



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:51 PM GMT

PDB ID : 4JK1
Title : X-ray crystal structure of Escherichia coli sigma70 holoenzyme in complex with Guanosine tetraphosphate (ppGpp)
Authors : Murakami, K.S.
Deposited on : 2013-03-09
Resolution : 3.90 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 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

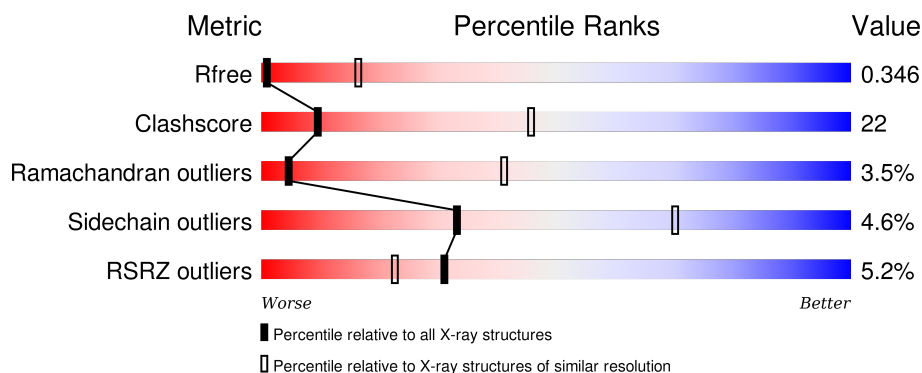
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>4%</div> <div>64%</div> <div>31%</div> <div>••</div> </div>
1	B	329	<div> <div>4%</div> <div>39%</div> <div>26%</div> <div>•</div> <div>33%</div> </div>
1	F	329	<div> <div>5%</div> <div>48%</div> <div>20%</div> <div>•</div> <div>30%</div> </div>
1	G	329	<div> <div>4%</div> <div>39%</div> <div>26%</div> <div>•</div> <div>34%</div> </div>
2	C	1342	<div> <div>3%</div> <div>55%</div> <div>39%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	1342	<div><div></div><div>6%</div><div>57%</div><div>38%</div><div>5%</div><div></div></div>
3	D	1407	<div><div></div><div>3%</div><div>43%</div><div>35%</div><div>5%</div><div>18%</div><div></div></div>
3	I	1407	<div><div></div><div>5%</div><div>44%</div><div>34%</div><div></div><div>18%</div><div></div></div>
4	E	91	<div><div></div><div>%</div><div>56%</div><div>38%</div><div></div><div></div><div></div></div>
4	J	91	<div><div></div><div>5%</div><div>45%</div><div>36%</div><div></div><div>16%</div><div></div></div>
5	X	613	<div><div></div><div>7%</div><div>51%</div><div>30%</div><div></div><div>16%</div><div></div></div>
5	Y	613	<div><div></div><div>5%</div><div>44%</div><div>28%</div><div></div><div>25%</div><div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 56126 atoms, of which 11 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			

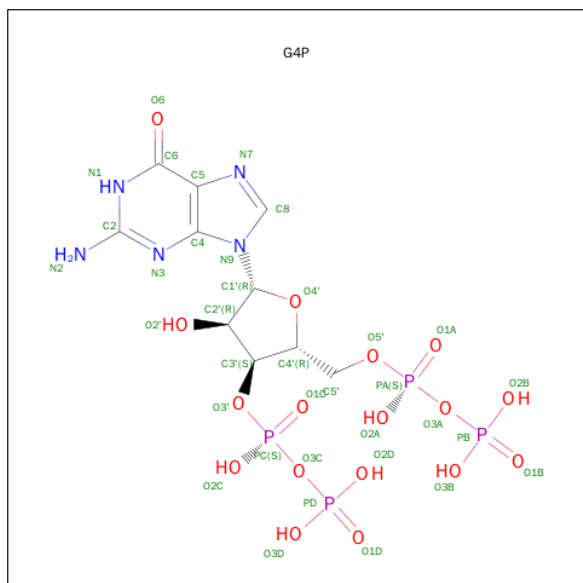
- Molecule 5 is a protein called Escherichia coli RNA polymerase sigma70 subunit.

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',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).

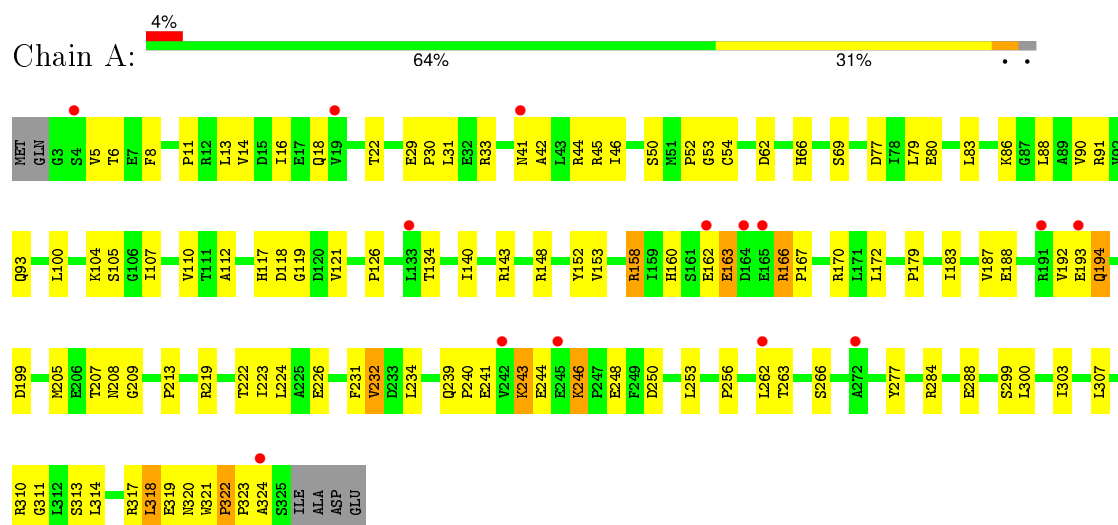


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	H	N	O	0	0
			47	10	11	5	17		

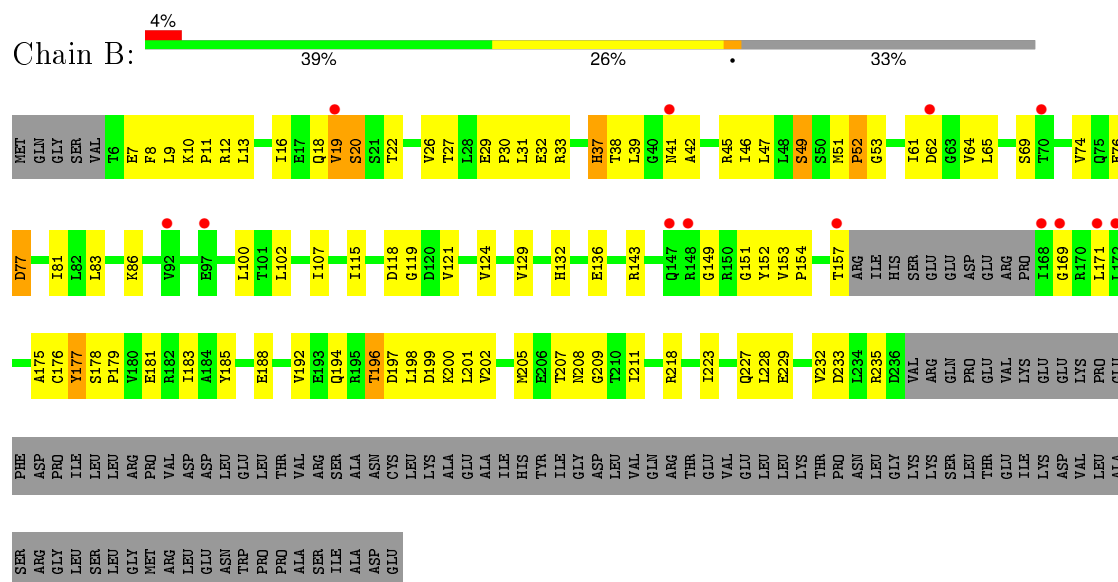
3 Residue-property plots

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

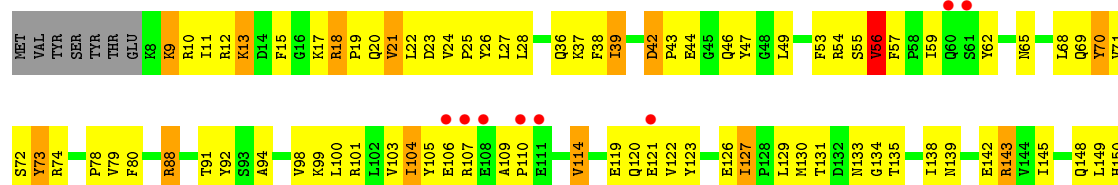
- Molecule 1: Escherichia coli RNA polymerase alpha subunit

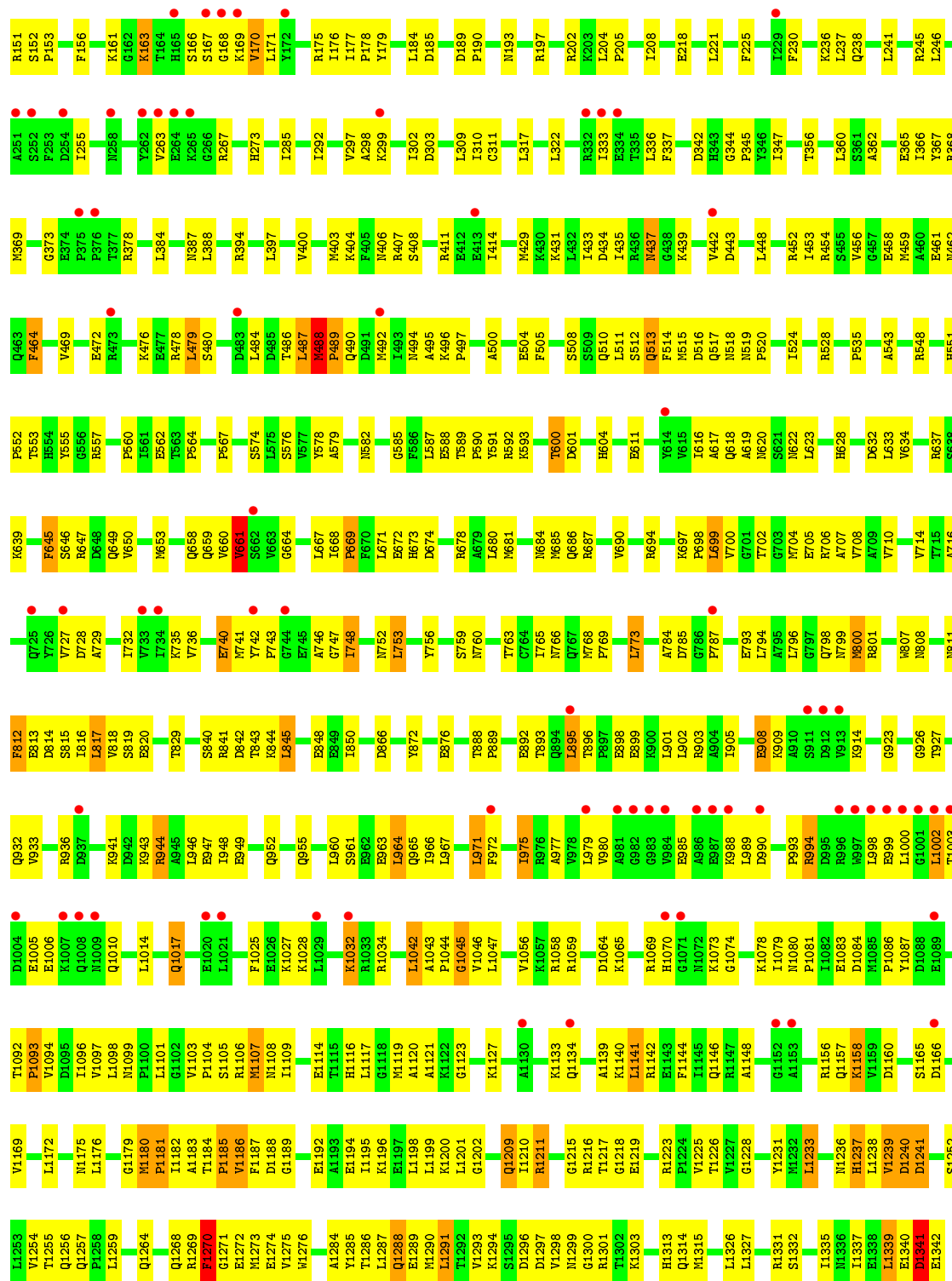


- Molecule 1: Escherichia coli RNA polymerase alpha subunit



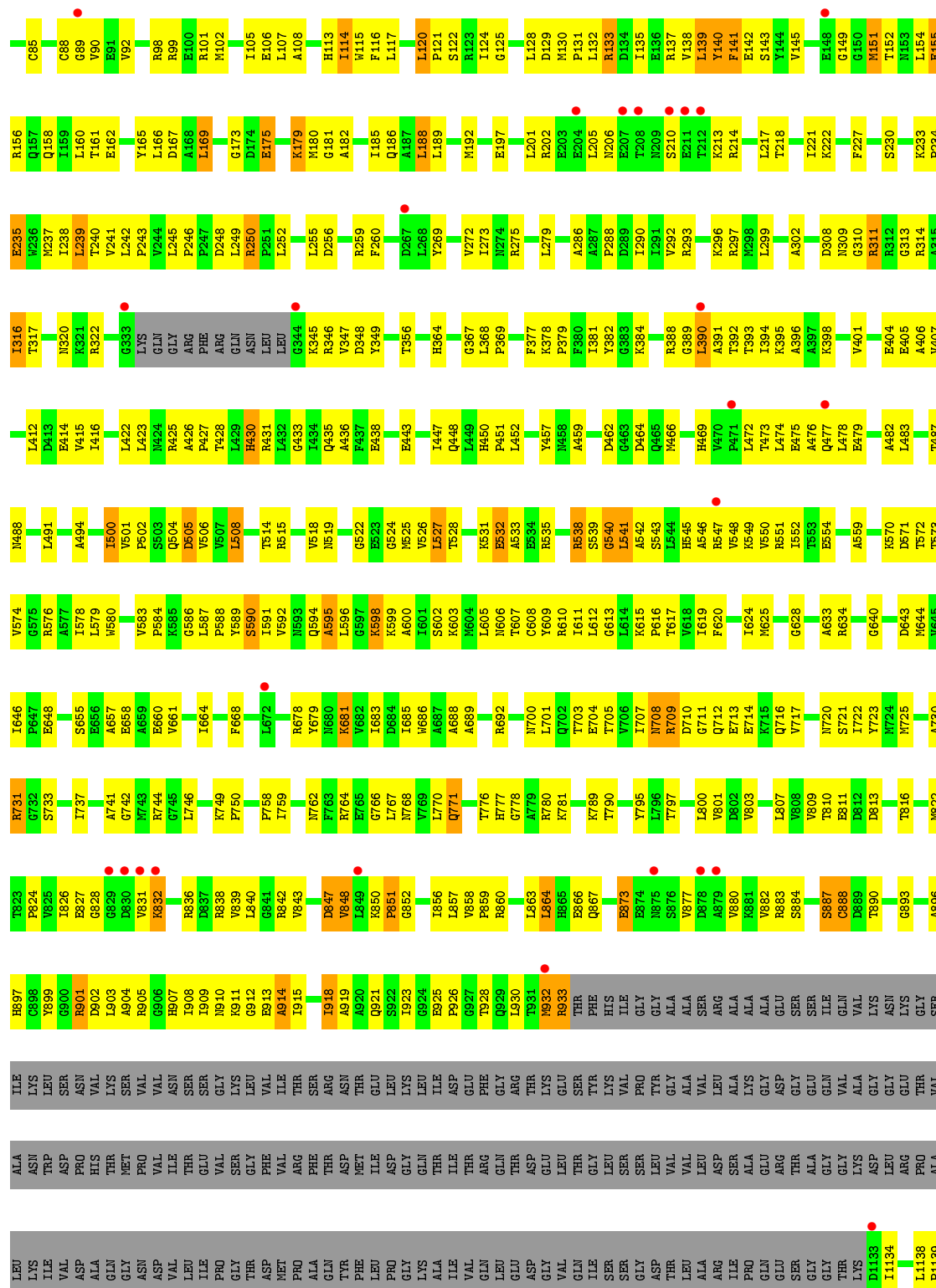
- Molecule 1: Escherichia coli RNA polymerase alpha subunit

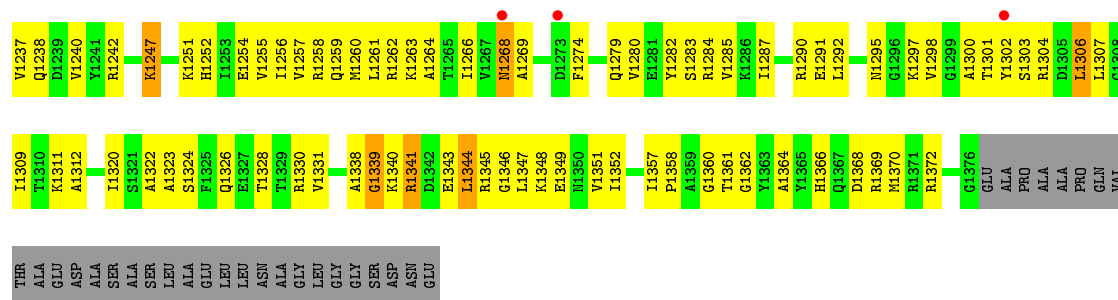




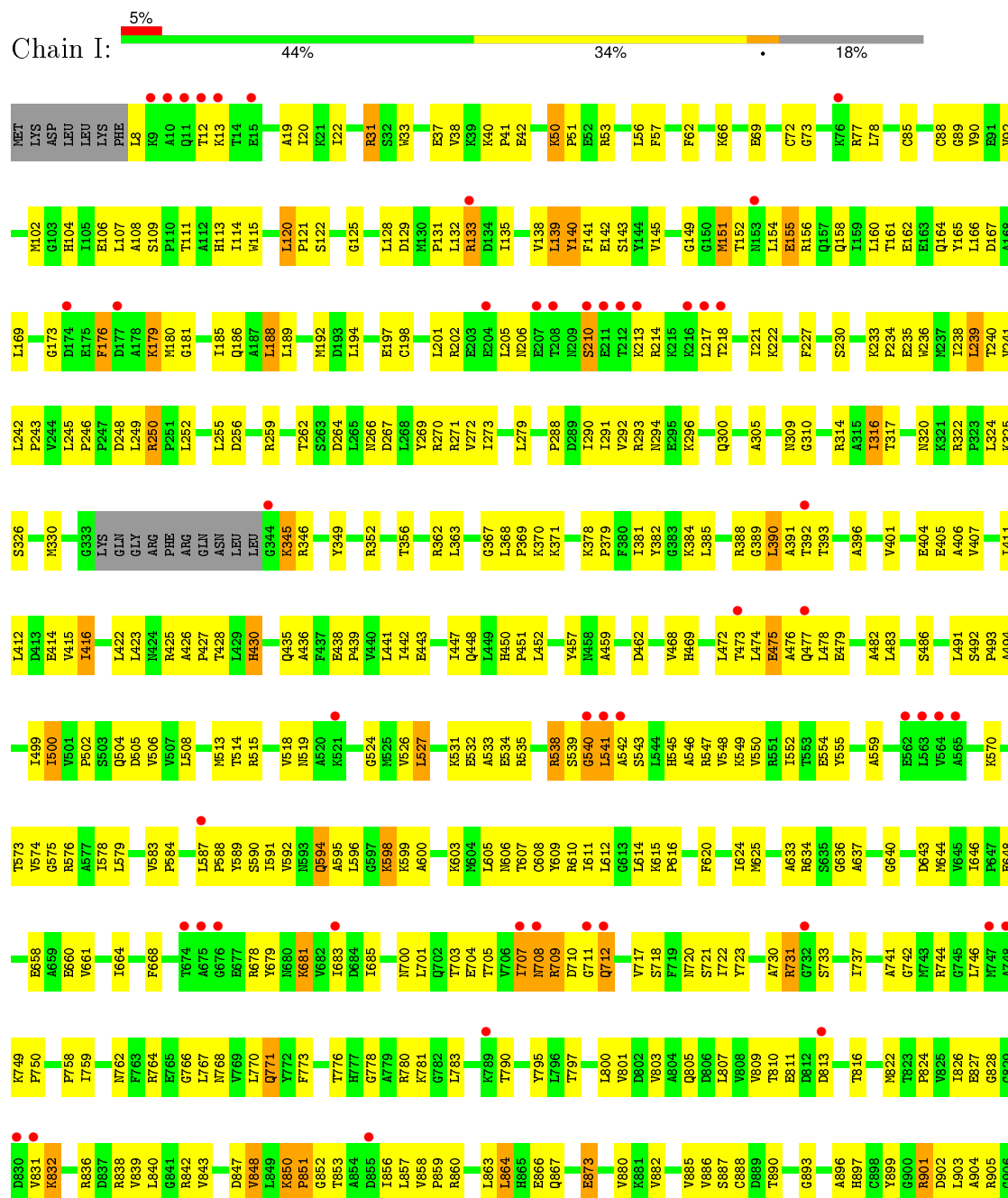
• Molecule 3: Escherichia coli RNA polymerase beta' subunit

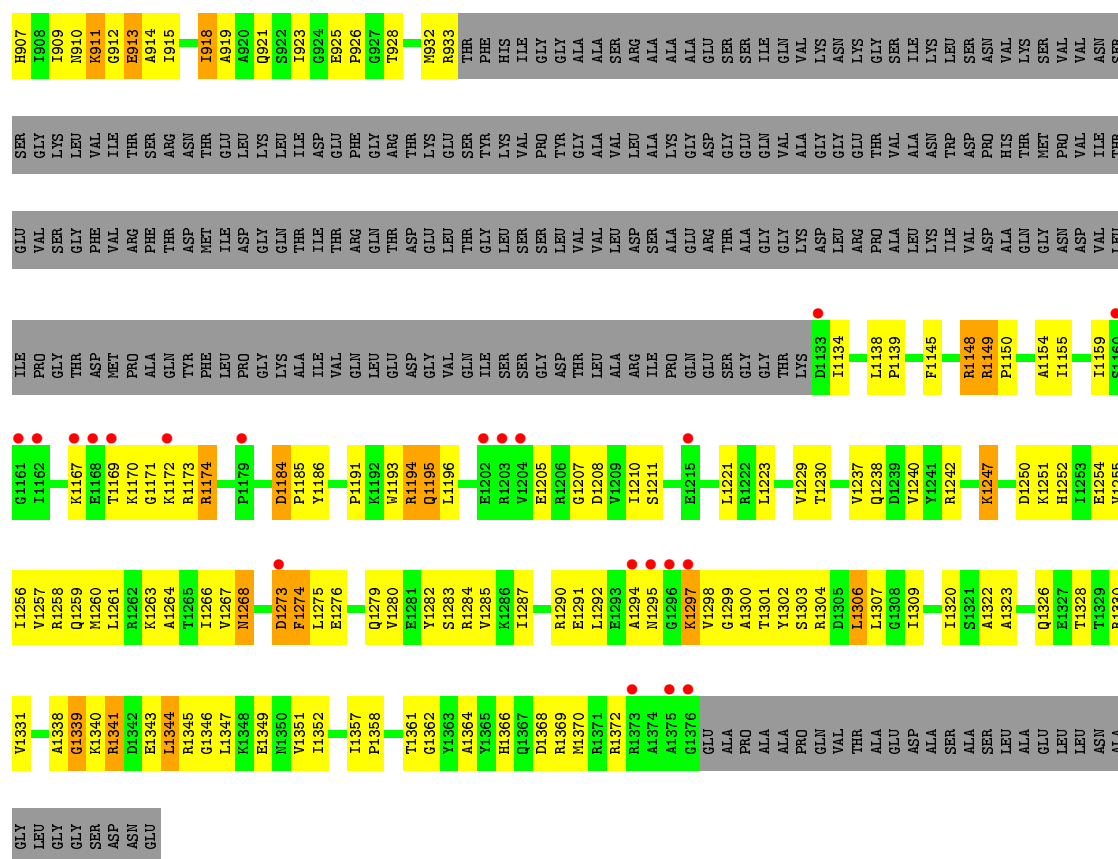




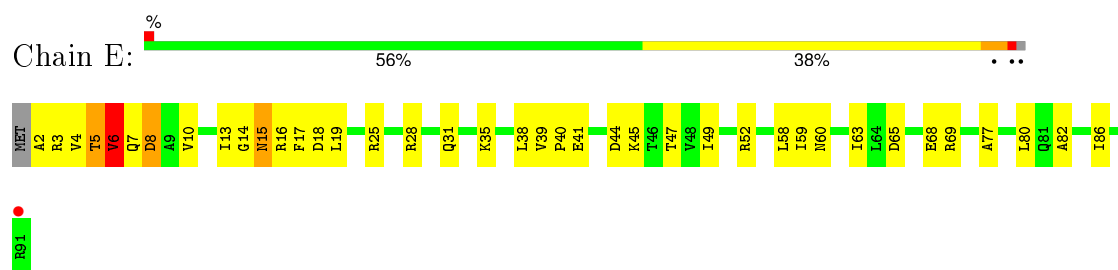


• Molecule 3: Escherichia coli RNA polymerase beta' subunit

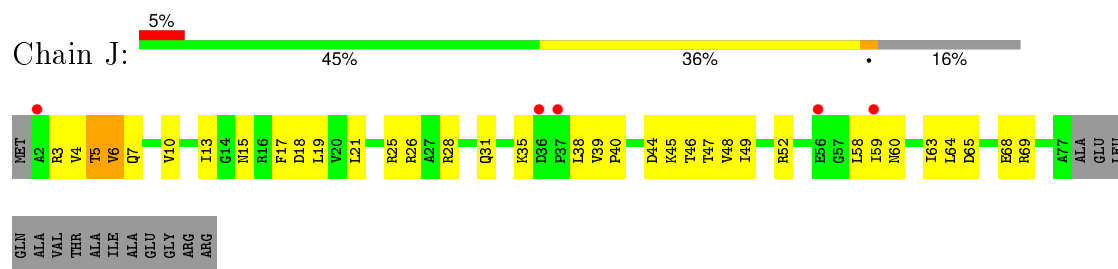




• Molecule 4: Escherichia coli RNA polymerase omega subunit

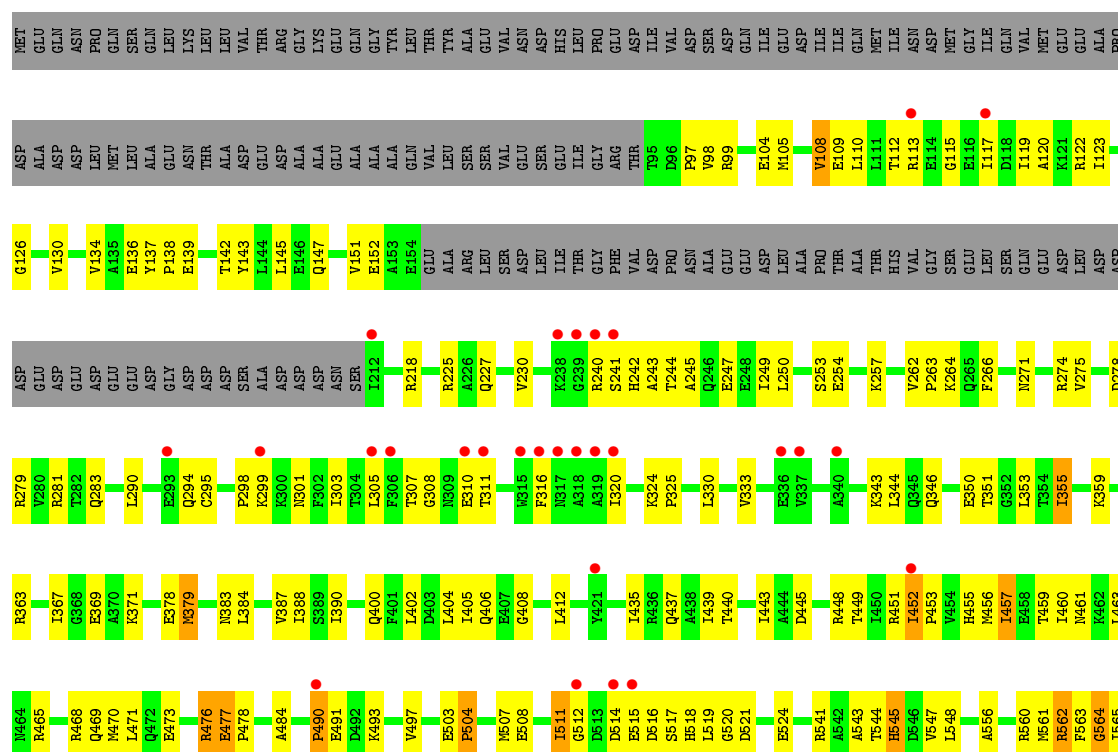
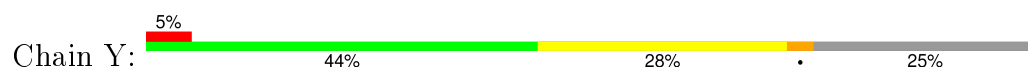
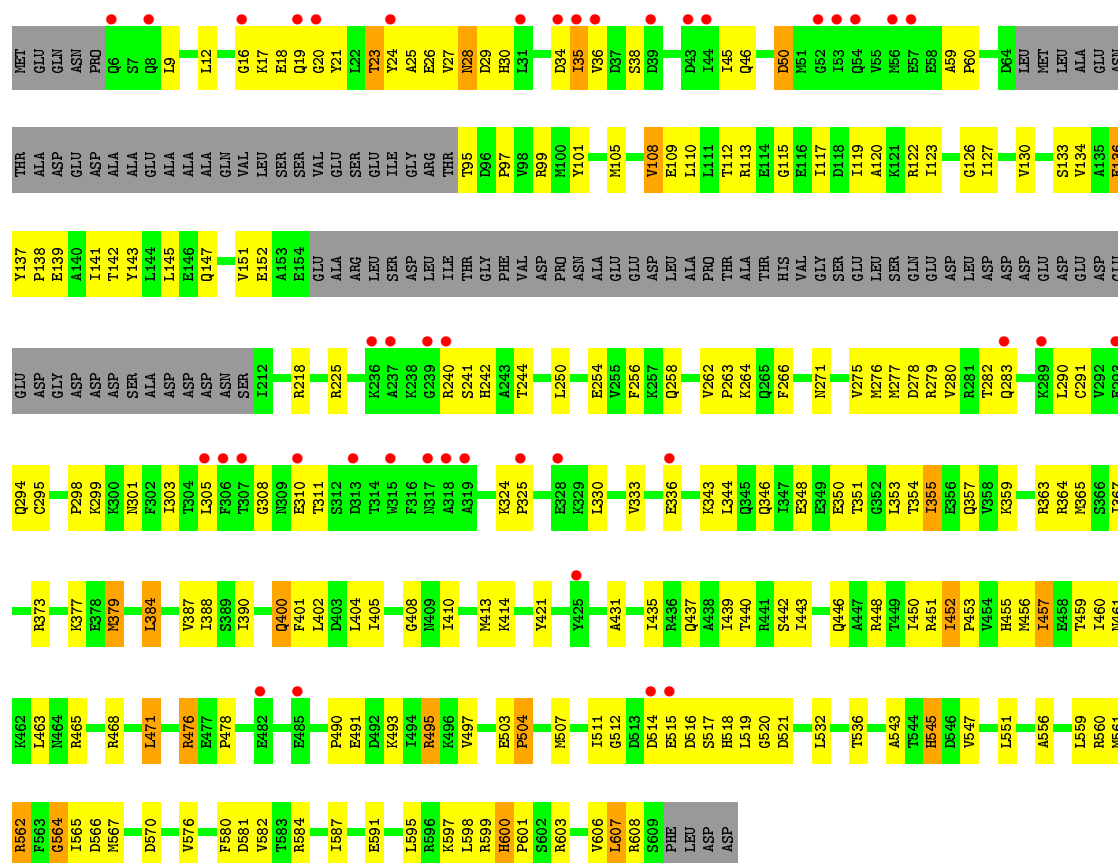


• Molecule 4: Escherichia coli RNA polymerase omega subunit



• Molecule 5: Escherichia coli RNA polymerase sigma70 subunit







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.57Å 203.82Å 307.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.90 29.84 – 3.85	Depositor EDS
% Data completeness (in resolution range)	89.6 (29.84-3.90) 82.4 (29.84-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.252 , 0.320 0.291 , 0.346	Depositor DCC
R_{free} test set	4728 reflections (5.58%)	DCC
Wilson B-factor (Å ²)	122.2	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 96273 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	56126	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: G4P, ZN

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	0.37	0/3454
1	B	0.19	0/1725	0.38	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	0.37	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	0.20	0/4253	0.36	0/5719
5	Y	0.20	0/3783	0.35	0/5083
All	All	0.20	0/56889	0.37	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	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1706	0	1738	89	0
1	F	1775	0	1800	62	0
1	G	1671	0	1706	84	0
2	C	10523	0	10546	517	0
2	H	10523	0	10546	501	0
3	D	9060	0	9257	530	0
3	I	9060	0	9257	511	0
4	E	708	0	719	40	0
4	J	605	0	612	32	0
5	X	4198	0	4250	169	0
5	Y	3732	0	3809	137	0
6	D	2	0	0	0	0
6	I	2	0	0	0	0
7	D	36	11	11	2	0
All	All	56115	11	56817	2538	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 22.

All (2538) 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	1.28	1.14
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.29	1.11
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.23	1.11
2:H:488:MET:HB2	2:H:490:GLN:H	1.14	1.05
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.38	1.02
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.42	1.01
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.41	1.01
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.43	1.00
1:B:12:ARG:H	1:B:30:PRO:HG2	1.27	0.99
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.42	0.98
2:C:54:ARG:H	2:C:55:SER:HB2	1.26	0.97
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.44	0.97
2:H:54:ARG:H	2:H:55:SER:HB2	1.25	0.97
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.44	0.96
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.47	0.94
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.50	0.94
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.47	0.94
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.48	0.93
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.50	0.92
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.50	0.92
2:H:488:MET:HB2	2:H:490:GLN:N	1.85	0.92
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.52	0.91
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.52	0.91
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.53	0.91
2:C:163:LYS:HD3	2:C:163:LYS:H	1.33	0.91
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.51	0.91
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	1.52	0.90
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.52	0.89
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.52	0.89
1:F:163:GLU:HG3	1:F:170:ARG:HH12	1.39	0.88
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.55	0.88
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.51	0.88
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.56	0.88
3:D:546:ALA:H	3:D:547:ARG:HA	1.37	0.88
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.57	0.87
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.55	0.87
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.04	0.87
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.55	0.86
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.04	0.86
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.58	0.86
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.57	0.86
3:I:546:ALA:H	3:I:547:ARG:HA	1.40	0.86
3:I:1247:LYS:H	3:I:1247:LYS:HD3	1.40	0.86
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.58	0.85
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.56	0.85
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.58	0.85
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.56	0.85
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.05	0.85
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.56	0.85
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.59	0.84
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.59	0.84
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.41	0.84
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.59	0.83
2:H:1101:LEU:HD21	3:I:508:LEU:HD12	1.60	0.83
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.60	0.83
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.58	0.83
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.60	0.82
3:D:128:LEU:HD21	3:D:188:LEU:HD13	1.60	0.82
3:D:643:ASP:O	3:D:720:ASN:ND2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:908:GLU:HG2	2:H:909:LYS:H	1.44	0.81
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.59	0.81
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.46	0.81
2:C:1101:LEU:HD21	3:D:508:LEU:HD12	1.62	0.81
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.45	0.81
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.62	0.81
2:C:131:THR:HG21	2:C:135:THR:HG22	1.62	0.81
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.62	0.81
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.61	0.81
4:E:5:THR:HA	4:E:6:VAL:CB	2.09	0.81
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.43	0.81
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.61	0.81
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.63	0.81
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.62	0.81
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.63	0.80
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.61	0.80
3:D:541:LEU:HD23	3:D:541:LEU:H	1.46	0.80
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.62	0.80
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.06	0.80
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.64	0.80
2:H:163:LYS:HD3	2:H:163:LYS:H	1.46	0.80
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.64	0.80
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	1.64	0.79
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.64	0.79
5:X:240:ARG:HD3	5:X:244:THR:HB	1.64	0.79
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.62	0.79
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.65	0.79
2:H:38:PHE:HE2	2:H:49:LEU:HD12	1.47	0.78
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.65	0.78
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.46	0.78
3:I:541:LEU:H	3:I:541:LEU:HD23	1.48	0.78
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.64	0.78
3:D:828:GLY:HA2	3:D:832:LYS:H	1.47	0.78
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.66	0.78
3:D:1247:LYS:H	3:D:1247:LYS:HD3	1.48	0.78
3:D:316:ILE:HG23	3:D:317:THR:H	1.49	0.78
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.66	0.77
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.19	0.77
5:X:35:ILE:HG13	5:X:36:VAL:H	1.47	0.77
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.66	0.77
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.66	0.77
2:C:800:MET:HA	2:C:800:MET:HE2	1.66	0.77
3:I:643:ASP:O	3:I:720:ASN:ND2	2.14	0.77
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	1.66	0.77
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	1.65	0.77
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.67	0.77
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.67	0.76
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.68	0.76
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.19	0.76
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.66	0.76
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.68	0.76
2:H:54:ARG:N	2:H:55:SER:HB2	2.00	0.76
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	1.66	0.76
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.65	0.76
3:D:230:SER:HB2	3:D:1339:GLY:H	1.51	0.76
2:C:131:THR:CG2	2:C:135:THR:HG22	2.16	0.75
4:J:5:THR:HA	4:J:6:VAL:CB	2.16	0.75
2:C:54:ARG:N	2:C:55:SER:HB2	2.01	0.75
3:D:1149:ARG:H	3:D:1149:ARG:HD3	1.50	0.75
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.67	0.75
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.69	0.75
2:H:800:MET:HE2	2:H:800:MET:HA	1.68	0.75
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.69	0.74
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.69	0.74
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.68	0.74
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.69	0.74
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.70	0.74
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.69	0.74
2:H:131:THR:HG21	2:H:135:THR:HG22	1.70	0.74
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.69	0.74
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.53	0.73
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.71	0.73
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.70	0.73
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.70	0.73
2:H:131:THR:CG2	2:H:135:THR:HG22	2.18	0.73
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.69	0.73
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.70	0.73
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.71	0.73
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.70	0.73
2:C:403:MET:HG3	2:C:414:ILE:HB	1.71	0.73
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.69	0.73
3:I:850:LYS:O	3:I:852:GLY:N	2.21	0.73
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.51	0.73
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.71	0.73
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.23	0.73
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.70	0.72
5:Y:448:ARG:HD2	5:Y:452:ILE:HD12	1.70	0.72
3:I:230:SER:HB2	3:I:1339:GLY:H	1.52	0.72
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.71	0.72
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.54	0.72
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.70	0.72
4:E:5:THR:HA	4:E:6:VAL:HB	1.71	0.72
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.24	0.72
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.25	0.72
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.70	0.72
4:J:15:ASN:HD21	4:J:17:PHE:HB2	1.53	0.72
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	1.71	0.71
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.73	0.71
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.71	0.71
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.20	0.71
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.72	0.71
3:D:546:ALA:H	3:D:547:ARG:CA	2.04	0.71
2:C:309:LEU:HD23	2:C:309:LEU:H	1.55	0.71
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.54	0.71
2:H:660:VAL:HG22	2:H:661:VAL:H	1.54	0.71
1:B:49:SER:HA	1:B:151:GLY:HA2	1.73	0.71
1:G:45:ARG:O	3:I:538:ARG:NH2	2.23	0.71
3:I:828:GLY:HA2	3:I:832:LYS:H	1.56	0.71
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.71	0.71
1:G:12:ARG:H	1:G:30:PRO:HG2	1.55	0.71
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.72	0.71
2:C:660:VAL:HG22	2:C:661:VAL:H	1.56	0.71
3:D:546:ALA:N	3:D:547:ARG:HA	2.05	0.71
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.73	0.71
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.55	0.71
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.71	0.71
3:D:828:GLY:HA2	3:D:832:LYS:N	2.06	0.70
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.24	0.70
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.24	0.70
4:E:5:THR:HA	4:E:6:VAL:HG12	1.72	0.70
2:H:142:GLU:HG2	2:H:515:MET:SD	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.73	0.70
2:C:690:VAL:HG22	2:C:691:PRO:HD2	1.73	0.70
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.56	0.70
3:D:850:LYS:O	3:D:852:GLY:N	2.25	0.70
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.72	0.70
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.56	0.70
2:C:37:LYS:HE3	2:C:37:LYS:HA	1.74	0.70
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.74	0.70
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.74	0.70
3:D:487:THR:HG21	4:E:4:VAL:HG12	1.73	0.70
3:I:546:ALA:N	3:I:547:ARG:HA	2.06	0.70
5:X:511:ILE:HG23	5:X:512:GLY:H	1.57	0.70
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.27	0.70
2:C:127:ILE:HD13	2:C:127:ILE:H	1.55	0.69
1:G:65:LEU:HD23	1:G:65:LEU:H	1.56	0.69
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.73	0.69
2:H:127:ILE:HD13	2:H:127:ILE:H	1.56	0.69
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.73	0.69
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.20	0.69
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.75	0.69
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.73	0.69
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.73	0.69
2:H:600:THR:HG22	2:H:601:ASP:H	1.56	0.69
2:C:54:ARG:H	2:C:55:SER:CB	2.04	0.69
1:B:41:ASN:HD21	2:C:1217:THR:HG22	1.57	0.69
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.73	0.69
2:C:1042:LEU:H	2:C:1042:LEU:HD13	1.58	0.69
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.73	0.69
2:H:309:LEU:HD23	2:H:309:LEU:H	1.55	0.69
5:X:108:VAL:HG23	5:X:109:GLU:H	1.58	0.69
2:H:1042:LEU:H	2:H:1042:LEU:HD13	1.58	0.69
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.75	0.69
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.27	0.69
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.75	0.69
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.92	0.69
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.22	0.69
2:C:170:VAL:HG23	2:C:171:LEU:H	1.57	0.69
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.24	0.68
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.72	0.68
3:I:128:LEU:HD11	3:I:188:LEU:HD22	1.75	0.68
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.75	0.68
2:C:528:ARG:NH2	2:C:576:SER:O	2.27	0.68
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.56	0.68
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.58	0.68
2:H:487:LEU:CB	2:H:488:MET:HA	2.23	0.68
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.23	0.68
3:I:828:GLY:HA2	3:I:832:LYS:N	2.08	0.68
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.09	0.68
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.76	0.68
5:X:139:GLU:HA	5:X:142:THR:HG22	1.76	0.68
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.76	0.68
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.76	0.68
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.76	0.68
2:H:403:MET:HG3	2:H:414:ILE:HB	1.75	0.68
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.23	0.68
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.58	0.68
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.94	0.68
3:I:546:ALA:H	3:I:547:ARG:CA	2.06	0.68
4:E:5:THR:HA	4:E:6:VAL:CG1	2.23	0.68
3:D:422:LEU:HA	3:D:436:ALA:HA	1.75	0.68
2:H:151:ARG:HH22	2:H:175:ARG:HH11	1.42	0.67
2:H:54:ARG:H	2:H:55:SER:CB	2.02	0.67
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.77	0.67
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.27	0.67
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.77	0.67
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.76	0.67
2:H:487:LEU:HB3	2:H:488:MET:HA	1.76	0.67
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.29	0.67
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.25	0.67
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.77	0.67
2:C:845:LEU:H	2:C:845:LEU:HD13	1.58	0.67
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.75	0.67
5:X:101:TYR:HE2	5:X:388:ILE:HD11	1.59	0.67
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.24	0.67
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.76	0.67
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.58	0.67
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.76	0.67
1:B:45:ARG:O	3:D:538:ARG:NH2	2.28	0.67
5:X:112:THR:HG22	5:X:113:ARG:H	1.59	0.67
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.77	0.67
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:5:THR:HB	4:E:7:GLN:HB2	1.76	0.67
5:X:476:ARG:H	5:X:476:ARG:HD2	1.60	0.67
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.77	0.67
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.28	0.67
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.28	0.67
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.77	0.67
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.75	0.67
2:H:845:LEU:H	2:H:845:LEU:HD13	1.58	0.66
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.28	0.66
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.77	0.66
2:H:55:SER:CB	2:H:56:VAL:HG22	2.26	0.66
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.77	0.66
2:H:131:THR:HG23	2:H:133:ASN:H	1.59	0.66
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.24	0.66
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.77	0.66
2:C:600:THR:HG22	2:C:601:ASP:H	1.60	0.66
3:D:259:ARG:HH21	5:X:504:PRO:HB2	1.60	0.66
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.78	0.66
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.75	0.66
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.78	0.66
2:H:170:VAL:HG23	2:H:171:LEU:H	1.61	0.66
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.31	0.66
5:X:457:ILE:O	5:X:461:ASN:ND2	2.28	0.66
2:H:484:LEU:H	2:H:484:LEU:HD22	1.60	0.66
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.24	0.66
3:D:836:ARG:HH12	3:D:839:VAL:HB	1.60	0.66
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.78	0.66
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.78	0.66
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.77	0.66
3:D:822:MET:SD	3:D:838:ARG:NH1	2.69	0.66
3:I:133:ARG:O	3:I:133:ARG:NH2	2.27	0.66
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.78	0.66
1:B:29:GLU:HA	1:B:200:LYS:CB	2.26	0.66
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.78	0.66
2:H:1252:SER:OG	2:H:1255:THR:O	2.14	0.66
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.78	0.66
5:X:448:ARG:HD2	5:X:452:ILE:HD12	1.78	0.65
2:H:241:LEU:HD22	2:H:285:ILE:HD13	1.79	0.65
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.78	0.65
2:H:488:MET:HE3	2:H:489:PRO:HA	1.78	0.65
2:H:488:MET:H	2:H:489:PRO:HA	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:SER:CB	2:C:56:VAL:HG22	2.26	0.65
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.77	0.65
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.79	0.65
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.29	0.65
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.28	0.65
3:I:422:LEU:HA	3:I:436:ALA:HA	1.79	0.65
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.61	0.65
2:C:1288:GLN:HE21	2:C:1288:GLN:HA	1.61	0.65
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.77	0.65
4:J:5:THR:CA	4:J:6:VAL:HB	2.27	0.65
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.78	0.65
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.27	0.65
3:I:145:VAL:HG22	3:I:180:MET:SD	2.37	0.65
1:G:49:SER:OG	3:I:538:ARG:NH2	2.30	0.65
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.62	0.65
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.77	0.65
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.79	0.65
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.78	0.65
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.12	0.65
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.79	0.65
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.78	0.64
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.63	0.64
2:C:106:GLU:N	2:C:107:ARG:HA	2.11	0.64
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.62	0.64
2:C:699:LEU:H	2:C:799:ASN:HD21	1.45	0.64
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.79	0.64
3:I:246:PRO:HB2	3:I:249:LEU:HD13	1.79	0.64
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.62	0.64
2:H:678:ARG:HE	2:H:1106:ARG:HG2	1.61	0.64
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.63	0.64
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.12	0.64
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.31	0.64
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.79	0.64
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.61	0.64
3:D:590:SER:O	3:D:594:GLN:N	2.31	0.64
2:C:488:MET:N	2:C:489:PRO:HD3	2.13	0.64
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.80	0.64
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.29	0.64
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.33	0.64
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.27	0.64
2:C:38:PHE:CE2	2:C:49:LEU:HD12	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.80	0.64
3:I:527:LEU:HD13	3:I:531:LYS:HB3	1.80	0.64
2:C:20:GLN:O	2:C:22:LEU:N	2.31	0.64
2:C:131:THR:HG23	2:C:133:ASN:H	1.63	0.64
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.81	0.63
5:Y:476:ARG:HD2	5:Y:476:ARG:H	1.63	0.63
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.13	0.63
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.78	0.63
1:F:68:TYR:HB3	2:H:756:TYR:CD1	2.33	0.63
2:C:714:VAL:HG23	2:C:787:PRO:HD2	1.78	0.63
3:D:438:GLU:OE1	4:E:3:ARG:NH1	2.32	0.63
3:D:128:LEU:HA	3:D:192:MET:HE1	1.79	0.63
4:J:5:THR:HA	4:J:6:VAL:HB	1.78	0.63
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.79	0.63
1:G:191:ARG:HH12	3:I:443:GLU:HG2	1.64	0.63
2:H:1288:GLN:HE21	2:H:1288:GLN:HA	1.61	0.63
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.31	0.63
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.31	0.63
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.13	0.63
3:I:151:MET:N	3:I:151:MET:SD	2.71	0.63
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.80	0.63
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.81	0.63
3:D:932:MET:O	3:D:933:ARG:HG3	1.97	0.63
2:H:21:VAL:HG13	2:H:22:LEU:H	1.64	0.63
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.29	0.63
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.81	0.63
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.31	0.63
2:H:69:GLN:HE22	2:H:101:ARG:HH21	1.46	0.63
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.80	0.63
2:C:189:ASP:OD1	2:C:193:ASN:N	2.25	0.63
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.80	0.63
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.31	0.62
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.81	0.62
3:I:644:MET:O	3:I:764:ARG:NH1	2.32	0.62
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.17	0.62
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.81	0.62
2:C:1239:VAL:O	2:C:1241:ASP:N	2.31	0.62
2:C:557:ARG:HB3	2:C:587:LEU:HD23	1.80	0.62
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.14	0.62
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.34	0.62
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.32	0.62
2:H:528:ARG:NH2	2:H:576:SER:O	2.32	0.62
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.81	0.62
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.63	0.62
3:I:720:ASN:O	3:I:722:ILE:N	2.32	0.62
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.80	0.62
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.81	0.62
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.81	0.62
3:I:1287:ILE:HG22	3:I:1290:ARG:HE	1.64	0.62
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	1.81	0.62
2:H:106:GLU:N	2:H:107:ARG:HA	2.13	0.62
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.14	0.62
1:A:11:PRO:HB3	1:A:31:LEU:CD2	2.29	0.62
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.81	0.62
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.82	0.62
4:J:5:THR:HA	4:J:6:VAL:HG12	1.82	0.62
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.29	0.62
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.64	0.62
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.64	0.62
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.81	0.62
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.82	0.62
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.81	0.62
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.24	0.62
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.24	0.62
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.32	0.62
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.64	0.62
2:H:487:LEU:HB3	2:H:488:MET:CA	2.29	0.61
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.82	0.61
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.64	0.61
2:H:800:MET:HA	2:H:800:MET:CE	2.30	0.61
3:D:252:LEU:HD23	3:D:252:LEU:H	1.66	0.61
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.65	0.61
3:D:588:PRO:CG	3:D:591:ILE:HD11	2.30	0.61
3:D:588:PRO:HG2	3:D:591:ILE:HD11	1.82	0.61
3:I:139:LEU:HD13	3:I:140:TYR:N	2.15	0.61
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.80	0.61
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.30	0.61
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.64	0.61
3:D:151:MET:N	3:D:151:MET:SD	2.73	0.61
3:I:213:LYS:O	3:I:217:LEU:HG	2.00	0.61
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1237:HIS:O	2:H:1238:LEU:HG	2.00	0.61
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.81	0.61
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.35	0.61
3:I:827:GLU:O	3:I:831:VAL:HG12	1.99	0.61
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.81	0.61
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.81	0.61
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.65	0.61
1:B:227:GLN:O	1:B:228:LEU:HG	1.99	0.61
2:C:699:LEU:HD12	2:C:1121:ALA:HB1	1.83	0.61
3:D:77:ARG:HG3	3:D:78:LEU:H	1.64	0.61
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.66	0.61
3:I:1341:ARG:NH2	3:I:1343:GLU:OE1	2.34	0.61
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.82	0.61
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.65	0.61
2:H:91:THR:HG22	2:H:139:ASN:H	1.65	0.61
5:X:503:GLU:N	5:X:504:PRO:HA	2.15	0.61
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.16	0.61
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.66	0.61
2:C:1237:HIS:O	2:C:1238:LEU:HG	2.00	0.61
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.82	0.61
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.36	0.61
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.83	0.61
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.31	0.61
4:E:10:VAL:CG2	4:E:16:ARG:HG2	2.31	0.61
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.83	0.61
3:D:1297:LYS:HA	3:D:1297:LYS:HZ2	1.64	0.61
2:H:646:SER:HB2	2:H:649:GLN:HG3	1.83	0.61
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.83	0.61
3:I:252:LEU:HD23	3:I:252:LEU:H	1.65	0.61
2:H:684:ASN:HA	2:H:687:ARG:HD3	1.83	0.61
5:X:517:SER:O	5:X:518:HIS:ND1	2.34	0.61
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.83	0.60
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.16	0.60
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.83	0.60
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.01	0.60
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.30	0.60
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.83	0.60
2:H:94:ALA:N	2:H:126:GLU:OE2	2.25	0.60
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.82	0.60
2:H:487:LEU:HB3	2:H:488:MET:CG	2.32	0.60
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.83	0.60
3:D:720:ASN:O	3:D:722:ILE:N	2.34	0.60
2:C:562:GLU:HG2	2:C:574:SER:CB	2.32	0.60
3:D:711:GLY:O	3:D:712:GLN:HG2	2.00	0.60
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.36	0.60
5:Y:585:GLU:HB3	5:Y:589:GLN:NE2	2.15	0.60
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.17	0.60
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.82	0.60
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.35	0.60
3:I:514:THR:HG23	3:I:576:ARG:HE	1.66	0.60
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.30	0.60
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.17	0.60
2:H:543:ALA:HB1	2:H:548:ARG:HD2	1.83	0.60
1:B:65:LEU:HA	1:B:169:GLY:HA2	1.83	0.60
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.82	0.60
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.82	0.60
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.27	0.60
3:D:500:ILE:H	3:D:500:ILE:HD13	1.66	0.60
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.82	0.60
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.82	0.60
4:J:15:ASN:HD22	4:J:18:ASP:H	1.49	0.60
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.83	0.60
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.37	0.60
1:A:232:VAL:HA	1:B:218:ARG:HG3	1.84	0.60
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.83	0.60
3:D:589:TYR:O	3:D:591:ILE:N	2.34	0.60
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.67	0.60
3:I:50:LYS:NZ	3:I:50:LYS:HB3	2.16	0.60
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.83	0.60
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.84	0.60
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.34	0.60
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.31	0.60
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.02	0.60
2:C:897:PRO:HB3	5:X:564:GLY:O	2.02	0.60
2:H:1239:VAL:O	2:H:1241:ASP:N	2.35	0.60
1:A:318:LEU:O	1:A:320:ASN:N	2.30	0.60
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.84	0.60
2:H:152:SER:HG	2:H:404:LYS:HZ2	1.43	0.60
3:D:213:LYS:O	3:D:217:LEU:HG	2.01	0.59
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.31	0.59
3:I:1268:ASN:HB3	3:I:1300:ALA:CB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:142:GLU:HG2	3:D:293:ARG:HB2	1.83	0.59
2:H:618:GLN:OE1	2:H:637:ARG:NH1	2.34	0.59
4:E:8:ASP:OD1	4:E:8:ASP:N	2.35	0.59
2:C:646:SER:HB2	2:C:649:GLN:HG3	1.84	0.59
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.84	0.59
2:C:1273:MET:HB3	3:D:428:THR:HB	1.83	0.59
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.85	0.59
3:I:768:ASN:O	3:I:771:GLN:NE2	2.35	0.59
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.67	0.59
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.67	0.59
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.68	0.59
3:D:827:GLU:O	3:D:831:VAL:HG12	2.02	0.59
2:C:387:ASN:HB3	2:C:394:ARG:HG3	1.85	0.59
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.68	0.59
5:X:584:ARG:O	5:X:587:ILE:HG22	2.02	0.59
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.38	0.59
4:E:5:THR:CA	4:E:6:VAL:HB	2.31	0.59
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.85	0.59
3:D:768:ASN:O	3:D:771:GLN:NE2	2.35	0.59
3:I:836:ARG:HH12	3:I:839:VAL:HB	1.67	0.59
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.82	0.59
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.37	0.59
3:I:1191:PRO:O	3:I:1193:TRP:N	2.34	0.59
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.67	0.59
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.35	0.59
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.85	0.59
2:H:20:GLN:O	2:H:22:LEU:N	2.36	0.59
2:H:616:ILE:HB	2:H:637:ARG:HB2	1.85	0.59
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.84	0.59
3:D:405:GLU:O	3:D:407:VAL:N	2.35	0.59
4:J:15:ASN:ND2	4:J:18:ASP:H	2.01	0.59
4:E:14:GLY:O	4:E:15:ASN:ND2	2.36	0.59
2:H:408:SER:O	2:H:431:LYS:NZ	2.29	0.59
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.85	0.59
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.84	0.59
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.83	0.59
3:D:1191:PRO:O	3:D:1193:TRP:N	2.33	0.59
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.67	0.59
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.84	0.59
2:C:873:ILE:HD11	2:C:931:VAL:HG22	1.84	0.59
3:I:711:GLY:O	3:I:712:GLN:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.85	0.59
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.68	0.59
4:E:2:ALA:HB1	4:E:6:VAL:HG23	1.84	0.59
1:G:49:SER:HA	1:G:151:GLY:HA2	1.85	0.59
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.66	0.59
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.84	0.59
3:D:85:CYS:HB3	3:D:88:CYS:O	2.03	0.59
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.84	0.59
2:C:166:SER:O	2:C:168:GLY:N	2.33	0.59
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.84	0.59
2:C:202:ARG:HD3	5:X:35:ILE:HB	1.85	0.58
2:H:844:LYS:HB2	2:H:844:LYS:HZ3	1.68	0.58
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.68	0.58
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.68	0.58
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.36	0.58
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.85	0.58
3:I:77:ARG:HG3	3:I:78:LEU:H	1.67	0.58
4:E:5:THR:HB	4:E:7:GLN:H	1.68	0.58
1:F:134:THR:HG21	2:H:727:VAL:O	2.03	0.58
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.38	0.58
2:H:901:LEU:HD13	5:Y:563:PHE:HE2	1.68	0.58
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.85	0.58
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.67	0.58
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.26	0.58
2:H:55:SER:CB	2:H:56:VAL:HG13	2.30	0.58
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.85	0.58
3:I:128:LEU:HD12	3:I:192:MET:CE	2.33	0.58
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.67	0.58
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.17	0.58
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.84	0.58
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.68	0.58
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.84	0.58
2:H:901:LEU:O	2:H:905:ILE:HG13	2.03	0.58
3:D:125:GLY:O	3:D:129:ASP:N	2.37	0.58
2:C:901:LEU:HD13	5:X:559:LEU:HD22	1.86	0.58
5:X:240:ARG:O	5:X:242:HIS:N	2.36	0.58
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.35	0.58
3:I:822:MET:SD	3:I:838:ARG:NH1	2.76	0.58
3:I:107:LEU:HD12	3:I:107:LEU:H	1.67	0.58
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.68	0.58
3:D:18:ASP:HA	3:D:1369:ARG:HH22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.84	0.58
2:C:302:ILE:HA	2:C:309:LEU:HA	1.85	0.58
2:H:387:ASN:HB3	2:H:394:ARG:HG3	1.83	0.58
3:D:388:ARG:NH2	3:D:414:GLU:OE2	2.36	0.58
2:C:808:ASN:H	3:D:633:ALA:HB2	1.68	0.58
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.85	0.58
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.34	0.58
5:X:35:ILE:HG23	5:X:36:VAL:HG13	1.86	0.58
2:H:237:LEU:HD13	2:H:292:ILE:HD12	1.86	0.58
2:H:55:SER:HB3	2:H:56:VAL:CB	2.34	0.58
3:D:1369:ARG:NH1	3:D:1369:ARG:HB3	2.19	0.58
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.68	0.58
2:H:504:GLU:O	2:H:508:SER:HB3	2.03	0.58
3:I:681:LYS:HB2	3:I:681:LYS:NZ	2.19	0.58
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.39	0.58
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.86	0.58
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.86	0.58
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.19	0.58
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.84	0.58
3:D:107:LEU:HD12	3:D:107:LEU:H	1.69	0.58
2:C:91:THR:HG22	2:C:139:ASN:H	1.69	0.58
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.03	0.58
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.84	0.58
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.39	0.58
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.69	0.57
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	1.86	0.57
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.37	0.57
2:C:55:SER:CB	2:C:56:VAL:HG13	2.33	0.57
4:J:5:THR:HA	4:J:6:VAL:CG1	2.33	0.57
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.19	0.57
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.38	0.57
3:D:1362:GLY:O	3:D:1364:ALA:N	2.35	0.57
2:H:660:VAL:O	2:H:661:VAL:HG22	2.04	0.57
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.03	0.57
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.86	0.57
3:I:202:ARG:O	3:I:206:ASN:ND2	2.37	0.57
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.86	0.57
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.04	0.57
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.20	0.57
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.05	0.57
3:D:145:VAL:HG22	3:D:180:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:756:TYR:H	2:C:766:ASN:HB3	1.69	0.57
3:I:405:GLU:O	3:I:407:VAL:N	2.37	0.57
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.68	0.57
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.04	0.57
2:C:800:MET:HA	2:C:800:MET:CE	2.34	0.57
1:F:9:LEU:O	1:G:227:GLN:NE2	2.37	0.57
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.87	0.57
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.85	0.57
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.86	0.57
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.87	0.57
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.69	0.57
1:B:179:PRO:O	1:B:207:THR:OG1	2.19	0.57
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.85	0.57
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.68	0.57
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.86	0.57
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.20	0.57
3:I:824:PRO:O	3:I:826:ILE:HG13	2.05	0.57
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.19	0.57
2:H:1335:ILE:HD11	3:I:22:ILE:HG13	1.85	0.57
2:H:302:ILE:HG22	2:H:309:LEU:HB3	1.86	0.57
2:C:576:SER:HB3	2:C:579:ALA:HB2	1.87	0.57
2:C:1252:SER:OG	2:C:1255:THR:O	2.21	0.57
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.68	0.57
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.87	0.57
5:Y:585:GLU:O	5:Y:589:GLN:N	2.36	0.57
1:B:86:LYS:NZ	3:D:526:VAL:O	2.37	0.57
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.38	0.57
2:C:1200:LYS:O	2:C:1202:GLY:N	2.35	0.57
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.87	0.57
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.05	0.57
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.35	0.57
2:C:1255:THR:O	2:C:1257:GLN:N	2.37	0.57
3:D:202:ARG:O	3:D:206:ASN:ND2	2.38	0.57
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.86	0.57
3:D:527:LEU:HD12	3:D:535:ARG:NE	2.18	0.56
1:B:227:GLN:O	1:B:229:GLU:N	2.31	0.56
1:A:80:GLU:HA	2:C:694:ARG:HH12	1.70	0.56
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.20	0.56
3:D:246:PRO:HB2	3:D:249:LEU:HD13	1.86	0.56
2:C:901:LEU:O	2:C:905:ILE:HG13	2.04	0.56
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.33	0.56
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.87	0.56
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.87	0.56
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.40	0.56
3:D:316:ILE:HG23	3:D:317:THR:N	2.17	0.56
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.40	0.56
1:B:33:ARG:HE	1:B:197:ASP:HB2	1.70	0.56
1:B:49:SER:OG	3:D:538:ARG:NH2	2.39	0.56
2:H:496:LYS:N	2:H:497:PRO:HD2	2.19	0.56
2:H:843:THR:HG22	2:H:844:LYS:H	1.70	0.56
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.05	0.56
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.87	0.56
3:I:85:CYS:HB3	3:I:88:CYS:O	2.05	0.56
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.87	0.56
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.86	0.56
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.88	0.56
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.88	0.56
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.06	0.56
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.70	0.56
3:D:487:THR:HG21	4:E:4:VAL:CG1	2.36	0.56
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.39	0.56
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.88	0.56
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.87	0.56
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.87	0.56
3:I:1345:ARG:HG2	3:I:1370:MET:HE1	1.87	0.56
2:C:843:THR:HG22	2:C:844:LYS:H	1.71	0.56
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.41	0.56
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.87	0.56
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.88	0.56
2:C:542:ARG:O	2:C:544:GLY:N	2.35	0.56
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.88	0.56
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.86	0.56
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.06	0.56
3:I:309:ASN:HD22	3:I:326:SER:HB3	1.71	0.56
2:H:548:ARG:NH2	2:H:567:PRO:O	2.38	0.56
5:X:561:MET:HA	5:X:567:MET:SD	2.45	0.56
3:I:1338:ALA:O	3:I:1340:LYS:N	2.39	0.56
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.86	0.56
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.36	0.56
5:X:503:GLU:HB3	5:X:504:PRO:O	2.06	0.56
3:D:245:LEU:O	3:D:250:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1200:LYS:O	2:H:1202:GLY:N	2.37	0.56
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.88	0.56
1:G:19:VAL:O	1:G:20:SER:OG	2.19	0.56
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.38	0.56
3:I:809:VAL:HG13	3:I:912:GLY:H	1.71	0.56
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.35	0.56
1:B:42:ALA:O	1:B:46:ILE:HG12	2.04	0.56
3:I:1362:GLY:O	3:I:1364:ALA:N	2.38	0.56
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.06	0.56
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.33	0.56
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.87	0.56
3:D:139:LEU:HD13	3:D:140:TYR:N	2.21	0.56
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.87	0.56
3:D:66:LYS:HG3	3:D:69:GLU:OE2	2.06	0.56
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.87	0.56
2:H:694:ARG:O	2:H:798:GLN:NE2	2.39	0.56
1:A:118:ASP:OD1	1:A:119:GLY:N	2.39	0.56
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.88	0.56
5:Y:387:VAL:HG13	5:Y:408:GLY:HA3	1.88	0.56
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.71	0.56
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.88	0.55
4:E:13:ILE:HD11	4:E:19:LEU:HD23	1.88	0.55
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.40	0.55
5:Y:283:GLN:NE2	5:Y:343:LYS:HD2	2.21	0.55
3:I:41:PRO:HB3	3:I:270:ARG:HG3	1.88	0.55
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.88	0.55
2:H:179:TYR:HE2	2:H:462:ASN:HD21	1.55	0.55
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.70	0.55
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.33	0.55
1:B:65:LEU:HD23	1:B:65:LEU:H	1.70	0.55
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.87	0.55
3:D:1338:ALA:O	3:D:1340:LYS:N	2.39	0.55
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.41	0.55
3:D:527:LEU:HD13	3:D:531:LYS:HB3	1.89	0.55
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.36	0.55
3:D:905:ARG:HG2	3:D:907:HIS:H	1.71	0.55
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.72	0.55
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.38	0.55
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.87	0.55
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.88	0.55
1:G:42:ALA:O	1:G:46:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:PRO:CG	1:G:228:LEU:H	2.19	0.55
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.19	0.55
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.22	0.55
3:I:412:LEU:O	3:I:416:ILE:HD12	2.07	0.55
3:I:72:CYS:SG	3:I:73:GLY:N	2.78	0.55
2:C:496:LYS:N	2:C:497:PRO:HD2	2.21	0.55
5:X:363:ARG:O	5:X:367:ILE:HG12	2.06	0.55
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.71	0.55
2:H:740:GLU:HB2	2:H:741:MET:SD	2.47	0.55
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.27	0.55
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.36	0.55
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.70	0.55
2:H:9:LYS:HD3	2:H:9:LYS:N	2.22	0.55
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.05	0.55
2:C:660:VAL:O	2:C:661:VAL:HG22	2.06	0.55
2:H:699:LEU:HD12	2:H:1121:ALA:HB1	1.87	0.55
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.41	0.55
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.22	0.55
3:I:125:GLY:O	3:I:129:ASP:N	2.39	0.55
7:D:1503:G4P:O1C	7:D:1503:G4P:O2'	2.21	0.55
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.36	0.55
3:D:450:HIS:NE2	3:D:625:MET:SD	2.80	0.55
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.89	0.55
2:C:740:GLU:HB2	2:C:741:MET:SD	2.47	0.55
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.39	0.55
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.89	0.55
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.71	0.55
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.89	0.55
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.72	0.55
3:D:389:GLY:O	3:D:391:ALA:N	2.40	0.55
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.88	0.55
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.89	0.55
1:B:64:VAL:HG13	1:B:69:SER:OG	2.06	0.55
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.89	0.55
3:I:450:HIS:CE1	3:I:452:LEU:HD12	2.42	0.55
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.69	0.55
2:C:634:VAL:H	2:C:645:PHE:HE2	1.53	0.55
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.41	0.55
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.88	0.55
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.70	0.55
2:C:55:SER:HB3	2:C:56:VAL:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1343:GLU:HA	3:D:1344:LEU:CB	2.34	0.55
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.32	0.55
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.89	0.55
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.40	0.55
2:C:752:ASN:O	2:C:753:LEU:HG	2.07	0.55
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.22	0.54
2:H:494:ASN:OD1	2:H:495:ALA:N	2.39	0.54
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.89	0.54
1:A:243:LYS:NZ	1:A:243:LYS:HB2	2.22	0.54
2:C:517:GLN:HE21	2:C:760:ASN:H	1.55	0.54
3:I:173:GLY:HA2	3:I:176:PHE:HE2	1.72	0.54
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.89	0.54
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.22	0.54
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.42	0.54
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.89	0.54
3:D:644:MET:O	3:D:764:ARG:NH1	2.40	0.54
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.07	0.54
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.72	0.54
3:I:709:ARG:O	3:I:711:GLY:N	2.41	0.54
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.90	0.54
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.88	0.54
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.40	0.54
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.23	0.54
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.89	0.54
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.72	0.54
2:C:898:GLU:N	2:C:898:GLU:OE1	2.37	0.54
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.89	0.54
2:C:1141:LEU:H	2:C:1141:LEU:CD1	2.20	0.54
3:I:491:LEU:HB2	3:I:904:ALA:HA	1.90	0.54
4:E:41:GLU:O	4:E:52:ARG:NH2	2.28	0.54
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.89	0.54
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.07	0.54
1:G:41:ASN:HD21	2:H:1217:THR:HG22	1.72	0.54
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.89	0.54
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.89	0.54
3:I:233:LYS:HD2	3:I:234:PRO:HD2	1.89	0.54
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.41	0.54
2:H:1339:LEU:H	2:H:1339:LEU:HD12	1.71	0.54
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.90	0.54
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.54
2:C:106:GLU:H	2:C:107:ARG:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.90	0.54
3:I:500:ILE:HD13	3:I:500:ILE:H	1.72	0.54
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.88	0.54
2:H:664:GLY:O	2:H:686:GLN:NE2	2.41	0.54
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.90	0.54
2:H:888:THR:O	2:H:914:LYS:N	2.33	0.54
2:H:510:GLN:O	2:H:513:GLN:NE2	2.40	0.54
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.89	0.54
2:C:149:LEU:HD12	2:C:452:ARG:O	2.08	0.54
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.90	0.54
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.90	0.54
5:Y:119:ILE:HG21	5:Y:379:MET:HG2	1.90	0.54
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.23	0.54
5:X:515:GLU:N	5:X:516:ASP:HA	2.22	0.54
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.73	0.54
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.90	0.54
3:I:1167:LYS:HB3	3:I:1170:LYS:HD2	1.89	0.54
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.20	0.54
3:D:72:CYS:SG	3:D:73:GLY:N	2.81	0.54
3:I:142:GLU:HG2	3:I:293:ARG:HB2	1.89	0.54
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.07	0.54
2:H:360:LEU:HD13	2:H:378:ARG:HH11	1.71	0.54
3:D:1297:LYS:HA	3:D:1297:LYS:NZ	2.23	0.54
3:I:88:CYS:O	3:I:90:VAL:N	2.41	0.54
2:H:753:LEU:HD12	2:H:753:LEU:O	2.08	0.54
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.90	0.54
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.90	0.54
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.23	0.54
3:D:1155:ILE:HG13	3:D:1210:ILE:CG2	2.33	0.53
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.08	0.53
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.88	0.53
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.27	0.53
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.90	0.53
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.08	0.53
1:G:179:PRO:O	1:G:207:THR:OG1	2.23	0.53
1:F:192:VAL:HG21	1:F:198:LEU:HD12	1.90	0.53
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.42	0.53
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.43	0.53
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.90	0.53
1:G:86:LYS:NZ	3:I:526:VAL:O	2.42	0.53
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1268:GLN:O	3:I:346:ARG:HA	2.09	0.53
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.90	0.53
3:D:573:THR:HG22	3:D:576:ARG:CG	2.38	0.53
3:I:905:ARG:HG2	3:I:907:HIS:H	1.74	0.53
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.72	0.53
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.44	0.53
3:I:294:ASN:ND2	5:Y:406:GLN:OE1	2.41	0.53
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.90	0.53
3:D:120:LEU:CB	3:D:121:PRO:CD	2.85	0.53
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.90	0.53
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.38	0.53
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.44	0.53
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.41	0.53
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.39	0.53
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.74	0.53
2:C:9:LYS:N	2:C:9:LYS:HD3	2.23	0.53
2:H:562:GLU:HG2	2:H:574:SER:CB	2.38	0.53
1:G:29:GLU:HA	1:G:200:LYS:CB	2.39	0.53
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.89	0.53
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.09	0.53
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.53
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.42	0.53
2:C:494:ASN:OD1	2:C:495:ALA:N	2.40	0.53
4:E:82:ALA:O	4:E:86:ILE:HG13	2.07	0.53
2:H:1119:MET:O	2:H:1123:GLY:N	2.40	0.53
2:C:311:CYS:SG	2:C:315:MET:HB2	2.49	0.53
3:D:42:GLU:HG3	5:X:451:ARG:HH21	1.74	0.53
2:C:768:MET:O	2:C:785:ASP:N	2.38	0.53
1:G:118:ASP:OD1	1:G:119:GLY:N	2.42	0.53
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.38	0.53
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.91	0.53
3:D:398:LYS:HD2	5:X:532:LEU:HD11	1.90	0.53
3:I:589:TYR:O	3:I:591:ILE:N	2.38	0.53
2:C:841:ARG:NH1	3:D:256:ASP:HB3	2.24	0.53
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.72	0.53
4:E:45:LYS:O	4:E:49:ILE:HG12	2.08	0.53
1:A:263:THR:HG23	1:A:266:SER:H	1.74	0.53
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.42	0.53
2:H:747:GLY:O	2:H:748:ILE:HG13	2.08	0.53
1:A:66:HIS:CE1	1:A:69:SER:HB2	2.44	0.53
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.38	0.53
2:C:21:VAL:HG13	2:C:22:LEU:H	1.73	0.53
3:D:1262:ARG:HH22	3:D:1312:ALA:HB1	1.73	0.53
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.89	0.53
3:I:679:TYR:CZ	3:I:683:ILE:HD11	2.44	0.53
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.44	0.53
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.90	0.53
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.38	0.53
2:C:41:GLN:CD	2:C:42:ASP:H	2.12	0.53
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.44	0.53
3:D:824:PRO:CB	3:D:836:ARG:HD3	2.39	0.53
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.44	0.53
2:H:741:MET:N	2:H:741:MET:SD	2.81	0.53
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.09	0.53
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.44	0.53
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.90	0.53
3:D:546:ALA:HB3	3:D:547:ARG:O	2.09	0.52
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.44	0.52
3:I:478:LEU:CD1	4:J:47:THR:HG23	2.38	0.52
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.73	0.52
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.24	0.52
1:B:61:ILE:HB	1:B:64:VAL:HB	1.91	0.52
2:C:753:LEU:O	2:C:753:LEU:HD12	2.09	0.52
2:C:747:GLY:O	2:C:748:ILE:HG13	2.08	0.52
3:I:550:VAL:HG23	3:I:552:ILE:HD11	1.91	0.52
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.91	0.52
2:C:42:ASP:O	2:C:44:GLU:HG2	2.10	0.52
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.73	0.52
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.73	0.52
5:Y:264:LYS:H	5:Y:264:LYS:HD2	1.75	0.52
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.09	0.52
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.73	0.52
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.73	0.52
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.90	0.52
2:C:975:ILE:HD13	2:C:975:ILE:O	2.09	0.52
3:D:709:ARG:O	3:D:711:GLY:N	2.42	0.52
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.91	0.52
3:I:264:ASP:HB3	3:I:324:LEU:HB3	1.90	0.52
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.45	0.52
5:X:402:LEU:HD13	5:X:405:ILE:HD11	1.91	0.52
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:4:VAL:O	4:J:5:THR:OG1	2.25	0.52
2:H:91:THR:HG22	2:H:139:ASN:N	2.24	0.52
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.44	0.52
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.91	0.52
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.44	0.52
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.25	0.52
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.91	0.52
3:I:1297:LYS:HA	3:I:1297:LYS:NZ	2.25	0.52
2:C:130:MET:SD	2:C:134:GLY:HA2	2.50	0.52
1:F:42:ALA:O	1:F:46:ILE:HG12	2.10	0.52
3:I:704:GLU:HB2	3:I:718:SER:OG	2.10	0.52
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.45	0.52
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.49	0.52
3:D:128:LEU:HD12	3:D:192:MET:CE	2.40	0.52
3:I:478:LEU:HD12	4:J:47:THR:HG23	1.90	0.52
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.90	0.52
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.91	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.42	0.52
5:Y:379:MET:CE	5:Y:379:MET:HA	2.40	0.52
5:X:17:LYS:N	5:X:18:GLU:HA	2.24	0.52
5:X:442:SER:OG	5:X:446:GLN:NE2	2.38	0.52
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.90	0.52
2:C:1244:HIS:HB3	2:C:1265:PHE:CD2	2.45	0.52
5:Y:576:VAL:HG12	5:Y:587:ILE:HG12	1.92	0.52
3:I:40:LYS:HB3	3:I:42:GLU:HG2	1.92	0.52
3:I:120:LEU:HD22	3:I:1330:ARG:HD3	1.92	0.52
2:H:1255:THR:O	2:H:1257:GLN:N	2.42	0.52
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.44	0.52
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.91	0.52
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.92	0.52
2:C:142:GLU:HG2	2:C:515:MET:SD	2.50	0.52
3:I:145:VAL:HG21	3:I:165:TYR:CD2	2.45	0.52
3:D:51:PRO:HB3	3:D:57:PHE:O	2.10	0.52
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.92	0.52
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.91	0.52
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.38	0.52
3:I:733:SER:O	3:I:737:ILE:HG12	2.09	0.52
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.92	0.52
2:C:134:GLY:O	2:C:527:LYS:NZ	2.43	0.52
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.92	0.52
2:C:892:GLU:O	2:C:893:THR:OG1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.91	0.52
3:D:1344:LEU:H	3:D:1345:ARG:HG3	1.75	0.52
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.45	0.52
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.91	0.52
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.44	0.52
3:D:810:THR:OG1	3:D:811:GLU:N	2.43	0.52
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.92	0.52
2:C:94:ALA:N	2:C:126:GLU:OE2	2.27	0.52
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.44	0.52
2:H:728:ASP:OD2	2:H:729:ALA:N	2.43	0.52
3:D:909:ILE:O	3:D:909:ILE:HD12	2.10	0.51
1:A:100:LEU:HD11	1:A:121:VAL:HG11	1.92	0.51
1:A:90:VAL:HG13	1:A:121:VAL:HG13	1.92	0.51
3:D:473:THR:HB	3:D:476:ALA:HB2	1.91	0.51
3:D:88:CYS:O	3:D:90:VAL:N	2.44	0.51
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.40	0.51
2:H:752:ASN:O	2:H:753:LEU:HG	2.10	0.51
5:X:355:ILE:HD13	5:X:355:ILE:O	2.10	0.51
3:I:292:VAL:HG22	3:I:296:LYS:HE3	1.92	0.51
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.25	0.51
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.32	0.51
3:D:141:PHE:O	3:D:297:ARG:HD3	2.10	0.51
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.43	0.51
3:D:395:LYS:HG3	5:X:536:THR:CG2	2.39	0.51
2:C:153:PRO:HD2	2:C:452:ARG:HD3	1.92	0.51
3:I:707:ILE:HG22	3:I:708:ASN:H	1.75	0.51
2:H:985:GLU:HG2	2:H:989:LEU:HD13	1.92	0.51
2:C:317:LEU:HD13	2:C:322:LEU:HD21	1.92	0.51
2:H:1273:MET:HB3	3:I:428:THR:HB	1.92	0.51
2:H:18:ARG:HD3	2:H:619:ALA:O	2.10	0.51
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.23	0.51
3:I:389:GLY:O	3:I:391:ALA:N	2.43	0.51
3:I:590:SER:O	3:I:594:GLN:N	2.43	0.51
3:I:611:ILE:HG13	3:I:612:LEU:HD23	1.91	0.51
3:D:152:THR:O	3:D:154:LEU:N	2.40	0.51
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.92	0.51
3:I:546:ALA:HB3	3:I:547:ARG:O	2.10	0.51
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.29	0.51
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.92	0.51
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.40	0.51
2:C:91:THR:HG22	2:C:138:ILE:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.26	0.51
2:H:189:ASP:OD1	2:H:193:ASN:N	2.34	0.51
2:C:936:ARG:HD2	2:C:1047:LEU:H	1.75	0.51
5:X:519:LEU:O	5:X:519:LEU:HD13	2.09	0.51
5:X:264:LYS:HD2	5:X:264:LYS:H	1.74	0.51
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.26	0.51
1:A:256:PRO:HA	1:A:277:TYR:HA	1.90	0.51
3:I:919:ALA:O	3:I:923:ILE:HG12	2.11	0.51
2:H:699:LEU:H	2:H:799:ASN:HD21	1.57	0.51
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	1.91	0.51
2:H:459:MET:SD	2:H:511:LEU:HD22	2.51	0.51
2:C:314:ASN:HD21	2:C:348:SER:HA	1.74	0.51
3:D:914:ALA:O	3:D:918:ILE:HG22	2.10	0.51
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.91	0.51
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.10	0.51
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.91	0.51
1:F:150:ARG:HH12	1:G:8:PHE:HA	1.74	0.51
2:H:138:ILE:HB	2:H:143:ARG:HD2	1.93	0.51
3:D:528:THR:HG22	3:D:551:ARG:HB2	1.92	0.51
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.92	0.51
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.92	0.51
2:H:963:GLU:O	2:H:967:LEU:HD13	2.11	0.51
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.75	0.51
2:C:728:ASP:OD2	2:C:729:ALA:N	2.43	0.51
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.91	0.51
1:B:33:ARG:NE	1:B:197:ASP:HB2	2.26	0.51
3:D:63:GLY:O	3:D:98:ARG:NH2	2.42	0.51
3:D:474:LEU:HD13	3:D:478:LEU:HD13	1.93	0.51
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.92	0.51
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	1.92	0.51
3:D:179:LYS:H	3:D:179:LYS:HD3	1.76	0.51
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.30	0.51
2:H:844:LYS:NZ	2:H:844:LYS:HB2	2.25	0.51
3:I:473:THR:HB	3:I:476:ALA:HB2	1.93	0.51
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.45	0.51
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.11	0.51
5:Y:519:LEU:O	5:Y:519:LEU:HD13	2.11	0.51
1:B:77:ASP:O	1:B:81:ILE:HG13	2.10	0.51
2:C:681:MET:O	2:C:685:MET:HG2	2.10	0.51
2:H:516:ASP:OD2	2:H:518:ASN:ND2	2.44	0.51
3:I:1261:LEU:CD2	3:I:1306:LEU:HD22	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:316:ILE:HG13	3:D:317:THR:N	2.26	0.51
1:A:80:GLU:HB2	2:C:694:ARG:NH2	2.24	0.51
1:B:41:ASN:ND2	2:C:1217:THR:HG22	2.25	0.51
5:X:384:LEU:HD13	5:X:384:LEU:O	2.10	0.51
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.11	0.51
3:I:325:LYS:HD3	5:Y:508:GLU:OE1	2.11	0.51
3:D:139:LEU:HD21	3:D:185:ILE:HD13	1.92	0.51
2:C:894:GLN:O	2:C:895:LEU:HB2	2.09	0.51
3:D:33:TRP:HB3	3:D:102:MET:HG3	1.91	0.51
1:F:118:ASP:OD1	1:F:119:GLY:N	2.44	0.51
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.92	0.51
3:D:1360:GLY:HA2	4:E:17:PHE:CZ	2.46	0.51
5:Y:283:GLN:CD	5:Y:343:LYS:HD2	2.31	0.51
2:C:1141:LEU:H	2:C:1141:LEU:HD13	1.76	0.51
2:C:946:LEU:O	2:C:949:GLU:HG3	2.10	0.51
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.93	0.51
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	1.92	0.51
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.09	0.51
2:C:12:ARG:O	2:C:13:LYS:HG2	2.11	0.50
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.46	0.50
3:I:910:ASN:HB3	4:J:15:ASN:OD1	2.11	0.50
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.11	0.50
5:X:600:HIS:H	5:X:601:PRO:HD2	1.75	0.50
2:H:989:LEU:HG	2:H:990:ASP:H	1.76	0.50
5:Y:445:ASP:N	5:Y:445:ASP:OD1	2.42	0.50
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.47	0.50
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.93	0.50
2:C:1288:GLN:CA	2:C:1288:GLN:HE21	2.24	0.50
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.11	0.50
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.93	0.50
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.46	0.50
1:A:250:ASP:HB3	1:A:253:LEU:HD13	1.93	0.50
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.93	0.50
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.12	0.50
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.46	0.50
3:I:546:ALA:N	3:I:547:ARG:CA	2.71	0.50
1:A:11:PRO:HD3	1:B:227:GLN:HG3	1.93	0.50
1:F:11:PRO:HG2	1:G:228:LEU:H	1.76	0.50
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.92	0.50
3:I:1280:VAL:HA	3:I:1283:SER:HB2	1.94	0.50
2:H:1252:SER:HA	5:Y:524:GLU:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.93	0.50
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.75	0.50
1:G:176:CYS:O	1:G:178:SER:N	2.42	0.50
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.11	0.50
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.47	0.50
1:A:104:LYS:HD3	1:A:105:SER:N	2.26	0.50
4:J:13:ILE:HD11	4:J:19:LEU:HD23	1.94	0.50
2:C:818:VAL:HG22	2:C:819:SER:H	1.75	0.50
2:H:590:PRO:O	2:H:659:GLN:NE2	2.45	0.50
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.94	0.50
3:D:546:ALA:N	3:D:547:ARG:CA	2.70	0.50
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.46	0.50
1:A:134:THR:HG21	2:C:727:VAL:O	2.12	0.50
1:B:118:ASP:OD1	1:B:119:GLY:N	2.44	0.50
2:C:639:LYS:HA	2:C:639:LYS:HE2	1.93	0.50
2:H:442:VAL:HG12	2:H:443:ASP:H	1.77	0.50
2:C:989:LEU:HG	2:C:990:ASP:H	1.76	0.50
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.94	0.50
3:I:504:GLN:HA	3:I:730:ALA:HA	1.92	0.50
3:I:1343:GLU:HA	3:I:1344:LEU:CB	2.38	0.50
5:X:457:ILE:HG23	5:X:461:ASN:HD21	1.77	0.50
1:B:9:LEU:H	1:B:9:LEU:HD23	1.77	0.50
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.94	0.50
2:C:1219:GLU:OE2	3:D:634:ARG:NH1	2.44	0.50
2:C:1086:PRO:HG2	2:C:1094:VAL:HG21	1.94	0.50
3:D:858:VAL:HB	3:D:859:PRO:CD	2.35	0.50
1:A:231:PHE:HZ	1:B:39:LEU:HD13	1.77	0.50
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.77	0.50
3:I:128:LEU:HD13	3:I:189:LEU:HD23	1.94	0.50
2:H:106:GLU:H	2:H:107:ARG:HA	1.77	0.50
3:I:50:LYS:HZ3	3:I:50:LYS:HB3	1.77	0.50
3:D:393:THR:HG23	3:D:396:ALA:H	1.77	0.50
1:A:226:GLU:HB3	1:B:10:LYS:NZ	2.27	0.50
1:B:19:VAL:O	1:B:20:SER:HB3	2.12	0.50
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.12	0.50
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.46	0.50
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.38	0.50
2:H:38:PHE:CE2	2:H:49:LEU:HD12	2.38	0.50
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.94	0.50
3:I:573:THR:HG22	3:I:576:ARG:CG	2.42	0.50
3:I:1266:ILE:HG13	3:I:1274:PHE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:CYS:O	1:B:178:SER:N	2.40	0.50
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.27	0.50
1:F:60:GLU:HG3	1:F:169:GLY:O	2.11	0.50
2:C:406:ASN:HB3	2:C:411:ARG:HB2	1.93	0.50
2:H:818:VAL:HG22	2:H:819:SER:H	1.76	0.50
3:D:610:ARG:CG	3:D:864:LEU:HD13	2.32	0.50
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.36	0.50
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.36	0.50
4:E:15:ASN:ND2	4:E:18:ASP:OD1	2.42	0.50
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.92	0.50
3:D:62:PHE:O	3:D:101:ARG:HG3	2.12	0.50
2:H:892:GLU:O	2:H:893:THR:OG1	2.25	0.50
1:G:16:ILE:HG12	1:G:26:VAL:HG22	1.93	0.50
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.12	0.50
2:C:163:LYS:HD3	2:C:163:LYS:N	2.16	0.50
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.11	0.50
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.41	0.50
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.94	0.50
3:I:918:ILE:HD13	3:I:919:ALA:N	2.27	0.50
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.94	0.50
3:I:843:VAL:HG11	3:I:897:HIS:HB3	1.94	0.50
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.26	0.50
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.12	0.50
2:C:820:GLU:HB2	2:C:1081:PRO:HA	1.94	0.49
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.42	0.49
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.94	0.49
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.94	0.49
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.46	0.49
2:C:741:MET:SD	2:C:741:MET:N	2.85	0.49
2:C:836:LEU:HB3	2:C:918:LEU:HD21	1.93	0.49
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.94	0.49
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.94	0.49
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.93	0.49
5:Y:279:ARG:NH2	5:Y:350:GLU:OE1	2.43	0.49
3:I:504:GLN:HG3	3:I:505:ASP:H	1.78	0.49
2:H:12:ARG:O	2:H:13:LYS:HG2	2.12	0.49
2:H:131:THR:HG22	2:H:135:THR:HG22	1.93	0.49
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.42	0.49
3:D:452:LEU:HG	3:D:625:MET:SD	2.52	0.49
3:D:932:MET:SD	3:D:932:MET:N	2.75	0.49
2:H:637:ARG:HE	3:I:770:LEU:HD23	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:660:GLU:O	3:I:664:ILE:HG12	2.12	0.49
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.93	0.49
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.77	0.49
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.94	0.49
3:D:33:TRP:O	3:D:102:MET:HB2	2.11	0.49
2:H:944:ARG:HD3	2:H:944:ARG:O	2.11	0.49
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.12	0.49
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.11	0.49
5:Y:278:ASP:OD1	5:Y:281:ARG:NH2	2.45	0.49
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.12	0.49
3:I:166:LEU:HD12	3:I:167:ASP:N	2.26	0.49
2:C:697:LYS:HZ3	2:C:791:LEU:HD11	1.77	0.49
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.38	0.49
2:C:27:LEU:O	2:C:528:ARG:NH1	2.44	0.49
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.95	0.49
3:I:1171:GLY:N	3:I:1172:LYS:O	2.45	0.49
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.94	0.49
1:B:22:THR:HG22	1:B:208:ASN:O	2.12	0.49
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.12	0.49
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.42	0.49
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.42	0.49
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.93	0.49
2:H:119:GLU:HG2	2:H:120:GLN:N	2.27	0.49
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.12	0.49
4:E:5:THR:CA	4:E:6:VAL:CB	2.86	0.49
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.93	0.49
1:A:243:LYS:HD3	1:A:243:LYS:N	2.28	0.49
3:I:552:ILE:HD13	3:I:570:LYS:HB2	1.94	0.49
3:I:648:GLU:N	3:I:648:GLU:OE2	2.45	0.49
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.78	0.49
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.27	0.49
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.45	0.49
2:H:384:LEU:O	2:H:388:LEU:HG	2.11	0.49
2:H:678:ARG:HD3	2:H:681:MET:HG3	1.94	0.49
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.95	0.49
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.36	0.49
2:C:96:LEU:HD22	2:C:127:ILE:HD12	1.94	0.49
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	1.95	0.49
2:C:1303:LYS:HA	2:C:1303:LYS:HE2	1.93	0.49
4:J:60:ASN:H	4:J:63:ILE:HB	1.77	0.49
2:C:402:ARG:NH2	2:C:419:ILE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ILE:O	1:A:307:LEU:HD13	2.11	0.49
3:I:152:THR:O	3:I:154:LEU:N	2.42	0.49
2:C:442:VAL:HG12	2:C:443:ASP:H	1.77	0.49
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.19	0.49
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.40	0.49
3:I:664:ILE:HD12	3:I:681:LYS:HE3	1.93	0.49
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.93	0.49
3:D:888:CYS:SG	3:D:890:THR:HB	2.53	0.49
5:X:400:GLN:O	5:X:404:LEU:HD13	2.12	0.49
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.93	0.49
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.28	0.49
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.27	0.49
2:H:639:LYS:HE2	2:H:639:LYS:HA	1.93	0.49
3:D:646:ILE:HD12	3:D:646:ILE:O	2.12	0.49
4:J:65:ASP:O	4:J:69:ARG:HG3	2.13	0.49
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.28	0.49
2:H:24:VAL:HG11	2:H:704:MET:HE1	1.94	0.49
5:X:143:TYR:O	5:X:147:GLN:HG2	2.13	0.49
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.45	0.49
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.95	0.49
2:H:1332:SER:O	3:I:243:PRO:HG2	2.12	0.49
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.94	0.49
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.94	0.49
3:D:797:THR:O	3:D:801:VAL:HG23	2.13	0.49
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.12	0.49
1:G:9:LEU:HD23	1:G:9:LEU:H	1.78	0.49
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.95	0.49
2:C:179:TYR:HE2	2:C:462:ASN:HD21	1.61	0.49
3:D:392:THR:HG22	5:X:603:ARG:HG2	1.94	0.49
5:Y:561:MET:HA	5:Y:567:MET:SD	2.53	0.49
4:J:5:THR:HB	4:J:7:GLN:H	1.78	0.49
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.47	0.49
2:C:127:ILE:HD13	2:C:127:ILE:N	2.27	0.49
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.48	0.49
3:D:608:CYS:O	3:D:612:LEU:HB2	2.13	0.49
3:D:648:GLU:N	3:D:648:GLU:OE2	2.45	0.49
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.47	0.49
3:D:856:ILE:HG13	3:D:857:LEU:O	2.12	0.49
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.48	0.49
2:H:524:ILE:HD12	2:H:708:VAL:HG13	1.93	0.49
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:516:ASP:OD1	2:C:518:ASN:ND2	2.45	0.49
2:C:384:LEU:O	2:C:388:LEU:HG	2.11	0.49
4:J:5:THR:HB	4:J:7:GLN:HB2	1.94	0.49
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.93	0.49
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.12	0.49
5:X:301:ASN:O	5:X:305:LEU:HD13	2.13	0.49
3:D:589:TYR:O	3:D:591:ILE:HG13	2.13	0.49
3:D:591:ILE:HD12	3:D:592:VAL:N	2.28	0.49
3:D:394:ILE:HG21	5:X:536:THR:HA	1.94	0.49
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.93	0.49
3:I:316:ILE:N	3:I:316:ILE:HD13	2.28	0.49
3:I:482:ALA:C	3:I:483:LEU:HD12	2.34	0.49
5:Y:400:GLN:O	5:Y:404:LEU:HD13	2.12	0.49
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.95	0.48
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	1.95	0.48
5:X:600:HIS:H	5:X:601:PRO:CD	2.26	0.48
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.94	0.48
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.78	0.48
3:D:515:ARG:HH22	3:D:717:VAL:C	2.16	0.48
3:I:810:THR:OG1	3:I:811:GLU:N	2.44	0.48
2:C:1119:MET:O	2:C:1123:GLY:N	2.43	0.48
5:Y:582:VAL:CB	5:Y:586:ARG:HG2	2.43	0.48
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.95	0.48
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.47	0.48
5:X:119:ILE:O	5:X:123:ILE:HG13	2.13	0.48
2:H:489:PRO:HB2	2:H:492:MET:CB	2.39	0.48
2:H:36:GLN:O	2:H:39:ILE:HG22	2.13	0.48
3:D:316:ILE:HD11	3:D:320:ASN:O	2.13	0.48
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.43	0.48
3:I:807:LEU:O	3:I:807:LEU:HD12	2.12	0.48
3:I:393:THR:HG23	3:I:396:ALA:H	1.78	0.48
3:I:197:GLU:O	3:I:201:LEU:HD23	2.12	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.12	0.48
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.43	0.48
5:X:310:GLU:O	5:X:344:LEU:HD23	2.14	0.48
2:H:1284:ALA:HB3	3:I:1361:THR:HB	1.94	0.48
3:I:363:LEU:O	3:I:363:LEU:HD23	2.13	0.48
3:D:166:LEU:HD12	3:D:167:ASP:N	2.28	0.48
2:C:106:GLU:HG2	2:C:109:ALA:H	1.78	0.48
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	1.95	0.48
2:H:756:TYR:H	2:H:766:ASN:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:THR:HG22	2:C:139:ASN:N	2.29	0.48
2:C:72:SER:O	2:C:98:VAL:HG23	2.13	0.48
3:I:161:THR:HG22	3:I:162:GLU:H	1.78	0.48
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.14	0.48
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.40	0.48
2:H:38:PHE:O	2:H:39:ILE:HB	2.12	0.48
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.46	0.48
5:X:28:ASN:HD22	5:X:29:ASP:N	2.11	0.48
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.48	0.48
2:H:149:LEU:HD12	2:H:452:ARG:O	2.13	0.48
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.44	0.48
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.27	0.48
1:B:107:ILE:HD11	1:B:136:GLU:HG2	1.95	0.48
1:A:207:THR:OG1	1:A:208:ASN:N	2.47	0.48
3:D:873:GLU:OE2	3:D:877:VAL:HB	2.13	0.48
5:X:493:LYS:O	5:X:497:VAL:HG23	2.13	0.48
3:I:1255:VAL:O	3:I:1258:ARG:HB3	2.12	0.48
2:H:808:ASN:H	3:I:633:ALA:HB2	1.78	0.48
5:X:390:ILE:HD11	5:X:435:ILE:CG2	2.41	0.48
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.49	0.48
2:C:844:LYS:NZ	2:C:844:LYS:HB2	2.28	0.48
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.44	0.48
3:I:245:LEU:O	3:I:250:ARG:NH1	2.45	0.48
3:I:56:LEU:HB3	3:I:250:ARG:NH2	2.28	0.48
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.14	0.48
1:G:196:THR:OG1	3:I:443:GLU:HG3	2.14	0.48
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.44	0.48
1:A:241:GLU:OE2	1:A:243:LYS:HE3	2.14	0.48
3:I:646:ILE:HD12	3:I:646:ILE:O	2.13	0.48
3:D:807:LEU:O	3:D:807:LEU:HD12	2.13	0.48
3:I:579:LEU:HD13	3:I:579:LEU:O	2.14	0.48
5:Y:437:GLN:HA	5:Y:440:THR:HG22	1.94	0.48
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.44	0.48
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.96	0.48
2:H:660:VAL:HG22	2:H:661:VAL:N	2.25	0.48
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.13	0.48
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.49	0.48
2:C:891:GLY:O	2:C:893:THR:HG23	2.14	0.48
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.49	0.48
3:I:513:MET:HE2	3:I:579:LEU:HB2	1.96	0.48
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.96	0.48
2:H:707:ALA:O	2:H:710:VAL:HG12	2.13	0.48
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.48	0.48
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.95	0.48
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.48	0.48
3:I:513:MET:O	3:I:575:GLY:HA3	2.14	0.48
2:C:1286:THR:N	3:D:479:GLU:OE2	2.45	0.48
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.78	0.48
1:G:33:ARG:HE	1:G:197:ASP:HB2	1.78	0.48
3:D:843:VAL:HG12	3:D:883:ARG:HD3	1.96	0.48
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.47	0.48
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	1.96	0.48
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.96	0.48
1:B:18:GLN:C	1:B:20:SER:H	2.17	0.48
2:H:932:GLN:HE22	2:H:952:GLN:HE22	1.62	0.48
4:J:45:LYS:O	4:J:49:ILE:HG12	2.13	0.48
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.13	0.48
3:D:778:GLY:HA2	3:D:781:LYS:HE3	1.96	0.48
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.96	0.48
2:H:163:LYS:CD	2:H:163:LYS:H	2.22	0.48
5:X:27:VAL:HA	5:X:30:HIS:HD2	1.78	0.48
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.29	0.48
2:H:1335:ILE:HD11	3:I:22:ILE:CG1	2.44	0.48
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.14	0.48
2:H:1339:LEU:N	2:H:1339:LEU:HD12	2.28	0.48
2:C:31:GLN:HG3	2:C:130:MET:HE1	1.94	0.48
2:H:73:TYR:HD2	2:H:74:ARG:H	1.58	0.48
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.95	0.48
1:A:192:VAL:O	1:A:194:GLN:N	2.46	0.48
3:I:349:TYR:CD1	3:I:472:LEU:HD11	2.47	0.47
2:H:766:ASN:H	2:H:787:PRO:HG3	1.79	0.47
2:H:152:SER:OG	2:H:404:LYS:NZ	2.24	0.47
3:I:41:PRO:HG3	3:I:273:ILE:HG22	1.96	0.47
5:X:24:TYR:O	5:X:26:GLU:N	2.45	0.47
3:D:840:LEU:O	3:D:840:LEU:HD12	2.14	0.47
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.96	0.47
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.96	0.47
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.96	0.47
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.49	0.47
2:H:908:GLU:HG2	2:H:909:LYS:N	2.22	0.47
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.96	0.47
2:C:843:THR:HB	2:C:845:LEU:HD22	1.96	0.47
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.14	0.47
3:D:919:ALA:O	3:D:923:ILE:HG12	2.14	0.47
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.14	0.47
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.94	0.47
5:Y:545:HIS:NE2	5:Y:566:ASP:OD2	2.35	0.47
5:X:130:VAL:O	5:X:134:VAL:HG23	2.14	0.47
3:D:613:GLY:O	3:D:617:THR:OG1	2.24	0.47
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.50	0.47
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.30	0.47
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.43	0.47
2:H:1117:LEU:HD21	2:H:1182:ILE:HG21	1.96	0.47
1:B:47:LEU:HD13	1:B:205:MET:HE2	1.96	0.47
3:D:161:THR:HG22	3:D:162:GLU:H	1.78	0.47
5:X:141:ILE:HG13	5:X:256:PHE:CD1	2.50	0.47
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.15	0.47
1:G:192:VAL:CG1	1:G:194:GLN:HG2	2.44	0.47
3:D:316:ILE:O	3:D:317:THR:OG1	2.28	0.47
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.95	0.47
3:I:450:HIS:NE2	3:I:625:MET:SD	2.87	0.47
2:C:1058:ARG:HD3	2:C:1240:ASP:OD1	2.14	0.47
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.45	0.47
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.30	0.47
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.27	0.47
2:H:898:GLU:N	2:H:898:GLU:OE1	2.38	0.47
2:H:1120:ALA:HB1	2:H:1198:LEU:HB3	1.96	0.47
2:H:706:ARG:HA	2:H:793:GLU:HA	1.96	0.47
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.97	0.47
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.14	0.47
2:H:702:THR:HA	2:H:1184:THR:O	2.14	0.47
2:H:17:LYS:NZ	2:H:1194:GLU:OE1	2.42	0.47
2:C:1106:ARG:O	2:C:1108:ASN:N	2.43	0.47
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.44	0.47
1:G:191:ARG:HH22	3:I:442:ILE:HA	1.80	0.47
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.96	0.47
3:I:608:CYS:O	3:I:612:LEU:HB2	2.14	0.47
3:I:316:ILE:H	3:I:316:ILE:HD13	1.79	0.47
3:I:840:LEU:HD12	3:I:840:LEU:O	2.14	0.47
2:C:839:VAL:HG13	2:C:1049:ILE:HG22	1.96	0.47
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.49	0.47
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.43	0.47
1:G:191:ARG:NH2	3:I:442:ILE:HA	2.30	0.47
3:D:789:LYS:HD2	3:D:932:MET:SD	2.54	0.47
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.95	0.47
2:H:634:VAL:H	2:H:645:PHE:HE2	1.62	0.47
3:I:811:GLU:OE2	3:I:890:THR:OG1	2.28	0.47
2:H:841:ARG:NH1	3:I:256:ASP:HB3	2.28	0.47
3:D:504:GLN:HG3	3:D:505:ASP:H	1.80	0.47
2:C:59:ILE:HD11	2:C:63:SER:OG	2.15	0.47
3:I:1196:LEU:HG	3:I:1210:ILE:HD11	1.95	0.47
2:C:403:MET:HG2	2:C:407:ARG:HH12	1.80	0.47
3:D:1292:LEU:HD21	3:I:1284:ARG:NH2	2.29	0.47
3:I:1287:ILE:HA	3:I:1290:ARG:HG2	1.97	0.47
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.45	0.47
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.96	0.47
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.15	0.47
3:I:591:ILE:HD12	3:I:592:VAL:N	2.28	0.47
5:X:595:LEU:O	5:X:599:ARG:NH1	2.46	0.47
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.30	0.47
3:I:290:ILE:O	3:I:293:ARG:HG3	2.15	0.47
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.96	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.65	0.47
3:D:482:ALA:C	3:D:483:LEU:HD12	2.34	0.47
3:D:133:ARG:NH2	3:D:133:ARG:HB2	2.30	0.47
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.14	0.47
2:C:963:GLU:O	2:C:966:ILE:HG22	2.15	0.47
2:C:510:GLN:O	2:C:511:LEU:HB2	2.15	0.47
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.95	0.47
2:C:119:GLU:HG2	2:C:120:GLN:N	2.29	0.47
1:G:31:LEU:HB2	1:G:199:ASP:O	2.15	0.47
2:H:263:VAL:HG22	2:H:273:HIS:CD2	2.49	0.47
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.80	0.47
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.97	0.47
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.96	0.47
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.44	0.47
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.28	0.47
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.78	0.47
3:I:370:LYS:HA	3:I:441:LEU:HD12	1.97	0.47
2:H:106:GLU:HG2	2:H:109:ALA:H	1.78	0.47
2:C:533:LEU:H	2:C:533:LEU:HD23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:552:ILE:HD13	3:D:570:LYS:HB2	1.97	0.47
2:C:205:PRO:O	2:C:208:ILE:HG22	2.15	0.47
2:H:130:MET:SD	2:H:134:GLY:HA2	2.54	0.47
2:C:751:TYR:HE1	2:C:783:LEU:HD12	1.79	0.47
1:A:42:ALA:O	1:A:46:ILE:HG12	2.14	0.47
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.14	0.47
3:D:832:LYS:HA	3:D:832:LYS:HZ1	1.79	0.47
2:C:127:ILE:HG22	2:C:502:VAL:HG11	1.97	0.47
3:I:120:LEU:CB	3:I:121:PRO:CD	2.90	0.47
5:X:452:ILE:HG21	5:X:457:ILE:HG12	1.97	0.47
2:H:669:PRO:HG2	2:H:1070:HIS:CE1	2.49	0.47
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.45	0.47
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.79	0.47
2:C:893:THR:O	2:C:895:LEU:N	2.40	0.47
5:X:346:GLN:O	5:X:350:GLU:HG3	2.15	0.47
5:X:545:HIS:NE2	5:X:566:ASP:OD2	2.48	0.47
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.38	0.47
3:I:227:PHE:O	3:I:230:SER:OG	2.25	0.47
1:F:45:ARG:NE	1:G:38:THR:OG1	2.49	0.47
3:D:41:PRO:HG3	3:D:273:ILE:HG22	1.96	0.47
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.80	0.47
3:D:660:GLU:O	3:D:664:ILE:HG12	2.15	0.47
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.35	0.47
5:X:115:GLY:O	5:X:119:ILE:HG12	2.15	0.47
3:I:8:LEU:N	3:I:8:LEU:HD23	2.30	0.47
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.97	0.47
2:H:356:THR:HG21	2:H:362:ALA:HA	1.96	0.47
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.41	0.46
3:D:56:LEU:HB3	3:D:250:ARG:HH21	1.80	0.46
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.81	0.46
2:C:756:TYR:H	2:C:766:ASN:CB	2.28	0.46
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.15	0.46
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.45	0.46
2:H:895:LEU:HD21	2:H:903:ARG:CZ	2.45	0.46
2:C:829:THR:HG22	2:C:1059:ARG:HG2	1.98	0.46
2:H:317:LEU:HD13	2:H:322:LEU:HD21	1.97	0.46
2:H:975:ILE:HD13	2:H:975:ILE:O	2.14	0.46
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.30	0.46
2:C:886:LYS:HD3	2:C:916:SER:O	2.15	0.46
2:C:434:ASP:HB3	2:C:439:LYS:HB2	1.97	0.46
2:C:53:PHE:HD1	2:C:57:PHE:CD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:511:ILE:HG23	5:X:512:GLY:N	2.28	0.46
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.45	0.46
2:C:487:LEU:CD1	2:C:488:MET:H	2.28	0.46
2:C:590:PRO:O	2:C:659:GLN:NE2	2.47	0.46
2:H:11:ILE:HG21	2:H:697:LYS:HZ2	1.80	0.46
2:H:555:TYR:OH	2:H:637:ARG:NH2	2.48	0.46
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.45	0.46
2:C:342:ASP:O	2:C:437:ASN:ND2	2.48	0.46
3:D:396:ALA:CB	5:X:606:VAL:HG11	2.46	0.46
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.27	0.46
3:D:8:LEU:HD23	3:D:8:LEU:N	2.30	0.46
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.98	0.46
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	1.97	0.46
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.96	0.46
3:D:227:PHE:O	3:D:230:SER:OG	2.26	0.46
2:C:1315:MET:HE2	3:D:473:THR:OG1	2.16	0.46
1:F:79:LEU:HD12	2:H:756:TYR:OH	2.16	0.46
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.15	0.46
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.96	0.46
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.97	0.46
3:I:797:THR:O	3:I:801:VAL:HG23	2.15	0.46
3:D:415:VAL:HG23	3:D:416:ILE:HG23	1.97	0.46
3:I:12:THR:O	3:I:13:LYS:HD2	2.15	0.46
3:D:240:THR:HG23	3:D:241:VAL:HG23	1.97	0.46
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.98	0.46
2:C:697:LYS:HG3	2:C:698:PRO:HD2	1.98	0.46
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.96	0.46
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.80	0.46
3:I:822:MET:HG2	3:I:839:VAL:HG22	1.96	0.46
3:D:27:PRO:O	3:D:31:ARG:HD3	2.15	0.46
5:X:556:ALA:O	5:X:560:ARG:HB2	2.16	0.46
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.14	0.46
1:A:243:LYS:HZ2	1:A:243:LYS:HB2	1.79	0.46
3:D:733:SER:O	3:D:737:ILE:HG12	2.15	0.46
5:X:271:ASN:O	5:X:275:VAL:HG23	2.14	0.46
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.15	0.46
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.75	0.46
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.15	0.46
3:D:850:LYS:HD2	3:D:851:PRO:CD	2.37	0.46
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.30	0.46
1:F:80:GLU:HA	2:H:694:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.46	0.46
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.28	0.46
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.49	0.46
5:X:379:MET:CE	5:X:379:MET:HA	2.46	0.46
3:I:1357:ILE:H	3:I:1357:ILE:HD12	1.80	0.46
4:J:3:ARG:NH2	4:J:44:ASP:OD2	2.49	0.46
2:H:178:PRO:HA	2:H:397:LEU:HD23	1.97	0.46
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	1.97	0.46
5:Y:105:MET:SD	5:Y:388:ILE:HD12	2.55	0.46
2:C:622:ASN:OD1	2:C:623:LEU:N	2.49	0.46
1:G:76:GLU:OE2	1:G:131:CYS:HA	2.16	0.46
5:Y:303:ILE:O	5:Y:307:THR:OG1	2.30	0.46
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.98	0.46
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.96	0.46
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.36	0.46
5:Y:608:ARG:HB3	5:Y:608:ARG:NH1	2.31	0.46
3:D:378:LYS:HD2	3:D:382:TYR:OH	2.14	0.46
2:H:1042:LEU:N	2:H:1042:LEU:HD13	2.27	0.46
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.45	0.46
3:D:514:THR:HG21	3:D:595:ALA:O	2.14	0.46
2:H:1142:ARG:HE	2:H:1169:VAL:HB	1.80	0.46
3:D:550:VAL:HG23	3:D:552:ILE:HD11	1.96	0.46
2:H:998:LEU:O	2:H:998:LEU:HD13	2.15	0.46
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.51	0.46
4:J:26:ARG:HD3	4:J:64:LEU:HD21	1.98	0.46
2:H:517:GLN:HE21	2:H:760:ASN:H	1.64	0.46
2:C:216:THR:O	2:C:220:ILE:HG13	2.15	0.46
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.48	0.46
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.30	0.46
2:H:902:LEU:HD11	5:Y:608:ARG:HA	1.97	0.46
1:G:227:GLN:C	1:G:228:LEU:HD23	2.36	0.46
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.16	0.46
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.26	0.46
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.98	0.46
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.97	0.46
3:I:154:LEU:HD21	3:I:160:LEU:HD21	1.98	0.46
2:H:1297:ASP:OD1	2:H:1300:GLY:HA3	2.16	0.46
3:I:856:ILE:HG13	3:I:857:LEU:O	2.14	0.46
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.98	0.46
3:I:1221:LEU:HD23	3:I:1229:VAL:HG11	1.97	0.46
2:C:131:THR:HG22	2:C:135:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1211:ARG:HB2	2:C:1220:GLN:HE21	1.80	0.46
3:I:245:LEU:CD1	3:I:246:PRO:HD2	2.45	0.46
3:D:233:LYS:CD	3:D:234:PRO:HD2	2.46	0.46
3:D:393:THR:HG21	5:X:607:LEU:HD22	1.97	0.46
2:C:682:GLY:HA2	2:C:685:MET:HG2	1.97	0.46
2:C:1335:ILE:HD11	3:D:22:ILE:HG13	1.98	0.46
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.15	0.46
3:I:33:TRP:O	3:I:102:MET:HB2	2.16	0.46
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.96	0.46
5:X:373:ARG:HG3	5:X:377:LYS:HE3	1.97	0.46
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.37	0.46
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.35	0.46
2:C:372:PRO:CB	5:X:34:ASP:HB3	2.45	0.46
1:B:178:SER:HA	1:B:179:PRO:HD3	1.85	0.46
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.97	0.46
1:G:110:VAL:HG11	1:G:140:ILE:HD11	1.98	0.46
1:B:31:LEU:HB2	1:B:199:ASP:O	2.16	0.46
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.46	0.46
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.16	0.46
1:G:191:ARG:NH2	3:I:441:LEU:O	2.49	0.46
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.51	0.46
3:D:66:LYS:HB2	3:D:69:GLU:HG2	1.97	0.46
2:C:966:ILE:HG23	2:C:967:LEU:HD12	1.98	0.46
3:D:416:ILE:O	3:D:416:ILE:HD12	2.16	0.46
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.15	0.46
3:D:114:ILE:HG21	3:D:308:ASP:HB3	1.98	0.46
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.97	0.46
2:H:1296:ASP:OD1	3:I:345:LYS:HD2	2.15	0.46
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.98	0.45
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.30	0.45
3:I:508:LEU:HD23	3:I:508:LEU:O	2.16	0.45
3:D:720:ASN:ND2	3:D:720:ASN:O	2.49	0.45
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.46	0.45
4:E:4:VAL:O	4:E:5:THR:OG1	2.20	0.45
3:I:909:ILE:O	3:I:909:ILE:HD12	2.16	0.45
1:F:10:LYS:HD2	1:G:226:GLU:O	2.16	0.45
1:A:88:LEU:HD22	1:A:90:VAL:HG23	1.98	0.45
2:H:127:ILE:N	2:H:127:ILE:HD13	2.28	0.45
3:D:572:THR:HG22	3:D:594:GLN:OE1	2.16	0.45
5:X:101:TYR:OH	5:X:384:LEU:HD11	2.16	0.45
2:C:876:GLU:N	2:C:876:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.80	0.45
3:D:809:VAL:HG13	3:D:912:GLY:H	1.80	0.45
5:X:437:GLN:HA	5:X:440:THR:HG22	1.97	0.45
1:B:16:ILE:HG12	1:B:26:VAL:HG22	1.97	0.45
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.97	0.45
3:I:1148:ARG:HB2	3:I:1148:ARG:NH2	2.32	0.45
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.81	0.45
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.98	0.45
3:D:767:LEU:HB3	3:D:771:GLN:NE2	2.31	0.45
2:H:21:VAL:HG13	2:H:22:LEU:N	2.30	0.45
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.79	0.45
5:Y:379:MET:HE2	5:Y:379:MET:HA	1.97	0.45
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	1.99	0.45
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.49	0.45
1:A:222:THR:O	1:A:226:GLU:HG3	2.17	0.45
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.46	0.45
2:H:893:THR:O	2:H:895:LEU:N	2.45	0.45
3:I:113:HIS:CE1	3:I:115:TRP:HB2	2.51	0.45
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.16	0.45
3:I:430:HIS:HA	3:I:921:GLN:HB3	1.97	0.45
1:A:5:VAL:O	1:A:6:THR:OG1	2.32	0.45
3:I:813:ASP:OD1	3:I:896:ALA:HB3	2.16	0.45
3:D:504:GLN:HA	3:D:730:ALA:HA	1.98	0.45
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.16	0.45
3:I:640:GLY:N	3:I:643:ASP:OD2	2.45	0.45
1:B:83:LEU:HD23	3:D:551:ARG:HG3	1.96	0.45
2:C:152:SER:HA	2:C:153:PRO:HD3	1.87	0.45
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.47	0.45
2:C:462:ASN:O	2:C:466:VAL:HG23	2.17	0.45
3:I:1251:LYS:O	3:I:1255:VAL:HG23	2.16	0.45
2:C:963:GLU:O	2:C:967:LEU:HD13	2.16	0.45
2:C:777:VAL:HG21	2:C:783:LEU:HD21	1.98	0.45
1:A:234:LEU:HD12	1:A:234:LEU:N	2.32	0.45
3:D:579:LEU:O	3:D:579:LEU:HD13	2.16	0.45
2:H:768:MET:O	2:H:785:ASP:N	2.47	0.45
5:X:250:LEU:O	5:X:254:GLU:HG2	2.16	0.45
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.48	0.45
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.98	0.45
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.98	0.45
3:I:524:GLY:HA2	3:I:548:VAL:HG23	1.99	0.45
2:C:43:PRO:HD3	2:C:47:TYR:HD2	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:660:VAL:HG22	2:C:661:VAL:N	2.27	0.45
3:D:655:SER:HA	3:D:658:GLU:HG2	1.96	0.45
1:F:79:LEU:O	1:F:83:LEU:HD13	2.17	0.45
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.36	0.45
4:E:44:ASP:HB2	4:E:52:ARG:HH21	1.82	0.45
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.98	0.45
2:H:73:TYR:CD2	2:H:73:TYR:N	2.85	0.45
2:H:680:LEU:HD13	3:I:783:LEU:HD12	1.98	0.45
2:C:580:GLN:HG2	2:C:581:THR:N	2.32	0.45
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.51	0.45
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.99	0.45
2:C:57:PHE:HE1	2:C:472:GLU:HA	1.80	0.45
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.16	0.45
3:D:526:VAL:HG12	3:D:549:LYS:O	2.16	0.45
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.44	0.45
3:I:51:PRO:HB3	3:I:57:PHE:O	2.16	0.45
2:H:876:GLU:N	2:H:876:GLU:OE2	2.49	0.45
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.15	0.45
3:D:915:ILE:O	3:D:918:ILE:HG23	2.17	0.45
2:H:972:PHE:HA	2:H:975:ILE:HG22	1.98	0.45
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.17	0.45
3:I:235:GLU:OE1	3:I:235:GLU:N	2.50	0.45
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.31	0.45
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.31	0.45
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.30	0.45
3:I:545:HIS:HA	3:I:546:ALA:HA	1.77	0.45
3:D:1287:ILE:HA	3:D:1290:ARG:HG2	1.98	0.45
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.32	0.45
3:D:260:PHE:O	5:X:504:PRO:HG2	2.16	0.45
2:H:1116:HIS:CE1	2:H:1226:THR:HG23	2.50	0.45
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.32	0.45
2:C:998:LEU:O	2:C:998:LEU:HD13	2.17	0.45
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.81	0.45
1:F:151:GLY:O	1:F:177:TYR:HB2	2.17	0.45
2:C:465:ARG:O	2:C:469:VAL:HG23	2.16	0.45
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.65	0.45
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.56	0.45
1:A:33:ARG:HG2	1:A:199:ASP:OD2	2.16	0.45
2:C:812:PHE:H	2:C:815:SER:HB2	1.81	0.45
2:H:908:GLU:CD	2:H:908:GLU:H	2.20	0.45
3:I:205:LEU:HB3	3:I:217:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.97	0.45
5:X:139:GLU:HG3	5:X:351:THR:HA	1.98	0.45
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.99	0.45
2:H:714:VAL:HG23	2:H:787:PRO:HD2	1.98	0.45
1:F:158:ARG:HE	1:F:172:LEU:HD13	1.81	0.45
2:H:818:VAL:HG22	2:H:819:SER:N	2.32	0.45
2:H:1006:GLU:H	2:H:1006:GLU:CD	2.20	0.45
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.97	0.45
5:Y:439:ILE:O	5:Y:443:ILE:HG13	2.15	0.45
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.17	0.45
1:F:166:ARG:HA	1:F:167:PRO:HD2	1.87	0.45
3:D:531:LYS:NZ	3:D:531:LYS:HB3	2.32	0.45
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.38	0.45
3:I:610:ARG:HG2	3:I:864:LEU:HD22	1.98	0.45
2:H:135:THR:OG1	2:H:143:ARG:O	2.29	0.45
2:H:1294:LYS:HE3	3:I:349:TYR:HB2	1.99	0.45
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.80	0.45
3:D:766:GLY:C	3:D:767:LEU:HD22	2.37	0.45
3:I:326:SER:O	3:I:330:MET:HG3	2.16	0.45
3:D:619:ILE:HD13	7:D:1503:G4P:O3D	2.17	0.45
2:C:868:SER:OG	2:C:942:ASP:OD1	2.28	0.45
1:G:47:LEU:HD13	1:G:205:MET:HE2	1.99	0.45
2:H:622:ASN:OD1	2:H:623:LEU:N	2.50	0.45
3:D:640:GLY:N	3:D:643:ASP:OD2	2.50	0.45
2:C:556:GLY:O	2:C:579:ALA:HB2	2.16	0.45
2:C:845:LEU:N	2:C:845:LEU:HD13	2.28	0.45
5:X:101:TYR:CE2	5:X:388:ILE:HD11	2.45	0.45
3:D:473:THR:HB	3:D:476:ALA:CB	2.47	0.45
3:I:325:LYS:HZ1	3:I:330:MET:HG2	1.82	0.45
5:X:120:ALA:CB	5:X:421:TYR:HB3	2.44	0.45
1:B:64:VAL:HG12	1:B:171:LEU:HD11	1.98	0.45
2:H:966:ILE:HG23	2:H:967:LEU:HD12	1.97	0.45
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.50	0.45
2:C:818:VAL:HG22	2:C:819:SER:N	2.32	0.45
5:X:123:ILE:O	5:X:127:ILE:HG12	2.17	0.45
1:B:183:ILE:HD11	1:B:205:MET:HE2	1.99	0.45
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.19	0.45
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.98	0.45
3:D:494:ALA:HA	3:D:1252:HIS:HE1	1.82	0.45
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.98	0.45
1:G:185:TYR:HA	1:G:202:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:824:PRO:O	3:D:826:ILE:HG13	2.16	0.45
3:I:1266:ILE:HA	3:I:1302:TYR:HA	1.99	0.45
1:A:317:ARG:C	1:A:318:LEU:HD13	2.37	0.45
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.99	0.45
1:G:100:LEU:HD21	1:G:121:VAL:HG21	1.98	0.45
2:C:964:LEU:HD12	2:C:1025:PHE:CG	2.52	0.45
3:D:657:ALA:HB2	3:D:689:ALA:HB2	1.99	0.45
2:H:1192:GLU:O	2:H:1196:LYS:HD3	2.17	0.45
4:E:5:THR:HB	4:E:7:GLN:N	2.29	0.44
2:H:143:ARG:NH1	2:H:512:SER:O	2.50	0.44
3:I:531:LYS:HB3	3:I:531:LYS:NZ	2.32	0.44
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.99	0.44
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.53	0.44
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.46	0.44
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.16	0.44
1:A:284:ARG:NH1	1:A:288:GLU:HG3	2.32	0.44
3:I:269:TYR:HA	3:I:272:VAL:HG12	1.99	0.44
1:G:195:ARG:HH21	1:G:198:LEU:HD21	1.81	0.44
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.99	0.44
3:I:909:ILE:H	3:I:909:ILE:HG13	1.56	0.44
3:I:860:ARG:HD3	3:I:866:GLU:OE2	2.17	0.44
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.81	0.44
2:H:946:LEU:O	2:H:949:GLU:HG3	2.16	0.44
3:I:911:LYS:O	3:I:911:LYS:HD2	2.17	0.44
2:H:1156:ARG:HH11	2:H:1157:GLN:H	1.64	0.44
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.98	0.44
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.18	0.44
1:A:53:GLY:HA3	1:A:179:PRO:HG3	1.98	0.44
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.98	0.44
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.97	0.44
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.33	0.44
3:D:217:LEU:O	3:D:221:ILE:HG12	2.16	0.44
3:I:1358:PRO:HB3	3:I:1366:HIS:CG	2.52	0.44
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.51	0.44
3:I:720:ASN:ND2	3:I:720:ASN:O	2.50	0.44
5:Y:451:ARG:O	5:Y:452:ILE:HG13	2.18	0.44
1:B:151:GLY:O	1:B:177:TYR:HB2	2.18	0.44
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.47	0.44
3:I:681:LYS:O	3:I:685:ILE:HG13	2.18	0.44
2:H:994:ARG:HD3	2:H:994:ARG:N	2.31	0.44
2:C:161:LYS:HB3	2:C:161:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.18	0.44
3:I:214:ARG:O	3:I:218:THR:HG22	2.17	0.44
5:X:277:MET:HE1	5:X:359:LYS:HE2	1.99	0.44
1:F:207:THR:HG23	1:F:209:GLY:H	1.82	0.44
2:C:702:THR:HA	2:C:1184:THR:O	2.17	0.44
2:C:813:GLU:HG2	3:D:504:GLN:NE2	2.31	0.44
3:I:221:ILE:HG13	3:I:222:LYS:N	2.33	0.44
3:I:899:TYR:CD2	3:I:909:ILE:HG12	2.53	0.44
5:Y:448:ARG:NH1	5:Y:452:ILE:HD12	2.32	0.44
3:D:252:LEU:HD23	3:D:252:LEU:N	2.32	0.44
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.16	0.44
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.33	0.44
1:A:223:ILE:HD13	1:B:8:PHE:CE1	2.52	0.44
3:D:356:THR:O	3:D:448:GLN:HA	2.17	0.44
1:F:182:ARG:NH1	2:H:1092:THR:HG22	2.33	0.44
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.31	0.44
3:D:154:LEU:HD21	3:D:160:LEU:HD21	1.99	0.44
1:G:33:ARG:NH1	2:H:820:GLU:OE2	2.51	0.44
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.80	0.44
2:H:1140:LYS:HE2	2:H:1166:ASP:HB3	1.99	0.44
5:Y:544:THR:O	5:Y:548:LEU:HG	2.17	0.44
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.38	0.44
3:I:240:THR:HG23	3:I:241:VAL:HG23	1.98	0.44
2:C:56:VAL:HB	2:C:57:PHE:H	1.51	0.44
3:D:525:MET:O	3:D:535:ARG:NH2	2.50	0.44
3:I:217:LEU:O	3:I:221:ILE:HG12	2.17	0.44
1:G:65:LEU:N	1:G:65:LEU:HD23	2.27	0.44
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.20	0.44
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.18	0.44
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.35	0.44
2:H:27:LEU:O	2:H:528:ARG:NH1	2.44	0.44
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.51	0.44
3:D:664:ILE:CD1	3:D:681:LYS:HE3	2.47	0.44
3:D:1195:GLN:N	3:D:1195:GLN:OE1	2.50	0.44
3:I:543:SER:O	3:I:574:VAL:HB	2.18	0.44
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.83	0.44
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.97	0.44
2:C:812:PHE:N	2:C:815:SER:HB2	2.31	0.44
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.99	0.44
3:I:131:PRO:CG	3:I:135:ILE:HD13	2.45	0.44
2:H:1042:LEU:HB2	2:H:1043:ALA:H	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:514:THR:HG23	3:D:576:ARG:HE	1.83	0.44
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.83	0.44
1:B:19:VAL:O	1:B:20:SER:CB	2.65	0.44
3:I:843:VAL:HG21	3:I:897:HIS:HA	1.99	0.44
3:I:885:VAL:O	3:I:1258:ARG:HD3	2.17	0.44
5:Y:130:VAL:O	5:Y:134:VAL:HG23	2.17	0.44
2:C:985:GLU:HG3	2:C:988:LYS:HB2	2.00	0.44
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.17	0.44
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.47	0.44
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.98	0.44
5:X:133:SER:OG	5:X:365:MET:HB2	2.17	0.44
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.99	0.44
3:D:1297:LYS:HE3	3:I:1267:VAL:HB	1.99	0.44
5:Y:586:ARG:HH22	5:Y:590:ILE:HD11	1.82	0.44
2:C:397:LEU:O	2:C:398:SER:OG	2.35	0.44
2:H:500:ALA:O	2:H:504:GLU:HB2	2.18	0.44
3:D:107:LEU:HD23	3:D:299:LEU:HD21	1.99	0.44
3:I:704:GLU:HB3	3:I:705:THR:H	1.72	0.44
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.18	0.44
2:H:71:VAL:O	2:H:72:SER:OG	2.29	0.44
5:Y:604:SER:HA	5:Y:607:LEU:HB2	2.00	0.44
3:D:539:SER:OG	3:D:540:GLY:N	2.51	0.44
2:C:707:ALA:O	2:C:710:VAL:HG12	2.18	0.44
2:C:475:VAL:HG23	2:C:492:MET:SD	2.58	0.44
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.41	0.44
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.17	0.44
3:D:1226:VAL:HA	3:D:1229:VAL:HG12	2.00	0.44
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.17	0.44
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	2.00	0.44
2:C:1244:HIS:HB3	2:C:1265:PHE:CG	2.53	0.44
2:H:551:HIS:CE1	2:H:553:THR:HG1	2.36	0.44
5:X:119:ILE:HD12	5:X:122:ARG:HH21	1.82	0.44
5:X:126:GLY:O	5:X:130:VAL:HG23	2.18	0.44
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.86	0.44
2:H:866:ASP:HA	2:H:872:TYR:OH	2.18	0.44
1:A:110:VAL:HG21	1:A:140:ILE:HD11	2.00	0.44
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.82	0.44
2:C:1212:LEU:HD11	2:C:1227:VAL:HG21	2.00	0.44
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.53	0.44
2:C:80:PHE:O	2:C:84:GLU:HB3	2.18	0.44
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:149:GLY:HA2	3:I:156:ARG:HG2	2.00	0.44
1:G:64:VAL:HG13	1:G:69:SER:OG	2.18	0.44
2:H:685:MET:CE	2:H:1073:LYS:HE2	2.48	0.44
2:H:681:MET:O	2:H:685:MET:HG2	2.17	0.44
3:D:221:ILE:HG13	3:D:222:LYS:N	2.33	0.44
2:C:475:VAL:O	2:C:479:LEU:HB2	2.18	0.44
1:G:227:GLN:C	1:G:229:GLU:H	2.21	0.44
2:H:505:PHE:O	2:H:512:SER:OG	2.30	0.44
1:A:88:LEU:HD22	1:A:90:VAL:CG2	2.48	0.44
2:C:1042:LEU:HB2	2:C:1043:ALA:H	1.70	0.44
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.33	0.44
3:I:526:VAL:CG1	3:I:549:LYS:HB2	2.48	0.44
5:Y:264:LYS:N	5:Y:264:LYS:HD2	2.33	0.44
2:C:1322:SER:OG	3:D:345:LYS:NZ	2.37	0.44
3:D:596:LEU:HD23	3:D:596:LEU:N	2.33	0.44
3:I:138:VAL:O	3:I:143:SER:HB3	2.18	0.44
4:E:60:ASN:H	4:E:63:ILE:HB	1.83	0.44
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.98	0.44
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.17	0.44
2:H:800:MET:HG2	2:H:1096:ILE:HD13	2.00	0.43
3:D:746:LEU:H	3:D:746:LEU:HD22	1.82	0.43
2:C:22:LEU:HD13	2:C:23:ASP:O	2.18	0.43
2:H:1109:ILE:HG12	3:I:644:MET:SD	2.58	0.43
3:D:580:TRP:HE1	3:D:589:TYR:HB3	1.82	0.43
3:D:1369:ARG:HB3	3:D:1369:ARG:HH11	1.83	0.43
3:I:800:LEU:O	3:I:803:VAL:HG12	2.18	0.43
3:I:317:THR:H	3:I:324:LEU:HD21	1.83	0.43
3:I:1297:LYS:HA	3:I:1297:LYS:HZ3	1.83	0.43
3:I:288:PRO:O	3:I:292:VAL:HG12	2.18	0.43
5:X:264:LYS:HD2	5:X:264:LYS:N	2.33	0.43
5:X:119:ILE:HG21	5:X:379:MET:HG2	1.98	0.43
1:A:300:LEU:HD13	1:A:300:LEU:O	2.18	0.43
1:A:313:SER:OG	1:A:314:LEU:N	2.50	0.43
4:J:48:VAL:O	4:J:52:ARG:HG3	2.18	0.43
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.47	0.43
2:H:365:GLU:OE2	2:H:368:ARG:NH2	2.51	0.43
2:C:801:ARG:NH1	2:C:1093:PRO:O	2.51	0.43
3:D:901:ARG:HB3	3:D:908:ILE:HA	2.00	0.43
3:D:1247:LYS:H	3:D:1247:LYS:CD	2.24	0.43
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.81	0.43
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.51	0.43
2:H:923:GLY:HA2	3:I:371:LYS:HE3	2.00	0.43
2:C:1332:SER:O	3:D:243:PRO:HG2	2.18	0.43
2:H:153:PRO:HD2	2:H:404:LYS:HZ1	1.82	0.43
3:D:99:ARG:HA	3:D:248:ASP:HB2	2.00	0.43
5:Y:584:ARG:O	5:Y:587:ILE:HG22	2.17	0.43
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.48	0.43
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.99	0.43
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.33	0.43
2:C:73:TYR:CD2	2:C:73:TYR:N	2.86	0.43
3:D:138:VAL:O	3:D:143:SER:HB3	2.18	0.43
3:I:205:LEU:HB3	3:I:217:LEU:HD13	2.00	0.43
3:D:488:ASN:HD21	4:E:6:VAL:CG1	2.32	0.43
5:X:35:ILE:HG23	5:X:36:VAL:N	2.33	0.43
3:D:450:HIS:HE2	3:D:625:MET:CE	2.30	0.43
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.53	0.43
3:I:252:LEU:N	3:I:252:LEU:HD23	2.31	0.43
3:I:1194:ARG:HD2	3:I:1194:ARG:N	2.33	0.43
3:I:589:TYR:O	3:I:591:ILE:HG13	2.19	0.43
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.82	0.43
2:C:442:VAL:HG12	2:C:443:ASP:N	2.33	0.43
3:I:363:LEU:O	3:I:486:SER:OG	2.22	0.43
2:C:71:VAL:O	2:C:72:SER:OG	2.32	0.43
2:C:1029:LEU:O	2:C:1032:LYS:HG3	2.18	0.43
1:A:310:ARG:HA	1:A:310:ARG:HE	1.83	0.43
2:H:964:LEU:HD12	2:H:1025:PHE:CG	2.53	0.43
2:H:1268:GLN:NE2	3:I:352:ARG:HD3	2.34	0.43
3:I:539:SER:OG	3:I:540:GLY:N	2.50	0.43
2:H:49:LEU:HG	2:H:461:GLU:HB2	2.01	0.43
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.54	0.43
4:E:16:ARG:O	4:E:19:LEU:HB3	2.18	0.43
3:I:832:LYS:HZ2	3:I:832:LYS:HB2	1.82	0.43
2:H:127:ILE:O	2:H:127:ILE:HG12	2.19	0.43
3:I:233:LYS:CD	3:I:234:PRO:HD2	2.47	0.43
2:H:1058:ARG:HD3	2:H:1240:ASP:OD1	2.19	0.43
3:D:290:ILE:O	3:D:293:ARG:HG3	2.18	0.43
5:Y:573:LEU:HD22	5:Y:588:ARG:HB2	1.99	0.43
1:A:311:GLY:O	5:X:599:ARG:NE	2.52	0.43
1:B:207:THR:OG1	1:B:208:ASN:N	2.51	0.43
2:H:735:LYS:HA	2:H:748:ILE:HA	2.01	0.43
3:D:1322:ALA:HB1	3:D:1326:GLN:HE21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:N	1:A:248:GLU:OE1	2.50	0.43
5:X:551:LEU:HD22	5:X:597:LYS:HD2	2.01	0.43
2:H:840:SER:HB3	2:H:850:ILE:HD11	2.00	0.43
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.53	0.43
1:G:51:MET:HA	1:G:52:PRO:HD3	1.87	0.43
2:H:1185:PRO:HB2	2:H:1186:VAL:H	1.64	0.43
2:H:812:PHE:CD2	2:H:813:GLU:HG3	2.53	0.43
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.85	0.43
3:I:766:GLY:C	3:I:767:LEU:HD22	2.39	0.43
2:C:21:VAL:HG13	2:C:22:LEU:N	2.33	0.43
1:F:51:MET:HA	1:F:52:PRO:HD3	1.82	0.43
2:C:221:LEU:HD21	2:C:314:ASN:HD22	1.83	0.43
5:Y:240:ARG:O	5:Y:242:HIS:N	2.51	0.43
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.53	0.43
3:D:1303:SER:HB2	3:I:1297:LYS:HG2	2.01	0.43
3:I:385:LEU:HD21	3:I:411:ILE:HG13	2.00	0.43
3:D:235:GLU:N	3:D:235:GLU:OE1	2.52	0.43
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.58	0.43
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.18	0.43
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.19	0.43
3:D:620:PHE:O	3:D:624:ILE:HG23	2.18	0.43
3:I:1343:GLU:CA	3:I:1344:LEU:HB2	2.43	0.43
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.80	0.43
3:I:423:LEU:HG	3:I:468:VAL:HG12	2.00	0.43
5:X:333:VAL:HG22	5:X:336:GLU:HB2	2.00	0.43
2:H:153:PRO:HD2	2:H:452:ARG:HD3	1.99	0.43
1:A:167:PRO:HG2	1:A:170:ARG:HG3	2.00	0.43
3:I:704:GLU:HB2	3:I:718:SER:HG	1.84	0.43
1:A:310:ARG:HA	1:A:310:ARG:NE	2.34	0.43
2:H:1027:LYS:HB2	2:H:1027:LYS:NZ	2.34	0.43
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.53	0.43
2:H:1276:TRP:HE3	2:H:1276:TRP:HA	1.84	0.43
2:C:888:THR:O	2:C:914:LYS:N	2.41	0.43
3:D:116:PHE:HB3	3:D:237:MET:CE	2.48	0.43
3:D:790:THR:HG22	3:D:928:THR:HG23	2.00	0.43
2:C:1340:GLU:OE2	3:D:1341:ARG:NH1	2.31	0.43
3:I:539:SER:O	3:I:541:LEU:N	2.52	0.43
3:I:746:LEU:H	3:I:746:LEU:HD22	1.84	0.43
3:I:1154:ALA:HB1	3:I:1211:SER:HB3	2.00	0.43
1:G:227:GLN:O	1:G:229:GLU:N	2.52	0.43
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:843:THR:HB	2:H:845:LEU:HD22	2.01	0.43
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.43
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	2.00	0.43
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.53	0.43
2:H:866:ASP:HA	2:H:872:TYR:CZ	2.54	0.43
3:D:239:LEU:HD12	3:D:239:LEU:O	2.19	0.43
5:X:439:ILE:O	5:X:443:ILE:HG13	2.18	0.43
1:A:79:LEU:O	1:A:83:LEU:HD13	2.18	0.43
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.19	0.43
3:I:1261:LEU:HD21	3:I:1306:LEU:CD2	2.36	0.43
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.46	0.43
3:I:205:LEU:HD13	3:I:217:LEU:CD2	2.48	0.43
1:A:11:PRO:HA	1:A:30:PRO:O	2.18	0.43
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.49	0.43
2:C:843:THR:HB	2:C:845:LEU:CD2	2.49	0.43
5:Y:562:ARG:HG3	5:Y:591:GLU:OE1	2.19	0.43
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.48	0.43
2:C:348:SER:O	2:C:352:ARG:HG3	2.19	0.43
3:I:161:THR:HG22	3:I:162:GLU:N	2.34	0.43
3:I:239:LEU:O	3:I:239:LEU:HD12	2.19	0.43
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.18	0.43
1:B:232:VAL:O	1:B:233:ASP:HB2	2.18	0.43
3:D:688:ALA:O	3:D:692:ARG:HG2	2.18	0.43
5:X:291:CYS:O	5:X:295:CYS:HB2	2.19	0.43
2:H:1287:LEU:O	2:H:1291:LEU:HB2	2.19	0.43
3:D:658:GLU:HA	3:D:661:VAL:CG1	2.48	0.43
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.52	0.43
2:H:617:ALA:HB2	2:H:650:VAL:HG21	1.99	0.43
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.49	0.43
3:D:173:GLY:O	3:D:175:GLU:HG3	2.18	0.43
5:Y:596:ARG:HH21	5:Y:599:ARG:CZ	2.32	0.43
2:H:1233:LEU:O	2:H:1233:LEU:HD12	2.19	0.43
3:I:596:LEU:HD23	3:I:596:LEU:N	2.33	0.43
5:X:465:ARG:O	5:X:468:ARG:HG2	2.19	0.43
2:C:408:SER:O	2:C:431:LYS:NZ	2.33	0.43
2:C:958:LYS:O	2:C:962:GLU:HG2	2.19	0.43
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.83	0.43
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.48	0.43
2:C:694:ARG:O	2:C:798:GLN:NE2	2.50	0.43
1:G:182:ARG:CG	1:G:206:GLU:HB3	2.48	0.43
5:Y:449:THR:HG23	5:Y:503:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.45	0.43
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.51	0.43
1:B:65:LEU:HD23	1:B:65:LEU:N	2.33	0.43
3:I:584:PRO:HD3	3:I:620:PHE:CD1	2.54	0.43
1:B:179:PRO:HB2	1:B:211:ILE:HG22	2.00	0.43
2:H:26:TYR:HE2	2:H:28:LEU:HB2	1.84	0.43
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.84	0.43
2:H:747:GLY:C	2:H:748:ILE:HG13	2.39	0.43
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.34	0.43
2:C:88:ARG:NH1	2:C:88:ARG:HB3	2.34	0.43
2:C:337:PHE:O	2:C:338:THR:OG1	2.30	0.43
5:X:608:ARG:HB3	5:X:608:ARG:NH1	2.33	0.43
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	2.01	0.43
3:D:501:VAL:HG21	3:D:602:SER:HB2	2.00	0.43
2:C:1258:PRO:HB3	3:D:348:ASP:OD2	2.19	0.43
2:C:345:PRO:O	2:C:349:GLU:HG2	2.18	0.43
2:C:270:THR:H	2:C:273:HIS:HD2	1.66	0.43
2:H:812:PHE:H	2:H:815:SER:HB2	1.84	0.42
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.40	0.42
3:D:1149:ARG:HA	3:D:1150:PRO:HD3	1.88	0.42
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.49	0.42
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.44	0.42
2:H:845:LEU:N	2:H:845:LEU:HD13	2.31	0.42
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.79	0.42
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.01	0.42
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.19	0.42
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.49	0.42
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.86	0.42
3:D:165:TYR:O	3:D:169:LEU:HB2	2.19	0.42
2:C:1027:LYS:HB2	2:C:1027:LYS:NZ	2.34	0.42
5:X:278:ASP:O	5:X:282:THR:OG1	2.24	0.42
2:C:1161:LEU:HD21	2:C:1172:LEU:HD11	2.01	0.42
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.35	0.42
5:X:108:VAL:HB	5:X:110:LEU:HG	2.01	0.42
1:G:83:LEU:HD11	3:I:527:LEU:O	2.19	0.42
5:X:456:MET:O	5:X:460:ILE:HG13	2.19	0.42
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.83	0.42
1:A:318:LEU:HD13	1:A:318:LEU:N	2.34	0.42
2:C:1086:PRO:HA	2:C:1213:TYR:O	2.19	0.42
2:H:362:ALA:O	2:H:366:ILE:HG13	2.19	0.42
1:G:110:VAL:HG21	1:G:140:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:210:SER:O	3:I:214:ARG:HG3	2.19	0.42
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.19	0.42
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.55	0.42
2:C:1336:ASN:HB2	3:D:25:ALA:HB2	2.01	0.42
1:F:190:ALA:HB2	1:F:200:LYS:HB3	2.01	0.42
1:F:44:ARG:HG3	1:F:183:ILE:HG22	2.01	0.42
2:H:469:VAL:O	2:H:472:GLU:HB3	2.19	0.42
2:H:56:VAL:HB	2:H:57:PHE:H	1.48	0.42
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.49	0.42
3:I:1345:ARG:HG2	3:I:1370:MET:CE	2.48	0.42
2:C:68:LEU:HG	2:C:100:LEU:HD23	2.01	0.42
5:X:9:LEU:HD22	5:X:60:PRO:HB3	2.00	0.42
3:D:573:THR:HG23	3:D:576:ARG:H	1.83	0.42
5:X:457:ILE:HG23	5:X:461:ASN:ND2	2.34	0.42
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.49	0.42
2:C:590:PRO:HB3	2:C:605:TYR:HE1	1.84	0.42
3:D:681:LYS:HB2	3:D:681:LYS:HZ2	1.82	0.42
3:D:1282:TYR:HA	3:D:1285:VAL:CG2	2.50	0.42
1:A:253:LEU:HB3	1:A:321:TRP:CH2	2.55	0.42
1:G:185:TYR:HB2	1:G:201:LEU:HD11	2.00	0.42
3:I:179:LYS:N	3:I:179:LYS:HD3	2.34	0.42
2:H:1219:GLU:OE2	3:I:634:ARG:NH1	2.52	0.42
3:D:378:LYS:HD2	3:D:382:TYR:CZ	2.54	0.42
5:X:451:ARG:O	5:X:452:ILE:HG13	2.20	0.42
2:H:42:ASP:HB2	2:H:47:TYR:CG	2.53	0.42
1:G:191:ARG:HA	1:G:191:ARG:HD3	1.88	0.42
3:I:573:THR:CG2	3:I:576:ARG:HG3	2.49	0.42
5:X:532:LEU:O	5:X:536:THR:HG23	2.20	0.42
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.42
3:D:681:LYS:O	3:D:685:ILE:HG13	2.19	0.42
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.83	0.42
3:D:607:THR:O	3:D:611:ILE:HG12	2.19	0.42
1:A:323:PRO:HA	1:A:324:ALA:HA	1.74	0.42
2:C:747:GLY:C	2:C:748:ILE:HG13	2.40	0.42
2:H:297:VAL:HB	2:H:317:LEU:HD21	2.01	0.42
2:C:73:TYR:O	2:C:74:ARG:HB2	2.19	0.42
2:H:161:LYS:HB3	2:H:161:LYS:NZ	2.33	0.42
5:X:543:ALA:O	5:X:547:VAL:HG23	2.19	0.42
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.20	0.42
5:Y:484:ALA:HB1	5:Y:490:PRO:O	2.20	0.42
1:B:51:MET:HA	1:B:52:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:238:ILE:HG13	3:I:238:ILE:O	2.19	0.42
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	2.02	0.42
2:H:812:PHE:N	2:H:815:SER:HB2	2.34	0.42
3:D:238:ILE:HG13	3:D:238:ILE:O	2.18	0.42
3:D:130:MET:HA	3:D:131:PRO:HD3	1.96	0.42
3:D:910:ASN:HB3	4:E:15:ASN:HA	2.02	0.42
3:D:857:LEU:HB2	3:D:860:ARG:HB2	2.02	0.42
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.84	0.42
3:D:435:GLN:HB2	3:D:457:TYR:OH	2.20	0.42
3:D:74:LYS:HB3	3:D:74:LYS:NZ	2.35	0.42
5:X:311:THR:HG21	5:X:348:GLU:CD	2.40	0.42
2:C:1105:SER:HB2	3:D:731:ARG:HD3	2.01	0.42
2:C:555:TYR:OH	2:C:654:ASP:OD2	2.36	0.42
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	2.02	0.42
1:F:163:GLU:HG3	1:F:170:ARG:NH1	2.20	0.42
3:I:1341:ARG:HD3	3:I:1343:GLU:CD	2.39	0.42
2:H:106:GLU:CB	2:H:107:ARG:HA	2.49	0.42
3:D:77:ARG:HD2	3:D:77:ARG:HA	1.76	0.42
2:C:896:THR:O	2:C:899:GLU:N	2.50	0.42
1:A:158:ARG:HH21	1:A:158:ARG:HB2	1.84	0.42
3:I:700:ASN:O	3:I:704:GLU:HG2	2.19	0.42
2:C:367:TYR:CD1	2:C:384:LEU:HD13	2.54	0.42
3:I:12:THR:C	3:I:13:LYS:HD2	2.40	0.42
1:G:110:VAL:HB	1:G:131:CYS:HB2	2.00	0.42
3:D:384:LYS:HD2	3:D:384:LYS:HA	1.85	0.42
2:C:1111:GLN:HG3	2:C:1230:MET:HE2	2.01	0.42
5:X:299:LYS:O	5:X:303:ILE:HG12	2.19	0.42
2:C:814:ASP:OD1	2:C:1106:ARG:NH1	2.50	0.42
1:A:29:GLU:O	1:A:31:LEU:N	2.52	0.42
2:C:96:LEU:HB2	2:C:127:ILE:CD1	2.49	0.42
3:I:378:LYS:HD2	3:I:382:TYR:OH	2.19	0.42
2:H:843:THR:HB	2:H:845:LEU:CD2	2.50	0.42
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.34	0.42
3:D:50:LYS:HB3	3:D:50:LYS:HZ2	1.85	0.42
3:D:1372:ARG:NH2	3:I:853:THR:HG21	2.35	0.42
3:I:1307:LEU:HD23	3:I:1307:LEU:N	2.35	0.42
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.54	0.42
2:H:593:LYS:HD2	2:H:604:HIS:NE2	2.35	0.42
2:H:632:ASP:O	2:H:633:LEU:HD23	2.20	0.42
3:D:535:ARG:HB3	3:D:541:LEU:HD11	2.02	0.42
2:C:49:LEU:HG	2:C:461:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1155:ILE:HG13	3:I:1210:ILE:CG2	2.43	0.42
2:H:91:THR:HG22	2:H:138:ILE:HA	2.02	0.42
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.79	0.42
2:H:620:ASN:ND2	3:I:768:ASN:HB2	2.35	0.42
3:I:370:LYS:HG3	3:I:371:LYS:H	1.84	0.42
2:H:1238:LEU:HD12	2:H:1239:VAL:N	2.34	0.42
2:H:59:ILE:HG12	2:H:65:ASN:O	2.20	0.42
1:B:22:THR:HB	1:B:207:THR:O	2.20	0.42
3:I:267:ASP:OD2	3:I:270:ARG:NH2	2.52	0.42
2:H:848:GLU:CD	2:H:888:THR:HG22	2.40	0.42
1:G:178:SER:HA	1:G:179:PRO:HD3	1.88	0.42
2:C:551:HIS:CE1	2:C:553:THR:HG1	2.37	0.42
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	2.00	0.42
2:H:72:SER:O	2:H:98:VAL:HG23	2.20	0.42
2:C:943:LYS:O	2:C:947:GLU:HG2	2.19	0.42
2:C:122:VAL:HG22	2:C:123:TYR:N	2.34	0.42
3:D:122:SER:HB2	3:D:132:LEU:HB2	2.00	0.42
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.34	0.42
2:H:685:MET:HE1	2:H:1073:LYS:HE2	2.00	0.42
1:F:167:PRO:HD2	1:F:170:ARG:NE	2.35	0.42
3:D:205:LEU:HB3	3:D:217:LEU:HB3	2.01	0.42
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.20	0.42
3:I:222:LYS:HZ1	3:I:1276:GLU:HB2	1.84	0.42
2:C:127:ILE:HG12	2:C:127:ILE:O	2.20	0.42
5:X:448:ARG:HD3	5:X:450:ILE:HG13	2.01	0.42
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.34	0.42
5:Y:343:LYS:O	5:Y:346:GLN:HB3	2.20	0.42
2:C:237:LEU:HB2	2:C:287:VAL:O	2.19	0.42
3:D:646:ILE:HG22	3:D:741:ALA:O	2.19	0.42
3:I:515:ARG:HH22	3:I:717:VAL:C	2.21	0.42
2:C:988:LYS:NZ	2:C:988:LYS:HB3	2.34	0.42
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.34	0.42
2:H:122:VAL:HG22	2:H:123:TYR:N	2.35	0.42
2:H:488:MET:HE3	2:H:490:GLN:N	2.35	0.42
3:D:1343:GLU:CA	3:D:1344:LEU:HB2	2.36	0.42
2:H:1269:ARG:N	2:H:1269:ARG:HD3	2.35	0.42
1:F:31:LEU:HB2	1:F:199:ASP:O	2.20	0.42
1:F:11:PRO:HA	1:F:30:PRO:O	2.20	0.42
1:A:80:GLU:HG3	2:C:694:ARG:HH12	1.85	0.42
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.20	0.42
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1146:GLN:CD	2:H:1160:ASP:HB2	2.41	0.42
3:I:31:ARG:HD2	3:I:104:HIS:CD2	2.55	0.42
2:H:1117:LEU:HD11	2:H:1182:ILE:HD13	2.02	0.42
3:D:161:THR:HG22	3:D:162:GLU:N	2.35	0.42
1:G:77:ASP:O	1:G:81:ILE:HG13	2.19	0.42
5:Y:99:ARG:HD3	5:Y:99:ARG:O	2.20	0.42
3:D:390:LEU:HD12	3:D:390:LEU:N	2.34	0.42
3:I:492:SER:HA	3:I:493:PRO:HD3	1.94	0.42
2:H:667:LEU:O	2:H:1069:ARG:NH2	2.53	0.42
3:D:543:SER:O	3:D:574:VAL:HB	2.20	0.42
3:D:313:GLY:H	5:X:38:SER:HB3	1.83	0.42
2:C:686:GLN:O	2:C:688:GLN:N	2.47	0.42
2:C:961:SER:O	2:C:965:GLN:HG3	2.20	0.42
2:C:429:MET:O	2:C:433:ILE:HG13	2.20	0.42
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.84	0.42
3:D:1290:ARG:HH22	3:I:1301:THR:HG22	1.85	0.41
1:A:45:ARG:NE	1:B:38:THR:OG1	2.53	0.41
3:I:356:THR:O	3:I:448:GLN:HA	2.20	0.41
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.45	0.41
2:C:669:PRO:HG2	2:C:1070:HIS:HE1	1.85	0.41
2:H:59:ILE:HB	2:H:480:SER:OG	2.20	0.41
3:D:800:LEU:O	3:D:803:VAL:HG12	2.20	0.41
1:F:182:ARG:HH11	2:H:1092:THR:HG22	1.83	0.41
3:D:66:LYS:HB3	3:D:66:LYS:NZ	2.35	0.41
2:C:221:LEU:HD13	2:C:298:ALA:HA	2.01	0.41
2:C:517:GLN:NE2	2:C:760:ASN:OD1	2.53	0.41
3:I:293:ARG:NH1	5:Y:104:GLU:HB2	2.34	0.41
2:C:1272:GLU:HG3	2:C:1276:TRP:CE2	2.55	0.41
3:I:109:SER:OG	3:I:296:LYS:HE2	2.20	0.41
1:A:246:LYS:N	1:A:246:LYS:HD3	2.35	0.41
1:A:299:SER:O	1:A:303:ILE:HG12	2.20	0.41
5:X:147:GLN:O	5:X:151:VAL:HG23	2.20	0.41
2:H:255:ILE:HD12	2:H:263:VAL:HB	2.02	0.41
2:C:208:ILE:HD11	2:C:365:GLU:HB3	2.01	0.41
1:G:52:PRO:HB2	1:G:53:GLY:H	1.59	0.41
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.35	0.41
3:D:822:MET:HG2	3:D:839:VAL:HG22	2.02	0.41
2:C:1211:ARG:HG3	2:C:1211:ARG:H	1.68	0.41
5:X:112:THR:HG22	5:X:113:ARG:N	2.31	0.41
3:D:789:LYS:HB3	3:D:932:MET:SD	2.60	0.41
3:I:305:ALA:O	3:I:309:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.34	0.41
5:Y:122:ARG:NH2	5:Y:378:GLU:OE2	2.50	0.41
3:I:607:THR:O	3:I:611:ILE:HG12	2.20	0.41
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.35	0.41
3:D:646:ILE:HG13	3:D:646:ILE:H	1.65	0.41
2:H:208:ILE:HD11	2:H:365:GLU:HB3	2.02	0.41
3:D:887:SER:HA	3:I:1292:LEU:HD23	2.02	0.41
3:I:492:SER:HB2	3:I:499:ILE:HB	2.01	0.41
2:C:1004:ASP:N	2:C:1004:ASP:OD1	2.53	0.41
3:I:605:LEU:HD13	3:I:605:LEU:O	2.20	0.41
3:D:26:SER:O	3:D:30:ILE:HG12	2.20	0.41
5:Y:316:PHE:CZ	5:Y:320:ILE:HD11	2.55	0.41
2:C:115:LYS:O	2:C:116:ASP:HB2	2.20	0.41
2:H:560:PRO:HA	3:I:780:ARG:NH2	2.35	0.41
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.31	0.41
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.55	0.41
2:C:51:ALA:C	2:C:53:PHE:H	2.23	0.41
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	2.02	0.41
3:D:382:TYR:CE1	3:D:401:VAL:HG21	2.56	0.41
2:H:773:LEU:CD1	2:H:773:LEU:H	2.32	0.41
3:I:50:LYS:HA	3:I:51:PRO:HD3	1.95	0.41
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.55	0.41
2:H:704:MET:HA	2:H:704:MET:HE2	2.02	0.41
2:H:1286:THR:N	3:I:479:GLU:OE2	2.50	0.41
3:I:646:ILE:H	3:I:646:ILE:HG13	1.66	0.41
5:X:279:ARG:NH2	5:X:350:GLU:OE1	2.50	0.41
1:A:183:ILE:HD11	1:A:205:MET:HG3	2.02	0.41
3:I:33:TRP:HB3	3:I:102:MET:HG3	2.02	0.41
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.20	0.41
3:D:532:GLU:OE1	3:D:578:ILE:HB	2.20	0.41
2:H:582:ASN:HB2	2:H:588:GLU:HG3	2.01	0.41
5:Y:143:TYR:O	5:Y:147:GLN:HG2	2.19	0.41
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.55	0.41
3:D:275:ARG:HD2	3:D:302:ALA:HB2	2.03	0.41
4:E:65:ASP:O	4:E:69:ARG:HG3	2.21	0.41
1:G:56:VAL:HG12	1:G:173:VAL:HG11	2.01	0.41
2:H:1195:ILE:O	2:H:1199:LEU:HG	2.21	0.41
3:I:899:TYR:CZ	3:I:915:ILE:HD12	2.55	0.41
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.46	0.41
3:D:905:ARG:NE	3:D:907:HIS:HB2	2.29	0.41
3:I:910:ASN:OD1	4:J:15:ASN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	2.01	0.41
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.03	0.41
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	2.02	0.41
5:X:145:LEU:HD11	5:X:225:ARG:HH21	1.83	0.41
3:I:325:LYS:HB3	5:Y:508:GLU:HG3	2.02	0.41
2:C:971:LEU:HD21	2:C:1017:GLN:HE22	1.85	0.41
5:X:453:PRO:HB2	5:X:455:HIS:CE1	2.55	0.41
2:H:148:GLN:HB2	2:H:511:LEU:HD21	2.02	0.41
3:I:591:ILE:HD12	3:I:592:VAL:HG13	2.03	0.41
5:X:598:LEU:O	5:X:599:ARG:HD2	2.19	0.41
2:C:773:LEU:C	2:C:773:LEU:HD22	2.41	0.41
3:I:809:VAL:CG1	3:I:913:GLU:H	2.34	0.41
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.35	0.41
3:D:377:PHE:O	3:D:381:ILE:HG13	2.20	0.41
3:I:1357:ILE:N	3:I:1357:ILE:HD12	2.35	0.41
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.20	0.41
3:D:533:ALA:HB2	3:D:578:ILE:HD13	2.02	0.41
3:D:1307:LEU:HD23	3:D:1307:LEU:N	2.35	0.41
5:X:276:MET:O	5:X:280:VAL:HG23	2.20	0.41
5:Y:383:ASN:HB2	5:Y:412:LEU:HD21	2.02	0.41
3:I:438:GLU:HA	3:I:439:PRO:HD3	1.87	0.41
3:D:700:ASN:O	3:D:704:GLU:HG2	2.21	0.41
3:I:1368:ASP:O	3:I:1372:ARG:HB2	2.19	0.41
3:I:850:LYS:NZ	3:I:873:GLU:HB3	2.36	0.41
2:H:57:PHE:HA	2:H:476:LYS:NZ	2.35	0.41
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.40	0.41
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.45	0.41
2:H:1313:HIS:HD2	3:I:474:LEU:HD23	1.86	0.41
2:C:1210:ILE:HG23	2:C:1211:ARG:NH1	2.35	0.41
3:I:233:LYS:HB3	3:I:236:TRP:CE2	2.55	0.41
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.48	0.41
5:X:290:LEU:O	5:X:294:GLN:HB3	2.20	0.41
3:I:473:THR:HB	3:I:476:ALA:CB	2.49	0.41
1:G:82:LEU:O	1:G:86:LYS:HG3	2.20	0.41
5:X:561:MET:SD	5:X:576:VAL:HG22	2.61	0.41
3:D:1257:VAL:HA	3:D:1260:MET:CB	2.50	0.41
3:D:803:VAL:HG11	3:D:1309:ILE:HG13	2.01	0.41
3:D:113:HIS:O	3:D:117:LEU:HB2	2.19	0.41
5:X:283:GLN:NE2	5:X:343:LYS:HD2	2.35	0.41
1:F:33:ARG:HA	1:F:33:ARG:HD3	1.89	0.41
5:X:45:ILE:HD12	5:X:45:ILE:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:605:LEU:O	3:D:605:LEU:HD13	2.21	0.41
2:H:1225:VAL:HG12	3:I:636:GLY:O	2.19	0.41
3:I:790:THR:HG22	3:I:928:THR:HG23	2.01	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.51	0.41
3:I:534:GLU:O	3:I:538:ARG:HB2	2.20	0.41
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.56	0.41
2:C:905:ILE:HG12	5:X:595:LEU:HD22	2.02	0.41
2:H:333:ILE:N	2:H:333:ILE:HD12	2.36	0.41
1:B:118:ASP:HB3	1:B:121:VAL:HB	2.03	0.41
3:I:679:TYR:O	3:I:683:ILE:HG13	2.19	0.41
1:G:33:ARG:NE	1:G:197:ASP:HB2	2.36	0.41
3:D:843:VAL:HG11	3:D:897:HIS:HB3	2.01	0.41
2:H:680:LEU:O	2:H:680:LEU:HD23	2.21	0.41
2:H:759:SER:HB3	2:H:763:THR:H	1.85	0.41
2:C:560:PRO:HB2	3:D:776:THR:OG1	2.20	0.41
2:H:453:ILE:HG23	2:H:453:ILE:O	2.21	0.41
2:H:896:THR:O	2:H:899:GLU:N	2.50	0.41
2:C:500:ALA:O	2:C:504:GLU:HB2	2.20	0.41
2:H:943:LYS:O	2:H:947:GLU:HG2	2.19	0.41
5:X:410:ILE:O	5:X:414:LYS:HG3	2.21	0.41
2:H:120:GLN:HG3	2:H:121:GLU:N	2.35	0.41
2:C:68:LEU:HD22	2:C:475:VAL:HG21	2.02	0.41
2:H:902:LEU:HD21	5:Y:608:ARG:CG	2.45	0.41
5:X:240:ARG:HD3	5:X:244:THR:CB	2.44	0.41
1:B:37:HIS:CE1	2:C:1216:ARG:HD3	2.56	0.41
3:I:450:HIS:CE1	3:I:452:LEU:HB2	2.55	0.41
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.50	0.41
1:B:7:GLU:O	1:B:8:PHE:CG	2.74	0.41
1:A:107:ILE:HG12	1:A:134:THR:O	2.21	0.41
3:I:362:ARG:HB3	3:I:363:LEU:H	1.65	0.41
3:I:646:ILE:HG22	3:I:741:ALA:O	2.21	0.41
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.21	0.41
2:H:453:ILE:HG22	2:H:585:GLY:O	2.21	0.41
2:C:177:ILE:HD12	2:C:177:ILE:N	2.36	0.41
2:H:1270:PHE:HB3	2:H:1271:GLY:H	1.61	0.41
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.21	0.41
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.48	0.41
5:X:113:ARG:O	5:X:117:ILE:HD13	2.21	0.41
2:H:69:GLN:HE22	2:H:101:ARG:NH2	2.13	0.41
3:D:478:LEU:CD1	4:E:47:THR:HG23	2.51	0.41
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1314:GLN:HG2	2:H:1315:MET:H	1.86	0.41
3:I:412:LEU:O	3:I:415:VAL:HG22	2.21	0.41
2:C:1293:VAL:HA	2:C:1297:ASP:HB3	2.02	0.41
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.02	0.41
3:I:479:GLU:O	3:I:483:LEU:HB2	2.21	0.41
3:I:1361:THR:O	4:J:21:LEU:HD21	2.20	0.41
2:H:263:VAL:HA	2:H:267:ARG:HH21	1.86	0.41
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.21	0.41
2:H:169:LYS:HD3	2:H:169:LYS:HA	1.81	0.41
2:C:529:ARG:HB2	2:C:529:ARG:NH1	2.35	0.41
3:D:288:PRO:O	3:D:292:VAL:HG12	2.20	0.41
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.93	0.41
2:H:429:MET:O	2:H:433:ILE:HG13	2.21	0.41
1:B:152:TYR:OH	3:D:535:ARG:NH1	2.47	0.41
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.38	0.41
1:G:152:TYR:OH	3:I:535:ARG:NH1	2.45	0.41
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.41	0.41
1:G:222:THR:O	1:G:226:GLU:HG2	2.21	0.41
5:Y:456:MET:O	5:Y:460:ILE:HG13	2.19	0.41
2:H:302:ILE:HA	2:H:309:LEU:HA	2.03	0.41
2:H:1043:ALA:C	2:H:1045:GLY:H	2.24	0.41
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.21	0.41
2:C:699:LEU:H	2:C:799:ASN:ND2	2.16	0.41
2:H:1169:VAL:HG23	2:H:1172:LEU:HD11	2.02	0.41
2:H:431:LYS:O	2:H:435:ILE:HG13	2.20	0.41
3:D:423:LEU:HB3	3:D:466:MET:CE	2.50	0.41
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.20	0.41
3:I:500:ILE:CD1	3:I:500:ILE:H	2.34	0.41
1:G:207:THR:OG1	1:G:208:ASN:N	2.53	0.41
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.86	0.41
2:H:205:PRO:O	2:H:208:ILE:HG22	2.21	0.41
2:H:177:ILE:N	2:H:177:ILE:HD12	2.36	0.41
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.86	0.41
2:H:225:PHE:CE2	2:H:347:ILE:HB	2.56	0.41
2:H:1107:MET:N	2:H:1107:MET:SD	2.94	0.41
3:I:390:LEU:HD12	3:I:390:LEU:N	2.34	0.41
2:C:453:ILE:HG23	2:C:453:ILE:O	2.21	0.41
1:B:74:VAL:HG12	1:B:76:GLU:H	1.85	0.41
2:H:221:LEU:HD22	2:H:336:LEU:HD11	2.02	0.41
2:H:176:ILE:HD12	2:H:184:LEU:HD23	2.02	0.41
2:H:999:GLU:HG2	2:H:1000:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:THR:O	1:F:226:GLU:HG3	2.21	0.41
5:Y:477:GLU:N	5:Y:477:GLU:OE1	2.53	0.41
2:C:521:LEU:HD22	2:C:667:LEU:HD12	2.02	0.41
2:H:961:SER:O	2:H:965:GLN:HG3	2.21	0.41
3:D:214:ARG:O	3:D:218:THR:HG22	2.21	0.41
2:C:980:VAL:O	2:C:984:VAL:HG22	2.21	0.41
3:D:12:THR:C	3:D:13:LYS:HD2	2.42	0.41
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.51	0.41
2:C:310:ILE:O	2:C:311:CYS:HB3	2.21	0.41
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.43	0.41
3:D:583:VAL:HG13	3:D:584:PRO:HD2	2.03	0.41
2:H:22:LEU:HD13	2:H:23:ASP:O	2.21	0.41
3:I:620:PHE:O	3:I:624:ILE:HG23	2.21	0.41
2:C:1331:ARG:HG3	3:D:33:TRP:CZ3	2.56	0.41
3:I:388:ARG:NH2	3:I:414:GLU:OE2	2.53	0.41
1:B:129:VAL:HG11	1:B:132:HIS:HE1	1.86	0.41
2:C:563:THR:HG21	3:D:780:ARG:CZ	2.50	0.41
2:H:145:ILE:CG2	2:H:456:VAL:HG22	2.51	0.41
2:C:54:ARG:HG2	2:C:55:SER:CB	2.49	0.40
2:H:816:ILE:HG13	2:H:1098:LEU:CD2	2.35	0.40
1:B:181:GLU:HG2	3:D:531:LYS:HD3	2.02	0.40
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.90	0.40
2:C:68:LEU:HA	2:C:68:LEU:HD12	1.91	0.40
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.56	0.40
3:D:746:LEU:N	3:D:746:LEU:HD22	2.36	0.40
5:X:431:ALA:O	5:X:435:ILE:HG13	2.21	0.40
3:D:52:GLU:OE1	5:X:451:ARG:HD2	2.21	0.40
3:I:139:LEU:C	3:I:139:LEU:HD22	2.41	0.40
2:H:94:ALA:O	2:H:126:GLU:HG2	2.21	0.40
2:H:202:ARG:NE	2:H:369:MET:HG2	2.36	0.40
1:G:183:ILE:HD11	1:G:205:MET:HE2	2.03	0.40
2:C:1092:THR:HA	2:C:1093:PRO:HD3	1.88	0.40
2:H:88:ARG:NH1	2:H:88:ARG:HB3	2.36	0.40
2:H:668:ILE:HD12	2:H:671:LEU:HD13	2.02	0.40
3:I:773:PHE:O	3:I:776:THR:HG22	2.21	0.40
3:I:194:LEU:O	3:I:198:CYS:HB2	2.21	0.40
1:F:82:LEU:O	1:F:86:LYS:HG3	2.21	0.40
2:H:54:ARG:N	2:H:55:SER:C	2.75	0.40
2:H:1108:ASN:O	2:H:1108:ASN:ND2	2.54	0.40
2:C:1108:ASN:ND2	2:C:1108:ASN:O	2.55	0.40
2:C:843:THR:HG22	2:C:844:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.86	0.40
3:I:475:GLU:H	3:I:475:GLU:HG2	1.74	0.40
2:C:619:ALA:HA	2:C:653:MET:HE2	2.02	0.40
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	2.02	0.40
3:D:1264:ALA:HB1	3:D:1303:SER:O	2.21	0.40
3:D:1266:ILE:HG22	3:D:1302:TYR:HB3	2.03	0.40
5:Y:281:ARG:HD3	5:Y:359:LYS:NZ	2.37	0.40
3:I:155:GLU:H	3:I:155:GLU:CD	2.25	0.40
3:I:810:THR:HG22	3:I:893:GLY:HA3	2.02	0.40
5:X:343:LYS:O	5:X:346:GLN:HB3	2.21	0.40
3:I:122:SER:OG	3:I:132:LEU:HD13	2.21	0.40
2:H:977:ALA:O	2:H:980:VAL:HG12	2.21	0.40
4:E:77:ALA:O	4:E:80:LEU:HD22	2.20	0.40
2:C:174:ALA:HB2	2:C:432:LEU:HD13	2.03	0.40
2:H:488:MET:HE2	2:H:488:MET:N	2.36	0.40
2:H:1106:ARG:O	2:H:1108:ASN:N	2.43	0.40
3:D:832:LYS:HB2	3:D:832:LYS:HZ2	1.86	0.40
1:B:154:PRO:O	1:B:157:THR:HG22	2.20	0.40
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.22	0.40
2:H:1241:ASP:N	2:H:1241:ASP:OD2	2.54	0.40
2:H:367:TYR:CD1	2:H:384:LEU:HD13	2.56	0.40
5:X:254:GLU:O	5:X:258:GLN:HG3	2.21	0.40
3:D:292:VAL:HG22	3:D:296:LYS:HE3	2.03	0.40
2:C:1060:ILE:H	2:C:1060:ILE:HG12	1.70	0.40
5:X:580:PHE:O	5:X:582:VAL:N	2.55	0.40
2:H:103:VAL:HG22	2:H:104:ILE:H	1.86	0.40
2:C:697:LYS:HD2	2:C:793:GLU:OE2	2.22	0.40
1:F:167:PRO:HG2	1:F:170:ARG:HG3	2.03	0.40
3:D:217:LEU:O	3:D:221:ILE:HG23	2.21	0.40
3:D:586:GLY:O	3:D:587:LEU:HB2	2.22	0.40
3:I:1290:ARG:HD2	3:I:1299:GLY:HA3	2.04	0.40
2:C:1166:ASP:C	2:C:1168:GLU:H	2.23	0.40
3:D:182:ALA:O	3:D:185:ILE:HG22	2.21	0.40
2:C:898:GLU:HG3	5:X:565:ILE:CD1	2.51	0.40
1:A:22:THR:HB	1:A:207:THR:O	2.21	0.40
3:I:801:VAL:O	3:I:805:GLN:HG2	2.21	0.40
1:B:52:PRO:HB2	1:B:53:GLY:H	1.61	0.40
3:D:704:GLU:O	3:D:705:THR:OG1	2.30	0.40
1:A:91:ARG:NH2	1:A:209:GLY:O	2.55	0.40
5:X:459:THR:O	5:X:463:LEU:HD13	2.21	0.40
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:310:GLY:O	3:D:314:ARG:HG2	2.20	0.40
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.51	0.40
3:D:42:GLU:HG3	5:X:451:ARG:NH2	2.37	0.40
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.48	0.40
2:H:773:LEU:HD22	2:H:773:LEU:O	2.22	0.40
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.85	0.40
3:D:428:THR:HG23	3:D:433:GLY:HA3	2.03	0.40
3:I:555:TYR:HD1	3:I:589:TYR:HE2	1.68	0.40
2:H:1314:GLN:O	3:I:473:THR:HG23	2.21	0.40
2:C:542:ARG:HG2	2:C:543:ALA:N	2.36	0.40
1:B:19:VAL:HG12	1:B:19:VAL:O	2.22	0.40
2:H:517:GLN:NE2	2:H:760:ASN:OD1	2.54	0.40
1:F:207:THR:OG1	1:F:208:ASN:N	2.54	0.40
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	2.02	0.40
5:X:295:CYS:SG	5:X:330:LEU:HD23	2.61	0.40
2:H:347:ILE:HD11	2:H:433:ILE:HD11	2.03	0.40
3:I:1195:GLN:OE1	3:I:1195:GLN:N	2.50	0.40
3:D:286:ALA:HB3	5:X:413:MET:SD	2.62	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%)	41 (13%)	14 (4%)	3	34
1	B	217/329 (66%)	186 (86%)	24 (11%)	7 (3%)	5	43
1	F	227/329 (69%)	196 (86%)	26 (12%)	5 (2%)	8	50
1	G	213/329 (65%)	188 (88%)	21 (10%)	4 (2%)	10	53
2	C	1333/1342 (99%)	1069 (80%)	213 (16%)	51 (4%)	4	38
2	H	1333/1342 (99%)	1070 (80%)	213 (16%)	50 (4%)	4	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1154/1407 (82%)	922 (80%)	189 (16%)	43 (4%)	4	39
3	I	1154/1407 (82%)	929 (80%)	183 (16%)	42 (4%)	4	40
4	E	88/91 (97%)	76 (86%)	8 (9%)	4 (4%)	3	33
4	J	74/91 (81%)	64 (86%)	6 (8%)	4 (5%)	2	30
5	X	511/613 (83%)	450 (88%)	45 (9%)	16 (3%)	5	44
5	Y	454/613 (74%)	411 (90%)	32 (7%)	11 (2%)	7	49
All	All	7079/8222 (86%)	5827 (82%)	1001 (14%)	251 (4%)	4	41

All (251) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	B	20	SER
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	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	406	ALA
3	D	710	ASP
3	D	847	ASP
3	D	1268	ASN
3	D	1344	LEU
4	E	6	VAL
5	X	241	SER
5	X	490	PRO
1	F	52	PRO
1	G	52	PRO
2	H	21	VAL

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Mol	Chain	Res	Type
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
3	I	120	LEU
3	I	406	ALA
3	I	710	ASP
3	I	847	ASP
3	I	851	PRO
5	Y	241	SER
1	A	52	PRO
1	B	19	VAL
2	C	79	VAL
2	C	669	PRO
2	C	699	LEU
2	C	753	LEU
2	C	1239	VAL
2	C	1256	GLN
3	D	89	GLY
3	D	155	GLU
3	D	255	LEU
3	D	316	ILE
3	D	390	LEU
3	D	404	GLU
3	D	542	ALA
3	D	595	ALA
3	D	703	THR
3	D	708	ASN
3	D	721	SER
3	D	851	PRO
3	D	887	SER
3	D	901	ARG
3	D	913	GLU
3	D	1274	PHE
3	D	1339	GLY
4	E	35	LYS

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Mol	Chain	Res	Type
5	X	20	GLY
5	X	25	ALA
1	F	160	HIS
1	G	177	TYR
2	H	78	PRO
2	H	170	VAL
2	H	535	PRO
2	H	736	VAL
2	H	753	LEU
2	H	1186	VAL
3	I	53	ARG
3	I	89	GLY
3	I	155	GLU
3	I	390	LEU
3	I	404	GLU
3	I	540	GLY
3	I	542	ALA
3	I	595	ALA
3	I	707	ILE
3	I	708	ASN
3	I	721	SER
3	I	913	GLU
3	I	914	ALA
3	I	1268	ASN
3	I	1339	GLY
3	I	1344	LEU
4	J	6	VAL
4	J	35	LYS
5	Y	108	VAL
5	Y	490	PRO
1	A	14	VAL
1	A	193	GLU
1	B	177	TYR
1	B	235	ARG
2	C	53	PHE
2	C	56	VAL
2	C	78	PRO
2	C	143	ARG
2	C	437	ASN
2	C	487	LEU
2	C	740	GLU
2	C	908	GLU

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Mol	Chain	Res	Type
2	C	1107	MET
2	C	1236	ASN
2	C	1240	ASP
2	C	1270	PHE
3	D	53	ARG
3	D	559	ALA
3	D	707	ILE
3	D	902	ASP
5	X	23	THR
5	X	491	GLU
5	X	581	ASP
1	F	188	GLU
1	G	188	GLU
1	G	228	LEU
2	H	13	LYS
2	H	56	VAL
2	H	298	ALA
2	H	437	ASN
2	H	740	GLU
2	H	908	GLU
2	H	1236	ASN
2	H	1239	VAL
2	H	1240	ASP
2	H	1256	GLN
2	H	1270	PHE
3	I	255	LEU
3	I	345	LYS
3	I	559	ALA
3	I	703	THR
3	I	901	ARG
3	I	1195	GLN
5	Y	491	GLU
5	Y	504	PRO
5	Y	564	GLY
1	A	93	GLN
1	A	160	HIS
1	A	166	ARG
1	A	187	VAL
1	A	188	GLU
1	A	194	GLN
1	B	188	GLU
2	C	13	LYS

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Mol	Chain	Res	Type
2	C	44	GLU
2	C	69	GLN
2	C	167	SER
2	C	736	VAL
2	C	812	PHE
2	C	1080	ASN
2	C	1139	ALA
2	C	1237	HIS
3	D	731	ARG
3	D	848	VAL
3	D	914	ALA
3	D	1195	GLN
5	X	50	ASP
5	X	108	VAL
5	X	308	GLY
5	X	504	PRO
5	X	514	ASP
1	F	153	VAL
2	H	43	PRO
2	H	44	GLU
2	H	143	ARG
2	H	167	SER
2	H	699	LEU
2	H	812	PHE
2	H	895	LEU
2	H	1003	THR
2	H	1080	ASN
2	H	1093	PRO
2	H	1107	MET
2	H	1181	PRO
3	I	210	SER
3	I	731	ARG
3	I	848	VAL
3	I	887	SER
3	I	888	CYS
3	I	902	ASP
5	Y	308	GLY
5	Y	514	ASP
5	Y	581	ASP
2	C	298	ALA
2	C	746	ALA
2	C	895	LEU

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Mol	Chain	Res	Type
2	C	1093	PRO
2	C	1238	LEU
3	D	598	LYS
3	D	888	CYS
3	D	1174	ARG
4	E	5	THR
5	X	564	GLY
5	X	600	HIS
1	F	166	ARG
2	H	53	PHE
2	H	104	ILE
2	H	487	LEU
2	H	488	MET
2	H	1139	ALA
2	H	1237	HIS
3	I	62	PHE
3	I	1174	ARG
3	I	1194	ARG
3	I	1274	PHE
4	J	5	THR
5	Y	600	HIS
1	A	163	GLU
1	B	49	SER
2	C	543	ALA
3	D	62	PHE
3	D	210	SER
3	D	590	SER
3	D	1173	ARG
3	D	1184	ASP
3	D	1194	ARG
4	E	59	ILE
2	H	746	ALA
3	I	598	LYS
3	I	712	GLN
4	J	59	ILE
1	A	232	VAL
1	A	322	PRO
2	C	104	ILE
3	D	540	GLY
2	H	1045	GLY
3	I	1184	ASP
3	D	742	GLY

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Mol	Chain	Res	Type
5	X	97	PRO
3	I	742	GLY
5	Y	97	PRO
2	C	373	GLY
2	H	373	GLY
2	C	117	ILE
2	C	1045	GLY
5	X	35	ILE
2	H	489	PRO
1	A	153	VAL
3	I	850	LYS
2	C	1181	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/286 (98%)	274 (98%)	7 (2%)	55	82
1	B	189/286 (66%)	185 (98%)	4 (2%)	61	85
1	F	197/286 (69%)	192 (98%)	5 (2%)	55	82
1	G	185/286 (65%)	180 (97%)	5 (3%)	52	80
2	C	1150/1157 (99%)	1087 (94%)	63 (6%)	27	66
2	H	1150/1157 (99%)	1092 (95%)	58 (5%)	30	68
3	D	971/1168 (83%)	919 (95%)	52 (5%)	27	67
3	I	971/1168 (83%)	921 (95%)	50 (5%)	29	68
4	E	74/75 (99%)	71 (96%)	3 (4%)	37	73
4	J	65/75 (87%)	65 (100%)	0	100	100
5	X	460/540 (85%)	442 (96%)	18 (4%)	39	74
5	Y	407/540 (75%)	391 (96%)	16 (4%)	39	74
All	All	6100/7024 (87%)	5819 (95%)	281 (5%)	33	70

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	117	HIS
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	77	ASP
1	B	196	THR
2	C	9	LYS
2	C	15	PHE
2	C	18	ARG
2	C	32	LEU
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL
2	C	70	TYR
2	C	73	TYR
2	C	80	PHE
2	C	88	ARG
2	C	114	VAL
2	C	121	GLU
2	C	127	ILE
2	C	133	ASN
2	C	150	HIS
2	C	163	LYS
2	C	479	LEU
2	C	487	LEU
2	C	514	PHE
2	C	554	HIS
2	C	600	THR
2	C	645	PHE
2	C	661	VAL
2	C	690	VAL
2	C	741	MET
2	C	773	LEU
2	C	800	MET
2	C	807	TRP
2	C	817	LEU
2	C	845	LEU

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Mol	Chain	Res	Type
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
2	C	994	ARG
2	C	1002	LEU
2	C	1010	GLN
2	C	1011	LEU
2	C	1017	GLN
2	C	1032	LYS
2	C	1042	LEU
2	C	1106	ARG
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1211	ARG
2	C	1233	LEU
2	C	1248	THR
2	C	1259	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1276	TRP
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	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	141	PHE
3	D	151	MET

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Mol	Chain	Res	Type
3	D	169	LEU
3	D	175	GLU
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
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	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	816	THR
3	D	832	LYS
3	D	847	ASP
3	D	864	LEU
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	1227	HIS
3	D	1247	LYS
3	D	1306	LEU
3	D	1341	ARG
4	E	6	VAL

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Mol	Chain	Res	Type
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	384	LEU
5	X	400	GLN
5	X	401	PHE
5	X	452	ILE
5	X	457	ILE
5	X	471	LEU
5	X	476	ARG
5	X	495	ARG
5	X	545	HIS
5	X	562	ARG
5	X	607	LEU
1	F	37	HIS
1	F	77	ASP
1	F	158	ARG
1	F	160	HIS
1	F	163	GLU
1	G	13	LEU
1	G	37	HIS
1	G	88	LEU
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

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Mol	Chain	Res	Type
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	600	THR
2	H	645	PHE
2	H	661	VAL
2	H	690	VAL
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
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	1034	ARG
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	1241	ASP
2	H	1264	GLN
2	H	1270	PHE
2	H	1288	GLN

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Mol	Chain	Res	Type
2	H	1291	LEU
2	H	1326	LEU
2	H	1339	LEU
2	H	1341	ASP
3	I	31	ARG
3	I	50	LYS
3	I	92	VAL
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	176	PHE
3	I	179	LYS
3	I	188	LEU
3	I	239	LEU
3	I	248	ASP
3	I	250	ARG
3	I	316	ILE
3	I	416	ILE
3	I	430	HIS
3	I	475	GLU
3	I	500	ILE
3	I	527	LEU
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
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	816	THR
3	I	832	LYS
3	I	864	LEU
3	I	867	GLN
3	I	873	GLU
3	I	911	LYS

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Mol	Chain	Res	Type
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	1273	ASP
3	I	1297	LYS
3	I	1306	LEU
3	I	1341	ARG
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	477	GLU
5	Y	511	ILE
5	Y	545	HIS
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 (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	239	GLN
1	B	41	ASN
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

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Mol	Chain	Res	Type
2	C	510	GLN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	649	GLN
2	C	673	HIS
2	C	799	ASN
2	C	894	GLN
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	1220	GLN
2	C	1264	GLN
2	C	1288	GLN
2	C	1313	HIS
3	D	94	GLN
3	D	164	GLN
3	D	300	GLN
3	D	504	GLN
3	D	519	ASN
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	46	GLN
5	X	54	GLN
5	X	301	ASN
5	X	406	GLN
5	X	437	GLN
5	X	461	ASN
5	X	469	GLN
2	H	46	GLN
2	H	69	GLN
2	H	238	GLN
2	H	462	ASN

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Mol	Chain	Res	Type
2	H	510	GLN
2	H	513	GLN
2	H	517	GLN
2	H	649	GLN
2	H	684	ASN
2	H	894	GLN
2	H	922	ASN
2	H	952	GLN
2	H	1010	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
2	H	1313	HIS
3	I	94	GLN
3	I	274	ASN
3	I	300	GLN
3	I	309	ASN
3	I	504	GLN
3	I	519	ASN
4	J	15	ASN
4	J	31	GLN
5	Y	242	HIS
5	Y	301	ASN
5	Y	342	GLN
5	Y	400	GLN
5	Y	437	GLN
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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	G4P	D	1503	-	29,38,38	2.27	6 (20%)	40,61,61	1.70	7 (17%)

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	G4P	D	1503	-	-	0/23/43/43	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1503	G4P	C6-N1	-4.01	1.31	1.36
7	D	1503	G4P	C5-C4	-3.82	1.31	1.40
7	D	1503	G4P	C2'-C3'	-3.54	1.45	1.53
7	D	1503	G4P	C8-N7	2.24	1.38	1.34
7	D	1503	G4P	C2-N3	5.25	1.39	1.33
7	D	1503	G4P	C2-N2	6.80	1.42	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1503	G4P	C4'-O4'-C1'	-6.35	102.75	109.72
7	D	1503	G4P	PC-O3C-PD	-4.63	117.16	132.67
7	D	1503	G4P	PA-O3A-PB	-3.45	121.10	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1503	G4P	C4-C5-N7	2.21	111.51	109.48
7	D	1503	G4P	O3A-PA-O5'	2.37	109.22	102.94
7	D	1503	G4P	O4'-C1'-N9	2.67	113.69	108.10
7	D	1503	G4P	O3C-PC-O3'	3.03	112.34	103.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1503	G4P	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	323/329 (98%)	0.02	14 (4%)	39	28	1, 73, 178, 299	0
1	B	221/329 (67%)	0.31	13 (5%)	26	17	5, 98, 204, 259	0
1	F	229/329 (69%)	0.32	16 (6%)	19	13	27, 123, 199, 278	0
1	G	217/329 (65%)	0.36	13 (5%)	25	17	34, 118, 187, 236	0
2	C	1335/1342 (99%)	-0.12	42 (3%)	52	40	0, 48, 170, 262	0
2	H	1335/1342 (99%)	0.12	81 (6%)	25	16	0, 88, 203, 293	0
3	D	1160/1407 (82%)	-0.02	43 (3%)	45	34	0, 42, 158, 289	0
3	I	1160/1407 (82%)	0.12	71 (6%)	25	16	0, 60, 192, 317	0
4	E	90/91 (98%)	-0.24	1 (1%)	82	74	1, 52, 121, 158	0
4	J	76/91 (83%)	0.28	5 (6%)	22	14	10, 89, 165, 211	0
5	X	517/613 (84%)	0.13	42 (8%)	15	10	0, 101, 226, 326	0
5	Y	458/613 (74%)	0.17	30 (6%)	22	14	1, 109, 234, 357	0
All	All	7121/8222 (86%)	0.07	371 (5%)	31	22	0, 73, 197, 357	0

All (371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	10	ALA	12.8
5	Y	239	GLY	9.2
3	I	212	THR	9.0
3	I	11	GLN	8.4
3	I	1161	GLY	7.5
3	D	1171	GLY	6.9
2	C	311	CYS	6.9
1	F	162	GLU	6.8
2	H	1001	GLY	6.6
3	I	1203	ARG	6.6
2	H	999	GLU	6.4

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Mol	Chain	Res	Type	RSRZ
3	I	208	THR	6.3
1	F	161	SER	6.2
2	H	1000	LEU	6.0
5	X	35	ILE	6.0
2	C	251	ALA	5.9
5	Y	315	TRP	5.9
3	I	9	LYS	5.9
3	I	12	THR	5.8
5	Y	319	ALA	5.8
2	H	987	GLU	5.8
5	X	36	VAL	5.7
5	Y	337	VAL	5.7
2	H	986	ALA	5.5
3	I	213	LYS	5.5
2	H	1002	LEU	5.3
5	Y	212	ILE	5.3
5	Y	318	ALA	5.2
5	X	56	MET	5.2
2	H	998	LEU	5.2
5	X	24	TYR	5.1
2	H	334	GLU	5.1
2	H	996	ARG	5.1
1	F	148	ARG	5.0
1	G	96	ASP	5.0
2	C	231	GLU	5.0
5	X	237	ALA	5.0
1	B	169	GLY	5.0
5	X	319	ALA	4.9
2	H	264	GLU	4.7
1	F	194	GLN	4.7
2	H	1003	THR	4.6
3	I	1375	ALA	4.6
5	Y	293	GLU	4.6
5	X	318	ALA	4.5
3	I	218	THR	4.5
2	H	983	GLY	4.5
5	Y	311	THR	4.4
2	H	912	ASP	4.4
2	H	990	ASP	4.4
3	I	708	ASN	4.4
5	X	305	LEU	4.4
3	I	1162	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
2	H	61	SER	4.3
3	I	1376	GLY	4.3
2	H	981	ALA	4.3
2	H	988	LYS	4.3
5	X	43	ASP	4.2
1	G	172	LEU	4.2
2	C	232	ILE	4.2
1	B	41	ASN	4.1
3	I	830	ASP	4.1
3	D	1170	LYS	4.1
3	I	13	LYS	4.1
5	Y	317	ASN	4.1
1	G	75	GLN	4.1
2	C	282	VAL	4.1
5	Y	421	TYR	4.0
3	I	675	ALA	4.0
3	I	732	GLY	4.0
2	H	60	GLN	4.0
1	A	165	GLU	4.0
2	H	982	GLY	4.0
3	D	211	GLU	3.9
3	D	1203	ARG	3.9
3	D	1133	ASP	3.9
5	X	34	ASP	3.9
5	Y	340	ALA	3.9
5	Y	336	GLU	3.8
3	D	1172	LYS	3.8
1	A	4	SER	3.8
1	A	162	GLU	3.8
2	C	116	ASP	3.8
5	X	306	PHE	3.8
2	H	744	GLY	3.8
5	Y	316	PHE	3.7
5	Y	320	ILE	3.7
5	Y	240	ARG	3.7
3	I	676	GLY	3.7
3	I	1160	SER	3.7
5	X	310	GLU	3.6
4	J	2	ALA	3.6
1	A	41	ASN	3.6
3	D	80	HIS	3.6
3	D	89	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
3	D	1199	PHE	3.6
2	H	1020	GLU	3.5
3	D	831	VAL	3.5
2	C	271	ALA	3.5
1	F	193	GLU	3.5
2	C	331	LYS	3.4
2	C	270	THR	3.4
5	X	19	GLN	3.4
5	X	53	ILE	3.4
2	C	252	SER	3.4
1	B	168	ILE	3.4
3	D	1273	ASP	3.4
2	C	238	GLN	3.4
3	I	1273	ASP	3.3
2	C	165	HIS	3.3
5	X	293	GLU	3.3
5	X	315	TRP	3.3
3	D	333	GLY	3.3
2	C	1002	LEU	3.3
3	D	1151	LYS	3.3
2	C	310	ILE	3.3
1	B	171	LEU	3.3
3	I	204	GLU	3.3
2	C	332	ARG	3.3
2	H	742	TYR	3.2
5	X	6	GLN	3.2
5	X	313	ASP	3.2
2	C	996	ARG	3.2
2	H	262	TYR	3.2
3	I	540	GLY	3.2
2	H	979	LEU	3.2
2	H	332	ARG	3.2
3	I	216	LYS	3.2
3	I	521	LYS	3.2
3	I	712	GLN	3.2
2	C	1000	LEU	3.2
5	X	54	GLN	3.2
2	C	77	GLU	3.2
5	Y	310	GLU	3.2
1	A	324	ALA	3.2
2	H	913	VAL	3.2
2	C	164	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	96	ASP	3.1
5	X	236	LYS	3.1
2	H	263	VAL	3.1
5	X	485	GLU	3.1
2	H	1070	HIS	3.1
3	D	1198	VAL	3.1
2	C	233	ARG	3.1
5	Y	241	SER	3.1
2	H	165	HIS	3.1
3	I	1204	VAL	3.1
5	X	44	ILE	3.1
1	A	193	GLU	3.1
2	H	1008	GLN	3.1
1	B	147	GLN	3.1
2	H	258	ASN	3.1
3	D	212	THR	3.1
3	I	1167	LYS	3.1
2	C	230	PHE	3.0
2	C	999	GLU	3.0
4	J	59	ILE	3.0
4	J	56	GLU	3.0
3	D	875	ASN	3.0
2	H	1009	ASN	3.0
1	F	163	GLU	3.0
3	I	1172	LYS	3.0
3	D	1302	TYR	3.0
2	H	252	SER	3.0
2	C	236	LYS	3.0
3	I	477	GLN	2.9
2	C	483	ASP	2.9
2	H	167	SER	2.9
3	D	344	GLY	2.9
2	H	375	PRO	2.9
2	H	251	ALA	2.9
3	I	855	ASP	2.9
1	G	13	LEU	2.9
5	X	515	GLU	2.9
3	I	210	SER	2.9
3	I	541	LEU	2.9
2	H	108	GLU	2.9
2	H	727	VAL	2.8
3	I	1373	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	1007	LYS	2.8
1	G	173	VAL	2.8
5	X	8	GLN	2.8
5	X	317	ASN	2.8
3	D	210	SER	2.8
2	H	172	TYR	2.8
2	H	229	ILE	2.8
3	I	748	ALA	2.8
3	D	477	GLN	2.8
2	C	266	GLY	2.8
2	H	911	SER	2.8
3	I	831	VAL	2.8
1	F	192	VAL	2.8
1	B	97	GLU	2.8
5	Y	578	LYS	2.8
1	F	191	ARG	2.7
3	D	832	LYS	2.7
1	A	245	GLU	2.7
2	H	1032	LYS	2.7
1	A	272	ALA	2.7
3	I	562	GLU	2.7
2	H	1021	LEU	2.7
2	C	305	SER	2.7
3	D	878	ASP	2.7
2	H	614	TYR	2.7
2	C	908	GLU	2.7
2	H	107	ARG	2.7
3	D	830	ASP	2.7
4	J	37	PRO	2.7
2	C	172	TYR	2.7
1	F	147	GLN	2.7
2	H	725	GLN	2.6
3	I	564	VAL	2.6
1	F	160	HIS	2.6
2	C	1001	GLY	2.6
3	I	1169	THR	2.6
5	X	425	TYR	2.6
1	G	24	ALA	2.6
2	H	473	ARG	2.6
3	I	211	GLU	2.6
5	X	283	GLN	2.6
5	X	328	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	299	LYS	2.6
3	D	471	PRO	2.6
2	C	257	ALA	2.6
2	H	254	ASP	2.6
2	H	984	VAL	2.6
3	I	1133	ASP	2.6
2	H	121	GLU	2.6
5	Y	574	GLU	2.6
3	D	207	GLU	2.6
2	H	787	PRO	2.6
1	B	157	THR	2.5
2	H	168	GLY	2.5
3	D	879	ALA	2.5
5	X	482	GLU	2.5
1	B	172	LEU	2.5
1	G	106	GLY	2.5
3	I	217	LEU	2.5
3	D	1185	PRO	2.5
2	H	1134	GLN	2.5
5	X	31	LEU	2.5
1	G	18	GLN	2.5
5	X	57	GLU	2.5
2	H	895	LEU	2.5
1	F	95	LYS	2.5
5	Y	305	LEU	2.5
1	G	107	ILE	2.5
1	B	70	THR	2.5
1	F	149	GLY	2.5
5	Y	113	ARG	2.5
2	C	120	GLN	2.5
2	H	111	GLU	2.5
4	J	36	ASP	2.5
3	I	133	ARG	2.5
3	D	932	MET	2.5
2	H	1152	GLY	2.5
2	H	1130	ALA	2.5
2	H	1153	ALA	2.5
3	I	1294	ALA	2.4
2	H	972	PHE	2.4
3	I	207	GLU	2.4
5	Y	238	LYS	2.4
5	Y	117	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	I	1215	GLU	2.4
3	D	208	THR	2.4
3	I	392	THR	2.4
2	H	413	GLU	2.4
3	I	542	ALA	2.4
3	D	1186	TYR	2.4
1	G	171	LEU	2.4
5	X	240	ARG	2.4
3	I	1202	GLU	2.4
2	H	106	GLU	2.4
3	I	177	ASP	2.4
5	X	39	ASP	2.4
5	Y	514	ASP	2.4
5	X	20	GLY	2.4
3	D	68	TYR	2.4
5	X	307	THR	2.4
2	H	1071	GLY	2.4
3	I	707	ILE	2.4
2	C	987	GLU	2.3
2	C	304	GLU	2.3
3	I	174	ASP	2.3
5	X	325	PRO	2.3
2	H	1089	GLU	2.3
1	G	23	HIS	2.3
2	H	333	ILE	2.3
5	X	289	LYS	2.3
3	I	1168	GLU	2.3
2	C	267	ARG	2.3
1	A	164	ASP	2.3
1	B	148	ARG	2.3
3	I	1297	LYS	2.3
5	Y	306	PHE	2.3
1	F	184	ALA	2.3
1	G	205	MET	2.2
1	A	19	VAL	2.2
5	Y	515	GLU	2.2
3	I	747	MET	2.2
2	H	376	PRO	2.2
2	C	261	VAL	2.2
4	E	91	ARG	2.2
5	X	514	ASP	2.2
2	H	1166	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1215	GLU	2.2
1	B	19	VAL	2.2
3	D	547	ARG	2.2
3	I	1296	GLY	2.2
1	A	262	LEU	2.2
3	I	1295	ASN	2.2
5	X	52	GLY	2.2
5	X	336	GLU	2.2
2	H	733	VAL	2.2
3	I	344	GLY	2.2
3	I	565	ALA	2.2
1	B	62	ASP	2.2
3	D	390	LEU	2.2
3	I	15	GLU	2.2
1	G	12	ARG	2.2
3	D	1268	ASN	2.2
2	H	997	TRP	2.2
3	I	563	LEU	2.1
3	I	789	LYS	2.1
5	X	16	GLY	2.1
2	C	272	ARG	2.1
2	H	110	PRO	2.1
2	H	937	ASP	2.1
3	I	1179	PRO	2.1
1	A	191	ARG	2.1
2	H	734	ILE	2.1
3	D	76	LYS	2.1
2	H	483	ASP	2.1
2	H	265	LYS	2.1
2	H	1029	LEU	2.1
3	D	829	GLY	2.1
2	C	625	GLU	2.1
3	D	849	LEU	2.1
5	Y	452	ILE	2.1
3	I	473	THR	2.1
1	A	133	LEU	2.1
3	I	153	ASN	2.1
3	D	204	GLU	2.1
3	I	587	LEU	2.1
2	C	258	ASN	2.1
2	H	442	VAL	2.1
2	H	169	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	674	THR	2.1
2	C	844	LYS	2.1
3	I	813	ASP	2.1
3	D	672	LEU	2.1
5	X	239	GLY	2.1
5	Y	299	LYS	2.1
2	H	662	SER	2.1
3	D	148	GLU	2.1
1	F	19	VAL	2.0
2	C	1134	GLN	2.0
2	H	1004	ASP	2.0
3	I	76	LYS	2.0
2	C	264	GLU	2.0
3	I	711	GLY	2.0
2	H	492	MET	2.0
1	B	92	VAL	2.0
2	C	237	LEU	2.0
5	Y	490	PRO	2.0
1	A	242	VAL	2.0
1	F	214	GLU	2.0
3	D	82	GLY	2.0
5	Y	512	GLY	2.0
3	D	267	ASP	2.0
3	I	683	ILE	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, 95th 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(\AA^2)	Q<0.9
7	G4P	D	1503	36/36	0.83	0.20	-0.66	31,56,93,118	0
6	ZN	D	1502	1/1	0.99	0.18	-0.70	8,8,8,8	0
6	ZN	I	1502	1/1	0.98	0.15	-0.77	49,49,49,49	0
6	ZN	I	1501	1/1	0.97	0.07	-1.48	60,60,60,60	0
6	ZN	D	1501	1/1	0.98	0.08	-1.51	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.