



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 02:55 PM UTC

PDB ID : 4JK1 / pdb_00004jk1
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

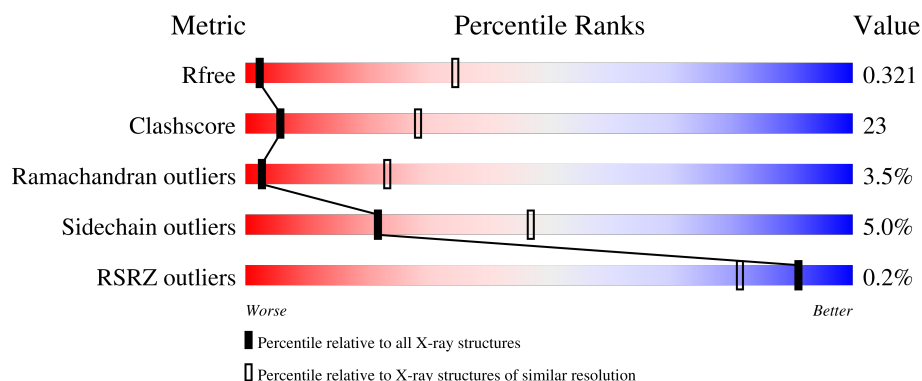
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.



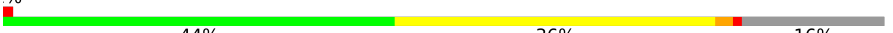
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	329	64% 30% • •
1	B	329	39% 26% • 33%
1	F	329	48% 20% • 30%
1	G	329	39% 26% • 34%
2	C	1342	54% 40% 6% •

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Mol	Chain	Length	Quality of chain
2	H	1342	 55% 38% 6% .
3	D	1407	 41% 37% 5% 18%
3	I	1407	 43% 36% . 18%
4	E	91	 53% 41% . .
4	J	91	 % 44% 36% . . 16%
5	X	613	 50% 31% . 16%
5	Y	613	 43% 29% . 25%

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			

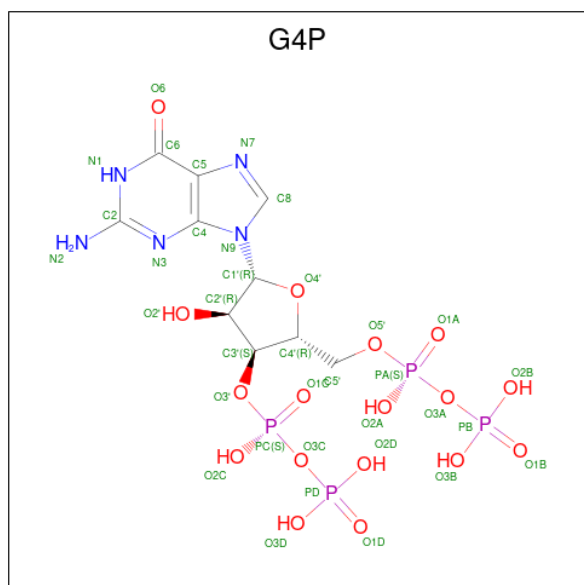
- Molecule 5 is a protein called Escherichia coli RNA polymerase sigma70 subunit.

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).

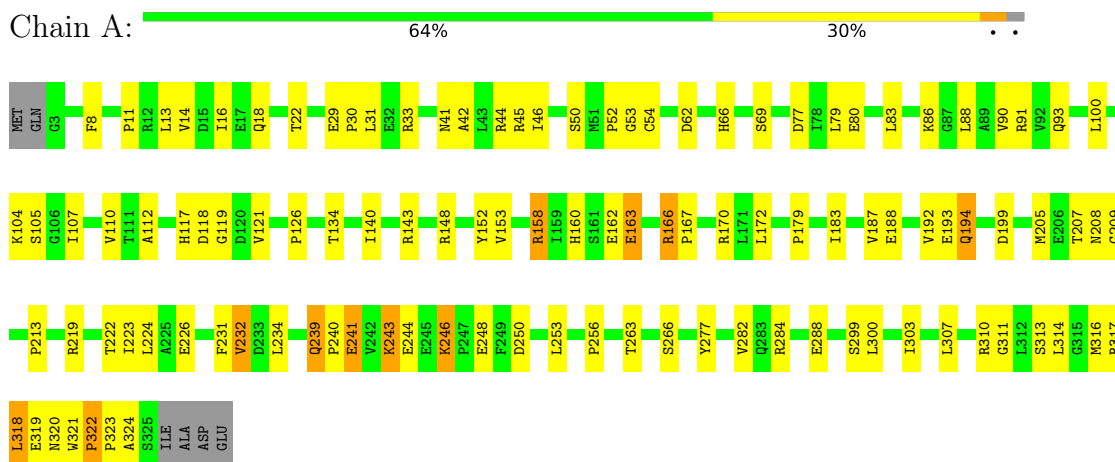


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	H	N	O	0	0
			47	10	11	5	17		

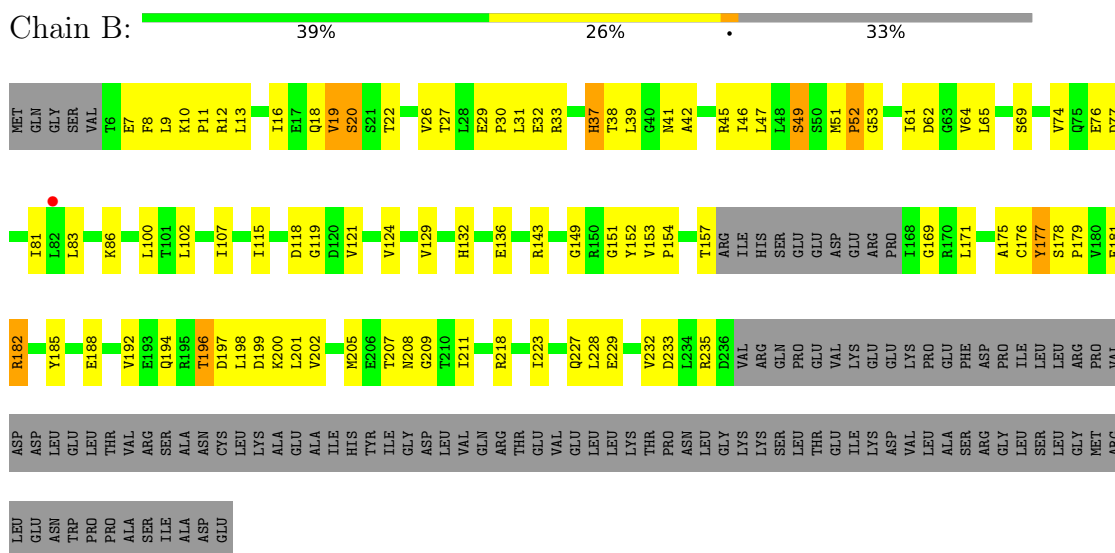
3 Residue-property plots

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

- Molecule 1: Escherichia coli RNA polymerase alpha subunit

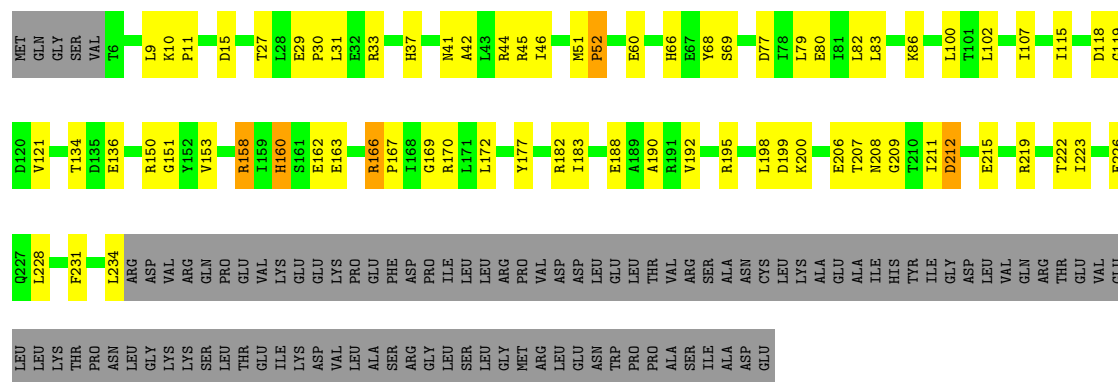


- Molecule 1: Escherichia coli RNA polymerase alpha subunit

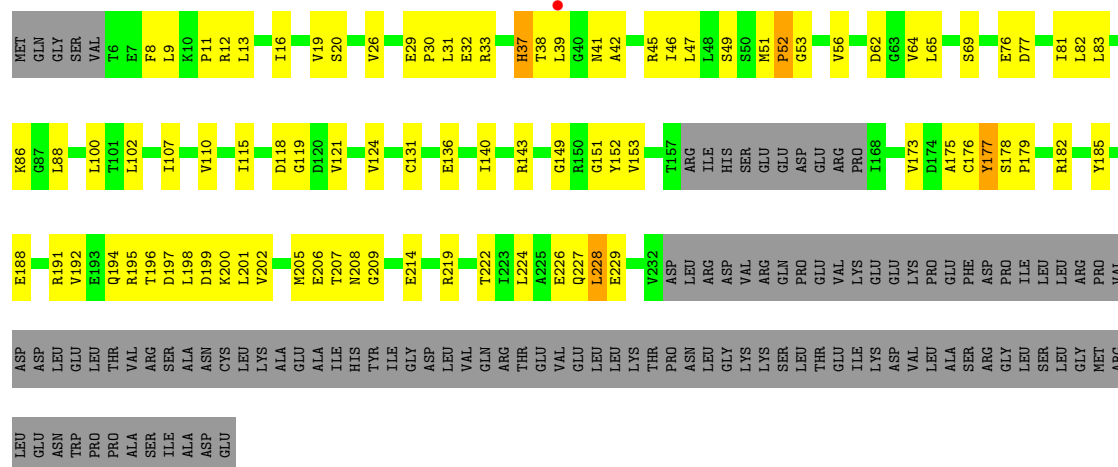


- Molecule 1: Escherichia coli RNA polymerase alpha subunit

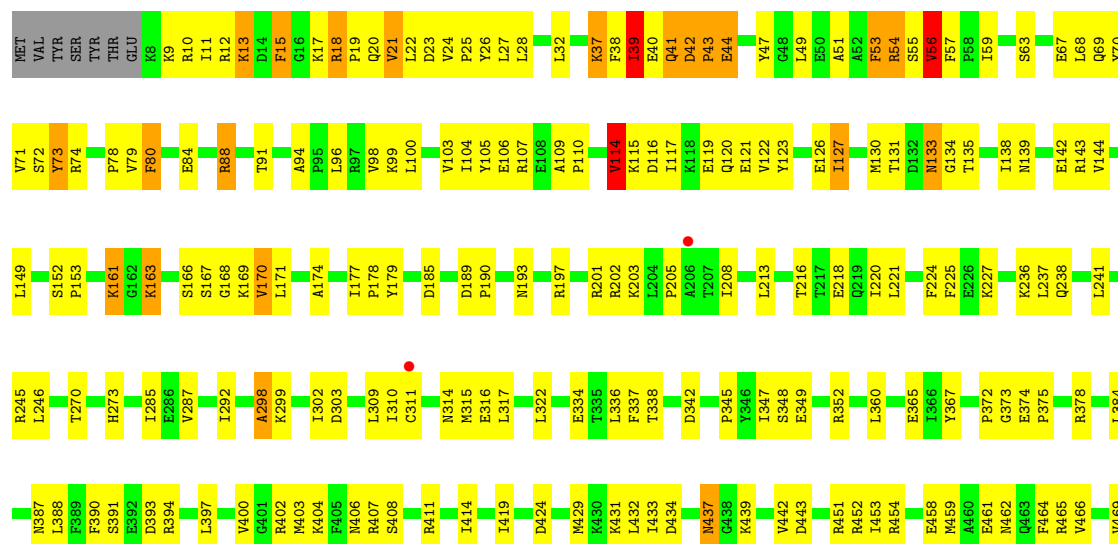


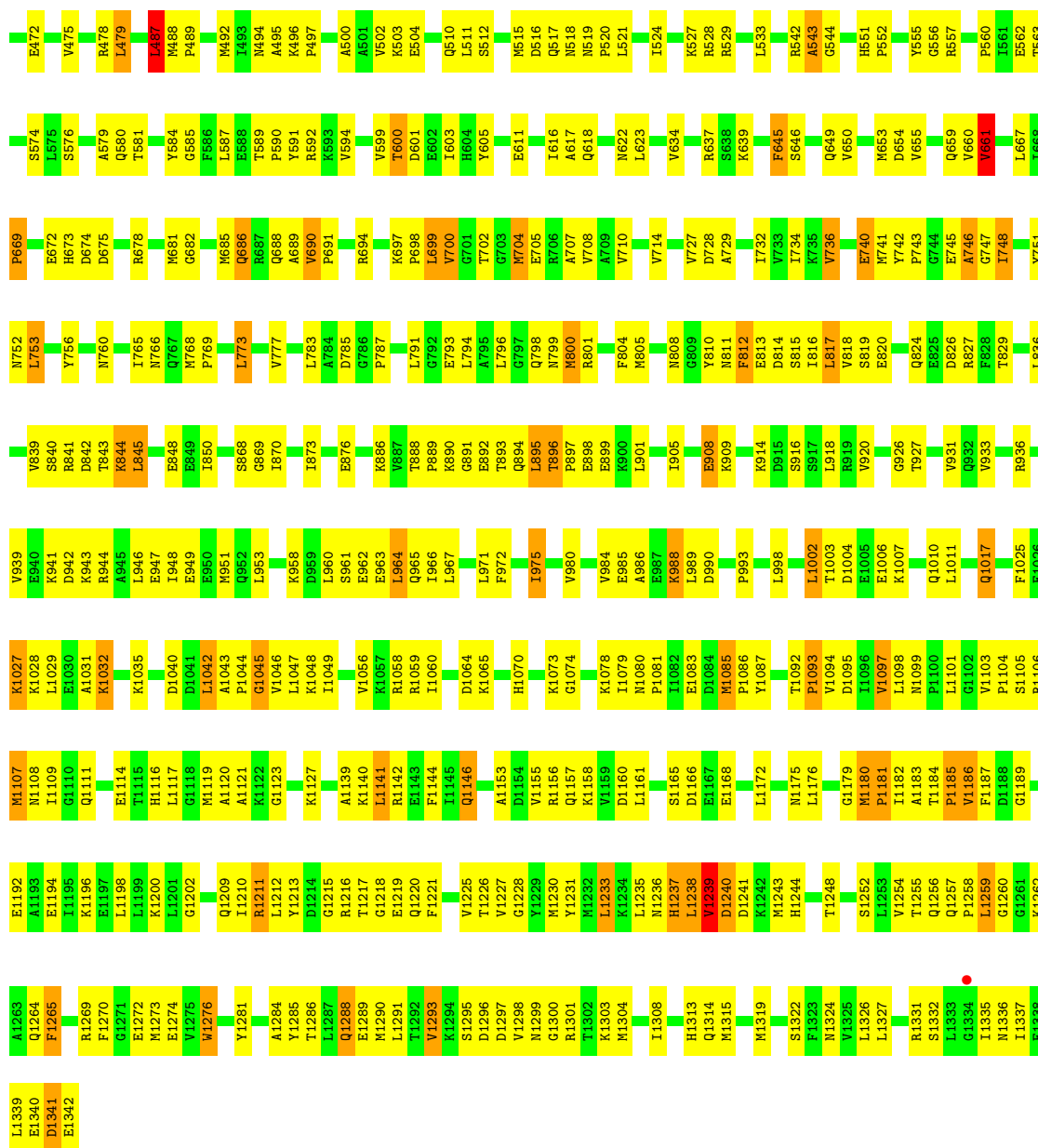


• Molecule 1: Escherichia coli RNA polymerase alpha subunit



• Molecule 2: Escherichia coli RNA polymerase beta subunit





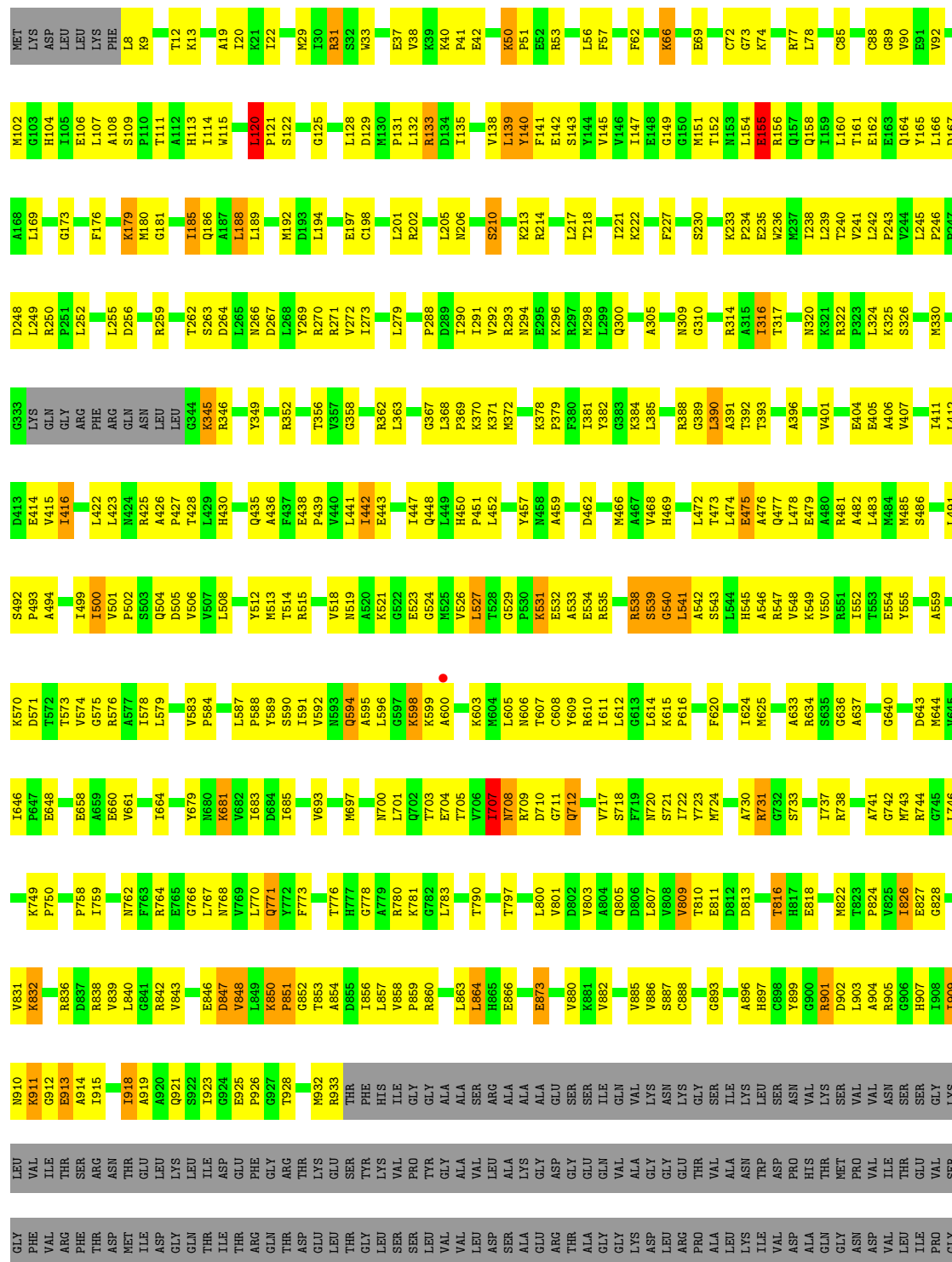


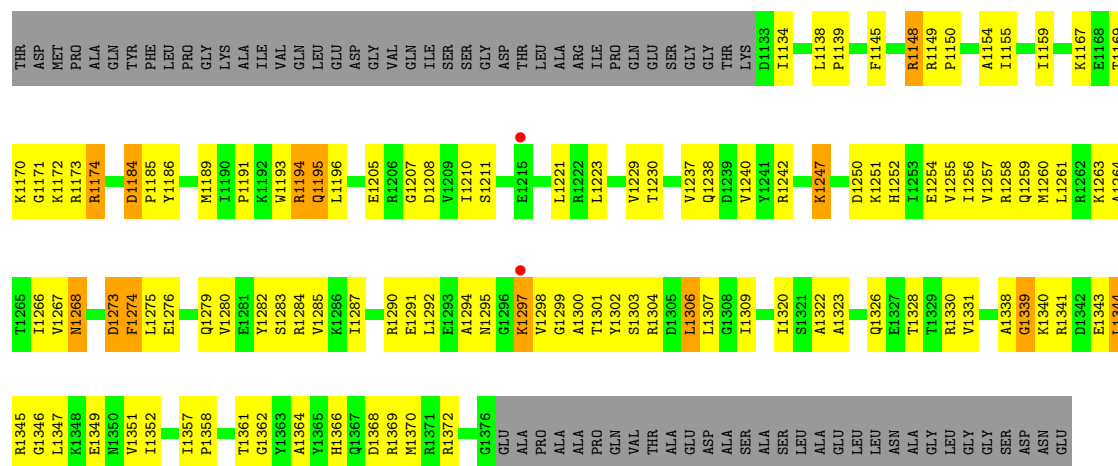


SER
LEU
GLU
ALA
LEU
LEU
LEU
LYS
ASN
ALA
GLY
GLY
GLY
SER
ASP
ASN
GLU

● Molecule 3: Escherichia coli RNA polymerase beta' subunit

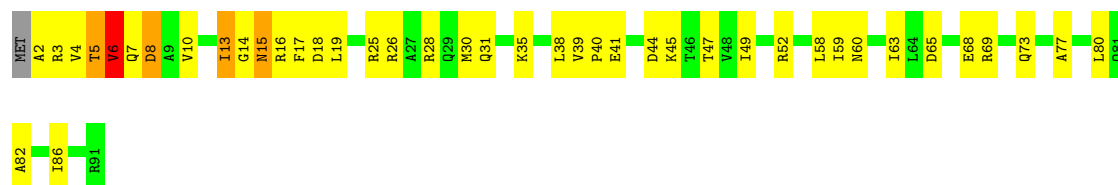
Chain I: 43% 36% 18%





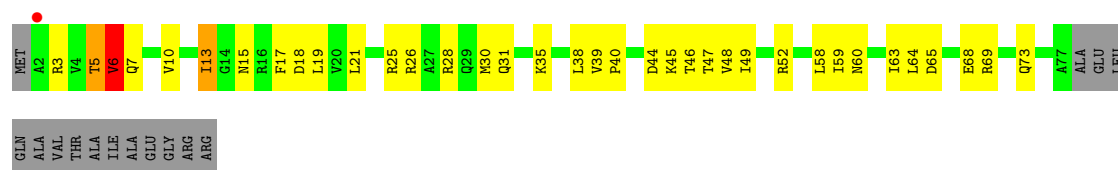
• Molecule 4: Escherichia coli RNA polymerase omega subunit

Chain E: 53% 41%



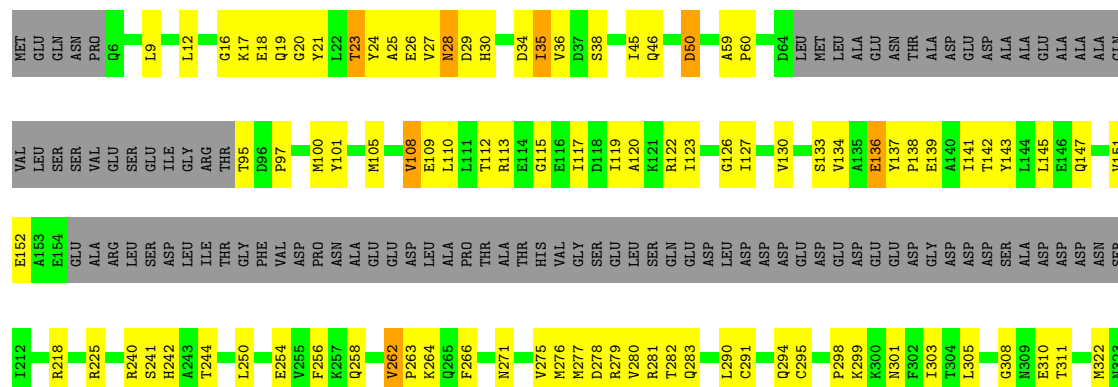
• Molecule 4: Escherichia coli RNA polymerase omega subunit

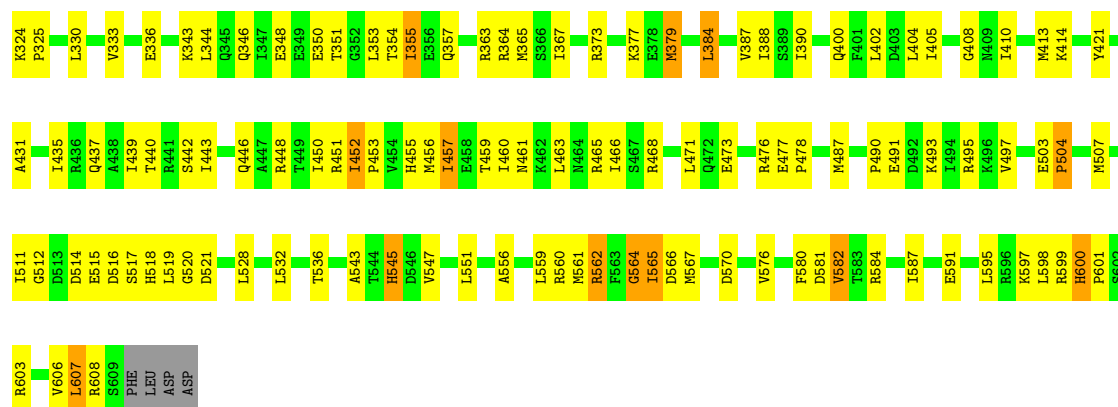
Chain J: 44% 36% 16%



• Molecule 5: Escherichia coli RNA polymerase sigma70 subunit

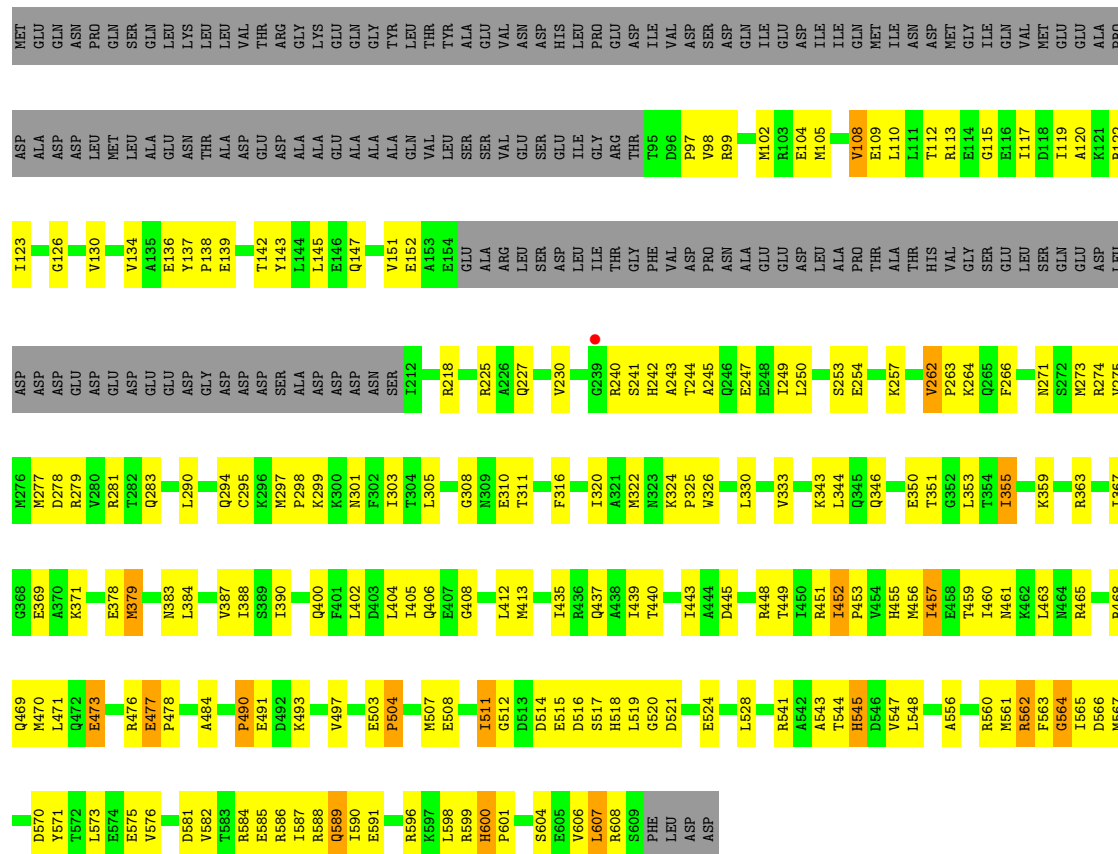
Chain X: 50% 31% 16%





● Molecule 5: Escherichia coli RNA polymerase sigma70 subunit

Chain Y: 43% 29% 25%



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 – 3.90	Depositor EDS
% Data completeness (in resolution range)	89.6 (29.84-3.90) 84.0 (29.84-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.252 , 0.320 0.254 , 0.321	Depositor DCC
R_{free} test set	4799 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	124.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, G4P

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	0.25	0/2548	0.70	1/3454 (0.0%)
1	B	0.24	0/1725	0.70	0/2337
1	F	0.25	0/1797	0.74	2/2436 (0.1%)
1	G	0.24	0/1690	0.70	0/2290
2	C	0.25	0/10690	0.72	8/14423 (0.1%)
2	H	0.25	0/10690	0.72	7/14423 (0.0%)
3	D	0.26	0/9198	0.73	7/12413 (0.1%)
3	I	0.26	0/9198	0.73	8/12413 (0.1%)
4	E	0.26	0/710	0.70	0/956
4	J	0.25	0/607	0.71	0/817
5	X	0.25	0/4253	0.69	0/5719
5	Y	0.24	0/3783	0.69	0/5083
All	All	0.25	0/56889	0.72	33/76764 (0.0%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	42	ASP	CA-C-N	6.62	128.11	119.84
2	C	42	ASP	C-N-CA	6.62	128.11	119.84
3	I	120	LEU	CA-C-N	-6.25	113.24	119.99
3	I	120	LEU	C-N-CA	-6.25	113.24	119.99
3	D	120	LEU	CA-C-N	-5.97	113.54	119.99
3	D	120	LEU	C-N-CA	-5.97	113.54	119.99
2	H	896	THR	CA-C-N	5.97	127.31	119.84
2	H	896	THR	C-N-CA	5.97	127.31	119.84
2	C	54	ARG	N-CA-C	5.88	121.90	114.31
2	C	896	THR	CA-C-N	5.87	127.17	119.84
2	C	896	THR	C-N-CA	5.87	127.17	119.84
1	F	212	ASP	CA-C-N	5.75	125.61	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	212	ASP	C-N-CA	5.75	125.61	119.28
3	I	529	GLY	CA-C-N	5.70	126.08	119.47
3	I	529	GLY	C-N-CA	5.70	126.08	119.47
2	C	1085	MET	CA-C-N	5.62	126.87	119.84
2	C	1085	MET	C-N-CA	5.62	126.87	119.84
3	D	539	SER	CB-CA-C	-5.58	110.16	116.63
3	I	539	SER	CB-CA-C	-5.58	110.13	116.54
3	D	529	GLY	CA-C-N	5.55	125.65	119.32
3	D	529	GLY	C-N-CA	5.55	125.65	119.32
2	H	54	ARG	N-CA-C	5.55	121.47	114.31
2	H	986	ALA	CB-CA-C	-5.42	110.34	116.63
3	I	854	ALA	CB-CA-C	-5.31	110.47	116.63
3	D	854	ALA	CB-CA-C	-5.27	110.52	116.63
2	C	986	ALA	CB-CA-C	-5.21	110.59	116.63
3	D	904	ALA	N-CA-C	-5.13	106.53	112.89
1	A	241	GLU	CB-CA-C	-5.12	110.27	117.23
2	H	1085	MET	CA-C-N	5.09	126.20	119.84
2	H	1085	MET	C-N-CA	5.09	126.20	119.84
3	I	358	GLY	CA-C-N	5.05	124.65	119.05
3	I	358	GLY	C-N-CA	5.05	124.65	119.05
2	H	1323	PHE	N-CA-C	-5.02	108.90	114.62

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	98	0
1	B	1706	0	1738	92	0
1	F	1775	0	1800	62	0
1	G	1671	0	1706	84	0
2	C	10523	0	10546	539	0
2	H	10523	0	10546	520	0
3	D	9060	0	9257	554	0
3	I	9060	0	9257	529	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	708	0	719	41	0
4	J	605	0	612	33	0
5	X	4198	0	4250	180	0
5	Y	3732	0	3809	148	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	2636	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 23.

All (2636) 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
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:H	2:C:163:LYS:HD3	1.33	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.58	0.86
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.62	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
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.61	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
2:H:800:MET:HA	2:H:800:MET:HE3	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
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.64	0.80
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.06	0.80
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.64	0.80
2:H:163:LYS:H	2:H:163:LYS:HD3	1.46	0.80
2:H:488:MET:HE3	2:H:489:PRO:HA	1.63	0.80
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:H:902:LEU:HD21	5:Y:608:ARG:HG3	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:HD23	3:I:541:LEU:H	1.48	0.78
2:C:800:MET:HA	2:C:800:MET:HE3	1.63	0.78
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.64	0.78
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.66	0.78
3:D:828:GLY:HA2	3:D:832:LYS:H	1.47	0.78
3:D:316:ILE:HG23	3:D:317:THR:H	1.49	0.78
3:D:1247:LYS:HD3	3:D:1247:LYS:H	1.48	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
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.66	0.77
5:X:35:ILE:HG13	5:X:36:VAL:H	1.47	0.77
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.66	0.77
3:D:925:GLU:HB3	3:D:926:PRO:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.49	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
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.68	0.76
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.66	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:HD3	3:D:1149:ARG:H	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
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:D:848:VAL:HG11	3:D:880:VAL:HA	1.69	0.74
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.68	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
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.71	0.73
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.53	0.73
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.70	0.73
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.70	0.73
2:H:131:THR:CG2	2:H:135:THR:HG22	2.18	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
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.69	0.73
2:C:403:MET:HG3	2:C:414:ILE:HB	1.71	0.73
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.70	0.73
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.53	0.73
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.51	0.73
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1111:GLN:HE21	2:C:1230:MET:HE1	1.55	0.71
2:C:1243:MET:HE3	3:D:372:MET:HB2	1.72	0.71
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	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
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
2:C:309:LEU:HD23	2:C:309:LEU:H	1.55	0.71
3:D:546:ALA:H	3:D:547:ARG:CA	2.04	0.71
1:A:80:GLU:HB2	2:C:694:ARG:HH22	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
2:H:660:VAL:HG22	2:H:661:VAL:H	1.54	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
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.72	0.71
1:G:12:ARG:H	1:G:30:PRO:HG2	1.55	0.71
2:C:660:VAL:HG22	2:C:661:VAL:H	1.56	0.71
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.73	0.71
3:D:546:ALA:N	3:D:547:ARG:HA	2.05	0.71
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.71	0.71
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.55	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
4:E:5:THR:HA	4:E:6:VAL:HG12	1.72	0.70
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.24	0.70
2:H:142:GLU:HG2	2:H:515:MET:SD	2.32	0.70
2:C:690:VAL:HG22	2:C:691:PRO:HD2	1.73	0.70
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.73	0.70
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.72	0.70
3:D:850:LYS:O	3:D:852:GLY:N	2.25	0.70
2:C:37:LYS:HA	2:C:37:LYS:HE3	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
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.56	0.70
3:D:487:THR:HG21	4:E:4:VAL:HG12	1.73	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
3:I:546:ALA:N	3:I:547:ARG:HA	2.06	0.70
2:C:127:ILE:H	2:C:127:ILE:HD13	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:C:1211:ARG:O	2:C:1211:ARG:NE	2.20	0.69
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.73	0.69
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.75	0.69
2:H:127:ILE:H	2:H:127:ILE:HD13	1.56	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
1:B:41:ASN:HD21	2:C:1217:THR:HG22	1.57	0.69
2:C:54:ARG:H	2:C:55:SER:CB	2.04	0.69
2:C:1042:LEU:HD13	2:C:1042:LEU:H	1.58	0.69
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.73	0.69
5:X:108:VAL:HG23	5:X:109:GLU:H	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
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.75	0.69
2:H:1042:LEU:HD13	2:H:1042:LEU:H	1.58	0.69
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.75	0.69
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.27	0.69
2:C:170:VAL:HG23	2:C:171:LEU:H	1.57	0.69
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.22	0.69
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.92	0.69
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.72	0.68
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.24	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
2:C:528:ARG:NH2	2:C:576:SER:O	2.27	0.68
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.75	0.68
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.56	0.68
3:D:142:GLU:HA	3:D:180:MET:HE2	1.75	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:426:ALA:HB3	3:D:427:PRO:HD3	1.76	0.68
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	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:422:LEU:HA	3:D:436:ALA:HA	1.75	0.68
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.94	0.68
4:E:5:THR:HA	4:E:6:VAL:CG1	2.23	0.68
3:I:546:ALA:H	3:I:547:ARG:CA	2.06	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
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
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.29	0.67
2:H:487:LEU:HB3	2:H:488:MET:HA	1.76	0.67
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.75	0.67
2:C:845:LEU:HD13	2:C:845:LEU:H	1.58	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
1:B:45:ARG:O	3:D:538:ARG:NH2	2.28	0.67
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.76	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
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.28	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.25	0.67
3:I:263:SER:HB2	5:Y:507:MET:HE2	1.76	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:512:TYR:HD2	3:D:724:MET:HE1	1.59	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
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:845:LEU:HD13	2:H:845:LEU:H	1.58	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: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
3:D:573:THR:HG22	3:D:576: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
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:128:LEU:HA	3:D:192:MET:HE1	1.76	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
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.78	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
1:B:29:GLU:HA	1:B:200:LYS:CB	2.26	0.66
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.78	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
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:C:55:SER:CB	2:C:56:VAL:HG22	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:488:MET:H	2:H:489:PRO:HA	1.60	0.65
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.28	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
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
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.29	0.65
2:C:1288:GLN:HA	2:C:1288:GLN:HE21	1.61	0.65
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.77	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
4:J:5:THR:CA	4:J:6:VAL:HB	2.27	0.65
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.77	0.65
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.62	0.65
1:G:49:SER:OG	3:I:538:ARG:NH2	2.30	0.65
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.78	0.65
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.79	0.65
3:D:1260:MET:HE2	3:D:1306:LEU:HD11	1.77	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
2:C:106:GLU:N	2:C:107:ARG:HA	2.11	0.64
2:C:699:LEU:H	2:C:799:ASN:HD21	1.45	0.64
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.63	0.64
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.79	0.64
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.31	0.64
3:I:246:PRO:HB2	3:I:249:LEU:HD13	1.79	0.64
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.62	0.64
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.62	0.64
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.12	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
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.31	0.64
3:D:590:SER:O	3:D:594:GLN:N	2.31	0.64
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.61	0.64
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.29	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
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.33	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:55:SER:HB3	2:C:56:VAL:CG1	2.27	0.64
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:C:39:ILE:HG22	2:C:40:GLU:HG2	1.78	0.63
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.81	0.63
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.13	0.63
5:Y:476:ARG:H	5:Y:476:ARG:HD2	1.63	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
1:F:68:TYR:HB3	2:H:756:TYR:CD1	2.33	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
4:J:5:THR:HA	4:J:6:VAL:HB	1.78	0.63
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.31	0.63
2:C:800:MET:HE1	2:C:827:ARG:HD3	1.81	0.63
2:H:1288:GLN:HA	2:H:1288:GLN:HE21	1.61	0.63
3:D:1173:ARG:HG2	3:D:1189:MET:HE1	1.81	0.63
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.31	0.63
2:C:11:ILE:HD13	2:C:697:LYS:HZ2	1.63	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
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.13	0.63
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.80	0.63
2:H:21:VAL:HG13	2:H:22:LEU:H	1.64	0.63
3:I:151:MET:SD	3:I:151:MET:N	2.71	0.63
2:C:189:ASP:OD1	2:C:193:ASN:N	2.25	0.63
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.29	0.63
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.80	0.63
2:H:69:GLN:HE22	2:H:101:ARG:HH21	1.46	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
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.80	0.63
2:C:557:ARG:HB3	2:C:587:LEU:HD23	1.80	0.62
2:C:1239:VAL:O	2:C:1241:ASP:N	2.31	0.62
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.17	0.62
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
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.81	0.62
3:I:644:MET:O	3:I:764:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.34	0.62
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.14	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
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.29	0.62
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.32	0.62
2:H:1085:MET:HE2	2:H:1094:VAL:HG23	1.80	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:720:ASN:O	3:I:722:ILE:N	2.32	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
3:I:1287:ILE:HG22	3:I:1290:ARG:HE	1.64	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
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.81	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:108:ALA:HB3	3:I:279:LEU:HD12	1.81	0.62
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.64	0.62
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.82	0.62
4:J:5:THR:HA	4:J:6:VAL:HG12	1.82	0.62
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.24	0.62
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.64	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
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.64	0.61
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.82	0.61
2:H:487:LEU:HB3	2:H:488:MET:CA	2.29	0.61
3:D:252:LEU:HD23	3:D:252:LEU:H	1.66	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
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.80	0.61
2:H:800:MET:HA	2:H:800:MET:CE	2.30	0.61
3:I:139:LEU:HD13	3:I:140:TYR:N	2.15	0.61
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.65	0.61
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.30	0.61
3:D:151:MET:SD	3:D:151:MET:N	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.64	0.61
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.33	0.61
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.35	0.61
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.81	0.61
2:H:1237:HIS:O	2:H:1238:LEU:HG	2.00	0.61
3:I:213:LYS:O	3:I:217:LEU:HG	2.00	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
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: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
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.66	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
3:I:1341:ARG:NH2	3:I:1343:GLU:OE1	2.34	0.61
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.66	0.61
5:X:503:GLU:N	5:X:504:PRO:HA	2.15	0.61
2:H:91:THR:HG22	2:H:139:ASN:H	1.65	0.61
2:H:1111:GLN:HE21	2:H:1230:MET:HE1	1.65	0.61
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.16	0.61
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.36	0.61
2:C:1237:HIS:O	2:C:1238:LEU:HG	2.00	0.61
3:D:29:MET:HA	3:D:29:MET:HE3	1.83	0.61
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.82	0.61
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.83	0.61
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.83	0.61
4:E:10:VAL:CG2	4:E:16:ARG:HG2	2.31	0.61
2:H:646:SER:HB2	2:H:649:GLN:HG3	1.83	0.61
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.31	0.61
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.83	0.61
5:X:517:SER:O	5:X:518:HIS:ND1	2.34	0.61
2:H:684:ASN:HA	2:H:687:ARG:HD3	1.83	0.61
3:I:252:LEU:H	3:I:252:LEU:HD23	1.65	0.61
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
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
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.82	0.60
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.30	0.60
2:H:94:ALA:N	2:H:126:GLU:OE2	2.25	0.60
5:Y:305:LEU:HD21	5:Y:322:MET:HE1	1.83	0.60
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.83	0.60
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.34	0.60
2:H:487:LEU:HB3	2:H:488:MET:CG	2.32	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:720:ASN:O	3:D:722:ILE:N	2.34	0.60
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.36	0.60
1:B:65:LEU:HA	1:B:169:GLY:HA2	1.83	0.60
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.30	0.60
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.35	0.60
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.82	0.60
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.17	0.60
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.82	0.60
2:H:543:ALA:HB1	2:H:548:ARG:HD2	1.83	0.60
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.82	0.60
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.17	0.60
3:I:514:THR:HG23	3:I:576:ARG:HE	1.66	0.60
5:Y:585:GLU:HB3	5:Y:589:GLN:NE2	2.15	0.60
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.82	0.60
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.82	0.60
3:D:500:ILE:H	3:D:500:ILE:HD13	1.66	0.60
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.27	0.60
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.83	0.60
4:J:15:ASN:HD22	4:J:18:ASP:H	1.49	0.60
1:A:232:VAL:HA	1:B:218:ARG:HG3	1.84	0.60
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.37	0.60
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.34	0.60
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.83	0.60
3:D:589:TYR:O	3:D:591:ILE:N	2.34	0.60
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.83	0.60
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.67	0.60
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.84	0.60
3:I:50:LYS:HB3	3:I:50:LYS:NZ	2.16	0.60
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.27	0.60
1:A:318:LEU:O	1:A:320:ASN:N	2.30	0.60
2:C:897:PRO:HB3	5:X:564:GLY:O	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.02	0.60
2:H:1239:VAL:O	2:H:1241:ASP:N	2.35	0.60
2:C:1304:MET:HE1	3:D:472:LEU:HD13	1.83	0.59
3:D:142:GLU:HG2	3:D:293:ARG:HB2	1.83	0.59
3:D:213:LYS:O	3:D:217:LEU:HG	2.01	0.59
2:H:618:GLN:OE1	2:H:637:ARG:NH1	2.34	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
2:C:646:SER:HB2	2:C:649:GLN:HG3	1.84	0.59
2:C:1273:MET:HB3	3:D:428:THR:HB	1.83	0.59
4:E:8:ASP:N	4:E:8:ASP:OD1	2.35	0.59
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.84	0.59
2:H:1304:MET:HE1	3:I:472:LEU:HD13	1.84	0.59
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.67	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
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.67	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
3:D:827:GLU:O	3:D:831:VAL:HG12	2.02	0.59
5:X:584:ARG:O	5:X:587:ILE:HG22	2.02	0.59
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.68	0.59
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.82	0.59
3:D:768:ASN:O	3:D:771:GLN:NE2	2.35	0.59
4:E:5:THR:CA	4:E:6:VAL:HB	2.31	0.59
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.67	0.59
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.85	0.59
3:I:836:ARG:HH12	3:I:839:VAL:HB	1.67	0.59
3:I:1191:PRO:O	3:I:1193:TRP:N	2.34	0.59
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.37	0.59
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.38	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:C:1065:LYS:NZ	3:D:462:ASP:O	2.35	0.59
3:D:405:GLU:O	3:D:407:VAL:N	2.35	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:I:29:MET:HA	3:I:29:MET:HE3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:408:SER:O	2:H:431:LYS:NZ	2.29	0.59
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.83	0.59
2:C:873:ILE:HD11	2:C:931:VAL:HG22	1.84	0.59
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.85	0.59
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.84	0.59
3:D:1191:PRO:O	3:D:1193:TRP:N	2.33	0.59
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.84	0.59
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.67	0.59
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.68	0.59
3:I:711:GLY:O	3:I:712:GLN:HG2	2.03	0.59
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.85	0.59
2:C:166:SER:O	2:C:168:GLY:N	2.33	0.59
3:D:85:CYS:HB3	3:D:88:CYS:O	2.03	0.59
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.84	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
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.84	0.59
2:H:951:MET:HA	2:H:951:MET:HE3	1.84	0.59
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.84	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
2:C:202:ARG:HD3	5:X:35:ILE:HB	1.85	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
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
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.36	0.58
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.67	0.58
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.85	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
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.27	0.58
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.17	0.58
2:H:55:SER:CB	2:H:56:VAL:HG13	2.30	0.58
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.67	0.58
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.26	0.58
3:I:128:LEU:HD12	3:I:192:MET:CE	2.33	0.58
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.85	0.58
2:C:901:LEU:HD13	5:X:559:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:951:MET:HA	2:C:951:MET:HE3	1.86	0.58
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.84	0.58
3:D:125:GLY:O	3:D:129:ASP:N	2.37	0.58
2:H:901:LEU:O	2:H:905:ILE:HG13	2.03	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
3:D:18:ASP:HA	3:D:1369:ARG:HH22	1.69	0.58
5:X:240:ARG:O	5:X:242:HIS:N	2.36	0.58
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.68	0.58
3:I:107:LEU:H	3:I:107:LEU:HD12	1.67	0.58
3:I:822:MET:SD	3:I:838:ARG:NH1	2.76	0.58
2:C:302:ILE:HA	2:C:309:LEU:HA	1.85	0.58
2:C:808:ASN:H	3:D:633:ALA:HB2	1.68	0.58
3:D:388:ARG:NH2	3:D:414:GLU:OE2	2.36	0.58
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.85	0.58
2:H:387:ASN:HB3	2:H:394:ARG:HG3	1.83	0.58
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.84	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:1101:LEU:HD21	3:I:508:LEU:CD1	2.34	0.58
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.68	0.58
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.39	0.58
3:D:1369:ARG:HB3	3:D:1369:ARG:NH1	2.19	0.58
2:H:55:SER:HB3	2:H:56:VAL:CB	2.34	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:15:PHE:CE2	2:C:1182:ILE:HD11	2.39	0.58
2:C:41:GLN:CD	2:C:42:ASP:H	2.12	0.58
2:C:91:THR:HG22	2:C:139:ASN:H	1.69	0.58
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.86	0.58
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.19	0.58
3:D:107:LEU:H	3:D:107:LEU:HD12	1.69	0.58
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.84	0.58
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.86	0.58
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.84	0.58
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.03	0.58
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.37	0.57
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
2:C:55:SER:CB	2:C:56:VAL:HG13	2.33	0.57
2:C:1085:MET:HE2	2:C:1094:VAL:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1362:GLY:O	3:D:1364:ALA:N	2.35	0.57
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.38	0.57
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.19	0.57
4:J:5:THR:HA	4:J:6:VAL:CG1	2.33	0.57
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.86	0.57
2:H:660:VAL:O	2:H:661:VAL:HG22	2.04	0.57
3:I:202:ARG:O	3:I:206:ASN:ND2	2.37	0.57
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.86	0.57
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.03	0.57
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.20	0.57
2:C:756:TYR:H	2:C:766:ASN:HB3	1.69	0.57
3:D:145:VAL:HG22	3:D:180:MET:SD	2.44	0.57
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.68	0.57
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.05	0.57
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.04	0.57
3:I:405:GLU:O	3:I:407:VAL:N	2.37	0.57
2:C:800:MET:HA	2:C:800:MET:CE	2.34	0.57
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.04	0.57
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.69	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:D:709:ARG:HD2	3:D:714:GLU:HB2	1.87	0.57
1:F:9:LEU:O	1:G:227:GLN:NE2	2.37	0.57
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.87	0.57
1:B:179:PRO:O	1:B:207:THR:OG1	2.19	0.57
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.68	0.57
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.85	0.57
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.20	0.57
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.86	0.57
2:H:1335:ILE:HD11	3:I:22:ILE:HG13	1.85	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: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:302:ILE:HG22	2:H:309:LEU:HB3	1.86	0.57
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.87	0.57
1:B:47:LEU:HD13	1:B:205:MET:HE2	1.86	0.57
1:B:86:LYS:NZ	3:D:526:VAL:O	2.37	0.57
2:C:1200:LYS:O	2:C:1202:GLY:N	2.35	0.57
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:Y:585:GLU:O	5:Y:589:GLN:N	2.36	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:D:545:HIS:HB2	3:D:546:ALA:CB	2.35	0.57
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.86	0.57
1:A:80:GLU:HA	2:C:694:ARG:HH12	1.70	0.56
1:B:227:GLN:O	1:B:229:GLU:N	2.31	0.56
2:C:901:LEU:O	2:C:905:ILE:HG13	2.04	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
3:D:527:LEU:HD12	3:D:535:ARG:NE	2.18	0.56
3:I:363:LEU:O	3:I:486:SER:OG	2.22	0.56
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.05	0.56
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.33	0.56
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.40	0.56
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.87	0.56
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.87	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:C:105:TYR:CD1	2:C:106:GLU:HB2	2.40	0.56
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.86	0.56
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.87	0.56
3:D:316:ILE:HG23	3:D:317:THR:N	2.17	0.56
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.87	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
3:I:85:CYS:HB3	3:I:88:CYS:O	2.05	0.56
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.88	0.56
5:Y:379:MET:HE2	5:Y:379:MET:HA	1.87	0.56
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.88	0.56
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.05	0.56
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.87	0.56
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.39	0.56
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.06	0.56
3:D:487:THR:HG21	4:E:4:VAL:CG1	2.36	0.56
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.88	0.56
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.87	0.56
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.70	0.56
2:C:542:ARG:O	2:C:544:GLY:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:1345:ARG:HG2	3:I:1370:MET:HE1	1.87	0.56
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.06	0.56
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.86	0.56
5:X:561:MET:HA	5:X:567:MET:SD	2.45	0.56
2:H:548:ARG:NH2	2:H:567:PRO:O	2.38	0.56
3:I:309:ASN:HD22	3:I:326:SER:HB3	1.71	0.56
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.86	0.56
3:I:1338:ALA:O	3:I:1340:LYS:N	2.39	0.56
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.36	0.56
3:D:245:LEU:O	3:D:250:ARG:NH1	2.39	0.56
5:X:503:GLU:HB3	5:X:504:PRO:O	2.06	0.56
2:H:1200:LYS:O	2:H:1202:GLY:N	2.37	0.56
1:B:42:ALA:O	1:B:46:ILE:HG12	2.04	0.56
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.06	0.56
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.38	0.56
1:G:19:VAL:O	1:G:20:SER:OG	2.19	0.56
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.88	0.56
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.35	0.56
3:I:809:VAL:HG13	3:I:912:GLY:H	1.71	0.56
3:I:1362:GLY:O	3:I:1364:ALA:N	2.38	0.56
1:A:118:ASP:OD1	1:A:119:GLY:N	2.39	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:66:LYS:HG3	3:D:69:GLU:OE2	2.06	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
2:H:694:ARG:O	2:H:798:GLN:NE2	2.39	0.56
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.87	0.56
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.88	0.56
3:D:481:ARG:HA	3:D:485:MET:HE2	1.88	0.56
3:D:697:MET:HE1	3:D:738:ARG:HA	1.87	0.56
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.71	0.56
5:Y:387:VAL:HG13	5:Y:408:GLY:HA3	1.88	0.56
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.88	0.55
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.40	0.55
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.30	0.55
4:E:13:ILE:HD11	4:E:19:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:179:TYR:HE2	2:H:462:ASN:HD21	1.55	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
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.70	0.55
5:Y:283:GLN:NE2	5:Y:343:LYS:HD2	2.21	0.55
1:B:65:LEU:HD23	1:B:65:LEU:H	1.70	0.55
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.33	0.55
2:C:704:MET:HE3	2:C:704:MET:HA	1.87	0.55
3:D:1338:ALA:O	3:D:1340:LYS:N	2.39	0.55
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.87	0.55
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.87	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
1:G:42:ALA:O	1:G:46:ILE:HG12	2.06	0.55
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.38	0.55
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.88	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
1:F:11:PRO:CG	1:G:228:LEU:H	2.19	0.55
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.22	0.55
2:H:704:MET:HA	2:H:704:MET:HE3	1.88	0.55
2:H:740:GLU:HB2	2:H:741:MET:SD	2.47	0.55
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.71	0.55
2:H:1141:LEU:H	2:H:1141:LEU:CD1	2.19	0.55
3:I:72:CYS:SG	3:I:73:GLY:N	2.78	0.55
3:I:412:LEU:O	3:I:416:ILE:HD12	2.07	0.55
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.70	0.55
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.05	0.55
2:H:9:LYS:HD3	2:H:9:LYS:N	2.22	0.55
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.36	0.55
2:C:660:VAL:O	2:C:661:VAL:HG22	2.06	0.55
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.22	0.55
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.41	0.55
3:D:1297:LYS:HA	3:D:1297:LYS:HZ3	1.71	0.55
7:D:1503:G4P:O1C	7:D:1503:G4P:O2'	2.21	0.55
2:H:699:LEU:HD12	2:H:1121:ALA:HB1	1.87	0.55
3:I:125:GLY:O	3:I:129:ASP:N	2.39	0.55
1:A:282:VAL:CG2	1:A:316:MET:HE2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:740:GLU:HB2	2:C:741:MET:SD	2.47	0.55
2:C:1274:GLU:OE1	2:C:1274:GLU:N	2.39	0.55
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.89	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:810:THR:HG22	3:D:893:GLY:HA3	1.89	0.55
1:B:64:VAL:HG13	1:B:69:SER:OG	2.06	0.55
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.72	0.55
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.71	0.55
3:D:389:GLY:O	3:D:391:ALA:N	2.40	0.55
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.89	0.55
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.89	0.55
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.88	0.55
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.70	0.55
2:C:634:VAL:H	2:C:645:PHE:HE2	1.53	0.55
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.69	0.55
3:I:450:HIS:CE1	3:I:452:LEU:HD12	2.42	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
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.89	0.55
2:C:55:SER:HB3	2:C:56:VAL:CB	2.37	0.55
2:C:752:ASN:O	2:C:753:LEU:HG	2.07	0.55
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.32	0.55
3:D:1343:GLU:HA	3:D:1344:LEU:CB	2.34	0.55
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.40	0.55
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.89	0.55
5:Y:283:GLN:CD	5:Y:343:LYS:HD2	2.31	0.55
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.22	0.54
2:C:517:GLN:HE21	2:C:760:ASN:H	1.55	0.54
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.89	0.54
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
3:I:173:GLY:HA2	3:I:176:PHE:HE2	1.72	0.54
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.89	0.54
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.42	0.54
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.89	0.54
3:D:644:MET:O	3:D:764:ARG:NH1	2.40	0.54
4:E:26:ARG:HE	4:E:30:MET:HE3	1.73	0.54
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.22	0.54
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.07	0.54
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:736:VAL:HG11	2:C:740:GLU:HA	1.89	0.54
2:C:805:MET:HE1	2:C:1221:PHE:CZ	2.42	0.54
2:C:898:GLU:OE1	2:C:898:GLU:N	2.37	0.54
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.72	0.54
2:C:1141:LEU:CD1	2:C:1141:LEU:H	2.20	0.54
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.89	0.54
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.40	0.54
4:E:41:GLU:O	4:E:52:ARG:NH2	2.28	0.54
1:G:41:ASN:HD21	2:H:1217:THR:HG22	1.72	0.54
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.23	0.54
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.89	0.54
3:I:491:LEU:HB2	3:I:904:ALA:HA	1.90	0.54
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.89	0.54
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.07	0.54
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.90	0.54
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.89	0.54
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.54
2:H:1339:LEU:H	2:H:1339:LEU:HD12	1.71	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
4:J:26:ARG:HE	4:J:30:MET:HE3	1.72	0.54
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.88	0.54
2:C:106:GLU:H	2:C:107:ARG:HA	1.72	0.54
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.90	0.54
2:H:664:GLY:O	2:H:686:GLN:NE2	2.41	0.54
3:I:325:LYS:HZ1	3:I:330:MET:HG2	1.72	0.54
3:I:500:ILE:HD13	3:I:500:ILE:H	1.72	0.54
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.90	0.54
2:H:510:GLN:O	2:H:513:GLN:NE2	2.40	0.54
2:H:888:THR:O	2:H:914:LYS:N	2.33	0.54
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.23	0.54
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.73	0.54
2:C:149:LEU:HD12	2:C:452:ARG:O	2.08	0.54
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.90	0.54
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.90	0.54
5:X:515:GLU:N	5:X:516:ASP:HA	2.22	0.54
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.90	0.54
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.89	0.54
3:I:1167:LYS:HB3	3:I:1170:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:119:ILE:HG21	5:Y:379:MET:HG2	1.90	0.54
3:D:72:CYS:SG	3:D:73:GLY:N	2.81	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:I:142:GLU:HG2	3:I:293:ARG:HB2	1.89	0.54
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.20	0.54
2:C:408:SER:O	2:C:431:LYS:NZ	2.33	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:1297:LYS:HA	3:D:1297:LYS:NZ	2.23	0.54
2:H:753:LEU:HD12	2:H:753:LEU:O	2.08	0.54
3:I:88:CYS:O	3:I:90:VAL:N	2.41	0.54
3:I:481:ARG:HA	3:I:485:MET:HE2	1.89	0.54
3:I:1260:MET:HE2	3:I:1306:LEU:HD11	1.90	0.54
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.90	0.54
3:D:1155:ILE:HG13	3:D:1210:ILE:CG2	2.33	0.53
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.90	0.53
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.88	0.53
1:F:192:VAL:HG21	1:F:198:LEU:HD12	1.90	0.53
1:G:179:PRO:O	1:G:207:THR:OG1	2.23	0.53
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.08	0.53
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.08	0.53
2:C:623:LEU:HD11	2:C:653:MET:HE1	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
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
3:I:288:PRO:HG2	5:Y:413:MET:HE2	1.90	0.53
3:I:482:ALA:C	3:I:483:LEU:HD12	2.34	0.53
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.42	0.53
3:D:515:ARG:HH22	3:D:717:VAL:C	2.16	0.53
3:D:573:THR:HG22	3:D:576:ARG:CG	2.38	0.53
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.44	0.53
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.72	0.53
2:H:1268:GLN:O	3:I:346:ARG:HA	2.09	0.53
3:I:128:LEU:HD12	3:I:192:MET:HE1	1.91	0.53
3:I:294:ASN:ND2	5:Y:406:GLN:OE1	2.41	0.53
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.90	0.53
3:I:905:ARG:HG2	3:I:907:HIS:H	1.74	0.53
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.90	0.53
1:B:18:GLN:C	1:B:20:SER:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.44	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:9:LYS:N	2:C:9:LYS:HD3	2.23	0.53
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.39	0.53
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.41	0.53
2:H:562:GLU:HG2	2:H:574:SER:CB	2.38	0.53
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.74	0.53
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.53
2:C:494:ASN:OD1	2:C:495:ALA:N	2.40	0.53
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.89	0.53
4:E:82:ALA:O	4:E:86:ILE:HG13	2.07	0.53
1:G:29:GLU:HA	1:G:200:LYS:CB	2.39	0.53
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.42	0.53
2:H:800:MET:HE1	2:H:827:ARG:HD3	1.91	0.53
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.09	0.53
2:C:311:CYS:SG	2:C:315:MET:HB2	2.49	0.53
2:C:768:MET:O	2:C:785:ASP:N	2.38	0.53
3:D:42:GLU:HG3	5:X:451:ARG:HH21	1.74	0.53
1:G:118:ASP:OD1	1:G:119:GLY:N	2.42	0.53
2:H:1119:MET:O	2:H:1123:GLY:N	2.40	0.53
1:A:66:HIS:CE1	1:A:69:SER:HB2	2.44	0.53
1:A:263:THR:HG23	1:A:266:SER:H	1.74	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
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.43	0.53
3:D:398:LYS:HD2	5:X:532:LEU:HD11	1.90	0.53
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.91	0.53
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.38	0.53
4:E:45:LYS:O	4:E:49:ILE:HG12	2.08	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
3:I:589:TYR:O	3:I:591:ILE:N	2.38	0.53
3:I:697:MET:HE1	3:I:738:ARG:HA	1.90	0.53
2:C:21:VAL:HG13	2:C:22:LEU:H	1.73	0.53
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.90	0.53
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.90	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
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.44	0.53
3:I:50:LYS:HB3	3:I:50:LYS:HZ3	1.74	0.53
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.38	0.53
3:I:679:TYR:CZ	3:I:683:ILE:HD11	2.44	0.53
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.44	0.53
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.90	0.53
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.09	0.53
3:D:824:PRO:CB	3:D:836:ARG:HD3	2.39	0.53
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.44	0.53
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.44	0.53
2:H:741:MET:SD	2:H:741:MET:N	2.81	0.53
1:B:61:ILE:HB	1:B:64:VAL:HB	1.91	0.52
2:C:747:GLY:O	2:C:748:ILE:HG13	2.08	0.52
2:C:753:LEU:O	2:C:753:LEU:HD12	2.09	0.52
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.44	0.52
3:D:546:ALA:HB3	3:D:547:ARG:O	2.09	0.52
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.24	0.52
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.73	0.52
3:I:478:LEU:CD1	4:J:47:THR:HG23	2.38	0.52
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.91	0.52
3:I:550:VAL:HG23	3:I:552:ILE:HD11	1.91	0.52
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.09	0.52
2:C:42:ASP:O	2:C:44:GLU:HG2	2.10	0.52
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.73	0.52
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.90	0.52
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.73	0.52
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.73	0.52
5:Y:264:LYS:HD2	5:Y:264:LYS:H	1.75	0.52
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.73	0.52
2:C:975:ILE:O	2:C:975:ILE:HD13	2.09	0.52
3:D:709:ARG:O	3:D:711:GLY:N	2.42	0.52
5:X:402:LEU:HD13	5:X:405:ILE:HD11	1.91	0.52
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.45	0.52
3:I:264:ASP:HB3	3:I:324:LEU:HB3	1.90	0.52
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.91	0.52
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.34	0.52
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.91	0.52
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.44	0.52
2:H:91:THR:HG22	2:H:139:ASN:N	2.24	0.52
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.45	0.52
2:C:130:MET:SD	2:C:134:GLY:HA2	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:108:ALA:HB3	3:D:279:LEU:HD12	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
1:F:42:ALA:O	1:F:46:ILE:HG12	2.10	0.52
2:H:17:LYS:NZ	2:H:1194:GLU:OE1	2.42	0.52
3:I:704:GLU:HB2	3:I:718:SER:OG	2.10	0.52
3:I:1297:LYS:HA	3:I:1297:LYS:NZ	2.25	0.52
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.49	0.52
2:C:1244:HIS:HB3	2:C:1265:PHE:CD2	2.45	0.52
3:D:128:LEU:HD12	3:D:192:MET:CE	2.40	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.42	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
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.91	0.52
3:I:478:LEU:HD12	4:J:47:THR:HG23	1.90	0.52
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.35	0.52
5:Y:379:MET:HA	5:Y:379:MET:CE	2.40	0.52
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.90	0.52
5:Y:576:VAL:HG12	5:Y:587:ILE:HG12	1.92	0.52
2:C:142:GLU:HG2	2:C:515:MET:SD	2.50	0.52
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.91	0.52
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.44	0.52
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.92	0.52
2:H:1255:THR:O	2:H:1257:GLN:N	2.42	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
3:I:832:LYS:HZ1	3:I:832:LYS:HA	1.73	0.52
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.38	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:145:VAL:HG21	3:I:165:TYR:CD2	2.45	0.52
3:I:733:SER:O	3:I:737:ILE:HG12	2.09	0.52
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.91	0.52
2:C:134:GLY:O	2:C:527:LYS:NZ	2.43	0.52
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.92	0.52
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.92	0.52
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.44	0.52
2:C:94:ALA:N	2:C:126:GLU:OE2	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:868:SER:OG	2:C:942:ASP:OD1	2.28	0.52
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.44	0.52
3:D:482:ALA:C	3:D:483:LEU:HD12	2.34	0.52
3:D:810:THR:OG1	3:D:811:GLU:N	2.43	0.52
3:D:1344:LEU:H	3:D:1345:ARG:HG3	1.75	0.52
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.92	0.52
2:H:728:ASP:OD2	2:H:729:ALA:N	2.43	0.52
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.91	0.52
1:A:90:VAL:HG13	1:A:121:VAL:HG13	1.92	0.51
1:A:100:LEU:HD11	1:A:121:VAL:HG11	1.92	0.51
3:D:88:CYS:O	3:D:90:VAL:N	2.44	0.51
3:D:141:PHE:O	3:D:297:ARG:HD3	2.10	0.51
3:D:473:THR:HB	3:D:476:ALA:HB2	1.91	0.51
3:D:909:ILE:HD12	3:D:909:ILE:O	2.10	0.51
5:X:355:ILE:O	5:X:355:ILE:HD13	2.10	0.51
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.40	0.51
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.32	0.51
2:H:752:ASN:O	2:H:753:LEU:HG	2.10	0.51
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.25	0.51
3:I:292:VAL:HG22	3:I:296:LYS:HE3	1.92	0.51
2:C:153:PRO:HD2	2:C:452:ARG:HD3	1.92	0.51
2:C:317:LEU:HD13	2:C:322:LEU:HD21	1.92	0.51
3:D:395:LYS:HG3	5:X:536:THR:CG2	2.39	0.51
2:H:985:GLU:HG2	2:H:989:LEU:HD13	1.92	0.51
2:H:1273:MET:HB3	3:I:428:THR:HB	1.92	0.51
3:I:707:ILE:HG22	3:I:708:ASN:H	1.75	0.51
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.43	0.51
3:I:1173:ARG:HG2	3:I:1189:MET:HE1	1.92	0.51
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.23	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
2:H:18:ARG:HD3	2:H:619:ALA:O	2.10	0.51
2:H:844:LYS:HB2	2:H:844:LYS:NZ	2.25	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
1:A:256:PRO:HA	1:A:277:TYR:HA	1.90	0.51
2:C:91:THR:HG22	2:C:138:ILE:HA	1.93	0.51
2:C:936:ARG:HD2	2:C:1047:LEU:H	1.75	0.51
5:X:264:LYS:H	5:X:264:LYS:HD2	1.74	0.51
5:X:519:LEU:O	5:X:519:LEU:HD13	2.09	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
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.92	0.51
2:H:189:ASP:OD1	2:H:193:ASN:N	2.34	0.51
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.29	0.51
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.26	0.51
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.40	0.51
3:I:546:ALA:HB3	3:I:547:ARG:O	2.10	0.51
3:I:919:ALA:O	3:I:923:ILE:HG12	2.11	0.51
2:C:314:ASN:HD21	2:C:348:SER:HA	1.74	0.51
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.91	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
1:F:150:ARG:HH12	1:G:8:PHE:HA	1.74	0.51
1:G:51:MET:HE1	1:G:219:ARG:HG2	1.93	0.51
2:H:459:MET:SD	2:H:511:LEU:HD22	2.51	0.51
2:H:699:LEU:H	2:H:799:ASN:HD21	1.57	0.51
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.10	0.51
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	1.91	0.51
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.92	0.51
2:C:728:ASP:OD2	2:C:729:ALA:N	2.43	0.51
3:D:528:THR:HG22	3:D:551:ARG:HB2	1.92	0.51
2:H:138:ILE:HB	2:H:143:ARG:HD2	1.93	0.51
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.75	0.51
2:H:963:GLU:O	2:H:967:LEU:HD13	2.11	0.51
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.92	0.51
1:B:33:ARG:NE	1:B:197:ASP:HB2	2.26	0.51
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	1.92	0.51
3:D:63:GLY:O	3:D:98:ARG:NH2	2.42	0.51
3:D:179:LYS:H	3:D:179:LYS:HD3	1.76	0.51
3:D:474:LEU:HD13	3:D:478:LEU:HD13	1.93	0.51
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.91	0.51
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.92	0.51
5:Y:277:MET:HE3	5:Y:281:ARG:HG3	1.93	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
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.45	0.51
3:I:473:THR:HB	3:I:476:ALA:HB2	1.93	0.51
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.11	0.51
5:Y:519:LEU:HD13	5:Y:519:LEU:O	2.11	0.51
1:A:80:GLU:HB2	2:C:694:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASN:ND2	2:C:1217:THR:HG22	2.25	0.51
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.11	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
3:D:139:LEU:HD21	3:D:185:ILE:HD13	1.92	0.51
3:D:316:ILE:HG13	3:D:317:THR:N	2.26	0.51
5:X:384:LEU:O	5:X:384:LEU:HD13	2.10	0.51
1:F:118:ASP:OD1	1:F:119:GLY:N	2.44	0.51
3:I:325:LYS:HD3	5:Y:508:GLU:OE1	2.11	0.51
3:I:1261:LEU:CD2	3:I:1306:LEU:HD22	2.32	0.51
2:C:946:LEU:O	2:C:949:GLU:HG3	2.10	0.51
2:C:1141:LEU:H	2:C:1141:LEU:HD13	1.76	0.51
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.09	0.51
3:D:832:LYS:HB2	3:D:832:LYS:HZ2	1.76	0.51
3:D:1360:GLY:HA2	4:E:17:PHE:CZ	2.46	0.51
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.36	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
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.92	0.51
1:B:182:ARG:HD3	3:D:581:MET:HE1	1.92	0.50
2:C:12:ARG:O	2:C:13:LYS:HG2	2.11	0.50
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.47	0.50
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.46	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
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.11	0.50
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.35	0.50
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.93	0.50
3:I:910:ASN:HB3	4:J:15:ASN:OD1	2.11	0.50
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.42	0.50
1:A:250:ASP:HB3	1:A:253:LEU:HD13	1.93	0.50
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.46	0.50
2:C:1288:GLN:HE21	2:C:1288:GLN:CA	2.24	0.50
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.11	0.50
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.46	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
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.93	0.50
1:A:11:PRO:HD3	1:B:227:GLN:HG3	1.93	0.50
1:A:104:LYS:HD3	1:A:105:SER:N	2.26	0.50
2:C:818:VAL:HG22	2:C:819:SER:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.47	0.50
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.92	0.50
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.75	0.50
1:F:11:PRO:HG2	1:G:228:LEU:H	1.76	0.50
1:G:176:CYS:O	1:G:178:SER:N	2.42	0.50
2:H:590:PRO:O	2:H:659:GLN:NE2	2.45	0.50
2:H:1252:SER:HA	5:Y:524:GLU:HA	1.93	0.50
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.93	0.50
3:I:546:ALA:N	3:I:547:ARG:CA	2.71	0.50
3:I:1280:VAL:HA	3:I:1283:SER:HB2	1.94	0.50
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.11	0.50
4:J:13:ILE:HD11	4:J:19:LEU:HD23	1.94	0.50
1:A:134:THR:HG21	2:C:727:VAL:O	2.12	0.50
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.94	0.50
1:B:118:ASP:OD1	1:B:119:GLY:N	2.44	0.50
2:C:639:LYS:HE2	2:C:639:LYS:HA	1.93	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: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
2:H:442:VAL:HG12	2:H:443:ASP:H	1.77	0.50
1:A:317:ARG:C	1:A:318:LEU:HD13	2.37	0.50
1:B:9:LEU:H	1:B:9:LEU:HD23	1.77	0.50
2:C:1086:PRO:HG2	2:C:1094:VAL:HG21	1.94	0.50
2:C:1219:GLU:OE2	3:D:634:ARG:NH1	2.44	0.50
5:X:457:ILE:HG23	5:X:461:ASN:HD21	1.77	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:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.94	0.50
1:A:226:GLU:HB3	1:B:10:LYS:NZ	2.27	0.50
1:A:231:PHE:HZ	1:B:39:LEU:HD13	1.77	0.50
1:B:19:VAL:O	1:B:20:SER:HB3	2.12	0.50
3:D:393:THR:HG23	3:D:396:ALA:H	1.77	0.50
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.12	0.50
3:D:858:VAL:HB	3:D:859:PRO:CD	2.35	0.50
2:H:106:GLU:H	2:H:107:ARG:HA	1.77	0.50
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.46	0.50
3:I:128:LEU:HD13	3:I:189:LEU:HD23	1.94	0.50
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.77	0.50
1:B:176:CYS:O	1:B:178:SER:N	2.40	0.50
2:C:406:ASN:HB3	2:C:411:ARG:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.38	0.50
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.27	0.50
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.94	0.50
1:F:60:GLU:HG3	1:F:169:GLY:O	2.11	0.50
2:H:38:PHE:CE2	2:H:49:LEU:HD12	2.38	0.50
2:H:818:VAL:HG22	2:H:819:SER:H	1.76	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
3:D:62:PHE:O	3:D:101:ARG:HG3	2.12	0.50
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.92	0.50
3:D:610:ARG:CG	3:D:864:LEU:HD13	2.32	0.50
4:E:15:ASN:ND2	4:E:18:ASP:OD1	2.42	0.50
1:G:16:ILE:HG12	1:G:26:VAL:HG22	1.93	0.50
2:H:892:GLU:O	2:H:893:THR:OG1	2.25	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
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.26	0.50
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.94	0.50
2:C:163:LYS:HD3	2:C:163:LYS:N	2.16	0.50
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.41	0.50
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.12	0.50
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.11	0.50
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.12	0.50
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.94	0.50
3:I:843:VAL:HG11	3:I:897:HIS:HB3	1.94	0.50
3:I:918:ILE:HD13	3:I:919:ALA:N	2.27	0.50
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.94	0.49
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.94	0.49
2:C:741:MET:SD	2:C:741:MET:N	2.85	0.49
2:C:799:ASN:O	2:C:800:MET:HE3	2.12	0.49
2:C:820:GLU:HB2	2:C:1081:PRO:HA	1.94	0.49
2:C:836:LEU:HB3	2:C:918:LEU:HD21	1.93	0.49
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.19	0.49
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.93	0.49
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.36	0.49
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.94	0.49
2:H:908:GLU:H	2:H:908:GLU:CD	2.20	0.49
2:H:1006:GLU:H	2:H:1006:GLU:CD	2.20	0.49
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.94	0.49
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.46	0.49
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:279:ARG:NH2	5:Y:350:GLU:OE1	2.43	0.49
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.77	0.49
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.42	0.49
3:D:33:TRP:O	3:D:102:MET:HB2	2.11	0.49
3:D:452:LEU:HG	3:D:625:MET:SD	2.52	0.49
3:D:766:GLY:C	3:D:767:LEU:HD22	2.37	0.49
3:D:932:MET:SD	3:D:932:MET:N	2.75	0.49
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.93	0.49
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.11	0.49
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.12	0.49
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.94	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:H:637:ARG:HE	3:I:770:LEU:HD23	1.77	0.49
2:H:944:ARG:O	2:H:944:ARG:HD3	2.11	0.49
3:I:166:LEU:HD12	3:I:167:ASP:N	2.26	0.49
3:I:504:GLN:HG3	3:I:505:ASP:H	1.78	0.49
3:I:660:GLU:O	3:I:664:ILE:HG12	2.12	0.49
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.12	0.49
5:Y:278:ASP:OD1	5:Y:281:ARG:NH2	2.45	0.49
1:B:22:THR:HG22	1:B:208:ASN:O	2.12	0.49
2:C:27:LEU:O	2:C:528:ARG:NH1	2.44	0.49
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.94	0.49
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.42	0.49
3:D:613:GLY:O	3:D:617:THR:OG1	2.24	0.49
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.38	0.49
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.12	0.49
1:G:227:GLN:C	1:G:228:LEU:HD23	2.36	0.49
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.95	0.49
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.93	0.49
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.42	0.49
3:I:1171:GLY:N	3:I:1172:LYS:O	2.45	0.49
1:A:243:LYS:HD3	1:A:243:LYS:N	2.28	0.49
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.27	0.49
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.12	0.49
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.93	0.49
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.78	0.49
5:X:466:ILE:HD12	5:X:487:MET:HE2	1.94	0.49
2:H:384:LEU:O	2:H:388:LEU:HG	2.11	0.49
3:I:552:ILE:HD13	3:I:570:LYS:HB2	1.94	0.49
3:I:648:GLU:OE2	3:I:648:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.45	0.49
1:A:303:ILE:O	1:A:307:LEU:HD13	2.11	0.49
2:C:96:LEU:HD22	2:C:127:ILE:HD12	1.94	0.49
2:C:402:ARG:NH2	2:C:419:ILE:O	2.46	0.49
2:C:442:VAL:HG12	2:C:443:ASP:H	1.77	0.49
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	1.95	0.49
2:C:1303:LYS:HE2	2:C:1303:LYS:HA	1.93	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:H:678:ARG:HD3	2:H:681:MET:HG3	1.94	0.49
3:I:152:THR:O	3:I:154:LEU:N	2.42	0.49
4:J:60:ASN:H	4:J:63:ILE:HB	1.77	0.49
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.19	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:H:742:TYR:CB	2:H:743:PRO:HD3	2.40	0.49
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.93	0.49
3:I:664:ILE:HD12	3:I:681:LYS:HE3	1.93	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
2:C:1289:GLU:HB3	2:C:1315:MET:HE2	1.94	0.49
3:D:646:ILE:HD12	3:D:646:ILE:O	2.12	0.49
5:X:143:TYR:O	5:X:147:GLN:HG2	2.13	0.49
2:H:24:VAL:HG11	2:H:704:MET:HE1	1.95	0.49
2:H:639:LYS:HA	2:H:639:LYS:HE2	1.93	0.49
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.27	0.49
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.28	0.49
4:J:65:ASP:O	4:J:69:ARG:HG3	2.13	0.49
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.45	0.49
2:C:179:TYR:HE2	2:C:462:ASN:HD21	1.61	0.49
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.38	0.49
3:D:392:THR:HG22	5:X:603:ARG:HG2	1.94	0.49
3:D:797:THR:O	3:D:801:VAL:HG23	2.13	0.49
1:G:9:LEU:HD23	1:G:9:LEU:H	1.78	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
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.12	0.49
2:H:1332:SER:O	3:I:243:PRO:HG2	2.12	0.49
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.95	0.49
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.95	0.49
5:Y:561:MET:HA	5:Y:567:MET:SD	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.48	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
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.48	0.49
2:C:384:LEU:O	2:C:388:LEU:HG	2.11	0.49
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.48	0.49
2:C:516:ASP:OD1	2:C:518:ASN:ND2	2.45	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
3:D:856:ILE:HG13	3:D:857:LEU:O	2.12	0.49
2:H:524:ILE:HD12	2:H:708:VAL:HG13	1.93	0.49
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.20	0.49
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.47	0.49
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.45	0.49
4:J:5:THR:HB	4:J:7:GLN:H	1.78	0.49
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.93	0.49
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.93	0.49
3:D:394:ILE:HG21	5:X:536:THR:HA	1.94	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
5:X:301:ASN:O	5:X:305:LEU:HD13	2.13	0.49
3:I:316:ILE:HD13	3:I:316:ILE:N	2.28	0.49
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.12	0.49
4:J:5:THR:HB	4:J:7:GLN:HB2	1.94	0.49
5:Y:400:GLN:O	5:Y:404:LEU:HD13	2.12	0.49
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.78	0.48
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.95	0.48
5:X:600:HIS:H	5:X:601:PRO:CD	2.26	0.48
3:I:810:THR:OG1	3:I:811:GLU:N	2.44	0.48
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.94	0.48
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	1.95	0.48
2:C:1119:MET:O	2:C:1123:GLY:N	2.43	0.48
5:X:119:ILE:O	5:X:123:ILE:HG13	2.13	0.48
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.47	0.48
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.95	0.48
5:Y:582:VAL:CB	5:Y:586:ARG:HG2	2.43	0.48
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.43	0.48
3:D:166:LEU:HD12	3:D:167:ASP:N	2.28	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:310:GLU:O	5:X:344:LEU:HD23	2.14	0.48
2:H:36:GLN:O	2:H:39:ILE:HG22	2.13	0.48
2:H:119:GLU:HG2	2:H:120:GLN:N	2.27	0.48
2:H:489:PRO:HB2	2:H:492:MET:CB	2.39	0.48
2:H:1284:ALA:HB3	3:I:1361:THR:HB	1.94	0.48
3:I:197:GLU:O	3:I:201:LEU:HD23	2.12	0.48
3:I:363:LEU:O	3:I:363:LEU:HD23	2.13	0.48
3:I:393:THR:HG23	3:I:396:ALA:H	1.78	0.48
3:I:807:LEU:HD12	3:I:807:LEU:O	2.12	0.48
2:C:72:SER:O	2:C:98:VAL:HG23	2.13	0.48
2:C:91:THR:HG22	2:C:139:ASN:N	2.29	0.48
2:C:106:GLU:HG2	2:C:109:ALA:H	1.78	0.48
2:H:756:TYR:H	2:H:766:ASN:HB3	1.78	0.48
3:I:161:THR:HG22	3:I:162:GLU:H	1.78	0.48
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	1.95	0.48
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.14	0.48
1:A:207:THR:OG1	1:A:208:ASN:N	2.47	0.48
1:B:107:ILE:HD11	1:B:136:GLU:HG2	1.95	0.48
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.44	0.48
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.48	0.48
3:D:873:GLU:OE2	3:D:877:VAL:HB	2.13	0.48
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.27	0.48
5:X:28:ASN:HD22	5:X:29:ASP:N	2.11	0.48
5:X:493:LYS:O	5:X:497:VAL:HG23	2.13	0.48
1:G:227:GLN:C	1:G:229:GLU:H	2.21	0.48
2:H:38:PHE:O	2:H:39:ILE:HB	2.12	0.48
2:H:149:LEU:HD12	2:H:452:ARG:O	2.13	0.48
2:H:808:ASN:H	3:I:633:ALA:HB2	1.78	0.48
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.46	0.48
3:I:1255:VAL:O	3:I:1258:ARG:HB3	2.12	0.48
1:A:241:GLU:OE2	1:A:243:LYS:HE3	2.14	0.48
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.42	0.48
2:C:844:LYS:HB2	2:C:844:LYS:NZ	2.28	0.48
3:D:807:LEU:HD12	3:D:807:LEU:O	2.13	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
1:G:196:THR:OG1	3:I:443:GLU:HG3	2.14	0.48
3:I:56:LEU:HB3	3:I:250:ARG:NH2	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:385:LEU:CD2	3:I:411:ILE:HG13	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:579:LEU:O	3:I:579:LEU:HD13	2.14	0.48
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.44	0.48
3:I:646:ILE:HD12	3:I:646:ILE:O	2.13	0.48
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.14	0.48
5:Y:437:GLN:HA	5:Y:440:THR:HG22	1.94	0.48
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.96	0.48
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.49	0.48
2:C:891:GLY:O	2:C:893:THR:HG23	2.14	0.48
3:D:263:SER:HB2	5:X:507:MET:HE2	1.96	0.48
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.49	0.48
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.96	0.48
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.13	0.48
2:H:660:VAL:HG22	2:H:661:VAL:N	2.25	0.48
2:H:707:ALA:O	2:H:710:VAL:HG12	2.13	0.48
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.95	0.48
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.95	0.48
2:C:1286:THR:N	3:D:479:GLU:OE2	2.45	0.48
3:D:843:VAL:HG12	3:D:883:ARG:HD3	1.96	0.48
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.48	0.48
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.48	0.48
1:G:33:ARG:HE	1:G:197:ASP:HB2	1.78	0.48
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.78	0.48
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.47	0.48
3:I:513:MET:O	3:I:575:GLY:HA3	2.14	0.48
3:I:766:GLY:C	3:I:767:LEU:HD22	2.39	0.48
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.96	0.48
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.13	0.48
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	1.96	0.48
3:D:778:GLY:HA2	3:D:781:LYS:HE3	1.96	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
5:Y:297:MET:HE2	5:Y:326:TRP:CZ3	2.48	0.48
1:A:192:VAL:O	1:A:194:GLN:N	2.46	0.48
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.96	0.48
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.29	0.48
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.95	0.48
5:X:27:VAL:HA	5:X:30:HIS:HD2	1.78	0.48
2:H:73:TYR:HD2	2:H:74:ARG:H	1.58	0.48
2:H:163:LYS:H	2:H:163:LYS:CD	2.22	0.48
2:H:1335:ILE:HD11	3:I:22:ILE:CG1	2.44	0.48
2:H:1339:LEU:HD12	2:H:1339:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.14	0.48
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.96	0.47
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.96	0.47
3:D:840:LEU:HD12	3:D:840:LEU:O	2.14	0.47
5:X:24:TYR:O	5:X:26:GLU:N	2.45	0.47
2:H:152:SER:OG	2:H:404:LYS:NZ	2.24	0.47
2:H:459:MET:HE2	2:H:505:PHE:HE1	1.79	0.47
2:H:747:GLY:C	2:H:748:ILE:HG13	2.39	0.47
2:H:766:ASN:H	2:H:787:PRO:HG3	1.79	0.47
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.96	0.47
3:I:41:PRO:HG3	3:I:273:ILE:HG22	1.96	0.47
3:I:349:TYR:CD1	3:I:472:LEU:HD11	2.47	0.47
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.95	0.47
2:C:843:THR:HB	2:C:845:LEU:HD22	1.96	0.47
3:D:298:MET:HE3	5:X:402:LEU:HB3	1.95	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
5:X:130:VAL:O	5:X:134:VAL:HG23	2.14	0.47
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.94	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:H:1243:MET:HE3	3:I:372:MET:HB2	1.96	0.47
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.14	0.47
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.96	0.47
5:Y:545:HIS:NE2	5:Y:566:ASP:OD2	2.35	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:161:THR:HG22	3:D:162:GLU:H	1.78	0.47
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.43	0.47
5:X:141:ILE:HG13	5:X:256:PHE:CD1	2.50	0.47
5:X:277:MET:HE3	5:X:281:ARG:HG3	1.96	0.47
2:H:1117:LEU:HD21	2:H:1182:ILE:HG21	1.96	0.47
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.30	0.47
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.45	0.47
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.97	0.47
2:C:1058:ARG:HD3	2:C:1240:ASP:OD1	2.14	0.47
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.95	0.47
1:G:192:VAL:CG1	1:G:194:GLN:HG2	2.44	0.47
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.15	0.47
2:H:702:THR:HA	2:H:1184:THR:O	2.14	0.47
2:H:706:ARG:HA	2:H:793:GLU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:898:GLU:OE1	2:H:898:GLU:N	2.38	0.47
2:H:1120:ALA:HB1	2:H:1198:LEU:HB3	1.96	0.47
3:I:142:GLU:HA	3:I:180:MET:HE2	1.97	0.47
3:I:450:HIS:NE2	3:I:625:MET:SD	2.87	0.47
3:I:512:TYR:HD2	3:I:724:MET:HE1	1.78	0.47
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.27	0.47
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.14	0.47
2:C:839:VAL:HG13	2:C:1049:ILE:HG22	1.96	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:102:LEU:HG	1:G:115:ILE:HG12	1.96	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:316:ILE:HD13	3:I:316:ILE:H	1.79	0.47
3:I:608:CYS:O	3:I:612:LEU:HB2	2.14	0.47
3:I:840:LEU:HD12	3:I:840:LEU:O	2.14	0.47
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.49	0.47
3:D:789:LYS:HD2	3:D:932:MET:SD	2.54	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
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
2:H:841:ARG:NH1	3:I:256:ASP:HB3	2.28	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.65	0.47
2:C:59:ILE:HD11	2:C:63:SER:OG	2.15	0.47
2:C:119:GLU:HG2	2:C:120:GLN:N	2.29	0.47
2:C:403:MET:HG2	2:C:407:ARG:HH12	1.80	0.47
2:C:510:GLN:O	2:C:511:LEU:HB2	2.15	0.47
2:C:963:GLU:O	2:C:966:ILE:HG22	2.15	0.47
3:D:133:ARG:HB2	3:D:133:ARG:NH2	2.30	0.47
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.45	0.47
3:D:504:GLN:HG3	3:D:505:ASP:H	1.80	0.47
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.96	0.47
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.30	0.47
3:D:1292:LEU:HD21	3:I:1284:ARG:NH2	2.29	0.47
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.14	0.47
5:X:311:THR:HG21	5:X:348:GLU:CD	2.40	0.47
5:X:595:LEU:O	5:X:599:ARG:NH1	2.46	0.47
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.96	0.47
3:I:290:ILE:O	3:I:293:ARG:HG3	2.15	0.47
3:I:591:ILE:HD12	3:I:592:VAL:N	2.28	0.47
3:I:1196:LEU:HG	3:I:1210:ILE:HD11	1.95	0.47
3:I:1287:ILE:HA	3:I:1290:ARG:HG2	1.97	0.47
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.15	0.47
1:A:42:ALA:O	1:A:46:ILE:HG12	2.14	0.47
2:C:205:PRO:O	2:C:208:ILE:HG22	2.15	0.47
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.44	0.47
2:C:533:LEU:HD23	2:C:533:LEU:H	1.80	0.47
2:C:751:TYR:HE1	2:C:783:LEU:HD12	1.79	0.47
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.28	0.47
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.80	0.47
3:D:552:ILE:HD13	3:D:570:LYS:HB2	1.97	0.47
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.97	0.47
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.14	0.47
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.96	0.47
2:H:106:GLU:HG2	2:H:109:ALA:H	1.78	0.47
2:H:130:MET:SD	2:H:134:GLY:HA2	2.54	0.47
3:I:370:LYS:HA	3:I:441:LEU:HD12	1.97	0.47
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.78	0.47
3:I:1341:ARG:HD3	3:I:1343:GLU:CD	2.39	0.47
2:C:127:ILE:HG22	2:C:502:VAL:HG11	1.97	0.47
2:C:747:GLY:C	2:C:748:ILE:HG13	2.40	0.47
2:C:893:THR:O	2:C:895:LEU:N	2.40	0.47
3:D:316:ILE:O	3:D:317:THR:OG1	2.28	0.47
5:X:346:GLN:O	5:X:350:GLU:HG3	2.15	0.47
5:X:452:ILE:HG21	5:X:457:ILE:HG12	1.97	0.47
5:X:545:HIS:NE2	5:X:566:ASP:OD2	2.48	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
3:I:120:LEU:CB	3:I:121:PRO:CD	2.90	0.47
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.38	0.47
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.79	0.47
3:D:41:PRO:HG3	3:D:273:ILE:HG22	1.96	0.47
3:D:660:GLU:O	3:D:664:ILE:HG12	2.15	0.47
5:X:115:GLY:O	5:X:119:ILE:HG12	2.15	0.47
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.80	0.47
1:F:45:ARG:NE	1:G:38:THR:OG1	2.49	0.47
2:H:356:THR:HG21	2:H:362:ALA:HA	1.96	0.47
2:H:848:GLU:CD	2:H:888:THR:HG22	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.97	0.47
3:I:8:LEU:HD23	3:I:8:LEU:N	2.30	0.47
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.40	0.46
2:C:434:ASP:HB3	2:C:439:LYS:HB2	1.97	0.46
2:C:756:TYR:H	2:C:766:ASN:CB	2.28	0.46
2:C:829:THR:HG22	2:C:1059:ARG:HG2	1.98	0.46
2:C:886:LYS:HD3	2:C:916:SER:O	2.15	0.46
3:D:56:LEU:HB3	3:D:250:ARG:HH21	1.80	0.46
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.30	0.46
2:H:317:LEU:HD13	2:H:322:LEU:HD21	1.97	0.46
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.81	0.46
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.41	0.46
2:H:895:LEU:HD21	2:H:903:ARG:CZ	2.45	0.46
2:H:975:ILE:HD13	2:H:975:ILE:O	2.14	0.46
3:I:515:ARG:HH22	3:I:717:VAL:C	2.21	0.46
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.45	0.46
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.15	0.46
2:C:53:PHE:HD1	2:C:57:PHE:CD2	2.33	0.46
2:C:342:ASP:O	2:C:437:ASN:ND2	2.48	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
3:D:8:LEU:HD23	3:D:8:LEU:N	2.30	0.46
3:D:396:ALA:CB	5:X:606:VAL:HG11	2.46	0.46
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.45	0.46
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.98	0.46
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.96	0.46
5:X:511:ILE:HG23	5:X:512:GLY:N	2.28	0.46
1:G:47:LEU:HD13	1:G:205:MET:HE2	1.97	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:227:PHE:O	3:I:230:SER:OG	2.25	0.46
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.45	0.46
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	1.97	0.46
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.27	0.46
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.98	0.46
3:D:240:THR:HG23	3:D:241:VAL:HG23	1.97	0.46
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.97	0.46
3:D:415:VAL:HG23	3:D:416:ILE:HG23	1.97	0.46
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.15	0.46
1:F:79:LEU:HD12	2:H:756:TYR:OH	2.16	0.46
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:12:THR:O	3:I:13:LYS:HD2	2.15	0.46
3:I:12:THR:C	3:I:13:LYS:HD2	2.40	0.46
3:I:797:THR:O	3:I:801:VAL:HG23	2.15	0.46
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.15	0.46
2:C:697:LYS:HG3	2:C:698:PRO:HD2	1.98	0.46
2:C:1166:ASP:C	2:C:1168:GLU:H	2.23	0.46
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.14	0.46
3:D:27:PRO:O	3:D:31:ARG:HD3	2.15	0.46
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.80	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
5:X:556:ALA:O	5:X:560:ARG:HB2	2.16	0.46
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.96	0.46
3:I:822:MET:HG2	3:I:839:VAL:HG22	1.96	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
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.28	0.46
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.98	0.46
2:C:51:ALA:C	2:C:53:PHE:H	2.23	0.46
2:C:622:ASN:OD1	2:C:623:LEU:N	2.49	0.46
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.46	0.46
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.49	0.46
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	1.97	0.46
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.30	0.46
3:D:850:LYS:HD2	3:D:851:PRO:CD	2.37	0.46
5:X:379:MET:CE	5:X:379:MET:HA	2.46	0.46
1:F:80:GLU:HA	2:H:694:ARG:HH22	1.80	0.46
1:G:76:GLU:OE2	1:G:131:CYS:HA	2.16	0.46
2:H:178:PRO:HA	2:H:397:LEU:HD23	1.97	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
5:Y:105:MET:SD	5:Y:388:ILE:HD12	2.55	0.46
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.48	0.46
2:C:216:THR:O	2:C:220:ILE:HG13	2.15	0.46
2:C:773:LEU:C	2:C:773:LEU:HD22	2.41	0.46
3:D:378:LYS:HD2	3:D:382:TYR:OH	2.14	0.46
3:D:514:THR:HG21	3:D:595:ALA:O	2.14	0.46
3:D:550:VAL:HG23	3:D:552:ILE:HD11	1.96	0.46
2:H:517:GLN:HE21	2:H:760:ASN:H	1.64	0.46
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.51	0.46
2:H:998:LEU:O	2:H:998:LEU:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1042:LEU:HD13	2:H:1042:LEU:N	2.27	0.46
2:H:1142:ARG:HE	2:H:1169:VAL:HB	1.80	0.46
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.30	0.46
3:I:298:MET:HE3	5:Y:402:LEU:HB3	1.98	0.46
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.45	0.46
3:I:704:GLU:HB2	3:I:718:SER:HG	1.81	0.46
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.96	0.46
4:J:26:ARG:HD3	4:J:64:LEU:HD21	1.98	0.46
5:Y:608:ARG:HB3	5:Y:608:ARG:NH1	2.31	0.46
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.98	0.46
2:C:804:PHE:O	3:D:638:SER:OG	2.31	0.46
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.98	0.46
3:D:143:SER:HB2	5:X:100:MET:HE2	1.96	0.46
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.97	0.46
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.16	0.46
5:X:45:ILE:C	5:X:45:ILE:HD12	2.41	0.46
2:H:902:LEU:HD11	5:Y:608:ARG:HA	1.97	0.46
2:H:1297:ASP:OD1	2:H:1300:GLY:HA3	2.16	0.46
3:I:154:LEU:HD21	3:I:160:LEU:HD21	1.98	0.46
3:I:856:ILE:HG13	3:I:857:LEU:O	2.14	0.46
3:I:1221:LEU:HD23	3:I:1229:VAL:HG11	1.97	0.46
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.26	0.46
2:C:131:THR:HG22	2:C:135:THR:HG22	1.96	0.46
2:C:682:GLY:HA2	2:C:685:MET:HG2	1.97	0.46
2:C:1211:ARG:HB2	2:C:1220:GLN:HE21	1.80	0.46
2:C:1335:ILE:HD11	3:D:22:ILE:HG13	1.98	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
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.15	0.46
5:X:278:ASP:O	5:X:282:THR:OG1	2.24	0.46
5:X:373:ARG:HG3	5:X:377:LYS:HE3	1.97	0.46
5:X:379:MET:HA	5:X:379:MET:HE2	1.98	0.46
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.96	0.46
3:I:33:TRP:O	3:I:102:MET:HB2	2.16	0.46
3:I:245:LEU:CD1	3:I:246:PRO:HD2	2.45	0.46
1:B:31:LEU:HB2	1:B:199:ASP:O	2.16	0.46
1:B:178:SER:HA	1:B:179:PRO:HD3	1.85	0.46
2:C:372:PRO:CB	5:X:34:ASP:HB3	2.45	0.46
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:966:ILE:HG23	2:C:967:LEU:HD12	1.98	0.46
3:D:66:LYS:HB2	3:D:69:GLU:HG2	1.97	0.46
3:D:114:ILE:HG21	3:D:308:ASP:HB3	1.98	0.46
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.46	0.46
3:D:416:ILE:HD12	3:D:416:ILE:O	2.16	0.46
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.16	0.46
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.15	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
2:H:799:ASN:O	2:H:800:MET:HE3	2.16	0.46
2:H:1296:ASP:OD1	3:I:345:LYS:HD2	2.15	0.46
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.97	0.46
1:A:88:LEU:HD22	1:A:90:VAL:HG23	1.98	0.45
1:B:16:ILE:HG12	1:B:26:VAL:HG22	1.97	0.45
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.80	0.45
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.98	0.45
2:C:876:GLU:N	2:C:876:GLU:OE2	2.49	0.45
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.46	0.45
3:D:572:THR:HG22	3:D:594:GLN:OE1	2.16	0.45
3:D:720:ASN:ND2	3:D:720:ASN:O	2.49	0.45
3:D:809:VAL:HG13	3:D:912:GLY:H	1.80	0.45
4:E:4:VAL:O	4:E:5:THR:OG1	2.20	0.45
5:X:101:TYR:OH	5:X:384:LEU:HD11	2.16	0.45
5:X:437:GLN:HA	5:X:440:THR:HG22	1.97	0.45
1:F:10:LYS:HD2	1:G:226:GLU:O	2.16	0.45
2:H:127:ILE:HD13	2:H:127:ILE:N	2.28	0.45
2:H:1146:GLN:CD	2:H:1160:ASP:HB2	2.41	0.45
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.30	0.45
3:I:508:LEU:O	3:I:508:LEU:HD23	2.16	0.45
3:I:909:ILE:HD12	3:I:909:ILE:O	2.16	0.45
1:A:222:THR:O	1:A:226:GLU:HG3	2.17	0.45
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.79	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
3:D:12:THR:C	3:D:13:LYS:HD2	2.42	0.45
3:D:512:TYR:CD2	3:D:724:MET:HE1	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.97	0.45
3:I:113:HIS:CE1	3:I:115:TRP:HB2	2.51	0.45
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.81	0.45
3:I:430:HIS:HA	3:I:921:GLN:HB3	1.97	0.45
3:I:813:ASP:OD1	3:I:896:ALA:HB3	2.16	0.45
3:I:1148:ARG:NH2	3:I:1148:ARG:HB2	2.32	0.45
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.16	0.45
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.48	0.45
1:A:234:LEU:N	1:A:234:LEU:HD12	2.32	0.45
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.98	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
2:C:462:ASN:O	2:C:466:VAL:HG23	2.17	0.45
2:C:777:VAL:HG21	2:C:783:LEU:HD21	1.98	0.45
2:C:963:GLU:O	2:C:967:LEU:HD13	2.16	0.45
3:D:423:LEU:HB3	3:D:466:MET:HE2	1.99	0.45
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.47	0.45
3:D:504:GLN:HA	3:D:730:ALA:HA	1.98	0.45
3:D:579:LEU:O	3:D:579:LEU:HD13	2.16	0.45
5:X:250:LEU:O	5:X:254:GLU:HG2	2.16	0.45
5:X:477:GLU:CD	5:X:477:GLU:H	2.25	0.45
2:H:768:MET:O	2:H:785:ASP:N	2.47	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
3:I:640:GLY:N	3:I:643:ASP:OD2	2.45	0.45
3:I:1251:LYS:O	3:I:1255:VAL:HG23	2.16	0.45
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.16	0.45
2:C:43:PRO:HD3	2:C:47:TYR:HD2	1.78	0.45
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.51	0.45
2:C:580:GLN:HG2	2:C:581:THR:N	2.32	0.45
2:C:660:VAL:HG22	2:C:661:VAL:N	2.27	0.45
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.98	0.45
3:D:655:SER:HA	3:D:658:GLU:HG2	1.96	0.45
4:E:44:ASP:HB2	4:E:52:ARG:HH21	1.82	0.45
1:F:79:LEU:O	1:F:83:LEU:HD13	2.17	0.45
2:H:73:TYR:N	2:H:73:TYR:CD2	2.85	0.45
2:H:680:LEU:HD13	3:I:783:LEU:HD12	1.98	0.45
3:I:139:LEU:C	3:I:139:LEU:HD22	2.41	0.45
2:C:57:PHE:HE1	2:C:472:GLU:HA	1.80	0.45
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.44	0.45
3:D:526:VAL:HG12	3:D:549:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:915:ILE:O	3:D:918:ILE:HG23	2.17	0.45
2:H:54:ARG:N	2:H:55:SER:C	2.75	0.45
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.99	0.45
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.31	0.45
2:H:876:GLU:N	2:H:876:GLU:OE2	2.49	0.45
2:H:972:PHE:HA	2:H:975:ILE:HG22	1.98	0.45
3:I:51:PRO:HB3	3:I:57:PHE:O	2.16	0.45
3:I:155:GLU:CD	3:I:155:GLU:H	2.25	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
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.16	0.45
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.15	0.45
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.17	0.45
1:A:33:ARG:HG2	1:A:199:ASP:OD2	2.16	0.45
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.32	0.45
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.32	0.45
2:C:465:ARG:O	2:C:469:VAL:HG23	2.16	0.45
2:C:998:LEU:HD13	2:C:998:LEU:O	2.17	0.45
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.81	0.45
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.65	0.45
2:C:1319:MET:HE3	2:C:1324:ASN:HB2	1.98	0.45
3:D:260:PHE:O	5:X:504:PRO:HG2	2.16	0.45
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.30	0.45
3:D:1287:ILE:HA	3:D:1290:ARG:HG2	1.98	0.45
1:F:151:GLY:O	1:F:177:TYR:HB2	2.17	0.45
2:H:1116:HIS:CE1	2:H:1226:THR:HG23	2.50	0.45
3:I:545:HIS:HA	3:I:546:ALA:HA	1.77	0.45
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.56	0.45
2:C:812:PHE:H	2:C:815:SER:HB2	1.81	0.45
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.97	0.45
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.99	0.45
5:X:139:GLU:HG3	5:X:351:THR:HA	1.98	0.45
1:F:158:ARG:HE	1:F:172:LEU:HD13	1.81	0.45
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.97	0.45
2:H:714:VAL:HG23	2:H:787:PRO:HD2	1.98	0.45
2:H:818:VAL:HG22	2:H:819:SER:N	2.32	0.45
3:I:205:LEU:HB3	3:I:217:LEU:HB3	1.99	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
3:D:531:LYS:HB3	3:D:531:LYS:NZ	2.32	0.45
3:D:619:ILE:HD13	7:D:1503:G4P:O3D	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.80	0.45
1:F:166:ARG:HA	1:F:167:PRO:HD2	1.87	0.45
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.38	0.45
2:H:135:THR:OG1	2:H:143:ARG:O	2.29	0.45
2:H:622:ASN:OD1	2:H:623:LEU:N	2.50	0.45
2:H:1294:LYS:HE3	3:I:349:TYR:HB2	1.99	0.45
3:I:326:SER:O	3:I:330:MET:HG3	2.16	0.45
3:I:610:ARG:HG2	3:I:864:LEU:HD22	1.98	0.45
3:I:693:VAL:HG21	3:I:743:MET:HE3	1.97	0.45
1:A:282:VAL:HG22	1:A:316:MET:HE2	1.98	0.45
1:B:64:VAL:HG12	1:B:171:LEU:HD11	1.98	0.45
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.45
2:C:556:GLY:O	2:C:579:ALA:HB2	2.16	0.45
2:C:800:MET:HE2	2:C:1095:ASP:OD2	2.17	0.45
2:C:818:VAL:HG22	2:C:819:SER:N	2.32	0.45
2:C:845:LEU:HD13	2:C:845:LEU:N	2.28	0.45
3:D:473:THR:HB	3:D:476:ALA:CB	2.47	0.45
3:D:494:ALA:HA	3:D:1252:HIS:HE1	1.82	0.45
3:D:640:GLY:N	3:D:643:ASP:OD2	2.50	0.45
5:X:101:TYR:CE2	5:X:388:ILE:HD11	2.45	0.45
5:X:120:ALA:CB	5:X:421:TYR:HB3	2.44	0.45
5:X:123:ILE:O	5:X:127:ILE:HG12	2.17	0.45
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.98	0.45
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.98	0.45
1:G:185:TYR:HA	1:G:202:VAL:O	2.17	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: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
3:D:824:PRO:O	3:D:826:ILE:HG13	2.16	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:H:1192:GLU:O	2:H:1196:LYS:HD3	2.17	0.45
3:I:457:TYR:CE2	3:I:466:MET:HE1	2.52	0.45
3:I:1266:ILE:HA	3:I:1302:TYR:HA	1.99	0.45
5:Y:562:ARG:HG3	5:Y:591:GLU:CD	2.42	0.45
1:A:284:ARG:NH1	1:A:288:GLU:HG3	2.32	0.44
1:B:228:LEU:C	1:B:228:LEU:HD12	2.43	0.44
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.46	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:269:TYR:HA	3:I:272:VAL:HG12	1.99	0.44
3:I:531:LYS:HB3	3:I:531:LYS:NZ	2.32	0.44
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.16	0.44
1:A:53:GLY:HA3	1:A:179:PRO:HG3	1.98	0.44
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.18	0.44
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.99	0.44
1:G:195:ARG:HH21	1:G:198:LEU:HD21	1.81	0.44
2:H:946:LEU:O	2:H:949:GLU:HG3	2.16	0.44
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.98	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
3:I:860:ARG:HD3	3:I:866:GLU:OE2	2.17	0.44
3:I:909:ILE:H	3:I:909:ILE:HG13	1.56	0.44
3:I:911:LYS:HD2	3:I:911:LYS:O	2.17	0.44
1:B:151:GLY:O	1:B:177:TYR:HB2	2.18	0.44
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.33	0.44
2:C:161:LYS:NZ	2:C:161:LYS:HB3	2.32	0.44
2:C:702:THR:HA	2:C:1184:THR:O	2.17	0.44
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.97	0.44
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.47	0.44
3:D:139:LEU:C	3:D:139:LEU:HD22	2.42	0.44
3:D:217:LEU:O	3:D:221:ILE:HG12	2.16	0.44
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.51	0.44
1:F:207:THR:HG23	1:F:209:GLY:H	1.82	0.44
2:H:685:MET:HE1	2:H:1073:LYS:HE2	1.98	0.44
2:H:994:ARG:HD3	2:H:994:ARG:N	2.31	0.44
3:I:214:ARG:O	3:I:218:THR:HG22	2.17	0.44
3:I:681:LYS:O	3:I:685:ILE:HG13	2.18	0.44
3:I:720:ASN:ND2	3:I:720:ASN:O	2.50	0.44
3:I:1358:PRO:HB3	3:I:1366:HIS:CG	2.52	0.44
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.18	0.44
5:Y:451:ARG:O	5:Y:452:ILE:HG13	2.18	0.44
1:A:223:ILE:HD13	1:B:8:PHE:CE1	2.52	0.44
1:B:227:GLN:C	1:B:229:GLU:H	2.20	0.44
2:C:169:LYS:HD3	2:C:169:LYS:HA	1.80	0.44
2:C:813:GLU:HG2	3:D:504:GLN:NE2	2.31	0.44
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.33	0.44
3:D:154:LEU:HD21	3:D:160:LEU:HD21	1.99	0.44
3:D:252:LEU:HD23	3:D:252:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:356:THR:O	3:D:448:GLN:HA	2.17	0.44
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.31	0.44
1:F:182:ARG:NH1	2:H:1092:THR:HG22	2.33	0.44
1:G:33:ARG:NH1	2:H:820:GLU:OE2	2.51	0.44
2:H:693:LEU:HD13	2:H:693:LEU:C	2.41	0.44
2:H:1140:LYS:HE2	2:H:1166:ASP:HB3	1.99	0.44
3:I:221:ILE:HG13	3:I:222:LYS:N	2.33	0.44
3:I:240:THR:HG23	3:I:241:VAL:HG23	1.98	0.44
3:I:899:TYR:CD2	3:I:909:ILE:HG12	2.53	0.44
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.16	0.44
5:Y:448:ARG:NH1	5:Y:452:ILE:HD12	2.32	0.44
5:Y:544:THR:O	5:Y:548:LEU:HG	2.17	0.44
2:C:56:VAL:HB	2:C:57:PHE:H	1.51	0.44
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.51	0.44
3:D:525:MET:O	3:D:535:ARG:NH2	2.50	0.44
3:D:664:ILE:CD1	3:D:681:LYS:HE3	2.47	0.44
3:D:678:ARG:HD2	3:D:678:ARG:C	2.43	0.44
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.50	0.44
1:G:65:LEU:HD23	1:G:65:LEU:N	2.27	0.44
2:H:27:LEU:O	2:H:528:ARG:NH1	2.44	0.44
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.35	0.44
2:H:773:LEU:C	2:H:773:LEU:HD22	2.42	0.44
2:H:1166:ASP:C	2:H:1168:GLU:H	2.25	0.44
3:I:217:LEU:O	3:I:221:ILE:HG12	2.17	0.44
3:I:543:SER:O	3:I:574:VAL:HB	2.18	0.44
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.18	0.44
1:B:19:VAL:O	1:B:20:SER:CB	2.65	0.44
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.99	0.44
2:C:740:GLU:CD	2:C:740:GLU:H	2.26	0.44
2:C:812:PHE:N	2:C:815:SER:HB2	2.31	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:19:ALA:HB1	3:D:1343:GLU:HB3	1.97	0.44
3:D:514:THR:HG23	3:D:576:ARG:HE	1.83	0.44
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.47	0.44
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.83	0.44
5:X:133:SER:OG	5:X:365:MET:HB2	2.17	0.44
5:X:283:GLN:CD	5:X:343:LYS:HD2	2.42	0.44
5:X:305:LEU:HD21	5:X:322:MET:HE1	1.98	0.44
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.83	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)
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.98	0.44
3:I:131:PRO:CG	3:I:135:ILE:HD13	2.45	0.44
3:I:512:TYR:CD2	3:I:724:MET:HE1	2.53	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:707:ALA:O	2:C:710:VAL:HG12	2.18	0.44
3:D:107:LEU:HD23	3:D:299:LEU:HD21	1.99	0.44
3:D:539:SER:OG	3:D:540:GLY:N	2.51	0.44
3:D:1297:LYS:HE3	3:I:1267:VAL:HB	1.99	0.44
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.99	0.44
2:H:71:VAL:O	2:H:72:SER:OG	2.29	0.44
2:H:500:ALA:O	2:H:504:GLU:HB2	2.18	0.44
2:H:892:GLU:C	2:H:894:GLN:H	2.26	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
5:Y:586:ARG:HH22	5:Y:590:ILE:HD11	1.82	0.44
5:Y:604:SER:HA	5:Y:607:LEU:HB2	2.00	0.44
1:A:110:VAL:HG21	1:A:140:ILE:HD11	2.00	0.44
2:C:80:PHE:O	2:C:84:GLU:HB3	2.18	0.44
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.53	0.44
2:C:475:VAL:HG23	2:C:492:MET:SD	2.58	0.44
2:C:1212:LEU:HD11	2:C:1227:VAL:HG21	2.00	0.44
2:C:1244:HIS:HB3	2:C:1265:PHE:CG	2.53	0.44
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.17	0.44
3:D:1226:VAL:HA	3:D:1229:VAL:HG12	2.00	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
1:G:64:VAL:HG13	1:G:69:SER:OG	2.18	0.44
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.41	0.44
2:H:866:ASP:HA	2:H:872:TYR:OH	2.18	0.44
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.18	0.44
3:I:149:GLY:HA2	3:I:156:ARG:HG2	2.00	0.44
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.86	0.44
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.82	0.44
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	2.00	0.44
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.17	0.44
1:A:88:LEU:HD22	1:A:90:VAL:CG2	2.48	0.44
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.98	0.44
2:C:475:VAL:O	2:C:479:LEU:HB2	2.18	0.44
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1042:LEU:HB2	2:C:1043:ALA:H	1.70	0.44
2:C:1322:SER:OG	3:D:345:LYS:NZ	2.37	0.44
3:D:221:ILE:HG13	3:D:222:LYS:N	2.33	0.44
3:D:596:LEU:N	3:D:596:LEU:HD23	2.33	0.44
4:E:60:ASN:H	4:E:63:ILE:HB	1.83	0.44
2:H:505:PHE:O	2:H:512:SER:OG	2.30	0.44
2:H:681:MET:O	2:H:685:MET:HG2	2.17	0.44
2:H:685:MET:CE	2:H:1073:LYS:HE2	2.48	0.44
2:H:1043:ALA:C	2:H:1045:GLY:H	2.24	0.44
3:I:138:VAL:O	3:I:143:SER:HB3	2.18	0.44
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.17	0.44
3:I:526:VAL:CG1	3:I:549:LYS:HB2	2.48	0.44
5:Y:264:LYS:HD2	5:Y:264:LYS:N	2.33	0.44
1:A:300:LEU:O	1:A:300:LEU:HD13	2.18	0.43
1:A:313:SER:OG	1:A:314:LEU:N	2.50	0.43
2:C:22:LEU:HD13	2:C:23:ASP:O	2.18	0.43
2:C:801:ARG:NH1	2:C:1093:PRO:O	2.51	0.43
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.47	0.43
3:D:580:TRP:HE1	3:D:589:TYR:HB3	1.82	0.43
3:D:746:LEU:H	3:D:746:LEU:HD22	1.82	0.43
3:D:1369:ARG:HB3	3:D:1369:ARG:HH11	1.83	0.43
5:X:119:ILE:HG21	5:X:379:MET:HG2	1.98	0.43
5:X:264:LYS:HD2	5:X:264:LYS:N	2.33	0.43
2:H:365:GLU:OE2	2:H:368:ARG:NH2	2.51	0.43
2:H:582:ASN:HD22	2:H:588:GLU:CD	2.26	0.43
2:H:800:MET:HG2	2:H:1096:ILE:HD13	2.00	0.43
2:H:1109:ILE:HG12	3:I:644:MET:SD	2.58	0.43
3:I:288:PRO:O	3:I:292:VAL:HG12	2.18	0.43
3:I:317:THR:H	3:I:324:LEU:HD21	1.83	0.43
3:I:800:LEU:O	3:I:803:VAL:HG12	2.18	0.43
4:J:48:VAL:O	4:J:52:ARG:HG3	2.18	0.43
2:C:73:TYR:N	2:C:73:TYR:CD2	2.86	0.43
2:C:1332:SER:O	3:D:243:PRO:HG2	2.18	0.43
3:D:99:ARG:HA	3:D:248:ASP:HB2	2.00	0.43
3:D:138:VAL:O	3:D:143:SER:HB3	2.18	0.43
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.81	0.43
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.48	0.43
3:D:425:ARG:NH2	3:D:464:ASP:OD2	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
2:H:153:PRO:HD2	2:H:404:LYS:HZ1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:923:GLY:HA2	3:I:371:LYS:HE3	2.00	0.43
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.33	0.43
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.99	0.43
5:Y:584:ARG:O	5:Y:587:ILE:HG22	2.17	0.43
1:A:310:ARG:HA	1:A:310:ARG:HE	1.83	0.43
2:C:71:VAL:O	2:C:72:SER:OG	2.32	0.43
2:C:442:VAL:HG12	2:C:443:ASP:N	2.33	0.43
2:C:1029:LEU:O	2:C:1032:LYS:HG3	2.18	0.43
3:D:318:GLY:C	3:D:320:ASN:H	2.26	0.43
3:D:450:HIS:HE2	3:D:625:MET:CE	2.30	0.43
3:D:488:ASN:HD21	4:E:6:VAL:CG1	2.32	0.43
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.82	0.43
5:X:35:ILE:HG23	5:X:36:VAL:N	2.33	0.43
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.53	0.43
2:H:964:LEU:HD12	2:H:1025:PHE:CG	2.53	0.43
3:I:205:LEU:HB3	3:I:217:LEU:HD13	2.00	0.43
3:I:252:LEU:HD23	3:I:252:LEU:N	2.31	0.43
3:I:589:TYR:O	3:I:591:ILE:HG13	2.19	0.43
3:I:1194:ARG:N	3:I:1194:ARG:HD2	2.33	0.43
1:A:248:GLU:OE1	1:A:248:GLU:N	2.50	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
3:D:155:GLU:H	3:D:155:GLU:CD	2.25	0.43
3:D:290:ILE:O	3:D:293:ARG:HG3	2.18	0.43
3:D:1322:ALA:HB1	3:D:1326:GLN:HE21	1.82	0.43
4:E:16:ARG:O	4:E:19:LEU:HB3	2.18	0.43
5:X:551:LEU:HD22	5:X:597:LYS:HD2	2.01	0.43
1:G:51:MET:HA	1:G:52:PRO:HD3	1.87	0.43
2:H:49:LEU:HG	2:H:461:GLU:HB2	2.01	0.43
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.53	0.43
2:H:735:LYS:HA	2:H:748:ILE:HA	2.01	0.43
2:H:840:SER:HB3	2:H:850:ILE:HD11	2.00	0.43
2:H:1058:ARG:HD3	2:H:1240:ASP:OD1	2.19	0.43
2:H:1268:GLN:NE2	3:I:352:ARG:HD3	2.34	0.43
3:I:233:LYS:CD	3:I:234:PRO:HD2	2.47	0.43
3:I:539:SER:OG	3:I:540:GLY:N	2.50	0.43
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.54	0.43
5:Y:281:ARG:HD3	5:Y:359:LYS:HZ3	1.84	0.43
5:Y:573:LEU:HD22	5:Y:588:ARG:HB2	1.99	0.43
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.58	0.43
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:VAL:HG13	2:C:22:LEU:N	2.33	0.43
2:C:221:LEU:HD21	2:C:314:ASN:HD22	1.83	0.43
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.53	0.43
3:D:235:GLU:OE1	3:D:235:GLU:N	2.52	0.43
3:D:620:PHE:O	3:D:624:ILE:HG23	2.18	0.43
3:D:1303:SER:HB2	3:I:1297:LYS:HG2	2.01	0.43
1:F:51:MET:HA	1:F:52:PRO:HD3	1.82	0.43
2:H:51:ALA:C	2:H:53:PHE:H	2.25	0.43
2:H:812:PHE:CD2	2:H:813:GLU:HG3	2.53	0.43
2:H:1185:PRO:HB2	2:H:1186:VAL:H	1.64	0.43
3:I:385:LEU:HD21	3:I:411:ILE:HG13	2.00	0.43
5:Y:240:ARG:O	5:Y:242:HIS:N	2.51	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
1:A:167:PRO:HG2	1:A:170:ARG:HG3	2.00	0.43
1:A:310:ARG:HA	1:A:310:ARG:NE	2.34	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
3:D:1341:ARG:HH21	3:D:1343:GLU:CD	2.25	0.43
5:X:333:VAL:HG22	5:X:336:GLU:HB2	2.00	0.43
2:H:127:ILE:O	2:H:127:ILE:HG12	2.19	0.43
2:H:153:PRO:HD2	2:H:452:ARG:HD3	1.99	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:HA	2:H:1276:TRP:HE3	1.84	0.43
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.80	0.43
3:I:147:ILE:HG23	3:I:156:ARG:C	2.44	0.43
3:I:423:LEU:HG	3:I:468:VAL:HG12	2.00	0.43
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.31	0.43
1:A:79:LEU:O	1:A:83:LEU:HD13	2.18	0.43
2:C:510:GLN:C	2:C:512:SER:H	2.27	0.43
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.53	0.43
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	2.00	0.43
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.19	0.43
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.43
2:C:1340:GLU:OE2	3:D:1341:ARG:NH1	2.31	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:G:227:GLN:O	1:G:229:GLU:N	2.52	0.43
2:H:843:THR:HB	2:H:845:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:866:ASP:HA	2:H:872:TYR:CZ	2.54	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:A:11:PRO:HA	1:A:30:PRO:O	2.18	0.43
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.46	0.43
1:B:232:VAL:O	1:B:233:ASP:HB2	2.18	0.43
2:C:348:SER:O	2:C:352:ARG:HG3	2.19	0.43
2:C:843:THR:HB	2:C:845:LEU:CD2	2.49	0.43
3:D:688:ALA:O	3:D:692:ARG:HG2	2.18	0.43
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.48	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:I:161:THR:HG22	3:I:162:GLU:N	2.34	0.43
3:I:205:LEU:HD13	3:I:217:LEU:CD2	2.48	0.43
3:I:239:LEU:HD12	3:I:239:LEU:O	2.19	0.43
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.49	0.43
3:I:1261:LEU:HD21	3:I:1306:LEU:CD2	2.36	0.43
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.18	0.43
5:Y:562:ARG:HG3	5:Y:591:GLU:OE1	2.19	0.43
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.52	0.43
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.49	0.43
2:C:958:LYS:O	2:C:962:GLU:HG2	2.19	0.43
3:D:173:GLY:O	3:D:175:GLU:HG3	2.18	0.43
3:D:658:GLU:HA	3:D:661:VAL:CG1	2.48	0.43
5:X:465:ARG:O	5:X:468:ARG:HG2	2.19	0.43
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.83	0.43
2:H:617:ALA:HB2	2:H:650:VAL:HG21	1.99	0.43
2:H:1233:LEU:HD12	2:H:1233:LEU:O	2.19	0.43
3:I:596:LEU:N	3:I:596:LEU:HD23	2.33	0.43
5:Y:596:ARG:HH21	5:Y:599:ARG:CZ	2.32	0.43
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.84	0.43
1:B:65:LEU:HD23	1:B:65:LEU:N	2.33	0.43
1:B:179:PRO:HB2	1:B:211:ILE:HG22	2.00	0.43
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.45	0.43
2:C:88:ARG:HB3	2:C:88:ARG:NH1	2.34	0.43
2:C:270:THR:H	2:C:273:HIS:HD2	1.66	0.43
2:C:337:PHE:O	2:C:338:THR:OG1	2.30	0.43
2:C:345:PRO:O	2:C:349:GLU:HG2	2.18	0.43
2:C:694:ARG:O	2:C:798:GLN:NE2	2.50	0.43
2:C:892:GLU:C	2:C:894:GLN:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1258:PRO:HB3	3:D:348:ASP:OD2	2.19	0.43
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.48	0.43
3:D:501:VAL:HG21	3:D:602:SER:HB2	2.00	0.43
3:D:1297:LYS:HZ3	3:D:1297:LYS:CA	2.31	0.43
5:X:608:ARG:NH1	5:X:608:ARG:HB3	2.33	0.43
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.34	0.43
1:G:182:ARG:CG	1:G:206:GLU:HB3	2.48	0.43
2:H:26:TYR:HE2	2:H:28:LEU:HB2	1.84	0.43
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	2.01	0.43
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.51	0.43
2:H:1259:LEU:C	2:H:1259:LEU:HD12	2.44	0.43
3:I:584:PRO:HD3	3:I:620:PHE:CD1	2.54	0.43
5:Y:134:VAL:HG22	5:Y:273:MET:HE1	2.01	0.43
5:Y:449:THR:HG23	5:Y:503:GLU:OE1	2.19	0.43
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.40	0.42
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.19	0.42
2:C:1027:LYS:HB2	2:C:1027:LYS:NZ	2.34	0.42
2:C:1161:LEU:HD21	2:C:1172:LEU:HD11	2.01	0.42
3:D:165:TYR:O	3:D:169:LEU:HB2	2.19	0.42
3:D:1149:ARG:HA	3:D:1150:PRO:HD3	1.88	0.42
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.86	0.42
2:H:478:ARG:HG2	2:H:492:MET:HE2	2.01	0.42
2:H:812:PHE:H	2:H:815:SER:HB2	1.84	0.42
2:H:845:LEU:HD13	2:H:845:LEU:N	2.31	0.42
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.79	0.42
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.49	0.42
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.49	0.42
5:Y:102:MET:HE1	5:Y:388:ILE:HG21	2.01	0.42
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.01	0.42
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.44	0.42
1:A:318:LEU:HD13	1:A:318:LEU:N	2.34	0.42
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.83	0.42
2:C:1086:PRO:HA	2:C:1213:TYR:O	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
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
5:X:456:MET:O	5:X:460:ILE:HG13	2.19	0.42
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.19	0.42
1:F:44:ARG:HG3	1:F:183:ILE:HG22	2.01	0.42
1:F:190:ALA:HB2	1:F:200:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:LEU:HD11	3:I:527:LEU:O	2.19	0.42
1:G:110:VAL:HG21	1:G:140:ILE:HD11	2.00	0.42
2:H:362:ALA:O	2:H:366:ILE:HG13	2.19	0.42
3:I:128:LEU:HD12	3:I:192:MET:HE3	2.02	0.42
3:I:210:SER:O	3:I:214:ARG:HG3	2.19	0.42
1:A:226:GLU:HB3	1:B:10:LYS:HZ3	1.84	0.42
1:A:253:LEU:HB3	1:A:321:TRP:CH2	2.55	0.42
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.49	0.42
2:C:68:LEU:HG	2:C:100:LEU:HD23	2.01	0.42
2:C:590:PRO:HB3	2:C:605:TYR:HE1	1.84	0.42
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.49	0.42
2:C:1043:ALA:C	2:C:1045:GLY:H	2.26	0.42
3:D:227:PHE:O	3:D:230:SER:OG	2.26	0.42
3:D:573:THR:HG23	3:D:576:ARG:H	1.83	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
5:X:9:LEU:HD22	5:X:60:PRO:HB3	2.00	0.42
5:X:457:ILE:HG23	5:X:461:ASN:ND2	2.34	0.42
1:G:185:TYR:HB2	1:G:201:LEU:HD11	2.00	0.42
2:H:56:VAL:HB	2:H:57:PHE:H	1.48	0.42
2:H:469:VAL:O	2:H:472:GLU:HB3	2.19	0.42
2:H:1219:GLU:OE2	3:I:634:ARG:NH1	2.52	0.42
3:I:179:LYS:HD3	3:I:179:LYS:N	2.34	0.42
3:I:1345:ARG:HG2	3:I:1370:MET:CE	2.48	0.42
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.83	0.42
1:A:323:PRO:HA	1:A:324:ALA:HA	1.74	0.42
1:B:51:MET:HA	1:B:52:PRO:HD3	1.87	0.42
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.20	0.42
3:D:378:LYS:HD2	3:D:382:TYR:CZ	2.54	0.42
3:D:607:THR:O	3:D:611:ILE:HG12	2.19	0.42
3:D:681:LYS:O	3:D:685:ILE:HG13	2.19	0.42
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.42
5:X:451:ARG:O	5:X:452:ILE:HG13	2.20	0.42
5:X:532:LEU:O	5:X:536:THR:HG23	2.20	0.42
5:X:543:ALA:O	5:X:547:VAL:HG23	2.19	0.42
1:G:191:ARG:HD3	1:G:191:ARG:HA	1.88	0.42
2:H:42:ASP:HB2	2:H:47:TYR:CG	2.53	0.42
2:H:161:LYS:NZ	2:H:161:LYS:HB3	2.33	0.42
2:H:297:VAL:HB	2:H:317:LEU:HD21	2.01	0.42
3:I:573:THR:CG2	3:I:576:ARG:HG3	2.49	0.42
5:Y:484:ALA:HB1	5:Y:490:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:555:TYR:OH	2:C:654:ASP:OD2	2.36	0.42
2:C:752:ASN:C	2:C:753:LEU:HG	2.44	0.42
2:C:1105:SER:HB2	3:D:731:ARG:HD3	2.01	0.42
3:D:74:LYS:HB3	3:D:74:LYS:NZ	2.35	0.42
3:D:130:MET:HA	3:D:131:PRO:HD3	1.96	0.42
3:D:238:ILE:O	3:D:238:ILE:HG13	2.18	0.42
3:D:435:GLN:HB2	3:D:457:TYR:OH	2.20	0.42
3:D:857:LEU:HB2	3:D:860:ARG:HB2	2.02	0.42
3:D:910:ASN:HB3	4:E:15:ASN:HA	2.02	0.42
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	2.02	0.42
5:X:528:LEU:C	5:X:528:LEU:HD12	2.45	0.42
2:H:812:PHE:N	2:H:815:SER:HB2	2.34	0.42
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.84	0.42
3:I:238:ILE:O	3:I:238:ILE:HG13	2.19	0.42
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	2.02	0.42
1:A:158:ARG:HB2	1:A:158:ARG:HH21	1.84	0.42
2:C:367:TYR:CD1	2:C:384:LEU:HD13	2.54	0.42
2:C:892:GLU:O	2:C:893:THR:OG1	2.27	0.42
2:C:896:THR:O	2:C:899:GLU:N	2.50	0.42
3:D:77:ARG:HA	3:D:77:ARG:HD2	1.76	0.42
3:D:384:LYS:HA	3:D:384:LYS:HD2	1.85	0.42
5:X:299:LYS:O	5:X:303:ILE:HG12	2.19	0.42
1:F:163:GLU:HG3	1:F:170:ARG:NH1	2.20	0.42
1:G:110:VAL:HB	1:G:131:CYS:HB2	2.00	0.42
2:H:106:GLU:CB	2:H:107:ARG:HA	2.49	0.42
3:I:700:ASN:O	3:I:704:GLU:HG2	2.19	0.42
4:J:19:LEU:HD13	4:J:19:LEU:C	2.45	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
2:C:814:ASP:OD1	2:C:1106:ARG:NH1	2.50	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
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
2:H:740:GLU:H	2:H:740:GLU:CD	2.27	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:I:378:LYS:HD2	3:I:382:TYR:OH	2.19	0.42
3:I:1307:LEU:N	3:I:1307:LEU:HD23	2.35	0.42
1:B:22:THR:HB	1:B:207:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:LEU:HG	2:C:461:GLU:HB2	2.02	0.42
2:C:122:VAL:HG22	2:C:123:TYR:N	2.34	0.42
2:C:943:LYS:O	2:C:947:GLU:HG2	2.19	0.42
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.34	0.42
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	2.00	0.42
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.79	0.42
3:D:122:SER:HB2	3:D:132:LEU:HB2	2.00	0.42
3:D:535:ARG:HB3	3:D:541:LEU:HD11	2.02	0.42
1:G:178:SER:HA	1:G:179:PRO:HD3	1.88	0.42
2:H:59:ILE:HG12	2:H:65:ASN:O	2.20	0.42
2:H:72:SER:O	2:H:98:VAL:HG23	2.20	0.42
2:H:91:THR:HG22	2:H:138:ILE:HA	2.02	0.42
2:H:620:ASN:ND2	3:I:768:ASN:HB2	2.35	0.42
2:H:1158:LYS:HD2	2:H:1158:LYS:C	2.44	0.42
2:H:1192:GLU:CD	3:I:764:ARG:HE	2.28	0.42
2:H:1238:LEU:HD12	2:H:1239:VAL:N	2.34	0.42
3:I:267:ASP:OD2	3:I:270:ARG:NH2	2.52	0.42
3:I:370:LYS:HG3	3:I:371:LYS:H	1.84	0.42
3:I:1155:ILE:HG13	3:I:1210:ILE:CG2	2.43	0.42
2:C:127:ILE:O	2:C:127:ILE:HG12	2.20	0.42
2:C:237:LEU:HB2	2:C:287:VAL:O	2.19	0.42
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.34	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
3:D:205:LEU:HB3	3:D:217:LEU:HB3	2.01	0.42
3:D:646:ILE:HG22	3:D:741:ALA:O	2.19	0.42
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.20	0.42
5:X:448:ARG:HD3	5:X:450:ILE:HG13	2.01	0.42
1:F:167:PRO:HD2	1:F:170:ARG:NE	2.35	0.42
3:I:222:LYS:HZ1	3:I:1276:GLU:HB2	1.84	0.42
5:Y:343:LYS:O	5:Y:346:GLN:HB3	2.20	0.42
1:A:80:GLU:HG3	2:C:694:ARG:HH12	1.85	0.42
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.84	0.42
2:C:429:MET:O	2:C:433:ILE:HG13	2.20	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:1238:LEU:HD12	2:C:1239:VAL:O	2.20	0.42
3:D:161:THR:HG22	3:D:162:GLU:N	2.35	0.42
3:D:313:GLY:H	5:X:38:SER:HB3	1.83	0.42
3:D:390:LEU:N	3:D:390:LEU:HD12	2.34	0.42
3:D:543:SER:O	3:D:574:VAL:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1343:GLU:CA	3:D:1344:LEU:HB2	2.36	0.42
1:F:11:PRO:HA	1:F:30:PRO:O	2.20	0.42
1:F:31:LEU:HB2	1:F:199:ASP:O	2.20	0.42
1:G:77:ASP:O	1:G:81:ILE:HG13	2.19	0.42
2:H:122:VAL:HG22	2:H:123:TYR:N	2.35	0.42
2:H:667:LEU:O	2:H:1069:ARG:NH2	2.53	0.42
2:H:1117:LEU:HD11	2:H:1182:ILE:HD13	2.02	0.42
2:H:1269:ARG:HD3	2:H:1269:ARG:N	2.35	0.42
3:I:31:ARG:HD2	3:I:104:HIS:CD2	2.55	0.42
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.85	0.42
3:I:492:SER:HA	3:I:493:PRO:HD3	1.94	0.42
5:Y:99:ARG:O	5:Y:99:ARG:HD3	2.20	0.42
1:A:45:ARG:NE	1:B:38:THR:OG1	2.53	0.41
1:A:246:LYS:HD3	1:A:246:LYS:N	2.35	0.41
1:A:299:SER:O	1:A:303:ILE:HG12	2.20	0.41
2:C:208:ILE:HD11	2:C:365:GLU:HB3	2.01	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
2:C:669:PRO:HG2	2:C:1070:HIS:HE1	1.85	0.41
2:C:1272:GLU:HG3	2:C:1276:TRP:CE2	2.55	0.41
3:D:66:LYS:NZ	3:D:66:LYS:HB3	2.35	0.41
3:D:800:LEU:O	3:D:803:VAL:HG12	2.20	0.41
3:D:1290:ARG:HH22	3:I:1301:THR:HG22	1.85	0.41
5:X:147:GLN:O	5:X:151:VAL:HG23	2.20	0.41
1:F:182:ARG:HH11	2:H:1092:THR:HG22	1.83	0.41
1:G:52:PRO:HB2	1:G:53:GLY:H	1.59	0.41
2:H:59:ILE:HB	2:H:480:SER:OG	2.20	0.41
2:H:255:ILE:HD12	2:H:263:VAL:HB	2.02	0.41
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.35	0.41
3:I:109:SER:OG	3:I:296:LYS:HE2	2.20	0.41
3:I:293:ARG:NH1	5:Y:104:GLU:HB2	2.34	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
3:I:644:MET:HE2	3:I:644:MET:HB3	1.94	0.41
2:C:73:TYR:O	2:C:74:ARG:HB2	2.19	0.41
2:C:115:LYS:O	2:C:116:ASP:HB2	2.20	0.41
2:C:402:ARG:HH12	2:C:424:ASP:CG	2.28	0.41
2:C:1004:ASP:OD1	2:C:1004:ASP:N	2.53	0.41
2:C:1211:ARG:H	2:C:1211:ARG:HG3	1.68	0.41
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.34	0.41
3:D:26:SER:O	3:D:30:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:646:ILE:H	3:D:646:ILE:HG13	1.65	0.41
3:D:789:LYS:HB3	3:D:932:MET:SD	2.60	0.41
3:D:822:MET:HG2	3:D:839:VAL:HG22	2.02	0.41
3:D:887:SER:HA	3:I:1292:LEU:HD23	2.02	0.41
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.35	0.41
5:X:112:THR:HG22	5:X:113:ARG:N	2.31	0.41
2:H:208:ILE:HD11	2:H:365:GLU:HB3	2.02	0.41
2:H:560:PRO:HA	3:I:780:ARG:NH2	2.35	0.41
2:H:752:ASN:C	2:H:753:LEU:HG	2.45	0.41
3:I:305:ALA:O	3:I:309:ASN:ND2	2.53	0.41
3:I:492:SER:HB2	3:I:499:ILE:HB	2.01	0.41
3:I:605:LEU:O	3:I:605:LEU:HD13	2.20	0.41
3:I:607:THR:O	3:I:611:ILE:HG12	2.20	0.41
5:Y:122:ARG:NH2	5:Y:378:GLU:OE2	2.50	0.41
5:Y:316:PHE:CZ	5:Y:320:ILE:HD11	2.55	0.41
1:A:183:ILE:HD11	1:A:205:MET:HG3	2.02	0.41
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.55	0.41
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.55	0.41
2:C:705:GLU:H	2:C:705:GLU:CD	2.28	0.41
2:C:971:LEU:C	2:C:971:LEU:HD13	2.44	0.41
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.55	0.41
3:D:275:ARG:HD2	3:D:302:ALA:HB2	2.03	0.41
3:D:382:TYR:CE1	3:D:401:VAL:HG21	2.56	0.41
3:D:532:GLU:OE1	3:D:578:ILE:HB	2.20	0.41
4:E:65:ASP:O	4:E:69:ARG:HG3	2.21	0.41
5:X:279:ARG:NH2	5:X:350:GLU:OE1	2.50	0.41
1:G:56:VAL:HG12	1:G:173:VAL:HG11	2.01	0.41
2:H:459:MET:HE1	2:H:511:LEU:HD22	2.02	0.41
2:H:582:ASN:HB2	2:H:588:GLU:HG3	2.01	0.41
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	2.02	0.41
2:H:773:LEU:CD1	2:H:773:LEU:H	2.32	0.41
2:H:1195:ILE:O	2:H:1199:LEU:HG	2.21	0.41
2:H:1286:THR:N	3:I:479:GLU:OE2	2.50	0.41
3:I:33:TRP:HB3	3:I:102:MET:HG3	2.02	0.41
3:I:50:LYS:HA	3:I:51:PRO:HD3	1.95	0.41
3:I:646:ILE:H	3:I:646:ILE:HG13	1.66	0.41
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.31	0.41
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.20	0.41
5:Y:143:TYR:O	5:Y:147:GLN:HG2	2.19	0.41
5:Y:297:MET:HE2	5:Y:326:TRP:CE3	2.56	0.41
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.35	0.41
2:C:971:LEU:HD21	2:C:1017:GLN:HE22	1.85	0.41
3:D:377:PHE:O	3:D:381:ILE:HG13	2.20	0.41
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.03	0.41
3:D:533:ALA:HB2	3:D:578:ILE:HD13	2.02	0.41
3:D:700:ASN:O	3:D:704:GLU:HG2	2.21	0.41
3:D:905:ARG:NE	3:D:907:HIS:HB2	2.29	0.41
3:D:1307:LEU:N	3:D:1307:LEU:HD23	2.35	0.41
5:X:145:LEU:HD11	5:X:225:ARG:HH21	1.83	0.41
5:X:276:MET:O	5:X:280:VAL:HG23	2.20	0.41
5:X:453:PRO:HB2	5:X:455:HIS:CE1	2.55	0.41
5:X:598:LEU:O	5:X:599:ARG:HD2	2.19	0.41
2:H:148:GLN:HB2	2:H:511:LEU:HD21	2.02	0.41
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	2.01	0.41
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	2.02	0.41
3:I:325:LYS:HB3	5:Y:508:GLU:HG3	2.02	0.41
3:I:438:GLU:HA	3:I:439:PRO:HD3	1.87	0.41
3:I:513:MET:HE2	3:I:579:LEU:HB2	2.02	0.41
3:I:591:ILE:HD12	3:I:592:VAL:HG13	2.03	0.41
3:I:809:VAL:CG1	3:I:913:GLU:H	2.34	0.41
3:I:899:TYR:CZ	3:I:915:ILE:HD12	2.55	0.41
3:I:910:ASN:OD1	4:J:15:ASN:HA	2.21	0.41
3:I:1357:ILE:HD12	3:I:1357:ILE:N	2.35	0.41
3:I:1368:ASP:O	3:I:1372:ARG:HB2	2.19	0.41
5:Y:383:ASN:HB2	5:Y:412:LEU:HD21	2.02	0.41
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.20	0.41
5:Y:528:LEU:C	5:Y:528:LEU:HD12	2.45	0.41
2:C:391:SER:OG	2:C:393:ASP:OD1	2.35	0.41
2:C:848:GLU:CD	2:C:888:THR:HG22	2.46	0.41
2:C:1210:ILE:HG23	2:C:1211:ARG:NH1	2.35	0.41
3:D:113:HIS:O	3:D:117:LEU:HB2	2.19	0.41
3:D:605:LEU:O	3:D:605:LEU:HD13	2.21	0.41
3:D:803:VAL:HG11	3:D:1309:ILE:HG13	2.01	0.41
3:D:1257:VAL:HA	3:D:1260:MET:CB	2.50	0.41
5:X:283:GLN:NE2	5:X:343:LYS:HD2	2.35	0.41
5:X:290:LEU:O	5:X:294:GLN:HB3	2.20	0.41
5:X:561:MET:SD	5:X:576:VAL:HG22	2.61	0.41
1:F:33:ARG:HA	1:F:33:ARG:HD3	1.89	0.41
1:G:82:LEU:O	1:G:86:LYS:HG3	2.20	0.41
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.40	0.41
2:H:57:PHE:HA	2:H:476:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1225:VAL:HG12	3:I:636:GLY:O	2.19	0.41
2:H:1313:HIS:HD2	3:I:474:LEU:HD23	1.86	0.41
3:I:233:LYS:HB3	3:I:236:TRP:CE2	2.55	0.41
3:I:473:THR:HB	3:I:476:ALA:CB	2.49	0.41
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.48	0.41
3:I:790:THR:HG22	3:I:928:THR:HG23	2.01	0.41
3:I:850:LYS:NZ	3:I:873:GLU:HB3	2.36	0.41
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.45	0.41
1:B:118:ASP:HB3	1:B:121:VAL:HB	2.03	0.41
2:C:99:LYS:C	2:C:100:LEU:HD12	2.45	0.41
2:C:500:ALA:O	2:C:504:GLU:HB2	2.20	0.41
2:C:560:PRO:HB2	3:D:776:THR:OG1	2.20	0.41
2:C:905:ILE:HG12	5:X:595:LEU:HD22	2.02	0.41
3:D:843:VAL:HG11	3:D:897:HIS:HB3	2.01	0.41
3:D:1296:GLY:C	3:D:1297:LYS:HZ3	2.28	0.41
5:X:410:ILE:O	5:X:414:LYS:HG3	2.21	0.41
1:G:33:ARG:NE	1:G:197:ASP:HB2	2.36	0.41
2:H:333:ILE:N	2:H:333:ILE:HD12	2.36	0.41
2:H:391:SER:OG	2:H:393:ASP:OD1	2.36	0.41
2:H:453:ILE:O	2:H:453:ILE:HG23	2.21	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:H:896:THR:O	2:H:899:GLU:N	2.50	0.41
2:H:943:LYS:O	2:H:947:GLU:HG2	2.19	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.51	0.41
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.56	0.41
3:I:534:GLU:O	3:I:538:ARG:HB2	2.20	0.41
3:I:679:TYR:O	3:I:683:ILE:HG13	2.19	0.41
1:A:107:ILE:HG12	1:A:134:THR:O	2.21	0.41
1:B:7:GLU:O	1:B:8:PHE:CG	2.74	0.41
1:B:37:HIS:CE1	2:C:1216:ARG:HD3	2.56	0.41
2:C:68:LEU:HD22	2:C:475:VAL:HG21	2.02	0.41
2:C:177:ILE:HD12	2:C:177:ILE:N	2.36	0.41
2:C:805:MET:HE1	2:C:1221:PHE:CE1	2.55	0.41
5:X:240:ARG:HD3	5:X:244:THR:CB	2.44	0.41
2:H:120:GLN:HG3	2:H:121:GLU:N	2.35	0.41
2:H:453:ILE:HG22	2:H:585:GLY:O	2.21	0.41
2:H:902:LEU:HD21	5:Y:608:ARG:CG	2.45	0.41
2:H:1270:PHE:HB3	2:H:1271:GLY:H	1.61	0.41
3:I:362:ARG:HB3	3:I:363:LEU:H	1.65	0.41
3:I:450:HIS:CE1	3:I:452:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:646:ILE:HG22	3:I:741:ALA:O	2.21	0.41
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.50	0.41
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.21	0.41
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.21	0.41
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.02	0.41
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.93	0.41
2:C:529:ARG:HB2	2:C:529:ARG:NH1	2.35	0.41
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.48	0.41
2:C:1293:VAL:HA	2:C:1297:ASP:HB3	2.02	0.41
3:D:288:PRO:O	3:D:292:VAL:HG12	2.20	0.41
3:D:478:LEU:CD1	4:E:47:THR:HG23	2.51	0.41
4:E:19:LEU:HD13	4:E:19:LEU:C	2.46	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
2:H:169:LYS:HD3	2:H:169:LYS:HA	1.81	0.41
2:H:263:VAL:HA	2:H:267:ARG:HH21	1.86	0.41
2:H:429:MET:O	2:H:433:ILE:HG13	2.21	0.41
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.21	0.41
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.35	0.41
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
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
1:B:74:VAL:HG12	1:B:76:GLU:H	1.85	0.41
1:B:152:TYR:OH	3:D:535:ARG:NH1	2.47	0.41
2:C:453:ILE:O	2:C:453:ILE:HG23	2.21	0.41
2:C:521:LEU:HD22	2:C:667:LEU:HD12	2.02	0.41
2:C:699:LEU:H	2:C:799:ASN:ND2	2.16	0.41
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.20	0.41
2:C:980:VAL:O	2:C:984:VAL:HG22	2.21	0.41
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.86	0.41
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.38	0.41
3:D:214:ARG:O	3:D:218:THR:HG22	2.21	0.41
3:D:423:LEU:HB3	3:D:466:MET:CE	2.50	0.41
3:D:706:VAL:C	3:D:707:ILE:HG13	2.45	0.41
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.86	0.41
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.21	0.41
1:F:222:THR:O	1:F:226:GLU:HG3	2.21	0.41
1:G:152:TYR:OH	3:I:535:ARG:NH1	2.45	0.41
1:G:207:THR:OG1	1:G:208:ASN:N	2.53	0.41
1:G:222:THR:O	1:G:226:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:ILE:HD12	2:H:184:LEU:HD23	2.02	0.41
2:H:177:ILE:HD12	2:H:177:ILE:N	2.36	0.41
2:H:205:PRO:O	2:H:208:ILE:HG22	2.21	0.41
2:H:221:LEU:HD22	2:H:336:LEU:HD11	2.02	0.41
2:H:225:PHE:CE2	2:H:347:ILE:HB	2.56	0.41
2:H:302:ILE:HA	2:H:309:LEU:HA	2.03	0.41
2:H:431:LYS:O	2:H:435:ILE:HG13	2.20	0.41
2:H:961:SER:O	2:H:965:GLN:HG3	2.21	0.41
2:H:999:GLU:HG2	2:H:1000:LEU:H	1.85	0.41
2:H:1107:MET:N	2:H:1107:MET:SD	2.94	0.41
2:H:1169:VAL:HG23	2:H:1172:LEU:HD11	2.02	0.41
3:I:390:LEU:N	3:I:390:LEU:HD12	2.34	0.41
3:I:500:ILE:H	3:I:500:ILE:CD1	2.34	0.41
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.41	0.41
5:Y:456:MET:O	5:Y:460:ILE:HG13	2.19	0.41
5:Y:477:GLU:OE1	5:Y:477:GLU:N	2.53	0.41
1:B:129:VAL:HG11	1:B:132:HIS:HE1	1.86	0.41
2:C:310:ILE:O	2:C:311:CYS:HB3	2.21	0.41
2:C:563:THR:HG21	3:D:780:ARG:CZ	2.50	0.41
2:C:1331:ARG:HG3	3:D:33:TRP:CZ3	2.56	0.41
3:D:155:GLU:CD	3:D:158:GLN:HB2	2.45	0.41
3:D:583:VAL:HG13	3:D:584:PRO:HD2	2.03	0.41
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.43	0.41
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.51	0.41
2:H:22:LEU:HD13	2:H:23:ASP:O	2.21	0.41
2:H:145:ILE:CG2	2:H:456:VAL:HG22	2.51	0.41
3:I:388:ARG:NH2	3:I:414:GLU:OE2	2.53	0.41
3:I:620:PHE:O	3:I:624:ILE:HG23	2.21	0.41
3:I:846:GLU:O	3:I:847:ASP:C	2.64	0.41
1:B:181:GLU:HG2	3:D:531:LYS:HD3	2.02	0.40
2:C:54:ARG:HG2	2:C:55:SER:CB	2.49	0.40
2:C:68:LEU:HD12	2:C:68:LEU:HA	1.91	0.40
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.56	0.40
2:C:1092:THR:HA	2:C:1093:PRO:HD3	1.88	0.40
3:D:52:GLU:OE1	5:X:451:ARG:HD2	2.21	0.40
3:D:746:LEU:HD22	3:D:746:LEU:N	2.36	0.40
5:X:431:ALA:O	5:X:435:ILE:HG13	2.21	0.40
1:F:82:LEU:O	1:F:86:LYS:HG3	2.21	0.40
2:H:88:ARG:NH1	2:H:88:ARG:HB3	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:668:ILE:HD12	2:H:671:LEU:HD13	2.02	0.40
2:H:816:ILE:HG13	2:H:1098:LEU:CD2	2.35	0.40
3:I:194:LEU:O	3:I:198:CYS:HB2	2.21	0.40
3:I:773:PHE:O	3:I:776:THR:HG22	2.21	0.40
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.90	0.40
2:C:174:ALA:HB2	2:C:432:LEU:HD13	2.03	0.40
2:C:843:THR:HG22	2:C:844:LYS:N	2.36	0.40
2:C:1108:ASN:O	2:C:1108:ASN:ND2	2.55	0.40
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.86	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
4:E:77:ALA:O	4:E:80:LEU:HD22	2.20	0.40
5:X:343:LYS:O	5:X:346:GLN:HB3	2.21	0.40
5:X:532:LEU:C	5:X:532:LEU:HD13	2.46	0.40
2:H:977:ALA:O	2:H:980:VAL:HG12	2.21	0.40
2:H:1108:ASN:O	2:H:1108:ASN:ND2	2.54	0.40
3:I:122:SER:OG	3:I:132:LEU:HD13	2.21	0.40
3:I:475:GLU:HG2	3:I:475:GLU:H	1.74	0.40
3:I:810:THR:HG22	3:I:893:GLY:HA3	2.02	0.40
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	2.02	0.40
5:Y:281:ARG:HD3	5:Y:359:LYS:NZ	2.37	0.40
1:B:154:PRO:O	1:B:157:THR:HG22	2.20	0.40
2:C:1060:ILE:H	2:C:1060:ILE:HG12	1.70	0.40
3:D:292:VAL:HG22	3:D:296:LYS:HE3	2.03	0.40
5:X:145:LEU:HD13	5:X:145:LEU:C	2.46	0.40
5:X:254:GLU:O	5:X:258:GLN:HG3	2.21	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:H:138:ILE:O	2:H:141:THR:OG1	2.33	0.40
2:H:367:TYR:CD1	2:H:384:LEU:HD13	2.56	0.40
2:H:1106:ARG:O	2:H:1108:ASN:N	2.43	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
3:I:1171:GLY:CA	3:I:1172:LYS:C	2.95	0.40
1:A:22:THR:HB	1:A:207:THR:O	2.21	0.40
1:A:91:ARG:NH2	1:A:209:GLY:O	2.55	0.40
1:B:52:PRO:HB2	1:B:53:GLY:H	1.61	0.40
2:C:697:LYS:HD2	2:C:793:GLU:OE2	2.22	0.40
2:C:869:GLY:C	2:C:870:ILE:HD12	2.46	0.40
2:C:898:GLU:HG3	5:X:565:ILE:CD1	2.51	0.40
3:D:161:THR:HG22	3:D:162:GLU:CD	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:182:ALA:O	3:D:185:ILE:HG22	2.21	0.40
3:D:217:LEU:O	3:D:221:ILE:HG23	2.21	0.40
3:D:704:GLU:O	3:D:705:THR:OG1	2.30	0.40
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.22	0.40
5:X:459:THR:O	5:X:463:LEU:HD13	2.21	0.40
1:F:167:PRO:HG2	1:F:170:ARG:HG3	2.03	0.40
3:I:801:VAL:O	3:I:805:GLN:HG2	2.21	0.40
3:I:1290:ARG:HD2	3:I:1299:GLY:HA3	2.04	0.40
1:B:19:VAL:O	1:B:19:VAL:HG12	2.22	0.40
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.85	0.40
2:C:542:ARG:HG2	2:C:543:ALA:N	2.36	0.40
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	2.02	0.40
3:D:42:GLU:HG3	5:X:451:ARG:NH2	2.37	0.40
3:D:286:ALA:HB3	5:X:413:MET:SD	2.62	0.40
3:D:310:GLY:O	3:D:314:ARG:HG2	2.20	0.40
3:D:428:THR:HG23	3:D:433:GLY:HA3	2.03	0.40
5:X:295:CYS:SG	5:X:330:LEU:HD23	2.61	0.40
1:F:207:THR:OG1	1:F:208:ASN:N	2.54	0.40
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.51	0.40
2:H:347:ILE:HD11	2:H:433:ILE:HD11	2.03	0.40
2:H:517:GLN:NE2	2:H:760:ASN:OD1	2.54	0.40
2:H:773:LEU:HD22	2:H:773:LEU:O	2.22	0.40
2:H:1314:GLN:O	3:I:473:THR:HG23	2.21	0.40
3:I:555:TYR:HD1	3:I:589:TYR:HE2	1.68	0.40
3:I:816:THR:OG1	3:I:818:GLU:OE1	2.30	0.40
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.48	0.40
3:I:1195:GLN:OE1	3:I:1195:GLN:N	2.50	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%)	2	20
1	B	217/329 (66%)	186 (86%)	24 (11%)	7 (3%)	3	25
1	F	227/329 (69%)	196 (86%)	26 (12%)	5 (2%)	5	31
1	G	213/329 (65%)	188 (88%)	21 (10%)	4 (2%)	6	33
2	C	1333/1342 (99%)	1069 (80%)	213 (16%)	51 (4%)	2	21
2	H	1333/1342 (99%)	1070 (80%)	213 (16%)	50 (4%)	2	21
3	D	1154/1407 (82%)	922 (80%)	189 (16%)	43 (4%)	2	22
3	I	1154/1407 (82%)	929 (80%)	183 (16%)	42 (4%)	2	23
4	E	88/91 (97%)	76 (86%)	8 (9%)	4 (4%)	2	19
4	J	74/91 (81%)	64 (86%)	6 (8%)	4 (5%)	1	17
5	X	511/613 (83%)	450 (88%)	45 (9%)	16 (3%)	3	25
5	Y	454/613 (74%)	411 (90%)	32 (7%)	11 (2%)	4	29
All	All	7079/8222 (86%)	5827 (82%)	1001 (14%)	251 (4%)	3	23

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	42	62
1	B	189/286 (66%)	185 (98%)	4 (2%)	47	65
1	F	197/286 (69%)	193 (98%)	4 (2%)	48	65
1	G	185/286 (65%)	182 (98%)	3 (2%)	55	69
2	C	1150/1157 (99%)	1080 (94%)	70 (6%)	17	43
2	H	1150/1157 (99%)	1086 (94%)	64 (6%)	19	45
3	D	971/1168 (83%)	915 (94%)	56 (6%)	18	44
3	I	971/1168 (83%)	918 (94%)	53 (6%)	19	45
4	E	74/75 (99%)	69 (93%)	5 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	65/75 (87%)	62 (95%)	3 (5%)	24	48
5	X	460/540 (85%)	444 (96%)	16 (4%)	32	54
5	Y	407/540 (75%)	390 (96%)	17 (4%)	26	50
All	All	6100/7024 (87%)	5798 (95%)	302 (5%)	22	47

All (302) 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	239	GLN
1	A	243	LYS
1	A	246	LYS
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	182	ARG
1	B	196	THR
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	161	LYS
2	C	163	LYS
2	C	203	LYS
2	C	479	LEU
2	C	487	LEU
2	C	600	THR
2	C	603	ILE

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Mol	Chain	Res	Type
2	C	645	PHE
2	C	661	VAL
2	C	690	VAL
2	C	700	VAL
2	C	704	MET
2	C	734	ILE
2	C	773	LEU
2	C	791	LEU
2	C	800	MET
2	C	817	LEU
2	C	844	LYS
2	C	845	LEU
2	C	890	LYS
2	C	908	GLU
2	C	909	LYS
2	C	920	VAL
2	C	941	LYS
2	C	953	LEU
2	C	964	LEU
2	C	975	ILE
2	C	988	LYS
2	C	1002	LEU
2	C	1010	GLN
2	C	1011	LEU
2	C	1017	GLN
2	C	1027	LYS
2	C	1032	LYS
2	C	1042	LEU
2	C	1097	VAL
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1211	ARG
2	C	1233	LEU
2	C	1239	VAL
2	C	1248	THR
2	C	1259	LEU
2	C	1262	LYS
2	C	1264	GLN
2	C	1265	PHE

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Mol	Chain	Res	Type
2	C	1276	TRP
2	C	1288	GLN
2	C	1291	LEU
2	C	1293	VAL
2	C	1326	LEU
2	C	1339	LEU
3	D	9	LYS
3	D	13	LYS
3	D	20	ILE
3	D	50	LYS
3	D	66	LYS
3	D	74	LYS
3	D	92	VAL
3	D	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	155	GLU
3	D	169	LEU
3	D	179	LYS
3	D	185	ILE
3	D	188	LEU
3	D	235	GLU
3	D	309	ASN
3	D	442	ILE
3	D	475	GLU
3	D	500	ILE
3	D	501	VAL
3	D	505	ASP
3	D	506	VAL
3	D	508	LEU
3	D	521	LYS
3	D	523	GLU
3	D	527	LEU
3	D	531	LYS
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	571	ASP
3	D	668	PHE
3	D	681	LYS
3	D	707	ILE

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Mol	Chain	Res	Type
3	D	713	GLU
3	D	771	GLN
3	D	809	VAL
3	D	816	THR
3	D	826	ILE
3	D	832	LYS
3	D	864	LEU
3	D	867	GLN
3	D	873	GLU
3	D	909	ILE
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	1188	GLU
3	D	1247	LYS
3	D	1297	LYS
3	D	1306	LEU
4	E	6	VAL
4	E	8	ASP
4	E	13	ILE
4	E	15	ASN
4	E	73	GLN
5	X	21	TYR
5	X	28	ASN
5	X	136	GLU
5	X	262	VAL
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	384	LEU
5	X	452	ILE
5	X	457	ILE
5	X	473	GLU
5	X	545	HIS
5	X	562	ARG
5	X	565	ILE
5	X	582	VAL
5	X	607	LEU
1	F	37	HIS

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Mol	Chain	Res	Type
1	F	77	ASP
1	F	158	ARG
1	F	160	HIS
1	G	13	LEU
1	G	37	HIS
1	G	88	LEU
2	H	9	LYS
2	H	18	ARG
2	H	37	LYS
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	99	LYS
2	H	127	ILE
2	H	161	LYS
2	H	311	CYS
2	H	442	VAL
2	H	479	LEU
2	H	484	LEU
2	H	488	MET
2	H	513	GLN
2	H	514	PHE
2	H	600	THR
2	H	603	ILE
2	H	645	PHE
2	H	661	VAL
2	H	690	VAL
2	H	700	VAL
2	H	704	MET
2	H	734	ILE
2	H	773	LEU
2	H	791	LEU
2	H	800	MET
2	H	817	LEU
2	H	844	LYS
2	H	845	LEU
2	H	890	LYS
2	H	909	LYS

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Mol	Chain	Res	Type
2	H	920	VAL
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	988	LYS
2	H	1002	LEU
2	H	1005	GLU
2	H	1010	GLN
2	H	1017	GLN
2	H	1027	LYS
2	H	1032	LYS
2	H	1042	LEU
2	H	1060	ILE
2	H	1097	VAL
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1210	ILE
2	H	1211	ARG
2	H	1233	LEU
2	H	1239	VAL
2	H	1262	LYS
2	H	1264	GLN
2	H	1288	GLN
2	H	1291	LEU
2	H	1326	LEU
2	H	1339	LEU
3	I	9	LYS
3	I	31	ARG
3	I	50	LYS
3	I	66	LYS
3	I	74	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	155	GLU
3	I	169	LEU
3	I	179	LYS

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Mol	Chain	Res	Type
3	I	185	ILE
3	I	188	LEU
3	I	248	ASP
3	I	316	ILE
3	I	416	ILE
3	I	442	ILE
3	I	475	GLU
3	I	500	ILE
3	I	501	VAL
3	I	521	LYS
3	I	523	GLU
3	I	527	LEU
3	I	531	LYS
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	571	ASP
3	I	594	GLN
3	I	681	LYS
3	I	707	ILE
3	I	771	GLN
3	I	809	VAL
3	I	816	THR
3	I	826	ILE
3	I	832	LYS
3	I	864	LEU
3	I	873	GLU
3	I	909	ILE
3	I	911	LYS
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1247	LYS
3	I	1273	ASP
3	I	1297	LYS
3	I	1306	LEU
3	I	1369	ARG
4	J	6	VAL
4	J	13	ILE
4	J	73	GLN

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Mol	Chain	Res	Type
5	Y	136	GLU
5	Y	262	VAL
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	473	GLU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	227	GLN
1	A	239	GLN
1	B	84	ASN
1	B	132	HIS
2	C	69	GLN
2	C	139	ASN
2	C	219	GLN
2	C	238	GLN
2	C	273	HIS
2	C	314	ASN
2	C	450	ASN
2	C	462	ASN
2	C	510	GLN
2	C	513	GLN
2	C	517	GLN
2	C	573	ASN
2	C	582	ASN
2	C	673	HIS
2	C	799	ASN
2	C	894	GLN

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Mol	Chain	Res	Type
2	C	955	GLN
2	C	1010	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1134	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	209	ASN
3	D	300	GLN
3	D	465	GLN
3	D	504	GLN
3	D	519	ASN
3	D	680	ASN
3	D	690	ASN
3	D	739	GLN
3	D	875	ASN
3	D	907	HIS
3	D	1268	ASN
3	D	1367	GLN
4	E	31	GLN
5	X	19	GLN
5	X	30	HIS
5	X	54	GLN
5	X	301	ASN
5	X	317	ASN
5	X	383	ASN
5	X	406	GLN
5	X	437	GLN
5	X	461	ASN
5	X	469	GLN
1	F	84	ASN
1	G	41	ASN
2	H	46	GLN
2	H	69	GLN
2	H	238	GLN
2	H	462	ASN
2	H	510	GLN

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Mol	Chain	Res	Type
2	H	513	GLN
2	H	517	GLN
2	H	573	ASN
2	H	582	ASN
2	H	628	HIS
2	H	673	HIS
2	H	684	ASN
2	H	686	GLN
2	H	799	ASN
2	H	834	GLN
2	H	922	ASN
2	H	932	GLN
2	H	1010	GLN
2	H	1038	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	209	ASN
3	I	300	GLN
3	I	309	ASN
3	I	320	ASN
3	I	504	GLN
3	I	519	ASN
3	I	680	ASN
3	I	690	ASN
3	I	739	GLN
3	I	777	HIS
3	I	1244	GLN
3	I	1367	GLN
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

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Mol	Chain	Res	Type
5	Y	469	GLN
5	Y	589	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	G4P	D	1503	-	36,38,38	1.93	12 (33%)	56,61,61	1.43	9 (16%)

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	-	-	8/27/43/43	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1503	G4P	C5-N7	-5.13	1.28	1.39
7	D	1503	G4P	C6-N1	-4.10	1.31	1.38
7	D	1503	G4P	C2'-C3'	-3.64	1.45	1.53
7	D	1503	G4P	C2-N2	3.46	1.42	1.34
7	D	1503	G4P	PC-O3C	-2.77	1.56	1.59
7	D	1503	G4P	C2-N3	2.76	1.39	1.33
7	D	1503	G4P	C2'-C1'	-2.45	1.45	1.53
7	D	1503	G4P	C5-C4	-2.35	1.31	1.38
7	D	1503	G4P	C8-N7	2.27	1.38	1.32
7	D	1503	G4P	C1'-N9	-2.21	1.41	1.47
7	D	1503	G4P	C3'-C4'	-2.17	1.47	1.52
7	D	1503	G4P	C8-N9	2.01	1.42	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1503	G4P	C5-C4-N3	-4.40	121.39	128.39
7	D	1503	G4P	N9-C8-N7	-3.61	106.71	113.40
7	D	1503	G4P	O4'-C1'-C2'	-3.05	100.09	106.62
7	D	1503	G4P	C4'-O4'-C1'	-3.04	102.75	109.47
7	D	1503	G4P	C2-N1-C6	-2.61	120.39	125.11
7	D	1503	G4P	O4'-C1'-N9	2.35	113.69	108.36
7	D	1503	G4P	C5-C4-N9	2.31	109.79	105.66
7	D	1503	G4P	C5-C6-N1	2.25	118.97	113.25
7	D	1503	G4P	O6-C6-C5	-2.24	120.61	126.53

There are no chirality outliers.

All (8) torsion outliers are listed below:

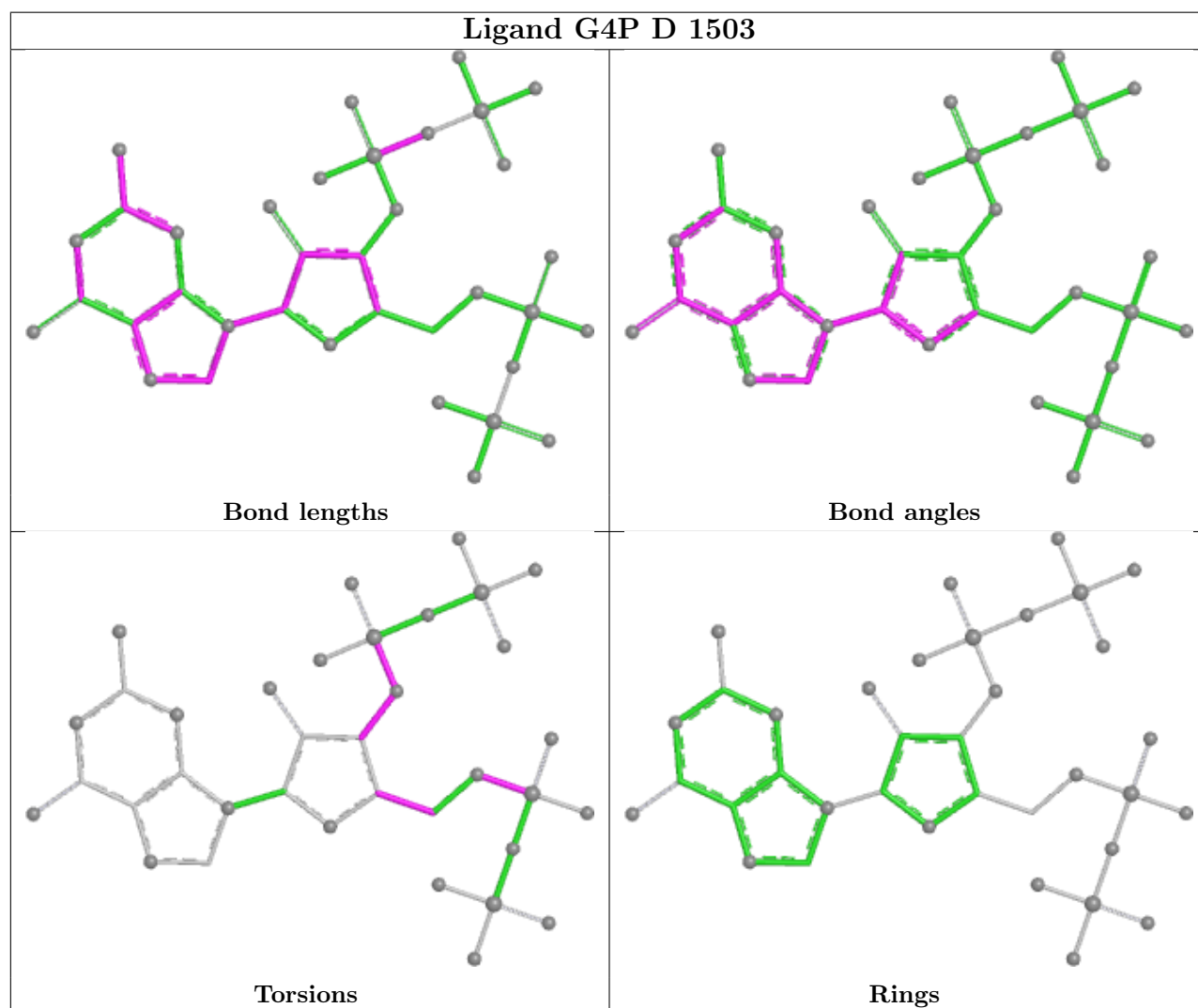
Mol	Chain	Res	Type	Atoms
7	D	1503	G4P	C5'-O5'-PA-O3A
7	D	1503	G4P	C5'-O5'-PA-O1A
7	D	1503	G4P	C5'-O5'-PA-O2A
7	D	1503	G4P	O4'-C4'-C5'-O5'
7	D	1503	G4P	C3'-C4'-C5'-O5'
7	D	1503	G4P	C4'-C3'-O3'-PC
7	D	1503	G4P	C2'-C3'-O3'-PC
7	D	1503	G4P	C3'-O3'-PC-O2C

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	-0.55	0 100 100	1, 73, 178, 299	0
1	B	221/329 (67%)	-0.37	1 (0%) 87 72	5, 98, 204, 259	0
1	F	229/329 (69%)	-0.41	0 100 100	27, 123, 199, 278	0
1	G	217/329 (65%)	-0.48	1 (0%) 87 72	34, 118, 187, 236	0
2	C	1335/1342 (99%)	-0.55	3 (0%) 91 81	0, 48, 170, 262	0
2	H	1335/1342 (99%)	-0.50	4 (0%) 90 78	0, 88, 203, 293	0
3	D	1160/1407 (82%)	-0.51	3 (0%) 90 78	0, 42, 158, 289	0
3	I	1160/1407 (82%)	-0.45	3 (0%) 90 78	0, 60, 192, 317	0
4	E	90/91 (98%)	-0.57	0 100 100	1, 52, 121, 158	0
4	J	76/91 (83%)	-0.51	1 (1%) 75 54	10, 89, 165, 211	0
5	X	517/613 (84%)	-0.51	0 100 100	0, 101, 226, 326	0
5	Y	458/613 (74%)	-0.52	1 (0%) 91 81	1, 109, 234, 357	0
All	All	7121/8222 (86%)	-0.50	17 (0%) 91 81	0, 73, 197, 357	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	1215	GLU	3.7
2	H	1072	ASN	3.1
3	D	1273	ASP	3.1
1	G	39	LEU	2.9
3	D	344	GLY	2.8
3	I	1297	LYS	2.6
2	C	206	ALA	2.3
2	H	1060	ILE	2.3
4	J	2	ALA	2.3
2	H	269	ILE	2.3
2	C	1334	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	2.2
2	H	1071	GLY	2.2
3	I	600	ALA	2.1
2	C	311	CYS	2.1
3	D	1171	GLY	2.0
5	Y	239	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

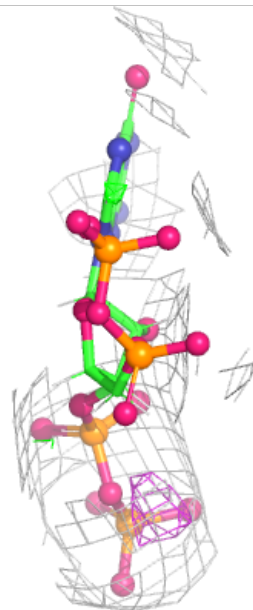
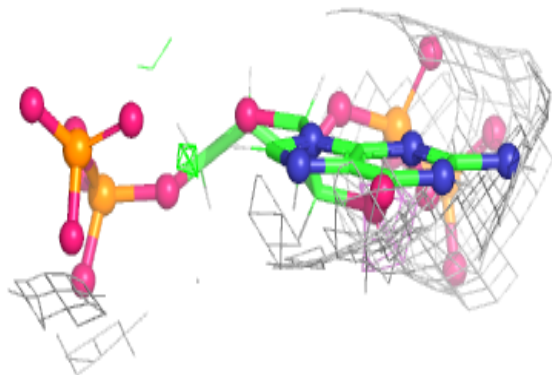
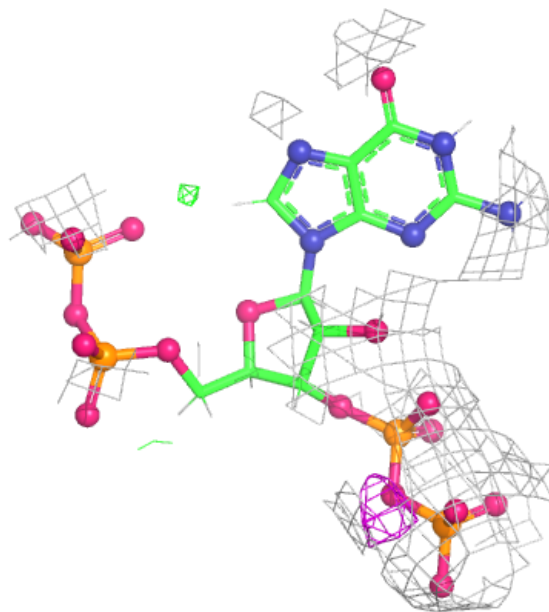
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	G4P	D	1503	36/36	0.80	0.08	31,56,93,118	0
6	ZN	I	1501	1/1	0.98	0.04	60,60,60,60	0
6	ZN	D	1501	1/1	1.00	0.03	54,54,54,54	0
6	ZN	I	1502	1/1	1.00	0.06	49,49,49,49	0
6	ZN	D	1502	1/1	1.00	0.05	8,8,8,8	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G4P D 1503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.