:464:ASP:O	2.19	0.42
2:H:302:ILE:HA	2:H:309:LEU:HA	2.01	0.42
3:D:909:ILE:HG13	3:D:909:ILE:H	1.56	0.42
2:H:59:ILE:HG12	2:H:65:ASN:O	2.20	0.42
5:Y:469:GLN:O	5:Y:473:GLU:HB2	2.19	0.42
1:A:152:TYR:CD1	1:A:154:PRO:HD3	2.54	0.42
3:I:678:ARG:O	3:I:682:VAL:HG13	2.20	0.42
3:D:114:ILE:CG2	3:D:308:ASP:HB3	2.50	0.42
3:I:403:ARG:O	3:I:405:GLU:N	2.53	0.42
3:I:1282:TYR:HA	3:I:1285:VAL:CG2	2.49	0.42
2:C:51:ALA:C	2:C:53:PHE:H	2.22	0.42
2:C:890:LYS:NZ	2:C:890:LYS:HB3	2.33	0.42
3:I:58:CYS:SG	3:I:61:ILE:HG13	2.60	0.42
2:H:81:ASP:OD1	2:H:83:GLN:HG2	2.19	0.42
2:H:1225:VAL:HG12	3:I:636:GLY:O	2.19	0.42
3:D:58:CYS:SG	3:D:61:ILE:HG13	2.58	0.42
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	2.02	0.42
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.30	0.42
3:I:370:LYS:HG3	3:I:371:LYS:H	1.84	0.42
3:D:252:LEU:HG	3:D:252:LEU:O	2.20	0.42
3:D:425:ARG:CZ	3:D:459:ALA:HA	2.49	0.42
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	2.00	0.42
2:H:27:LEU:O	2:H:528:ARG:NH1	2.49	0.42
2:H:1285:TYR:CG	3:I:475:GLU:HG3	2.54	0.42
1:A:311:GLY:O	5:X:599:ARG:NE	2.52	0.42
2:H:94:ALA:O	2:H:126:GLU:HG2	2.19	0.42
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.02	0.42
2:C:1029:LEU:O	2:C:1032:LYS:HG3	2.18	0.42
2:C:184:LEU:HD13	2:C:389:PHE:CZ	2.54	0.42
2:H:896:THR:O	2:H:899:GLU:N	2.48	0.42
3:I:313:GLY:O	3:I:314:ARG:HB2	2.20	0.42
5:Y:532:LEU:O	5:Y:536:THR:HG23	2.19	0.42
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.55	0.42
1:B:153:VAL:O	1:B:175:ALA:N	2.52	0.42
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.54	0.42
2:C:68:LEU:HD22	2:C:475:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:LEU:HD13	2:H:23:ASP:O	2.19	0.42
2:C:487:LEU:H	2:C:487:LEU:HD12	1.84	0.42
5:X:139:GLU:HA	5:X:142:THR:CG2	2.48	0.42
2:H:1314:GLN:HG3	4:J:28:ARG:HH12	1.83	0.42
2:H:1166:ASP:C	2:H:1168:GLU:H	2.23	0.42
3:D:77:ARG:CG	3:D:78:LEU:H	2.31	0.42
2:C:748:ILE:HD12	2:C:748:ILE:C	2.39	0.42
3:I:796:LEU:O	3:I:800:LEU:HD23	2.19	0.42
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.42
3:I:607:THR:O	3:I:611:ILE:HG12	2.19	0.42
5:Y:278:ASP:O	5:Y:282:THR:OG1	2.24	0.42
2:C:342:ASP:O	2:C:437:ASN:ND2	2.52	0.42
3:D:159:ILE:N	3:D:159:ILE:HD12	2.34	0.42
3:D:558:ASP:OD1	3:D:559:ALA:N	2.52	0.42
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.52	0.42
3:I:1324:SER:CB	3:I:1348:LYS:HD3	2.48	0.42
2:H:1268:GLN:O	3:I:346:ARG:HA	2.20	0.42
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.85	0.42
3:I:397:ALA:O	3:I:401:VAL:HG13	2.20	0.42
1:G:191:ARG:HH12	3:I:443:GLU:HG2	1.84	0.42
2:H:553:THR:O	2:H:557:ARG:HD3	2.19	0.42
3:I:534:GLU:O	3:I:538:ARG:HB2	2.20	0.42
3:I:474:LEU:HB3	4:J:28:ARG:HH21	1.85	0.42
3:I:1297:LYS:CA	3:I:1297:LYS:NZ	2.82	0.42
3:D:490:ILE:HG23	3:D:500:ILE:HD11	2.01	0.42
3:I:66:LYS:HB3	3:I:66:LYS:NZ	2.34	0.42
3:I:147:ILE:HG13	3:I:149:GLY:H	1.84	0.42
2:C:1270:PHE:CE1	2:C:1290:MET:HG2	2.55	0.42
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.55	0.42
2:C:104:ILE:HD11	2:C:115:LYS:HB2	2.02	0.42
2:H:17:LYS:HD2	2:H:17:LYS:N	2.35	0.42
2:C:836:LEU:HB3	2:C:918:LEU:HD21	2.02	0.42
5:X:439:ILE:O	5:X:443:ILE:HG13	2.19	0.42
3:I:491:LEU:HB2	3:I:904:ALA:HA	2.01	0.42
2:H:431:LYS:O	2:H:435:ILE:HG13	2.19	0.42
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.50	0.42
2:H:1073:LYS:HD3	3:I:462:ASP:CB	2.21	0.42
3:D:619:ILE:O	3:D:623:GLN:HG2	2.19	0.42
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.48	0.42
2:H:1146:GLN:CD	2:H:1160:ASP:HB2	2.40	0.42
2:H:766:ASN:H	2:H:787:PRO:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:382:TYR:CE1	3:D:401:VAL:HG21	2.55	0.42
5:Y:119:ILE:CD1	5:Y:122:ARG:HH21	2.33	0.42
2:C:99:LYS:HZ3	2:C:99:LYS:HB3	1.83	0.42
2:C:348:SER:O	2:C:352:ARG:HG3	2.20	0.42
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.67	0.42
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.20	0.42
3:I:105:ILE:HG13	3:I:244:VAL:CG2	2.50	0.42
5:X:316:PHE:CZ	5:X:334:SER:HA	2.55	0.42
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.50	0.42
2:C:632:ASP:O	2:C:633:LEU:HD23	2.20	0.42
2:H:560:PRO:HA	3:I:780:ARG:NH2	2.34	0.42
3:I:1343:GLU:HA	3:I:1344:LEU:CB	2.35	0.42
5:X:448:ARG:HD3	5:X:450:ILE:HG13	2.01	0.42
3:D:583:VAL:HG13	3:D:584:PRO:HD2	2.01	0.42
3:I:1148:ARG:HB2	3:I:1148:ARG:NH2	2.35	0.42
5:Y:262:VAL:HG12	5:Y:264:LYS:H	1.84	0.42
3:D:466:MET:HB3	3:D:466:MET:HE2	1.88	0.42
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.19	0.42
2:C:1315:MET:HE2	3:D:473:THR:OG1	2.20	0.42
3:D:154:LEU:HD22	3:D:176:PHE:HE1	1.83	0.42
3:D:843:VAL:HG21	3:D:897:HIS:HA	2.02	0.42
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.20	0.42
5:X:24:TYR:O	5:X:26:GLU:N	2.52	0.42
5:X:608:ARG:HB3	5:X:608:ARG:NH1	2.35	0.42
2:H:80:PHE:O	2:H:84:GLU:HB3	2.19	0.42
2:C:768:MET:O	2:C:785:ASP:N	2.48	0.42
5:X:373:ARG:HG3	5:X:377:LYS:HE3	2.00	0.42
1:G:52:PRO:HG3	1:G:150:ARG:HH12	1.84	0.42
3:I:269:TYR:HA	3:I:272:VAL:HG12	2.02	0.42
3:D:901:ARG:CB	3:D:908:ILE:HA	2.50	0.42
1:G:227:GLN:C	1:G:229:GLU:H	2.23	0.42
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.54	0.42
5:X:262:VAL:HG12	5:X:264:LYS:H	1.85	0.42
1:A:45:ARG:HG2	2:C:1083:GLU:OE1	2.20	0.42
2:H:1252:SER:HB3	2:H:1259:LEU:CD2	2.50	0.42
1:F:234:LEU:HD12	1:F:234:LEU:N	2.35	0.42
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.37	0.42
2:C:80:PHE:HB3	2:C:85:CYS:SG	2.59	0.42
2:H:92:TYR:CD1	2:H:129:LEU:HB2	2.55	0.42
5:X:477:GLU:H	5:X:477:GLU:CD	2.23	0.42
3:D:574:VAL:O	3:D:578:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:52:GLY:O	5:X:53:ILE:HB	2.20	0.42
2:H:1161:LEU:HD21	2:H:1172:LEU:HD11	2.02	0.42
2:H:549:ASP:OD1	2:H:550:VAL:N	2.53	0.42
2:H:122:VAL:HG22	2:H:123:TYR:N	2.34	0.41
2:C:56:VAL:HB	2:C:57:PHE:H	1.51	0.41
2:H:54:ARG:N	2:H:55:SER:C	2.74	0.41
2:H:699:LEU:HD12	2:H:1121:ALA:HB1	2.01	0.41
3:I:746:LEU:H	3:I:746:LEU:HD22	1.85	0.41
2:H:303:ASP:HB2	2:H:310:ILE:CD1	2.46	0.41
3:I:131:PRO:CG	3:I:135:ILE:HD13	2.46	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.85	0.41
3:I:326:SER:O	3:I:330:MET:HG3	2.19	0.41
3:I:532:GLU:OE1	3:I:578:ILE:HB	2.20	0.41
3:D:141:PHE:HD2	3:D:141:PHE:HA	1.71	0.41
2:H:469:VAL:O	2:H:472:GLU:HB3	2.20	0.41
3:D:18:ASP:HA	3:D:1369:ARG:HH22	1.84	0.41
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.19	0.41
5:Y:363:ARG:HE	5:Y:363:ARG:HA	1.84	0.41
3:I:33:TRP:HB3	3:I:102:MET:HG3	2.02	0.41
2:C:72:SER:O	2:C:98:VAL:HG23	2.20	0.41
1:B:22:THR:HB	1:B:207:THR:O	2.19	0.41
3:D:1180:VAL:HG22	3:D:1185:PRO:HA	2.02	0.41
2:H:481:LEU:C	2:H:481:LEU:HD13	2.40	0.41
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.20	0.41
2:C:988:LYS:NZ	2:C:988:LYS:HB3	2.34	0.41
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.79	0.41
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	2.02	0.41
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.87	0.41
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.35	0.41
1:F:167:PRO:HD2	1:F:170:ARG:NE	2.35	0.41
3:I:298:MET:CE	5:Y:402:LEU:HB3	2.50	0.41
3:D:591:ILE:HD12	3:D:592:VAL:HG13	2.02	0.41
3:I:1292:LEU:HD12	3:I:1292:LEU:N	2.36	0.41
3:I:382:TYR:HE1	3:I:401:VAL:CG2	2.33	0.41
1:B:228:LEU:C	1:B:228:LEU:HD12	2.41	0.41
2:H:170:VAL:HG23	2:H:171:LEU:N	2.31	0.41
2:H:1335:ILE:CD1	3:I:22:ILE:HD11	2.49	0.41
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.85	0.41
3:I:290:ILE:O	3:I:293:ARG:HG3	2.20	0.41
2:H:1323:PHE:O	2:H:1327:LEU:HG	2.20	0.41
3:I:500:ILE:CD1	3:I:500:ILE:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:992:LEU:HD23	2:H:996:ARG:CG	2.50	0.41
2:H:985:GLU:HG2	2:H:989:LEU:HD13	2.01	0.41
3:I:73:GLY:O	3:I:76:LYS:HE3	2.19	0.41
3:I:843:VAL:HG11	3:I:897:HIS:HB3	2.02	0.41
2:H:103:VAL:HG22	2:H:104:ILE:N	2.34	0.41
5:Y:133:SER:OG	5:Y:365:MET:HB2	2.20	0.41
2:C:135:THR:OG1	2:C:142:GLU:HG3	2.20	0.41
2:H:513:GLN:HA	2:H:513:GLN:NE2	2.24	0.41
2:C:1142:ARG:O	2:C:1146:GLN:HB2	2.20	0.41
3:I:120:LEU:HD12	3:I:120:LEU:N	2.35	0.41
3:D:1284:ARG:HA	3:D:1287:ILE:CG1	2.47	0.41
2:C:1333:LEU:HB2	2:C:1335:ILE:HG22	2.03	0.41
2:H:263:VAL:HA	2:H:267:ARG:HH21	1.86	0.41
3:I:141:PHE:O	3:I:297:ARG:HD3	2.21	0.41
2:H:896:THR:HG23	2:H:897:PRO:HD2	2.02	0.41
5:Y:316:PHE:CZ	5:Y:334:SER:HA	2.55	0.41
1:B:207:THR:OG1	1:B:208:ASN:N	2.54	0.41
2:C:230:PHE:HB2	2:C:333:ILE:HB	2.01	0.41
2:H:964:LEU:HD12	2:H:1025:PHE:CG	2.55	0.41
2:C:943:LYS:O	2:C:947:GLU:HG2	2.20	0.41
2:C:82:VAL:HG13	2:C:83:GLN:N	2.36	0.41
2:C:81:ASP:OD1	2:C:83:GLN:HG2	2.21	0.41
2:C:1283:ALA:HB1	2:C:1286:THR:HB	2.02	0.41
1:B:31:LEU:HB2	1:B:199:ASP:O	2.19	0.41
1:B:86:LYS:NZ	3:D:526:VAL:O	2.48	0.41
2:H:843:THR:HB	2:H:845:LEU:HD22	2.02	0.41
2:C:170:VAL:HG23	2:C:171:LEU:N	2.28	0.41
2:H:619:ALA:HA	2:H:653:MET:CE	2.51	0.41
2:C:812:PHE:CE1	3:D:451:PRO:HB2	2.55	0.41
1:A:45:ARG:NH1	2:C:1084:ASP:HB3	2.36	0.41
2:H:142:GLU:O	2:H:143:ARG:HB2	2.21	0.41
2:H:1239:VAL:HG12	2:H:1240:ASP:N	2.34	0.41
2:C:27:LEU:O	2:C:528:ARG:NH1	2.52	0.41
3:D:369:PRO:HB2	3:D:372:MET:HB2	2.01	0.41
2:C:697:LYS:HE2	2:C:697:LYS:HB2	1.89	0.41
1:A:22:THR:O	1:A:207:THR:N	2.50	0.41
3:D:805:GLN:HB2	3:D:805:GLN:HE21	1.72	0.41
2:H:518:ASN:ND2	2:H:761:GLN:HG2	2.35	0.41
1:F:222:THR:O	1:F:226:GLU:HG3	2.20	0.41
3:I:219:LYS:O	3:I:223:LEU:HG	2.20	0.41
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1199:LEU:HD13	2:H:1206:THR:HA	2.02	0.41
3:D:1149:ARG:HA	3:D:1150:PRO:HD3	1.90	0.41
3:I:217:LEU:O	3:I:221:ILE:HG23	2.21	0.41
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.85	0.41
1:F:46:ILE:O	1:F:50:SER:HB2	2.20	0.41
3:I:135:ILE:O	3:I:139:LEU:HD12	2.20	0.41
3:D:363:LEU:HA	3:D:450:HIS:ND1	2.36	0.41
3:D:678:ARG:HD2	3:D:678:ARG:C	2.41	0.41
1:F:190:ALA:N	1:F:198:LEU:O	2.48	0.41
3:I:279:LEU:HD23	3:I:295:GLU:HB3	2.02	0.41
1:A:166:ARG:HG3	1:A:166:ARG:O	2.21	0.41
3:I:1193:TRP:CD1	3:I:1194:ARG:HD2	2.55	0.41
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.55	0.41
3:I:479:GLU:O	3:I:483:LEU:HB2	2.21	0.41
1:B:47:LEU:HD13	1:B:205:MET:HE2	2.03	0.41
2:C:546:GLU:O	2:C:548:ARG:N	2.48	0.41
2:C:317:LEU:HD13	2:C:322:LEU:HD21	2.01	0.41
5:Y:528:LEU:O	5:Y:528:LEU:HD12	2.20	0.41
3:I:303:VAL:O	3:I:307:LEU:HG	2.20	0.41
5:X:133:SER:OG	5:X:365:MET:HB2	2.21	0.41
3:D:128:LEU:HA	3:D:192:MET:CE	2.49	0.41
3:D:214:ARG:HA	3:D:217:LEU:HD12	2.02	0.41
3:I:392:THR:HG22	5:Y:606:VAL:HG11	2.01	0.41
4:E:16:ARG:O	4:E:19:LEU:HB3	2.20	0.41
3:I:130:MET:HA	3:I:131:PRO:HD3	1.96	0.41
1:A:45:ARG:HH12	2:C:1216:ARG:HA	1.86	0.41
2:C:397:LEU:O	2:C:398:SER:OG	2.33	0.41
2:H:1165:SER:O	2:H:1168:GLU:HB3	2.21	0.41
2:C:1087:TYR:CE2	2:C:1215:GLY:HA2	2.50	0.41
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.56	0.41
5:Y:343:LYS:O	5:Y:346:GLN:HB3	2.19	0.41
3:D:269:TYR:CG	3:D:306:LEU:HD11	2.54	0.41
5:Y:582:VAL:CB	5:Y:586:ARG:HG2	2.50	0.41
5:X:45:ILE:HD12	5:X:45:ILE:C	2.40	0.41
3:D:649:LYS:O	3:D:653:ILE:HG12	2.21	0.41
3:I:1229:VAL:O	3:I:1233:ILE:HG13	2.20	0.41
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.98	0.41
5:Y:453:PRO:CD	5:Y:456:MET:HB2	2.42	0.41
2:H:843:THR:HB	2:H:845:LEU:CD2	2.51	0.41
3:D:555:TYR:HD1	3:D:589:TYR:HE2	1.69	0.41
3:I:382:TYR:CE1	3:I:398:LYS:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.84	0.41
3:I:473:THR:HB	3:I:476:ALA:CB	2.49	0.41
2:C:901:LEU:HD13	5:X:559:LEU:HD22	2.02	0.41
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.55	0.41
3:I:1322:ALA:O	3:I:1326:GLN:HG3	2.21	0.41
5:X:363:ARG:HE	5:X:363:ARG:HA	1.85	0.41
5:Y:476:ARG:HB2	5:Y:477:GLU:OE1	2.20	0.41
3:I:494:ALA:HA	3:I:1252:HIS:CE1	2.53	0.41
2:C:99:LYS:HA	2:C:121:GLU:HA	2.02	0.41
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	2.03	0.41
3:D:532:GLU:OE1	3:D:578:ILE:HB	2.21	0.41
2:H:680:LEU:HD23	2:H:680:LEU:O	2.21	0.41
3:D:45:ASN:OD1	3:D:46:TYR:N	2.54	0.41
2:C:869:GLY:C	2:C:870:ILE:HD12	2.41	0.41
1:F:89:ALA:HB3	1:F:124:VAL:HB	2.03	0.41
3:D:746:LEU:H	3:D:746:LEU:HD22	1.85	0.41
2:H:811:ASN:HA	2:H:815:SER:HB2	2.03	0.41
3:D:609:TYR:HA	3:D:617:THR:OG1	2.21	0.41
5:X:35:ILE:HG13	5:X:36:VAL:N	2.21	0.41
3:D:1149:ARG:CD	3:D:1149:ARG:H	2.23	0.41
3:I:422:LEU:O	3:I:422:LEU:HD12	2.20	0.41
2:C:820:GLU:HB2	2:C:1081:PRO:HA	2.02	0.41
5:Y:112:THR:HG22	5:Y:113:ARG:N	2.30	0.41
2:H:1285:TYR:HA	2:H:1288:GLN:HB3	2.02	0.41
3:D:27:PRO:HD3	3:D:236:TRP:CE3	2.56	0.41
2:C:975:ILE:O	2:C:978:VAL:HG12	2.21	0.41
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	2.01	0.41
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.20	0.41
5:Y:105:MET:SD	5:Y:388:ILE:HD12	2.61	0.41
2:C:429:MET:O	2:C:433:ILE:HG13	2.20	0.41
2:C:177:ILE:HG13	2:C:183:TRP:CZ3	2.56	0.41
1:G:76:GLU:OE2	1:G:131:CYS:HA	2.20	0.41
3:I:873:GLU:HG3	3:I:873:GLU:H	1.64	0.41
2:H:103:VAL:HG22	2:H:104:ILE:H	1.86	0.41
5:X:261:LEU:HD12	5:X:261:LEU:N	2.36	0.41
3:D:53:ARG:HA	3:D:53:ARG:HD2	1.96	0.41
5:Y:261:LEU:HD12	5:Y:261:LEU:N	2.36	0.41
5:X:270:VAL:HA	5:X:273:MET:HE3	2.01	0.41
2:H:977:ALA:O	2:H:980:VAL:HG12	2.20	0.41
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	2.03	0.41
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1173:ARG:CA	3:I:1174:ARG:CB	2.86	0.41
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.56	0.41
3:D:128:LEU:HD12	3:D:192:MET:CE	2.35	0.41
3:I:746:LEU:HD22	3:I:746:LEU:N	2.36	0.41
5:Y:456:MET:O	5:Y:460:ILE:HG13	2.20	0.41
1:A:80:GLU:HG3	2:C:694:ARG:NH1	2.35	0.41
2:C:773:LEU:HD22	2:C:773:LEU:C	2.41	0.41
2:H:127:ILE:HA	2:H:128:PRO:HD3	1.89	0.41
2:H:618:GLN:HG2	2:H:637:ARG:NH2	2.36	0.41
5:X:262:VAL:HG13	5:X:263:PRO:CD	2.48	0.41
3:I:116:PHE:HB3	3:I:237:MET:HE3	2.03	0.41
2:C:752:ASN:C	2:C:753:LEU:HG	2.40	0.41
3:I:552:ILE:HD13	3:I:570:LYS:HB2	2.03	0.41
3:I:526:VAL:HG12	3:I:549:LYS:O	2.20	0.41
2:C:122:VAL:CG2	5:X:472:GLN:HE21	2.34	0.41
3:D:647:PRO:HG3	3:D:697:MET:HA	2.03	0.41
2:C:442:VAL:HG12	2:C:443:ASP:N	2.36	0.41
2:C:688:GLN:O	2:C:1236:ASN:N	2.54	0.41
3:I:155:GLU:H	3:I:155:GLU:CD	2.24	0.41
2:H:1287:LEU:O	2:H:1291:LEU:HB2	2.21	0.41
3:D:1161:GLY:HA2	3:D:1181:ASP:HB2	2.01	0.41
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.03	0.41
2:C:103:VAL:HG22	2:C:104:ILE:N	2.36	0.41
3:D:155:GLU:CD	3:D:158:GLN:HB2	2.41	0.41
2:C:82:VAL:O	2:C:86:GLN:HG3	2.20	0.41
2:H:690:VAL:HA	2:H:691:PRO:HD3	1.91	0.41
2:H:374:GLU:HA	2:H:375:PRO:HD3	1.93	0.41
2:H:1138:VAL:O	2:H:1139:ALA:HB3	2.20	0.41
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.20	0.41
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.55	0.41
5:Y:374:ARG:O	5:Y:378:GLU:HG3	2.21	0.41
2:H:97:ARG:HA	2:H:122:VAL:O	2.20	0.41
2:C:1287:LEU:O	2:C:1291:LEU:HB2	2.21	0.41
2:H:812:PHE:H	2:H:815:SER:HB2	1.86	0.41
2:C:661:VAL:HG23	2:C:662:SER:O	2.22	0.41
3:I:527:LEU:HB3	3:I:528:THR:H	1.72	0.41
3:I:903:LEU:HD11	3:I:909:ILE:CG2	2.45	0.41
3:D:681:LYS:HD3	3:D:682:VAL:N	2.36	0.41
3:I:128:LEU:HD12	3:I:192:MET:HE1	2.02	0.41
2:H:1142:ARG:O	2:H:1146:GLN:HB2	2.20	0.41
3:D:409:TRP:O	3:D:412:LEU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:492:ASP:HA	5:Y:495:ARG:HG3	2.01	0.41
2:H:31:GLN:HG3	2:H:130:MET:HE1	2.03	0.41
4:E:15:ASN:HD21	4:E:18:ASP:CB	2.32	0.41
2:H:698:PRO:HB3	2:H:1231:TYR:CE1	2.56	0.41
1:B:176:CYS:C	1:B:178:SER:N	2.74	0.41
4:J:39:VAL:CG1	4:J:40:PRO:HD2	2.50	0.41
2:C:892:GLU:C	2:C:894:GLN:H	2.24	0.41
3:D:1292:LEU:HD12	3:D:1292:LEU:N	2.35	0.41
2:C:84:GLU:HG3	2:C:88:ARG:HD3	2.03	0.41
3:I:856:ILE:HD12	3:I:857:LEU:H	1.86	0.41
2:C:931:VAL:HG21	2:C:944:ARG:CZ	2.52	0.41
2:C:1272:GLU:O	2:C:1275:VAL:HG22	2.21	0.41
3:D:361:LEU:HD22	3:D:361:LEU:N	2.36	0.41
2:C:516:ASP:OD1	2:C:518:ASN:ND2	2.54	0.41
3:D:1266:ILE:HG22	3:D:1302:TYR:HB3	2.02	0.41
1:G:110:VAL:HG11	1:G:140:ILE:HD11	2.02	0.41
2:H:691:PRO:HA	2:H:788:SER:OG	2.21	0.41
2:C:1243:MET:SD	3:D:445:LYS:HB3	2.61	0.41
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.21	0.40
3:D:217:LEU:O	3:D:221:ILE:HG23	2.20	0.40
3:I:545:HIS:HB2	3:I:546:ALA:CA	2.51	0.40
5:Y:448:ARG:HD3	5:Y:450:ILE:HG13	2.02	0.40
2:C:1165:SER:O	2:C:1168:GLU:HB3	2.21	0.40
5:Y:591:GLU:O	5:Y:595:LEU:HG	2.21	0.40
2:H:892:GLU:C	2:H:894:GLN:H	2.24	0.40
2:H:130:MET:HG3	2:H:134:GLY:HA2	2.03	0.40
3:D:1274:PHE:CD2	3:D:1275:LEU:HG	2.50	0.40
2:H:740:GLU:CD	2:H:740:GLU:H	2.24	0.40
2:C:73:TYR:HA	2:C:98:VAL:HA	2.02	0.40
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.56	0.40
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.02	0.40
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.86	0.40
2:C:854:ILE:HB	2:C:857:VAL:HG11	2.03	0.40
1:B:16:ILE:HG12	1:B:26:VAL:HG22	2.02	0.40
1:F:59:VAL:HG21	1:F:85:LEU:HD13	2.03	0.40
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.40
2:C:1269:ARG:HD2	3:D:344:GLY:N	2.35	0.40
2:H:844:LYS:HB2	2:H:844:LYS:HZ3	1.86	0.40
3:D:836:ARG:HA	3:D:836:ARG:HD2	1.88	0.40
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.31	0.40
3:I:519:ASN:HD21	3:I:707:ILE:CG2	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:618:GLN:HG2	2:C:637:ARG:HH22	1.86	0.40
3:D:707:ILE:HG22	3:D:708:ASN:H	1.86	0.40
5:Y:558:VAL:O	5:Y:562:ARG:HB2	2.21	0.40
1:A:323:PRO:HA	1:A:324:ALA:HA	1.77	0.40
3:D:697:MET:SD	3:D:741:ALA:HB3	2.62	0.40
3:D:1282:TYR:HA	3:D:1285:VAL:CG2	2.52	0.40
3:D:857:LEU:HB2	3:D:860:ARG:HB2	2.03	0.40
2:C:538:LEU:HD12	2:C:538:LEU:H	1.86	0.40
3:I:385:LEU:HD23	3:I:411:ILE:HG13	2.03	0.40
2:H:821:ARG:HB2	2:H:1082:ILE:HD13	2.04	0.40
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	2.03	0.40
2:H:870:ILE:HD12	2:H:870:ILE:N	2.36	0.40
5:X:253:SER:O	5:X:257:LYS:HG3	2.21	0.40
2:C:848:GLU:HG2	2:C:888:THR:HA	2.02	0.40
2:H:219:GLN:O	2:H:223:LEU:HG	2.21	0.40
1:A:67:GLU:HA	1:A:78:ILE:HG21	2.03	0.40
2:C:1163:THR:HG22	2:C:1164:PHE:H	1.86	0.40
5:X:551:LEU:HD22	5:X:597:LYS:HD2	2.02	0.40
1:A:102:LEU:HD12	1:A:115:ILE:HG12	2.03	0.40
3:D:1341:ARG:HD3	3:D:1343:GLU:CD	2.42	0.40
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.49	0.40
3:I:545:HIS:HA	3:I:546:ALA:HA	1.80	0.40
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.51	0.40
2:C:1259:LEU:HD12	2:C:1259:LEU:C	2.40	0.40
2:C:517:GLN:HG3	2:C:759:SER:OG	2.21	0.40
3:D:395:LYS:NZ	5:X:607:LEU:O	2.50	0.40
3:D:1256:ILE:O	3:D:1260:MET:HB2	2.22	0.40
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.55	0.40
2:H:1214:ASP:HB3	2:H:1218:GLY:H	1.86	0.40
5:X:283:GLN:CD	5:X:343:LYS:HD2	2.41	0.40
2:C:18:ARG:HG3	2:C:19:PRO:HD2	2.03	0.40
2:C:1004:ASP:OD1	2:C:1004:ASP:N	2.55	0.40
3:I:1243:LEU:O	3:I:1243:LEU:HD23	2.22	0.40
1:A:313:SER:OG	1:A:314:LEU:N	2.53	0.40
3:I:510:LEU:HD12	3:I:601:ILE:HD11	2.03	0.40
5:Y:292:VAL:HG13	5:Y:297:MET:O	2.21	0.40
3:D:1158:GLU:HA	3:D:1223:LEU:CD2	2.50	0.40
3:D:746:LEU:N	3:D:746:LEU:HD22	2.36	0.40
3:D:205:LEU:HB3	3:D:217:LEU:HD22	2.04	0.40
3:D:588:PRO:O	3:D:589:TYR:HB2	2.21	0.40
3:I:325:LYS:NZ	3:I:325:LYS:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:591:ILE:CD1	3:I:592:VAL:HG13	2.52	0.40
5:X:559:LEU:HD23	5:X:559:LEU:HA	1.90	0.40
1:B:27:THR:HG22	1:B:202:VAL:HG22	2.03	0.40
1:B:61:ILE:HB	1:B:64:VAL:HB	2.03	0.40
3:D:483:LEU:HD11	4:E:20:VAL:HG21	2.03	0.40
3:D:679:TYR:O	3:D:683:ILE:HG13	2.21	0.40
2:C:505:PHE:HA	2:C:509:SER:HB3	2.04	0.40
3:I:310:GLY:HA2	3:I:314:ARG:HG2	2.04	0.40
5:X:469:GLN:HE21	5:X:473:GLU:HG3	1.87	0.40
2:C:115:LYS:O	2:C:116:ASP:HB2	2.21	0.40
2:H:623:LEU:HD12	2:H:623:LEU:N	2.36	0.40
2:H:1212:LEU:HD12	2:H:1225:VAL:HG21	2.03	0.40
5:X:410:ILE:O	5:X:414:LYS:HG3	2.22	0.40
3:D:147:ILE:HD12	3:D:178:ALA:HB2	2.03	0.40
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.85	0.40
2:C:409:LEU:HD11	2:C:428:VAL:HA	2.04	0.40
3:I:529:GLY:HA3	3:I:530:PRO:HD3	1.91	0.40
3:I:609:TYR:HE2	3:I:614:LEU:HD13	1.86	0.40
3:I:1278:GLU:HG3	3:I:1279:GLN:N	2.37	0.40
3:I:915:ILE:O	3:I:918:ILE:HG23	2.22	0.40
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.86	0.40
2:C:59:ILE:HG12	2:C:65:ASN:O	2.20	0.40
2:C:936:ARG:HB3	2:C:939:VAL:HG21	2.04	0.40
3:D:355:ILE:HG21	3:D:466:MET:SD	2.61	0.40
2:C:178:PRO:HA	2:C:397:LEU:CD2	2.46	0.40
3:D:678:ARG:O	3:D:682:VAL:HG13	2.21	0.40
5:X:558:VAL:O	5:X:562:ARG:HB2	2.22	0.40
3:D:709:ARG:O	3:D:712:GLN:N	2.53	0.40
3:D:412:LEU:HA	3:D:415:VAL:HG22	2.04	0.40
2:H:1108:ASN:O	2:H:1108:ASN:ND2	2.52	0.40
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.56	0.40
2:H:894:GLN:NE2	3:I:77:ARG:HD3	2.32	0.40
1:A:50:SER:HA	1:A:150:ARG:HD2	2.02	0.40
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.84	0.40
2:H:1329:GLU:O	2:H:1332:SER:HB3	2.21	0.40
5:X:400:GLN:HE21	5:X:403:ASP:CG	2.25	0.40
3:I:887:SER:O	3:I:888:CYS:HB3	2.21	0.40
2:C:1195:ILE:O	2:C:1199:LEU:HG	2.22	0.40
2:C:465:ARG:O	2:C:469:VAL:HG23	2.21	0.40
5:X:374:ARG:HH21	5:X:377:LYS:HD2	1.87	0.40
5:X:530:LEU:H	5:X:530:LEU:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:84:ILE:H	3:D:84:ILE:HG13	1.76	0.40
3:I:417:ARG:NH1	4:J:43:ASN:O	2.55	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	321/329 (98%)	266 (83%)	40 (12%)	15 (5%)	3	33
1	B	217/329 (66%)	187 (86%)	22 (10%)	8 (4%)	4	40
1	F	227/329 (69%)	193 (85%)	28 (12%)	6 (3%)	7	47
1	G	213/329 (65%)	186 (87%)	22 (10%)	5 (2%)	8	50
2	C	1333/1342 (99%)	1073 (80%)	208 (16%)	52 (4%)	4	37
2	H	1333/1342 (99%)	1078 (81%)	206 (16%)	49 (4%)	4	40
3	D	1154/1407 (82%)	926 (80%)	182 (16%)	46 (4%)	4	37
3	I	1154/1407 (82%)	925 (80%)	184 (16%)	45 (4%)	4	37
4	E	88/91 (97%)	77 (88%)	6 (7%)	5 (6%)	2	28
4	J	74/91 (81%)	64 (86%)	6 (8%)	4 (5%)	2	30
5	X	511/613 (83%)	450 (88%)	46 (9%)	15 (3%)	6	45
5	Y	454/613 (74%)	409 (90%)	34 (8%)	11 (2%)	7	49
All	All	7079/8222 (86%)	5834 (82%)	984 (14%)	261 (4%)	4	40

All (261) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	B	20	SER

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Mol	Chain	Res	Type
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	669	PRO
2	C	686	GLN
2	C	748	ILE
2	C	993	PRO
2	C	1185	PRO
2	C	1186	VAL
2	C	1341	ASP
3	D	120	LEU
3	D	311	ARG
3	D	390	LEU
3	D	404	GLU
3	D	406	ALA
3	D	708	ASN
3	D	710	ASP
3	D	847	ASP
3	D	1268	ASN
3	D	1339	GLY
3	D	1344	LEU
5	X	241	SER
5	X	490	PRO
1	F	52	PRO
1	G	52	PRO
1	G	177	TYR
2	H	21	VAL
2	H	39	ILE
2	H	79	VAL
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL
2	H	669	PRO
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO
2	H	1341	ASP

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Mol	Chain	Res	Type
3	I	120	LEU
3	I	390	LEU
3	I	404	GLU
3	I	710	ASP
3	I	847	ASP
3	I	1339	GLY
5	Y	241	SER
1	A	52	PRO
1	A	160	HIS
1	A	187	VAL
1	A	193	GLU
1	B	19	VAL
1	B	177	TYR
2	C	56	VAL
2	C	78	PRO
2	C	79	VAL
2	C	753	LEU
2	C	1236	ASN
2	C	1239	VAL
2	C	1240	ASP
3	D	89	GLY
3	D	155	GLU
3	D	316	ILE
3	D	542	ALA
3	D	595	ALA
3	D	721	SER
3	D	887	SER
3	D	901	ARG
3	D	913	GLU
3	D	914	ALA
4	E	6	VAL
4	E	35	LYS
5	X	20	GLY
2	H	56	VAL
2	H	78	PRO
2	H	170	VAL
2	H	298	ALA
2	H	535	PRO
2	H	753	LEU
2	H	1186	VAL
2	H	1239	VAL
2	H	1240	ASP

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Mol	Chain	Res	Type
2	H	1256	GLN
3	I	89	GLY
3	I	155	GLU
3	I	345	LYS
3	I	406	ALA
3	I	540	GLY
3	I	542	ALA
3	I	707	ILE
3	I	708	ASN
3	I	731	ARG
3	I	851	PRO
3	I	901	ARG
3	I	913	GLU
3	I	914	ALA
3	I	1268	ASN
3	I	1344	LEU
4	J	6	VAL
4	J	35	LYS
5	Y	490	PRO
5	Y	564	GLY
1	A	14	VAL
1	B	235	ARG
2	C	44	GLU
2	C	53	PHE
2	C	143	ARG
2	C	437	ASN
2	C	699	LEU
2	C	740	GLU
2	C	812	PHE
2	C	1107	MET
2	C	1256	GLN
3	D	559	ALA
3	D	703	THR
3	D	707	ILE
3	D	731	ARG
3	D	848	VAL
3	D	851	PRO
3	D	902	ASP
5	X	23	THR
5	X	308	GLY
5	X	514	ASP
5	X	581	ASP

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Mol	Chain	Res	Type
1	F	160	HIS
1	F	188	GLU
1	G	188	GLU
1	G	228	LEU
2	H	13	LYS
2	H	44	GLU
2	H	53	PHE
2	H	437	ASN
2	H	740	GLU
2	H	812	PHE
2	H	1107	MET
2	H	1236	ASN
3	I	53	ARG
3	I	132	LEU
3	I	559	ALA
3	I	595	ALA
3	I	703	THR
3	I	721	SER
3	I	887	SER
3	I	1195	GLN
5	Y	108	VAL
5	Y	308	GLY
5	Y	491	GLU
5	Y	581	ASP
1	A	166	ARG
1	A	188	GLU
1	A	194	GLN
1	B	188	GLU
2	C	298	ALA
2	C	1080	ASN
2	C	1139	ALA
3	D	53	ARG
3	D	132	LEU
3	D	598	LYS
3	D	728	SER
3	D	855	ASP
3	D	888	CYS
3	D	1195	GLN
3	D	1363	TYR
4	E	5	THR
5	X	50	ASP
5	X	108	VAL

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Mol	Chain	Res	Type
5	X	504	PRO
1	F	153	VAL
1	F	166	ARG
2	H	43	PRO
2	H	143	ARG
2	H	699	LEU
2	H	739	ASP
2	H	895	LEU
2	H	1003	THR
2	H	1080	ASN
2	H	1093	PRO
2	H	1270	PHE
3	I	598	LYS
3	I	728	SER
3	I	848	VAL
3	I	855	ASP
3	I	888	CYS
5	Y	504	PRO
5	Y	514	ASP
1	A	93	GLN
1	A	163	GLU
1	A	195	ARG
2	C	13	LYS
2	C	487	LEU
2	C	543	ALA
2	C	746	ALA
2	C	895	LEU
2	C	1093	PRO
2	C	1237	HIS
2	C	1238	LEU
2	C	1270	PHE
3	D	62	PHE
3	D	210	SER
3	D	540	GLY
3	D	1167	LYS
5	X	25	ALA
5	X	491	GLU
5	X	564	GLY
5	X	600	HIS
1	F	33	ARG
2	H	488	MET
2	H	746	ALA

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Mol	Chain	Res	Type
2	H	1045	GLY
2	H	1237	HIS
3	I	62	PHE
3	I	210	SER
3	I	902	ASP
4	J	5	THR
5	Y	600	HIS
1	A	153	VAL
1	B	49	SER
1	B	228	LEU
2	C	59	ILE
2	C	69	GLN
2	C	739	ASP
2	C	1003	THR
2	C	1315	MET
3	D	417	ARG
3	D	742	GLY
3	D	1173	ARG
4	E	15	ASN
4	E	59	ILE
1	G	49	SER
2	H	1139	ALA
2	H	1238	LEU
3	I	108	ALA
3	I	443	GLU
3	I	712	GLN
3	I	742	GLY
3	I	1167	LYS
4	J	59	ILE
1	A	232	VAL
2	C	104	ILE
2	H	59	ILE
2	H	104	ILE
2	C	1045	GLY
3	I	850	LYS
1	A	322	PRO
2	C	373	GLY
3	D	850	LYS
2	H	373	GLY
5	X	35	ILE
3	I	316	ILE
5	Y	97	PRO

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Mol	Chain	Res	Type
2	C	117	ILE
3	D	471	PRO
3	D	1184	ASP
3	I	471	PRO
2	H	489	PRO
2	H	1181	PRO
2	C	1181	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/286 (98%)	273 (97%)	8 (3%)	51	80
1	B	189/286 (66%)	186 (98%)	3 (2%)	70	88
1	F	197/286 (69%)	194 (98%)	3 (2%)	72	89
1	G	185/286 (65%)	182 (98%)	3 (2%)	70	88
2	C	1150/1157 (99%)	1094 (95%)	56 (5%)	31	69
2	H	1150/1157 (99%)	1097 (95%)	53 (5%)	33	70
3	D	971/1168 (83%)	921 (95%)	50 (5%)	29	68
3	I	971/1168 (83%)	918 (94%)	53 (6%)	27	66
4	E	74/75 (99%)	72 (97%)	2 (3%)	52	80
4	J	65/75 (87%)	65 (100%)	0	100	100
5	X	460/540 (85%)	447 (97%)	13 (3%)	51	80
5	Y	407/540 (75%)	392 (96%)	15 (4%)	41	75
All	All	6100/7024 (87%)	5841 (96%)	259 (4%)	36	72

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	79	LEU
1	A	117	HIS

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Mol	Chain	Res	Type
1	A	158	ARG
1	A	243	LYS
1	A	246	LYS
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	182	ARG
2	C	9	LYS
2	C	15	PHE
2	C	18	ARG
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL
2	C	70	TYR
2	C	80	PHE
2	C	88	ARG
2	C	121	GLU
2	C	127	ILE
2	C	150	HIS
2	C	163	LYS
2	C	479	LEU
2	C	487	LEU
2	C	514	PHE
2	C	603	ILE
2	C	645	PHE
2	C	661	VAL
2	C	690	VAL
2	C	693	LEU
2	C	773	LEU
2	C	800	MET
2	C	807	TRP
2	C	817	LEU
2	C	845	LEU
2	C	908	GLU
2	C	941	LYS
2	C	944	ARG
2	C	953	LEU
2	C	955	GLN
2	C	964	LEU
2	C	975	ILE

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Mol	Chain	Res	Type
2	C	994	ARG
2	C	1002	LEU
2	C	1010	GLN
2	C	1017	GLN
2	C	1032	LYS
2	C	1042	LEU
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1211	ARG
2	C	1233	LEU
2	C	1241	ASP
2	C	1259	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1288	GLN
2	C	1291	LEU
2	C	1326	LEU
2	C	1339	LEU
2	C	1341	ASP
3	D	13	LYS
3	D	20	ILE
3	D	31	ARG
3	D	50	LYS
3	D	92	VAL
3	D	104	HIS
3	D	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	141	PHE
3	D	151	MET
3	D	169	LEU
3	D	179	LYS
3	D	188	LEU
3	D	235	GLU
3	D	239	LEU
3	D	250	ARG
3	D	309	ASN
3	D	430	HIS

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Mol	Chain	Res	Type
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	527	LEU
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	614	LEU
3	D	668	PHE
3	D	678	ARG
3	D	681	LYS
3	D	709	ARG
3	D	713	GLU
3	D	771	GLN
3	D	795	TYR
3	D	805	GLN
3	D	816	THR
3	D	832	LYS
3	D	867	GLN
3	D	873	GLU
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1149	ARG
3	D	1188	GLU
3	D	1247	LYS
3	D	1306	LEU
4	E	8	ASP
4	E	15	ASN
5	X	21	TYR
5	X	28	ASN
5	X	99	ARG
5	X	136	GLU
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	452	ILE
5	X	476	ARG
5	X	495	ARG

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Mol	Chain	Res	Type
5	X	545	HIS
5	X	562	ARG
5	X	607	LEU
1	F	158	ARG
1	F	160	HIS
1	F	163	GLU
1	G	37	HIS
1	G	218	ARG
1	G	228	LEU
2	H	9	LYS
2	H	15	PHE
2	H	18	ARG
2	H	37	LYS
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	99	LYS
2	H	127	ILE
2	H	150	HIS
2	H	163	LYS
2	H	311	CYS
2	H	464	PHE
2	H	479	LEU
2	H	488	MET
2	H	513	GLN
2	H	514	PHE
2	H	645	PHE
2	H	661	VAL
2	H	690	VAL
2	H	711	ASP
2	H	773	LEU
2	H	800	MET
2	H	807	TRP
2	H	817	LEU
2	H	845	LEU
2	H	941	LYS
2	H	944	ARG
2	H	955	GLN

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Mol	Chain	Res	Type
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	994	ARG
2	H	1002	LEU
2	H	1005	GLU
2	H	1010	GLN
2	H	1017	GLN
2	H	1032	LYS
2	H	1042	LEU
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1211	ARG
2	H	1233	LEU
2	H	1264	GLN
2	H	1288	GLN
2	H	1291	LEU
2	H	1341	ASP
3	I	31	ARG
3	I	50	LYS
3	I	92	VAL
3	I	104	HIS
3	I	114	ILE
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	141	PHE
3	I	151	MET
3	I	169	LEU
3	I	179	LYS
3	I	188	LEU
3	I	235	GLU
3	I	239	LEU
3	I	248	ASP
3	I	250	ARG
3	I	309	ASN
3	I	316	ILE
3	I	325	LYS
3	I	416	ILE
3	I	430	HIS

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Mol	Chain	Res	Type
3	I	475	GLU
3	I	500	ILE
3	I	505	ASP
3	I	527	LEU
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	571	ASP
3	I	594	GLN
3	I	668	PHE
3	I	678	ARG
3	I	681	LYS
3	I	709	ARG
3	I	771	GLN
3	I	795	TYR
3	I	805	GLN
3	I	816	THR
3	I	832	LYS
3	I	867	GLN
3	I	873	GLU
3	I	911	LYS
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1149	ARG
3	I	1247	LYS
3	I	1297	LYS
3	I	1306	LEU
3	I	1369	ARG
5	Y	136	GLU
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET
5	Y	384	LEU
5	Y	452	ILE
5	Y	457	ILE
5	Y	476	ARG
5	Y	495	ARG
5	Y	545	HIS

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Mol	Chain	Res	Type
5	Y	562	ARG
5	Y	565	ILE
5	Y	589	GLN
5	Y	607	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	227	GLN
1	A	239	GLN
1	B	66	HIS
1	B	84	ASN
2	C	41	GLN
2	C	69	GLN
2	C	238	GLN
2	C	273	HIS
2	C	314	ASN
2	C	462	ASN
2	C	510	GLN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	554	HIS
2	C	673	HIS
2	C	799	ASN
2	C	955	GLN
2	C	1010	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1134	GLN
2	C	1146	GLN
2	C	1175	ASN
2	C	1264	GLN
2	C	1288	GLN
3	D	94	GLN
3	D	419	HIS
3	D	477	GLN
3	D	488	ASN
3	D	504	GLN
3	D	519	ASN
3	D	623	GLN

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Mol	Chain	Res	Type
3	D	875	ASN
3	D	907	HIS
3	D	1197	ASN
3	D	1268	ASN
3	D	1350	ASN
4	E	31	GLN
5	X	30	HIS
5	X	54	GLN
5	X	258	GLN
5	X	301	ASN
5	X	400	GLN
5	X	406	GLN
5	X	437	GLN
5	X	446	GLN
5	X	461	ASN
5	X	469	GLN
1	G	37	HIS
1	G	41	ASN
1	G	66	HIS
2	H	46	GLN
2	H	69	GLN
2	H	238	GLN
2	H	462	ASN
2	H	510	GLN
2	H	513	GLN
2	H	517	GLN
2	H	673	HIS
2	H	799	ASN
2	H	894	GLN
2	H	955	GLN
2	H	1010	GLN
2	H	1017	GLN
2	H	1108	ASN
2	H	1111	GLN
2	H	1134	GLN
2	H	1175	ASN
2	H	1220	GLN
2	H	1264	GLN
2	H	1288	GLN
3	I	94	GLN
3	I	274	ASN
3	I	300	GLN

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Mol	Chain	Res	Type
3	I	419	HIS
3	I	477	GLN
3	I	504	GLN
3	I	519	ASN
3	I	1227	HIS
3	I	1350	ASN
4	J	15	ASN
4	J	31	GLN
5	Y	301	ASN
5	Y	342	GLN
5	Y	400	GLN
5	Y	437	GLN
5	Y	461	ASN
5	Y	469	GLN
5	Y	589	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	0O2	D	1503	-	31,42,42	2.05	9 (29%)	46,68,68	2.32	10 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	0O2	D	1503	-	-	0/29/49/49	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1503	0O2	O2'-C2'	-4.34	1.32	1.43
7	D	1503	0O2	C6-C5	-3.06	1.35	1.41
7	D	1503	0O2	O4'-C1'	-2.74	1.37	1.41
7	D	1503	0O2	C2'-C3'	-2.61	1.47	1.53
7	D	1503	0O2	O4'-C4'	-2.53	1.39	1.45
7	D	1503	0O2	PC-O3'	-2.22	1.54	1.60
7	D	1503	0O2	C8-N7	3.38	1.41	1.34
7	D	1503	0O2	C2-N2	4.41	1.43	1.34
7	D	1503	0O2	O6-C6	4.98	1.36	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1503	0O2	C4'-O4'-C1'	-9.46	99.33	109.72
7	D	1503	0O2	PB-O3A-PA	-6.98	113.14	132.73
7	D	1503	0O2	PC-O3C-PD	-5.48	114.28	132.67
7	D	1503	0O2	N3-C2-N1	-3.07	122.77	127.44
7	D	1503	0O2	PB-O3B-PG	-2.43	124.52	132.67
7	D	1503	0O2	O2G-PG-O1G	-2.31	103.14	110.58
7	D	1503	0O2	O4'-C4'-C3'	2.26	110.06	104.86
7	D	1503	0O2	C1'-N9-C4	2.31	130.43	126.94
7	D	1503	0O2	O3G-PG-O3B	2.47	116.28	105.09
7	D	1503	0O2	O3'-C3'-C2'	2.58	121.55	111.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1503	0O2	9	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	323/329 (98%)	-0.18	4 (1%) 81 73	0, 55, 172, 230	0
1	B	221/329 (67%)	-0.01	7 (3%) 51 39	0, 86, 193, 260	0
1	F	229/329 (69%)	0.02	13 (5%) 27 20	2, 123, 212, 293	0
1	G	217/329 (65%)	0.06	5 (2%) 64 53	5, 113, 204, 271	0
2	C	1335/1342 (99%)	-0.28	23 (1%) 73 63	0, 38, 168, 304	0
2	H	1335/1342 (99%)	-0.11	40 (2%) 54 42	0, 78, 206, 346	0
3	D	1160/1407 (82%)	-0.20	18 (1%) 74 65	0, 28, 152, 297	0
3	I	1160/1407 (82%)	-0.08	43 (3%) 45 35	0, 54, 183, 316	0
4	E	90/91 (98%)	-0.20	0 100 100	0, 33, 116, 167	0
4	J	76/91 (83%)	0.08	1 (1%) 79 71	12, 83, 181, 230	0
5	X	517/613 (84%)	-0.09	19 (3%) 45 35	0, 98, 238, 341	0
5	Y	458/613 (74%)	-0.07	18 (3%) 43 33	1, 100, 216, 296	0
All	All	7121/8222 (86%)	-0.13	191 (2%) 58 47	0, 63, 198, 346	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	10	ALA	9.8
2	H	982	GLY	9.5
2	H	981	ALA	8.6
3	I	521	LYS	8.5
2	H	983	GLY	7.6
3	I	9	LYS	6.9
3	I	1376	GLY	6.1
3	I	208	THR	5.8
3	I	1294	ALA	5.2
5	Y	309	ASN	5.2
1	F	162	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
5	Y	311	THR	4.8
1	F	193	GLU	4.7
2	H	1020	GLU	4.6
3	I	207	GLU	4.6
3	I	12	THR	4.6
5	X	35	ILE	4.4
3	D	1171	GLY	4.4
1	F	148	ARG	4.4
3	D	1133	ASP	4.3
5	X	34	ASP	4.3
2	C	251	ALA	4.3
3	I	1295	ASN	4.2
3	I	11	GLN	4.2
2	H	1008	GLN	4.1
2	H	1009	ASN	4.0
3	I	1375	ALA	4.0
5	Y	239	GLY	4.0
2	C	266	GLY	3.9
3	I	13	LYS	3.9
1	A	196	THR	3.8
2	H	172	TYR	3.8
5	X	328	GLU	3.8
2	C	165	HIS	3.8
5	X	240	ARG	3.7
1	F	195	ARG	3.6
2	C	252	SER	3.6
3	D	1170	LYS	3.6
3	D	1199	PHE	3.6
5	Y	305	LEU	3.6
2	C	1166	ASP	3.5
2	H	1019	ASP	3.5
3	I	1167	LYS	3.4
5	Y	315	TRP	3.4
2	H	113	THR	3.3
3	I	1203	ARG	3.3
2	C	272	ARG	3.2
5	Y	478	PRO	3.2
1	F	194	GLN	3.2
2	H	305	SER	3.2
2	H	987	GLU	3.1
2	H	1000	LEU	3.1
2	C	282	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	164	ASP	3.1
3	I	1161	GLY	3.1
3	I	212	THR	3.1
1	F	161	SER	3.0
2	H	1012	GLU	3.0
2	H	376	PRO	3.0
5	X	318	ALA	3.0
3	I	855	ASP	3.0
2	H	988	LYS	3.0
5	X	16	GLY	3.0
3	I	676	GLY	3.0
1	B	73	GLY	2.9
5	X	36	VAL	2.9
2	H	332	ARG	2.9
1	B	169	GLY	2.9
2	H	1001	GLY	2.9
1	A	191	ARG	2.9
2	H	742	TYR	2.9
1	B	74	VAL	2.8
2	C	265	LYS	2.8
2	H	375	PRO	2.8
2	H	60	GLN	2.8
2	H	115	LYS	2.8
2	H	999	GLU	2.8
5	Y	307	THR	2.8
2	H	1003	THR	2.7
1	B	75	GLN	2.7
3	I	667	GLN	2.7
5	Y	310	GLU	2.7
2	C	311	CYS	2.7
2	H	980	VAL	2.7
3	I	1133	ASP	2.7
5	X	64	ASP	2.7
1	B	147	GLN	2.7
1	F	192	VAL	2.7
2	H	996	ARG	2.6
5	X	56	MET	2.6
5	X	315	TRP	2.6
2	C	267	ARG	2.6
5	X	153	ALA	2.6
3	I	1172	LYS	2.6
2	C	250	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	310	ILE	2.6
3	I	677	GLU	2.6
5	X	420	GLU	2.6
5	Y	212	ILE	2.6
5	X	423	ARG	2.6
5	X	339	ARG	2.6
2	C	238	GLN	2.6
5	X	239	GLY	2.6
3	I	175	GLU	2.6
3	D	81	ARG	2.6
3	I	708	ASN	2.5
2	H	105	TYR	2.5
5	Y	308	GLY	2.5
2	C	305	SER	2.5
1	G	96	ASP	2.5
2	H	979	LEU	2.5
3	I	675	ALA	2.5
5	Y	240	ARG	2.5
3	I	520	ALA	2.5
5	X	20	GLY	2.5
1	G	18	GLN	2.5
2	C	233	ARG	2.5
3	D	1376	GLY	2.5
3	I	205	LEU	2.5
2	H	1002	LEU	2.5
3	D	1168	GLU	2.5
1	F	113	ALA	2.5
3	I	1204	VAL	2.5
3	D	1172	LYS	2.5
3	D	212	THR	2.5
2	H	781	ASP	2.5
2	C	306	THR	2.5
3	I	209	ASN	2.4
2	H	169	LYS	2.4
5	Y	304	THR	2.4
1	F	163	GLU	2.4
2	C	258	ASN	2.4
2	H	986	ALA	2.4
3	I	876	SER	2.4
3	D	834	PRO	2.4
3	I	14	THR	2.4
5	Y	600	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	1316	GLU	2.4
3	I	1213	GLY	2.4
5	X	57	GLU	2.4
3	D	89	GLY	2.4
3	I	151	MET	2.4
5	X	305	LEU	2.3
2	C	981	ALA	2.3
2	C	1002	LEU	2.3
5	Y	321	ALA	2.3
2	H	984	VAL	2.3
3	I	174	ASP	2.3
3	I	564	VAL	2.3
3	D	1134	ILE	2.3
5	Y	578	LYS	2.3
3	I	709	ARG	2.3
2	H	912	ASP	2.3
1	F	196	THR	2.3
5	Y	154	GLU	2.3
1	F	33	ARG	2.2
5	Y	312	SER	2.2
1	G	148	ARG	2.2
1	B	136	GLU	2.2
2	C	375	PRO	2.2
3	D	80	HIS	2.2
3	I	91	GLU	2.2
2	H	782	VAL	2.2
3	D	211	GLU	2.2
2	H	990	ASP	2.2
2	C	164	THR	2.1
3	D	676	GLY	2.1
3	D	333	GLY	2.1
3	I	1160	SER	2.1
3	D	208	THR	2.1
2	H	1258	PRO	2.1
3	I	1170	LYS	2.1
4	J	35	LYS	2.1
1	G	157	THR	2.1
2	H	1023	HIS	2.1
2	C	1001	GLY	2.1
3	I	1171	GLY	2.1
5	X	24	TYR	2.1
1	A	190	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	831	VAL	2.1
1	G	24	ALA	2.1
5	Y	423	ARG	2.1
1	F	95	LYS	2.0
2	H	1134	GLN	2.0
1	A	4	SER	2.0
2	C	597	GLY	2.0
2	H	163	LYS	2.0
3	I	1201	GLY	2.0
1	B	105	SER	2.0
3	I	1162	ILE	2.0
3	I	834	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	ZN	I	1502	1/1	0.99	0.17	-0.72	49,49,49,49	0
6	ZN	D	1502	1/1	0.97	0.18	-0.94	8,8,8,8	0
6	ZN	D	1501	1/1	0.99	0.05	-1.65	54,54,54,54	0
6	ZN	I	1501	1/1	0.97	0.04	-1.83	60,60,60,60	0
7	0O2	D	1503	40/40	0.90	0.16	-1.91	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.