Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 08:29 AM EDT

PDB ID	:	4ERP / pdb_00004erp
Title	:	Crystal structure of a gemcitabine-diphosphate inhibited E. coli class Ia ribonucleotide reductase complex
Authors	:	Zimanyi, C.M.; Drennan, C.L.
Deposited on	:	2012-04-20
Resolution	:	4.45 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 (i) 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 (i)) were used in the production of this report:

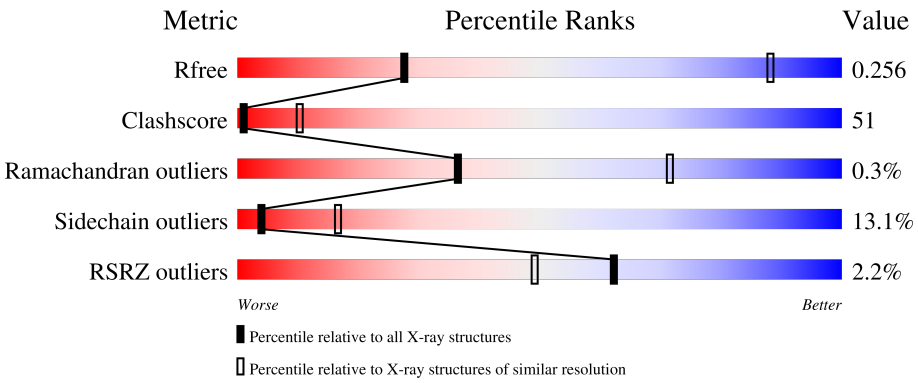
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.45 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	1119 (5.02-3.90)
Clashscore	190562	1024 (5.00-3.92)
Ramachandran outliers	187476	1055 (5.02-3.90)
Sidechain outliers	187428	1038 (5.02-3.90)
RSRZ outliers	180081	1114 (5.02-3.90)

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 <=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	761	2%, 34%, 52%, 10%, •
1	B	761	3%, 34%, 52%, 10%, •
1	C	761	2%, 36%, 48%, 11%, •, •
1	D	761	%, 33%, 53%, 11%, •
2	E	375	2%, 37%, 50%, 7%, 6%

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Mol	Chain	Length	Quality of chain
2	F	375	2% 39% 49% 7% 5%
2	G	375	2% 39% 48% 7% 5%
2	H	375	3% 35% 52% 8% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	B	801	-	-	X	-
3	ATP	C	801	-	-	X	-
3	ATP	D	801	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 35205 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

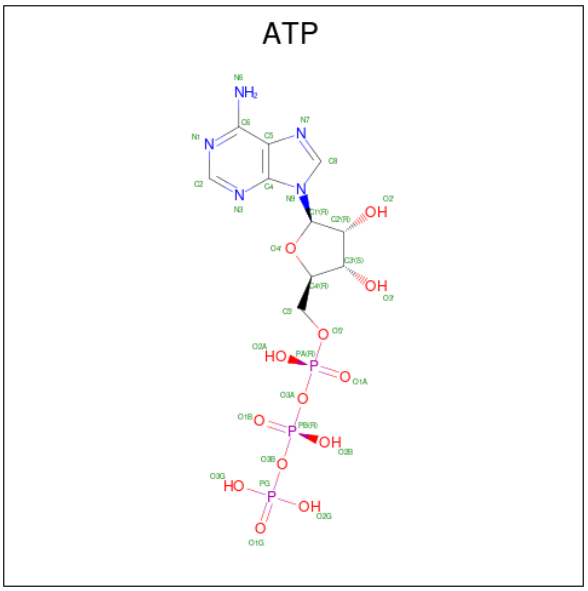
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	734	5845	3712	1004	1105	24	0	0	0
1	B	735	5850	3715	1005	1106	24	0	0	0
1	C	733	5841	3710	1003	1104	24	0	0	0
1	D	736	5859	3720	1007	1108	24	0	0	0

- Molecule 2 is a protein called Ribonucleoside-diphosphate reductase 1 subunit beta.

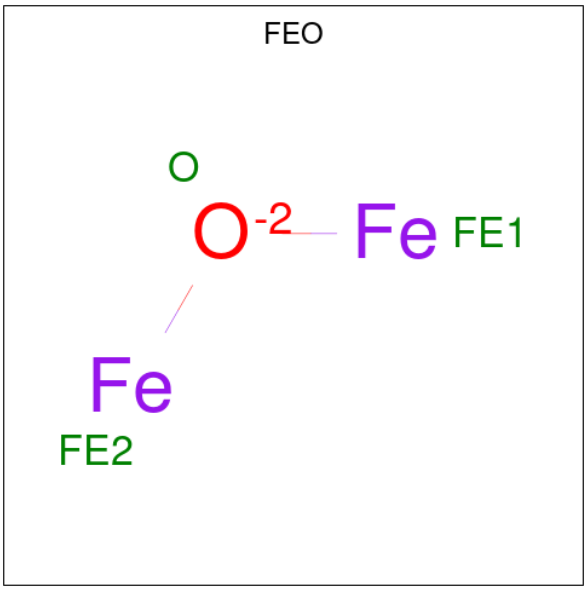
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	354	2900	1850	480	557	13	0	0	0
2	F	358	2930	1867	486	564	13	0	0	0
2	G	357	2922	1863	483	563	13	0	0	0
2	H	356	2914	1857	483	561	13	0	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe_2O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	O		
4	E	1	3	2	1	0	0
4	F	1	3	2	1	0	0
4	G	1	3	2	1	0	0
4	H	1	3	2	1	0	0

- Molecule 5 is water.

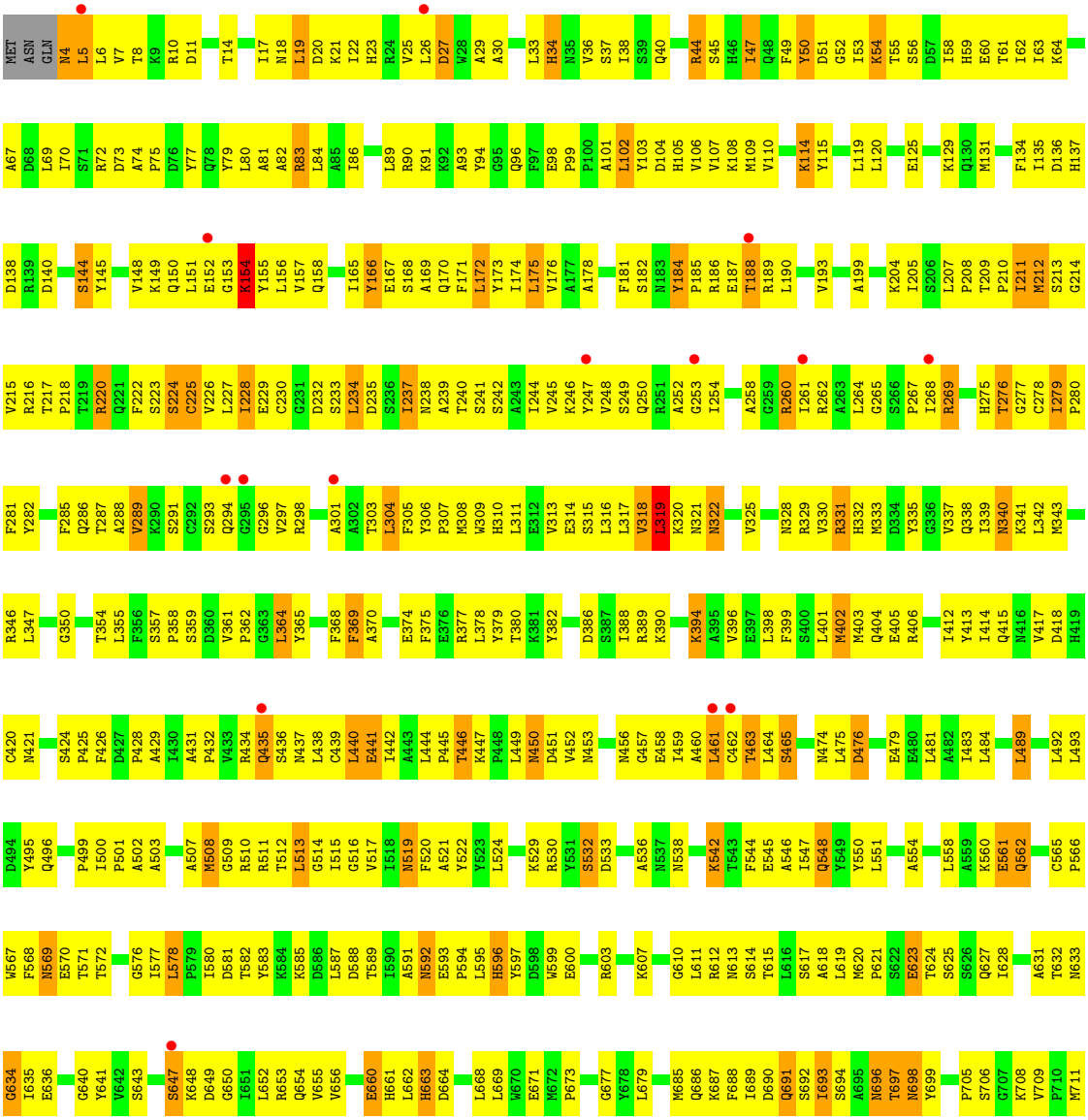
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	E	2	2	2	0	0
5	F	2	2	2	0	0
5	G	2	2	2	0	0
5	H	2	2	2	0	0

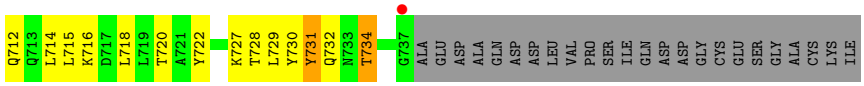
3 Residue-property plots (i)

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: Ribonucleoside-diphosphate reductase 1 subunit alpha

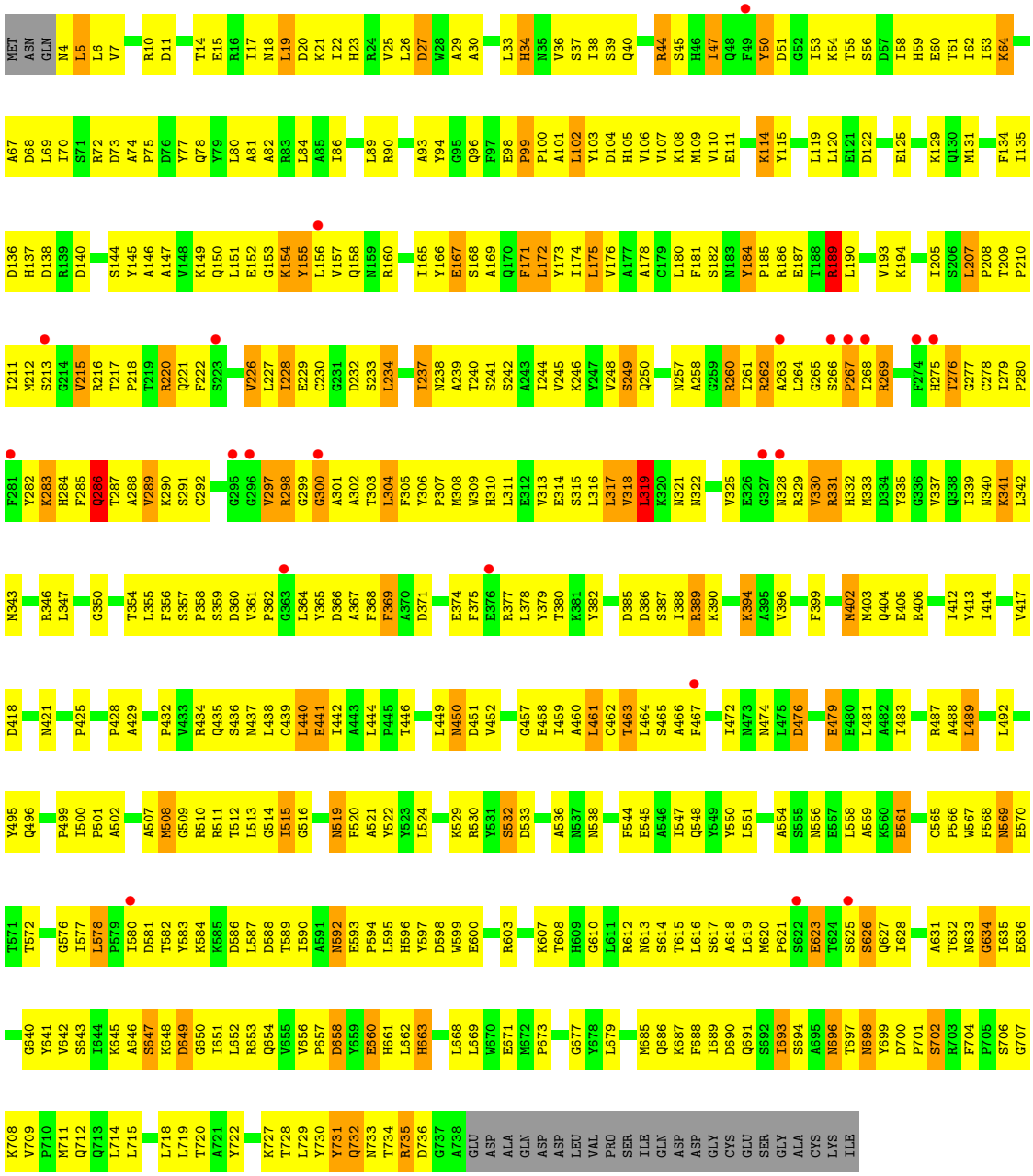
Chain A: 2% 34% 52% 10%





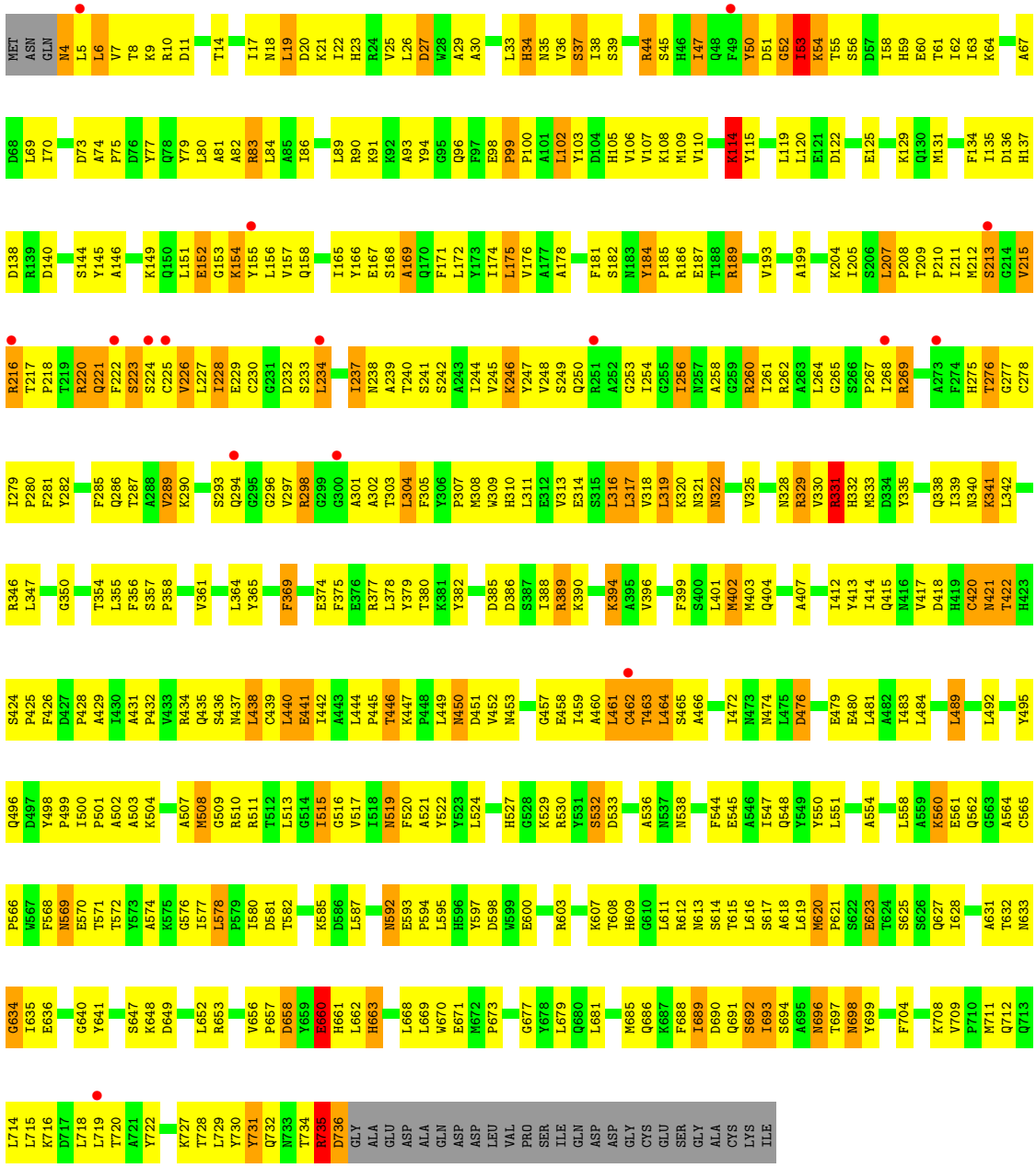
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

Chain B:



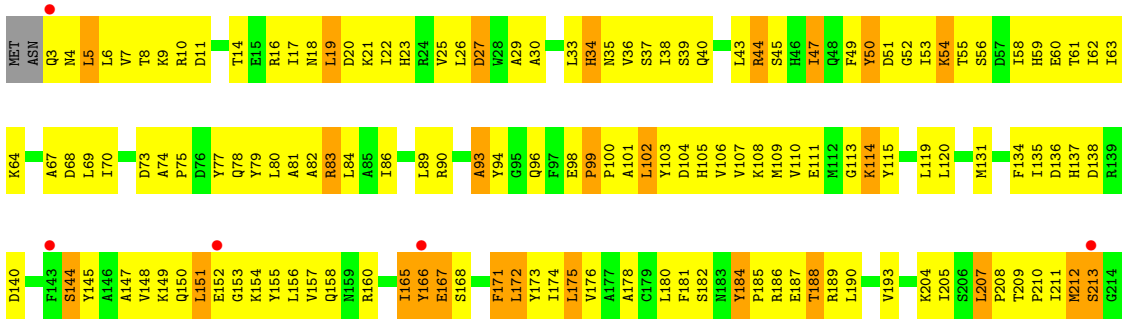
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

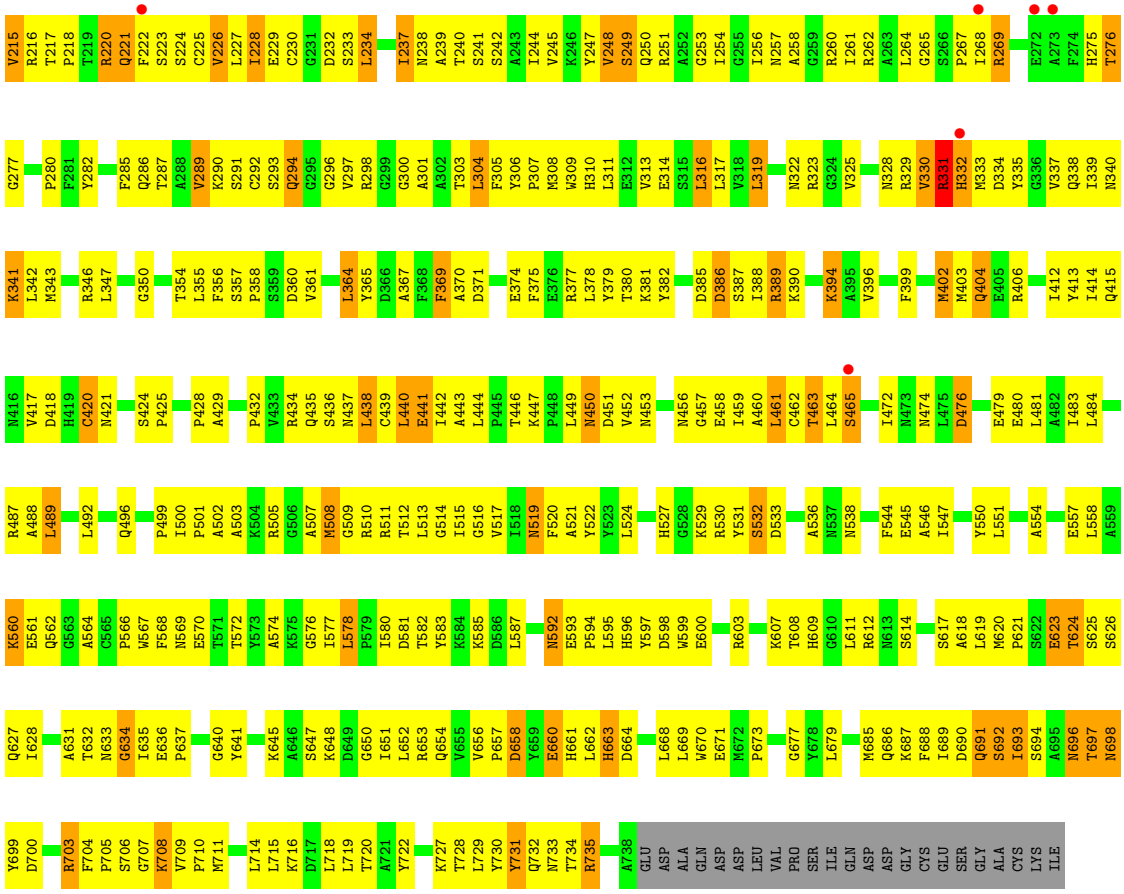
Chain C:



- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

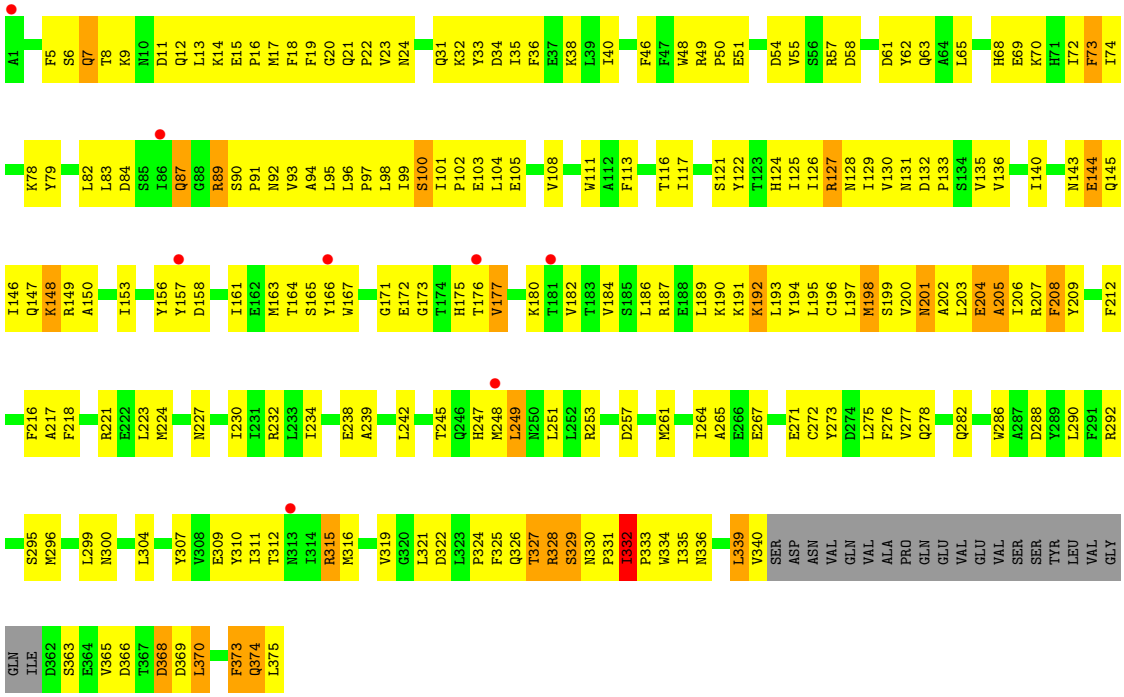
Chain D:





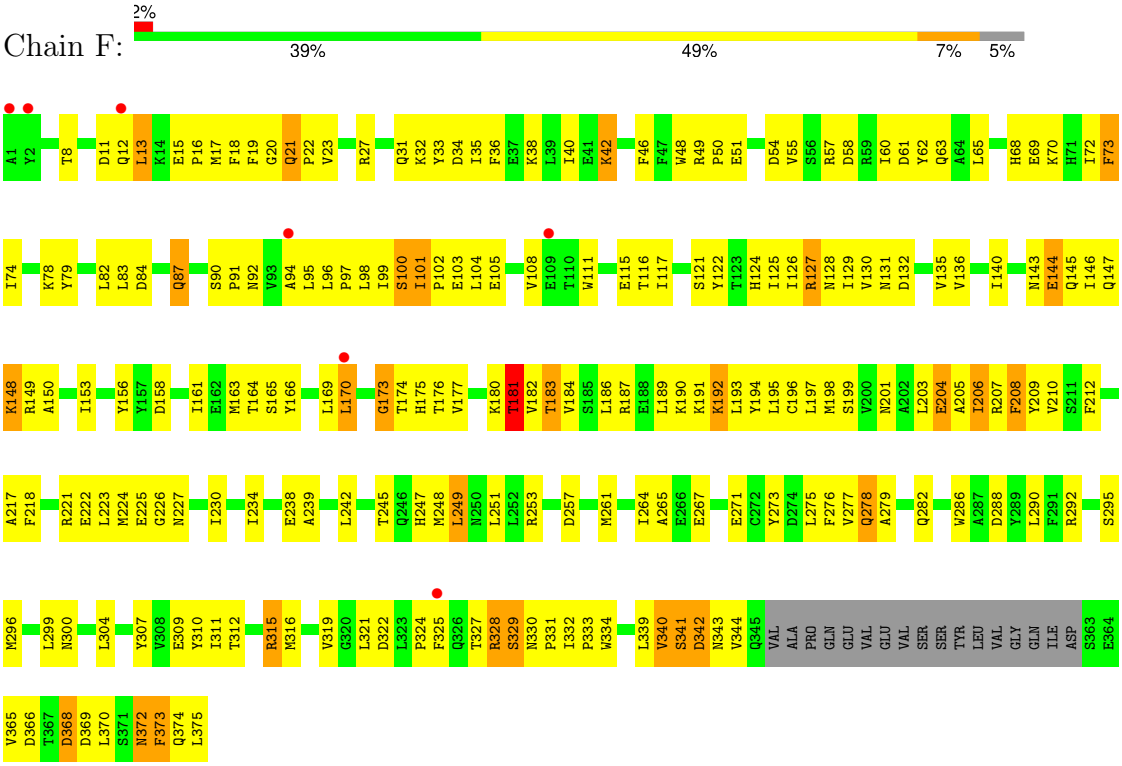
• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

Chain E:



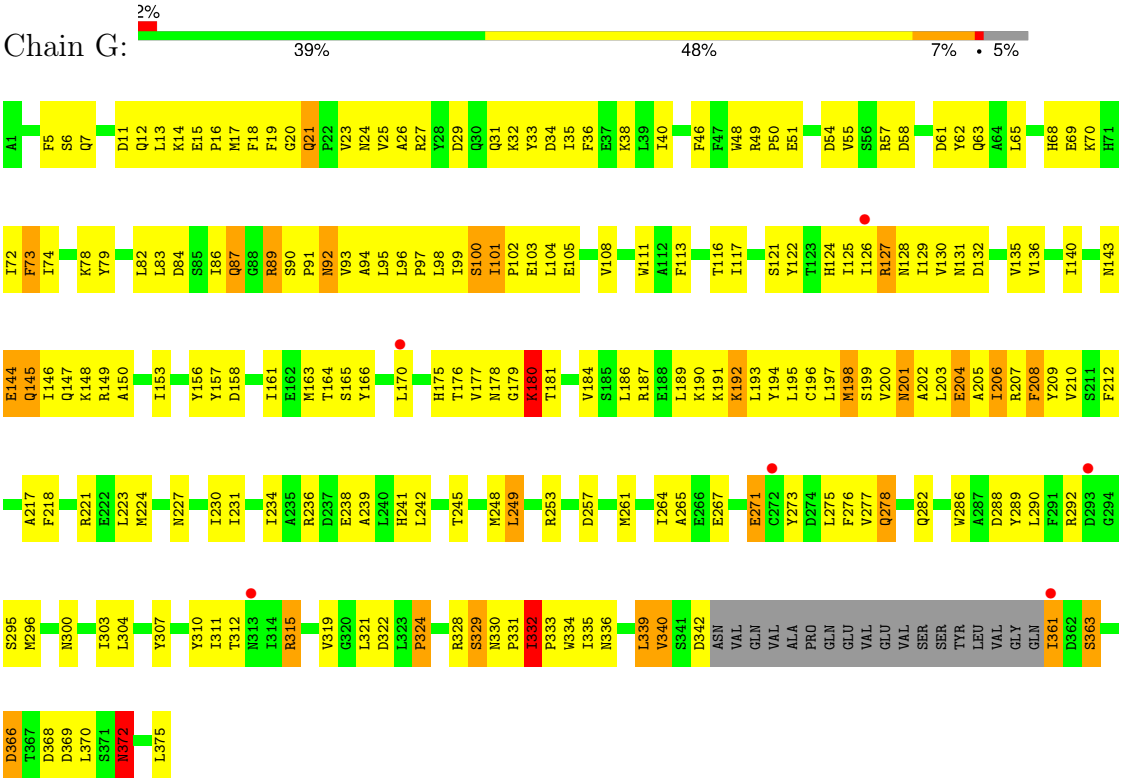
• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

Chain F:



• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

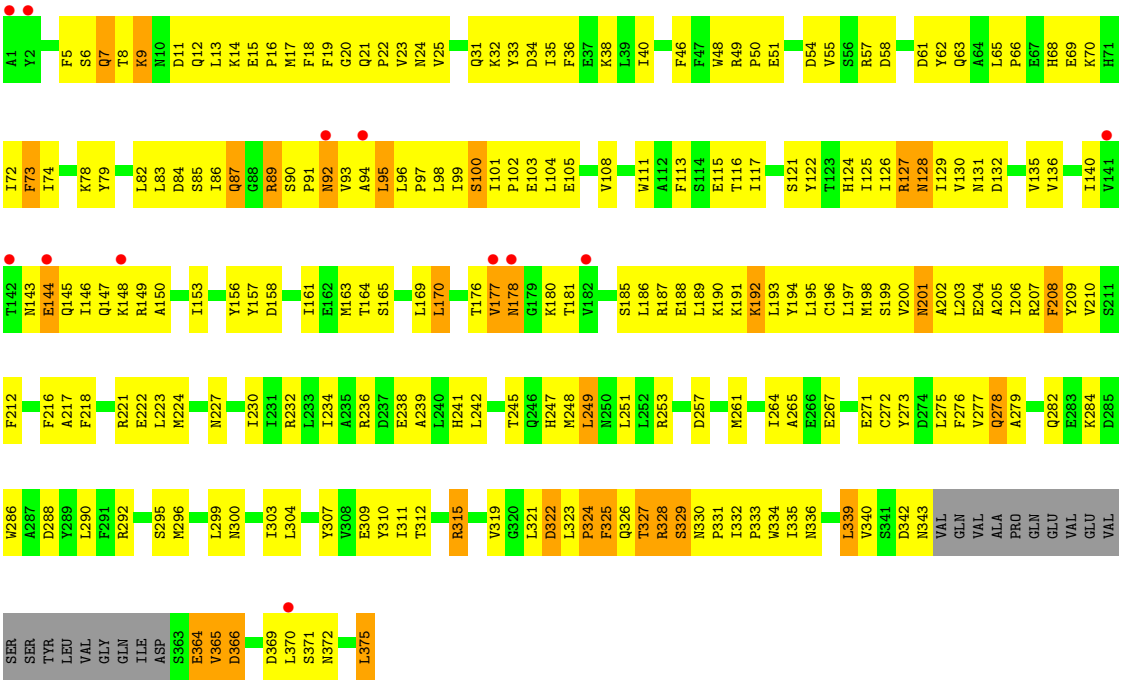
Chain G:



• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

Chain H:

3%
35%
52%
8%
5%


A1 Y2 F5 S6 Q7 T8 K9 N10 D11 Q12 L13 K14 E15 P16 M17 F18 F19 G20 Q21 P22 V23 N24 V25 Q31 K32 Y33 D34 I35 F36 E37 K38 L39 I40 F46 F47 W48 R49 P50 E51 D54 V55 S56 R57 D58 D61 Y62 Q63 A64 L65 P66 E67 H68 E69 K70 H71
I72 F73 I74 K78 Y79 L82 L83 D84 S85 I86 Q87 G88 R89 S90 P91 N92 V93 A94 L95 L96 P97 L98 I99 S100 I101 P102 E103 L104 E105 V108 W111 A112 F113 S114 E115 T116 I117 S121 Y122 T123 H124 I125 I126 R127 N128 I129 V130 N131 D132 V135 V136 I140 V141
T142 N143 E144 Q145 I146 Q147 K148 R149 A150 I153 Y156 Y157 D158 I161 E162 M163 T164 S165 L169 L170 T176 V177 N178 G179 K180 T181 V182 S185 L186 R187 E188 L189 K190 K191 K192 L193 Y194 L195 C196 L197 M198 S199 V200 N201 A202 L203 E204 A205 I206 R207 F208 Y209 V210 S211
F212 F216 A217 F218 R221 E222 L223 M224 N227 I230 I231 R232 L233 I234 A235 R236 D237 E238 A239 L240 H241 L242 T245 Q246 H247 M248 L249 N250 L251 L252 R253 D257 M261 I264 A265 E266 E267 E271 C272 Y273 D274 L275 F276 V277 Q278 A279 Q282 E283 K284 D285
W286 A287 D288 Y289 L290 F291 R292 S295 M296 L299 N300 I303 L304 Y307 V308 E309 Y310 I311 T312 R315 V319 G320 L321 D322 L323 P324 F325 Q326 T327 R328 S329 N330 P331 I332 P333 W334 I335 N336 L339 V340 S341 D342 N343 VAL GLN VAL ALA PRO GLN GLU VAL GLU VAL
SER SER TYR LEU VAL GLY GLN ILE ASP S363 E364 V365 D366 D369 L370 S371 N372 L375

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	128.67Å 398.91Å 319.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.45 50.00 – 4.45	Depositor EDS
% Data completeness (in resolution range)	82.3 (50.00-4.45) 82.2 (50.00-4.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 4.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.267 0.224 , 0.256	Depositor DCC
R_{free} test set	2334 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	108.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 166.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	35205	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.42	1/5973 (0.0%)	0.91	25/8090 (0.3%)
1	B	0.43	1/5978 (0.0%)	0.96	30/8097 (0.4%)
1	C	0.44	0/5969	0.97	34/8085 (0.4%)
1	D	0.42	0/5987	0.94	31/8109 (0.4%)
2	E	0.37	0/2964	0.88	9/4019 (0.2%)
2	F	0.41	2/2994 (0.1%)	0.91	8/4060 (0.2%)
2	G	0.41	0/2986	0.94	14/4049 (0.3%)
2	H	0.39	0/2978	0.89	6/4038 (0.1%)
All	All	0.42	4/35829 (0.0%)	0.93	157/48547 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	ASP	C-N	-8.89	1.23	1.33
2	F	173	GLY	C-N	7.59	1.43	1.33
2	F	181	THR	C-N	5.32	1.40	1.33
1	A	279	ILE	C-N	5.02	1.40	1.34

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	92	ASN	N-CA-C	13.79	126.03	111.14
1	C	187	GLU	N-CA-C	11.77	123.86	111.14
1	B	187	GLU	N-CA-C	11.63	123.70	111.14
2	H	92	ASN	N-CA-C	11.29	123.33	111.14
1	C	114	LYS	N-CA-C	10.91	122.92	111.14
1	D	332	HIS	N-CA-C	10.87	123.13	111.28
1	C	169	ALA	N-CA-C	10.72	123.97	111.11
1	A	114	LYS	N-CA-C	10.70	122.70	111.14
1	D	114	LYS	N-CA-C	10.69	122.68	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	596	HIS	N-CA-C	10.68	123.00	111.36
1	B	114	LYS	N-CA-C	10.63	122.62	111.14
2	G	73	PHE	N-CA-C	10.58	122.57	111.14
2	E	73	PHE	N-CA-C	10.49	122.47	111.14
2	H	73	PHE	N-CA-C	10.40	122.37	111.14
2	F	73	PHE	N-CA-C	10.37	122.34	111.14
1	B	189	ARG	N-CA-C	10.33	122.30	111.14
1	C	224	SER	N-CA-C	10.23	122.52	111.36
2	F	342	ASP	N-CA-C	9.28	124.85	112.88
2	G	144	GLU	N-CA-C	9.26	120.98	111.07
2	E	144	GLU	N-CA-C	9.24	120.95	111.07
2	F	144	GLU	N-CA-C	9.21	120.92	111.07
2	H	144	GLU	N-CA-C	9.13	120.84	111.07
1	D	532	SER	N-CA-C	9.08	120.79	111.07
1	C	532	SER	N-CA-C	9.07	120.94	111.14
1	B	532	SER	N-CA-C	9.05	120.75	111.07
2	F	341	SER	N-CA-C	8.80	123.38	111.24
1	A	532	SER	N-CA-C	8.78	120.63	111.14
1	D	456	ASN	N-CA-C	8.60	120.65	111.28
2	G	94	ALA	N-CA-C	8.39	120.50	111.36
1	A	456	ASN	N-CA-C	8.23	120.33	111.36
2	H	94	ALA	N-CA-C	7.85	119.92	111.36
1	D	370	ALA	N-CA-C	7.78	119.84	111.36
1	C	246	LYS	N-CA-C	7.78	119.39	111.07
1	B	155	TYR	N-CA-C	7.64	119.39	111.14
1	D	658	ASP	N-CA-C	7.57	121.50	111.28
1	B	658	ASP	N-CA-C	7.51	121.43	111.28
1	C	608	THR	N-CA-C	7.45	119.48	111.36
1	B	341	LYS	N-CA-C	7.40	118.98	111.07
1	C	316	LEU	N-CA-C	7.40	119.34	111.28
1	B	169	ALA	N-CA-C	7.35	118.94	111.07
1	D	341	LYS	N-CA-C	7.34	118.93	111.07
1	C	154	LYS	N-CA-C	7.30	119.24	111.28
1	D	316	LEU	N-CA-C	7.17	119.10	111.28
2	G	324	PRO	N-CA-C	7.16	127.23	112.47
1	D	166	TYR	N-CA-C	7.12	119.12	111.36
1	A	279	ILE	O-C-N	7.12	124.98	120.42
1	C	341	LYS	N-CA-C	7.02	118.58	111.07
1	D	608	THR	N-CA-C	7.01	119.00	111.36
1	B	608	THR	N-CA-C	6.95	118.93	111.36
1	C	369	PHE	N-CA-C	6.85	118.83	111.36
1	C	692	SER	N-CA-C	6.84	120.14	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	389	ARG	N-CA-C	-6.76	99.89	109.96
1	C	389	ARG	N-CA-C	-6.75	99.91	109.96
1	D	389	ARG	N-CA-C	-6.75	99.91	109.96
1	D	369	PHE	N-CA-C	6.69	118.36	111.14
1	D	331	ARG	N-CA-C	6.65	118.61	111.36
2	G	368	ASP	N-CA-C	6.63	118.51	111.28
1	D	660	GLU	N-CA-C	6.61	118.49	111.28
1	C	223	SER	N-CA-C	6.61	119.05	108.41
1	B	660	GLU	N-CA-C	6.57	118.10	111.07
1	C	660	GLU	N-CA-C	6.54	118.41	111.28
1	B	98	GLU	CA-C-N	6.46	124.37	119.66
1	B	98	GLU	C-N-CA	6.46	124.37	119.66
1	A	369	PHE	N-CA-C	6.43	118.37	111.36
1	C	98	GLU	CA-C-N	6.41	124.34	119.66
1	C	98	GLU	C-N-CA	6.41	124.34	119.66
2	G	201	ASN	N-CA-C	-6.41	104.56	112.38
1	D	98	GLU	CA-C-N	6.39	124.32	119.66
1	D	98	GLU	C-N-CA	6.39	124.32	119.66
1	A	98	GLU	CA-C-N	6.37	124.31	119.66
1	A	98	GLU	C-N-CA	6.37	124.31	119.66
1	C	249	SER	N-CA-C	-6.31	104.68	112.38
2	G	332	ILE	CA-C-N	6.27	126.18	119.28
2	G	332	ILE	C-N-CA	6.27	126.18	119.28
1	C	298	ARG	N-CA-C	6.27	119.76	108.17
2	G	176	THR	N-CA-C	-6.26	100.77	110.10
1	A	249	SER	N-CA-C	-6.26	104.74	112.38
2	E	332	ILE	CA-C-N	6.24	126.14	119.28
2	E	332	ILE	C-N-CA	6.24	126.14	119.28
1	B	215	VAL	N-CA-C	-6.20	101.00	109.37
1	D	692	SER	N-CA-C	6.17	119.17	110.23
2	E	201	ASN	N-CA-C	-6.14	104.89	112.38
1	D	215	VAL	N-CA-C	-6.13	101.09	109.37
2	E	373	PHE	N-CA-C	-6.06	101.07	110.10
2	H	201	ASN	N-CA-C	-6.05	105.00	112.38
2	E	205	ALA	N-CA-C	6.02	120.42	112.72
1	C	215	VAL	N-CA-C	-5.99	101.28	109.37
1	A	169	ALA	N-CA-C	5.97	117.59	111.14
1	B	360	ASP	O-C-N	-5.97	114.14	122.37
2	H	128	ASN	N-CA-C	5.96	117.78	111.28
1	B	508	MET	N-CA-C	-5.95	105.12	112.38
1	D	187	GLU	N-CA-C	5.95	117.84	111.36
2	E	93	VAL	N-CA-C	5.94	116.72	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	735	ARG	N-CA-C	5.93	117.42	111.07
2	G	372	ASN	N-CA-C	5.93	117.74	111.28
1	C	508	MET	N-CA-C	-5.92	105.16	112.38
1	A	508	MET	N-CA-C	-5.91	105.17	112.38
1	D	508	MET	N-CA-C	-5.88	105.21	112.38
1	C	152	GLU	N-CA-C	-5.87	104.96	111.71
1	A	166	TYR	N-CA-C	5.85	120.54	113.17
1	C	53	ILE	N-CA-C	-5.84	101.65	109.30
1	A	370	ALA	N-CA-C	5.83	120.43	112.68
1	C	421	ASN	N-CA-C	5.81	117.41	111.14
1	B	286	GLN	N-CA-C	5.80	117.68	111.36
1	D	709	VAL	N-CA-C	-5.79	102.65	108.96
1	D	99	PRO	O-C-N	5.75	123.95	121.31
1	B	99	PRO	O-C-N	5.74	123.95	121.31
1	A	187	GLU	N-CA-C	5.65	117.52	111.36
1	C	429	ALA	N-CA-C	5.62	117.40	111.28
1	C	99	PRO	O-C-N	5.60	123.89	121.31
1	B	429	ALA	N-CA-C	5.60	117.38	111.28
1	A	99	PRO	O-C-N	5.59	123.88	121.31
1	B	331	ARG	N-CA-C	5.57	119.77	112.92
1	A	429	ALA	N-CA-C	5.56	117.34	111.28
1	B	213	SER	N-CA-C	5.55	117.33	111.28
1	C	213	SER	N-CA-C	5.55	117.33	111.28
2	G	180	LYS	N-CA-C	5.54	117.27	108.79
1	A	254	ILE	N-CA-C	5.50	115.87	108.17
1	A	331	ARG	N-CA-C	5.50	117.27	111.28
1	A	154	LYS	N-CA-C	5.44	117.28	111.36
1	D	429	ALA	N-CA-C	5.44	117.28	111.36
1	B	561	GLU	N-CA-C	5.43	117.19	111.28
1	D	249	SER	N-CA-C	-5.42	105.37	111.28
1	D	213	SER	N-CA-C	5.41	117.18	111.28
1	B	648	LYS	N-CA-C	-5.35	105.45	111.28
2	F	206	ILE	N-CA-C	5.34	116.74	111.67
1	B	267	PRO	N-CA-CB	5.29	107.95	103.35
1	C	52	GLY	N-CA-C	5.28	122.07	115.21
2	G	206	ILE	N-CA-C	5.25	116.66	111.67
2	F	340	VAL	N-CA-C	5.25	115.13	107.88
1	A	319	LEU	N-CA-C	5.25	117.00	111.28
1	B	319	LEU	N-CA-C	5.23	116.98	111.28
1	C	267	PRO	N-CA-CB	5.23	107.90	103.35
1	A	267	PRO	N-CA-CB	5.22	107.90	103.35
1	D	267	PRO	N-CA-CB	5.20	107.87	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	368	ASP	N-CA-C	5.18	117.01	111.36
1	B	626	SER	N-CA-C	5.17	116.92	111.28
1	D	93	ALA	N-CA-C	5.17	117.00	111.36
1	D	99	PRO	CA-C-N	5.17	125.15	120.03
1	D	99	PRO	C-N-CA	5.17	125.15	120.03
1	C	658	ASP	N-CA-C	5.14	118.72	111.52
1	A	561	GLU	N-CA-C	5.14	116.96	111.36
1	C	331	ARG	N-CA-C	5.13	116.95	111.36
1	B	369	PHE	N-CA-C	5.12	116.94	111.36
1	B	99	PRO	CA-C-N	5.11	125.08	120.03
1	B	99	PRO	C-N-CA	5.11	125.08	120.03
1	B	154	LYS	N-CA-C	5.11	116.53	111.07
1	C	99	PRO	CA-C-N	5.08	125.06	120.03
1	C	99	PRO	C-N-CA	5.08	125.06	120.03
1	A	99	PRO	CA-C-N	5.05	125.03	120.03
1	A	99	PRO	C-N-CA	5.05	125.03	120.03
1	D	167	GLU	N-CA-C	5.05	117.35	109.52
2	E	198	MET	N-CA-C	-5.04	106.96	113.01
2	F	148	LYS	N-CA-C	5.03	116.76	111.28
1	A	664	ASP	N-CA-C	5.02	116.83	111.36
2	G	198	MET	N-CA-C	-5.02	106.99	113.01
1	D	626	SER	N-CA-C	5.00	116.74	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5845	0	5770	661	0
1	B	5850	0	5775	676	0
1	C	5841	0	5767	646	0
1	D	5859	0	5783	680	0
2	E	2900	0	2826	249	0
2	F	2930	0	2854	242	0
2	G	2922	0	2846	252	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2914	0	2837	288	0
3	A	31	0	12	4	0
3	B	31	0	12	9	0
3	C	31	0	11	15	0
3	D	31	0	12	10	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
5	E	2	0	0	1	0
5	F	2	0	0	1	0
5	G	2	0	0	1	0
5	H	2	0	0	0	0
All	All	35205	0	34505	3564	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 51.

All (3564) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:TYR:CE1	1:C:216:ARG:HD2	1.42	1.53
1:C:442:ILE:HD12	1:C:462:CYS:SG	1.48	1.51
1:D:114:LYS:HG3	1:D:166:TYR:CE2	1.45	1.50
1:B:222:PHE:CD2	1:B:492:LEU:HD11	1.44	1.49
1:A:5:LEU:HD12	1:A:17:ILE:CG1	1.41	1.49
1:D:89:LEU:CD2	1:D:152:GLU:HG3	1.53	1.38
2:H:232:ARG:HD3	2:H:342:ASP:CB	1.51	1.38
1:D:89:LEU:HD21	1:D:152:GLU:CG	1.52	1.38
2:F:38:LYS:HD3	2:F:344:VAL:CG1	1.53	1.36
1:D:172:LEU:HD23	1:D:216:ARG:NH2	1.37	1.34
1:D:215:VAL:O	1:D:216:ARG:HG2	1.25	1.33
1:A:172:LEU:HD23	1:A:216:ARG:CZ	1.60	1.32
1:B:258:ALA:HB3	1:B:282:TYR:CE2	1.62	1.32
2:H:55:VAL:HG21	2:H:128:ASN:ND2	1.39	1.31
1:A:5:LEU:CD1	1:A:17:ILE:HG12	1.59	1.30
2:E:322:ASP:O	2:E:324:PRO:HD3	1.27	1.29
1:B:258:ALA:HB3	1:B:282:TYR:CZ	1.70	1.26
2:H:232:ARG:CD	2:H:342:ASP:HB2	1.65	1.25
1:A:215:VAL:O	1:A:216:ARG:HG2	1.07	1.25
2:F:340:VAL:HG12	2:F:341:SER:OG	1.35	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:LEU:O	2:F:32:LYS:HD2	1.29	1.25
1:B:189:ARG:O	1:B:193:VAL:HG23	1.35	1.24
2:G:322:ASP:O	2:G:324:PRO:HD3	1.34	1.24
1:C:418:ASP:O	1:C:422:THR:HG23	1.32	1.23
1:C:442:ILE:CD1	1:C:462:CYS:SG	2.26	1.22
1:B:114:LYS:HE2	1:B:166:TYR:CE2	1.74	1.22
1:B:222:PHE:CD2	1:B:492:LEU:CD1	2.25	1.20
1:B:282:TYR:CE2	1:B:304:LEU:HD22	1.76	1.19
1:C:50:TYR:CE2	1:C:53:ILE:HB	1.79	1.18
1:B:619:LEU:HD12	1:B:693:ILE:CG2	1.72	1.18
1:C:115:TYR:CE1	1:C:216:ARG:CD	2.27	1.18
1:C:254:ILE:N	1:C:438:LEU:HD12	1.57	1.18
2:E:205:ALA:HB1	2:E:315:ARG:HD3	1.22	1.17
1:A:208:PRO:CG	1:A:211:ILE:HD13	1.72	1.17
1:B:619:LEU:HD12	1:B:693:ILE:HG22	1.26	1.17
1:B:711:MET:HB3	2:H:364:GLU:O	1.45	1.17
1:B:40:GLN:NE2	2:H:333:PRO:HG2	1.58	1.16
1:D:463:THR:O	1:D:464:LEU:HD23	1.43	1.16
1:A:317:LEU:HD12	1:A:401:LEU:HD23	1.25	1.15
1:C:17:ILE:HD12	3:C:801:ATP:C2	1.79	1.15
1:A:463:THR:CB	1:A:513:LEU:HD23	1.75	1.15
1:B:222:PHE:CE2	1:B:492:LEU:HD11	1.82	1.15
1:C:441:GLU:HG2	1:C:620:MET:CB	1.78	1.13
1:B:282:TYR:HE2	1:B:304:LEU:CD2	1.60	1.13
1:C:301:ALA:O	1:C:438:LEU:HD11	1.46	1.13
1:A:463:THR:OG1	1:A:513:LEU:HD23	1.47	1.13
1:C:617:SER:HB2	1:C:690:ASP:H	1.14	1.13
1:C:189:ARG:O	1:C:193:VAL:HG23	1.48	1.12
1:D:294:GLN:HB2	1:D:298:ARG:HG3	1.23	1.12
1:D:463:THR:C	1:D:464:LEU:HD23	1.73	1.12
1:A:463:THR:O	1:A:464:LEU:HD23	1.47	1.12
1:B:735:ARG:HG3	1:B:735:ARG:O	1.43	1.12
1:C:515:ILE:HD12	1:C:551:LEU:HD13	1.28	1.12
1:D:254:ILE:N	1:D:438:LEU:HD12	1.64	1.11
1:A:215:VAL:O	1:A:216:ARG:CG	1.97	1.11
1:C:317:LEU:HD11	1:C:401:LEU:CD2	1.80	1.11
1:C:317:LEU:HD11	1:C:401:LEU:HD21	1.11	1.11
1:C:317:LEU:HD12	1:C:318:VAL:HG13	1.29	1.11
1:B:618:ALA:N	1:B:689:ILE:HD11	1.66	1.10
1:B:44:ARG:HG3	1:B:69:LEU:HD21	1.12	1.10
1:B:317:LEU:CD1	1:B:402:MET:HA	1.80	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:LEU:CB	1:A:693:ILE:HG22	1.82	1.10
1:B:318:VAL:HG23	1:B:329:ARG:CZ	1.81	1.10
1:B:621:PRO:HD3	1:B:694:SER:CB	1.81	1.10
1:B:282:TYR:CE2	1:B:304:LEU:CD2	2.34	1.09
1:C:369:PHE:CE2	1:C:434:ARG:HD3	1.86	1.09
1:D:172:LEU:HD23	1:D:216:ARG:CZ	1.81	1.09
1:B:619:LEU:CD1	1:B:693:ILE:HG22	1.81	1.09
1:C:293:SER:HB2	1:C:296:GLY:HA2	1.35	1.08
1:A:489:LEU:HD22	1:A:513:LEU:HD22	1.14	1.08
1:A:619:LEU:HB2	1:A:693:ILE:CG2	1.83	1.08
1:C:222:PHE:CD2	1:C:492:LEU:HD11	1.88	1.08
2:F:332:ILE:HG22	2:F:334:TRP:HE1	1.06	1.08
1:B:258:ALA:CB	1:B:282:TYR:CE2	2.35	1.07
1:C:175:LEU:HD22	1:C:216:ARG:HD3	1.11	1.07
1:D:157:VAL:HG12	1:D:166:TYR:HD2	1.14	1.07
1:A:493:LEU:HD21	1:A:513:LEU:HD21	1.15	1.07
1:B:114:LYS:HE2	1:B:166:TYR:HE2	0.97	1.07
1:C:621:PRO:HD3	1:C:694:SER:HB2	1.33	1.07
1:D:301:ALA:O	1:D:438:LEU:HD11	1.55	1.07
1:C:735:ARG:O	1:C:736:ASP:HB3	1.53	1.06
1:A:647:SER:HB2	1:A:652:LEU:HG	1.37	1.06
1:D:44:ARG:HG3	1:D:69:LEU:HD21	1.30	1.06
1:D:150:GLN:HB3	1:D:154:LYS:HD3	1.38	1.06
1:C:441:GLU:HG2	1:C:620:MET:HB2	1.07	1.06
1:A:692:SER:HB2	1:A:727:LYS:HB2	1.36	1.06
1:B:44:ARG:CG	1:B:69:LEU:HD21	1.86	1.06
1:D:329:ARG:HD3	1:D:331:ARG:NH2	1.71	1.06
2:H:332:ILE:HG22	2:H:334:TRP:HE1	1.19	1.06
1:A:5:LEU:HD12	1:A:17:ILE:CD1	1.85	1.06
1:B:700:ASP:OD1	1:B:735:ARG:HD2	1.55	1.06
1:D:153:GLY:HA2	1:D:158:GLN:HE22	1.16	1.06
1:A:225:CYS:HB3	1:A:253:GLY:O	1.55	1.05
1:C:331:ARG:HG2	1:C:332:HIS:HD2	1.11	1.05
1:A:208:PRO:HG2	1:A:211:ILE:HD13	1.06	1.05
2:F:332:ILE:HG22	2:F:334:TRP:NE1	1.71	1.05
1:A:227:LEU:HB3	1:A:435:GLN:NE2	1.72	1.04
1:A:463:THR:C	1:A:464:LEU:HD23	1.81	1.04
1:C:513:LEU:HD11	1:C:616:LEU:HD23	1.36	1.04
1:D:685:MET:O	1:D:689:ILE:HG13	1.57	1.04
1:C:44:ARG:HG3	1:C:69:LEU:HD21	1.34	1.04
1:D:44:ARG:HA	1:D:44:ARG:HE	0.88	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:339:LEU:O	2:E:339:LEU:HD12	1.55	1.04
2:H:336:ASN:HA	2:H:339:LEU:HD11	1.34	1.04
1:C:513:LEU:HD11	1:C:616:LEU:CD2	1.88	1.04
1:A:207:LEU:HB2	1:A:212:MET:HE1	1.39	1.03
1:C:44:ARG:HA	1:C:44:ARG:HE	1.22	1.03
1:D:150:GLN:O	1:D:154:LYS:HG3	1.57	1.03
1:D:39:SER:HB3	2:G:332:ILE:HG22	1.40	1.03
1:D:114:LYS:CG	1:D:166:TYR:CE2	2.41	1.03
1:D:617:SER:HB2	1:D:690:ASP:H	1.19	1.03
1:B:220:ARG:O	1:B:496:GLN:HA	1.59	1.02
1:C:167:GLU:OE2	1:C:172:LEU:HD12	1.57	1.02
2:G:340:VAL:HG13	2:G:340:VAL:O	1.59	1.02
1:A:155:TYR:HD1	1:A:212:MET:CB	1.72	1.02
1:D:155:TYR:HE2	1:D:212:MET:HE2	1.22	1.02
1:B:286:GLN:NE2	1:B:332:HIS:HB2	1.72	1.02
2:F:38:LYS:HD3	2:F:344:VAL:HG11	1.03	1.01
1:A:172:LEU:CD2	1:A:216:ARG:NH1	2.23	1.01
1:B:619:LEU:CG	1:B:693:ILE:HG22	1.90	1.01
1:C:294:GLN:OE1	1:C:298:ARG:HD3	1.60	1.01
1:B:621:PRO:HD3	1:B:694:SER:HB2	1.37	1.01
1:C:175:LEU:CD2	1:C:216:ARG:HD3	1.90	1.01
1:D:44:ARG:HA	1:D:44:ARG:NE	1.66	1.00
1:D:157:VAL:HG12	1:D:166:TYR:CD2	1.96	1.00
2:G:273:TYR:CE2	2:G:324:PRO:HG3	1.96	1.00
1:A:172:LEU:CD2	1:A:216:ARG:CZ	2.37	1.00
1:A:298:ARG:HE	1:C:6:LEU:HD21	1.25	1.00
1:D:286:GLN:OE1	1:D:332:HIS:HB2	1.61	1.00
1:C:17:ILE:HD12	3:C:801:ATP:H2	1.24	1.00
1:A:5:LEU:HB2	1:A:17:ILE:CG2	1.92	1.00
1:B:258:ALA:CB	1:B:282:TYR:CZ	2.45	0.99
1:C:226:VAL:HG12	1:C:461:LEU:HD22	1.43	0.99
1:D:220:ARG:O	1:D:496:GLN:HA	1.62	0.99
1:B:286:GLN:HE21	1:B:332:HIS:HB2	1.21	0.99
1:C:157:VAL:HG23	1:C:216:ARG:HH12	1.26	0.99
1:D:711:MET:CB	2:G:363:SER:HB3	1.92	0.99
1:D:215:VAL:O	1:D:216:ARG:CG	2.11	0.99
1:B:318:VAL:CG2	1:B:329:ARG:NH1	2.26	0.98
1:B:466:ALA:HA	1:B:516:GLY:O	1.63	0.98
1:D:254:ILE:H	1:D:438:LEU:CD1	1.76	0.98
2:H:65:LEU:HD21	2:H:223:LEU:HD13	1.45	0.98
1:A:489:LEU:CD2	1:A:513:LEU:HD22	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:LEU:HB2	1:D:51:ASP:OD1	1.62	0.98
1:D:623:GLU:HG2	1:D:633:ASN:ND2	1.78	0.97
1:D:44:ARG:HE	1:D:44:ARG:CA	1.76	0.97
1:D:711:MET:HB3	2:G:363:SER:HB3	1.46	0.97
1:C:331:ARG:HG2	1:C:332:HIS:CD2	1.97	0.97
1:D:711:MET:H	2:G:363:SER:CB	1.76	0.97
1:A:208:PRO:HG2	1:A:211:ILE:CD1	1.94	0.97
1:C:369:PHE:HE2	1:C:434:ARG:HD3	1.22	0.97
2:H:55:VAL:CG2	2:H:128:ASN:ND2	2.27	0.97
1:D:316:LEU:O	1:D:319:LEU:HG	1.64	0.97
1:A:625:SER:O	1:A:628:ILE:HG22	1.65	0.96
2:E:65:LEU:HD21	2:E:223:LEU:HD13	1.47	0.96
1:B:109:MET:SD	1:B:166:TYR:HB3	2.05	0.96
1:D:37:SER:HB3	2:G:331:PRO:O	1.62	0.96
1:D:144:SER:O	1:D:148:VAL:HG23	1.65	0.96
1:A:317:LEU:HD12	1:A:401:LEU:CD2	1.96	0.96
2:F:92:ASN:HA	2:F:96:LEU:HD13	1.48	0.96
1:B:317:LEU:HD11	1:B:402:MET:HA	1.48	0.96
1:A:144:SER:O	1:A:148:VAL:HG23	1.66	0.96
1:A:341:LYS:HB2	1:A:722:TYR:OH	1.66	0.96
1:A:361:VAL:CG1	1:A:364:LEU:HB2	1.96	0.95
1:B:369:PHE:CD1	1:B:434:ARG:HA	2.02	0.95
1:C:464:LEU:HD13	1:C:620:MET:SD	2.05	0.95
2:F:322:ASP:O	2:F:324:PRO:HD3	1.65	0.95
1:A:618:ALA:HB2	1:A:691:GLN:HG3	1.46	0.95
1:C:207:LEU:HD11	1:C:212:MET:SD	2.05	0.95
2:G:149:ARG:HH12	2:G:286:TRP:HB2	1.32	0.95
1:D:89:LEU:HD21	1:D:152:GLU:CD	1.89	0.95
2:F:12:GLN:HE21	2:F:23:VAL:HG13	1.30	0.95
1:A:227:LEU:CB	1:A:435:GLN:NE2	2.29	0.95
1:D:114:LYS:HD3	1:D:114:LYS:N	1.81	0.94
1:A:109:MET:SD	1:A:166:TYR:HB3	2.07	0.94
1:D:625:SER:O	1:D:628:ILE:HG22	1.67	0.94
2:F:149:ARG:HH12	2:F:286:TRP:HB2	1.33	0.94
1:A:369:PHE:CE2	1:A:434:ARG:HD3	2.01	0.94
1:C:157:VAL:CG2	1:C:216:ARG:HH12	1.81	0.94
1:C:320:LYS:HE2	1:C:333:MET:O	1.66	0.94
1:A:413:TYR:OH	1:A:731:TYR:HE2	1.50	0.94
1:B:701:PRO:HD2	1:B:735:ARG:HG2	1.48	0.94
1:D:172:LEU:CD2	1:D:216:ARG:NH2	2.31	0.94
2:F:38:LYS:CD	2:F:344:VAL:HG11	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:SER:CB	1:B:689:ILE:HD12	1.97	0.93
1:D:168:SER:OG	1:D:171:PHE:HB2	1.68	0.93
1:B:226:VAL:HG12	1:B:461:LEU:HD22	1.50	0.93
1:C:109:MET:SD	1:C:166:TYR:HB3	2.09	0.93
2:H:111:TRP:HZ2	2:H:204:GLU:OE2	1.49	0.93
1:B:619:LEU:CB	1:B:693:ILE:HG22	1.97	0.93
1:C:625:SER:O	1:C:628:ILE:HG22	1.69	0.93
1:D:254:ILE:H	1:D:438:LEU:HD12	1.29	0.93
1:C:420:CYS:O	1:C:424:SER:HB2	1.68	0.92
1:A:623:GLU:HG2	1:A:633:ASN:ND2	1.84	0.92
1:D:205:ILE:HD11	1:D:481:LEU:HB3	1.51	0.92
1:C:17:ILE:CD1	3:C:801:ATP:H2	1.81	0.92
1:C:711:MET:HE2	1:C:715:LEU:HG	1.51	0.92
1:D:294:GLN:HB2	1:D:298:ARG:CG	1.98	0.92
1:D:364:LEU:O	1:D:364:LEU:HD13	1.69	0.92
2:H:149:ARG:HH12	2:H:286:TRP:HB2	1.33	0.92
1:B:37:SER:HB3	2:H:331:PRO:O	1.69	0.92
1:B:516:GLY:CA	1:B:620:MET:HE1	2.00	0.92
2:F:38:LYS:HD3	2:F:344:VAL:HG12	1.51	0.92
1:C:301:ALA:C	1:C:438:LEU:HD11	1.95	0.92
2:E:205:ALA:HB1	2:E:315:ARG:CD	2.00	0.91
1:B:315:SER:O	1:B:318:VAL:HG13	1.70	0.91
1:C:254:ILE:H	1:C:438:LEU:CD1	1.82	0.91
1:B:317:LEU:HD12	1:B:402:MET:HA	1.50	0.91
1:B:619:LEU:HB2	1:B:693:ILE:HA	1.53	0.91
2:H:55:VAL:HG21	2:H:128:ASN:HD21	1.20	0.91
1:A:425:PRO:HG2	1:A:690:ASP:HB3	1.49	0.91
1:D:89:LEU:HD21	1:D:152:GLU:HG3	0.91	0.91
1:B:145:TYR:HE2	1:B:652:LEU:HD23	1.36	0.91
2:H:232:ARG:NH1	2:H:343:ASN:H	1.69	0.91
1:C:53:ILE:CD1	1:C:58:ILE:HG12	2.01	0.91
1:A:5:LEU:HB2	1:A:17:ILE:HG21	1.51	0.91
1:C:369:PHE:HD2	1:C:434:ARG:NH1	1.67	0.91
1:C:157:VAL:CG2	1:C:216:ARG:NH1	2.33	0.91
1:D:168:SER:HG	1:D:171:PHE:HD2	0.92	0.91
1:B:297:VAL:HB	1:B:298:ARG:HE	1.35	0.90
1:C:361:VAL:CG1	1:C:364:LEU:HB2	2.01	0.90
1:C:254:ILE:N	1:C:438:LEU:CD1	2.34	0.90
2:G:273:TYR:HE2	2:G:324:PRO:HG3	1.32	0.90
1:D:157:VAL:O	1:D:166:TYR:HB2	1.72	0.90
1:D:294:GLN:CB	1:D:298:ARG:HG3	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:GLN:HG2	2:H:102:PRO:HD3	1.53	0.90
1:A:463:THR:HB	1:A:513:LEU:HD23	1.49	0.90
1:B:365:TYR:CZ	1:B:369:PHE:HE2	1.88	0.90
1:B:258:ALA:HB3	1:B:282:TYR:OH	1.72	0.90
1:C:685:MET:O	1:C:689:ILE:HG12	1.70	0.90
1:A:155:TYR:HD1	1:A:212:MET:HB3	1.35	0.90
1:B:215:VAL:HG22	1:B:222:PHE:CZ	2.06	0.90
1:D:716:LYS:HG2	2:G:370:LEU:HD21	1.54	0.90
2:F:340:VAL:CG1	2:F:341:SER:OG	2.20	0.90
2:G:92:ASN:HA	2:G:96:LEU:HD13	1.51	0.90
1:C:463:THR:C	1:C:464:LEU:HD23	1.96	0.89
1:C:447:LYS:HB2	1:C:458:GLU:H	1.36	0.89
2:H:111:TRP:CZ2	2:H:204:GLU:OE2	2.25	0.89
1:C:254:ILE:H	1:C:438:LEU:HD12	1.38	0.89
2:H:236:ARG:HD3	2:H:342:ASP:OD1	1.73	0.89
1:B:282:TYR:HA	1:B:285:PHE:HD2	1.36	0.89
2:F:87:GLN:O	2:F:91:PRO:CD	2.20	0.89
1:A:711:MET:HE2	1:A:715:LEU:HG	1.53	0.89
1:A:369:PHE:HD2	1:A:434:ARG:HH11	1.14	0.89
1:B:689:ILE:HG13	1:B:691:GLN:O	1.73	0.89
1:C:175:LEU:HD22	1:C:216:ARG:CD	2.01	0.89
1:B:205:ILE:HD11	1:B:481:LEU:HB3	1.55	0.89
1:B:619:LEU:CD1	1:B:693:ILE:CG2	2.43	0.89
1:C:89:LEU:HD21	1:C:152:GLU:HG3	1.54	0.89
2:E:87:GLN:O	2:E:91:PRO:CD	2.21	0.88
2:G:87:GLN:O	2:G:91:PRO:CD	2.21	0.88
1:C:317:LEU:CD1	1:C:401:LEU:HD21	2.02	0.88
2:H:87:GLN:O	2:H:91:PRO:CD	2.21	0.88
1:A:361:VAL:HG12	1:A:364:LEU:HB2	1.53	0.88
1:B:365:TYR:CE2	1:B:369:PHE:HE2	1.91	0.88
1:D:248:VAL:HG23	1:D:254:ILE:CG1	2.03	0.88
1:C:205:ILE:HD11	1:C:481:LEU:HB3	1.56	0.88
1:A:114:LYS:HE2	1:A:166:TYR:CE2	2.08	0.88
1:D:248:VAL:CG2	1:D:254:ILE:HG13	2.03	0.88
1:B:168:SER:OG	1:B:171:PHE:HB2	1.74	0.87
1:D:222:PHE:CD2	1:D:492:LEU:HD11	2.08	0.87
1:B:619:LEU:HD12	1:B:693:ILE:HG21	1.55	0.87
1:A:298:ARG:NE	1:C:6:LEU:HD21	1.89	0.87
2:H:332:ILE:HG22	2:H:334:TRP:NE1	1.88	0.87
1:C:81:ALA:HA	1:C:84:LEU:HD12	1.56	0.87
1:C:226:VAL:CG1	1:C:461:LEU:HD22	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:LEU:HD12	1:D:333:MET:SD	2.15	0.87
1:B:617:SER:HB2	1:B:690:ASP:H	1.38	0.87
2:H:206:ILE:O	2:H:210:VAL:HG23	1.75	0.87
1:A:712:GLN:HE21	2:F:370:LEU:HD23	1.40	0.86
1:D:81:ALA:HA	1:D:84:LEU:HD12	1.56	0.86
1:B:222:PHE:CG	1:B:492:LEU:HD11	2.09	0.86
1:B:617:SER:HB3	1:B:689:ILE:HD12	1.54	0.86
1:D:711:MET:H	2:G:363:SER:HB2	1.37	0.86
2:E:55:VAL:HG21	2:E:128:ASN:ND2	1.91	0.86
1:D:172:LEU:HD23	1:D:216:ARG:HH22	1.37	0.86
2:G:12:GLN:OE1	2:G:27:ARG:HD3	1.76	0.86
1:A:565:CYS:HB3	1:A:568:PHE:HB2	1.58	0.85
1:B:711:MET:HE2	1:B:715:LEU:HG	1.58	0.85
1:D:39:SER:CB	2:G:332:ILE:HG22	2.05	0.85
2:E:92:ASN:HA	2:E:96:LEU:HD13	1.58	0.85
1:B:522:TYR:CE1	1:B:662:LEU:HD11	2.10	0.85
2:F:332:ILE:CG2	2:F:334:TRP:NE1	2.40	0.85
1:A:619:LEU:HB2	1:A:693:ILE:HG22	0.92	0.85
2:F:12:GLN:NE2	2:F:23:VAL:HG13	1.91	0.85
1:B:261:ILE:HB	1:B:278:CYS:SG	2.16	0.85
1:D:150:GLN:HB3	1:D:154:LYS:CD	2.07	0.85
1:A:81:ALA:HA	1:A:84:LEU:HD12	1.59	0.85
1:B:114:LYS:CE	1:B:166:TYR:CE2	2.60	0.85
1:A:248:VAL:HG21	1:A:289:VAL:HA	1.59	0.85
1:B:686:GLN:HA	1:B:689:ILE:HG22	1.57	0.85
1:D:50:TYR:CE2	1:D:53:ILE:HD12	2.11	0.85
1:A:615:THR:HG21	1:A:691:GLN:NE2	1.91	0.85
1:C:317:LEU:CD1	1:C:401:LEU:CD2	2.53	0.85
1:B:516:GLY:HA3	1:B:620:MET:HE1	1.57	0.84
1:C:258:ALA:HB1	1:C:261:ILE:HD12	1.58	0.84
1:D:5:LEU:HD12	1:D:17:ILE:HG12	1.59	0.84
1:D:37:SER:CB	2:G:331:PRO:O	2.25	0.84
1:B:301:ALA:CB	1:B:438:LEU:CD2	2.56	0.84
1:C:441:GLU:CG	1:C:620:MET:HB2	2.01	0.84
1:C:568:PHE:CE2	1:C:574:ALA:HB2	2.12	0.84
2:F:13:LEU:O	2:F:32:LYS:CD	2.21	0.84
2:F:187:ARG:HG2	2:F:191:LYS:HE3	1.60	0.84
2:E:322:ASP:O	2:E:324:PRO:CD	2.21	0.84
1:B:318:VAL:HG23	1:B:329:ARG:NH1	1.91	0.84
2:F:332:ILE:CG2	2:F:334:TRP:HE1	1.89	0.84
2:G:322:ASP:C	2:G:324:PRO:HD3	2.01	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:ASP:HA	2:H:161:ILE:HD12	1.59	0.84
1:A:689:ILE:CG2	1:A:691:GLN:O	2.25	0.84
1:C:560:LYS:HD3	1:C:609:HIS:CG	2.12	0.84
1:D:157:VAL:H	1:D:167:GLU:HG2	1.42	0.84
1:A:153:GLY:HA2	1:A:158:GLN:HE22	1.42	0.84
1:A:615:THR:HG21	1:A:691:GLN:HE22	1.42	0.84
2:F:38:LYS:CD	2:F:344:VAL:CG1	2.48	0.84
1:C:50:TYR:HE2	1:C:53:ILE:HB	1.39	0.84
1:B:248:VAL:HG11	1:B:289:VAL:HA	1.59	0.84
1:B:301:ALA:CB	1:B:438:LEU:HD21	2.08	0.84
1:D:172:LEU:CD2	1:D:216:ARG:CZ	2.56	0.84
2:E:177:VAL:HG23	2:E:180:LYS:O	1.78	0.84
1:A:204:LYS:HE3	1:A:481:LEU:HD21	1.60	0.84
2:G:177:VAL:HB	2:G:180:LYS:O	1.78	0.84
2:H:187:ARG:HG2	2:H:191:LYS:HE3	1.59	0.84
2:H:203:LEU:HA	2:H:207:ARG:HB2	1.58	0.84
1:A:562:GLN:O	1:A:562:GLN:HG3	1.77	0.83
1:B:222:PHE:CE2	1:B:492:LEU:CD1	2.52	0.83
1:B:318:VAL:HG21	1:B:329:ARG:NH1	1.91	0.83
1:D:248:VAL:HG23	1:D:254:ILE:HG13	1.59	0.83
1:A:155:TYR:CD1	1:A:212:MET:CB	2.59	0.83
1:D:301:ALA:C	1:D:438:LEU:HD11	2.01	0.83
2:H:206:ILE:HD11	2:H:315:ARG:HG2	1.57	0.83
1:A:618:ALA:HB2	1:A:691:GLN:CG	2.08	0.83
1:B:618:ALA:CA	1:B:689:ILE:HD11	2.08	0.83
1:C:369:PHE:CD2	1:C:434:ARG:HG2	2.13	0.83
1:A:689:ILE:HG22	1:A:691:GLN:O	1.79	0.83
1:C:316:LEU:O	1:C:319:LEU:HG	1.78	0.83
2:F:309:GLU:HG2	2:F:325:PHE:CD1	2.12	0.83
1:A:516:GLY:HA3	1:A:620:MET:HE1	1.61	0.83
1:B:81:ALA:HA	1:B:84:LEU:HD12	1.60	0.83
1:B:686:GLN:CD	1:B:727:LYS:HG3	2.04	0.83
1:D:114:LYS:HG3	1:D:166:TYR:CZ	2.13	0.83
1:D:329:ARG:HD3	1:D:331:ARG:HH21	1.40	0.83
1:C:317:LEU:HD13	1:C:401:LEU:HG	1.61	0.82
2:G:55:VAL:HG21	2:G:128:ASN:ND2	1.92	0.82
1:D:703:ARG:O	1:D:703:ARG:HG3	1.78	0.82
2:E:322:ASP:C	2:E:324:PRO:HD3	2.04	0.82
1:B:258:ALA:HB3	1:B:282:TYR:HE2	1.44	0.82
1:C:39:SER:HB3	2:E:332:ILE:HG22	1.60	0.82
1:C:515:ILE:HD12	1:C:551:LEU:CD1	2.07	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:322:ASP:O	2:G:324:PRO:CD	2.24	0.82
1:A:205:ILE:HD11	1:A:481:LEU:HB3	1.59	0.82
1:A:463:THR:CB	1:A:513:LEU:CD2	2.58	0.82
1:A:618:ALA:HB2	1:A:691:GLN:HB2	1.60	0.82
1:C:464:LEU:CD1	1:C:620:MET:SD	2.67	0.82
1:A:172:LEU:HD23	1:A:216:ARG:NH2	1.93	0.82
1:B:619:LEU:CG	1:B:693:ILE:CG2	2.57	0.82
1:A:615:THR:CB	1:A:691:GLN:NE2	2.43	0.82
1:C:37:SER:HB3	2:E:331:PRO:O	1.79	0.82
1:D:711:MET:HE2	1:D:715:LEU:HG	1.62	0.82
2:E:339:LEU:HD13	2:E:340:VAL:HG23	1.62	0.82
1:B:222:PHE:HB3	1:B:492:LEU:HD21	1.61	0.82
1:B:301:ALA:HB3	1:B:438:LEU:CD2	2.10	0.82
1:D:689:ILE:HD13	1:D:693:ILE:HG23	1.60	0.82
1:C:560:LYS:HD3	1:C:609:HIS:CE1	2.15	0.81
2:E:187:ARG:HG2	2:E:191:LYS:HE3	1.59	0.81
1:A:569:ASN:HD22	1:A:570:GLU:H	1.28	0.81
1:B:222:PHE:CB	1:B:492:LEU:HD21	2.11	0.81
1:C:317:LEU:HD12	1:C:318:VAL:CG1	2.09	0.81
1:A:207:LEU:HB2	1:A:212:MET:CE	2.09	0.81
1:C:50:TYR:O	1:C:53:ILE:HG22	1.80	0.81
1:D:316:LEU:HA	1:D:319:LEU:HD11	1.62	0.81
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.63	0.81
1:C:6:LEU:HD12	1:C:51:ASP:OD2	1.81	0.81
1:C:157:VAL:HG23	1:C:216:ARG:NH1	1.93	0.81
1:D:228:ILE:HD11	1:D:459:ILE:HG12	1.62	0.81
1:C:44:ARG:HA	1:C:44:ARG:NE	1.94	0.81
2:G:158:ASP:HA	2:G:161:ILE:HD12	1.62	0.81
1:A:6:LEU:HD11	1:C:298:ARG:NE	1.95	0.81
1:C:293:SER:CB	1:C:296:GLY:HA2	2.09	0.81
1:C:513:LEU:HD12	1:C:616:LEU:HA	1.60	0.81
1:D:207:LEU:HG	1:D:212:MET:SD	2.21	0.81
2:G:187:ARG:HG2	2:G:191:LYS:HE3	1.61	0.81
2:G:206:ILE:O	2:G:210:VAL:HG23	1.81	0.81
1:B:686:GLN:NE2	1:B:689:ILE:CG2	2.44	0.81
2:H:12:GLN:HE21	2:H:23:VAL:HG13	1.44	0.81
1:C:222:PHE:CD2	1:C:492:LEU:CD1	2.64	0.81
1:B:226:VAL:CG1	1:B:461:LEU:HD22	2.09	0.80
1:A:692:SER:CB	1:A:727:LYS:HB2	2.10	0.80
1:B:228:ILE:HD11	1:B:459:ILE:HG12	1.60	0.80
1:D:59:HIS:HB2	3:D:801:ATP:H5'1	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:339:LEU:HD12	2:E:339:LEU:C	2.06	0.80
1:D:244:ILE:O	1:D:248:VAL:HB	1.81	0.80
1:B:282:TYR:HE2	1:B:304:LEU:HD21	1.46	0.80
1:B:289:VAL:HG11	1:B:302:ALA:HB2	1.63	0.80
1:C:153:GLY:HA2	1:C:158:GLN:HE22	1.45	0.80
1:D:248:VAL:CG2	1:D:254:ILE:CG1	2.60	0.80
1:D:447:LYS:HB2	1:D:458:GLU:H	1.46	0.80
2:F:158:ASP:HA	2:F:161:ILE:HD12	1.64	0.80
1:A:6:LEU:CD1	1:C:298:ARG:CZ	2.60	0.80
1:C:172:LEU:CD2	1:C:212:MET:HE3	2.12	0.80
1:B:37:SER:CB	2:H:331:PRO:O	2.29	0.80
1:C:316:LEU:HA	1:C:319:LEU:HD11	1.63	0.80
1:C:361:VAL:HG11	1:C:364:LEU:HB2	1.64	0.80
2:F:206:ILE:HD11	2:F:315:ARG:HG2	1.62	0.80
1:A:369:PHE:CZ	1:A:434:ARG:HB3	2.17	0.80
1:B:625:SER:O	1:B:628:ILE:HG22	1.80	0.80
1:C:155:TYR:HD1	1:C:212:MET:HB2	1.47	0.80
1:C:290:LYS:HD2	1:C:296:GLY:O	1.81	0.80
1:D:93:ALA:HB2	1:D:165:ILE:HG22	1.62	0.80
1:D:93:ALA:HB2	1:D:165:ILE:O	1.82	0.80
1:C:685:MET:O	1:C:689:ILE:CD1	2.30	0.80
1:B:282:TYR:CE2	1:B:304:LEU:HD21	2.17	0.80
1:C:712:GLN:HE21	2:E:370:LEU:HD21	1.47	0.80
1:D:309:TRP:CH2	1:D:364:LEU:HD12	2.17	0.80
1:A:617:SER:HB2	1:A:690:ASP:H	1.44	0.79
1:A:618:ALA:CB	1:A:691:GLN:HB2	2.11	0.79
1:A:6:LEU:O	1:A:7:VAL:HG23	1.82	0.79
2:E:205:ALA:CB	2:E:315:ARG:HD3	2.11	0.79
1:A:19:LEU:HD12	1:A:19:LEU:H	1.47	0.79
1:B:569:ASN:HD22	1:B:570:GLU:H	1.29	0.79
1:A:692:SER:CB	1:A:727:LYS:CB	2.61	0.79
1:C:53:ILE:HD11	1:C:58:ILE:HG12	1.64	0.79
1:C:207:LEU:CD1	1:C:212:MET:SD	2.70	0.79
2:E:203:LEU:HA	2:E:207:ARG:HB2	1.64	0.79
2:E:339:LEU:CD1	2:E:340:VAL:HG23	2.12	0.79
2:G:12:GLN:HG2	2:G:102:PRO:HD3	1.64	0.79
1:C:228:ILE:HD11	1:C:459:ILE:HG12	1.63	0.79
1:D:93:ALA:CB	1:D:165:ILE:O	2.29	0.79
1:A:447:LYS:HB2	1:A:458:GLU:H	1.47	0.79
1:C:561:GLU:HG2	1:C:562:GLN:HG3	1.65	0.79
1:B:369:PHE:CE1	1:B:434:ARG:HA	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ARG:CG	1:C:69:LEU:HD21	2.12	0.79
1:D:568:PHE:CE2	1:D:574:ALA:HB2	2.18	0.79
2:G:179:GLY:O	2:G:180:LYS:CD	2.30	0.79
1:A:228:ILE:HD11	1:A:459:ILE:HG12	1.62	0.79
1:C:114:LYS:HG3	1:C:166:TYR:CD2	2.18	0.79
1:C:341:LYS:HB2	1:C:722:TYR:OH	1.83	0.79
1:D:39:SER:HB3	2:G:332:ILE:CG2	2.12	0.79
1:D:364:LEU:HD13	1:D:364:LEU:C	2.07	0.79
2:E:204:GLU:HG2	2:E:238:GLU:CD	2.08	0.79
1:B:522:TYR:HE1	1:B:662:LEU:HD11	1.47	0.78
1:D:155:TYR:CE2	1:D:212:MET:HE2	2.13	0.78
2:F:55:VAL:HG21	2:F:128:ASN:ND2	1.97	0.78
2:F:203:LEU:HA	2:F:207:ARG:HB2	1.65	0.78
2:G:12:GLN:HE21	2:G:23:VAL:HG13	1.46	0.78
1:C:685:MET:O	1:C:689:ILE:CG1	2.30	0.78
1:D:258:ALA:HB1	1:D:261:ILE:HD12	1.65	0.78
1:D:463:THR:O	1:D:464:LEU:CD2	2.30	0.78
1:A:615:THR:HB	1:A:691:GLN:NE2	1.98	0.78
1:A:692:SER:HB2	1:A:727:LYS:CB	2.11	0.78
1:B:189:ARG:O	1:B:193:VAL:CG2	2.26	0.78
2:E:204:GLU:HG2	2:E:238:GLU:OE1	1.83	0.78
1:A:420:CYS:O	1:A:424:SER:HB2	1.83	0.78
1:B:303:THR:OG1	1:B:438:LEU:HD12	1.83	0.78
1:C:215:VAL:O	1:C:216:ARG:HB3	1.81	0.78
1:C:513:LEU:CD1	1:C:616:LEU:HD23	2.11	0.78
1:C:569:ASN:HD22	1:C:570:GLU:H	1.27	0.78
1:D:114:LYS:HG3	1:D:166:TYR:HE2	1.43	0.78
1:A:615:THR:CG2	1:A:691:GLN:NE2	2.47	0.78
1:C:301:ALA:O	1:C:438:LEU:CD1	2.29	0.78
1:C:730:TYR:O	1:C:731:TYR:O	2.02	0.78
1:D:329:ARG:CD	1:D:331:ARG:HH21	1.97	0.78
1:D:420:CYS:O	1:D:424:SER:HB2	1.83	0.78
1:A:167:GLU:OE1	1:A:172:LEU:HA	1.84	0.78
1:A:215:VAL:C	1:A:216:ARG:HG2	2.08	0.78
1:A:322:ASN:HA	1:A:331:ARG:HE	1.49	0.78
1:A:369:PHE:CE1	1:A:434:ARG:HA	2.19	0.78
1:A:463:THR:HB	1:A:513:LEU:CD2	2.13	0.78
2:E:12:GLN:HE21	2:E:23:VAL:HG13	1.48	0.78
1:B:93:ALA:HB2	1:B:165:ILE:O	1.82	0.78
1:C:621:PRO:HD3	1:C:694:SER:CB	2.13	0.78
1:A:565:CYS:HB2	1:A:611:LEU:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:206:ILE:HD11	2:G:315:ARG:HG2	1.65	0.78
2:H:339:LEU:HD13	2:H:339:LEU:H	1.47	0.78
1:A:172:LEU:HD21	1:A:216:ARG:NH1	1.97	0.78
1:B:19:LEU:HD22	2:H:295:SER:O	1.84	0.78
1:B:145:TYR:CZ	1:B:149:LYS:HG2	2.19	0.78
1:B:619:LEU:HB2	1:B:693:ILE:HG22	1.64	0.78
2:E:87:GLN:O	2:E:91:PRO:HD2	1.83	0.78
1:B:93:ALA:CB	1:B:165:ILE:O	2.32	0.78
1:B:282:TYR:HA	1:B:285:PHE:CD2	2.19	0.78
2:E:158:ASP:HA	2:E:161:ILE:HD12	1.66	0.78
2:G:340:VAL:O	2:G:340:VAL:CG1	2.30	0.78
2:F:206:ILE:O	2:F:210:VAL:HG23	1.84	0.77
1:C:6:LEU:HD12	1:C:51:ASP:CG	2.09	0.77
1:D:248:VAL:HG23	1:D:254:ILE:CD1	2.14	0.77
1:D:560:LYS:HD3	1:D:609:HIS:CG	2.19	0.77
2:G:87:GLN:O	2:G:91:PRO:HD2	1.83	0.77
1:B:361:VAL:CG1	1:B:364:LEU:HB2	2.14	0.77
1:B:617:SER:C	1:B:689:ILE:CD1	2.57	0.77
1:C:19:LEU:H	1:C:19:LEU:HD12	1.47	0.77
2:F:87:GLN:O	2:F:91:PRO:HD2	1.83	0.77
2:G:203:LEU:HA	2:G:207:ARG:HB2	1.65	0.77
2:H:87:GLN:O	2:H:91:PRO:HD2	1.83	0.77
1:A:275:HIS:CD2	1:A:277:GLY:H	2.03	0.77
1:D:730:TYR:O	1:D:731:TYR:O	2.03	0.77
1:C:560:LYS:HD3	1:C:609:HIS:ND1	2.00	0.77
1:D:297:VAL:O	1:D:297:VAL:HG12	1.83	0.77
1:D:561:GLU:HG2	1:D:562:GLN:HG3	1.65	0.77
1:B:301:ALA:HB3	1:B:438:LEU:HD22	1.66	0.77
1:A:619:LEU:HD12	1:A:693:ILE:HG21	1.66	0.77
1:B:275:HIS:CD2	1:B:277:GLY:H	2.03	0.77
1:C:369:PHE:O	1:C:421:ASN:CG	2.27	0.77
1:D:227:LEU:HD23	1:D:435:GLN:HG3	1.66	0.77
1:C:623:GLU:O	1:C:627:GLN:HG2	1.84	0.76
2:H:92:ASN:HA	2:H:96:LEU:HD13	1.65	0.76
1:C:157:VAL:HG21	1:C:216:ARG:NH1	2.00	0.76
1:C:275:HIS:CD2	1:C:277:GLY:H	2.03	0.76
1:D:44:ARG:HG3	1:D:69:LEU:CD2	2.13	0.76
1:D:621:PRO:HD3	1:D:694:SER:CB	2.15	0.76
1:B:301:ALA:HB1	1:B:438:LEU:HD21	1.68	0.76
1:D:49:PHE:HD1	1:D:53:ILE:HD13	1.50	0.76
1:D:560:LYS:HE2	1:D:609:HIS:CE1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ASN:HD21	1:B:439:CYS:HB2	1.51	0.76
1:D:5:LEU:HB2	1:D:17:ILE:HG12	1.65	0.76
1:D:275:HIS:CD2	1:D:277:GLY:H	2.03	0.76
1:A:5:LEU:CG	1:A:17:ILE:HG12	2.16	0.76
1:B:59:HIS:HB2	3:B:801:ATP:H4'	1.65	0.76
1:B:730:TYR:O	1:B:731:TYR:O	2.03	0.76
1:C:313:VAL:O	1:C:317:LEU:HD23	1.86	0.76
1:C:428:PRO:O	1:C:432:PRO:HB3	1.85	0.76
1:D:108:LYS:HE3	1:D:109:MET:HE2	1.68	0.76
1:A:276:THR:HG23	1:A:280:PRO:HG2	1.66	0.76
1:B:155:TYR:HD1	1:B:212:MET:HB2	1.51	0.76
1:C:369:PHE:CE2	1:C:434:ARG:CD	2.66	0.76
1:D:719:LEU:HD22	2:G:375:LEU:HD21	1.68	0.76
2:H:336:ASN:CA	2:H:339:LEU:HD11	2.13	0.76
1:A:5:LEU:CD1	1:A:17:ILE:CD1	2.64	0.76
1:A:440:LEU:HD12	1:A:728:THR:HB	1.68	0.76
1:B:466:ALA:CA	1:B:516:GLY:O	2.33	0.76
1:C:17:ILE:CD1	3:C:801:ATP:C2	2.60	0.76
1:D:421:ASN:O	1:D:428:PRO:HG3	1.86	0.76
1:D:89:LEU:HD22	1:D:152:GLU:HG3	1.64	0.75
1:D:489:LEU:HD22	1:D:513:LEU:HD22	1.68	0.75
1:A:167:GLU:OE1	1:A:172:LEU:HB2	1.86	0.75
1:B:40:GLN:HE22	2:H:333:PRO:HG2	1.51	0.75
1:D:175:LEU:HD22	1:D:216:ARG:HD2	1.67	0.75
1:D:406:ARG:NH1	1:D:697:THR:HG23	2.01	0.75
2:G:179:GLY:O	2:G:180:LYS:HD3	1.86	0.75
2:H:309:GLU:HG2	2:H:325:PHE:CD1	2.22	0.75
1:D:275:HIS:HD2	1:D:277:GLY:H	1.34	0.75
1:A:297:VAL:CG1	1:C:4:ASN:ND2	2.50	0.75
1:A:562:GLN:HG2	1:A:612:ARG:CZ	2.16	0.75
1:C:418:ASP:O	1:C:422:THR:CG2	2.27	0.75
1:A:529:LYS:HB3	1:A:536:ALA:HB2	1.66	0.75
1:C:53:ILE:HD13	1:C:58:ILE:HG12	1.67	0.75
1:C:94:TYR:HE2	1:C:168:SER:HB2	1.52	0.75
1:C:457:GLY:O	1:C:502:ALA:HB1	1.87	0.75
1:C:716:LYS:HG2	2:E:370:LEU:HD13	1.69	0.75
2:F:239:ALA:CB	2:F:342:ASP:OD2	2.35	0.75
1:B:617:SER:C	1:B:689:ILE:HD11	2.11	0.74
1:D:168:SER:OG	1:D:171:PHE:HD2	1.67	0.74
1:A:5:LEU:HD12	1:A:17:ILE:HG12	0.78	0.74
1:A:618:ALA:HB2	1:A:691:GLN:CB	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:TYR:CZ	1:B:369:PHE:CE2	2.75	0.74
1:B:464:LEU:HA	1:B:514:GLY:O	1.86	0.74
1:B:275:HIS:HD2	1:B:277:GLY:H	1.34	0.74
1:C:437:ASN:HD21	1:C:439:CYS:HB2	1.52	0.74
1:A:227:LEU:HD23	1:A:435:GLN:HG2	1.70	0.74
1:B:108:LYS:HE3	1:B:109:MET:HE2	1.68	0.74
1:C:361:VAL:HG12	1:C:364:LEU:HB2	1.67	0.74
2:H:336:ASN:HA	2:H:339:LEU:CD1	2.14	0.74
1:D:316:LEU:O	1:D:319:LEU:CG	2.34	0.74
1:A:489:LEU:HD22	1:A:513:LEU:CD2	2.07	0.74
1:A:716:LYS:HG2	2:F:370:LEU:HD11	1.69	0.74
1:B:19:LEU:HB2	2:H:295:SER:HB3	1.69	0.74
1:B:316:LEU:O	1:B:319:LEU:CD1	2.35	0.74
1:B:361:VAL:HG12	1:B:364:LEU:HB2	1.68	0.74
1:C:204:LYS:HE3	1:C:481:LEU:HD21	1.69	0.74
2:E:12:GLN:HG2	2:E:102:PRO:HD3	1.68	0.74
1:A:437:ASN:HD21	1:A:439:CYS:HB2	1.52	0.74
1:A:647:SER:HB2	1:A:652:LEU:CG	2.17	0.74
1:D:19:LEU:HD22	2:G:295:SER:O	1.88	0.74
2:G:201:ASN:O	2:G:205:ALA:HB3	1.87	0.74
1:A:6:LEU:HD11	1:C:298:ARG:CZ	2.18	0.74
1:A:315:SER:O	1:A:318:VAL:CG2	2.35	0.74
1:A:475:LEU:HD11	1:A:542:LYS:HE2	1.69	0.74
1:A:623:GLU:HG2	1:A:633:ASN:HD22	1.49	0.74
1:B:227:LEU:HD23	1:B:435:GLN:HG3	1.67	0.74
1:B:208:PRO:HD3	1:B:464:LEU:O	1.88	0.74
1:D:157:VAL:CG1	1:D:166:TYR:HD2	1.97	0.74
1:D:623:GLU:HG2	1:D:633:ASN:HD22	1.50	0.74
1:B:700:ASP:OD1	1:B:735:ARG:CD	2.36	0.73
2:F:372:ASN:HD22	2:F:372:ASN:H	1.35	0.73
2:H:310:TYR:N	2:H:328:ARG:HD3	2.04	0.73
1:B:341:LYS:HB2	1:B:722:TYR:OH	1.88	0.73
2:H:85:SER:O	2:H:89:ARG:NH2	2.21	0.73
1:A:421:ASN:O	1:A:428:PRO:HG3	1.87	0.73
1:B:40:GLN:NE2	2:H:333:PRO:CG	2.45	0.73
1:B:286:GLN:NE2	1:B:332:HIS:CB	2.51	0.73
1:C:44:ARG:HG3	1:C:69:LEU:CD2	2.14	0.73
1:C:59:HIS:HB2	3:C:801:ATP:H5'2	1.68	0.73
1:D:260:ARG:HG3	1:D:365:TYR:CZ	2.24	0.73
2:F:316:MET:SD	2:F:324:PRO:HG3	2.29	0.73
2:H:201:ASN:O	2:H:205:ALA:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:VAL:HG23	1:D:254:ILE:HD11	1.69	0.73
2:H:12:GLN:CG	2:H:102:PRO:HD3	2.19	0.73
2:G:65:LEU:HD21	2:G:223:LEU:HD13	1.69	0.73
1:A:89:LEU:HD21	1:A:152:GLU:HG3	1.70	0.73
1:B:145:TYR:HE2	1:B:652:LEU:CD2	2.02	0.73
1:D:167:GLU:CD	1:D:172:LEU:HB2	2.14	0.73
1:A:625:SER:O	1:A:628:ILE:CG2	2.37	0.73
1:C:425:PRO:HG2	1:C:690:ASP:HB3	1.69	0.73
1:D:286:GLN:CD	1:D:332:HIS:ND1	2.46	0.73
1:A:232:ASP:CG	1:A:262:ARG:HE	1.97	0.73
1:A:369:PHE:HD2	1:A:434:ARG:NH1	1.86	0.73
1:C:232:ASP:OD2	1:C:262:ARG:NE	2.20	0.73
2:E:310:TYR:N	2:E:328:ARG:HD3	2.04	0.73
2:F:87:GLN:O	2:F:91:PRO:HD3	1.89	0.73
2:F:201:ASN:O	2:F:205:ALA:HB3	1.89	0.73
1:A:155:TYR:HD1	1:A:212:MET:HB2	1.54	0.72
1:A:319:LEU:HA	1:A:329:ARG:HG3	1.71	0.72
1:B:234:LEU:HD22	1:B:234:LEU:H	1.53	0.72
1:C:94:TYR:CE2	1:C:168:SER:HB2	2.24	0.72
1:C:560:LYS:HE2	1:C:609:HIS:CE1	2.24	0.72
2:E:316:MET:SD	2:E:324:PRO:HG2	2.28	0.72
1:A:279:ILE:HD13	1:A:319:LEU:HD21	1.70	0.72
1:C:275:HIS:HD2	1:C:277:GLY:H	1.35	0.72
1:C:513:LEU:HD11	1:C:616:LEU:HD22	1.71	0.72
2:F:204:GLU:HG2	2:F:238:GLU:OE1	1.89	0.72
1:D:19:LEU:HD12	1:D:19:LEU:H	1.53	0.72
1:D:437:ASN:HD21	1:D:439:CYS:HB2	1.54	0.72
1:A:275:HIS:HD2	1:A:277:GLY:H	1.35	0.72
1:C:108:LYS:HE3	1:C:109:MET:HE2	1.72	0.72
1:C:115:TYR:HE1	1:C:216:ARG:HD2	0.95	0.72
2:G:201:ASN:O	2:G:205:ALA:CB	2.37	0.72
1:A:167:GLU:OE1	1:A:172:LEU:CA	2.38	0.72
1:A:234:LEU:H	1:A:234:LEU:HD22	1.54	0.72
1:B:440:LEU:HD12	1:B:728:THR:HB	1.71	0.72
1:C:696:ASN:HD22	1:C:696:ASN:H	1.37	0.72
1:D:293:SER:OG	1:D:296:GLY:HA2	1.89	0.72
1:D:329:ARG:CG	1:D:331:ARG:HH21	2.03	0.72
2:G:204:GLU:HG2	2:G:238:GLU:CD	2.15	0.72
1:A:320:LYS:HE2	1:A:333:MET:O	1.90	0.72
1:A:463:THR:HG1	1:A:513:LEU:HD23	1.51	0.72
1:B:19:LEU:H	1:B:19:LEU:HD12	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:GLN:NE2	1:B:727:LYS:HE3	2.05	0.72
1:C:232:ASP:CG	1:C:262:ARG:HE	1.97	0.72
2:F:204:GLU:HG2	2:F:238:GLU:CD	2.15	0.72
1:A:705:PRO:O	1:A:706:SER:HB2	1.90	0.71
1:D:658:ASP:O	1:D:658:ASP:CG	2.32	0.71
1:C:106:VAL:O	1:C:110:VAL:HG23	1.89	0.71
1:D:34:HIS:O	1:D:35:ASN:HB2	1.91	0.71
2:F:312:THR:HB	2:F:325:PHE:CD2	2.24	0.71
1:C:735:ARG:O	1:C:736:ASP:CB	2.34	0.71
2:E:339:LEU:O	2:E:340:VAL:HB	1.91	0.71
2:F:65:LEU:HD21	2:F:223:LEU:HD13	1.72	0.71
2:H:176:THR:OG1	2:H:181:THR:HG22	1.89	0.71
1:A:227:LEU:HB3	1:A:435:GLN:HE22	1.52	0.71
1:B:711:MET:HB3	2:H:364:GLU:C	2.15	0.71
1:C:316:LEU:O	1:C:319:LEU:CD1	2.38	0.71
2:H:232:ARG:HD3	2:H:342:ASP:HB2	0.75	0.71
1:A:108:LYS:HE3	1:A:109:MET:HE2	1.73	0.71
1:B:529:LYS:H	1:B:529:LYS:HD2	1.54	0.71
1:C:248:VAL:HG21	1:C:289:VAL:HA	1.72	0.71
1:D:234:LEU:H	1:D:234:LEU:HD22	1.55	0.71
2:F:177:VAL:N	2:F:180:LYS:O	2.21	0.71
2:H:87:GLN:O	2:H:91:PRO:HD3	1.90	0.71
1:A:298:ARG:HH21	1:C:6:LEU:HD21	1.54	0.71
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.73	0.71
1:C:222:PHE:CE2	1:C:492:LEU:HD11	2.25	0.71
2:E:87:GLN:O	2:E:91:PRO:HD3	1.90	0.71
1:A:369:PHE:HE2	1:A:434:ARG:HD3	1.50	0.71
1:C:621:PRO:CD	1:C:694:SER:HB2	2.18	0.71
2:H:178:ASN:CG	2:H:178:ASN:O	2.33	0.71
1:A:369:PHE:O	1:A:421:ASN:CG	2.34	0.71
1:B:54:LYS:O	1:B:58:ILE:HG13	1.91	0.71
1:D:150:GLN:O	1:D:154:LYS:CG	2.35	0.71
1:A:6:LEU:HD12	1:C:298:ARG:NH1	2.05	0.71
1:A:106:VAL:O	1:A:110:VAL:HG23	1.90	0.71
1:C:254:ILE:HG22	1:C:256:ILE:HG13	1.73	0.71
1:D:150:GLN:OE1	1:D:154:LYS:HD2	1.89	0.71
1:C:4:ASN:HD22	1:C:4:ASN:N	1.89	0.70
1:C:254:ILE:O	1:C:438:LEU:HG	1.91	0.70
1:C:545:GLU:HG3	1:C:595:LEU:HD23	1.73	0.70
1:C:663:HIS:ND1	1:C:663:HIS:N	2.39	0.70
1:D:254:ILE:N	1:D:438:LEU:CD1	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:205:ALA:HB1	2:F:315:ARG:HD3	1.73	0.70
1:B:39:SER:HB2	2:H:303:ILE:HG21	1.71	0.70
2:F:310:TYR:N	2:F:328:ARG:HD3	2.05	0.70
2:G:87:GLN:O	2:G:91:PRO:HD3	1.89	0.70
2:G:204:GLU:HG2	2:G:238:GLU:OE1	1.90	0.70
2:H:201:ASN:O	2:H:205:ALA:CB	2.39	0.70
1:A:692:SER:HB3	1:A:727:LYS:HD2	1.74	0.70
1:B:365:TYR:CE2	1:B:369:PHE:CE2	2.77	0.70
1:D:569:ASN:OD1	1:D:570:GLU:N	2.24	0.70
1:C:620:MET:O	1:C:620:MET:HG2	1.91	0.70
1:A:235:ASP:OD2	1:B:246:LYS:NZ	2.25	0.70
2:E:173:GLY:O	2:E:175:HIS:CE1	2.43	0.70
1:A:315:SER:O	1:A:318:VAL:HG23	1.92	0.70
1:B:106:VAL:O	1:B:110:VAL:HG23	1.91	0.70
1:B:301:ALA:HB1	1:B:438:LEU:CD2	2.21	0.70
1:B:701:PRO:CD	1:B:735:ARG:HG2	2.20	0.70
2:G:205:ALA:HB1	2:G:315:ARG:HD3	1.74	0.70
1:D:114:LYS:HG3	1:D:166:TYR:CD2	2.19	0.70
1:A:6:LEU:HD12	1:C:298:ARG:CZ	2.21	0.70
1:C:114:LYS:HD3	1:C:114:LYS:N	2.06	0.70
1:D:282:TYR:CE2	1:D:304:LEU:HD22	2.26	0.70
2:H:339:LEU:HD13	2:H:339:LEU:N	2.06	0.70
1:A:5:LEU:HB2	1:A:17:ILE:HG23	1.71	0.69
1:A:279:ILE:HD13	1:A:319:LEU:CD2	2.22	0.69
1:A:545:GLU:HG3	1:A:595:LEU:HD23	1.73	0.69
1:B:572:THR:HB	1:B:577:ILE:HD12	1.74	0.69
1:B:696:ASN:HD22	1:B:696:ASN:H	1.37	0.69
1:D:167:GLU:OE2	1:D:216:ARG:NH2	2.24	0.69
2:E:82:LEU:HD13	2:E:140:ILE:HG22	1.75	0.69
1:A:222:PHE:CD2	1:A:492:LEU:HD11	2.27	0.69
1:D:50:TYR:CD2	1:D:50:TYR:N	2.55	0.69
2:H:13:LEU:O	2:H:32:LYS:HD2	1.92	0.69
1:A:572:THR:HB	1:A:577:ILE:HD12	1.74	0.69
1:D:516:GLY:HA3	1:D:620:MET:HE1	1.74	0.69
2:H:232:ARG:NH1	2:H:343:ASN:N	2.40	0.69
1:B:441:GLU:HB3	1:B:619:LEU:O	1.92	0.69
1:C:115:TYR:CD1	1:C:216:ARG:CG	2.76	0.69
1:D:106:VAL:O	1:D:110:VAL:HG23	1.92	0.69
1:D:329:ARG:CB	1:D:331:ARG:HH21	2.04	0.69
1:D:696:ASN:H	1:D:696:ASN:HD22	1.37	0.69
2:E:206:ILE:CD1	2:E:312:THR:HG23	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:232:ARG:HH12	2:H:343:ASN:H	1.40	0.69
1:A:413:TYR:HH	1:A:731:TYR:HE2	0.73	0.69
1:D:153:GLY:HA2	1:D:158:GLN:NE2	2.00	0.69
2:F:309:GLU:HG2	2:F:325:PHE:CE1	2.27	0.69
2:H:89:ARG:HG2	2:H:90:SER:N	2.06	0.69
1:B:301:ALA:CB	1:B:438:LEU:HD22	2.22	0.69
2:E:333:PRO:O	2:E:336:ASN:ND2	2.25	0.69
2:G:82:LEU:HD13	2:G:140:ILE:HG22	1.75	0.69
2:H:309:GLU:OE2	2:H:325:PHE:CD1	2.46	0.69
1:A:167:GLU:CD	1:A:172:LEU:HB2	2.17	0.69
1:A:208:PRO:HG3	1:A:211:ILE:HD13	1.72	0.69
1:A:298:ARG:HH21	1:C:6:LEU:CD2	2.05	0.69
1:A:298:ARG:NH2	1:C:6:LEU:HD21	2.08	0.69
1:B:40:GLN:HE21	2:H:333:PRO:HG2	1.53	0.69
1:B:168:SER:HG	1:B:171:PHE:HD2	1.41	0.69
1:B:593:GLU:OE2	1:B:596:HIS:NE2	2.26	0.69
1:C:227:LEU:HD23	1:C:435:GLN:HG3	1.75	0.69
2:G:333:PRO:O	2:G:336:ASN:ND2	2.25	0.69
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.74	0.69
1:A:181:PHE:O	1:A:184:TYR:HB2	1.93	0.69
1:A:463:THR:O	1:A:464:LEU:CD2	2.34	0.69
1:A:510:ARG:HG3	1:A:567:TRP:HE3	1.58	0.69
1:C:369:PHE:CD2	1:C:434:ARG:HD3	2.26	0.69
1:D:49:PHE:CD1	1:D:53:ILE:HD13	2.27	0.69
1:C:692:SER:HB2	1:C:727:LYS:HB2	1.74	0.69
1:D:241:SER:O	1:D:245:VAL:HG23	1.93	0.69
1:D:329:ARG:HD3	1:D:331:ARG:HH22	1.56	0.69
1:D:517:VAL:HG12	1:D:619:LEU:HD22	1.75	0.69
1:D:705:PRO:O	1:D:706:SER:HB2	1.93	0.69
2:H:206:ILE:CD1	2:H:315:ARG:HG2	2.22	0.69
2:H:232:ARG:HD3	2:H:342:ASP:HB3	1.70	0.69
1:C:465:SER:O	1:C:515:ILE:HA	1.92	0.68
2:G:92:ASN:O	2:G:96:LEU:HB2	1.93	0.68
1:B:22:ILE:HD11	3:B:801:ATP:C2	2.28	0.68
1:B:250:GLN:HE22	1:B:499:PRO:HG3	1.58	0.68
1:B:441:GLU:HG2	1:B:620:MET:CB	2.23	0.68
1:C:234:LEU:HD22	1:C:234:LEU:H	1.56	0.68
1:C:685:MET:O	1:C:689:ILE:HD11	1.93	0.68
1:D:567:TRP:O	1:D:569:ASN:N	2.26	0.68
2:F:197:LEU:HD12	2:F:198:MET:N	2.07	0.68
2:G:197:LEU:HD12	2:G:198:MET:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:277:VAL:HG22	2:H:324:PRO:HG3	1.76	0.68
1:A:226:VAL:CG1	1:A:461:LEU:HD22	2.22	0.68
1:A:309:TRP:CH2	1:A:364:LEU:HD12	2.27	0.68
1:B:239:ALA:HA	1:B:452:VAL:HG12	1.75	0.68
1:B:711:MET:CB	2:H:364:GLU:O	2.33	0.68
1:C:685:MET:C	1:C:689:ILE:HD11	2.19	0.68
2:G:366:ASP:CG	2:G:366:ASP:O	2.36	0.68
1:B:689:ILE:CG1	1:B:691:GLN:O	2.40	0.68
1:D:55:THR:HA	1:D:58:ILE:HD12	1.76	0.68
2:H:82:LEU:HD13	2:H:140:ILE:HG22	1.74	0.68
2:H:332:ILE:CG2	2:H:334:TRP:HE1	2.02	0.68
1:B:19:LEU:HD22	2:H:295:SER:C	2.18	0.68
1:C:7:VAL:HG21	3:C:801:ATP:N1	2.09	0.68
1:A:226:VAL:HG12	1:A:461:LEU:HD22	1.76	0.68
1:B:735:ARG:O	1:B:735:ARG:CG	2.30	0.68
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.76	0.68
1:C:228:ILE:C	1:C:435:GLN:HE22	2.01	0.68
1:C:276:THR:HG21	1:D:291:SER:O	1.94	0.68
1:C:686:GLN:CD	1:C:727:LYS:HG3	2.19	0.68
1:D:22:ILE:HD12	1:D:22:ILE:H	1.58	0.68
1:B:22:ILE:H	1:B:22:ILE:HD12	1.59	0.68
1:B:318:VAL:HG21	1:B:329:ARG:HH12	1.56	0.68
1:D:440:LEU:HD12	1:D:728:THR:HB	1.75	0.68
2:H:5:PHE:CD1	2:H:24:ASN:O	2.45	0.68
2:H:205:ALA:HB1	2:H:315:ARG:HD3	1.76	0.68
1:A:59:HIS:HB2	3:A:801:ATP:H4'	1.76	0.68
1:D:135:ILE:HD11	1:D:174:ILE:HG21	1.76	0.68
1:D:522:TYR:HE1	1:D:662:LEU:HD11	1.59	0.68
1:A:361:VAL:HG11	1:A:364:LEU:HG	1.74	0.68
1:B:145:TYR:CE2	1:B:652:LEU:HD23	2.26	0.68
1:C:420:CYS:O	1:C:424:SER:CB	2.42	0.68
2:E:197:LEU:HD12	2:E:198:MET:N	2.08	0.68
2:H:232:ARG:CD	2:H:342:ASP:CB	2.45	0.68
1:D:232:ASP:OD2	1:D:262:ARG:NE	2.23	0.67
1:D:572:THR:HB	1:D:577:ILE:HD12	1.74	0.67
1:D:686:GLN:CD	1:D:727:LYS:HG3	2.20	0.67
1:B:155:TYR:CE1	1:B:212:MET:SD	2.87	0.67
1:B:510:ARG:HG3	1:B:567:TRP:HE3	1.59	0.67
1:A:232:ASP:OD2	1:A:262:ARG:NE	2.27	0.67
1:A:696:ASN:H	1:A:696:ASN:HD22	1.43	0.67
1:D:306:TYR:OH	1:D:317:LEU:HD23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PRO:HG2	1:B:211:ILE:HD13	1.77	0.67
1:D:150:GLN:OE1	1:D:154:LYS:HE2	1.94	0.67
1:D:316:LEU:O	1:D:319:LEU:CD1	2.42	0.67
2:E:65:LEU:CD2	2:E:223:LEU:HD13	2.24	0.67
2:H:185:SER:HB3	2:H:188:GLU:HB2	1.75	0.67
1:A:406:ARG:NH1	1:A:732:GLN:HG3	2.10	0.67
1:C:222:PHE:CG	1:C:492:LEU:HD11	2.28	0.67
1:C:305:PHE:CE1	1:C:436:SER:O	2.48	0.67
1:C:316:LEU:O	1:C:319:LEU:CG	2.43	0.67
1:C:625:SER:O	1:C:628:ILE:CG2	2.41	0.67
1:D:44:ARG:CG	1:D:69:LEU:HD21	2.16	0.67
1:A:686:GLN:CD	1:A:727:LYS:HG3	2.19	0.67
1:B:286:GLN:HE21	1:B:332:HIS:CB	2.04	0.67
1:C:241:SER:O	1:C:245:VAL:HG23	1.93	0.67
1:C:442:ILE:HD11	1:C:462:CYS:SG	2.34	0.67
1:D:181:PHE:O	1:D:184:TYR:HB2	1.94	0.67
1:D:689:ILE:CD1	1:D:693:ILE:HG23	2.24	0.67
1:C:155:TYR:HD1	1:C:212:MET:CB	2.07	0.67
1:C:403:MET:HE1	1:C:718:LEU:HD22	1.77	0.67
1:C:440:LEU:HD12	1:C:728:THR:HB	1.74	0.67
1:D:114:LYS:HE3	1:D:166:TYR:OH	1.95	0.67
1:D:406:ARG:HH11	1:D:697:THR:HG23	1.59	0.67
1:D:711:MET:HB2	2:G:363:SER:HB3	1.75	0.67
2:E:177:VAL:CG2	2:E:180:LYS:O	2.42	0.67
1:A:465:SER:HB2	1:A:489:LEU:CD1	2.24	0.67
2:G:12:GLN:CG	2:G:102:PRO:HD3	2.25	0.67
2:H:197:LEU:HD12	2:H:198:MET:N	2.09	0.67
1:B:565:CYS:HB3	1:B:568:PHE:HB2	1.76	0.67
1:B:232:ASP:CG	1:B:262:ARG:HB3	2.19	0.66
1:B:258:ALA:CB	1:B:282:TYR:OH	2.41	0.66
1:C:114:LYS:HE2	1:C:166:TYR:CE2	2.29	0.66
1:C:254:ILE:HG21	1:C:256:ILE:HD11	1.75	0.66
1:C:369:PHE:CD2	1:C:434:ARG:CG	2.77	0.66
1:D:168:SER:OG	1:D:171:PHE:CD2	2.44	0.66
2:E:206:ILE:HD13	2:E:312:THR:OG1	1.94	0.66
2:H:307:TYR:O	2:H:311:ILE:HG22	1.96	0.66
1:B:403:MET:HE1	1:B:718:LEU:HD22	1.75	0.66
1:C:668:LEU:HB2	1:C:671:GLU:HG3	1.76	0.66
1:C:686:GLN:HA	1:C:689:ILE:CG1	2.25	0.66
2:H:332:ILE:CG2	2:H:334:TRP:NE1	2.57	0.66
1:A:493:LEU:HD21	1:A:513:LEU:CD2	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:TYR:HH	1:D:731:TYR:HE2	1.43	0.66
1:D:464:LEU:HD22	1:D:514:GLY:HA3	1.77	0.66
1:D:560:LYS:HD3	1:D:609:HIS:CE1	2.31	0.66
1:A:93:ALA:HB2	1:A:165:ILE:O	1.96	0.66
1:A:155:TYR:CD1	1:A:212:MET:HB3	2.25	0.66
2:E:328:ARG:CZ	2:E:328:ARG:HB3	2.26	0.66
1:A:155:TYR:CD1	1:A:212:MET:HB2	2.27	0.66
1:A:239:ALA:HA	1:A:452:VAL:HG12	1.76	0.66
1:A:301:ALA:CB	1:A:438:LEU:HD21	2.25	0.66
1:C:560:LYS:HD3	1:C:609:HIS:CD2	2.31	0.66
1:D:211:ILE:O	1:D:215:VAL:HG23	1.96	0.66
1:D:403:MET:HG2	1:D:711:MET:HE1	1.76	0.66
1:D:619:LEU:HB2	1:D:693:ILE:HG22	1.77	0.66
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.77	0.66
1:B:212:MET:O	1:B:216:ARG:NH1	2.29	0.66
1:C:216:ARG:HG2	1:C:216:ARG:O	1.94	0.66
1:C:517:VAL:HG12	1:C:619:LEU:HD22	1.76	0.66
1:D:663:HIS:ND1	1:D:663:HIS:N	2.38	0.66
2:E:149:ARG:HH12	2:E:286:TRP:HB2	1.60	0.66
2:H:55:VAL:HG21	2:H:128:ASN:CG	2.18	0.66
2:H:124:HIS:HA	2:H:127:ARG:HD3	1.77	0.66
1:A:522:TYR:HE1	1:A:662:LEU:HD11	1.59	0.66
1:B:168:SER:OG	1:B:171:PHE:HD2	1.77	0.66
1:B:227:LEU:HD11	1:B:437:ASN:HB3	1.76	0.66
1:C:712:GLN:HE21	2:E:370:LEU:CD2	2.08	0.66
1:A:40:GLN:NE2	2:F:333:PRO:HG2	2.10	0.66
1:A:241:SER:O	1:A:245:VAL:HG23	1.95	0.66
1:A:369:PHE:CE2	1:A:434:ARG:HB3	2.31	0.66
1:A:512:THR:HB	1:A:615:THR:OG1	1.96	0.66
1:B:168:SER:HG	1:B:171:PHE:HB2	1.60	0.66
1:D:37:SER:HB2	1:D:40:GLN:HB2	1.77	0.66
2:F:307:TYR:O	2:F:311:ILE:HG22	1.95	0.66
1:C:302:ALA:HA	1:C:438:LEU:HD11	1.78	0.66
1:A:403:MET:HG2	1:A:711:MET:HE1	1.77	0.65
1:A:517:VAL:HG12	1:A:619:LEU:HD22	1.78	0.65
1:B:425:PRO:HG2	1:B:690:ASP:HB3	1.78	0.65
1:C:181:PHE:O	1:C:184:TYR:HB2	1.94	0.65
2:E:12:GLN:CG	2:E:102:PRO:HD3	2.26	0.65
1:B:181:PHE:O	1:B:184:TYR:HB2	1.96	0.65
1:B:686:GLN:NE2	1:B:689:ILE:HG23	2.11	0.65
1:D:208:PRO:HG2	1:D:211:ILE:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:13:LEU:O	2:E:32:LYS:HD2	1.96	0.65
2:H:330:ASN:OD1	2:H:331:PRO:HD2	1.96	0.65
1:B:621:PRO:CD	1:B:694:SER:CB	2.69	0.65
2:F:35:ILE:HG23	2:F:36:PHE:H	1.61	0.65
1:A:79:TYR:O	1:A:83:ARG:HG2	1.97	0.65
1:A:493:LEU:HD11	1:A:513:LEU:HD11	1.77	0.65
1:D:286:GLN:OE1	1:D:332:HIS:CB	2.41	0.65
1:D:307:PRO:HG2	1:D:310:HIS:HB2	1.78	0.65
1:A:692:SER:HB3	1:A:727:LYS:CB	2.24	0.65
1:B:464:LEU:CA	1:B:514:GLY:O	2.44	0.65
1:B:513:LEU:HG	1:B:613:ASN:ND2	2.11	0.65
1:B:513:LEU:HG	1:B:613:ASN:HD22	1.61	0.65
1:D:154:LYS:HE2	1:D:624:THR:CG2	2.26	0.65
1:D:560:LYS:HE2	1:D:609:HIS:ND1	2.11	0.65
2:F:94:ALA:O	2:F:95:LEU:HD23	1.96	0.65
2:H:35:ILE:HG23	2:H:36:PHE:H	1.62	0.65
1:A:297:VAL:CG1	1:A:297:VAL:O	2.44	0.65
1:B:241:SER:O	1:B:245:VAL:HG23	1.95	0.65
1:D:239:ALA:HA	1:D:452:VAL:HG12	1.78	0.65
2:F:372:ASN:H	2:F:372:ASN:ND2	1.95	0.65
1:D:147:ALA:O	1:D:151:LEU:HG	1.97	0.65
1:D:167:GLU:OE2	1:D:172:LEU:HB2	1.97	0.65
1:D:184:TYR:O	1:D:189:ARG:NH2	2.29	0.65
1:C:513:LEU:HD12	1:C:513:LEU:O	1.96	0.65
1:A:184:TYR:O	1:A:189:ARG:NH2	2.29	0.65
1:B:167:GLU:HG3	1:B:168:SER:N	2.12	0.65
1:C:79:TYR:O	1:C:83:ARG:HG2	1.96	0.65
2:F:328:ARG:HB3	2:F:328:ARG:CZ	2.27	0.65
2:H:207:ARG:HH22	2:H:282:GLN:CD	2.04	0.65
1:A:131:MET:HE3	1:A:193:VAL:HG11	1.79	0.65
1:B:619:LEU:HB2	1:B:693:ILE:CG2	2.26	0.65
1:B:686:GLN:NE2	1:B:727:LYS:HG3	2.11	0.65
1:C:544:PHE:HE2	1:C:685:MET:HE2	1.61	0.65
1:D:253:GLY:C	1:D:438:LEU:HD12	2.21	0.65
1:C:322:ASN:HA	1:C:331:ARG:HH21	1.62	0.64
1:A:93:ALA:CB	1:A:165:ILE:O	2.45	0.64
1:C:22:ILE:H	1:C:22:ILE:HD12	1.61	0.64
2:E:20:GLY:CA	2:E:100:SER:HB3	2.27	0.64
2:E:62:TYR:O	2:E:70:LYS:HE2	1.98	0.64
1:C:6:LEU:HD12	1:C:51:ASP:OD1	1.97	0.64
1:C:716:LYS:HG2	2:E:370:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:GLY:CA	1:D:158:GLN:HE22	2.01	0.64
1:D:208:PRO:HD3	1:D:464:LEU:O	1.98	0.64
1:A:298:ARG:CZ	1:C:6:LEU:HD21	2.27	0.64
1:B:315:SER:O	1:B:318:VAL:CG1	2.45	0.64
1:B:516:GLY:HA3	1:B:620:MET:CE	2.26	0.64
1:B:656:VAL:O	1:B:657:PRO:C	2.40	0.64
1:C:232:ASP:OD2	1:C:262:ARG:NH2	2.29	0.64
2:H:328:ARG:HB3	2:H:328:ARG:CZ	2.28	0.64
1:B:619:LEU:HG	1:B:693:ILE:CG2	2.28	0.64
1:D:227:LEU:HD11	1:D:437:ASN:HB3	1.80	0.64
1:D:625:SER:O	1:D:628:ILE:CG2	2.41	0.64
1:B:215:VAL:HG22	1:B:222:PHE:HZ	1.63	0.64
1:B:464:LEU:CB	1:B:514:GLY:O	2.46	0.64
1:D:560:LYS:HD3	1:D:609:HIS:CD2	2.33	0.64
1:D:656:VAL:O	1:D:657:PRO:C	2.39	0.64
2:E:35:ILE:HG23	2:E:36:PHE:H	1.62	0.64
2:E:90:SER:HB2	2:E:91:PRO:HD3	1.79	0.64
2:G:361:ILE:HD13	2:G:361:ILE:N	2.13	0.64
2:G:372:ASN:OD1	2:G:372:ASN:N	2.30	0.64
1:A:145:TYR:OH	1:A:149:LYS:HE3	1.98	0.64
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.78	0.64
1:C:617:SER:HB2	1:C:690:ASP:N	1.99	0.64
1:D:145:TYR:OH	1:D:149:LYS:HE3	1.98	0.64
1:A:297:VAL:HG11	1:C:4:ASN:HD22	1.62	0.64
1:A:329:ARG:HD3	1:A:331:ARG:NH1	2.13	0.64
1:C:572:THR:HB	1:C:577:ILE:HD12	1.79	0.64
1:D:150:GLN:OE1	1:D:154:LYS:CD	2.45	0.64
1:D:558:LEU:HD11	1:D:562:GLN:NE2	2.12	0.64
2:H:177:VAL:O	2:H:178:ASN:ND2	2.30	0.64
1:B:307:PRO:HG2	1:B:310:HIS:HB2	1.79	0.64
1:C:209:THR:HB	1:C:210:PRO:HD3	1.80	0.64
1:D:297:VAL:O	1:D:297:VAL:CG1	2.45	0.63
2:E:177:VAL:HG21	2:E:182:VAL:HG23	1.78	0.63
2:F:369:ASP:O	2:F:372:ASN:ND2	2.31	0.63
2:G:307:TYR:O	2:G:311:ILE:HG22	1.97	0.63
2:H:90:SER:HB2	2:H:91:PRO:HD3	1.79	0.63
1:A:301:ALA:HB3	1:A:438:LEU:HD21	1.79	0.63
1:A:689:ILE:HG21	1:A:691:GLN:O	1.98	0.63
1:B:211:ILE:O	1:B:215:VAL:HG23	1.99	0.63
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.79	0.63
1:C:211:ILE:O	1:C:215:VAL:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ILE:HG22	1:C:256:ILE:CG1	2.27	0.63
1:C:278:CYS:HB3	1:C:282:TYR:CE1	2.33	0.63
2:F:90:SER:HB2	2:F:91:PRO:HD3	1.81	0.63
2:G:334:TRP:O	2:G:335:ILE:C	2.42	0.63
1:A:516:GLY:HA2	1:A:618:ALA:O	1.98	0.63
1:A:619:LEU:HD12	1:A:693:ILE:CG2	2.28	0.63
1:B:6:LEU:HB2	1:B:51:ASP:OD1	1.98	0.63
1:C:55:THR:HA	1:C:58:ILE:HD12	1.80	0.63
1:C:208:PRO:HG2	1:C:211:ILE:HD13	1.78	0.63
1:C:558:LEU:HD11	1:C:562:GLN:NE2	2.14	0.63
1:D:375:PHE:O	1:D:379:TYR:HB2	1.98	0.63
2:G:35:ILE:HG23	2:G:36:PHE:H	1.63	0.63
1:A:94:TYR:HE2	1:A:168:SER:HB2	1.63	0.63
1:B:441:GLU:CB	1:B:619:LEU:O	2.46	0.63
2:F:12:GLN:NE2	2:F:23:VAL:CG1	2.60	0.63
1:A:6:LEU:HD22	1:A:14:THR:HG22	1.81	0.63
1:A:297:VAL:HG11	1:C:4:ASN:ND2	2.13	0.63
1:A:544:PHE:HE2	1:A:685:MET:HE2	1.64	0.63
1:B:37:SER:HB2	1:B:40:GLN:HB2	1.78	0.63
1:B:145:TYR:CE2	1:B:652:LEU:CD2	2.82	0.63
1:B:234:LEU:HA	1:B:237:ILE:HD12	1.80	0.63
1:C:465:SER:O	1:C:516:GLY:N	2.30	0.63
1:C:513:LEU:CD2	1:C:613:ASN:ND2	2.62	0.63
2:H:55:VAL:CG2	2:H:128:ASN:CG	2.71	0.63
1:A:307:PRO:HG2	1:A:310:HIS:HB2	1.81	0.63
1:A:319:LEU:HB3	1:A:330:VAL:H	1.64	0.63
1:A:463:THR:OG1	1:A:513:LEU:CD2	2.36	0.63
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.80	0.63
1:C:239:ALA:HA	1:C:452:VAL:HG12	1.80	0.63
1:D:544:PHE:HE2	1:D:685:MET:HE2	1.64	0.63
2:H:65:LEU:CD2	2:H:223:LEU:HD13	2.23	0.63
1:D:441:GLU:HG2	1:D:620:MET:CB	2.29	0.63
1:D:597:TYR:O	1:D:598:ASP:C	2.41	0.63
1:A:522:TYR:CE1	1:A:662:LEU:HD11	2.34	0.63
1:C:463:THR:CA	1:C:464:LEU:HD23	2.28	0.63
1:D:153:GLY:O	1:D:160:ARG:NH2	2.31	0.63
1:D:172:LEU:CD2	1:D:216:ARG:NH1	2.61	0.63
1:D:560:LYS:CE	1:D:609:HIS:ND1	2.62	0.63
2:E:205:ALA:HB2	2:E:242:LEU:HD13	1.79	0.63
2:F:62:TYR:O	2:F:70:LYS:HE2	1.99	0.63
1:B:318:VAL:CG2	1:B:329:ARG:CZ	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:GLN:HE22	1:C:499:PRO:HG3	1.63	0.63
2:E:65:LEU:O	2:E:70:LYS:HG3	1.98	0.63
2:E:173:GLY:O	2:E:175:HIS:NE2	2.31	0.63
2:F:82:LEU:HD13	2:F:140:ILE:HG22	1.79	0.63
2:G:13:LEU:O	2:G:32:LYS:HD2	1.98	0.63
2:H:6:SER:OG	2:H:21:GLN:NE2	2.27	0.63
1:A:474:ASN:ND2	1:A:476:ASP:HB2	2.14	0.62
1:B:558:LEU:HD12	1:B:561:GLU:HB3	1.81	0.62
2:F:94:ALA:C	2:F:95:LEU:HD23	2.24	0.62
2:H:273:TYR:OH	2:H:324:PRO:HB3	1.99	0.62
2:H:329:SER:O	2:H:330:ASN:C	2.40	0.62
1:A:5:LEU:CD1	1:A:17:ILE:CG1	2.38	0.62
1:A:176:VAL:HG13	1:A:215:VAL:HG11	1.81	0.62
1:A:305:PHE:CE1	1:A:436:SER:O	2.53	0.62
1:C:361:VAL:HG11	1:C:364:LEU:CB	2.29	0.62
1:D:155:TYR:HE1	1:D:209:THR:HG23	1.64	0.62
1:A:226:VAL:HG21	1:A:247:TYR:CD2	2.35	0.62
1:A:686:GLN:NE2	1:A:727:LYS:HE3	2.15	0.62
1:C:238:ASN:OD1	1:D:242:SER:HA	1.99	0.62
2:E:20:GLY:O	2:E:21:GLN:C	2.43	0.62
2:F:206:ILE:CD1	2:F:315:ARG:HG2	2.30	0.62
2:H:195:LEU:HD13	2:H:271:GLU:HG2	1.82	0.62
1:A:232:ASP:OD2	1:A:262:ARG:NH2	2.31	0.62
1:B:155:TYR:CD1	1:B:212:MET:HB2	2.31	0.62
1:C:157:VAL:HG21	1:C:216:ARG:HH11	1.65	0.62
1:C:435:GLN:CD	1:C:446:THR:HG21	2.24	0.62
2:F:239:ALA:HB2	2:F:342:ASP:OD2	1.99	0.62
1:A:227:LEU:HD11	1:A:437:ASN:HB3	1.81	0.62
1:B:305:PHE:CZ	1:B:436:SER:O	2.52	0.62
1:C:305:PHE:CZ	1:C:436:SER:O	2.52	0.62
1:D:234:LEU:HA	1:D:237:ILE:HD12	1.82	0.62
1:B:209:THR:HB	1:B:210:PRO:HD3	1.82	0.62
1:B:375:PHE:O	1:B:379:TYR:HB2	1.98	0.62
1:C:474:ASN:ND2	1:C:476:ASP:HB2	2.15	0.62
1:D:25:VAL:HG21	3:D:801:ATP:H3'	1.82	0.62
2:F:99:ILE:HD11	2:F:108:VAL:HG21	1.79	0.62
1:A:167:GLU:OE1	1:A:172:LEU:CB	2.47	0.62
1:B:317:LEU:HD11	1:B:402:MET:CA	2.28	0.62
1:D:341:LYS:HB2	1:D:722:TYR:OH	2.00	0.62
2:E:334:TRP:O	2:E:335:ILE:C	2.43	0.62
2:F:12:GLN:OE1	2:F:27:ARG:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:90:SER:HB2	2:G:91:PRO:HD3	1.81	0.62
2:H:62:TYR:O	2:H:70:LYS:HE2	1.99	0.62
1:A:227:LEU:CG	1:A:435:GLN:NE2	2.62	0.62
1:B:278:CYS:HB3	1:B:282:TYR:CE1	2.35	0.62
1:D:428:PRO:O	1:D:432:PRO:HB3	2.00	0.62
2:H:65:LEU:O	2:H:70:LYS:HG3	1.99	0.62
1:A:234:LEU:HA	1:A:237:ILE:HD12	1.82	0.62
1:B:474:ASN:ND2	1:B:476:ASP:HB2	2.15	0.62
1:C:227:LEU:HD11	1:C:437:ASN:HB3	1.81	0.62
1:C:330:VAL:HB	1:C:335:TYR:OH	1.99	0.62
1:C:522:TYR:HE1	1:C:662:LEU:HD11	1.63	0.62
1:C:569:ASN:HD22	1:C:570:GLU:N	1.96	0.62
1:D:79:TYR:O	1:D:83:ARG:HG2	1.98	0.62
2:E:331:PRO:C	2:E:333:PRO:HD3	2.25	0.62
2:F:201:ASN:O	2:F:205:ALA:CB	2.47	0.62
1:A:406:ARG:HH11	1:A:732:GLN:HG3	1.64	0.62
1:A:647:SER:O	1:A:650:GLY:N	2.33	0.62
1:C:560:LYS:CD	1:C:609:HIS:CE1	2.83	0.62
1:D:227:LEU:HB2	1:D:460:ALA:HB3	1.81	0.62
1:D:286:GLN:NE2	1:D:332:HIS:ND1	2.48	0.62
2:F:312:THR:HB	2:F:325:PHE:HD2	1.62	0.62
1:B:232:ASP:OD2	1:B:262:ARG:HB3	2.00	0.61
1:B:701:PRO:HD2	1:B:735:ARG:CG	2.25	0.61
1:B:702:SER:HB3	1:B:735:ARG:HD3	1.81	0.61
1:C:167:GLU:OE2	1:C:172:LEU:CD1	2.43	0.61
1:C:307:PRO:HG2	1:C:310:HIS:HB2	1.79	0.61
2:G:236:ARG:HG3	2:G:340:VAL:HG23	1.82	0.61
2:G:331:PRO:C	2:G:333:PRO:HD3	2.25	0.61
1:A:228:ILE:HG21	1:A:240:THR:HG23	1.81	0.61
1:A:440:LEU:HD12	1:A:728:THR:CB	2.30	0.61
1:A:716:LYS:HG2	2:F:370:LEU:HD21	1.82	0.61
1:B:62:ILE:HD12	1:B:84:LEU:HD22	1.82	0.61
1:B:369:PHE:CE1	1:B:434:ARG:CA	2.83	0.61
1:C:131:MET:HE3	1:C:193:VAL:HG11	1.81	0.61
1:C:302:ALA:N	1:C:438:LEU:HD21	2.15	0.61
2:F:221:ARG:NH1	2:F:296:MET:HE3	2.14	0.61
1:C:59:HIS:HB2	3:C:801:ATP:C5'	2.30	0.61
1:C:686:GLN:NE2	1:C:727:LYS:HE3	2.14	0.61
1:D:50:TYR:CD2	1:D:53:ILE:HD12	2.35	0.61
2:F:329:SER:O	2:F:330:ASN:C	2.40	0.61
2:F:330:ASN:OD1	2:F:331:PRO:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:SER:O	1:A:691:GLN:HG2	1.99	0.61
1:B:513:LEU:CD1	1:B:613:ASN:ND2	2.63	0.61
1:C:114:LYS:HG3	1:C:166:TYR:CE2	2.35	0.61
1:D:157:VAL:N	1:D:167:GLU:HG2	2.14	0.61
2:E:307:TYR:O	2:E:311:ILE:HG22	1.99	0.61
2:F:339:LEU:O	2:F:340:VAL:HG23	2.00	0.61
1:A:49:PHE:HD1	1:A:53:ILE:HD13	1.65	0.61
1:A:50:TYR:O	1:A:53:ILE:HB	2.00	0.61
1:A:250:GLN:HE22	1:A:499:PRO:HG3	1.65	0.61
1:B:82:ALA:O	1:B:86:ILE:HG12	1.99	0.61
1:C:320:LYS:CE	1:C:333:MET:O	2.46	0.61
1:C:375:PHE:O	1:C:379:TYR:HB2	2.00	0.61
1:D:150:GLN:HE22	1:D:645:LYS:NZ	1.99	0.61
1:D:150:GLN:CD	1:D:154:LYS:HD2	2.26	0.61
1:A:569:ASN:HD22	1:A:570:GLU:N	1.97	0.61
1:B:663:HIS:ND1	1:B:663:HIS:N	2.47	0.61
1:C:305:PHE:CE2	1:C:436:SER:HB3	2.36	0.61
1:C:521:ALA:HB3	1:C:632:THR:HG21	1.82	0.61
1:C:686:GLN:HA	1:C:689:ILE:HG13	1.83	0.61
1:D:158:GLN:HB3	1:D:165:ILE:CD1	2.30	0.61
1:D:465:SER:HB2	1:D:489:LEU:CD1	2.30	0.61
1:A:211:ILE:O	1:A:215:VAL:HG23	2.00	0.61
1:A:428:PRO:O	1:A:432:PRO:HB3	2.01	0.61
1:D:114:LYS:N	1:D:114:LYS:CD	2.57	0.61
1:D:290:LYS:NZ	1:D:300:GLY:O	2.30	0.61
2:E:177:VAL:CB	2:E:180:LYS:O	2.49	0.61
2:G:12:GLN:NE2	2:G:23:VAL:HG13	2.15	0.61
1:A:227:LEU:HB3	1:A:435:GLN:CD	2.26	0.61
1:B:569:ASN:HD22	1:B:570:GLU:N	1.98	0.61
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.82	0.61
1:C:253:GLY:C	1:C:438:LEU:HD12	2.26	0.61
2:E:207:ARG:HH22	2:E:282:GLN:CD	2.09	0.61
2:H:99:ILE:HD11	2:H:108:VAL:HG21	1.83	0.61
2:H:232:ARG:HH11	2:H:343:ASN:N	1.99	0.61
1:A:150:GLN:O	1:A:154:LYS:HB2	2.00	0.61
1:A:209:THR:HB	1:A:210:PRO:HD3	1.83	0.61
1:B:262:ARG:NH1	1:B:267:PRO:O	2.33	0.61
1:D:511:ARG:HD3	1:D:612:ARG:O	2.01	0.61
1:D:696:ASN:H	1:D:696:ASN:ND2	1.99	0.61
2:H:310:TYR:CE2	2:H:330:ASN:CG	2.79	0.61
1:A:225:CYS:CB	1:A:253:GLY:O	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:VAL:HG11	1:A:364:LEU:CG	2.31	0.61
1:C:711:MET:HG2	2:E:365:VAL:HG22	1.81	0.61
1:D:59:HIS:O	1:D:62:ILE:HG12	2.01	0.61
2:G:62:TYR:O	2:G:70:LYS:HE2	2.01	0.61
2:G:195:LEU:HD13	2:G:271:GLU:HG2	1.81	0.61
2:H:310:TYR:CD2	2:H:330:ASN:OD1	2.54	0.61
1:A:305:PHE:CZ	1:A:436:SER:O	2.54	0.60
1:A:361:VAL:HG11	1:A:364:LEU:HB2	1.81	0.60
1:B:428:PRO:O	1:B:432:PRO:HB3	2.01	0.60
1:C:621:PRO:CD	1:C:694:SER:CB	2.79	0.60
1:D:6:LEU:CB	1:D:51:ASP:OD1	2.44	0.60
1:D:522:TYR:CE1	1:D:662:LEU:HD11	2.36	0.60
2:E:36:PHE:HE1	2:E:248:MET:HE2	1.65	0.60
1:D:474:ASN:ND2	1:D:476:ASP:HB2	2.16	0.60
2:E:89:ARG:HG2	2:E:90:SER:N	2.16	0.60
1:A:172:LEU:HD21	1:A:216:ARG:HH12	1.65	0.60
1:A:375:PHE:O	1:A:379:TYR:HB2	2.01	0.60
1:B:587:LEU:HD23	1:B:590:ILE:HD11	1.84	0.60
1:C:234:LEU:HA	1:C:237:ILE:HD12	1.83	0.60
1:C:332:HIS:O	1:C:333:MET:CG	2.49	0.60
2:E:31:GLN:CD	2:E:31:GLN:N	2.60	0.60
2:G:36:PHE:HE1	2:G:248:MET:HE2	1.66	0.60
2:H:20:GLY:CA	2:H:100:SER:HB3	2.31	0.60
1:D:131:MET:HE3	1:D:193:VAL:HG11	1.82	0.60
1:D:623:GLU:HG2	1:D:633:ASN:HD21	1.63	0.60
1:A:82:ALA:O	1:A:86:ILE:HG12	2.02	0.60
1:A:567:TRP:O	1:A:569:ASN:ND2	2.34	0.60
1:B:617:SER:C	1:B:689:ILE:HD12	2.26	0.60
1:C:515:ILE:HD13	1:C:551:LEU:HD22	1.82	0.60
1:D:39:SER:CB	2:G:332:ILE:CG2	2.74	0.60
2:G:179:GLY:C	2:G:180:LYS:HG2	2.26	0.60
1:C:172:LEU:HD21	1:C:212:MET:HE3	1.80	0.60
1:D:521:ALA:HB3	1:D:632:THR:HG21	1.84	0.60
1:D:696:ASN:HD22	1:D:696:ASN:N	1.99	0.60
2:E:104:LEU:O	2:E:108:VAL:HG23	2.02	0.60
2:E:195:LEU:HD13	2:E:271:GLU:HG2	1.83	0.60
1:A:208:PRO:CG	1:A:211:ILE:CD1	2.64	0.60
1:A:369:PHE:CE2	1:A:434:ARG:CD	2.80	0.60
1:B:316:LEU:HA	1:B:319:LEU:HD11	1.83	0.60
1:B:544:PHE:HE2	1:B:685:MET:HE2	1.64	0.60
1:D:5:LEU:HD12	1:D:17:ILE:CG1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:VAL:HB	1:D:335:TYR:OH	2.01	0.60
2:F:205:ALA:HB1	2:F:315:ARG:CD	2.31	0.60
1:A:293:SER:HB2	1:A:298:ARG:O	2.01	0.60
1:C:17:ILE:HD12	3:C:801:ATP:N1	2.15	0.60
1:C:714:LEU:HD22	1:C:732:GLN:HE22	1.67	0.60
2:E:206:ILE:HD13	2:E:312:THR:CB	2.32	0.60
2:F:20:GLY:O	2:F:21:GLN:C	2.42	0.60
2:H:20:GLY:O	2:H:21:GLN:C	2.43	0.60
1:A:663:HIS:ND1	1:A:663:HIS:N	2.39	0.60
1:B:283:LYS:HG2	1:B:330:VAL:HG22	1.82	0.60
1:B:319:LEU:HA	1:B:329:ARG:HG2	1.84	0.60
1:C:716:LYS:CG	2:E:370:LEU:HD22	2.32	0.60
1:D:19:LEU:HD22	2:G:295:SER:C	2.27	0.60
1:D:560:LYS:HD3	1:D:609:HIS:ND1	2.17	0.60
2:E:74:ILE:O	2:E:78:LYS:HG3	2.01	0.60
2:H:36:PHE:HE1	2:H:248:MET:HE2	1.67	0.60
1:B:282:TYR:CD2	1:B:304:LEU:CD2	2.84	0.60
1:C:155:TYR:CZ	1:C:628:ILE:HD12	2.37	0.60
1:D:82:ALA:O	1:D:86:ILE:HG12	2.02	0.60
2:H:91:PRO:O	2:H:95:LEU:HG	2.01	0.60
2:H:205:ALA:HB1	2:H:315:ARG:CD	2.32	0.60
1:A:278:CYS:HB3	1:A:282:TYR:CE1	2.37	0.59
1:A:521:ALA:HB3	1:A:632:THR:HG21	1.83	0.59
1:B:105:HIS:NE2	1:B:109:MET:HE3	2.17	0.59
1:B:131:MET:HE3	1:B:193:VAL:HG11	1.84	0.59
1:B:587:LEU:O	1:B:589:THR:N	2.34	0.59
1:B:708:LYS:O	1:B:709:VAL:C	2.45	0.59
1:C:39:SER:CB	2:E:332:ILE:HG22	2.31	0.59
1:C:167:GLU:HG2	1:C:168:SER:N	2.17	0.59
1:D:305:PHE:CZ	1:D:436:SER:O	2.54	0.59
1:D:686:GLN:NE2	1:D:727:LYS:HE3	2.16	0.59
2:E:5:PHE:HE2	2:E:7:GLN:NE2	2.00	0.59
2:H:31:GLN:CD	2:H:31:GLN:N	2.60	0.59
1:B:587:LEU:C	1:B:589:THR:H	2.09	0.59
1:D:209:THR:HB	1:D:210:PRO:HD3	1.83	0.59
1:D:364:LEU:C	1:D:364:LEU:CD1	2.76	0.59
2:E:12:GLN:NE2	2:E:23:VAL:HG13	2.17	0.59
2:E:99:ILE:HD11	2:E:108:VAL:HG21	1.83	0.59
2:H:104:LEU:O	2:H:108:VAL:HG23	2.02	0.59
1:A:22:ILE:O	1:A:26:LEU:HG	2.02	0.59
1:A:449:LEU:HD21	1:A:502:ALA:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ASN:ND2	1:A:570:GLU:H	2.00	0.59
1:B:228:ILE:HG21	1:B:240:THR:HG23	1.83	0.59
1:B:305:PHE:CE1	1:B:436:SER:O	2.55	0.59
1:B:597:TYR:O	1:B:598:ASP:C	2.42	0.59
1:D:6:LEU:HD12	1:D:51:ASP:OD1	2.02	0.59
1:D:147:ALA:HB2	1:D:627:GLN:O	2.02	0.59
1:D:730:TYR:O	1:D:731:TYR:C	2.46	0.59
2:E:167:TRP:NE1	2:E:172:GLU:OE2	2.34	0.59
1:B:286:GLN:NE2	1:B:332:HIS:ND1	2.50	0.59
1:C:82:ALA:O	1:C:86:ILE:HG12	2.01	0.59
1:C:207:LEU:N	1:C:207:LEU:HD23	2.17	0.59
1:D:708:LYS:O	1:D:710:PRO:HD3	2.03	0.59
2:G:205:ALA:HB1	2:G:315:ARG:CD	2.32	0.59
1:A:303:THR:OG1	1:A:438:LEU:HD12	2.02	0.59
1:B:617:SER:O	1:B:691:GLN:HG3	2.03	0.59
1:B:730:TYR:O	1:B:731:TYR:C	2.46	0.59
1:D:52:GLY:C	1:D:53:ILE:HG22	2.28	0.59
1:D:595:LEU:HD22	1:D:599:TRP:NE1	2.18	0.59
2:G:20:GLY:O	2:G:21:GLN:C	2.42	0.59
1:B:262:ARG:HG2	1:B:275:HIS:CE1	2.38	0.59
1:D:689:ILE:HG22	1:D:691:GLN:O	2.03	0.59
1:D:703:ARG:O	1:D:703:ARG:CG	2.51	0.59
1:D:711:MET:CB	2:G:363:SER:CB	2.75	0.59
2:E:217:ALA:HB1	2:E:296:MET:HE1	1.84	0.59
2:G:99:ILE:HD11	2:G:108:VAL:HG21	1.84	0.59
2:G:217:ALA:HB1	2:G:296:MET:HE1	1.84	0.59
1:A:425:PRO:CG	1:A:690:ASP:HB3	2.27	0.59
1:B:414:ILE:HB	1:B:729:LEU:HD12	1.83	0.59
1:C:59:HIS:O	1:C:62:ILE:HG12	2.03	0.59
1:C:105:HIS:NE2	1:C:109:MET:HE3	2.18	0.59
1:C:216:ARG:CG	1:C:216:ARG:O	2.51	0.59
1:D:361:VAL:CG1	1:D:364:LEU:HB2	2.33	0.59
1:A:403:MET:HE1	1:A:718:LEU:HD22	1.85	0.59
1:D:5:LEU:HB2	1:D:17:ILE:CG1	2.32	0.59
1:D:567:TRP:O	1:D:568:PHE:C	2.45	0.59
1:D:685:MET:O	1:D:689:ILE:CG1	2.44	0.59
2:E:111:TRP:CD1	2:E:111:TRP:C	2.80	0.59
2:G:206:ILE:CD1	2:G:315:ARG:HG2	2.32	0.59
1:A:316:LEU:HA	1:A:319:LEU:HD11	1.85	0.59
1:A:716:LYS:HA	2:F:370:LEU:HD11	1.84	0.59
1:D:207:LEU:N	1:D:207:LEU:HD23	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:193:LEU:O	2:E:197:LEU:HG	2.02	0.59
2:F:38:LYS:CD	2:F:344:VAL:HG12	2.25	0.59
2:G:20:GLY:CA	2:G:100:SER:HB3	2.33	0.59
2:G:149:ARG:NH1	2:G:286:TRP:HB2	2.13	0.59
2:H:12:GLN:NE2	2:H:23:VAL:HG13	2.15	0.59
1:B:37:SER:OG	2:H:331:PRO:O	2.20	0.59
1:C:569:ASN:ND2	1:C:570:GLU:H	1.98	0.59
1:C:670:TRP:CE2	1:C:735:ARG:HG3	2.38	0.59
1:C:696:ASN:H	1:C:696:ASN:ND2	2.00	0.59
1:C:708:LYS:O	1:C:709:VAL:C	2.45	0.59
2:E:147:GLN:O	2:E:150:ALA:HB3	2.03	0.59
1:A:6:LEU:HD11	1:C:298:ARG:CD	2.32	0.58
1:A:545:GLU:CD	1:A:596:HIS:H	2.11	0.58
1:C:44:ARG:HE	1:C:44:ARG:CA	2.07	0.58
1:C:417:VAL:HG23	1:C:418:ASP:N	2.18	0.58
1:C:529:LYS:HB3	1:C:536:ALA:HB2	1.84	0.58
1:C:619:LEU:HB2	1:C:693:ILE:HG22	1.85	0.58
1:D:43:LEU:HD12	2:G:334:TRP:NE1	2.18	0.58
2:F:73:PHE:HB2	2:F:218:PHE:CE2	2.38	0.58
2:H:193:LEU:O	2:H:197:LEU:HG	2.03	0.58
1:A:417:VAL:HG23	1:A:418:ASP:N	2.18	0.58
1:B:595:LEU:HD22	1:B:599:TRP:NE1	2.18	0.58
1:C:34:HIS:O	1:C:35:ASN:HB2	2.03	0.58
1:C:403:MET:HG2	1:C:711:MET:HE1	1.83	0.58
1:D:50:TYR:H	1:D:50:TYR:HD2	1.50	0.58
1:D:305:PHE:CE1	1:D:436:SER:O	2.56	0.58
1:D:617:SER:HB2	1:D:690:ASP:N	2.04	0.58
2:F:74:ILE:O	2:F:78:LYS:HG3	2.03	0.58
2:F:115:GLU:OE1	2:F:115:GLU:HA	2.03	0.58
2:G:31:GLN:N	2:G:31:GLN:CD	2.61	0.58
2:G:193:LEU:O	2:G:197:LEU:HG	2.03	0.58
2:H:6:SER:CB	2:H:21:GLN:HE21	2.16	0.58
1:B:86:ILE:HG21	1:B:140:ASP:HB3	1.85	0.58
1:B:567:TRP:O	1:B:569:ASN:ND2	2.36	0.58
1:B:712:GLN:NE2	2:H:369:ASP:HB3	2.18	0.58
1:D:592:ASN:O	1:D:594:PRO:HD3	2.04	0.58
2:F:104:LEU:O	2:F:108:VAL:HG23	2.02	0.58
1:B:276:THR:HG23	1:B:280:PRO:HG2	1.84	0.58
1:B:286:GLN:NE2	1:B:332:HIS:CG	2.71	0.58
1:B:521:ALA:HB3	1:B:632:THR:HG21	1.84	0.58
1:C:449:LEU:HD21	1:C:502:ALA:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:167:TRP:CD1	2:E:172:GLU:OE2	2.57	0.58
2:F:207:ARG:HH22	2:F:282:GLN:CD	2.11	0.58
1:A:621:PRO:HD3	1:A:694:SER:CB	2.33	0.58
1:B:511:ARG:HD3	1:B:612:ARG:O	2.03	0.58
1:B:592:ASN:O	1:B:594:PRO:HD3	2.03	0.58
2:E:20:GLY:HA3	2:E:100:SER:HB3	1.85	0.58
2:F:31:GLN:CD	2:F:31:GLN:N	2.61	0.58
2:F:195:LEU:HD13	2:F:271:GLU:HG2	1.84	0.58
2:H:143:ASN:CG	2:H:146:ILE:HD13	2.28	0.58
1:A:227:LEU:CB	1:A:435:GLN:HE22	2.08	0.58
1:A:511:ARG:HD3	1:A:612:ARG:O	2.03	0.58
2:F:83:LEU:HD22	2:F:203:LEU:HG	1.85	0.58
1:D:692:SER:HB2	1:D:727:LYS:HB2	1.86	0.58
2:G:74:ILE:O	2:G:78:LYS:HG3	2.04	0.58
2:H:309:GLU:HG2	2:H:325:PHE:CE1	2.38	0.58
1:A:176:VAL:HA	1:A:215:VAL:HG11	1.84	0.58
1:A:474:ASN:HD21	1:A:476:ASP:HB2	1.69	0.58
1:A:621:PRO:HD3	1:A:694:SER:HB2	1.86	0.58
1:B:10:ARG:H	1:B:55:THR:CG2	2.16	0.58
1:B:412:ILE:HD12	1:B:412:ILE:N	2.19	0.58
1:C:474:ASN:HD21	1:C:476:ASP:HB2	1.69	0.58
1:D:329:ARG:CD	1:D:331:ARG:NH2	2.53	0.58
1:D:564:ALA:HA	1:D:611:LEU:O	2.03	0.58
2:H:221:ARG:NH1	2:H:296:MET:HE3	2.19	0.58
1:B:440:LEU:HD12	1:B:728:THR:CB	2.33	0.58
1:C:545:GLU:HG3	1:C:595:LEU:CD2	2.33	0.58
1:C:730:TYR:O	1:C:731:TYR:C	2.46	0.58
2:H:336:ASN:O	2:H:340:VAL:HG23	2.03	0.58
1:A:10:ARG:H	1:A:55:THR:CG2	2.16	0.58
1:A:22:ILE:H	1:A:22:ILE:HD12	1.68	0.58
1:A:52:GLY:C	1:A:53:ILE:HG22	2.28	0.58
1:A:513:LEU:O	1:A:615:THR:O	2.22	0.58
1:B:696:ASN:H	1:B:696:ASN:ND2	2.01	0.58
2:F:92:ASN:O	2:F:96:LEU:HB2	2.04	0.58
2:H:364:GLU:OE1	2:H:364:GLU:HA	2.04	0.58
1:B:10:ARG:CG	1:B:56:SER:HB2	2.34	0.57
1:D:150:GLN:OE1	1:D:154:LYS:CE	2.52	0.57
1:D:286:GLN:O	1:D:289:VAL:HG22	2.03	0.57
1:C:522:TYR:CE1	1:C:662:LEU:HD11	2.39	0.57
1:D:406:ARG:HH11	1:D:697:THR:CG2	2.17	0.57
2:E:191:LYS:HG2	2:E:264:ILE:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:273:TYR:O	2:E:277:VAL:HG23	2.04	0.57
1:C:515:ILE:CD1	1:C:551:LEU:HD22	2.34	0.57
1:D:441:GLU:HG2	1:D:620:MET:HB3	1.86	0.57
2:G:191:LYS:HG2	2:G:264:ILE:HG23	1.86	0.57
2:G:207:ARG:HH22	2:G:282:GLN:CD	2.13	0.57
1:A:86:ILE:HG21	1:A:140:ASP:HB3	1.85	0.57
1:A:167:GLU:OE2	1:A:216:ARG:NH2	2.36	0.57
1:A:520:PHE:CE2	1:A:524:LEU:HD11	2.39	0.57
1:B:59:HIS:O	1:B:62:ILE:HG12	2.04	0.57
1:B:245:VAL:O	1:B:249:SER:HB3	2.04	0.57
1:C:560:LYS:CE	1:C:609:HIS:CE1	2.87	0.57
2:F:20:GLY:CA	2:F:100:SER:HB3	2.34	0.57
2:H:328:ARG:HB3	2:H:328:ARG:NH1	2.20	0.57
1:A:414:ILE:HB	1:A:729:LEU:HD12	1.86	0.57
1:A:696:ASN:H	1:A:696:ASN:ND2	2.02	0.57
1:B:260:ARG:O	1:B:261:ILE:C	2.41	0.57
1:B:515:ILE:HB	1:B:616:LEU:O	2.05	0.57
1:C:260:ARG:HD3	1:C:365:TYR:CE2	2.39	0.57
1:D:207:LEU:CG	1:D:212:MET:SD	2.92	0.57
1:D:361:VAL:CG1	1:D:382:TYR:CE2	2.87	0.57
2:E:83:LEU:HD22	2:E:203:LEU:HG	1.86	0.57
2:H:230:ILE:O	2:H:234:ILE:HG12	2.04	0.57
1:A:576:GLY:HA3	1:A:607:LYS:HE2	1.87	0.57
1:B:309:TRP:CH2	1:B:364:LEU:HD12	2.39	0.57
1:B:413:TYR:HB3	1:B:729:LEU:O	2.04	0.57
1:C:317:LEU:HD13	1:C:401:LEU:CG	2.34	0.57
1:D:62:ILE:HD12	1:D:84:LEU:HD22	1.86	0.57
1:D:152:GLU:HA	1:D:156:LEU:HD12	1.86	0.57
2:F:230:ILE:O	2:F:234:ILE:HG12	2.05	0.57
2:G:132:ASP:OD2	2:G:135:VAL:HG13	2.05	0.57
1:A:696:ASN:HD22	1:A:696:ASN:N	2.01	0.57
1:B:207:LEU:N	1:B:207:LEU:HD23	2.19	0.57
1:B:268:ILE:O	1:B:269:ARG:HB3	2.05	0.57
1:C:513:LEU:CD1	1:C:616:LEU:HA	2.33	0.57
1:D:316:LEU:CA	1:D:319:LEU:HD11	2.35	0.57
1:D:329:ARG:HB3	1:D:331:ARG:HE	1.70	0.57
1:D:447:LYS:HB2	1:D:458:GLU:N	2.19	0.57
1:D:576:GLY:HA3	1:D:607:LYS:HE2	1.87	0.57
2:E:339:LEU:C	2:E:339:LEU:CD1	2.77	0.57
1:B:318:VAL:HG23	1:B:329:ARG:NH2	2.18	0.57
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLN:O	1:C:289:VAL:HG22	2.04	0.57
1:D:86:ILE:HG21	1:D:140:ASP:HB3	1.87	0.57
1:D:276:THR:HG23	1:D:280:PRO:HG2	1.87	0.57
2:E:143:ASN:CG	2:E:146:ILE:HD13	2.29	0.57
2:F:277:VAL:HG22	2:F:324:PRO:HB3	1.86	0.57
2:H:206:ILE:O	2:H:210:VAL:CG2	2.51	0.57
1:A:317:LEU:CD1	1:A:401:LEU:HD23	2.16	0.57
1:C:155:TYR:CD1	1:C:212:MET:HB2	2.35	0.57
1:C:174:ILE:HG23	1:C:175:LEU:N	2.20	0.57
1:D:268:ILE:O	1:D:269:ARG:HB3	2.05	0.57
2:E:148:LYS:HG2	2:E:149:ARG:N	2.19	0.57
2:F:72:ILE:HG23	2:F:290:LEU:HD23	1.87	0.57
2:H:96:LEU:HA	2:H:99:ILE:HD12	1.86	0.57
1:C:10:ARG:CG	1:C:56:SER:HB2	2.35	0.57
1:C:369:PHE:CD2	1:C:434:ARG:CD	2.88	0.57
1:C:511:ARG:HD3	1:C:612:ARG:O	2.05	0.57
1:D:254:ILE:H	1:D:438:LEU:HD11	1.64	0.57
2:E:132:ASP:OD2	2:E:135:VAL:HG13	2.05	0.57
1:A:6:LEU:O	1:A:7:VAL:CG2	2.52	0.56
1:A:615:THR:CG2	1:A:691:GLN:HE22	2.14	0.56
1:B:316:LEU:O	1:B:319:LEU:HD12	2.05	0.56
1:B:515:ILE:HD13	1:B:551:LEU:CD1	2.35	0.56
1:D:150:GLN:CB	1:D:154:LYS:CD	2.82	0.56
1:D:282:TYR:CD2	1:D:304:LEU:HD13	2.40	0.56
1:D:294:GLN:CG	1:D:298:ARG:HG3	2.34	0.56
1:D:309:TRP:CZ2	1:D:364:LEU:CD1	2.88	0.56
2:G:15:GLU:OE1	2:G:20:GLY:HA3	2.05	0.56
2:G:83:LEU:HD22	2:G:203:LEU:HG	1.87	0.56
2:G:273:TYR:O	2:G:277:VAL:HG23	2.05	0.56
1:A:182:SER:O	1:A:189:ARG:CZ	2.53	0.56
1:A:268:ILE:O	1:A:269:ARG:HB3	2.05	0.56
1:A:712:GLN:HE21	2:F:370:LEU:CD2	2.15	0.56
1:B:10:ARG:NH2	3:B:801:ATP:O2A	2.34	0.56
1:C:369:PHE:CE2	1:C:434:ARG:CG	2.88	0.56
1:D:176:VAL:HG13	1:D:215:VAL:HG21	1.87	0.56
2:E:328:ARG:HB3	2:E:328:ARG:NH1	2.20	0.56
2:G:111:TRP:CD1	2:G:111:TRP:C	2.81	0.56
2:G:111:TRP:HD1	2:G:111:TRP:O	1.88	0.56
1:A:190:LEU:H	1:A:190:LEU:HD22	1.71	0.56
1:A:369:PHE:CZ	1:A:434:ARG:CB	2.88	0.56
1:A:516:GLY:CA	1:A:620:MET:HE1	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HD22	1:B:167:GLU:HG2	1.87	0.56
1:B:417:VAL:HG23	1:B:418:ASP:N	2.20	0.56
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.87	0.56
1:B:522:TYR:CD1	1:B:662:LEU:HD11	2.39	0.56
1:B:625:SER:O	1:B:628:ILE:CG2	2.52	0.56
1:C:10:ARG:H	1:C:55:THR:CG2	2.18	0.56
1:C:527:HIS:O	1:C:529:LYS:HD2	2.05	0.56
1:C:560:LYS:CD	1:C:609:HIS:ND1	2.68	0.56
1:C:656:VAL:O	1:C:657:PRO:C	2.46	0.56
1:D:50:TYR:HE2	1:D:53:ILE:HD12	1.64	0.56
1:D:68:ASP:OD2	1:D:651:ILE:HG21	2.05	0.56
1:D:303:THR:HA	1:D:334:ASP:O	2.05	0.56
1:D:711:MET:N	2:G:363:SER:CB	2.59	0.56
2:E:295:SER:OG	2:E:300:ASN:HB3	2.05	0.56
2:F:42:LYS:HG3	2:F:344:VAL:HG23	1.87	0.56
2:G:143:ASN:CG	2:G:146:ILE:HD13	2.29	0.56
2:G:310:TYR:CE2	2:G:330:ASN:HB2	2.39	0.56
2:H:72:ILE:HG23	2:H:290:LEU:HD23	1.87	0.56
2:H:74:ILE:O	2:H:78:LYS:HG3	2.04	0.56
2:H:149:ARG:NH1	2:H:286:TRP:HB2	2.14	0.56
1:A:459:ILE:HD11	1:A:502:ALA:HB3	1.86	0.56
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.87	0.56
1:C:592:ASN:O	1:C:594:PRO:HD3	2.05	0.56
1:D:5:LEU:CD1	1:D:17:ILE:HG12	2.34	0.56
1:D:55:THR:HA	1:D:58:ILE:CD1	2.35	0.56
1:D:464:LEU:HD22	1:D:514:GLY:CA	2.35	0.56
1:D:474:ASN:HD21	1:D:476:ASP:HB2	1.70	0.56
2:F:111:TRP:HZ2	2:F:204:GLU:OE2	1.89	0.56
2:F:143:ASN:CG	2:F:146:ILE:HD13	2.30	0.56
2:F:191:LYS:HG2	2:F:264:ILE:HG23	1.87	0.56
2:F:217:ALA:HB1	2:F:296:MET:HE1	1.87	0.56
2:H:309:GLU:OE2	2:H:325:PHE:HD1	1.89	0.56
1:A:59:HIS:O	1:A:62:ILE:HG12	2.06	0.56
1:A:592:ASN:O	1:A:594:PRO:HD3	2.04	0.56
1:B:669:LEU:HD11	1:B:698:ASN:ND2	2.21	0.56
1:C:222:PHE:HE2	1:C:495:TYR:CD2	2.24	0.56
1:C:230:CYS:SG	1:C:237:ILE:HA	2.46	0.56
1:C:440:LEU:HD12	1:C:728:THR:CB	2.34	0.56
1:C:576:GLY:HA3	1:C:607:LYS:HE2	1.87	0.56
1:D:222:PHE:HB2	1:D:492:LEU:HD21	1.86	0.56
2:F:111:TRP:C	2:F:111:TRP:CD1	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:104:LEU:O	2:G:108:VAL:HG23	2.04	0.56
1:C:115:TYR:CD1	1:C:216:ARG:CD	2.88	0.56
1:C:228:ILE:HG21	1:C:240:THR:HG23	1.87	0.56
1:C:242:SER:HA	1:D:238:ASN:OD1	2.06	0.56
1:D:74:ALA:HB1	1:D:77:TYR:HD2	1.70	0.56
1:D:154:LYS:HE2	1:D:624:THR:HG22	1.87	0.56
2:F:295:SER:OG	2:F:300:ASN:HB3	2.05	0.56
2:H:96:LEU:HA	2:H:99:ILE:CD1	2.35	0.56
2:H:197:LEU:HD13	2:H:249:LEU:HG	1.87	0.56
2:H:217:ALA:HB1	2:H:296:MET:HE1	1.88	0.56
1:A:10:ARG:CG	1:A:56:SER:HB2	2.35	0.56
1:D:190:LEU:H	1:D:190:LEU:HD22	1.70	0.56
1:D:414:ILE:HB	1:D:729:LEU:HD12	1.88	0.56
2:H:5:PHE:CE1	2:H:24:ASN:O	2.59	0.56
2:H:191:LYS:HG2	2:H:264:ILE:HG23	1.87	0.56
1:A:29:ALA:HB1	1:A:80:LEU:HD12	1.88	0.56
1:B:449:LEU:HG	1:B:457:GLY:HA3	1.87	0.56
1:C:268:ILE:O	1:C:269:ARG:HB3	2.05	0.56
1:C:317:LEU:CD1	1:C:401:LEU:CG	2.84	0.56
1:C:560:LYS:CE	1:C:609:HIS:ND1	2.69	0.56
1:D:10:ARG:CG	1:D:56:SER:HB2	2.36	0.56
1:D:147:ALA:CB	1:D:628:ILE:HA	2.36	0.56
2:G:192:LYS:O	2:G:192:LYS:HE3	2.06	0.56
1:A:217:THR:HB	1:A:218:PRO:HD2	1.88	0.56
1:B:114:LYS:CE	1:B:166:TYR:HE2	1.91	0.56
1:B:316:LEU:O	1:B:319:LEU:HG	2.06	0.56
1:C:22:ILE:HD11	3:C:801:ATP:N3	2.21	0.56
1:C:254:ILE:CG2	1:C:256:ILE:HD11	2.36	0.56
1:D:228:ILE:HG21	1:D:240:THR:HG23	1.87	0.56
2:E:96:LEU:HA	2:E:99:ILE:CD1	2.36	0.56
2:F:111:TRP:CZ2	2:F:204:GLU:OE2	2.59	0.56
2:F:193:LEU:O	2:F:197:LEU:HG	2.05	0.56
2:G:230:ILE:O	2:G:234:ILE:HG12	2.06	0.56
2:G:334:TRP:O	2:G:336:ASN:N	2.38	0.56
1:A:538:ASN:ND2	1:A:593:GLU:HB2	2.20	0.56
1:A:618:ALA:O	1:A:619:LEU:HD23	2.06	0.56
1:B:109:MET:CE	1:B:166:TYR:O	2.54	0.56
1:C:247:TYR:CE1	1:C:499:PRO:HD2	2.41	0.56
2:F:273:TYR:O	2:F:277:VAL:HG23	2.05	0.56
2:G:6:SER:OG	2:G:24:ASN:HB3	2.06	0.56
2:G:125:ILE:O	2:G:129:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:132:ASP:OD2	2:H:135:VAL:HG13	2.06	0.56
1:B:222:PHE:CD2	1:B:492:LEU:CG	2.89	0.55
1:D:105:HIS:NE2	1:D:109:MET:HE3	2.21	0.55
1:D:115:TYR:CE1	1:D:216:ARG:HD2	2.41	0.55
1:D:417:VAL:HG23	1:D:418:ASP:N	2.21	0.55
2:E:15:GLU:OE1	2:E:20:GLY:HA3	2.06	0.55
2:F:19:PHE:CE2	2:F:190:LYS:HG2	2.41	0.55
2:F:111:TRP:O	2:F:111:TRP:HD1	1.88	0.55
2:F:197:LEU:HD13	2:F:249:LEU:HG	1.88	0.55
2:F:221:ARG:HH11	2:F:296:MET:HE3	1.70	0.55
2:H:273:TYR:O	2:H:277:VAL:HG23	2.06	0.55
1:A:228:ILE:N	1:A:435:GLN:HE22	2.04	0.55
1:A:708:LYS:O	1:A:709:VAL:C	2.45	0.55
1:C:62:ILE:HD12	1:C:84:LEU:HD22	1.87	0.55
1:D:157:VAL:C	1:D:166:TYR:HB2	2.30	0.55
1:D:217:THR:HB	1:D:218:PRO:HD2	1.87	0.55
2:E:111:TRP:O	2:E:111:TRP:HD1	1.89	0.55
2:G:329:SER:O	2:G:330:ASN:C	2.48	0.55
2:H:15:GLU:OE1	2:H:20:GLY:HA3	2.05	0.55
1:A:641:TYR:CE2	1:A:668:LEU:HD11	2.42	0.55
1:C:17:ILE:HA	3:C:801:ATP:N1	2.22	0.55
1:D:86:ILE:O	1:D:90:ARG:HG3	2.06	0.55
1:D:172:LEU:HD13	1:D:173:TYR:N	2.21	0.55
2:E:72:ILE:HG23	2:E:290:LEU:HD23	1.89	0.55
2:E:221:ARG:NH1	2:E:296:MET:HE3	2.22	0.55
1:A:227:LEU:CA	1:A:435:GLN:HE22	2.19	0.55
1:A:669:LEU:HD11	1:A:698:ASN:ND2	2.21	0.55
1:B:172:LEU:HD23	1:B:216:ARG:CZ	2.36	0.55
1:B:215:VAL:O	1:B:216:ARG:CG	2.54	0.55
1:A:224:SER:C	1:A:225:CYS:SG	2.89	0.55
1:A:227:LEU:HD23	1:A:435:GLN:CG	2.36	0.55
1:B:6:LEU:HD22	1:B:14:THR:HG22	1.88	0.55
1:B:647:SER:OG	1:B:652:LEU:HD11	2.05	0.55
1:D:232:ASP:CG	1:D:262:ARG:HE	2.13	0.55
1:D:303:THR:OG1	1:D:438:LEU:HA	2.07	0.55
1:D:420:CYS:O	1:D:424:SER:CB	2.53	0.55
1:D:668:LEU:HB2	1:D:671:GLU:HG3	1.89	0.55
2:G:62:TYR:HB2	2:G:224:MET:HE1	1.89	0.55
2:G:339:LEU:O	2:G:340:VAL:HG12	2.06	0.55
2:H:73:PHE:HB2	2:H:218:PHE:CE2	2.41	0.55
2:H:335:ILE:O	2:H:339:LEU:CD1	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:CE2	1:A:168:SER:HB2	2.41	0.55
1:A:224:SER:C	1:A:225:CYS:HG	2.15	0.55
1:B:94:TYR:CE2	1:B:168:SER:HB3	2.42	0.55
1:C:538:ASN:ND2	1:C:593:GLU:HB2	2.22	0.55
1:D:53:ILE:O	1:D:58:ILE:HD11	2.07	0.55
2:E:192:LYS:O	2:E:192:LYS:HE3	2.06	0.55
2:F:340:VAL:HG12	2:F:341:SER:CB	2.35	0.55
1:A:172:LEU:HD13	1:A:173:TYR:N	2.21	0.55
1:B:244:ILE:O	1:B:248:VAL:HG22	2.07	0.55
1:B:474:ASN:HD21	1:B:476:ASP:HB2	1.69	0.55
1:C:317:LEU:CD1	1:C:401:LEU:HG	2.33	0.55
1:C:378:LEU:HB3	1:C:382:TYR:HE2	1.71	0.55
1:C:513:LEU:HD21	1:C:613:ASN:ND2	2.21	0.55
1:D:182:SER:O	1:D:189:ARG:CZ	2.55	0.55
1:D:442:ILE:HG23	1:D:444:LEU:HG	1.88	0.55
2:E:177:VAL:HG21	2:E:182:VAL:CG2	2.36	0.55
2:G:96:LEU:HA	2:G:99:ILE:CD1	2.36	0.55
2:H:83:LEU:HD22	2:H:203:LEU:HG	1.87	0.55
1:A:4:ASN:OD1	1:C:297:VAL:CG1	2.54	0.55
1:B:168:SER:OG	1:B:171:PHE:CD2	2.55	0.55
1:B:686:GLN:HA	1:B:689:ILE:CG2	2.32	0.55
1:C:93:ALA:HB2	1:C:165:ILE:O	2.07	0.55
1:D:339:ILE:HD11	1:D:402:MET:HE1	1.89	0.55
1:D:516:GLY:HA2	1:D:618:ALA:O	2.07	0.55
2:F:15:GLU:OE1	2:F:20:GLY:HA3	2.06	0.55
2:F:16:PRO:HG2	2:F:18:PHE:O	2.07	0.55
2:G:95:LEU:O	2:G:99:ILE:HG13	2.06	0.55
2:G:178:ASN:C	2:G:180:LYS:H	2.15	0.55
1:A:420:CYS:O	1:A:424:SER:CB	2.53	0.55
1:D:74:ALA:HB1	1:D:77:TYR:CD2	2.42	0.55
2:G:16:PRO:HG2	2:G:18:PHE:O	2.07	0.55
2:G:96:LEU:HA	2:G:99:ILE:HD12	1.89	0.55
2:G:197:LEU:HD13	2:G:249:LEU:HG	1.88	0.55
1:A:286:GLN:HB2	1:A:333:MET:HE2	1.88	0.55
1:A:647:SER:O	1:A:648:LYS:C	2.48	0.55
1:B:115:TYR:CD1	1:B:216:ARG:HG3	2.42	0.55
1:B:174:ILE:HG23	1:B:175:LEU:N	2.22	0.55
1:D:223:SER:OG	1:D:461:LEU:HD11	2.07	0.55
1:D:619:LEU:HD12	1:D:693:ILE:CG2	2.37	0.55
2:E:197:LEU:HD13	2:E:249:LEU:HG	1.87	0.55
2:E:334:TRP:O	2:E:336:ASN:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:72:ILE:HG23	2:G:290:LEU:HD23	1.88	0.55
2:G:221:ARG:NH1	2:G:296:MET:HE3	2.21	0.55
1:C:29:ALA:HB1	1:C:80:LEU:HD12	1.89	0.54
1:C:86:ILE:HG21	1:C:140:ASP:HB3	1.89	0.54
1:C:115:TYR:CE1	1:C:216:ARG:CG	2.90	0.54
1:C:441:GLU:CD	1:C:442:ILE:HG12	2.32	0.54
1:C:513:LEU:HD23	1:C:613:ASN:ND2	2.23	0.54
1:D:22:ILE:HD11	3:D:801:ATP:N3	2.21	0.54
1:D:29:ALA:HB1	1:D:80:LEU:HD12	1.89	0.54
1:D:158:GLN:HB3	1:D:165:ILE:HD12	1.87	0.54
1:D:293:SER:HB2	1:D:298:ARG:O	2.06	0.54
1:D:465:SER:O	1:D:515:ILE:HA	2.07	0.54
1:D:568:PHE:CD2	1:D:574:ALA:HB2	2.41	0.54
2:E:122:TYR:HA	2:E:125:ILE:HD12	1.89	0.54
2:G:125:ILE:HD13	2:G:227:ASN:ND2	2.22	0.54
1:B:440:LEU:HB2	1:B:730:TYR:CE1	2.42	0.54
1:B:569:ASN:ND2	1:B:570:GLU:H	2.00	0.54
1:C:332:HIS:O	1:C:333:MET:HG2	2.07	0.54
1:C:714:LEU:CD2	1:C:732:GLN:HE22	2.19	0.54
1:D:412:ILE:HD12	1:D:412:ILE:N	2.23	0.54
2:E:62:TYR:HB2	2:E:224:MET:HE1	1.88	0.54
2:F:328:ARG:HB3	2:F:328:ARG:NH1	2.22	0.54
1:A:696:ASN:HB2	1:A:731:TYR:O	2.08	0.54
1:B:230:CYS:SG	1:B:237:ILE:HA	2.47	0.54
1:B:529:LYS:HB3	1:B:536:ALA:HB2	1.89	0.54
1:C:217:THR:HB	1:C:218:PRO:HD2	1.88	0.54
1:C:369:PHE:CE2	1:C:434:ARG:HB3	2.43	0.54
1:C:597:TYR:O	1:C:598:ASP:C	2.47	0.54
1:D:520:PHE:CE2	1:D:524:LEU:HD11	2.42	0.54
2:E:73:PHE:HB2	2:E:218:PHE:CE2	2.42	0.54
2:E:205:ALA:O	2:E:209:TYR:HB2	2.07	0.54
2:E:207:ARG:HH22	2:E:282:GLN:NE2	2.05	0.54
1:A:44:ARG:HA	1:A:44:ARG:HE	1.73	0.54
1:A:189:ARG:O	1:A:193:VAL:HG23	2.06	0.54
1:D:520:PHE:HB3	1:D:635:ILE:HA	1.88	0.54
2:F:322:ASP:O	2:F:324:PRO:CD	2.47	0.54
2:G:179:GLY:C	2:G:180:LYS:CG	2.81	0.54
2:H:65:LEU:HD21	2:H:223:LEU:CD1	2.30	0.54
1:A:55:THR:HA	1:A:58:ILE:HD12	1.88	0.54
1:A:212:MET:O	1:A:216:ARG:NH1	2.40	0.54
1:A:301:ALA:HB3	1:A:438:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:GLN:HE21	2:H:333:PRO:CG	2.16	0.54
1:B:89:LEU:HD21	1:B:152:GLU:HG3	1.88	0.54
1:B:286:GLN:O	1:B:289:VAL:HG22	2.07	0.54
1:C:278:CYS:O	1:C:282:TYR:HD1	1.90	0.54
1:C:464:LEU:HD12	1:C:620:MET:SD	2.47	0.54
1:D:538:ASN:ND2	1:D:593:GLU:HB2	2.22	0.54
1:D:641:TYR:CE2	1:D:668:LEU:HD11	2.42	0.54
1:D:658:ASP:HB3	1:D:662:LEU:HD12	1.90	0.54
2:E:84:ASP:HA	2:E:87:GLN:HB2	1.90	0.54
1:A:279:ILE:CD1	1:A:319:LEU:HD21	2.35	0.54
1:B:25:VAL:HG21	3:B:801:ATP:O2'	2.08	0.54
1:B:217:THR:HB	1:B:218:PRO:HD2	1.88	0.54
1:B:403:MET:HG2	1:B:711:MET:HE1	1.90	0.54
1:C:564:ALA:HA	1:C:611:LEU:O	2.07	0.54
2:G:24:ASN:ND2	2:G:25:VAL:HG12	2.22	0.54
1:A:151:LEU:O	1:A:156:LEU:HG	2.07	0.54
1:B:261:ILE:HG21	1:B:278:CYS:HA	1.89	0.54
1:B:576:GLY:HA3	1:B:607:LYS:HE2	1.89	0.54
1:B:641:TYR:CE2	1:B:668:LEU:HD11	2.43	0.54
1:C:25:VAL:HG21	3:C:801:ATP:O3'	2.08	0.54
1:C:686:GLN:HA	1:C:689:ILE:HG12	1.90	0.54
1:D:689:ILE:CG2	1:D:691:GLN:O	2.55	0.54
2:H:16:PRO:HG2	2:H:18:PHE:O	2.07	0.54
1:A:37:SER:HB3	1:A:40:GLN:HB2	1.89	0.54
1:A:596:HIS:HB3	1:A:597:TYR:CE2	2.42	0.54
1:B:658:ASP:O	1:B:662:LEU:HB2	2.08	0.54
1:D:172:LEU:CD2	1:D:216:ARG:HH22	2.08	0.54
1:D:174:ILE:HG23	1:D:175:LEU:N	2.22	0.54
1:D:568:PHE:CE2	1:D:574:ALA:CB	2.91	0.54
2:G:122:TYR:HA	2:G:125:ILE:HD12	1.88	0.54
2:H:12:GLN:O	2:H:14:LYS:N	2.41	0.54
1:A:174:ILE:HG23	1:A:175:LEU:N	2.21	0.54
1:A:226:VAL:HB	1:A:459:ILE:HG22	1.90	0.54
1:A:509:GLY:O	1:A:566:PRO:HB2	2.07	0.54
1:A:562:GLN:CG	1:A:612:ARG:CZ	2.85	0.54
1:B:36:VAL:HA	1:B:77:TYR:CE2	2.43	0.54
1:B:55:THR:HA	1:B:58:ILE:HD12	1.90	0.54
1:B:302:ALA:O	1:B:333:MET:HB3	2.08	0.54
1:B:618:ALA:O	1:B:619:LEU:HD23	2.08	0.54
1:D:5:LEU:CB	1:D:17:ILE:HG12	2.37	0.54
1:D:719:LEU:HD12	2:G:370:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:CD1	1:A:53:ILE:HD13	2.44	0.54
1:A:105:HIS:NE2	1:A:109:MET:HE3	2.23	0.54
1:A:230:CYS:SG	1:A:237:ILE:HA	2.49	0.54
1:A:693:ILE:N	1:A:693:ILE:HD12	2.23	0.54
1:B:22:ILE:HD12	1:B:22:ILE:N	2.23	0.54
1:B:569:ASN:HD22	1:B:569:ASN:N	2.06	0.54
1:B:702:SER:HB3	1:B:735:ARG:CD	2.38	0.54
1:C:21:LYS:O	1:C:25:VAL:HG23	2.08	0.54
1:D:441:GLU:CD	1:D:442:ILE:HG12	2.33	0.54
1:D:516:GLY:HA2	1:D:619:LEU:HD23	1.90	0.54
1:D:621:PRO:HD3	1:D:694:SER:HB2	1.89	0.54
2:H:125:ILE:O	2:H:129:ILE:HG12	2.08	0.54
2:H:125:ILE:HG21	2:H:227:ASN:HD22	1.73	0.54
2:H:192:LYS:HE3	2:H:192:LYS:O	2.08	0.54
1:A:340:ASN:HB3	1:A:368:PHE:CE1	2.42	0.53
1:A:413:TYR:OH	1:A:731:TYR:CE2	2.39	0.53
1:A:435:GLN:HG2	1:A:436:SER:N	2.19	0.53
1:D:22:ILE:HD12	1:D:22:ILE:N	2.24	0.53
2:E:329:SER:O	2:E:330:ASN:C	2.48	0.53
2:F:62:TYR:HB2	2:F:224:MET:HE1	1.90	0.53
2:G:73:PHE:HB2	2:G:218:PHE:CE2	2.43	0.53
1:B:4:ASN:ND2	1:B:5:LEU:HD22	2.24	0.53
1:B:538:ASN:ND2	1:B:593:GLU:HB2	2.23	0.53
1:B:686:GLN:HE21	1:B:727:LYS:HE3	1.71	0.53
1:C:617:SER:HB3	1:C:689:ILE:HA	1.89	0.53
1:D:509:GLY:O	1:D:566:PRO:HD2	2.07	0.53
1:D:711:MET:HB2	2:G:363:SER:CB	2.37	0.53
2:F:12:GLN:O	2:F:101:ILE:HG22	2.08	0.53
2:F:192:LYS:HE3	2:F:192:LYS:O	2.07	0.53
2:H:330:ASN:ND2	2:H:332:ILE:O	2.42	0.53
1:A:74:ALA:HB1	1:A:77:TYR:HD2	1.73	0.53
1:B:364:LEU:O	1:B:364:LEU:HD13	2.07	0.53
1:B:689:ILE:HG23	1:B:689:ILE:O	2.08	0.53
1:C:62:ILE:HG13	1:C:63:ILE:N	2.23	0.53
1:D:53:ILE:O	1:D:53:ILE:CG1	2.55	0.53
1:D:180:LEU:HD23	1:D:488:ALA:HB1	1.90	0.53
2:E:96:LEU:HD12	2:E:108:VAL:HG11	1.91	0.53
2:E:122:TYR:O	2:E:126:ILE:HG13	2.09	0.53
2:E:253:ARG:HG3	2:E:265:ALA:HB1	1.91	0.53
2:F:173:GLY:O	2:F:183:THR:HG23	2.08	0.53
2:G:34:ASP:O	2:G:38:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ALA:HB1	1:A:77:TYR:CD2	2.44	0.53
1:A:412:ILE:N	1:A:412:ILE:HD12	2.24	0.53
1:B:215:VAL:O	1:B:216:ARG:CB	2.56	0.53
1:B:365:TYR:O	1:B:368:PHE:N	2.41	0.53
1:C:412:ILE:N	1:C:412:ILE:HD12	2.23	0.53
1:C:712:GLN:HG3	2:E:370:LEU:HD21	1.89	0.53
1:D:147:ALA:HB1	1:D:628:ILE:HA	1.91	0.53
1:D:240:THR:HG22	1:D:244:ILE:HD11	1.90	0.53
2:F:36:PHE:HE1	2:F:248:MET:HE2	1.72	0.53
2:F:95:LEU:O	2:F:99:ILE:HG13	2.08	0.53
2:F:96:LEU:HA	2:F:99:ILE:CD1	2.39	0.53
2:F:132:ASP:OD2	2:F:135:VAL:HG13	2.08	0.53
2:H:125:ILE:HD13	2:H:227:ASN:ND2	2.23	0.53
1:A:18:ASN:O	1:A:19:LEU:C	2.51	0.53
1:B:211:ILE:HA	1:B:222:PHE:CE1	2.43	0.53
1:B:283:LYS:HG2	1:B:330:VAL:CG2	2.38	0.53
1:B:290:LYS:NZ	1:B:299:GLY:O	2.37	0.53
1:B:378:LEU:HB3	1:B:382:TYR:HE2	1.73	0.53
1:B:464:LEU:HB2	1:B:514:GLY:O	2.08	0.53
1:B:520:PHE:CE2	1:B:524:LEU:HD11	2.44	0.53
1:D:154:LYS:HE2	1:D:624:THR:HG21	1.89	0.53
1:D:517:VAL:HG12	1:D:619:LEU:CD2	2.38	0.53
2:E:125:ILE:O	2:E:129:ILE:HG12	2.08	0.53
2:E:195:LEU:HD11	2:E:275:LEU:HD11	1.90	0.53
2:E:273:TYR:HB2	2:E:321:LEU:HD22	1.90	0.53
2:E:273:TYR:CE2	2:E:324:PRO:HG3	2.43	0.53
2:F:149:ARG:NH1	2:F:286:TRP:HB2	2.14	0.53
2:F:309:GLU:HA	2:F:325:PHE:CD2	2.44	0.53
2:G:125:ILE:HG21	2:G:227:ASN:HD22	1.73	0.53
1:A:441:GLU:HG2	1:A:620:MET:CB	2.39	0.53
1:A:447:LYS:HB2	1:A:458:GLU:N	2.20	0.53
1:B:176:VAL:HG13	1:B:215:VAL:HG21	1.90	0.53
1:C:388:ILE:O	1:C:389:ARG:C	2.51	0.53
2:F:99:ILE:HD13	2:F:105:GLU:HA	1.90	0.53
2:F:177:VAL:HB	2:F:180:LYS:O	2.07	0.53
2:H:92:ASN:O	2:H:96:LEU:HB2	2.07	0.53
1:A:378:LEU:HB3	1:A:382:TYR:HE2	1.74	0.53
1:A:542:LYS:HG3	1:A:596:HIS:CD2	2.43	0.53
1:B:74:ALA:HB1	1:B:77:TYR:HD2	1.73	0.53
1:C:10:ARG:HG3	1:C:56:SER:HB2	1.91	0.53
1:C:237:ILE:HD13	1:C:281:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:THR:HG22	1:C:244:ILE:HD11	1.91	0.53
1:C:286:GLN:OE1	1:C:332:HIS:HB2	2.09	0.53
1:C:339:ILE:HD11	1:C:402:MET:HE1	1.90	0.53
1:D:43:LEU:CD1	2:G:334:TRP:CE2	2.91	0.53
1:D:47:ILE:C	1:D:47:ILE:HD13	2.33	0.53
1:D:249:SER:HB2	1:D:292:CYS:SG	2.49	0.53
2:E:230:ILE:O	2:E:234:ILE:HG12	2.07	0.53
2:E:310:TYR:CE2	2:E:330:ASN:HB2	2.43	0.53
2:E:332:ILE:N	2:E:333:PRO:HD3	2.24	0.53
2:G:277:VAL:HG22	2:G:324:PRO:CG	2.39	0.53
1:A:625:SER:C	1:A:628:ILE:HG22	2.34	0.53
1:B:86:ILE:O	1:B:90:ARG:HG3	2.09	0.53
1:B:711:MET:CB	2:H:364:GLU:H	2.22	0.53
1:C:226:VAL:CG1	1:C:461:LEU:CD2	2.84	0.53
1:C:301:ALA:C	1:C:438:LEU:CD1	2.78	0.53
1:D:519:ASN:HA	1:D:632:THR:OG1	2.09	0.53
1:D:711:MET:N	2:G:363:SER:HB2	2.17	0.53
2:E:95:LEU:O	2:E:99:ILE:HG13	2.08	0.53
2:H:122:TYR:HA	2:H:125:ILE:HD12	1.90	0.53
2:H:130:VAL:HG12	2:H:131:ASN:N	2.24	0.53
1:A:62:ILE:HG13	1:A:63:ILE:N	2.24	0.53
1:A:425:PRO:HG2	1:A:690:ASP:CB	2.33	0.53
1:B:339:ILE:HD11	1:B:402:MET:HE1	1.91	0.53
1:B:618:ALA:N	1:B:689:ILE:CD1	2.52	0.53
1:B:668:LEU:HB2	1:B:671:GLU:HG3	1.90	0.53
1:B:712:GLN:HE21	2:H:369:ASP:HB3	1.72	0.53
1:C:175:LEU:CD2	1:C:216:ARG:CD	2.75	0.53
1:C:449:LEU:HD21	1:C:502:ALA:HB2	1.91	0.53
1:D:20:ASP:HA	1:D:23:HIS:CD2	2.44	0.53
2:E:99:ILE:HD13	2:E:105:GLU:HA	1.91	0.53
2:G:328:ARG:NH1	2:G:328:ARG:HB3	2.23	0.53
1:A:96:GLN:NE2	1:D:386:ASP:OD2	2.42	0.53
1:A:242:SER:HA	1:B:238:ASN:OD1	2.08	0.53
1:B:19:LEU:CD2	2:H:295:SER:O	2.57	0.53
1:B:172:LEU:HD13	1:B:173:TYR:N	2.23	0.53
1:B:269:ARG:HG3	1:B:269:ARG:O	2.09	0.53
1:B:647:SER:HB2	1:B:652:LEU:HG	1.89	0.53
1:B:706:SER:O	1:B:708:LYS:HG3	2.09	0.53
1:C:222:PHE:CE2	1:C:492:LEU:CD1	2.90	0.53
1:D:21:LYS:O	1:D:25:VAL:HG23	2.08	0.53
1:D:157:VAL:O	1:D:166:TYR:CB	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:GLN:HB2	1:D:333:MET:HE3	1.91	0.53
1:D:388:ILE:O	1:D:389:ARG:C	2.50	0.53
2:F:96:LEU:HA	2:F:99:ILE:HD12	1.89	0.53
2:F:125:ILE:HD13	2:F:227:ASN:ND2	2.23	0.53
2:F:207:ARG:HH22	2:F:282:GLN:NE2	2.07	0.53
1:A:207:LEU:HB3	1:A:208:PRO:HD2	1.91	0.52
1:A:442:ILE:HG23	1:A:444:LEU:HG	1.91	0.52
1:B:6:LEU:HD12	1:B:51:ASP:OD1	2.08	0.52
1:B:94:TYR:HE2	1:B:168:SER:HB3	1.73	0.52
1:C:361:VAL:CG1	1:C:364:LEU:CB	2.81	0.52
1:C:442:ILE:HG23	1:C:444:LEU:HG	1.92	0.52
1:C:696:ASN:HD22	1:C:696:ASN:N	2.00	0.52
1:D:230:CYS:SG	1:D:237:ILE:HA	2.49	0.52
1:D:378:LEU:HB3	1:D:382:TYR:HE2	1.73	0.52
1:D:403:MET:HE1	1:D:718:LEU:HD22	1.91	0.52
2:F:34:ASP:O	2:F:38:LYS:HG3	2.09	0.52
2:H:253:ARG:HG3	2:H:265:ALA:HB1	1.91	0.52
1:A:322:ASN:HA	1:A:331:ARG:NE	2.23	0.52
1:B:74:ALA:HB1	1:B:77:TYR:CD2	2.43	0.52
1:C:47:ILE:HD13	1:C:47:ILE:C	2.34	0.52
1:C:463:THR:HG21	1:C:492:LEU:HD23	1.91	0.52
1:D:110:VAL:HG21	1:D:120:LEU:HD11	1.91	0.52
1:D:437:ASN:ND2	1:D:439:CYS:HB2	2.24	0.52
1:D:440:LEU:HD12	1:D:728:THR:CB	2.38	0.52
2:G:295:SER:OG	2:G:300:ASN:HB3	2.09	0.52
1:A:19:LEU:HD12	1:A:19:LEU:N	2.20	0.52
1:A:668:LEU:O	1:A:671:GLU:N	2.42	0.52
1:B:50:TYR:CE2	1:B:53:ILE:HD12	2.45	0.52
1:C:114:LYS:N	1:C:114:LYS:CD	2.73	0.52
1:D:149:LYS:HG3	1:D:652:LEU:HD21	1.91	0.52
1:D:215:VAL:O	1:D:216:ARG:CB	2.57	0.52
1:D:519:ASN:HD21	1:D:657:PRO:HG2	1.74	0.52
1:D:668:LEU:O	1:D:671:GLU:N	2.41	0.52
2:F:239:ALA:HA	2:F:242:LEU:HD21	1.92	0.52
2:G:130:VAL:HG12	2:G:131:ASN:N	2.25	0.52
2:H:295:SER:OG	2:H:300:ASN:HB3	2.09	0.52
1:A:22:ILE:HD11	3:A:801:ATP:C2	2.44	0.52
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.92	0.52
1:B:215:VAL:O	1:B:216:ARG:NH1	2.41	0.52
1:B:696:ASN:HD22	1:B:696:ASN:N	2.00	0.52
1:B:719:LEU:HD22	2:H:375:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ALA:HB1	1:C:77:TYR:HD2	1.74	0.52
1:D:301:ALA:O	1:D:438:LEU:CD1	2.44	0.52
2:E:5:PHE:CE2	2:E:7:GLN:NE2	2.77	0.52
2:E:16:PRO:HG2	2:E:18:PHE:O	2.09	0.52
2:F:84:ASP:HA	2:F:87:GLN:HB2	1.91	0.52
2:F:209:TYR:HA	2:F:212:PHE:CD2	2.45	0.52
2:G:332:ILE:N	2:G:333:PRO:HD3	2.25	0.52
2:H:6:SER:CB	2:H:21:GLN:NE2	2.71	0.52
2:H:34:ASP:O	2:H:38:LYS:HG3	2.09	0.52
1:A:286:GLN:O	1:A:289:VAL:HG22	2.08	0.52
1:A:449:LEU:HD21	1:A:502:ALA:HB2	1.91	0.52
1:B:70:ILE:O	1:B:653:ARG:HD2	2.10	0.52
1:B:592:ASN:H	1:B:592:ASN:ND2	2.07	0.52
1:C:6:LEU:CD1	1:C:51:ASP:OD2	2.56	0.52
1:D:592:ASN:ND2	1:D:592:ASN:H	2.08	0.52
2:F:273:TYR:HB2	2:F:321:LEU:HD22	1.90	0.52
2:H:169:LEU:O	2:H:170:LEU:HD23	2.09	0.52
2:H:195:LEU:HD11	2:H:275:LEU:HD11	1.91	0.52
2:H:336:ASN:O	2:H:339:LEU:HD22	2.10	0.52
1:A:62:ILE:HD12	1:A:84:LEU:HD22	1.91	0.52
1:A:621:PRO:HG3	1:A:730:TYR:CE2	2.45	0.52
1:B:21:LYS:O	1:B:25:VAL:HG23	2.10	0.52
1:B:150:GLN:HE22	1:B:645:LYS:NZ	2.08	0.52
1:B:619:LEU:HG	1:B:693:ILE:HG23	1.91	0.52
1:B:621:PRO:HD3	1:B:694:SER:OG	2.08	0.52
1:C:269:ARG:HG3	1:C:269:ARG:O	2.09	0.52
1:C:444:LEU:HD21	1:C:691:GLN:OE1	2.09	0.52
1:D:103:TYR:O	1:D:107:VAL:HG23	2.10	0.52
1:D:145:TYR:HE2	1:D:652:LEU:HD23	1.75	0.52
2:E:96:LEU:HA	2:E:99:ILE:HD12	1.91	0.52
2:F:99:ILE:CD1	2:F:108:VAL:HG21	2.40	0.52
2:F:122:TYR:HA	2:F:125:ILE:HD12	1.91	0.52
2:F:195:LEU:HD11	2:F:275:LEU:HD11	1.92	0.52
1:A:227:LEU:HG	1:A:435:GLN:HE21	1.73	0.52
1:A:269:ARG:O	1:A:269:ARG:HG3	2.09	0.52
1:A:369:PHE:CE2	1:A:434:ARG:CB	2.93	0.52
1:B:10:ARG:N	1:B:55:THR:HG22	2.25	0.52
1:B:62:ILE:HG13	1:B:63:ILE:N	2.24	0.52
1:B:519:ASN:ND2	1:B:632:THR:H	2.08	0.52
1:C:110:VAL:HG21	1:C:120:LEU:HD11	1.92	0.52
1:D:189:ARG:O	1:D:193:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:TYR:HB3	2:F:184:VAL:HG21	1.90	0.52
2:F:238:GLU:O	2:F:242:LEU:HD23	2.10	0.52
2:F:310:TYR:CE2	2:F:330:ASN:HB2	2.44	0.52
2:G:339:LEU:O	2:G:339:LEU:HD13	2.09	0.52
2:H:79:TYR:HB2	2:H:286:TRP:CH2	2.45	0.52
2:H:339:LEU:HD22	2:H:340:VAL:HG23	1.92	0.52
1:A:36:VAL:HA	1:A:77:TYR:CE2	2.45	0.52
1:A:37:SER:HB2	2:F:333:PRO:HD3	1.92	0.52
1:A:238:ASN:OD1	1:B:242:SER:HA	2.10	0.52
1:A:278:CYS:O	1:A:282:TYR:HD1	1.93	0.52
1:A:330:VAL:HB	1:A:335:TYR:OH	2.10	0.52
1:A:696:ASN:HB3	1:A:730:TYR:HB3	1.92	0.52
1:B:180:LEU:HD23	1:B:488:ALA:HB1	1.92	0.52
1:C:520:PHE:HB3	1:C:635:ILE:HA	1.91	0.52
1:D:220:ARG:O	1:D:496:GLN:CA	2.48	0.52
1:D:225:CYS:H	1:D:462:CYS:HB3	1.75	0.52
2:E:191:LYS:HG2	2:E:264:ILE:CG2	2.40	0.52
2:F:125:ILE:HG21	2:F:227:ASN:HD22	1.75	0.52
1:A:53:ILE:O	1:A:53:ILE:CG1	2.55	0.52
1:A:237:ILE:HD13	1:A:281:PHE:CE2	2.44	0.52
1:B:215:VAL:O	1:B:216:ARG:HG2	2.09	0.52
1:C:26:LEU:HB2	1:C:38:ILE:HG23	1.91	0.52
1:C:223:SER:HB2	1:C:461:LEU:HD11	1.92	0.52
1:D:338:GLN:HG2	1:D:415:GLN:NE2	2.25	0.52
1:D:595:LEU:HD22	1:D:599:TRP:HE1	1.75	0.52
2:E:339:LEU:O	2:E:340:VAL:CB	2.57	0.52
1:A:10:ARG:N	1:A:55:THR:HG22	2.25	0.52
1:A:595:LEU:HD22	1:A:599:TRP:NE1	2.25	0.52
1:B:406:ARG:NH1	1:B:732:GLN:HG3	2.25	0.52
1:B:442:ILE:HG23	1:B:444:LEU:HG	1.91	0.52
1:B:458:GLU:OE2	1:B:510:ARG:NH1	2.43	0.52
1:B:509:GLY:O	1:B:566:PRO:HB2	2.10	0.52
1:B:595:LEU:HD22	1:B:599:TRP:HE1	1.75	0.52
1:C:313:VAL:O	1:C:317:LEU:CD2	2.56	0.52
1:C:316:LEU:O	1:C:319:LEU:HD12	2.09	0.52
1:C:444:LEU:HD11	1:C:462:CYS:SG	2.49	0.52
1:C:565:CYS:SG	1:C:568:PHE:HB2	2.50	0.52
1:C:569:ASN:HD22	1:C:569:ASN:N	2.08	0.52
1:D:25:VAL:HG21	3:D:801:ATP:C3'	2.40	0.52
1:D:89:LEU:CD2	1:D:152:GLU:CG	2.38	0.52
1:D:248:VAL:HG11	1:D:289:VAL:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:SER:OG	2:E:24:ASN:HB3	2.09	0.52
2:E:92:ASN:CA	2:E:96:LEU:HD13	2.35	0.52
2:G:89:ARG:HG2	2:G:90:SER:N	2.25	0.52
2:H:284:LYS:HE3	2:H:325:PHE:CZ	2.46	0.52
1:A:20:ASP:HA	1:A:23:HIS:CD2	2.45	0.51
1:A:261:ILE:HD12	1:A:281:PHE:HD2	1.75	0.51
1:A:512:THR:HG22	1:A:614:SER:HB2	1.92	0.51
1:A:569:ASN:HD22	1:A:569:ASN:N	2.08	0.51
1:B:6:LEU:HD22	1:B:14:THR:CG2	2.39	0.51
1:B:374:GLU:HG3	1:B:378:LEU:HD11	1.92	0.51
1:C:44:ARG:HG3	1:C:69:LEU:HD11	1.91	0.51
1:C:74:ALA:HB1	1:C:77:TYR:CD2	2.44	0.51
1:C:103:TYR:O	1:C:107:VAL:HG23	2.10	0.51
1:D:145:TYR:CE2	1:D:652:LEU:HD23	2.45	0.51
1:D:465:SER:HB2	1:D:489:LEU:HD11	1.92	0.51
1:D:617:SER:O	1:D:691:GLN:HG3	2.09	0.51
2:E:130:VAL:HG12	2:E:131:ASN:N	2.25	0.51
2:H:5:PHE:HD1	2:H:24:ASN:O	1.91	0.51
1:A:47:ILE:HD13	1:A:47:ILE:C	2.34	0.51
1:A:338:GLN:HG2	1:A:415:GLN:NE2	2.24	0.51
1:A:562:GLN:HG2	1:A:612:ARG:NE	2.26	0.51
1:B:615:THR:HB	1:B:691:GLN:NE2	2.25	0.51
1:C:22:ILE:HD12	1:C:22:ILE:N	2.26	0.51
1:C:36:VAL:HA	1:C:77:TYR:CE2	2.45	0.51
1:C:519:ASN:ND2	1:C:632:THR:H	2.08	0.51
1:D:225:CYS:O	1:D:462:CYS:CB	2.59	0.51
1:D:309:TRP:CZ2	1:D:364:LEU:HD12	2.45	0.51
2:E:171:GLY:O	2:E:175:HIS:CE1	2.63	0.51
2:F:12:GLN:HE21	2:F:23:VAL:CG1	2.12	0.51
1:A:227:LEU:CA	1:A:435:GLN:NE2	2.73	0.51
1:A:475:LEU:CD1	1:A:542:LYS:HE2	2.39	0.51
1:A:655:VAL:HG12	1:A:656:VAL:O	2.10	0.51
1:B:110:VAL:HG21	1:B:120:LEU:HD11	1.91	0.51
1:B:228:ILE:C	1:B:435:GLN:HE22	2.18	0.51
1:C:282:TYR:CE2	1:C:304:LEU:HD22	2.44	0.51
1:C:459:ILE:HD11	1:C:502:ALA:HB3	1.92	0.51
1:C:568:PHE:CE2	1:C:574:ALA:CB	2.89	0.51
1:D:6:LEU:HD22	1:D:14:THR:HG22	1.91	0.51
1:D:36:VAL:HA	1:D:77:TYR:CE2	2.44	0.51
2:E:36:PHE:CE1	2:E:248:MET:HE2	2.44	0.51
1:B:20:ASP:HA	1:B:23:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:SER:O	1:B:145:TYR:C	2.52	0.51
1:B:282:TYR:CD2	1:B:304:LEU:HD22	2.37	0.51
1:C:86:ILE:O	1:C:90:ARG:HG3	2.11	0.51
1:C:517:VAL:HG12	1:C:619:LEU:CD2	2.39	0.51
1:D:167:GLU:CD	1:D:216:ARG:HH21	2.19	0.51
1:D:619:LEU:HD12	1:D:693:ILE:HG22	1.91	0.51
2:F:130:VAL:HG12	2:F:131:ASN:N	2.25	0.51
2:G:175:HIS:O	2:G:177:VAL:HG23	2.11	0.51
1:A:517:VAL:HG12	1:A:619:LEU:CD2	2.40	0.51
1:B:437:ASN:ND2	1:B:439:CYS:HB2	2.24	0.51
1:B:519:ASN:HD21	1:B:657:PRO:HG2	1.76	0.51
1:C:93:ALA:CB	1:C:165:ILE:O	2.59	0.51
1:C:286:GLN:HB2	1:C:333:MET:HE2	1.93	0.51
1:C:568:PHE:CD2	1:C:574:ALA:HB2	2.45	0.51
1:D:440:LEU:HB2	1:D:730:TYR:CE1	2.45	0.51
2:E:339:LEU:HD12	2:E:340:VAL:HG23	1.91	0.51
2:G:33:TYR:OH	2:G:257:ASP:HB2	2.11	0.51
2:G:253:ARG:HG3	2:G:265:ALA:HB1	1.93	0.51
2:H:62:TYR:HB2	2:H:224:MET:HE1	1.92	0.51
1:A:156:LEU:HB3	1:A:167:GLU:HG2	1.92	0.51
1:B:15:GLU:OE2	3:B:801:ATP:N6	2.41	0.51
1:B:103:TYR:O	1:B:107:VAL:HG23	2.10	0.51
1:B:262:ARG:HB2	1:B:359:SER:HB3	1.92	0.51
1:C:254:ILE:O	1:C:438:LEU:CG	2.59	0.51
1:D:217:THR:HB	1:D:218:PRO:CD	2.41	0.51
1:D:269:ARG:HG3	1:D:269:ARG:O	2.09	0.51
1:D:356:PHE:CE1	1:D:390:LYS:HB3	2.45	0.51
1:D:465:SER:HB2	1:D:489:LEU:HD12	1.92	0.51
2:E:12:GLN:O	2:E:14:LYS:N	2.44	0.51
2:G:221:ARG:HH11	2:G:296:MET:HE3	1.75	0.51
2:G:273:TYR:HB2	2:G:321:LEU:HD22	1.92	0.51
2:H:209:TYR:HA	2:H:212:PHE:CD2	2.45	0.51
2:H:273:TYR:HB2	2:H:321:LEU:HD22	1.92	0.51
1:B:263:ALA:HB3	1:B:357:SER:OG	2.11	0.51
1:B:388:ILE:O	1:B:389:ARG:C	2.51	0.51
1:C:50:TYR:CD2	1:C:53:ILE:HB	2.41	0.51
1:C:519:ASN:CG	1:C:631:ALA:HB1	2.35	0.51
1:C:569:ASN:ND2	1:C:569:ASN:N	2.57	0.51
1:D:8:THR:N	1:D:52:GLY:O	2.44	0.51
1:D:67:ALA:HA	1:D:70:ILE:HD11	1.92	0.51
1:D:234:LEU:O	1:D:237:ILE:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:ASN:ND2	1:D:632:THR:H	2.08	0.51
1:D:560:LYS:CE	1:D:609:HIS:CE1	2.92	0.51
2:E:209:TYR:HA	2:E:212:PHE:CD2	2.46	0.51
2:F:372:ASN:HD22	2:F:372:ASN:N	1.98	0.51
1:A:4:ASN:OD1	1:C:297:VAL:HG12	2.10	0.51
1:A:569:ASN:ND2	1:A:569:ASN:N	2.56	0.51
1:B:325:VAL:HG13	1:B:328:ASN:HB3	1.93	0.51
1:B:569:ASN:ND2	1:B:569:ASN:N	2.56	0.51
1:C:441:GLU:OE1	1:C:442:ILE:HG12	2.11	0.51
1:D:7:VAL:HG21	3:D:801:ATP:N1	2.26	0.51
1:D:62:ILE:HG13	1:D:63:ILE:N	2.23	0.51
1:D:282:TYR:HA	1:D:285:PHE:HD2	1.76	0.51
1:D:369:PHE:O	1:D:421:ASN:CG	2.54	0.51
1:D:487:ARG:HD3	1:D:558:LEU:HD22	1.92	0.51
2:E:33:TYR:OH	2:E:257:ASP:HB2	2.11	0.51
2:E:153:ILE:HD11	2:E:207:ARG:HE	1.76	0.51
1:A:617:SER:C	1:A:689:ILE:HG23	2.36	0.51
1:B:319:LEU:HB3	1:B:330:VAL:H	1.76	0.51
1:B:457:GLY:C	1:B:502:ALA:HB1	2.36	0.51
1:D:374:GLU:HG3	1:D:378:LEU:HD11	1.93	0.51
2:E:79:TYR:HB2	2:E:286:TRP:CH2	2.46	0.51
2:F:125:ILE:O	2:F:129:ILE:HG12	2.10	0.51
2:G:36:PHE:CE1	2:G:248:MET:HE2	2.46	0.51
2:G:99:ILE:HD13	2:G:105:GLU:HA	1.93	0.51
2:H:20:GLY:HA3	2:H:100:SER:HB3	1.92	0.51
2:H:207:ARG:HH22	2:H:282:GLN:NE2	2.08	0.51
1:A:22:ILE:HD11	3:A:801:ATP:N3	2.26	0.51
1:A:465:SER:HB2	1:A:489:LEU:HD12	1.93	0.51
1:A:542:LYS:HE3	1:A:596:HIS:NE2	2.26	0.51
1:B:26:LEU:HB2	1:B:38:ILE:HG23	1.92	0.51
1:B:131:MET:HA	1:B:134:PHE:CE2	2.46	0.51
1:B:234:LEU:HA	1:B:237:ILE:CD1	2.41	0.51
1:B:248:VAL:HG21	1:B:288:ALA:O	2.11	0.51
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.93	0.51
1:B:515:ILE:HD13	1:B:551:LEU:CD2	2.40	0.51
1:B:519:ASN:HA	1:B:632:THR:OG1	2.11	0.51
1:C:8:THR:OG1	1:C:52:GLY:O	2.28	0.51
1:C:356:PHE:CE1	1:C:390:LYS:HB3	2.46	0.51
1:D:444:LEU:HD22	1:D:512:THR:HG21	1.93	0.51
1:D:557:GLU:O	1:D:560:LYS:HB2	2.11	0.51
2:E:125:ILE:HG21	2:E:227:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:THR:CG2	2:F:181:THR:HB	2.41	0.51
2:H:319:VAL:HG23	2:H:321:LEU:H	1.76	0.51
1:A:8:THR:HB	1:A:54:LYS:HA	1.91	0.50
1:A:623:GLU:O	1:A:627:GLN:HG2	2.10	0.50
1:A:712:GLN:HE22	2:F:366:ASP:HB3	1.76	0.50
1:B:467:PHE:HE1	1:B:481:LEU:HB3	1.75	0.50
1:B:515:ILE:HD13	1:B:551:LEU:HD13	1.92	0.50
1:B:529:LYS:HD2	1:B:529:LYS:N	2.25	0.50
1:C:437:ASN:ND2	1:C:439:CYS:HB2	2.25	0.50
1:C:592:ASN:ND2	1:C:592:ASN:H	2.08	0.50
1:D:403:MET:CG	1:D:711:MET:HE1	2.40	0.50
2:G:191:LYS:HG2	2:G:264:ILE:CG2	2.41	0.50
1:A:21:LYS:O	1:A:25:VAL:HG23	2.11	0.50
1:A:361:VAL:HG11	1:A:364:LEU:CB	2.41	0.50
1:A:369:PHE:CD2	1:A:434:ARG:HD3	2.45	0.50
1:A:623:GLU:HG2	1:A:633:ASN:HD21	1.72	0.50
1:B:258:ALA:HB1	1:B:282:TYR:CZ	2.45	0.50
1:B:593:GLU:OE2	1:B:596:HIS:CE1	2.64	0.50
1:B:620:MET:SD	1:B:620:MET:O	2.69	0.50
1:C:10:ARG:N	1:C:55:THR:HG22	2.27	0.50
1:C:279:ILE:HD13	1:C:319:LEU:HD22	1.92	0.50
1:C:576:GLY:CA	1:C:607:LYS:HE2	2.41	0.50
1:D:8:THR:HB	1:D:54:LYS:HA	1.93	0.50
1:D:711:MET:HE3	1:D:714:LEU:HB2	1.93	0.50
2:E:149:ARG:NH1	2:E:286:TRP:HB2	2.26	0.50
2:G:161:ILE:O	2:G:165:SER:HB2	2.11	0.50
1:A:282:TYR:CD2	1:A:304:LEU:HD13	2.47	0.50
1:A:297:VAL:O	1:A:297:VAL:HG12	2.11	0.50
1:A:692:SER:HB3	1:A:727:LYS:HB3	1.93	0.50
1:B:86:ILE:HG22	1:B:90:ARG:HD2	1.94	0.50
1:B:262:ARG:HD3	1:B:266:SER:HB3	1.92	0.50
1:C:67:ALA:HA	1:C:70:ILE:HD11	1.94	0.50
1:C:513:LEU:O	1:C:615:THR:O	2.29	0.50
1:C:669:LEU:HD11	1:C:698:ASN:ND2	2.26	0.50
1:D:449:LEU:HD21	1:D:502:ALA:CB	2.42	0.50
2:E:79:TYR:HB2	2:E:286:TRP:CZ2	2.46	0.50
2:E:99:ILE:CD1	2:E:108:VAL:HG21	2.42	0.50
2:G:96:LEU:HD12	2:G:108:VAL:HG11	1.93	0.50
1:A:215:VAL:N	1:A:222:PHE:HE1	2.09	0.50
1:B:73:ASP:C	1:B:75:PRO:HD3	2.37	0.50
1:B:217:THR:HB	1:B:218:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:LYS:NZ	1:C:331:ARG:O	2.45	0.50
1:C:441:GLU:HG2	1:C:620:MET:HB3	1.87	0.50
1:D:73:ASP:C	1:D:75:PRO:HD3	2.36	0.50
1:D:325:VAL:HG13	1:D:328:ASN:HB3	1.93	0.50
2:G:166:TYR:HB3	2:G:184:VAL:HG21	1.93	0.50
2:H:12:GLN:O	2:H:13:LEU:C	2.54	0.50
2:H:221:ARG:HH11	2:H:296:MET:HE3	1.75	0.50
2:H:326:GLN:HG3	2:H:327:THR:O	2.11	0.50
1:A:5:LEU:C	1:A:17:ILE:HG23	2.37	0.50
1:A:19:LEU:HD22	2:F:295:SER:O	2.11	0.50
1:A:479:GLU:HA	1:A:550:TYR:HB3	1.94	0.50
1:B:147:ALA:CB	1:B:628:ILE:HA	2.41	0.50
1:C:176:VAL:HG13	1:C:215:VAL:HG21	1.93	0.50
1:C:185:PRO:O	1:C:189:ARG:CB	2.59	0.50
1:C:217:THR:HB	1:C:218:PRO:CD	2.41	0.50
1:D:285:PHE:O	1:D:289:VAL:HG13	2.12	0.50
1:D:686:GLN:OE1	1:D:693:ILE:HG13	2.12	0.50
2:E:92:ASN:HA	2:E:96:LEU:CD1	2.37	0.50
2:E:239:ALA:HA	2:E:242:LEU:HD21	1.93	0.50
2:E:319:VAL:HG23	2:E:321:LEU:H	1.76	0.50
2:F:122:TYR:O	2:F:126:ILE:HG13	2.11	0.50
2:F:288:ASP:O	2:F:292:ARG:HB2	2.12	0.50
2:G:27:ARG:HB2	2:G:29:ASP:OD1	2.12	0.50
2:G:209:TYR:HA	2:G:212:PHE:CD2	2.47	0.50
2:H:176:THR:HG23	2:H:180:LYS:C	2.37	0.50
2:H:206:ILE:HG21	2:H:312:THR:OG1	2.12	0.50
1:A:73:ASP:C	1:A:75:PRO:HD3	2.36	0.50
1:A:519:ASN:ND2	1:A:632:THR:H	2.09	0.50
1:B:522:TYR:CD1	1:B:662:LEU:CD1	2.95	0.50
1:B:587:LEU:O	1:B:588:ASP:C	2.51	0.50
1:C:144:SER:O	1:C:145:TYR:C	2.54	0.50
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.92	0.50
1:D:6:LEU:HD22	1:D:14:THR:CG2	2.42	0.50
1:D:333:MET:O	1:D:335:TYR:CE1	2.64	0.50
1:D:669:LEU:HD11	1:D:698:ASN:ND2	2.26	0.50
2:E:149:ARG:NH2	2:E:282:GLN:O	2.45	0.50
2:E:288:ASP:O	2:E:292:ARG:HB2	2.12	0.50
2:G:36:PHE:O	2:G:40:ILE:HG13	2.12	0.50
2:H:99:ILE:HD13	2:H:105:GLU:HA	1.93	0.50
1:A:285:PHE:O	1:A:289:VAL:HG13	2.12	0.50
1:A:459:ILE:CD1	1:A:502:ALA:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASN:CG	1:A:631:ALA:HB1	2.37	0.50
1:B:403:MET:HB3	1:B:711:MET:HE1	1.93	0.50
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.92	0.50
1:C:73:ASP:C	1:C:75:PRO:HD3	2.37	0.50
2:F:50:PRO:CG	2:F:121:SER:HB3	2.42	0.50
2:G:111:TRP:CD1	2:G:111:TRP:O	2.65	0.50
2:H:122:TYR:O	2:H:126:ILE:HG13	2.12	0.50
1:A:10:ARG:HG3	1:A:56:SER:HB2	1.93	0.50
1:B:303:THR:OG1	1:B:438:LEU:CD1	2.56	0.50
1:D:522:TYR:HB2	1:D:657:PRO:HG2	1.94	0.50
2:E:34:ASP:O	2:E:38:LYS:HG3	2.12	0.50
2:F:33:TYR:OH	2:F:257:ASP:HB2	2.11	0.50
2:F:96:LEU:HD12	2:F:108:VAL:HG11	1.93	0.50
2:F:194:TYR:CE1	2:F:249:LEU:HD23	2.47	0.50
1:A:332:HIS:O	1:A:333:MET:HG3	2.11	0.50
1:A:403:MET:CG	1:A:711:MET:HE1	2.40	0.50
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.92	0.50
1:B:640:GLY:HA2	1:B:668:LEU:HD13	1.94	0.50
1:C:338:GLN:HG2	1:C:415:GLN:NE2	2.27	0.50
1:D:576:GLY:CA	1:D:607:LYS:HE2	2.41	0.50
1:D:696:ASN:HB2	1:D:731:TYR:O	2.12	0.50
2:E:365:VAL:HG12	2:E:366:ASP:N	2.26	0.50
2:G:50:PRO:CG	2:G:121:SER:HB3	2.42	0.50
2:G:153:ILE:HD11	2:G:207:ARG:HE	1.77	0.50
2:H:288:ASP:O	2:H:292:ARG:HB2	2.12	0.50
1:A:227:LEU:HG	1:A:435:GLN:NE2	2.27	0.49
1:A:229:GLU:CD	1:A:434:ARG:HD2	2.36	0.49
1:C:86:ILE:HG22	1:C:90:ARG:HD2	1.93	0.49
1:C:102:LEU:O	1:C:106:VAL:HG23	2.12	0.49
1:C:282:TYR:CD2	1:C:304:LEU:HD13	2.46	0.49
1:D:30:ALA:HA	1:D:33:LEU:HD12	1.94	0.49
1:D:617:SER:HB3	1:D:689:ILE:HA	1.94	0.49
1:D:685:MET:HB2	1:D:689:ILE:HD11	1.93	0.49
2:E:125:ILE:HD13	2:E:227:ASN:ND2	2.27	0.49
2:F:153:ILE:HG23	2:F:199:SER:OG	2.12	0.49
2:F:153:ILE:HD11	2:F:207:ARG:HE	1.77	0.49
2:G:190:LYS:HB3	2:G:261:MET:SD	2.52	0.49
2:H:74:ILE:HG12	2:H:78:LYS:HE3	1.93	0.49
2:H:79:TYR:HB2	2:H:286:TRP:CZ2	2.46	0.49
2:H:161:ILE:O	2:H:165:SER:HB2	2.12	0.49
2:H:328:ARG:CZ	2:H:328:ARG:CB	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:ASN:ND2	1:A:592:ASN:H	2.09	0.49
1:A:730:TYR:O	1:A:731:TYR:C	2.54	0.49
1:B:102:LEU:O	1:B:106:VAL:HG23	2.11	0.49
1:B:700:ASP:OD2	1:B:735:ARG:NH1	2.44	0.49
1:B:711:MET:HE3	1:B:714:LEU:HB2	1.94	0.49
1:C:37:SER:CB	2:E:331:PRO:O	2.57	0.49
1:D:234:LEU:HA	1:D:237:ILE:CD1	2.42	0.49
1:D:316:LEU:C	1:D:319:LEU:HG	2.35	0.49
2:E:74:ILE:HG12	2:E:78:LYS:HE3	1.94	0.49
2:F:74:ILE:HG12	2:F:78:LYS:HE3	1.94	0.49
2:F:161:ILE:O	2:F:165:SER:HB2	2.11	0.49
2:G:84:ASP:HA	2:G:87:GLN:HB2	1.94	0.49
2:G:204:GLU:HG3	5:G:601:HOH:O	2.12	0.49
2:H:19:PHE:CE2	2:H:190:LYS:HG2	2.47	0.49
1:B:29:ALA:HB1	1:B:80:LEU:HD12	1.93	0.49
1:C:670:TRP:CZ2	1:C:735:ARG:HA	2.47	0.49
1:D:319:LEU:O	1:D:329:ARG:HG2	2.12	0.49
2:E:326:GLN:HG3	2:E:327:THR:O	2.11	0.49
1:A:461:LEU:HD23	1:A:503:ALA:HB1	1.93	0.49
1:B:22:ILE:HD11	3:B:801:ATP:N3	2.27	0.49
1:B:47:ILE:C	1:B:47:ILE:HD13	2.37	0.49
1:D:640:GLY:HA2	1:D:668:LEU:HD13	1.95	0.49
2:F:190:LYS:HB3	2:F:261:MET:SD	2.52	0.49
2:G:319:VAL:HG23	2:G:321:LEU:H	1.76	0.49
2:H:96:LEU:HD12	2:H:108:VAL:HG11	1.95	0.49
1:B:278:CYS:HB3	1:B:282:TYR:HE1	1.77	0.49
1:B:712:GLN:CD	2:H:366:ASP:OD1	2.56	0.49
1:C:414:ILE:HB	1:C:729:LEU:HD12	1.93	0.49
1:C:711:MET:HE3	1:C:714:LEU:HB2	1.93	0.49
1:D:119:LEU:HD12	1:D:119:LEU:N	2.26	0.49
2:E:36:PHE:O	2:E:40:ILE:HG13	2.12	0.49
2:E:92:ASN:O	2:E:96:LEU:HB2	2.12	0.49
2:F:319:VAL:HG23	2:F:321:LEU:H	1.77	0.49
2:F:372:ASN:HD22	2:F:373:PHE:H	1.61	0.49
2:G:178:ASN:C	2:G:180:LYS:N	2.70	0.49
2:G:310:TYR:N	2:G:328:ARG:HD3	2.28	0.49
2:G:311:ILE:HG23	2:G:312:THR:H	1.78	0.49
1:B:19:LEU:HD13	2:H:295:SER:H	1.77	0.49
1:B:175:LEU:HD22	1:B:216:ARG:HD2	1.94	0.49
1:B:222:PHE:CE2	1:B:492:LEU:HD12	2.46	0.49
1:C:18:ASN:O	1:C:19:LEU:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD12	1:C:19:LEU:N	2.21	0.49
1:D:53:ILE:O	1:D:54:LYS:C	2.55	0.49
1:D:131:MET:HA	1:D:134:PHE:CE2	2.48	0.49
1:D:229:GLU:CD	1:D:434:ARG:HD2	2.37	0.49
1:D:260:ARG:O	1:D:261:ILE:C	2.55	0.49
1:D:308:MET:HE1	1:D:399:PHE:CE1	2.47	0.49
1:D:658:ASP:O	1:D:658:ASP:OD2	2.31	0.49
1:D:670:TRP:HB3	1:D:735:ARG:HH12	1.78	0.49
2:F:177:VAL:CB	2:F:180:LYS:O	2.61	0.49
2:H:238:GLU:O	2:H:242:LEU:HD23	2.13	0.49
1:A:291:SER:O	1:B:280:PRO:HB3	2.12	0.49
1:B:145:TYR:CZ	1:B:149:LYS:CG	2.94	0.49
1:B:242:SER:O	1:B:246:LYS:HG2	2.13	0.49
1:B:264:LEU:HD12	1:B:265:GLY:N	2.28	0.49
1:B:700:ASP:HA	1:B:735:ARG:HB3	1.95	0.49
1:C:641:TYR:O	1:C:656:VAL:HG13	2.13	0.49
2:E:161:ILE:O	2:E:165:SER:HB2	2.12	0.49
2:G:201:ASN:O	2:G:205:ALA:HB2	2.13	0.49
2:G:239:ALA:HA	2:G:242:LEU:HD21	1.94	0.49
2:G:277:VAL:HG22	2:G:324:PRO:HG2	1.94	0.49
2:H:33:TYR:OH	2:H:257:ASP:HB2	2.13	0.49
1:A:110:VAL:HG21	1:A:120:LEU:HD11	1.95	0.49
1:A:217:THR:HB	1:A:218:PRO:CD	2.42	0.49
1:A:240:THR:HG22	1:A:244:ILE:HD11	1.94	0.49
1:A:576:GLY:CA	1:A:607:LYS:HE2	2.42	0.49
1:B:10:ARG:HG3	1:B:56:SER:HB2	1.93	0.49
1:B:234:LEU:O	1:B:237:ILE:HD12	2.13	0.49
1:B:297:VAL:HG21	1:B:298:ARG:HH21	1.77	0.49
1:B:339:ILE:HD11	1:B:414:ILE:HD12	1.93	0.49
1:B:463:THR:HB	1:B:489:LEU:CD2	2.43	0.49
1:B:519:ASN:CG	1:B:631:ALA:HB1	2.38	0.49
1:C:20:ASP:HA	1:C:23:HIS:CD2	2.48	0.49
1:C:119:LEU:N	1:C:119:LEU:HD12	2.28	0.49
1:C:131:MET:HA	1:C:134:PHE:CE2	2.47	0.49
1:C:285:PHE:O	1:C:289:VAL:HG13	2.12	0.49
1:C:426:PHE:HA	1:C:571:THR:HA	1.95	0.49
1:D:10:ARG:HG3	1:D:56:SER:HB2	1.93	0.49
1:D:19:LEU:HD12	1:D:19:LEU:N	2.26	0.49
1:D:150:GLN:HE22	1:D:645:LYS:HZ1	1.61	0.49
1:D:260:ARG:O	1:D:358:PRO:HG2	2.12	0.49
1:D:545:GLU:HG3	1:D:595:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:238:GLU:O	2:E:242:LEU:HD23	2.12	0.49
2:F:328:ARG:CZ	2:F:328:ARG:CB	2.90	0.49
2:G:122:TYR:O	2:G:126:ILE:HG13	2.12	0.49
2:G:339:LEU:O	2:G:339:LEU:CD1	2.61	0.49
1:A:5:LEU:HB2	1:A:17:ILE:HG12	1.94	0.49
1:A:264:LEU:HD12	1:A:265:GLY:N	2.28	0.49
1:B:479:GLU:HB3	1:B:550:TYR:CD1	2.48	0.49
1:C:276:THR:HG21	1:D:292:CYS:HA	1.93	0.49
1:C:294:GLN:C	1:C:296:GLY:N	2.71	0.49
1:C:394:LYS:HD3	1:C:394:LYS:H	1.78	0.49
1:D:26:LEU:HB2	1:D:38:ILE:HG23	1.94	0.49
1:D:109:MET:HB2	1:D:115:TYR:CD2	2.48	0.49
1:D:700:ASP:OD1	1:D:735:ARG:HD2	2.13	0.49
2:E:17:MET:HG2	2:E:257:ASP:OD2	2.13	0.49
2:E:177:VAL:HB	2:E:180:LYS:O	2.11	0.49
2:F:191:LYS:HG2	2:F:264:ILE:CG2	2.42	0.49
2:G:207:ARG:HH22	2:G:282:GLN:NE2	2.11	0.49
1:A:189:ARG:O	1:A:190:LEU:C	2.56	0.49
1:A:339:ILE:HD11	1:A:402:MET:HE1	1.94	0.49
1:B:22:ILE:H	1:B:22:ILE:CD1	2.26	0.49
1:B:222:PHE:CG	1:B:492:LEU:HD21	2.48	0.49
1:B:283:LYS:CG	1:B:330:VAL:HG22	2.43	0.49
1:B:297:VAL:HB	1:B:298:ARG:NE	2.16	0.49
1:B:530:ARG:HB2	1:B:533:ASP:OD2	2.13	0.49
1:C:140:ASP:CG	1:C:169:ALA:HB3	2.38	0.49
1:C:172:LEU:HD23	1:C:212:MET:HE3	1.94	0.49
1:C:254:ILE:O	1:C:438:LEU:CD1	2.61	0.49
1:D:86:ILE:HG22	1:D:90:ARG:HD2	1.93	0.49
2:E:186:LEU:HG	2:E:190:LYS:HE3	1.95	0.49
2:G:238:GLU:O	2:G:242:LEU:HD23	2.13	0.49
2:H:36:PHE:CE1	2:H:248:MET:HE2	2.47	0.49
1:A:369:PHE:CE2	1:A:434:ARG:CG	2.96	0.48
1:B:78:GLN:NE2	1:B:654:GLN:HA	2.28	0.48
1:B:119:LEU:HD12	1:B:119:LEU:N	2.27	0.48
1:B:215:VAL:HG22	1:B:222:PHE:CE1	2.47	0.48
1:C:19:LEU:HD22	2:E:295:SER:C	2.37	0.48
1:C:109:MET:HB2	1:C:115:TYR:CD2	2.48	0.48
2:E:12:GLN:O	2:E:13:LEU:C	2.56	0.48
2:H:84:ASP:HA	2:H:87:GLN:HB2	1.94	0.48
2:H:99:ILE:CD1	2:H:108:VAL:HG21	2.43	0.48
2:H:140:ILE:O	2:H:146:ILE:HG21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:THR:HG23	2:H:181:THR:HG23	1.95	0.48
1:A:154:LYS:HB3	1:A:155:TYR:CD2	2.48	0.48
1:A:246:LYS:HG3	1:A:500:ILE:HD11	1.95	0.48
1:B:109:MET:HB2	1:B:115:TYR:CD2	2.48	0.48
1:B:522:TYR:HB2	1:B:657:PRO:HG2	1.94	0.48
1:B:576:GLY:CA	1:B:607:LYS:HE2	2.44	0.48
1:C:232:ASP:OD2	1:C:262:ARG:CZ	2.61	0.48
1:D:39:SER:HB2	2:G:303:ILE:HG21	1.95	0.48
2:E:328:ARG:CZ	2:E:328:ARG:CB	2.90	0.48
2:F:36:PHE:O	2:F:40:ILE:HG13	2.12	0.48
2:G:195:LEU:HD11	2:G:275:LEU:HD11	1.94	0.48
1:A:6:LEU:HD22	1:A:14:THR:CG2	2.43	0.48
1:A:86:ILE:HG22	1:A:90:ARG:HD2	1.95	0.48
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.94	0.48
1:A:692:SER:HB3	1:A:727:LYS:CD	2.43	0.48
1:C:151:LEU:O	1:C:156:LEU:HG	2.13	0.48
2:E:50:PRO:CG	2:E:121:SER:HB3	2.44	0.48
2:H:36:PHE:O	2:H:40:ILE:HG13	2.14	0.48
1:A:7:VAL:HG23	1:A:17:ILE:HG22	1.96	0.48
1:A:10:ARG:H	1:A:55:THR:HG21	1.78	0.48
1:A:207:LEU:HD23	1:A:465:SER:OG	2.14	0.48
1:A:220:ARG:O	1:A:496:GLN:HA	2.13	0.48
1:A:234:LEU:O	1:A:237:ILE:HD12	2.13	0.48
1:A:298:ARG:CZ	1:C:6:LEU:HD11	2.44	0.48
1:A:322:ASN:C	1:A:331:ARG:HH11	2.21	0.48
1:A:441:GLU:CD	1:A:442:ILE:HG12	2.38	0.48
1:B:350:GLY:HA2	1:B:396:VAL:CG2	2.43	0.48
1:D:286:GLN:CD	1:D:332:HIS:HB2	2.32	0.48
2:F:46:PHE:O	2:F:48:TRP:HD1	1.97	0.48
2:G:99:ILE:CD1	2:G:108:VAL:HG21	2.43	0.48
1:A:208:PRO:HD3	1:A:464:LEU:O	2.13	0.48
1:A:227:LEU:HD23	1:A:435:GLN:CD	2.38	0.48
1:B:547:ILE:O	1:B:551:LEU:HG	2.12	0.48
1:C:264:LEU:HD12	1:C:265:GLY:N	2.28	0.48
1:D:339:ILE:HD11	1:D:414:ILE:HD12	1.94	0.48
2:E:156:TYR:HB3	2:E:196:CYS:SG	2.54	0.48
2:G:130:VAL:HG12	2:G:131:ASN:H	1.79	0.48
2:H:178:ASN:O	2:H:178:ASN:OD1	2.30	0.48
1:A:119:LEU:HD12	1:A:119:LEU:N	2.29	0.48
1:B:406:ARG:HD3	1:B:732:GLN:NE2	2.28	0.48
1:B:466:ALA:CB	1:B:516:GLY:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ILE:O	1:C:47:ILE:HG23	2.14	0.48
1:C:648:LYS:HE2	1:C:648:LYS:HB3	1.68	0.48
1:D:168:SER:OG	1:D:171:PHE:CB	2.52	0.48
1:D:222:PHE:CB	1:D:492:LEU:HD21	2.43	0.48
1:D:309:TRP:CH2	1:D:364:LEU:CD1	2.92	0.48
1:D:347:LEU:HD21	1:D:715:LEU:HD22	1.96	0.48
1:D:394:LYS:H	1:D:394:LYS:HD3	1.78	0.48
1:D:685:MET:CB	1:D:689:ILE:HD11	2.44	0.48
2:E:206:ILE:O	2:E:206:ILE:HG22	2.14	0.48
2:F:253:ARG:HG3	2:F:265:ALA:HB1	1.95	0.48
2:F:372:ASN:HD22	2:F:373:PHE:N	2.12	0.48
2:G:79:TYR:HB2	2:G:286:TRP:CH2	2.48	0.48
2:G:200:VAL:C	2:G:202:ALA:N	2.70	0.48
1:A:54:LYS:HD3	1:A:56:SER:HB3	1.95	0.48
1:A:479:GLU:HB2	1:A:550:TYR:CD1	2.48	0.48
1:B:54:LYS:HD3	1:B:56:SER:HB3	1.96	0.48
1:C:44:ARG:NE	1:C:44:ARG:CA	2.73	0.48
1:C:52:GLY:O	1:C:53:ILE:C	2.56	0.48
1:C:234:LEU:O	1:C:237:ILE:HD12	2.14	0.48
1:D:189:ARG:O	1:D:190:LEU:C	2.57	0.48
1:D:228:ILE:C	1:D:435:GLN:HE22	2.22	0.48
1:D:293:SER:CB	1:D:298:ARG:O	2.61	0.48
1:D:441:GLU:OE1	1:D:442:ILE:HG12	2.13	0.48
2:E:311:ILE:HG23	2:E:312:THR:H	1.78	0.48
2:G:12:GLN:O	2:G:14:LYS:N	2.47	0.48
2:G:69:GLU:HG2	2:G:296:MET:HG3	1.96	0.48
2:G:74:ILE:HG12	2:G:78:LYS:HE3	1.95	0.48
2:G:79:TYR:HB2	2:G:286:TRP:CZ2	2.49	0.48
2:G:82:LEU:HD22	2:G:146:ILE:HG23	1.96	0.48
1:A:322:ASN:O	1:A:331:ARG:NH1	2.47	0.48
1:B:668:LEU:O	1:B:671:GLU:N	2.41	0.48
1:D:18:ASN:O	1:D:19:LEU:C	2.56	0.48
1:D:19:LEU:HB2	2:G:295:SER:HB3	1.96	0.48
2:G:288:ASP:O	2:G:292:ARG:HB2	2.13	0.48
2:H:239:ALA:HA	2:H:242:LEU:HD21	1.96	0.48
1:A:247:TYR:CE1	1:A:499:PRO:HD2	2.48	0.48
1:A:388:ILE:O	1:A:389:ARG:C	2.57	0.48
1:B:153:GLY:HA2	1:B:158:GLN:HE22	1.78	0.48
1:C:19:LEU:HD22	2:E:295:SER:O	2.12	0.48
1:C:712:GLN:HE21	2:E:370:LEU:CG	2.26	0.48
1:D:33:LEU:HB2	1:D:36:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:SER:OG	2:G:331:PRO:O	2.31	0.48
1:D:406:ARG:NH1	1:D:697:THR:CG2	2.74	0.48
2:E:92:ASN:O	2:E:96:LEU:HD13	2.14	0.48
2:F:20:GLY:N	2:F:100:SER:HB3	2.29	0.48
2:G:5:PHE:CD1	2:G:24:ASN:O	2.67	0.48
2:G:20:GLY:N	2:G:100:SER:HB3	2.29	0.48
2:H:7:GLN:NE2	2:H:7:GLN:HA	2.29	0.48
1:A:311:LEU:HA	1:A:355:LEU:HB3	1.96	0.48
1:A:313:VAL:O	1:A:317:LEU:HG	2.14	0.48
1:A:464:LEU:HD22	1:A:514:GLY:O	2.14	0.48
1:A:615:THR:CG2	1:A:691:GLN:HE21	2.25	0.48
1:D:102:LEU:O	1:D:106:VAL:HG23	2.14	0.48
1:D:156:LEU:HD22	1:D:167:GLU:HG3	1.95	0.48
1:D:248:VAL:HG21	1:D:289:VAL:HA	1.96	0.48
1:D:294:GLN:HG2	1:D:298:ARG:HG3	1.96	0.48
1:D:323:ARG:HG3	2:F:292:ARG:CG	2.43	0.48
2:E:253:ARG:HG3	2:E:265:ALA:CB	2.44	0.48
2:F:340:VAL:CG1	2:F:341:SER:N	2.74	0.48
2:H:50:PRO:CG	2:H:121:SER:HB3	2.44	0.48
2:H:322:ASP:O	2:H:324:PRO:HD3	2.14	0.48
1:A:5:LEU:CB	1:A:17:ILE:HG12	2.43	0.47
1:A:6:LEU:C	1:A:7:VAL:HG23	2.39	0.47
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.96	0.47
1:A:86:ILE:O	1:A:90:ARG:HG3	2.14	0.47
1:A:306:TYR:CD2	1:A:316:LEU:HD13	2.49	0.47
1:A:325:VAL:HG13	1:A:328:ASN:HB3	1.94	0.47
1:A:350:GLY:HA2	1:A:396:VAL:CG2	2.44	0.47
1:A:692:SER:CB	1:A:727:LYS:HB3	2.41	0.47
1:A:711:MET:HE3	1:A:714:LEU:HB2	1.95	0.47
1:B:145:TYR:OH	1:B:149:LYS:CG	2.62	0.47
1:B:316:LEU:O	1:B:319:LEU:CG	2.62	0.47
1:B:441:GLU:CD	1:B:442:ILE:HG12	2.39	0.47
1:B:489:LEU:HD22	1:B:513:LEU:HD22	1.95	0.47
1:B:513:LEU:CG	1:B:613:ASN:ND2	2.76	0.47
1:C:685:MET:C	1:C:689:ILE:CG1	2.87	0.47
1:D:223:SER:OG	1:D:496:GLN:OE1	2.27	0.47
1:D:560:LYS:CD	1:D:609:HIS:CE1	2.97	0.47
2:E:194:TYR:CE1	2:E:249:LEU:HD23	2.50	0.47
2:G:194:TYR:CE1	2:G:249:LEU:HD23	2.49	0.47
2:H:253:ARG:HG3	2:H:265:ALA:CB	2.44	0.47
1:A:26:LEU:HB2	1:A:38:ILE:HG23	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ARG:HA	1:B:565:CYS:SG	2.53	0.47
1:B:696:ASN:HB2	1:B:731:TYR:O	2.14	0.47
1:C:229:GLU:CD	1:C:434:ARG:HD2	2.39	0.47
1:C:618:ALA:O	1:C:619:LEU:HD23	2.14	0.47
1:D:264:LEU:HD12	1:D:265:GLY:N	2.28	0.47
1:D:479:GLU:HA	1:D:550:TYR:HB3	1.96	0.47
2:E:374:GLN:O	2:E:375:LEU:HD23	2.14	0.47
2:F:17:MET:HG2	2:F:257:ASP:OD2	2.14	0.47
2:F:374:GLN:O	2:F:375:LEU:OXT	2.31	0.47
2:H:191:LYS:HG2	2:H:264:ILE:CG2	2.43	0.47
1:A:6:LEU:HB2	1:A:51:ASP:OD1	2.15	0.47
1:A:131:MET:HE3	1:A:193:VAL:CG1	2.45	0.47
1:A:339:ILE:HG22	1:A:340:ASN:N	2.29	0.47
1:A:357:SER:O	1:A:358:PRO:C	2.57	0.47
1:A:441:GLU:OE1	1:A:442:ILE:HG12	2.13	0.47
1:B:229:GLU:CD	1:B:434:ARG:HD2	2.40	0.47
2:E:190:LYS:HB3	2:E:261:MET:SD	2.54	0.47
2:E:221:ARG:HH11	2:E:296:MET:HE3	1.77	0.47
2:F:310:TYR:CA	2:F:328:ARG:HD3	2.44	0.47
2:G:19:PHE:CE2	2:G:190:LYS:HG2	2.49	0.47
2:H:130:VAL:HG12	2:H:131:ASN:H	1.78	0.47
1:A:301:ALA:HB1	1:A:438:LEU:HD21	1.95	0.47
1:A:339:ILE:HD11	1:A:414:ILE:HD12	1.96	0.47
1:A:617:SER:HB2	1:A:690:ASP:N	2.21	0.47
1:A:617:SER:CB	1:A:689:ILE:HA	2.44	0.47
1:A:693:ILE:HD12	1:A:693:ILE:H	1.80	0.47
1:A:699:TYR:CZ	1:A:714:LEU:HD23	2.49	0.47
1:B:4:ASN:HD22	1:B:5:LEU:HD22	1.80	0.47
1:B:479:GLU:HA	1:B:550:TYR:HB3	1.96	0.47
1:C:303:THR:OG1	1:C:438:LEU:HA	2.15	0.47
1:C:316:LEU:CA	1:C:319:LEU:HD11	2.37	0.47
1:C:699:TYR:CZ	1:C:714:LEU:HD23	2.50	0.47
1:D:625:SER:C	1:D:628:ILE:HG22	2.39	0.47
2:G:7:GLN:HA	2:G:7:GLN:NE2	2.30	0.47
1:A:374:GLU:HG3	1:A:378:LEU:HD11	1.96	0.47
1:A:615:THR:HB	1:A:691:GLN:HE21	1.76	0.47
1:B:33:LEU:HB2	1:B:36:VAL:HG21	1.96	0.47
1:B:147:ALA:HB2	1:B:627:GLN:O	2.14	0.47
1:B:167:GLU:OE2	1:B:172:LEU:HB2	2.15	0.47
1:B:356:PHE:CE1	1:B:390:LYS:HB3	2.50	0.47
1:B:361:VAL:HG11	1:B:364:LEU:HB2	1.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:LEU:C	1:B:589:THR:N	2.64	0.47
1:D:516:GLY:CA	1:D:620:MET:HE1	2.42	0.47
1:D:700:ASP:CG	1:D:735:ARG:HD2	2.39	0.47
2:E:16:PRO:HA	2:E:257:ASP:OD1	2.15	0.47
2:E:84:ASP:OD1	2:E:208:PHE:CE2	2.67	0.47
2:E:309:GLU:HB3	2:E:328:ARG:HD2	1.97	0.47
2:F:58:ASP:O	2:F:61:ASP:HB2	2.15	0.47
2:H:69:GLU:HG2	2:H:296:MET:HG3	1.95	0.47
2:H:186:LEU:HG	2:H:190:LYS:HE3	1.96	0.47
1:A:660:GLU:H	1:A:660:GLU:HG2	1.49	0.47
1:B:18:ASN:O	1:B:19:LEU:C	2.56	0.47
1:B:47:ILE:HG23	1:B:47:ILE:O	2.14	0.47
2:E:19:PHE:CE2	2:E:190:LYS:HG2	2.49	0.47
2:E:103:GLU:HG2	2:E:104:LEU:H	1.79	0.47
2:E:205:ALA:O	2:E:311:ILE:HD11	2.15	0.47
2:F:79:TYR:HB2	2:F:286:TRP:CH2	2.49	0.47
2:F:204:GLU:HG3	5:F:602:HOH:O	2.13	0.47
2:G:103:GLU:HG2	2:G:104:LEU:H	1.80	0.47
2:G:140:ILE:O	2:G:146:ILE:HG21	2.14	0.47
2:H:311:ILE:HG23	2:H:312:THR:H	1.79	0.47
1:A:67:ALA:HA	1:A:70:ILE:HD11	1.96	0.47
1:A:214:GLY:HA3	1:A:222:PHE:CE1	2.50	0.47
1:A:227:LEU:CD2	1:A:435:GLN:HG2	2.43	0.47
1:A:339:ILE:HG22	1:A:340:ASN:H	1.80	0.47
1:A:545:GLU:HG3	1:A:595:LEU:CD2	2.42	0.47
1:B:64:LYS:HG3	1:B:649:ASP:OD2	2.15	0.47
1:B:285:PHE:O	1:B:289:VAL:HG13	2.14	0.47
1:B:403:MET:CG	1:B:711:MET:HE1	2.44	0.47
1:B:545:GLU:HG3	1:B:595:LEU:HD23	1.96	0.47
1:C:308:MET:HE1	1:C:399:PHE:CE1	2.50	0.47
1:C:347:LEU:HD13	1:C:399:PHE:HB2	1.95	0.47
1:C:357:SER:O	1:C:358:PRO:C	2.57	0.47
1:C:479:GLU:HA	1:C:550:TYR:HB3	1.96	0.47
1:D:53:ILE:HG12	1:D:58:ILE:HG12	1.97	0.47
1:D:113:GLY:C	1:D:114:LYS:HD3	2.38	0.47
1:D:152:GLU:O	1:D:158:GLN:NE2	2.48	0.47
1:D:560:LYS:CD	1:D:609:HIS:ND1	2.77	0.47
1:D:647:SER:HB2	1:D:652:LEU:CD1	2.45	0.47
2:E:82:LEU:HD22	2:E:146:ILE:HG23	1.96	0.47
2:E:206:ILE:HD13	2:E:312:THR:HG23	1.95	0.47
2:F:82:LEU:HD22	2:F:146:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:11:ASP:OD2	2:G:13:LEU:HB2	2.14	0.47
2:G:20:GLY:HA3	2:G:100:SER:HB3	1.96	0.47
2:G:186:LEU:HG	2:G:190:LYS:HE3	1.96	0.47
2:H:9:LYS:H	2:H:9:LYS:HG3	1.60	0.47
2:H:89:ARG:HE	2:H:89:ARG:HB3	1.50	0.47
2:H:116:THR:OG1	2:H:117:ILE:HD12	2.14	0.47
2:H:124:HIS:O	2:H:128:ASN:ND2	2.47	0.47
2:H:194:TYR:CE1	2:H:249:LEU:HD23	2.50	0.47
1:A:10:ARG:H	1:A:55:THR:HG22	1.79	0.47
1:A:102:LEU:O	1:A:106:VAL:HG23	2.15	0.47
1:A:234:LEU:HA	1:A:237:ILE:CD1	2.44	0.47
1:B:115:TYR:CE1	1:B:216:ARG:HG3	2.49	0.47
1:D:510:ARG:HB3	1:D:614:SER:OG	2.14	0.47
1:D:530:ARG:HB2	1:D:533:ASP:OD2	2.14	0.47
2:H:46:PHE:O	2:H:48:TRP:HD1	1.98	0.47
2:H:82:LEU:HD22	2:H:146:ILE:HG23	1.95	0.47
1:A:369:PHE:CD1	1:A:434:ARG:HA	2.48	0.47
1:A:529:LYS:N	1:A:529:LYS:HD2	2.30	0.47
1:C:222:PHE:CB	1:C:492:LEU:HD21	2.44	0.47
1:C:317:LEU:CD1	1:C:318:VAL:HG13	2.20	0.47
1:C:325:VAL:HG13	1:C:328:ASN:HB3	1.96	0.47
1:C:496:GLN:HG3	1:C:496:GLN:O	2.15	0.47
1:C:520:PHE:CE2	1:C:524:LEU:HD11	2.49	0.47
1:D:114:LYS:O	1:D:217:THR:HG22	2.15	0.47
1:D:247:TYR:CZ	1:D:499:PRO:HD2	2.49	0.47
1:D:413:TYR:HB3	1:D:729:LEU:O	2.14	0.47
1:D:496:GLN:O	1:D:496:GLN:HG3	2.14	0.47
1:D:519:ASN:CG	1:D:631:ALA:HB1	2.40	0.47
2:E:84:ASP:OD1	2:E:208:PHE:HE2	1.96	0.47
2:F:69:GLU:HG2	2:F:296:MET:HG3	1.97	0.47
2:H:6:SER:HB2	2:H:21:GLN:NE2	2.29	0.47
1:A:94:TYR:C	1:A:96:GLN:H	2.23	0.47
1:A:308:MET:HE1	1:A:399:PHE:CE1	2.50	0.47
1:A:435:GLN:CG	1:A:436:SER:N	2.78	0.47
1:A:547:ILE:O	1:A:551:LEU:HG	2.15	0.47
1:B:114:LYS:HB3	1:B:157:VAL:HG11	1.96	0.47
1:B:357:SER:O	1:B:358:PRO:C	2.57	0.47
1:B:369:PHE:O	1:B:421:ASN:ND2	2.48	0.47
1:C:114:LYS:O	1:C:217:THR:HG22	2.15	0.47
1:C:696:ASN:HB2	1:C:731:TYR:O	2.15	0.47
1:D:157:VAL:O	1:D:166:TYR:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:LEU:HD13	1:D:399:PHE:HB2	1.95	0.47
2:E:68:HIS:O	2:E:72:ILE:HG13	2.15	0.47
2:F:111:TRP:CD1	2:F:111:TRP:O	2.67	0.47
2:G:16:PRO:HA	2:G:257:ASP:OD1	2.15	0.47
2:G:58:ASP:O	2:G:61:ASP:HB2	2.15	0.47
2:G:334:TRP:C	2:G:336:ASN:N	2.71	0.47
2:H:68:HIS:O	2:H:72:ILE:HG13	2.15	0.47
1:A:413:TYR:HE1	1:A:731:TYR:CD2	2.33	0.46
1:A:437:ASN:ND2	1:A:439:CYS:HB2	2.26	0.46
1:A:496:GLN:O	1:A:496:GLN:HG3	2.14	0.46
1:B:19:LEU:HD12	1:B:19:LEU:N	2.27	0.46
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.96	0.46
1:C:459:ILE:CD1	1:C:502:ALA:HB3	2.45	0.46
1:D:225:CYS:O	1:D:462:CYS:HB2	2.15	0.46
2:H:153:ILE:HG23	2:H:199:SER:OG	2.15	0.46
1:A:464:LEU:HD13	1:A:620:MET:HE2	1.97	0.46
1:A:648:LYS:HE2	1:A:648:LYS:HB3	1.76	0.46
1:D:131:MET:HE3	1:D:193:VAL:CG1	2.45	0.46
1:D:185:PRO:O	1:D:189:ARG:HB2	2.16	0.46
1:D:250:GLN:O	1:D:251:ARG:C	2.58	0.46
1:D:483:ILE:HA	1:D:554:ALA:HB1	1.97	0.46
2:E:217:ALA:CB	2:E:296:MET:HE1	2.45	0.46
2:F:16:PRO:HA	2:F:257:ASP:OD1	2.15	0.46
2:G:253:ARG:HG3	2:G:265:ALA:CB	2.45	0.46
2:H:201:ASN:O	2:H:205:ALA:HB2	2.15	0.46
1:A:185:PRO:O	1:A:189:ARG:HB2	2.16	0.46
1:A:282:TYR:CE2	1:A:304:LEU:HD22	2.50	0.46
1:A:341:LYS:HB2	1:A:722:TYR:HH	1.76	0.46
1:A:357:SER:O	1:A:359:SER:N	2.48	0.46
1:A:519:ASN:HA	1:A:632:THR:OG1	2.15	0.46
1:A:588:ASP:O	1:A:591:ALA:O	2.34	0.46
1:B:496:GLN:HG3	1:B:496:GLN:O	2.14	0.46
1:C:220:ARG:O	1:C:496:GLN:HA	2.15	0.46
1:C:282:TYR:HA	1:C:285:PHE:HD2	1.79	0.46
1:C:350:GLY:HA2	1:C:396:VAL:CG2	2.45	0.46
1:C:403:MET:HE1	1:C:718:LEU:CD2	2.44	0.46
1:D:47:ILE:HG23	1:D:47:ILE:O	2.15	0.46
1:D:286:GLN:CD	1:D:332:HIS:CG	2.93	0.46
1:D:339:ILE:HG22	1:D:340:ASN:N	2.31	0.46
1:D:623:GLU:CG	1:D:633:ASN:ND2	2.64	0.46
2:G:242:LEU:HD23	2:G:242:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:90:SER:CB	2:H:91:PRO:HD3	2.46	0.46
1:A:260:ARG:HD3	1:A:365:TYR:CE2	2.50	0.46
1:A:483:ILE:HA	1:A:554:ALA:HB1	1.97	0.46
1:B:45:SER:HB2	1:B:61:THR:HG22	1.96	0.46
1:B:67:ALA:HA	1:B:70:ILE:HD11	1.97	0.46
1:B:207:LEU:HD12	1:B:211:ILE:CG2	2.46	0.46
1:B:226:VAL:CG1	1:B:461:LEU:CD2	2.90	0.46
1:B:515:ILE:HD13	1:B:551:LEU:HD22	1.97	0.46
1:C:339:ILE:HD11	1:C:414:ILE:HD12	1.96	0.46
1:C:339:ILE:HG22	1:C:340:ASN:N	2.31	0.46
1:C:530:ARG:HB2	1:C:533:ASP:OD2	2.16	0.46
1:D:443:ALA:H	1:D:691:GLN:HB3	1.80	0.46
2:E:166:TYR:HB3	2:E:184:VAL:HG21	1.97	0.46
2:E:311:ILE:HG23	2:E:312:THR:N	2.31	0.46
2:F:222:GLU:O	2:F:223:LEU:HD23	2.15	0.46
2:F:309:GLU:HA	2:F:325:PHE:CG	2.50	0.46
2:H:70:LYS:O	2:H:74:ILE:HG22	2.15	0.46
2:H:111:TRP:CD1	2:H:241:HIS:CD2	3.04	0.46
1:A:246:LYS:CG	1:A:500:ILE:HD11	2.45	0.46
1:A:297:VAL:CG1	1:C:4:ASN:HD21	2.26	0.46
1:A:309:TRP:CZ3	1:A:364:LEU:HD12	2.50	0.46
1:A:340:ASN:OD1	1:A:343:MET:HG2	2.16	0.46
1:A:620:MET:SD	1:A:620:MET:N	2.78	0.46
1:B:240:THR:HG22	1:B:244:ILE:HD11	1.98	0.46
1:B:306:TYR:CD2	1:B:316:LEU:HD13	2.50	0.46
1:B:641:TYR:O	1:B:656:VAL:HG13	2.15	0.46
1:C:302:ALA:CA	1:C:438:LEU:HD11	2.46	0.46
1:D:594:PRO:O	1:D:596:HIS:CD2	2.69	0.46
2:E:58:ASP:O	2:E:61:ASP:HB2	2.15	0.46
2:E:130:VAL:HG12	2:E:131:ASN:H	1.79	0.46
2:F:372:ASN:ND2	2:F:372:ASN:N	2.58	0.46
2:G:25:VAL:HG22	2:G:26:ALA:N	2.30	0.46
1:A:214:GLY:C	1:A:222:PHE:HE1	2.24	0.46
1:A:647:SER:OG	1:A:652:LEU:HD11	2.16	0.46
1:B:10:ARG:H	1:B:55:THR:HG21	1.78	0.46
1:B:308:MET:HE1	1:B:399:PHE:CE1	2.51	0.46
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.97	0.46
1:C:75:PRO:HB2	1:C:660:GLU:OE2	2.16	0.46
1:C:413:TYR:HB3	1:C:729:LEU:O	2.15	0.46
1:D:94:TYR:C	1:D:96:GLN:H	2.23	0.46
1:D:151:LEU:HA	1:D:155:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:685:MET:C	1:D:689:ILE:HG13	2.33	0.46
2:E:11:ASP:OD2	2:E:13:LEU:HB2	2.16	0.46
2:E:247:HIS:O	2:E:251:LEU:HG	2.16	0.46
2:F:70:LYS:O	2:F:74:ILE:HG22	2.14	0.46
2:F:221:ARG:HH11	2:F:221:ARG:HG3	1.80	0.46
2:H:17:MET:HG2	2:H:257:ASP:OD2	2.14	0.46
2:H:200:VAL:C	2:H:202:ALA:N	2.72	0.46
2:H:277:VAL:CG2	2:H:324:PRO:HG3	2.44	0.46
1:A:361:VAL:CG1	1:A:364:LEU:CB	2.81	0.46
1:B:208:PRO:CD	1:B:464:LEU:O	2.62	0.46
1:B:483:ILE:HA	1:B:554:ALA:HB1	1.96	0.46
1:B:565:CYS:HA	1:B:566:PRO:HD3	1.83	0.46
1:C:4:ASN:ND2	1:C:4:ASN:N	2.59	0.46
1:C:54:LYS:HG2	1:C:56:SER:H	1.80	0.46
1:D:329:ARG:HB2	1:D:331:ARG:HH21	1.79	0.46
2:E:69:GLU:HG2	2:E:296:MET:HG3	1.98	0.46
2:E:206:ILE:CD1	2:E:312:THR:HA	2.46	0.46
2:F:68:HIS:O	2:F:72:ILE:HG13	2.16	0.46
2:G:124:HIS:HA	2:G:127:ARG:HD3	1.98	0.46
2:G:261:MET:SD	2:G:264:ILE:HD12	2.55	0.46
2:H:103:GLU:HG2	2:H:104:LEU:H	1.80	0.46
1:A:52:GLY:C	1:A:53:ILE:CG2	2.89	0.46
1:A:103:TYR:O	1:A:107:VAL:HG23	2.16	0.46
1:A:204:LYS:HG2	1:A:481:LEU:HD11	1.96	0.46
1:B:145:TYR:OH	1:B:149:LYS:HG2	2.16	0.46
1:B:513:LEU:O	1:B:615:THR:O	2.34	0.46
1:C:625:SER:C	1:C:628:ILE:HG22	2.37	0.46
1:D:260:ARG:HG3	1:D:365:TYR:CE2	2.50	0.46
1:D:647:SER:HB2	1:D:652:LEU:HD11	1.97	0.46
2:F:312:THR:HB	2:F:325:PHE:CE2	2.50	0.46
1:A:131:MET:HA	1:A:134:PHE:CE2	2.50	0.46
1:B:172:LEU:HD23	1:B:216:ARG:NH2	2.31	0.46
1:B:220:ARG:NH2	1:B:495:TYR:OH	2.48	0.46
1:B:339:ILE:HG22	1:B:340:ASN:N	2.31	0.46
1:B:646:ALA:HB1	1:B:650:GLY:HA2	1.98	0.46
1:B:679:LEU:HD22	1:B:720:THR:HB	1.98	0.46
1:C:19:LEU:HB2	2:E:295:SER:HB3	1.98	0.46
1:C:33:LEU:HB2	1:C:36:VAL:HG21	1.98	0.46
1:C:225:CYS:O	1:C:226:VAL:HG13	2.15	0.46
1:C:483:ILE:HA	1:C:554:ALA:HB1	1.98	0.46
1:D:350:GLY:HA2	1:D:396:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:GLU:OE2	1:D:377:ARG:HD3	2.16	0.46
2:E:191:LYS:C	2:E:193:LEU:H	2.24	0.46
2:E:310:TYR:CA	2:E:328:ARG:HD3	2.45	0.46
2:F:79:TYR:HB2	2:F:286:TRP:CZ2	2.50	0.46
2:F:242:LEU:HD23	2:F:242:LEU:H	1.81	0.46
2:H:16:PRO:HA	2:H:257:ASP:OD1	2.16	0.46
2:H:236:ARG:HD3	2:H:342:ASP:CG	2.40	0.46
1:A:47:ILE:HG23	1:A:47:ILE:O	2.15	0.46
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.51	0.46
1:A:315:SER:O	1:A:318:VAL:HG22	2.15	0.46
1:A:347:LEU:HD13	1:A:399:PHE:HB2	1.98	0.46
1:A:441:GLU:HG2	1:A:620:MET:HB3	1.98	0.46
1:B:72:ARG:HB3	1:B:642:VAL:HG13	1.98	0.46
1:B:711:MET:HB3	2:H:364:GLU:N	2.31	0.46
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.97	0.46
1:C:374:GLU:HG3	1:C:378:LEU:HD11	1.98	0.46
1:C:480:GLU:OE2	1:C:484:LEU:HD11	2.16	0.46
1:C:685:MET:CB	1:C:689:ILE:HD11	2.45	0.46
1:D:425:PRO:HG2	1:D:690:ASP:HB3	1.97	0.46
2:E:46:PHE:O	2:E:48:TRP:HD1	1.98	0.46
2:F:130:VAL:HG12	2:F:131:ASN:H	1.80	0.46
2:G:12:GLN:O	2:G:13:LEU:C	2.57	0.46
2:G:205:ALA:O	2:G:209:TYR:HB2	2.16	0.46
2:G:311:ILE:HG23	2:G:312:THR:N	2.31	0.46
2:H:365:VAL:O	2:H:365:VAL:HG22	2.15	0.46
1:A:228:ILE:H	1:A:435:GLN:HE22	1.63	0.45
1:B:27:ASP:OD1	1:B:38:ILE:HD13	2.16	0.45
1:B:516:GLY:HA3	1:B:620:MET:SD	2.57	0.45
2:E:111:TRP:CD1	2:E:111:TRP:O	2.68	0.45
2:F:175:HIS:O	2:F:181:THR:HA	2.15	0.45
2:H:84:ASP:OD1	2:H:208:PHE:HE2	1.99	0.45
1:B:94:TYR:C	1:B:96:GLN:H	2.24	0.45
1:B:365:TYR:O	1:B:366:ASP:C	2.57	0.45
1:B:463:THR:HG21	1:B:492:LEU:HD23	1.98	0.45
1:C:234:LEU:HA	1:C:237:ILE:CD1	2.45	0.45
1:C:619:LEU:HD12	1:C:693:ILE:CG2	2.47	0.45
1:D:699:TYR:CZ	1:D:714:LEU:HD23	2.51	0.45
2:E:140:ILE:O	2:E:146:ILE:HG21	2.16	0.45
2:E:264:ILE:HA	2:E:267:GLU:HG2	1.98	0.45
2:F:35:ILE:HG23	2:F:36:PHE:N	2.29	0.45
2:G:49:ARG:HB3	2:G:51:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:116:THR:OG1	2:G:117:ILE:HD12	2.15	0.45
2:G:203:LEU:HA	2:G:207:ARG:HD2	1.97	0.45
1:A:298:ARG:HE	1:C:6:LEU:CD2	2.11	0.45
1:A:513:LEU:HD12	1:A:613:ASN:ND2	2.31	0.45
1:A:585:LYS:C	1:A:587:LEU:H	2.24	0.45
1:A:633:ASN:O	1:A:634:GLY:C	2.59	0.45
1:A:647:SER:C	1:A:649:ASP:N	2.72	0.45
1:B:701:PRO:HD3	1:B:734:THR:HG22	1.98	0.45
1:C:447:LYS:HB2	1:C:458:GLU:N	2.17	0.45
2:F:340:VAL:CG1	2:F:341:SER:CB	2.93	0.45
2:G:127:ARG:H	2:G:127:ARG:HG2	1.60	0.45
2:H:190:LYS:HB3	2:H:261:MET:SD	2.55	0.45
2:H:242:LEU:HD23	2:H:242:LEU:H	1.81	0.45
1:A:37:SER:OG	2:F:331:PRO:O	2.27	0.45
1:A:320:LYS:CE	1:A:331:ARG:O	2.65	0.45
1:A:600:GLU:HA	1:A:603:ARG:HB3	1.98	0.45
1:B:152:GLU:O	1:B:152:GLU:HG2	2.17	0.45
1:B:699:TYR:CZ	1:B:714:LEU:HD23	2.51	0.45
1:C:99:PRO:HA	1:C:100:PRO:HD3	1.73	0.45
1:C:204:LYS:HG2	1:C:481:LEU:HD11	1.99	0.45
1:C:519:ASN:HA	1:C:632:THR:OG1	2.15	0.45
1:D:9:LYS:HB3	3:D:801:ATP:PG	2.57	0.45
1:D:222:PHE:CD2	1:D:492:LEU:CD1	2.92	0.45
1:D:367:ALA:O	1:D:371:ASP:O	2.34	0.45
2:E:203:LEU:HA	2:E:207:ARG:HD2	1.98	0.45
2:H:9:LYS:HB2	2:H:9:LYS:NZ	2.31	0.45
2:H:24:ASN:ND2	2:H:25:VAL:HG12	2.32	0.45
2:H:84:ASP:OD1	2:H:208:PHE:CE2	2.69	0.45
2:H:136:VAL:O	2:H:140:ILE:HG13	2.17	0.45
1:A:5:LEU:CB	1:A:17:ILE:HG21	2.36	0.45
1:A:6:LEU:CD1	1:C:298:ARG:NH1	2.73	0.45
1:B:211:ILE:HA	1:B:222:PHE:CD1	2.52	0.45
1:B:275:HIS:HD2	1:B:277:GLY:N	2.10	0.45
1:B:313:VAL:HG13	1:B:314:GLU:N	2.31	0.45
1:B:524:LEU:HD22	1:B:536:ALA:HB1	1.98	0.45
1:C:55:THR:HA	1:C:58:ILE:CD1	2.46	0.45
1:C:221:GLN:HE21	1:C:221:GLN:HB2	1.58	0.45
1:C:254:ILE:O	1:C:302:ALA:HA	2.17	0.45
1:C:714:LEU:CD2	1:C:732:GLN:NE2	2.78	0.45
1:D:114:LYS:CE	1:D:166:TYR:OH	2.62	0.45
1:D:316:LEU:HA	1:D:319:LEU:CD1	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:90:SER:HB3	2:E:157:TYR:CE1	2.52	0.45
2:G:68:HIS:O	2:G:72:ILE:HG13	2.16	0.45
2:H:90:SER:HB3	2:H:157:TYR:CE1	2.51	0.45
1:A:4:ASN:CG	1:C:297:VAL:HG11	2.41	0.45
1:A:282:TYR:HA	1:A:285:PHE:HD2	1.81	0.45
1:A:530:ARG:HB2	1:A:533:ASP:OD2	2.16	0.45
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.47	0.45
1:B:10:ARG:H	1:B:55:THR:HG22	1.80	0.45
1:B:592:ASN:ND2	1:B:592:ASN:N	2.64	0.45
1:B:719:LEU:HD22	2:H:375:LEU:HD21	1.99	0.45
1:C:44:ARG:CD	1:C:69:LEU:HD21	2.47	0.45
1:D:507:ALA:O	1:D:508:MET:C	2.60	0.45
2:E:242:LEU:HD23	2:E:242:LEU:H	1.82	0.45
2:G:46:PHE:O	2:G:48:TRP:HD1	1.99	0.45
2:H:58:ASP:O	2:H:61:ASP:HB2	2.16	0.45
2:H:278:GLN:NE2	2:H:279:ALA:N	2.65	0.45
2:H:311:ILE:HG23	2:H:312:THR:N	2.32	0.45
1:A:268:ILE:HD11	1:A:275:HIS:HA	1.99	0.45
1:A:308:MET:SD	1:A:343:MET:HE3	2.57	0.45
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.98	0.45
1:B:308:MET:SD	1:B:343:MET:HE3	2.57	0.45
1:B:515:ILE:HG21	1:B:551:LEU:HD11	1.98	0.45
1:C:290:LYS:HB3	1:C:296:GLY:HA3	1.99	0.45
1:C:342:LEU:HD11	1:C:346:ARG:HE	1.82	0.45
1:C:385:ASP:O	1:C:390:LYS:HE2	2.16	0.45
1:C:560:LYS:HD3	1:C:609:HIS:NE2	2.32	0.45
1:D:7:VAL:HG23	1:D:17:ILE:HG22	1.97	0.45
1:D:67:ALA:HA	1:D:70:ILE:CD1	2.47	0.45
1:D:99:PRO:HA	1:D:100:PRO:HD3	1.73	0.45
1:D:150:GLN:NE2	1:D:645:LYS:HZ1	2.15	0.45
1:D:693:ILE:O	1:D:693:ILE:HD12	2.17	0.45
2:E:204:GLU:HG3	5:E:602:HOH:O	2.15	0.45
2:E:206:ILE:HD13	2:E:312:THR:HA	1.97	0.45
2:E:245:THR:O	2:E:249:LEU:HD12	2.16	0.45
2:G:17:MET:HG2	2:G:257:ASP:OD2	2.17	0.45
2:G:35:ILE:HG23	2:G:36:PHE:N	2.31	0.45
2:G:136:VAL:O	2:G:140:ILE:HG13	2.17	0.45
2:G:156:TYR:HB3	2:G:196:CYS:SG	2.57	0.45
2:H:203:LEU:O	2:H:203:LEU:HD23	2.16	0.45
1:A:298:ARG:NH2	1:C:6:LEU:CG	2.80	0.45
1:A:303:THR:OG1	1:A:438:LEU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:PHE:CE2	1:A:610:GLY:HA2	2.52	0.45
1:B:55:THR:HG21	3:B:801:ATP:PB	2.57	0.45
1:B:623:GLU:OE1	1:B:623:GLU:HA	2.17	0.45
1:C:94:TYR:C	1:C:96:GLN:H	2.24	0.45
1:C:207:LEU:HD12	1:C:211:ILE:CG2	2.46	0.45
1:C:268:ILE:HD11	1:C:275:HIS:HA	1.99	0.45
1:C:519:ASN:HA	1:C:519:ASN:HD22	1.58	0.45
1:C:578:LEU:HD12	1:C:580:ILE:HD11	1.99	0.45
1:D:247:TYR:CE1	1:D:499:PRO:HD2	2.52	0.45
1:D:524:LEU:HD22	1:D:536:ALA:HB1	1.99	0.45
1:D:647:SER:O	1:D:650:GLY:N	2.50	0.45
2:E:153:ILE:HG23	2:E:199:SER:OG	2.17	0.45
2:F:140:ILE:O	2:F:146:ILE:HG21	2.16	0.45
2:G:153:ILE:HG23	2:G:199:SER:OG	2.16	0.45
1:B:394:LYS:H	1:B:394:LYS:HD3	1.82	0.45
1:C:9:LYS:HE2	3:C:801:ATP:O3G	2.16	0.45
1:C:114:LYS:HE2	1:C:166:TYR:HE2	1.80	0.45
1:D:39:SER:OG	2:G:332:ILE:HG22	2.17	0.45
1:D:150:GLN:NE2	1:D:645:LYS:NZ	2.63	0.45
1:D:337:VAL:HG11	1:D:402:MET:HE2	1.98	0.45
2:E:12:GLN:C	2:E:14:LYS:N	2.73	0.45
2:F:103:GLU:HG2	2:F:104:LEU:H	1.81	0.45
2:F:186:LEU:HG	2:F:190:LYS:HE3	1.99	0.45
2:F:261:MET:SD	2:F:264:ILE:HD12	2.57	0.45
2:G:84:ASP:OD1	2:G:208:PHE:HE2	2.00	0.45
2:H:49:ARG:HB3	2:H:51:GLU:OE1	2.17	0.45
2:H:310:TYR:CA	2:H:328:ARG:HD3	2.47	0.45
1:A:33:LEU:HB2	1:A:36:VAL:HG21	1.99	0.45
1:A:224:SER:O	1:A:252:ALA:HB1	2.16	0.45
1:A:689:ILE:HD13	1:A:693:ILE:HG23	1.99	0.45
1:B:44:ARG:HD3	1:B:44:ARG:HA	1.41	0.45
1:B:172:LEU:HD13	1:B:172:LEU:C	2.42	0.45
1:B:208:PRO:CG	1:B:211:ILE:HD13	2.46	0.45
1:B:403:MET:CB	1:B:711:MET:HE1	2.47	0.45
1:B:600:GLU:HA	1:B:603:ARG:HB3	1.98	0.45
1:B:617:SER:CA	1:B:689:ILE:HD12	2.45	0.45
1:C:7:VAL:HG11	3:C:801:ATP:C6	2.52	0.45
1:C:27:ASP:OD1	1:C:38:ILE:HD13	2.17	0.45
1:C:149:LYS:HG2	1:C:652:LEU:HD21	1.99	0.45
1:C:151:LEU:O	1:C:152:GLU:C	2.60	0.45
1:C:254:ILE:H	1:C:438:LEU:HD11	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LEU:HD22	1:D:167:GLU:O	2.16	0.45
1:D:425:PRO:HG3	1:D:690:ASP:OD1	2.17	0.45
1:D:545:GLU:OE2	1:D:597:TYR:CD2	2.69	0.45
2:E:200:VAL:C	2:E:202:ALA:N	2.71	0.45
2:F:20:GLY:HA3	2:F:100:SER:HB3	1.98	0.45
2:F:203:LEU:O	2:F:203:LEU:HD23	2.17	0.45
2:F:245:THR:O	2:F:249:LEU:HD12	2.17	0.45
2:F:311:ILE:HG23	2:F:312:THR:H	1.81	0.45
2:G:90:SER:CB	2:G:91:PRO:HD3	2.46	0.45
1:B:149:LYS:HD3	1:B:149:LYS:HA	1.87	0.44
1:B:268:ILE:HD11	1:B:275:HIS:HA	1.99	0.44
1:B:337:VAL:HB	1:B:414:ILE:HD13	1.99	0.44
1:B:626:SER:OG	1:B:633:ASN:HA	2.18	0.44
1:B:643:SER:HB3	1:B:654:GLN:HB3	1.99	0.44
1:C:34:HIS:O	1:C:35:ASN:CB	2.65	0.44
1:C:275:HIS:HD2	1:C:277:GLY:N	2.10	0.44
1:C:585:LYS:C	1:C:587:LEU:H	2.24	0.44
1:C:600:GLU:HA	1:C:603:ARG:HB3	1.99	0.44
1:D:5:LEU:HD12	1:D:17:ILE:CD1	2.47	0.44
1:D:17:ILE:HA	3:D:801:ATP:N1	2.32	0.44
1:D:78:GLN:NE2	1:D:654:GLN:HA	2.32	0.44
2:E:70:LYS:O	2:E:74:ILE:HG22	2.17	0.44
2:E:277:VAL:HG22	2:E:324:PRO:HB3	1.99	0.44
2:E:370:LEU:N	2:E:370:LEU:HD23	2.32	0.44
2:F:299:LEU:HD11	2:F:304:LEU:HD13	1.99	0.44
2:G:84:ASP:OD1	2:G:208:PHE:CE2	2.70	0.44
2:H:205:ALA:O	2:H:209:TYR:HB2	2.17	0.44
1:A:27:ASP:OD1	1:A:38:ILE:HD13	2.18	0.44
1:A:102:LEU:HG	1:A:135:ILE:CD1	2.47	0.44
1:A:232:ASP:OD2	1:A:262:ARG:CZ	2.64	0.44
1:B:249:SER:HA	1:B:292:CYS:SG	2.57	0.44
1:B:289:VAL:O	1:B:300:GLY:HA3	2.16	0.44
1:B:615:THR:HB	1:B:691:GLN:HE21	1.80	0.44
1:C:10:ARG:NH2	1:C:91:LYS:HG2	2.32	0.44
1:C:115:TYR:CD1	1:C:216:ARG:HG3	2.49	0.44
1:C:293:SER:HB2	1:C:296:GLY:CA	2.26	0.44
1:C:441:GLU:OE2	1:C:442:ILE:HG12	2.17	0.44
1:D:623:GLU:O	1:D:627:GLN:HG2	2.18	0.44
2:E:124:HIS:HA	2:E:127:ARG:HD3	2.00	0.44
2:F:16:PRO:O	2:F:100:SER:OG	2.33	0.44
2:F:330:ASN:CG	2:F:332:ILE:O	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:HH21	1:C:6:LEU:CG	2.30	0.44
1:A:699:TYR:O	1:A:734:THR:HG22	2.17	0.44
1:B:328:ASN:O	1:B:329:ARG:HG3	2.17	0.44
1:B:441:GLU:HG2	1:B:620:MET:HB3	1.96	0.44
1:B:556:ASN:O	1:B:559:ALA:HB3	2.17	0.44
1:C:222:PHE:HB3	1:C:492:LEU:HD21	1.99	0.44
1:C:248:VAL:C	1:C:250:GLN:N	2.74	0.44
1:C:633:ASN:O	1:C:634:GLY:C	2.59	0.44
1:C:679:LEU:HD22	1:C:720:THR:HB	1.99	0.44
1:D:22:ILE:H	1:D:22:ILE:CD1	2.27	0.44
1:D:44:ARG:HG3	1:D:69:LEU:HD11	1.99	0.44
1:D:136:ASP:O	1:D:137:HIS:C	2.60	0.44
1:D:204:LYS:HE3	1:D:481:LEU:HD21	1.98	0.44
1:D:207:LEU:HD12	1:D:211:ILE:CG2	2.47	0.44
1:D:319:LEU:HB3	1:D:330:VAL:H	1.83	0.44
1:D:578:LEU:HD12	1:D:580:ILE:HD11	1.99	0.44
1:D:585:LYS:C	1:D:587:LEU:H	2.25	0.44
2:F:277:VAL:HG22	2:F:324:PRO:CB	2.47	0.44
2:G:70:LYS:O	2:G:74:ILE:HG22	2.16	0.44
2:H:261:MET:SD	2:H:264:ILE:HD12	2.57	0.44
1:A:510:ARG:HG2	1:A:567:TRP:HB2	1.99	0.44
1:B:39:SER:CB	2:H:303:ILE:HG21	2.43	0.44
1:B:102:LEU:HG	1:B:135:ILE:CD1	2.48	0.44
1:C:320:LYS:CE	1:C:331:ARG:O	2.66	0.44
1:C:692:SER:HB2	1:C:727:LYS:CB	2.45	0.44
1:D:340:ASN:OD1	1:D:343:MET:HG2	2.18	0.44
1:D:361:VAL:HG11	1:D:364:LEU:HB2	1.99	0.44
1:D:633:ASN:O	1:D:634:GLY:C	2.60	0.44
2:F:49:ARG:HB3	2:F:51:GLU:OE1	2.18	0.44
2:G:25:VAL:CG2	2:G:26:ALA:N	2.81	0.44
2:H:339:LEU:CD1	2:H:339:LEU:N	2.77	0.44
1:A:262:ARG:CG	1:A:275:HIS:CE1	3.01	0.44
1:B:7:VAL:HG23	1:B:17:ILE:HG22	2.00	0.44
1:B:55:THR:HG21	3:B:801:ATP:O2B	2.18	0.44
1:B:367:ALA:O	1:B:371:ASP:O	2.36	0.44
1:B:593:GLU:CD	1:B:596:HIS:NE2	2.75	0.44
1:B:711:MET:CB	2:H:364:GLU:N	2.80	0.44
1:C:378:LEU:HB3	1:C:382:TYR:CE2	2.52	0.44
1:C:532:SER:CB	1:C:673:PRO:HD2	2.48	0.44
1:D:207:LEU:CD1	1:D:212:MET:SD	3.05	0.44
1:D:248:VAL:HG21	1:D:254:ILE:HG13	1.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:HIS:ND1	1:D:311:LEU:N	2.66	0.44
1:D:319:LEU:HA	1:D:329:ARG:HG3	1.98	0.44
1:D:337:VAL:HB	1:D:414:ILE:HD13	1.99	0.44
1:D:442:ILE:CG2	1:D:444:LEU:HG	2.48	0.44
2:E:90:SER:HB3	2:E:157:TYR:CZ	2.52	0.44
2:F:62:TYR:HA	2:F:65:LEU:HD12	2.00	0.44
2:G:143:ASN:HB3	2:G:146:ILE:HB	2.00	0.44
2:H:176:THR:HA	2:H:180:LYS:O	2.17	0.44
1:A:74:ALA:N	1:A:75:PRO:HD3	2.33	0.44
1:A:136:ASP:O	1:A:137:HIS:C	2.60	0.44
1:A:176:VAL:HA	1:A:215:VAL:CG1	2.46	0.44
1:B:516:GLY:HA2	1:B:620:MET:HE1	1.92	0.44
1:B:544:PHE:CE2	1:B:685:MET:HE2	2.49	0.44
1:C:136:ASP:O	1:C:137:HIS:C	2.59	0.44
1:D:9:LYS:HB3	3:D:801:ATP:O3G	2.17	0.44
1:D:52:GLY:C	1:D:53:ILE:CG2	2.89	0.44
2:E:12:GLN:CD	2:E:102:PRO:HD3	2.43	0.44
2:F:15:GLU:HB2	2:F:101:ILE:HG23	1.99	0.44
2:F:205:ALA:O	2:F:209:TYR:HB2	2.17	0.44
2:G:217:ALA:CB	2:G:296:MET:HE1	2.46	0.44
2:H:177:VAL:O	2:H:177:VAL:HG22	2.18	0.44
1:A:22:ILE:HD12	1:A:22:ILE:N	2.33	0.44
1:A:297:VAL:O	1:A:297:VAL:HG13	2.17	0.44
1:A:337:VAL:HB	1:A:414:ILE:HD13	2.00	0.44
1:B:50:TYR:HE2	1:B:53:ILE:CG1	2.30	0.44
1:B:168:SER:HG	1:B:171:PHE:CB	2.29	0.44
1:B:257:ASN:HD22	1:B:435:GLN:HB3	1.81	0.44
1:C:185:PRO:O	1:C:189:ARG:HB3	2.18	0.44
1:C:208:PRO:CG	1:C:211:ILE:HD13	2.47	0.44
1:C:369:PHE:O	1:C:421:ASN:OD1	2.36	0.44
1:C:544:PHE:CE2	1:C:685:MET:HE2	2.48	0.44
1:D:148:VAL:HA	1:D:151:LEU:CD1	2.47	0.44
1:D:545:GLU:HG3	1:D:595:LEU:CD2	2.48	0.44
2:E:221:ARG:HH11	2:E:221:ARG:HG3	1.83	0.44
2:E:334:TRP:C	2:E:336:ASN:N	2.72	0.44
2:H:90:SER:HB3	2:H:157:TYR:CZ	2.52	0.44
1:A:293:SER:OG	1:A:296:GLY:HA2	2.17	0.44
1:B:205:ILE:HG12	1:B:467:PHE:CD1	2.53	0.44
1:B:263:ALA:HB3	1:B:357:SER:CB	2.48	0.44
1:B:337:VAL:HG11	1:B:402:MET:HE2	2.00	0.44
1:B:369:PHE:O	1:B:421:ASN:CG	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:GLU:OE1	1:B:442:ILE:HG12	2.17	0.44
1:B:507:ALA:O	1:B:508:MET:C	2.60	0.44
1:B:689:ILE:CG2	1:B:689:ILE:O	2.64	0.44
1:C:45:SER:HB2	1:C:61:THR:HG22	1.99	0.44
1:C:302:ALA:HA	1:C:438:LEU:CD1	2.46	0.44
1:C:365:TYR:CE2	1:C:369:PHE:CE2	3.05	0.44
1:C:547:ILE:O	1:C:551:LEU:HG	2.17	0.44
1:D:54:LYS:HD3	1:D:56:SER:HB3	1.99	0.44
1:D:221:GLN:HE21	1:D:221:GLN:HB2	1.54	0.44
1:D:268:ILE:HD11	1:D:275:HIS:HA	1.99	0.44
1:D:275:HIS:HD2	1:D:277:GLY:N	2.10	0.44
1:D:461:LEU:HD23	1:D:503:ALA:HB1	1.99	0.44
2:E:203:LEU:HD23	2:E:203:LEU:O	2.18	0.44
2:F:98:LEU:CD1	2:F:193:LEU:HD13	2.48	0.44
2:F:177:VAL:HG21	2:F:182:VAL:HG23	2.00	0.44
2:F:253:ARG:HG3	2:F:265:ALA:CB	2.47	0.44
2:G:278:GLN:HE21	2:G:278:GLN:HB3	1.63	0.44
2:H:111:TRP:CD1	2:H:241:HIS:CE1	3.05	0.44
1:A:510:ARG:HG3	1:A:567:TRP:CE3	2.46	0.44
1:A:578:LEU:HD12	1:A:580:ILE:HD11	2.00	0.44
1:B:20:ASP:O	1:B:21:LYS:C	2.61	0.44
1:B:99:PRO:HA	1:B:100:PRO:HD3	1.73	0.44
1:B:633:ASN:O	1:B:634:GLY:C	2.59	0.44
1:C:102:LEU:HG	1:C:135:ILE:CD1	2.48	0.44
1:C:464:LEU:HD23	1:C:464:LEU:N	2.32	0.44
1:C:524:LEU:HB3	1:C:529:LYS:O	2.18	0.44
1:C:716:LYS:HG2	2:E:370:LEU:CD1	2.45	0.44
1:D:441:GLU:OE2	1:D:442:ILE:HG12	2.17	0.44
1:D:600:GLU:HA	1:D:603:ARG:HB3	1.99	0.44
2:E:35:ILE:HG23	2:E:36:PHE:N	2.31	0.44
2:E:90:SER:CB	2:E:91:PRO:HD3	2.46	0.44
2:F:8:THR:HB	2:F:21:GLN:NE2	2.32	0.44
2:F:90:SER:CB	2:F:91:PRO:HD3	2.45	0.44
2:F:203:LEU:HA	2:F:207:ARG:HD2	2.00	0.44
2:F:209:TYR:CE2	2:F:339:LEU:CD2	3.01	0.44
2:G:15:GLU:HB2	2:G:101:ILE:HG23	2.00	0.44
1:A:18:ASN:O	1:A:20:ASP:N	2.51	0.43
1:A:114:LYS:HB3	1:A:157:VAL:HG11	2.00	0.43
1:A:592:ASN:ND2	1:A:592:ASN:N	2.66	0.43
1:A:617:SER:HB3	1:A:689:ILE:HA	2.00	0.43
1:B:131:MET:HE3	1:B:193:VAL:CG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:SER:O	1:B:146:ALA:N	2.50	0.43
1:B:147:ALA:HB1	1:B:628:ILE:HA	2.00	0.43
1:B:250:GLN:NE2	1:B:499:PRO:HG3	2.31	0.43
1:B:330:VAL:HB	1:B:335:TYR:OH	2.18	0.43
1:C:10:ARG:H	1:C:55:THR:HG21	1.81	0.43
1:C:77:TYR:HA	1:C:80:LEU:HB3	2.00	0.43
1:C:309:TRP:CH2	1:C:364:LEU:HD12	2.52	0.43
1:C:451:ASP:CG	1:C:452:VAL:N	2.76	0.43
1:C:507:ALA:O	1:C:508:MET:C	2.60	0.43
1:D:50:TYR:CD2	1:D:53:ILE:HB	2.53	0.43
1:D:257:ASN:HD22	1:D:435:GLN:HB3	1.83	0.43
1:D:357:SER:O	1:D:358:PRO:C	2.60	0.43
2:F:164:THR:OG1	2:F:189:LEU:HD11	2.17	0.43
2:F:311:ILE:HG23	2:F:312:THR:N	2.33	0.43
2:G:90:SER:HB3	2:G:157:TYR:CZ	2.53	0.43
2:H:309:GLU:HG2	2:H:325:PHE:CG	2.53	0.43
1:A:5:LEU:HD12	1:A:17:ILE:HD13	1.90	0.43
1:A:134:PHE:CD1	1:A:134:PHE:N	2.86	0.43
1:B:72:ARG:H	1:B:72:ARG:HG2	1.63	0.43
1:B:374:GLU:OE2	1:B:377:ARG:HD3	2.17	0.43
1:B:465:SER:O	1:B:515:ILE:HA	2.18	0.43
1:B:522:TYR:CE1	1:B:662:LEU:CD1	2.94	0.43
1:B:657:PRO:O	1:B:662:LEU:HD12	2.18	0.43
1:C:17:ILE:HD11	3:C:801:ATP:H2	1.77	0.43
1:C:67:ALA:HA	1:C:70:ILE:CD1	2.48	0.43
1:C:89:LEU:CD2	1:C:152:GLU:HG3	2.37	0.43
1:D:232:ASP:OD2	1:D:262:ARG:NH2	2.51	0.43
1:D:447:LYS:HB3	1:D:457:GLY:HA2	2.00	0.43
1:D:618:ALA:O	1:D:619:LEU:HD23	2.18	0.43
1:D:648:LYS:HB3	1:D:648:LYS:HE2	1.61	0.43
2:F:60:ILE:H	2:F:60:ILE:HG13	1.66	0.43
2:F:136:VAL:O	2:F:140:ILE:HG13	2.18	0.43
2:H:98:LEU:CD1	2:H:193:LEU:HD13	2.48	0.43
2:H:156:TYR:HB3	2:H:196:CYS:SG	2.58	0.43
2:H:284:LYS:HZ1	2:H:325:PHE:HE1	1.61	0.43
1:A:93:ALA:HB1	1:A:165:ILE:O	2.18	0.43
1:A:178:ALA:O	1:A:182:SER:N	2.51	0.43
1:A:374:GLU:OE2	1:A:377:ARG:HD3	2.19	0.43
1:A:465:SER:O	1:A:515:ILE:HA	2.19	0.43
1:B:4:ASN:ND2	1:B:5:LEU:H	2.15	0.43
1:B:248:VAL:HG11	1:B:289:VAL:CA	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:HD11	1:B:346:ARG:HE	1.83	0.43
1:B:510:ARG:CG	1:B:567:TRP:HE3	2.27	0.43
1:C:174:ILE:HG23	1:C:175:LEU:H	1.83	0.43
1:C:719:LEU:HB3	2:E:375:LEU:CD2	2.49	0.43
1:D:27:ASP:OD1	1:D:38:ILE:HD13	2.18	0.43
1:D:249:SER:C	1:D:251:ARG:H	2.26	0.43
1:D:658:ASP:OD2	1:D:662:LEU:HD12	2.19	0.43
2:G:12:GLN:C	2:G:14:LYS:N	2.75	0.43
1:A:90:ARG:NH2	1:A:137:HIS:HB3	2.33	0.43
1:A:447:LYS:HB3	1:A:457:GLY:HA2	2.01	0.43
1:B:107:VAL:O	1:B:110:VAL:HB	2.19	0.43
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.48	0.43
1:C:313:VAL:HG13	1:C:314:GLU:N	2.34	0.43
1:C:403:MET:CG	1:C:711:MET:HE1	2.47	0.43
1:C:510:ARG:HB3	1:C:614:SER:OG	2.18	0.43
1:C:592:ASN:ND2	1:C:592:ASN:N	2.65	0.43
1:D:8:THR:O	1:D:54:LYS:HA	2.19	0.43
1:D:316:LEU:O	1:D:319:LEU:HD12	2.17	0.43
1:D:365:TYR:CE2	1:D:369:PHE:HE2	2.36	0.43
2:E:21:GLN:HA	2:E:22:PRO:HD3	1.85	0.43
2:E:116:THR:OG1	2:E:117:ILE:HD12	2.16	0.43
2:F:92:ASN:CA	2:F:96:LEU:HD13	2.35	0.43
2:H:12:GLN:CD	2:H:102:PRO:HD3	2.43	0.43
1:A:519:ASN:HA	1:A:519:ASN:HD22	1.59	0.43
1:B:319:LEU:HG	1:B:319:LEU:H	1.46	0.43
1:B:500:ILE:HG23	1:B:501:PRO:HD2	2.01	0.43
1:B:513:LEU:HD11	1:B:613:ASN:ND2	2.34	0.43
1:B:719:LEU:HD22	2:H:375:LEU:HD22	2.01	0.43
1:C:498:TYR:HB2	1:C:504:LYS:HB2	2.01	0.43
1:D:172:LEU:HD13	1:D:172:LEU:C	2.44	0.43
1:D:185:PRO:HB2	1:D:188:THR:OG1	2.18	0.43
1:D:207:LEU:HD12	1:D:211:ILE:HG21	2.01	0.43
1:D:342:LEU:HD11	1:D:346:ARG:HE	1.83	0.43
1:D:507:ALA:C	1:D:509:GLY:N	2.74	0.43
1:D:595:LEU:HD13	1:D:599:TRP:CD1	2.54	0.43
1:D:620:MET:N	1:D:620:MET:SD	2.79	0.43
1:D:652:LEU:C	1:D:653:ARG:HG2	2.44	0.43
1:D:714:LEU:HD22	1:D:732:GLN:NE2	2.34	0.43
2:F:83:LEU:HD22	2:F:203:LEU:CG	2.47	0.43
2:G:164:THR:OG1	2:G:189:LEU:HD11	2.19	0.43
2:G:203:LEU:HD23	2:G:203:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:ASP:OD2	2:H:13:LEU:HB2	2.19	0.43
1:A:172:LEU:HD13	1:A:172:LEU:C	2.44	0.43
1:A:342:LEU:HD11	1:A:346:ARG:HE	1.82	0.43
1:B:54:LYS:CD	1:B:56:SER:HB3	2.49	0.43
1:B:150:GLN:NE2	1:B:645:LYS:NZ	2.67	0.43
1:B:190:LEU:HD22	1:B:190:LEU:N	2.33	0.43
1:B:510:ARG:HG2	1:B:567:TRP:HB2	2.00	0.43
1:B:532:SER:HA	1:B:677:GLY:HA3	2.01	0.43
1:C:74:ALA:N	1:C:75:PRO:HD3	2.33	0.43
1:C:394:LYS:HD3	1:C:394:LYS:N	2.33	0.43
1:C:545:GLU:HA	1:C:688:PHE:CD1	2.53	0.43
2:F:36:PHE:CE1	2:F:248:MET:HE2	2.52	0.43
1:A:101:ALA:HB3	1:A:104:ASP:OD2	2.19	0.43
1:C:122:ASP:O	1:C:189:ARG:NH2	2.50	0.43
1:C:361:VAL:HG11	1:C:364:LEU:HG	2.00	0.43
1:D:311:LEU:HA	1:D:355:LEU:HB3	1.99	0.43
1:D:361:VAL:HG12	1:D:364:LEU:HB2	2.00	0.43
1:D:527:HIS:O	1:D:529:LYS:HD2	2.19	0.43
1:D:714:LEU:HD22	1:D:732:GLN:HE22	1.83	0.43
2:F:84:ASP:OD1	2:F:208:PHE:CE2	2.71	0.43
2:G:191:LYS:C	2:G:193:LEU:H	2.26	0.43
2:H:85:SER:O	2:H:89:ARG:CZ	2.66	0.43
1:A:532:SER:CB	1:A:673:PRO:HD2	2.48	0.43
1:A:583:TYR:CG	1:A:687:LYS:HG3	2.53	0.43
1:A:617:SER:O	1:A:691:GLN:CG	2.65	0.43
1:B:34:HIS:C	1:B:36:VAL:H	2.26	0.43
1:B:50:TYR:HE2	1:B:53:ILE:HD12	1.82	0.43
1:B:207:LEU:HD12	1:B:211:ILE:HG21	2.00	0.43
1:B:568:PHE:CE2	1:B:610:GLY:HA2	2.54	0.43
1:C:321:ASN:O	1:C:329:ARG:HG2	2.19	0.43
1:C:519:ASN:HD21	1:C:657:PRO:HG2	1.83	0.43
1:C:670:TRP:CD2	1:C:735:ARG:HG3	2.54	0.43
1:D:20:ASP:O	1:D:21:LYS:C	2.61	0.43
1:D:34:HIS:O	1:D:35:ASN:CB	2.65	0.43
1:D:154:LYS:CE	1:D:624:THR:HG21	2.49	0.43
1:D:547:ILE:O	1:D:551:LEU:HG	2.19	0.43
1:D:641:TYR:O	1:D:656:VAL:HG13	2.18	0.43
2:E:136:VAL:O	2:E:140:ILE:HG13	2.19	0.43
2:E:191:LYS:HE2	2:E:267:GLU:OE2	2.19	0.43
2:F:295:SER:OG	2:F:296:MET:N	2.52	0.43
2:H:95:LEU:N	2:H:95:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:342:ASP:OD1	2:H:342:ASP:O	2.37	0.43
1:A:45:SER:HB2	1:A:61:THR:HG22	2.00	0.43
1:A:291:SER:O	1:B:280:PRO:CB	2.67	0.43
1:A:722:TYR:HD2	2:F:375:LEU:HD22	1.84	0.43
1:B:136:ASP:O	1:B:137:HIS:C	2.60	0.43
1:C:403:MET:HE3	1:C:715:LEU:HD23	2.00	0.43
1:C:515:ILE:HD13	1:C:551:LEU:CD2	2.48	0.43
1:C:617:SER:CB	1:C:689:ILE:HA	2.49	0.43
1:D:50:TYR:HD2	1:D:53:ILE:HB	1.83	0.43
1:D:313:VAL:HG13	1:D:314:GLU:N	2.33	0.43
1:D:385:ASP:OD1	1:D:387:SER:OG	2.31	0.43
2:E:98:LEU:CD1	2:E:193:LEU:HD13	2.49	0.43
2:F:116:THR:OG1	2:F:117:ILE:HD12	2.18	0.43
2:F:309:GLU:HB3	2:F:328:ARG:HD2	2.01	0.43
2:G:206:ILE:O	2:G:210:VAL:CG2	2.61	0.43
2:G:277:VAL:HG22	2:G:324:PRO:CB	2.49	0.43
2:H:20:GLY:N	2:H:100:SER:HB3	2.32	0.43
1:A:75:PRO:HB2	1:A:660:GLU:OE2	2.19	0.43
1:A:237:ILE:H	1:A:237:ILE:HG13	1.51	0.43
1:A:451:ASP:CG	1:A:452:VAL:N	2.77	0.43
1:A:452:VAL:HG23	1:A:453:ASN:ND2	2.33	0.43
1:B:464:LEU:C	1:B:464:LEU:HD12	2.44	0.43
1:B:578:LEU:HD12	1:B:580:ILE:HD11	2.01	0.43
1:B:734:THR:HG22	1:B:735:ARG:H	1.83	0.43
1:C:686:GLN:CA	1:C:689:ILE:HG12	2.48	0.43
1:D:165:ILE:HD13	1:D:165:ILE:HA	1.78	0.43
1:D:237:ILE:H	1:D:237:ILE:HG13	1.51	0.43
1:D:308:MET:HE1	1:D:399:PHE:CD1	2.54	0.43
2:E:94:ALA:O	2:E:97:PRO:HD2	2.19	0.43
2:E:369:ASP:OD2	2:E:370:LEU:HD23	2.19	0.43
2:G:91:PRO:HA	2:G:95:LEU:CD1	2.49	0.43
2:G:117:ILE:HD12	2:G:117:ILE:N	2.34	0.43
2:H:339:LEU:HD22	2:H:339:LEU:C	2.43	0.43
1:A:172:LEU:CD2	1:A:216:ARG:NH2	2.68	0.42
1:A:447:LYS:CB	1:A:457:GLY:HA2	2.49	0.42
1:A:711:MET:HE3	1:A:711:MET:HA	2.01	0.42
1:B:114:LYS:O	1:B:217:THR:HG22	2.18	0.42
1:B:374:GLU:HG3	1:B:378:LEU:CD1	2.49	0.42
1:B:440:LEU:HB2	1:B:730:TYR:CD1	2.54	0.42
1:C:115:TYR:CD1	1:C:216:ARG:HG2	2.53	0.42
1:C:258:ALA:HB1	1:C:261:ILE:CD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ALA:HA	1:C:516:GLY:O	2.19	0.42
1:D:150:GLN:CB	1:D:154:LYS:HD2	2.49	0.42
1:D:357:SER:HB3	1:D:360:ASP:CG	2.44	0.42
1:D:531:TYR:CE2	1:D:637:PRO:HD3	2.53	0.42
2:E:277:VAL:HG22	2:E:324:PRO:CG	2.49	0.42
2:G:332:ILE:HD12	2:G:332:ILE:O	2.18	0.42
2:H:117:ILE:HD12	2:H:117:ILE:N	2.34	0.42
1:A:114:LYS:O	1:A:217:THR:HG22	2.19	0.42
1:A:417:VAL:HG23	1:A:418:ASP:H	1.83	0.42
1:A:513:LEU:HD12	1:A:613:ASN:HD22	1.83	0.42
1:A:714:LEU:HD22	1:A:732:GLN:NE2	2.35	0.42
1:B:617:SER:HB2	1:B:690:ASP:N	2.20	0.42
1:C:276:THR:HG23	1:C:280:PRO:HG2	2.00	0.42
1:C:369:PHE:O	1:C:421:ASN:ND2	2.52	0.42
1:C:524:LEU:HD22	1:C:536:ALA:HB1	2.01	0.42
1:D:107:VAL:O	1:D:110:VAL:HB	2.19	0.42
1:D:134:PHE:N	1:D:134:PHE:CD1	2.86	0.42
1:D:567:TRP:C	1:D:569:ASN:N	2.72	0.42
2:E:177:VAL:N	2:E:180:LYS:O	2.50	0.42
2:F:191:LYS:C	2:F:193:LEU:H	2.26	0.42
2:F:217:ALA:CB	2:F:296:MET:HE1	2.49	0.42
2:H:21:GLN:HA	2:H:22:PRO:HD3	1.85	0.42
2:H:86:ILE:O	2:H:87:GLN:C	2.62	0.42
2:H:309:GLU:HB3	2:H:328:ARG:HD2	2.00	0.42
1:A:215:VAL:N	1:A:222:PHE:CE1	2.86	0.42
1:A:320:LYS:HE2	1:A:331:ARG:O	2.19	0.42
1:A:524:LEU:HD22	1:A:536:ALA:HB1	2.00	0.42
1:B:34:HIS:ND1	1:B:34:HIS:N	2.65	0.42
1:B:147:ALA:O	1:B:151:LEU:HG	2.19	0.42
1:B:153:GLY:O	1:B:160:ARG:NH2	2.46	0.42
1:C:20:ASP:O	1:C:21:LYS:C	2.60	0.42
1:C:500:ILE:HG23	1:C:501:PRO:HD2	2.00	0.42
1:D:74:ALA:N	1:D:75:PRO:HD3	2.35	0.42
2:F:264:ILE:HA	2:F:267:GLU:HG2	2.00	0.42
2:G:90:SER:HB3	2:G:157:TYR:CE1	2.54	0.42
2:G:204:GLU:CD	2:G:241:HIS:HB3	2.44	0.42
2:H:9:LYS:NZ	2:H:9:LYS:CB	2.83	0.42
2:H:12:GLN:C	2:H:14:LYS:N	2.75	0.42
2:H:336:ASN:HA	2:H:339:LEU:HD21	2.00	0.42
1:A:204:LYS:HG2	1:A:481:LEU:CD1	2.49	0.42
1:A:288:ALA:HB2	1:B:284:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ALA:C	1:A:509:GLY:N	2.74	0.42
1:A:548:GLN:HE21	1:A:548:GLN:CA	2.32	0.42
1:B:167:GLU:CD	1:B:172:LEU:HB2	2.45	0.42
1:B:222:PHE:H	1:B:496:GLN:HB2	1.85	0.42
1:B:507:ALA:C	1:B:509:GLY:N	2.74	0.42
1:B:545:GLU:HG3	1:B:595:LEU:CD2	2.50	0.42
1:C:69:LEU:HB2	1:C:77:TYR:CD1	2.54	0.42
1:C:167:GLU:CG	1:C:168:SER:N	2.82	0.42
1:C:212:MET:O	1:C:216:ARG:NH2	2.52	0.42
1:C:220:ARG:NH2	1:C:495:TYR:OH	2.52	0.42
1:C:279:ILE:HD13	1:C:319:LEU:CD2	2.49	0.42
1:C:407:ALA:CA	1:C:732:GLN:OE1	2.67	0.42
1:D:90:ARG:NH2	1:D:137:HIS:HB3	2.34	0.42
2:E:143:ASN:HB3	2:E:146:ILE:HB	2.02	0.42
2:F:21:GLN:HA	2:F:22:PRO:HD3	1.85	0.42
2:G:113:PHE:HA	2:G:116:THR:HG23	2.02	0.42
2:G:310:TYR:HB2	2:G:328:ARG:HG3	2.01	0.42
2:H:247:HIS:O	2:H:251:LEU:HG	2.19	0.42
1:A:53:ILE:O	1:A:58:ILE:HD11	2.19	0.42
1:A:313:VAL:HG13	1:A:314:GLU:N	2.33	0.42
1:B:77:TYR:HA	1:B:80:LEU:HB3	2.00	0.42
1:B:462:CYS:O	1:B:462:CYS:SG	2.77	0.42
1:B:467:PHE:CE1	1:B:481:LEU:HB3	2.55	0.42
1:B:519:ASN:CB	1:B:631:ALA:HB1	2.50	0.42
1:B:583:TYR:CG	1:B:687:LYS:HG3	2.54	0.42
1:C:178:ALA:O	1:C:182:SER:N	2.52	0.42
1:D:256:ILE:HB	1:D:304:LEU:HG	2.00	0.42
1:D:385:ASP:O	1:D:390:LYS:HE2	2.20	0.42
1:D:519:ASN:CB	1:D:631:ALA:HB1	2.49	0.42
2:E:261:MET:SD	2:E:264:ILE:HD12	2.59	0.42
2:G:62:TYR:HA	2:G:65:LEU:HD12	2.00	0.42
2:H:96:LEU:CB	2:H:97:PRO:HD3	2.50	0.42
1:A:10:ARG:NH2	1:A:91:LYS:HG2	2.35	0.42
1:A:34:HIS:ND1	1:A:34:HIS:N	2.65	0.42
1:A:215:VAL:C	1:A:216:ARG:CG	2.79	0.42
1:A:308:MET:HE1	1:A:399:PHE:CD1	2.54	0.42
1:A:378:LEU:HB3	1:A:382:TYR:CE2	2.54	0.42
1:B:185:PRO:O	1:B:189:ARG:CB	2.67	0.42
1:B:364:LEU:HD13	1:B:364:LEU:C	2.45	0.42
1:B:385:ASP:OD1	1:B:387:SER:OG	2.31	0.42
1:C:347:LEU:HD22	1:C:399:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ASP:C	1:C:660:GLU:N	2.76	0.42
1:C:670:TRP:CE2	1:C:735:ARG:CG	3.02	0.42
1:C:685:MET:HB3	1:C:689:ILE:HD11	2.01	0.42
1:D:293:SER:OG	1:D:296:GLY:CA	2.65	0.42
1:D:347:LEU:HD22	1:D:399:PHE:CG	2.54	0.42
1:D:532:SER:CB	1:D:673:PRO:HD2	2.49	0.42
2:E:99:ILE:HG21	2:E:105:GLU:HB2	2.01	0.42
2:E:164:THR:OG1	2:E:189:LEU:HD11	2.19	0.42
2:F:84:ASP:OD1	2:F:208:PHE:HE2	2.02	0.42
2:F:96:LEU:CB	2:F:97:PRO:HD3	2.49	0.42
2:G:295:SER:OG	2:G:296:MET:N	2.53	0.42
2:G:366:ASP:OD1	2:G:369:ASP:HB3	2.19	0.42
2:H:222:GLU:O	2:H:223:LEU:HD23	2.20	0.42
2:H:264:ILE:HA	2:H:267:GLU:HG2	2.01	0.42
1:A:507:ALA:O	1:A:508:MET:C	2.60	0.42
1:B:258:ALA:C	1:B:282:TYR:OH	2.63	0.42
1:B:347:LEU:HD13	1:B:399:PHE:HB2	2.01	0.42
1:B:532:SER:CB	1:B:673:PRO:HD2	2.50	0.42
1:B:704:PHE:O	1:B:707:GLY:N	2.51	0.42
1:C:308:MET:HE1	1:C:399:PHE:CD1	2.55	0.42
1:C:548:GLN:CA	1:C:548:GLN:HE21	2.33	0.42
1:D:394:LYS:HD3	1:D:394:LYS:N	2.35	0.42
2:E:206:ILE:HD13	2:E:312:THR:CG2	2.50	0.42
2:E:325:PHE:O	2:E:326:GLN:C	2.61	0.42
2:H:245:THR:O	2:H:249:LEU:HD12	2.19	0.42
1:A:52:GLY:O	1:A:53:ILE:CG2	2.68	0.42
1:A:199:ALA:HB2	1:A:484:LEU:HD13	2.01	0.42
1:A:298:ARG:NH2	1:C:6:LEU:HG	2.35	0.42
1:A:394:LYS:H	1:A:394:LYS:HD3	1.84	0.42
1:A:532:SER:HA	1:A:677:GLY:HA3	2.01	0.42
1:B:451:ASP:CG	1:B:452:VAL:N	2.78	0.42
1:B:584:LYS:HG3	1:B:586:ASP:H	1.85	0.42
1:C:167:GLU:OE1	1:C:172:LEU:HA	2.20	0.42
1:C:184:TYR:HB3	1:C:189:ARG:HB2	2.02	0.42
1:C:369:PHE:CE2	1:C:434:ARG:CB	3.03	0.42
1:C:374:GLU:OE2	1:C:377:ARG:HD3	2.20	0.42
1:C:452:VAL:HG23	1:C:453:ASN:ND2	2.34	0.42
1:D:37:SER:OG	2:G:333:PRO:HD3	2.19	0.42
1:D:447:LYS:CB	1:D:457:GLY:HA2	2.50	0.42
1:D:621:PRO:HD3	1:D:694:SER:OG	2.20	0.42
2:G:98:LEU:CD1	2:G:193:LEU:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:ASN:HB3	2:H:146:ILE:HB	2.00	0.42
1:A:714:LEU:HD22	1:A:732:GLN:HE22	1.84	0.42
1:B:55:THR:HG21	3:B:801:ATP:O1B	2.20	0.42
1:B:282:TYR:O	1:B:285:PHE:HB2	2.20	0.42
1:B:441:GLU:HG2	1:B:620:MET:HB2	1.99	0.42
1:B:515:ILE:O	1:B:618:ALA:O	2.37	0.42
1:B:545:GLU:HA	1:B:688:PHE:CD1	2.54	0.42
1:B:696:ASN:ND2	1:B:696:ASN:N	2.63	0.42
1:C:22:ILE:H	1:C:22:ILE:CD1	2.29	0.42
1:C:207:LEU:HD12	1:C:211:ILE:HG21	2.01	0.42
1:C:319:LEU:HB3	1:C:330:VAL:H	1.85	0.42
1:C:450:ASN:N	1:C:450:ASN:ND2	2.67	0.42
1:C:507:ALA:C	1:C:509:GLY:N	2.75	0.42
1:D:52:GLY:O	1:D:53:ILE:CG2	2.68	0.42
1:D:500:ILE:HG23	1:D:501:PRO:HD2	2.01	0.42
2:G:200:VAL:O	2:G:201:ASN:C	2.60	0.42
2:G:264:ILE:HA	2:G:267:GLU:HG2	2.01	0.42
2:H:217:ALA:CB	2:H:296:MET:HE1	2.48	0.42
2:H:295:SER:OG	2:H:296:MET:N	2.52	0.42
1:A:248:VAL:C	1:A:250:GLN:N	2.74	0.42
1:A:500:ILE:HG23	1:A:501:PRO:HD2	2.01	0.42
1:A:643:SER:HB3	1:A:654:GLN:HB3	2.02	0.42
1:B:50:TYR:HE2	1:B:53:ILE:CD1	2.33	0.42
1:B:50:TYR:HE2	1:B:53:ILE:HG13	1.84	0.42
1:B:134:PHE:HB3	1:B:194:LYS:HG3	2.02	0.42
1:B:145:TYR:O	1:B:146:ALA:C	2.63	0.42
1:B:369:PHE:CE1	1:B:434:ARG:O	2.72	0.42
1:B:621:PRO:CD	1:B:694:SER:OG	2.67	0.42
1:C:479:GLU:HG3	1:C:550:TYR:CD1	2.54	0.42
1:C:519:ASN:HD22	1:C:632:THR:H	1.66	0.42
1:D:452:VAL:HG23	1:D:453:ASN:ND2	2.34	0.42
2:F:156:TYR:HB3	2:F:196:CYS:SG	2.60	0.42
2:G:36:PHE:CE1	2:G:104:LEU:HD13	2.55	0.42
2:G:83:LEU:HD22	2:G:203:LEU:CG	2.49	0.42
2:G:336:ASN:HA	2:G:339:LEU:HD11	2.01	0.42
1:A:69:LEU:HB2	1:A:77:TYR:CD1	2.55	0.41
1:A:320:LYS:NZ	1:A:331:ARG:O	2.53	0.41
1:A:413:TYR:HB3	1:A:729:LEU:O	2.19	0.41
1:B:583:TYR:HB3	1:B:687:LYS:HG3	2.02	0.41
1:C:131:MET:HA	1:C:134:PHE:CD2	2.55	0.41
1:D:45:SER:HB2	1:D:61:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:TYR:HA	1:D:80:LEU:HB3	2.02	0.41
1:D:545:GLU:HA	1:D:688:PHE:CD1	2.55	0.41
2:F:124:HIS:HA	2:F:127:ARG:HD3	2.00	0.41
2:G:245:THR:O	2:G:249:LEU:HD12	2.20	0.41
2:H:203:LEU:HA	2:H:207:ARG:HD2	2.02	0.41
1:A:77:TYR:HA	1:A:80:LEU:HB3	2.02	0.41
1:A:426:PHE:HA	1:A:571:THR:HA	2.01	0.41
1:A:696:ASN:ND2	1:A:696:ASN:N	2.64	0.41
1:A:730:TYR:O	1:A:731:TYR:O	2.37	0.41
1:B:178:ALA:O	1:B:182:SER:N	2.53	0.41
1:B:463:THR:HB	1:B:489:LEU:HD21	2.02	0.41
1:B:686:GLN:OE1	1:B:727:LYS:HG3	2.19	0.41
1:C:131:MET:HE3	1:C:193:VAL:CG1	2.46	0.41
1:D:55:THR:CG2	1:D:56:SER:N	2.84	0.41
1:D:308:MET:SD	1:D:343:MET:HE3	2.60	0.41
1:D:545:GLU:OE2	1:D:597:TYR:HD2	2.03	0.41
2:E:49:ARG:HB3	2:E:51:GLU:OE1	2.20	0.41
2:E:132:ASP:HA	2:E:133:PRO:HD3	1.91	0.41
2:E:200:VAL:O	2:E:201:ASN:C	2.62	0.41
2:F:147:GLN:HA	2:F:150:ALA:HB3	2.02	0.41
2:G:86:ILE:O	2:G:87:GLN:C	2.62	0.41
2:G:92:ASN:CA	2:G:96:LEU:HD13	2.37	0.41
1:A:185:PRO:HB2	1:A:188:THR:OG1	2.21	0.41
1:A:220:ARG:NH2	1:A:495:TYR:OH	2.53	0.41
1:A:244:ILE:O	1:A:248:VAL:HG23	2.19	0.41
1:B:38:ILE:HB	2:H:303:ILE:HD11	2.02	0.41
1:B:101:ALA:HB3	1:B:104:ASP:OD2	2.20	0.41
1:C:134:PHE:CD1	1:C:134:PHE:N	2.86	0.41
1:C:226:VAL:C	1:C:227:LEU:HD12	2.45	0.41
1:C:254:ILE:CG2	1:C:256:ILE:CG1	2.95	0.41
1:C:652:LEU:C	1:C:653:ARG:HG2	2.44	0.41
1:D:3:GLN:N	1:D:5:LEU:HD21	2.35	0.41
1:D:69:LEU:HB2	1:D:77:TYR:CD1	2.55	0.41
1:D:101:ALA:HB3	1:D:104:ASP:OD2	2.19	0.41
1:D:463:THR:HB	1:D:489:LEU:CD2	2.51	0.41
1:D:505:ARG:HG2	1:D:505:ARG:HH11	1.86	0.41
2:E:216:PHE:HZ	2:E:232:ARG:HA	1.85	0.41
2:F:102:PRO:HG2	2:F:103:GLU:H	1.86	0.41
2:H:111:TRP:CD1	2:H:241:HIS:NE2	2.88	0.41
2:H:164:THR:OG1	2:H:189:LEU:HD11	2.20	0.41
2:H:191:LYS:C	2:H:193:LEU:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:HA	1:A:70:ILE:CD1	2.50	0.41
1:A:125:GLU:HG2	1:A:129:LYS:HD2	2.02	0.41
1:A:276:THR:HG21	1:B:291:SER:O	2.20	0.41
1:A:435:GLN:OE1	1:A:446:THR:HG21	2.20	0.41
1:A:440:LEU:HB2	1:A:730:TYR:CE1	2.55	0.41
1:A:567:TRP:C	1:A:569:ASN:ND2	2.79	0.41
1:B:131:MET:HA	1:B:134:PHE:CD2	2.56	0.41
1:B:134:PHE:CD1	1:B:134:PHE:N	2.86	0.41
1:B:220:ARG:CZ	1:B:495:TYR:CE1	3.03	0.41
1:B:569:ASN:ND2	1:B:570:GLU:N	2.65	0.41
1:B:595:LEU:HD13	1:B:599:TRP:CD1	2.55	0.41
1:C:519:ASN:CB	1:C:631:ALA:HB1	2.51	0.41
1:D:5:LEU:N	1:D:5:LEU:HD23	2.35	0.41
1:D:37:SER:OG	2:G:333:PRO:CD	2.68	0.41
1:D:463:THR:C	1:D:464:LEU:CD2	2.67	0.41
1:D:532:SER:HA	1:D:677:GLY:HA3	2.01	0.41
1:D:718:LEU:HD13	1:D:729:LEU:HD11	2.02	0.41
2:F:169:LEU:HB2	2:F:170:LEU:HG	2.02	0.41
1:A:5:LEU:O	1:A:17:ILE:HG23	2.20	0.41
1:A:107:VAL:O	1:A:110:VAL:HB	2.19	0.41
1:A:172:LEU:C	1:A:172:LEU:HD22	2.45	0.41
1:A:652:LEU:C	1:A:653:ARG:HG2	2.45	0.41
1:B:74:ALA:N	1:B:75:PRO:HD3	2.34	0.41
1:B:122:ASP:O	1:B:189:ARG:NH2	2.50	0.41
1:B:245:VAL:HA	1:B:248:VAL:HG22	2.02	0.41
1:B:258:ALA:C	1:B:260:ARG:N	2.79	0.41
1:B:263:ALA:HB3	1:B:357:SER:HB2	2.02	0.41
1:B:263:ALA:CB	1:B:357:SER:OG	2.67	0.41
1:B:347:LEU:HD21	1:B:715:LEU:HD22	2.03	0.41
1:B:548:GLN:CA	1:B:548:GLN:HE21	2.34	0.41
1:B:617:SER:HB3	1:B:689:ILE:CD1	2.39	0.41
1:B:700:ASP:OD1	1:B:735:ARG:CG	2.68	0.41
1:B:722:TYR:HD2	2:H:375:LEU:HB3	1.85	0.41
1:C:107:VAL:O	1:C:110:VAL:HB	2.20	0.41
1:C:304:LEU:HD12	1:C:333:MET:SD	2.60	0.41
1:C:407:ALA:HB2	1:C:732:GLN:OE1	2.20	0.41
1:C:681:LEU:O	1:C:685:MET:HG3	2.21	0.41
1:D:178:ALA:O	1:D:182:SER:N	2.54	0.41
2:E:295:SER:OG	2:E:296:MET:N	2.52	0.41
2:G:102:PRO:HG2	2:G:103:GLU:H	1.86	0.41
1:A:214:GLY:C	1:A:222:PHE:CE1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:HD13	1:A:319:LEU:HD22	2.02	0.41
1:B:226:VAL:C	1:B:227:LEU:HD12	2.45	0.41
1:B:510:ARG:HB3	1:B:614:SER:OG	2.21	0.41
1:C:155:TYR:O	1:C:172:LEU:HD11	2.20	0.41
1:C:407:ALA:HA	1:C:732:GLN:OE1	2.20	0.41
1:C:532:SER:HA	1:C:677:GLY:HA3	2.01	0.41
1:D:9:LYS:HE2	3:D:801:ATP:O1G	2.21	0.41
1:D:519:ASN:HD22	1:D:632:THR:H	1.66	0.41
1:D:546:ALA:O	1:D:547:ILE:C	2.64	0.41
1:D:679:LEU:HD22	1:D:720:THR:HB	2.02	0.41
2:F:278:GLN:NE2	2:F:279:ALA:N	2.69	0.41
2:G:96:LEU:CB	2:G:97:PRO:HD3	2.50	0.41
2:H:299:LEU:HD11	2:H:304:LEU:HD13	2.02	0.41
2:H:370:LEU:O	2:H:371:SER:C	2.64	0.41
1:A:19:LEU:HD22	2:F:295:SER:C	2.46	0.41
1:A:83:ARG:HG2	1:A:83:ARG:H	1.63	0.41
1:A:442:ILE:CG2	1:A:444:LEU:HG	2.50	0.41
1:B:62:ILE:CD1	1:B:84:LEU:HD22	2.48	0.41
1:B:712:GLN:OE1	2:H:366:ASP:OD1	2.38	0.41
1:C:145:TYR:O	1:C:146:ALA:C	2.62	0.41
1:D:131:MET:HA	1:D:134:PHE:CD2	2.56	0.41
1:D:286:GLN:OE1	1:D:332:HIS:CG	2.74	0.41
1:D:310:HIS:O	1:D:355:LEU:HD22	2.21	0.41
1:D:378:LEU:HB3	1:D:382:TYR:CE2	2.52	0.41
1:D:444:LEU:HD12	1:D:460:ALA:HB1	2.03	0.41
1:D:451:ASP:CG	1:D:452:VAL:N	2.79	0.41
2:E:91:PRO:HA	2:E:95:LEU:CD1	2.50	0.41
2:G:99:ILE:HG21	2:G:105:GLU:HB2	2.03	0.41
1:A:8:THR:O	1:A:54:LYS:HA	2.21	0.41
1:A:298:ARG:NH2	1:C:6:LEU:CD2	2.74	0.41
1:A:321:ASN:HB2	1:A:405:GLU:OE1	2.20	0.41
1:A:369:PHE:CD2	1:A:434:ARG:HG2	2.55	0.41
1:A:716:LYS:HG2	2:F:370:LEU:CD1	2.44	0.41
1:B:67:ALA:HA	1:B:70:ILE:CD1	2.51	0.41
1:B:220:ARG:CZ	1:B:495:TYR:HE1	2.34	0.41
1:B:450:ASN:ND2	1:B:450:ASN:N	2.66	0.41
1:B:689:ILE:HD12	1:B:689:ILE:HA	1.91	0.41
1:B:712:GLN:NE2	2:H:366:ASP:OD1	2.53	0.41
1:C:10:ARG:N	3:C:801:ATP:O2G	2.54	0.41
1:C:125:GLU:HG2	1:C:129:LYS:HD2	2.03	0.41
1:C:207:LEU:CG	1:C:212:MET:SD	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:LEU:HB2	1:C:580:ILE:HG12	2.02	0.41
1:C:640:GLY:HA2	1:C:668:LEU:HD13	2.03	0.41
1:C:658:ASP:C	1:C:660:GLU:H	2.28	0.41
1:D:4:ASN:HB3	1:D:16:ARG:NH1	2.35	0.41
1:D:172:LEU:HD11	1:D:212:MET:HG2	2.03	0.41
1:D:374:GLU:HG3	1:D:378:LEU:CD1	2.51	0.41
1:D:583:TYR:CG	1:D:687:LYS:HG3	2.55	0.41
2:E:83:LEU:HD22	2:E:203:LEU:CG	2.48	0.41
2:G:177:VAL:HG12	2:G:178:ASN:N	2.36	0.41
1:A:40:GLN:HE21	2:F:333:PRO:HG2	1.82	0.41
1:A:223:SER:OG	1:A:496:GLN:OE1	2.33	0.41
1:A:369:PHE:CZ	1:A:434:ARG:CA	3.04	0.41
1:A:431:ALA:HB1	1:A:445:PRO:CG	2.51	0.41
1:A:450:ASN:N	1:A:450:ASN:ND2	2.67	0.41
1:A:519:ASN:HD22	1:A:632:THR:H	1.69	0.41
1:A:545:GLU:HA	1:A:688:PHE:CD1	2.56	0.41
1:A:699:TYR:HB2	1:A:734:THR:HG22	2.03	0.41
1:B:90:ARG:NH2	1:B:137:HIS:HB3	2.36	0.41
1:B:510:ARG:NH1	1:B:567:TRP:CZ3	2.89	0.41
1:B:617:SER:HB2	1:B:689:ILE:HD12	1.94	0.41
1:B:645:LYS:O	1:B:652:LEU:HB2	2.21	0.41
1:C:115:TYR:HE1	1:C:216:ARG:HH11	1.67	0.41
1:C:278:CYS:O	1:C:282:TYR:CD1	2.71	0.41
1:C:361:VAL:HG11	1:C:364:LEU:CG	2.50	0.41
1:D:55:THR:O	1:D:56:SER:C	2.63	0.41
1:D:148:VAL:HA	1:D:151:LEU:HD12	2.03	0.41
1:D:151:LEU:HG	1:D:151:LEU:H	1.63	0.41
1:D:417:VAL:HG23	1:D:418:ASP:H	1.86	0.41
1:D:450:ASN:N	1:D:450:ASN:ND2	2.66	0.41
1:D:617:SER:CB	1:D:689:ILE:HA	2.50	0.41
1:D:707:GLY:O	1:D:708:LYS:HD2	2.21	0.41
2:E:50:PRO:HB3	2:E:121:SER:HB3	2.02	0.41
2:E:96:LEU:CB	2:E:97:PRO:HD3	2.51	0.41
2:E:113:PHE:HA	2:E:116:THR:HG23	2.03	0.41
2:F:143:ASN:HB3	2:F:146:ILE:HB	2.03	0.41
2:G:65:LEU:CD2	2:G:223:LEU:HD13	2.47	0.41
2:G:179:GLY:O	2:G:180:LYS:HD2	2.17	0.41
2:G:231:ILE:O	2:G:234:ILE:HB	2.21	0.41
2:G:304:LEU:HD12	2:G:304:LEU:HA	1.93	0.41
2:H:147:GLN:HA	2:H:150:ALA:HB3	2.02	0.41
2:H:198:MET:HE2	2:H:272:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:216:PHE:HZ	2:H:232:ARG:HA	1.86	0.41
2:H:278:GLN:HE21	2:H:278:GLN:HB3	1.64	0.41
1:A:34:HIS:C	1:A:36:VAL:H	2.27	0.41
1:A:258:ALA:C	1:A:260:ARG:N	2.77	0.41
1:A:465:SER:HB3	1:A:515:ILE:HG23	2.03	0.41
1:A:697:THR:HG1	1:A:699:TYR:HE1	1.68	0.41
1:B:68:ASP:OD2	1:B:651:ILE:HG21	2.21	0.41
1:B:333:MET:O	1:B:335:TYR:CE1	2.74	0.41
1:C:228:ILE:CD1	1:C:459:ILE:HG12	2.42	0.41
1:C:417:VAL:HG23	1:C:418:ASP:H	1.85	0.41
1:C:417:VAL:CG2	1:C:418:ASP:N	2.83	0.41
1:C:461:LEU:HD23	1:C:503:ALA:HB1	2.03	0.41
1:D:172:LEU:C	1:D:172:LEU:HD22	2.46	0.41
1:D:480:GLU:OE2	1:D:484:LEU:HD11	2.21	0.41
1:D:529:LYS:HD2	1:D:529:LYS:H	1.86	0.41
1:A:5:LEU:CD1	1:A:17:ILE:HD13	2.47	0.40
1:A:596:HIS:CB	1:A:597:TYR:CE2	3.04	0.40
1:B:340:ASN:OD1	1:B:343:MET:HG2	2.20	0.40
1:C:247:TYR:CZ	1:C:499:PRO:HD2	2.55	0.40
1:C:302:ALA:CA	1:C:438:LEU:HD21	2.51	0.40
1:C:305:PHE:CZ	1:C:436:SER:HB3	2.57	0.40
1:D:7:VAL:HG11	3:D:801:ATP:C6	2.56	0.40
1:D:226:VAL:HG12	1:D:461:LEU:HD22	2.03	0.40
1:D:583:TYR:HB3	1:D:687:LYS:HG3	2.03	0.40
2:E:273:TYR:HE2	2:E:324:PRO:HG3	1.85	0.40
2:E:368:ASP:O	2:E:369:ASP:C	2.63	0.40
2:F:127:ARG:H	2:F:127:ARG:HG2	1.59	0.40
2:F:225:GLU:O	2:F:226:GLY:C	2.64	0.40
2:H:113:PHE:HA	2:H:116:THR:HG23	2.03	0.40
2:H:191:LYS:HE2	2:H:267:GLU:OE2	2.22	0.40
1:A:308:MET:HE2	1:A:398:LEU:HD23	2.03	0.40
1:A:369:PHE:CE1	1:A:434:ARG:CA	2.99	0.40
1:A:699:TYR:HB2	1:A:734:THR:CG2	2.51	0.40
1:B:321:ASN:HB2	1:B:405:GLU:OE1	2.20	0.40
1:B:487:ARG:HD3	1:B:558:LEU:HD22	2.03	0.40
1:C:19:LEU:H	1:C:19:LEU:CD1	2.16	0.40
1:C:199:ALA:HB2	1:C:484:LEU:HD13	2.04	0.40
1:C:254:ILE:CA	1:C:438:LEU:HD12	2.43	0.40
1:C:569:ASN:ND2	1:C:570:GLU:N	2.65	0.40
1:D:150:GLN:O	1:D:154:LYS:N	2.49	0.40
1:D:208:PRO:CG	1:D:211:ILE:HD13	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:GLY:CA	1:D:438:LEU:CD1	3.00	0.40
1:D:325:VAL:HG13	1:D:328:ASN:CB	2.51	0.40
2:E:299:LEU:HD11	2:E:304:LEU:HD13	2.03	0.40
2:G:177:VAL:CB	2:G:180:LYS:O	2.59	0.40
2:G:191:LYS:C	2:G:193:LEU:N	2.80	0.40
2:H:99:ILE:HG21	2:H:105:GLU:HB2	2.03	0.40
1:A:569:ASN:ND2	1:A:570:GLU:N	2.65	0.40
1:B:208:PRO:HG2	1:B:211:ILE:CD1	2.49	0.40
1:B:286:GLN:HE22	1:B:332:HIS:CG	2.35	0.40
1:B:316:LEU:CA	1:B:319:LEU:HD11	2.48	0.40
1:C:144:SER:O	1:C:146:ALA:N	2.55	0.40
1:C:431:ALA:HB1	1:C:445:PRO:CG	2.52	0.40
1:C:463:THR:HB	1:C:489:LEU:CD2	2.50	0.40
1:C:509:GLY:O	1:C:566:PRO:HD2	2.22	0.40
1:C:558:LEU:HD23	1:C:612:ARG:HG2	2.03	0.40
1:D:208:PRO:HG2	1:D:211:ILE:CD1	2.50	0.40
1:D:404:GLN:HE21	1:D:404:GLN:HB2	1.69	0.40
1:D:544:PHE:CE2	1:D:685:MET:HE2	2.49	0.40
1:D:578:LEU:HB2	1:D:580:ILE:HG12	2.03	0.40
1:D:592:ASN:ND2	1:D:592:ASN:N	2.65	0.40
1:D:670:TRP:HB3	1:D:735:ARG:NH1	2.36	0.40
2:F:247:HIS:O	2:F:251:LEU:HG	2.21	0.40
2:F:277:VAL:CG2	2:F:324:PRO:HB3	2.50	0.40
2:G:147:GLN:HA	2:G:150:ALA:HB3	2.03	0.40
2:G:336:ASN:O	2:G:339:LEU:HD12	2.21	0.40
1:A:34:HIS:C	1:A:36:VAL:N	2.79	0.40
1:A:55:THR:HG21	3:A:801:ATP:O2B	2.22	0.40
1:A:155:TYR:CE1	1:A:212:MET:HG2	2.55	0.40
1:A:288:ALA:HB2	1:B:284:HIS:HE1	1.85	0.40
1:A:546:ALA:O	1:A:547:ILE:C	2.64	0.40
1:B:69:LEU:HB2	1:B:77:TYR:CD1	2.56	0.40
1:B:94:TYR:CD1	1:B:100:PRO:HD2	2.57	0.40
1:B:125:GLU:HG2	1:B:129:LYS:HD2	2.04	0.40
1:B:228:ILE:CD1	1:B:459:ILE:HG12	2.41	0.40
1:B:513:LEU:HD11	1:B:613:ASN:HD21	1.86	0.40
1:B:519:ASN:HD22	1:B:632:THR:H	1.69	0.40
1:B:567:TRP:C	1:B:569:ASN:ND2	2.79	0.40
1:C:185:PRO:O	1:C:189:ARG:HB2	2.22	0.40
1:C:204:LYS:HG2	1:C:481:LEU:CD1	2.52	0.40
1:D:361:VAL:HG13	1:D:382:TYR:CE2	2.57	0.40
1:D:378:LEU:O	1:D:381:LYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:198:MET:HE2	2:E:272:CYS:SG	2.62	0.40
2:E:339:LEU:CD1	2:E:340:VAL:CG2	2.90	0.40
2:F:117:ILE:HD12	2:F:117:ILE:N	2.37	0.40
2:G:145:GLN:HG2	2:G:289:TYR:CG	2.57	0.40
2:H:65:LEU:HA	2:H:66:PRO:HD3	1.86	0.40
2:H:115:GLU:OE1	2:H:115:GLU:HA	2.22	0.40
2:H:279:ALA:HA	2:H:282:GLN:OE1	2.21	0.40
2:H:332:ILE:O	2:H:332:ILE:HG13	2.21	0.40
1:A:337:VAL:HG11	1:A:402:MET:HE2	2.03	0.40
1:A:596:HIS:HB3	1:A:597:TYR:CD2	2.57	0.40
1:A:679:LEU:HD22	1:A:720:THR:HB	2.02	0.40
1:D:67:ALA:O	1:D:653:ARG:HG3	2.22	0.40
1:D:207:LEU:HD11	1:D:212:MET:SD	2.62	0.40
2:E:310:TYR:CZ	2:E:330:ASN:HB2	2.57	0.40
2:F:11:ASP:OD1	2:F:13:LEU:HD12	2.22	0.40
2:G:200:VAL:C	2:G:202:ALA:H	2.28	0.40
2:H:13:LEU:O	2:H:32:LYS:CD	2.66	0.40
2:H:370:LEU:O	2:H:372:ASN:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	732/761 (96%)	672 (92%)	57 (8%)	3 (0%)	30	67
1	B	733/761 (96%)	679 (93%)	50 (7%)	4 (0%)	24	63
1	C	731/761 (96%)	681 (93%)	48 (7%)	2 (0%)	36	71
1	D	734/761 (96%)	673 (92%)	59 (8%)	2 (0%)	36	71
2	E	350/375 (93%)	325 (93%)	25 (7%)	0	100	100
2	F	354/375 (94%)	326 (92%)	28 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	353/375 (94%)	328 (93%)	25 (7%)	0	100	100
2	H	352/375 (94%)	327 (93%)	24 (7%)	1 (0%)	36	71
All	All	4339/4544 (96%)	4011 (92%)	316 (7%)	12 (0%)	36	71

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	731	TYR
1	C	731	TYR
1	D	731	TYR
1	B	300	GLY
2	H	324	PRO
1	A	634	GLY
1	A	731	TYR
1	B	634	GLY
1	D	634	GLY
1	C	634	GLY
1	B	362	PRO
1	A	362	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	629/651 (97%)	538 (86%)	91 (14%)	3	14
1	B	629/651 (97%)	543 (86%)	86 (14%)	3	15
1	C	629/651 (97%)	535 (85%)	94 (15%)	3	14
1	D	630/651 (97%)	541 (86%)	89 (14%)	3	15
2	E	321/340 (94%)	287 (89%)	34 (11%)	6	22
2	F	325/340 (96%)	292 (90%)	33 (10%)	7	23
2	G	324/340 (95%)	290 (90%)	34 (10%)	6	22
2	H	323/340 (95%)	286 (88%)	37 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3810/3964 (96%)	3312 (87%)	498 (13%)	4 16

All (498) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	5	LEU
1	A	11	ASP
1	A	19	LEU
1	A	27	ASP
1	A	34	HIS
1	A	44	ARG
1	A	47	ILE
1	A	50	TYR
1	A	54	LYS
1	A	60	GLU
1	A	64	LYS
1	A	72	ARG
1	A	83	ARG
1	A	102	LEU
1	A	138	ASP
1	A	144	SER
1	A	154	LYS
1	A	170	GLN
1	A	171	PHE
1	A	172	LEU
1	A	175	LEU
1	A	184	TYR
1	A	186	ARG
1	A	188	THR
1	A	211	ILE
1	A	212	MET
1	A	213	SER
1	A	220	ARG
1	A	224	SER
1	A	225	CYS
1	A	228	ILE
1	A	233	SER
1	A	234	LEU
1	A	237	ILE
1	A	260	ARG
1	A	269	ARG

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Mol	Chain	Res	Type
1	A	276	THR
1	A	287	THR
1	A	289	VAL
1	A	294	GLN
1	A	304	LEU
1	A	318	VAL
1	A	319	LEU
1	A	322	ASN
1	A	340	ASN
1	A	354	THR
1	A	364	LEU
1	A	380	THR
1	A	386	ASP
1	A	390	LYS
1	A	394	LYS
1	A	402	MET
1	A	404	GLN
1	A	435	GLN
1	A	440	LEU
1	A	441	GLU
1	A	446	THR
1	A	450	ASN
1	A	461	LEU
1	A	462	CYS
1	A	463	THR
1	A	465	SER
1	A	476	ASP
1	A	489	LEU
1	A	513	LEU
1	A	519	ASN
1	A	542	LYS
1	A	548	GLN
1	A	560	LYS
1	A	561	GLU
1	A	562	GLN
1	A	569	ASN
1	A	578	LEU
1	A	581	ASP
1	A	582	THR
1	A	589	THR
1	A	592	ASN
1	A	623	GLU

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Mol	Chain	Res	Type
1	A	624	THR
1	A	636	GLU
1	A	647	SER
1	A	660	GLU
1	A	661	HIS
1	A	663	HIS
1	A	691	GLN
1	A	693	ILE
1	A	696	ASN
1	A	697	THR
1	A	698	ASN
1	A	734	THR
1	B	5	LEU
1	B	11	ASP
1	B	19	LEU
1	B	27	ASP
1	B	34	HIS
1	B	44	ARG
1	B	47	ILE
1	B	50	TYR
1	B	60	GLU
1	B	64	LYS
1	B	102	LEU
1	B	111	GLU
1	B	138	ASP
1	B	154	LYS
1	B	167	GLU
1	B	171	PHE
1	B	172	LEU
1	B	175	LEU
1	B	184	TYR
1	B	186	ARG
1	B	189	ARG
1	B	207	LEU
1	B	220	ARG
1	B	221	GLN
1	B	226	VAL
1	B	228	ILE
1	B	233	SER
1	B	234	LEU
1	B	237	ILE
1	B	249	SER

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Mol	Chain	Res	Type
1	B	260	ARG
1	B	262	ARG
1	B	269	ARG
1	B	276	THR
1	B	283	LYS
1	B	286	GLN
1	B	287	THR
1	B	289	VAL
1	B	297	VAL
1	B	298	ARG
1	B	304	LEU
1	B	317	LEU
1	B	318	VAL
1	B	319	LEU
1	B	322	ASN
1	B	330	VAL
1	B	331	ARG
1	B	354	THR
1	B	380	THR
1	B	386	ASP
1	B	394	LYS
1	B	402	MET
1	B	404	GLN
1	B	440	LEU
1	B	441	GLU
1	B	446	THR
1	B	450	ASN
1	B	461	LEU
1	B	463	THR
1	B	472	ILE
1	B	476	ASP
1	B	479	GLU
1	B	489	LEU
1	B	515	ILE
1	B	519	ASN
1	B	569	ASN
1	B	578	LEU
1	B	581	ASP
1	B	582	THR
1	B	592	ASN
1	B	623	GLU
1	B	636	GLU

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Mol	Chain	Res	Type
1	B	647	SER
1	B	649	ASP
1	B	660	GLU
1	B	661	HIS
1	B	663	HIS
1	B	693	ILE
1	B	696	ASN
1	B	697	THR
1	B	698	ASN
1	B	702	SER
1	B	732	GLN
1	B	733	ASN
1	B	735	ARG
1	B	736	ASP
1	C	4	ASN
1	C	5	LEU
1	C	6	LEU
1	C	11	ASP
1	C	14	THR
1	C	19	LEU
1	C	27	ASP
1	C	34	HIS
1	C	37	SER
1	C	44	ARG
1	C	47	ILE
1	C	50	TYR
1	C	53	ILE
1	C	54	LYS
1	C	60	GLU
1	C	64	LYS
1	C	83	ARG
1	C	102	LEU
1	C	114	LYS
1	C	138	ASP
1	C	154	LYS
1	C	171	PHE
1	C	175	LEU
1	C	184	TYR
1	C	186	ARG
1	C	189	ARG
1	C	207	LEU
1	C	213	SER

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Mol	Chain	Res	Type
1	C	216	ARG
1	C	220	ARG
1	C	221	GLN
1	C	226	VAL
1	C	228	ILE
1	C	233	SER
1	C	234	LEU
1	C	237	ILE
1	C	246	LYS
1	C	256	ILE
1	C	260	ARG
1	C	269	ARG
1	C	276	THR
1	C	287	THR
1	C	289	VAL
1	C	304	LEU
1	C	317	LEU
1	C	319	LEU
1	C	322	ASN
1	C	329	ARG
1	C	331	ARG
1	C	354	THR
1	C	380	THR
1	C	386	ASP
1	C	394	LYS
1	C	402	MET
1	C	404	GLN
1	C	420	CYS
1	C	422	THR
1	C	438	LEU
1	C	440	LEU
1	C	441	GLU
1	C	446	THR
1	C	450	ASN
1	C	461	LEU
1	C	462	CYS
1	C	463	THR
1	C	464	LEU
1	C	472	ILE
1	C	476	ASP
1	C	489	LEU
1	C	515	ILE

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Mol	Chain	Res	Type
1	C	519	ASN
1	C	560	LYS
1	C	569	ASN
1	C	578	LEU
1	C	581	ASP
1	C	582	THR
1	C	592	ASN
1	C	620	MET
1	C	623	GLU
1	C	636	GLU
1	C	647	SER
1	C	649	ASP
1	C	660	GLU
1	C	661	HIS
1	C	663	HIS
1	C	689	ILE
1	C	693	ILE
1	C	696	ASN
1	C	697	THR
1	C	698	ASN
1	C	704	PHE
1	C	734	THR
1	C	735	ARG
1	C	736	ASP
1	D	5	LEU
1	D	11	ASP
1	D	19	LEU
1	D	27	ASP
1	D	34	HIS
1	D	44	ARG
1	D	47	ILE
1	D	50	TYR
1	D	54	LYS
1	D	60	GLU
1	D	64	LYS
1	D	83	ARG
1	D	102	LEU
1	D	111	GLU
1	D	138	ASP
1	D	144	SER
1	D	151	LEU
1	D	165	ILE

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Mol	Chain	Res	Type
1	D	171	PHE
1	D	172	LEU
1	D	175	LEU
1	D	184	TYR
1	D	186	ARG
1	D	188	THR
1	D	207	LEU
1	D	212	MET
1	D	213	SER
1	D	220	ARG
1	D	221	GLN
1	D	224	SER
1	D	226	VAL
1	D	228	ILE
1	D	233	SER
1	D	234	LEU
1	D	237	ILE
1	D	248	VAL
1	D	269	ARG
1	D	276	THR
1	D	287	THR
1	D	289	VAL
1	D	294	GLN
1	D	304	LEU
1	D	319	LEU
1	D	322	ASN
1	D	330	VAL
1	D	331	ARG
1	D	354	THR
1	D	364	LEU
1	D	380	THR
1	D	386	ASP
1	D	394	LYS
1	D	402	MET
1	D	404	GLN
1	D	420	CYS
1	D	438	LEU
1	D	440	LEU
1	D	441	GLU
1	D	446	THR
1	D	450	ASN
1	D	461	LEU

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Mol	Chain	Res	Type
1	D	463	THR
1	D	465	SER
1	D	472	ILE
1	D	476	ASP
1	D	489	LEU
1	D	519	ASN
1	D	560	LYS
1	D	578	LEU
1	D	581	ASP
1	D	582	THR
1	D	592	ASN
1	D	623	GLU
1	D	624	THR
1	D	636	GLU
1	D	660	GLU
1	D	661	HIS
1	D	663	HIS
1	D	664	ASP
1	D	691	GLN
1	D	693	ILE
1	D	696	ASN
1	D	697	THR
1	D	698	ASN
1	D	703	ARG
1	D	704	PHE
1	D	708	LYS
1	D	733	ASN
1	D	734	THR
1	D	735	ARG
2	E	7	GLN
2	E	8	THR
2	E	9	LYS
2	E	54	ASP
2	E	57	ARG
2	E	63	GLN
2	E	87	GLN
2	E	89	ARG
2	E	100	SER
2	E	101	ILE
2	E	127	ARG
2	E	144	GLU
2	E	145	GLN

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Mol	Chain	Res	Type
2	E	148	LYS
2	E	163	MET
2	E	176	THR
2	E	177	VAL
2	E	192	LYS
2	E	204	GLU
2	E	208	PHE
2	E	249	LEU
2	E	276	PHE
2	E	278	GLN
2	E	315	ARG
2	E	327	THR
2	E	328	ARG
2	E	329	SER
2	E	332	ILE
2	E	339	LEU
2	E	363	SER
2	E	368	ASP
2	E	370	LEU
2	E	373	PHE
2	E	374	GLN
2	F	13	LEU
2	F	21	GLN
2	F	42	LYS
2	F	54	ASP
2	F	57	ARG
2	F	63	GLN
2	F	87	GLN
2	F	100	SER
2	F	101	ILE
2	F	127	ARG
2	F	144	GLU
2	F	145	GLN
2	F	148	LYS
2	F	163	MET
2	F	170	LEU
2	F	176	THR
2	F	181	THR
2	F	183	THR
2	F	192	LYS
2	F	204	GLU
2	F	208	PHE

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Mol	Chain	Res	Type
2	F	249	LEU
2	F	276	PHE
2	F	278	GLN
2	F	315	ARG
2	F	327	THR
2	F	328	ARG
2	F	329	SER
2	F	343	ASN
2	F	365	VAL
2	F	368	ASP
2	F	372	ASN
2	F	373	PHE
2	G	21	GLN
2	G	54	ASP
2	G	57	ARG
2	G	63	GLN
2	G	87	GLN
2	G	89	ARG
2	G	93	VAL
2	G	100	SER
2	G	101	ILE
2	G	127	ARG
2	G	144	GLU
2	G	145	GLN
2	G	148	LYS
2	G	163	MET
2	G	170	LEU
2	G	180	LYS
2	G	181	THR
2	G	192	LYS
2	G	204	GLU
2	G	208	PHE
2	G	249	LEU
2	G	271	GLU
2	G	276	PHE
2	G	278	GLN
2	G	315	ARG
2	G	329	SER
2	G	332	ILE
2	G	339	LEU
2	G	340	VAL
2	G	342	ASP

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Mol	Chain	Res	Type
2	G	361	ILE
2	G	363	SER
2	G	366	ASP
2	G	372	ASN
2	H	7	GLN
2	H	8	THR
2	H	9	LYS
2	H	54	ASP
2	H	57	ARG
2	H	63	GLN
2	H	87	GLN
2	H	89	ARG
2	H	93	VAL
2	H	95	LEU
2	H	100	SER
2	H	101	ILE
2	H	127	ARG
2	H	144	GLU
2	H	145	GLN
2	H	148	LYS
2	H	163	MET
2	H	170	LEU
2	H	177	VAL
2	H	178	ASN
2	H	192	LYS
2	H	208	PHE
2	H	249	LEU
2	H	276	PHE
2	H	278	GLN
2	H	315	ARG
2	H	322	ASP
2	H	323	LEU
2	H	325	PHE
2	H	327	THR
2	H	328	ARG
2	H	329	SER
2	H	339	LEU
2	H	364	GLU
2	H	365	VAL
2	H	366	ASP
2	H	375	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	78	GLN
1	A	150	GLN
1	A	158	GLN
1	A	191	GLN
1	A	221	GLN
1	A	250	GLN
1	A	275	HIS
1	A	328	ASN
1	A	338	GLN
1	A	404	GLN
1	A	415	GLN
1	A	421	ASN
1	A	435	GLN
1	A	450	ASN
1	A	453	ASN
1	A	519	ASN
1	A	569	ASN
1	A	592	ASN
1	A	613	ASN
1	A	630	ASN
1	A	686	GLN
1	A	696	ASN
1	A	712	GLN
1	A	713	GLN
1	B	4	ASN
1	B	59	HIS
1	B	78	GLN
1	B	88	HIS
1	B	130	GLN
1	B	150	GLN
1	B	158	GLN
1	B	191	GLN
1	B	221	GLN
1	B	250	GLN
1	B	257	ASN
1	B	275	HIS
1	B	286	GLN
1	B	328	ASN
1	B	338	GLN
1	B	404	GLN
1	B	415	GLN

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Mol	Chain	Res	Type
1	B	435	GLN
1	B	450	ASN
1	B	453	ASN
1	B	519	ASN
1	B	569	ASN
1	B	592	ASN
1	B	613	ASN
1	B	686	GLN
1	B	691	GLN
1	B	696	ASN
1	B	698	ASN
1	B	712	GLN
1	B	713	GLN
1	C	4	ASN
1	C	59	HIS
1	C	78	GLN
1	C	88	HIS
1	C	150	GLN
1	C	158	GLN
1	C	191	GLN
1	C	221	GLN
1	C	250	GLN
1	C	275	HIS
1	C	328	ASN
1	C	332	HIS
1	C	338	GLN
1	C	404	GLN
1	C	415	GLN
1	C	421	ASN
1	C	450	ASN
1	C	453	ASN
1	C	519	ASN
1	C	569	ASN
1	C	592	ASN
1	C	613	ASN
1	C	696	ASN
1	C	698	ASN
1	C	712	GLN
1	C	713	GLN
1	D	78	GLN
1	D	150	GLN
1	D	158	GLN

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Mol	Chain	Res	Type
1	D	191	GLN
1	D	221	GLN
1	D	257	ASN
1	D	275	HIS
1	D	328	ASN
1	D	338	GLN
1	D	404	GLN
1	D	415	GLN
1	D	435	GLN
1	D	450	ASN
1	D	453	ASN
1	D	519	ASN
1	D	592	ASN
1	D	613	ASN
1	D	627	GLN
1	D	630	ASN
1	D	686	GLN
1	D	696	ASN
1	D	698	ASN
1	D	713	GLN
1	D	733	ASN
2	E	7	GLN
2	E	76	ASN
2	E	124	HIS
2	E	128	ASN
2	E	227	ASN
2	E	246	GLN
2	E	278	GLN
2	E	313	ASN
2	E	317	GLN
2	E	336	ASN
2	F	7	GLN
2	F	21	GLN
2	F	76	ASN
2	F	124	HIS
2	F	128	ASN
2	F	227	ASN
2	F	246	GLN
2	F	278	GLN
2	F	313	ASN
2	F	317	GLN
2	F	372	ASN

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Mol	Chain	Res	Type
2	G	7	GLN
2	G	76	ASN
2	G	92	ASN
2	G	124	HIS
2	G	128	ASN
2	G	227	ASN
2	G	246	GLN
2	G	278	GLN
2	G	313	ASN
2	G	317	GLN
2	G	336	ASN
2	H	7	GLN
2	H	76	ASN
2	H	124	HIS
2	H	128	ASN
2	H	227	ASN
2	H	246	GLN
2	H	278	GLN
2	H	317	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	FEO	F	501	2,5	0,2,2	-	-	-		
3	ATP	A	801	-	32,33,33	2.01	9 (28%)	48,52,52	2.01	13 (27%)
3	ATP	B	801	-	32,33,33	2.02	9 (28%)	48,52,52	2.01	13 (27%)
3	ATP	C	801	-	32,33,33	2.02	10 (31%)	48,52,52	1.98	13 (27%)
4	FEO	G	501	2,5	0,2,2	-	-	-		
4	FEO	H	501	2,5	0,2,2	-	-	-		
3	ATP	D	801	-	32,33,33	2.03	10 (31%)	48,52,52	1.91	10 (20%)
4	FEO	E	501	2,5	0,2,2	-	-	-		

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
3	ATP	B	801	-	-	4/22/38/38	0/3/3/3
3	ATP	C	801	-	-	6/22/38/38	0/3/3/3
3	ATP	D	801	-	-	5/22/38/38	0/3/3/3
3	ATP	A	801	-	-	4/22/38/38	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	ATP	C6-N6	6.23	1.50	1.34
3	B	801	ATP	C6-N6	6.19	1.50	1.34
3	A	801	ATP	C6-N6	6.17	1.50	1.34
3	C	801	ATP	C6-N6	6.15	1.49	1.34
3	C	801	ATP	C2'-C3'	-4.44	1.41	1.53
3	D	801	ATP	C2'-C3'	-4.43	1.41	1.53
3	A	801	ATP	C2'-C3'	-4.43	1.41	1.53
3	B	801	ATP	C2'-C3'	-4.42	1.41	1.53
3	D	801	ATP	PA-O3A	-3.11	1.56	1.59
3	D	801	ATP	PB-O3A	-3.11	1.56	1.59
3	C	801	ATP	PB-O3A	-3.09	1.56	1.59
3	B	801	ATP	PB-O3A	-2.96	1.56	1.59
3	C	801	ATP	O4'-C1'	2.95	1.48	1.42
3	C	801	ATP	PA-O3A	-2.95	1.56	1.59
3	D	801	ATP	O4'-C1'	2.90	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	ATP	O4'-C1'	2.88	1.48	1.42
3	A	801	ATP	O4'-C1'	2.86	1.48	1.42
3	A	801	ATP	PB-O3A	-2.86	1.56	1.59
3	C	801	ATP	O4'-C4'	-2.85	1.38	1.45
3	A	801	ATP	PA-O3A	-2.83	1.56	1.59
3	B	801	ATP	PA-O3A	-2.82	1.56	1.59
3	B	801	ATP	O4'-C4'	-2.80	1.38	1.45
3	A	801	ATP	O4'-C4'	-2.76	1.38	1.45
3	D	801	ATP	O4'-C4'	-2.66	1.39	1.45
3	A	801	ATP	C5-N7	-2.55	1.34	1.39
3	B	801	ATP	C5-N7	-2.53	1.34	1.39
3	C	801	ATP	C5-N7	-2.53	1.34	1.39
3	C	801	ATP	O3'-C3'	-2.51	1.36	1.43
3	D	801	ATP	C5-N7	-2.46	1.34	1.39
3	D	801	ATP	O3'-C3'	-2.45	1.36	1.43
3	B	801	ATP	C8-N9	-2.42	1.33	1.37
3	A	801	ATP	O3'-C3'	-2.41	1.37	1.43
3	B	801	ATP	O3'-C3'	-2.41	1.37	1.43
3	A	801	ATP	C8-N9	-2.39	1.33	1.37
3	D	801	ATP	C8-N9	-2.28	1.33	1.37
3	D	801	ATP	PB-O3B	-2.21	1.57	1.59
3	C	801	ATP	PB-O3B	-2.15	1.57	1.59
3	C	801	ATP	C8-N9	-2.15	1.33	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	ATP	O4'-C1'-N9	5.41	118.47	108.09
3	B	801	ATP	O4'-C1'-N9	5.41	118.47	108.09
3	D	801	ATP	C5-C4-N3	-5.33	119.38	126.72
3	B	801	ATP	C5-C4-N3	-5.27	119.46	126.72
3	A	801	ATP	C5-C4-N3	-5.27	119.46	126.72
3	C	801	ATP	C5-C4-N3	-5.17	119.60	126.72
3	C	801	ATP	N3-C2-N1	-4.84	121.25	128.58
3	B	801	ATP	N3-C2-N1	-4.72	121.43	128.58
3	A	801	ATP	N3-C2-N1	-4.72	121.44	128.58
3	D	801	ATP	N3-C2-N1	-4.72	121.44	128.58
3	D	801	ATP	O4'-C1'-N9	4.44	116.61	108.09
3	D	801	ATP	N3-C4-N9	4.02	134.00	127.17
3	C	801	ATP	O4'-C1'-N9	4.02	115.80	108.09
3	C	801	ATP	N3-C4-N9	3.99	133.94	127.17
3	C	801	ATP	C2'-C1'-N9	-3.96	103.46	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	ATP	N3-C4-N9	3.91	133.81	127.17
3	B	801	ATP	N3-C4-N9	3.90	133.80	127.17
3	D	801	ATP	C2-N3-C4	3.62	120.67	111.83
3	A	801	ATP	C2-N3-C4	3.58	120.57	111.83
3	C	801	ATP	C2-N3-C4	3.57	120.55	111.83
3	B	801	ATP	C2-N3-C4	3.56	120.52	111.83
3	C	801	ATP	N9-C8-N7	-3.55	108.90	113.94
3	D	801	ATP	N9-C8-N7	-3.51	108.96	113.94
3	A	801	ATP	N9-C8-N7	-3.44	109.06	113.94
3	B	801	ATP	N9-C8-N7	-3.42	109.09	113.94
3	C	801	ATP	C4-N9-C8	3.00	108.88	105.74
3	D	801	ATP	C4-N9-C8	2.95	108.83	105.74
3	A	801	ATP	C4-N9-C8	2.85	108.73	105.74
3	B	801	ATP	C4-N9-C8	2.84	108.72	105.74
3	D	801	ATP	C5-N7-C8	2.67	107.64	103.45
3	B	801	ATP	O5'-C5'-C4'	2.65	118.03	108.99
3	A	801	ATP	O5'-C5'-C4'	2.64	118.00	108.99
3	C	801	ATP	C5-N7-C8	2.61	107.55	103.45
3	A	801	ATP	C5-N7-C8	2.60	107.54	103.45
3	B	801	ATP	C5-N7-C8	2.58	107.50	103.45
3	A	801	ATP	C3'-C2'-C1'	2.57	106.32	101.46
3	B	801	ATP	C3'-C2'-C1'	2.56	106.30	101.46
3	D	801	ATP	O5'-C5'-C4'	2.45	117.32	108.99
3	D	801	ATP	C4-C5-N7	-2.31	107.94	110.58
3	A	801	ATP	C4-C5-N7	-2.30	107.95	110.58
3	B	801	ATP	C4-C5-N7	-2.30	107.95	110.58
3	A	801	ATP	C2'-C3'-C4'	2.21	106.89	102.61
3	B	801	ATP	C2'-C3'-C4'	2.21	106.88	102.61
3	C	801	ATP	C2'-C3'-C4'	2.16	106.78	102.61
3	B	801	ATP	O2'-C2'-C1'	-2.14	102.72	110.10
3	A	801	ATP	O2'-C2'-C1'	-2.13	102.77	110.10
3	C	801	ATP	O5'-C5'-C4'	2.11	116.16	108.99
3	C	801	ATP	O3'-C3'-C4'	-2.09	105.07	111.08
3	C	801	ATP	C4-C5-N7	-2.07	108.22	110.58

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	ATP	PB-O3A-PA-O5'
3	B	801	ATP	PB-O3A-PA-O5'
3	C	801	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	801	ATP	C5'-O5'-PA-O2A
3	C	801	ATP	C5'-O5'-PA-O3A
3	D	801	ATP	C5'-O5'-PA-O1A
3	D	801	ATP	C5'-O5'-PA-O2A
3	D	801	ATP	C5'-O5'-PA-O3A
3	D	801	ATP	O4'-C4'-C5'-O5'
3	D	801	ATP	C3'-C4'-C5'-O5'
3	A	801	ATP	O4'-C4'-C5'-O5'
3	A	801	ATP	C3'-C4'-C5'-O5'
3	B	801	ATP	O4'-C4'-C5'-O5'
3	B	801	ATP	C3'-C4'-C5'-O5'
3	C	801	ATP	O4'-C4'-C5'-O5'
3	C	801	ATP	C3'-C4'-C5'-O5'
3	C	801	ATP	PB-O3A-PA-O5'
3	A	801	ATP	PG-O3B-PB-O2B
3	B	801	ATP	PG-O3B-PB-O2B

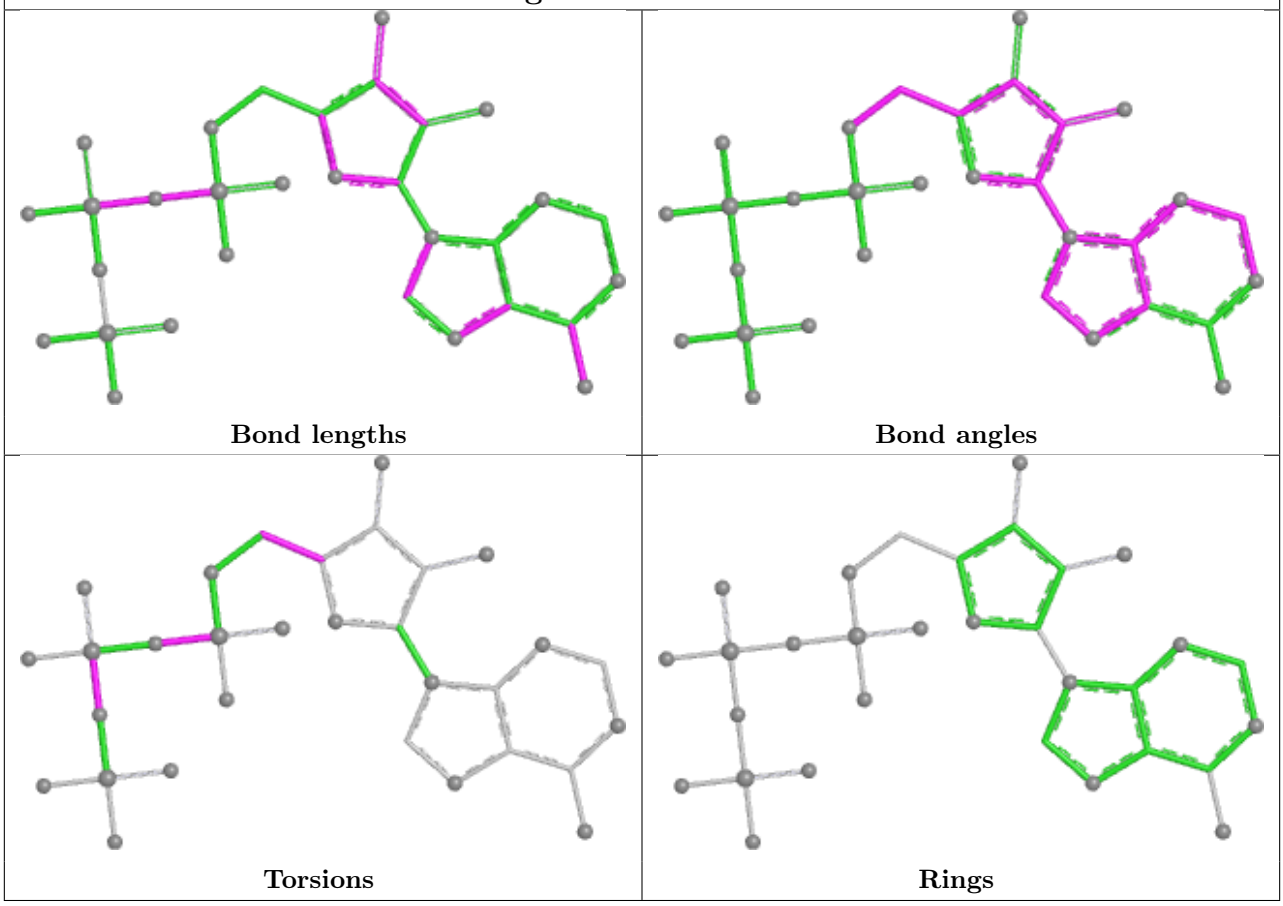
There are no ring outliers.

4 monomers are involved in 38 short contacts:

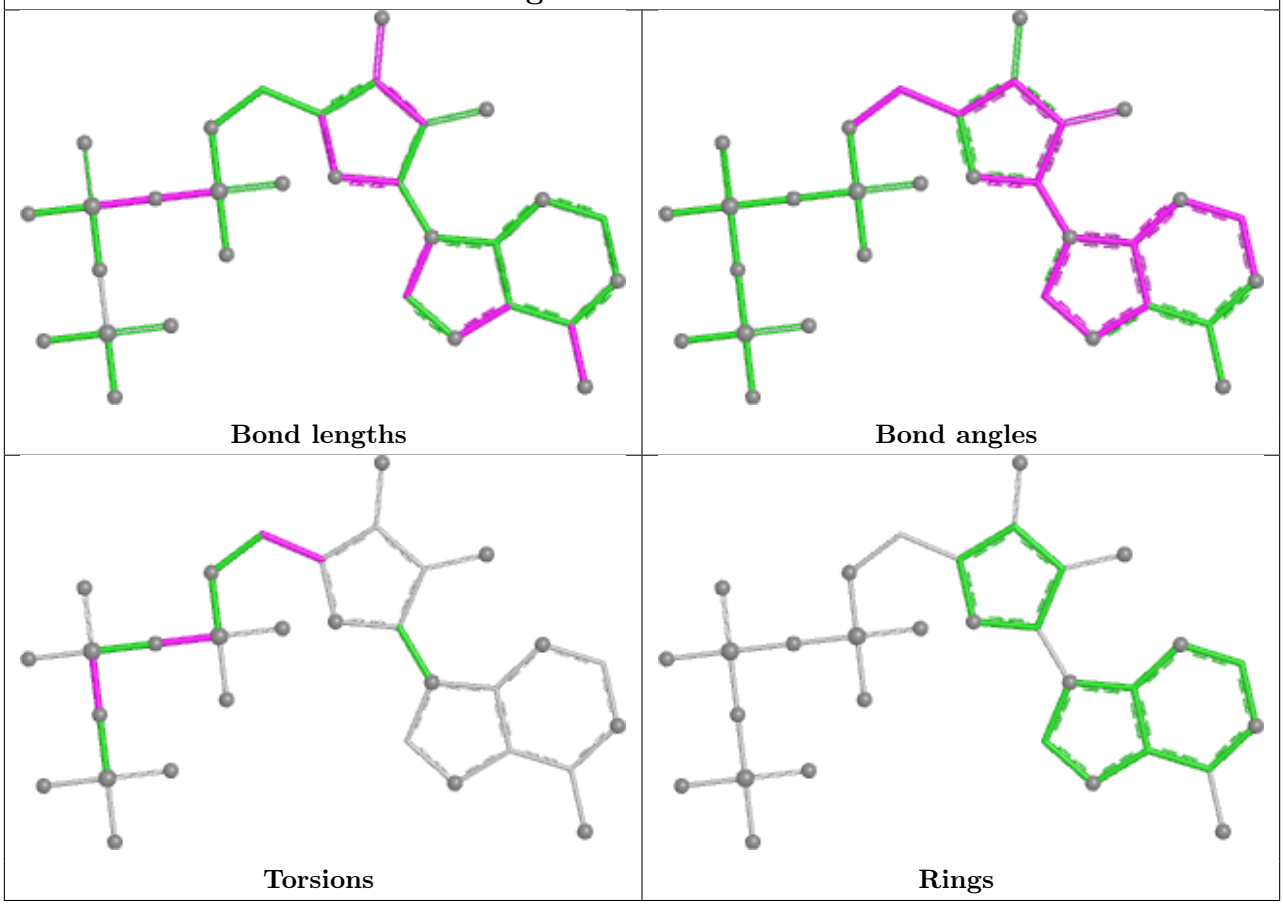
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	ATP	4	0
3	B	801	ATP	9	0
3	C	801	ATP	15	0
3	D	801	ATP	10	0

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 then 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.

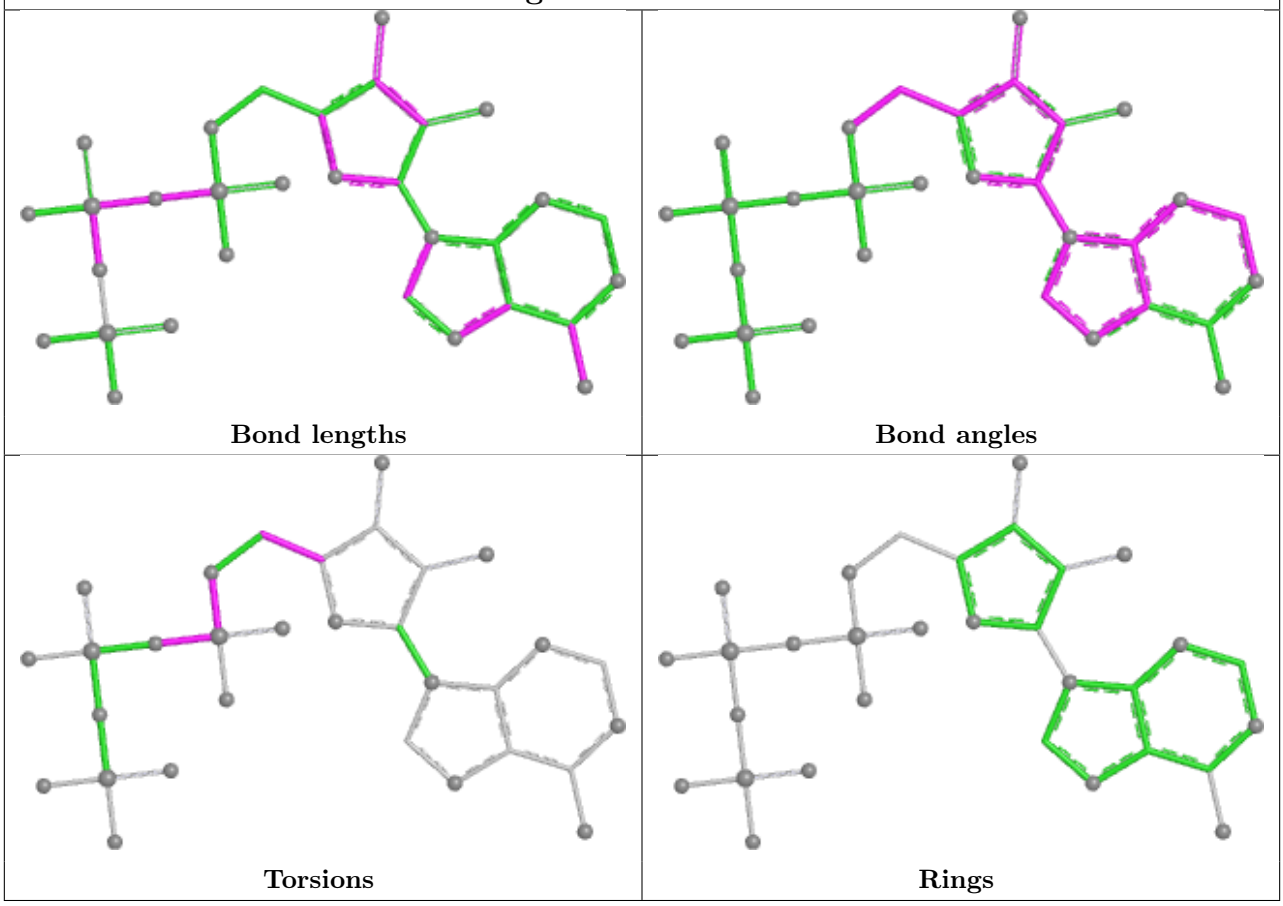
Ligand ATP A 801



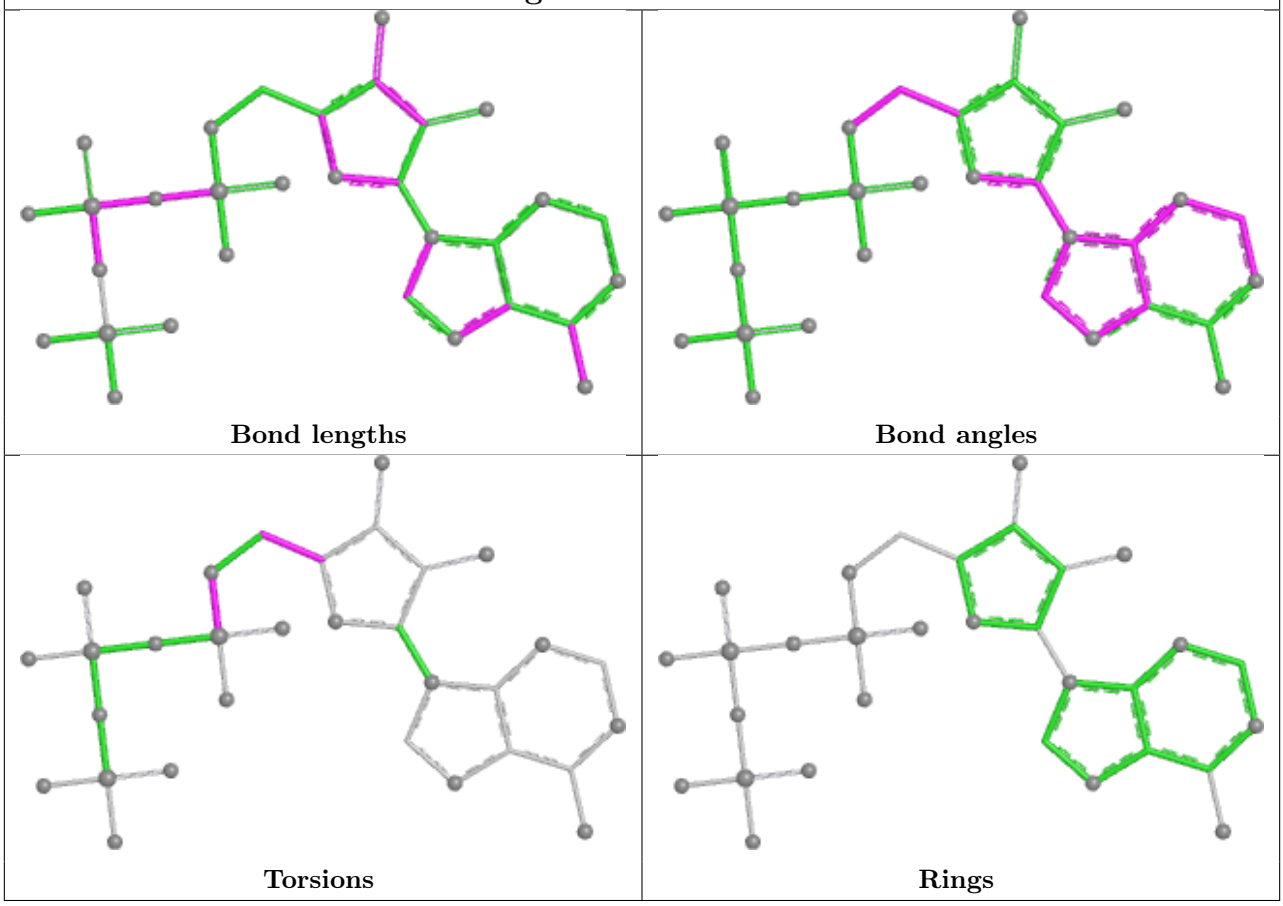
Ligand ATP B 801



Ligand ATP C 801



Ligand ATP D 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	734/761 (96%)	0.32	16 (2%)	62	49	62, 120, 165, 251	0
1	B	735/761 (96%)	0.41	22 (2%)	52	41	76, 152, 200, 256	0
1	C	733/761 (96%)	0.34	16 (2%)	62	49	63, 128, 171, 261	0
1	D	736/761 (96%)	0.36	11 (1%)	72	57	68, 133, 187, 253	0
2	E	354/375 (94%)	0.44	8 (2%)	61	48	77, 152, 210, 243	0
2	F	358/375 (95%)	0.46	7 (1%)	65	51	74, 151, 209, 256	0
2	G	357/375 (95%)	0.43	6 (1%)	69	55	96, 162, 207, 255	0
2	H	356/375 (94%)	0.37	12 (3%)	48	39	117, 172, 208, 267	0
All	All	4363/4544 (96%)	0.38	98 (2%)	62	49	62, 141, 198, 267	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	PHE	4.8
1	D	268	ILE	4.2
1	D	222	PHE	4.1
2	F	170	LEU	3.9
1	D	152	GLU	3.8
2	F	12	GLN	3.7
2	E	157	TYR	3.2
2	F	94	ALA	3.2
1	C	294	GLN	3.2
1	B	281	PHE	3.2
1	B	275	HIS	3.1
2	E	1	ALA	3.0
1	D	273	ALA	3.0
1	B	296	GLY	3.0
1	C	462	CYS	2.9
1	A	26	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	325	PHE	2.9
2	E	181	THR	2.8
1	B	49	PHE	2.8
1	A	647	SER	2.8
1	C	224	SER	2.8
2	H	2	TYR	2.8
1	B	622	SER	2.8
1	D	465	SER	2.7
2	G	361	ILE	2.7
2	E	176	THR	2.6
1	A	737	GLY	2.6
1	B	267	PRO	2.6
1	A	261	ILE	2.5
1	A	268	ILE	2.5
1	B	223	SER	2.5
1	B	328	ASN	2.5
2	G	126	ILE	2.5
1	B	327	GLY	2.5
1	B	295	GLY	2.5
1	B	467	PHE	2.4
1	C	213	SER	2.4
1	A	253	GLY	2.4
1	C	300	GLY	2.4
2	H	94	ALA	2.4
2	H	370	LEU	2.4
2	G	272	CYS	2.4
1	D	3	GLN	2.4
1	B	213	SER	2.4
1	B	268	ILE	2.4
2	H	144	GLU	2.3
2	H	1	ALA	2.3
1	B	156	LEU	2.3
2	H	92	ASN	2.3
1	A	294	GLN	2.3
1	A	461	LEU	2.3
1	C	155	TYR	2.3
1	B	263	ALA	2.3
1	C	268	ILE	2.3
1	B	266	SER	2.3
2	F	109	GLU	2.3
2	G	293	ASP	2.3
2	H	142	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	2.3
2	H	177	VAL	2.3
2	E	313	ASN	2.2
2	G	313	ASN	2.2
2	H	141	VAL	2.2
1	A	435	GLN	2.2
2	E	86	ILE	2.2
1	A	462	CYS	2.2
2	E	248	MET	2.2
2	H	148	LYS	2.2
1	D	143	PHE	2.2
1	D	213	SER	2.2
1	C	5	LEU	2.2
1	C	719	LEU	2.2
1	B	300	GLY	2.2
1	B	274	PHE	2.2
1	A	301	ALA	2.2
2	G	170	LEU	2.2
1	B	580	ILE	2.1
1	A	188	THR	2.1
1	A	247	TYR	2.1
1	A	152	GLU	2.1
1	B	376	GLU	2.1
2	H	178	ASN	2.1
1	C	216	ARG	2.1
1	C	225	CYS	2.1
1	B	363	GLY	2.1
1	C	49	PHE	2.1
1	C	273	ALA	2.1
2	F	1	ALA	2.1
1	A	295	GLY	2.1
1	D	332	HIS	2.1
2	H	182	VAL	2.1
1	D	166	TYR	2.0
2	E	166	TYR	2.0
1	C	234	LEU	2.0
2	F	2	TYR	2.0
1	C	251	ARG	2.0
1	D	272	GLU	2.0
1	B	625	SER	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)

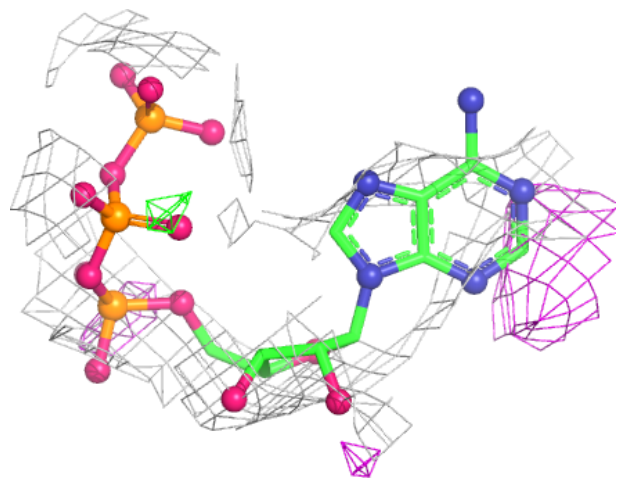
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

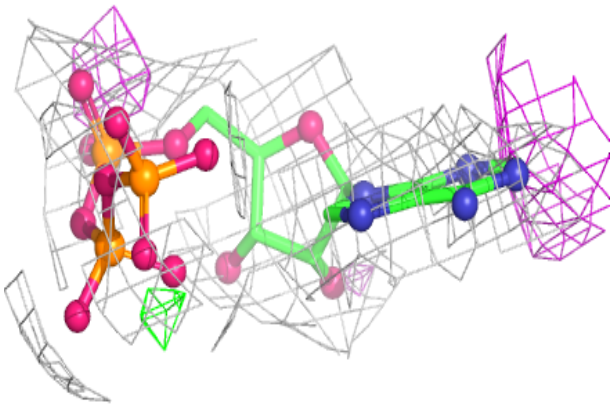
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ATP	C	801	31/31	0.86	0.16	138,138,138,138	0
3	ATP	D	801	31/31	0.88	0.12	195,195,195,195	0
3	ATP	B	801	31/31	0.89	0.09	225,225,225,225	0
3	ATP	A	801	31/31	0.93	0.11	126,126,126,126	0
4	FEO	F	501	3/3	0.98	0.09	106,106,106,106	0
4	FEO	E	501	3/3	0.99	0.07	119,119,119,119	0
4	FEO	G	501	3/3	0.99	0.07	124,124,124,124	0
4	FEO	H	501	3/3	0.99	0.07	133,133,133,133	0

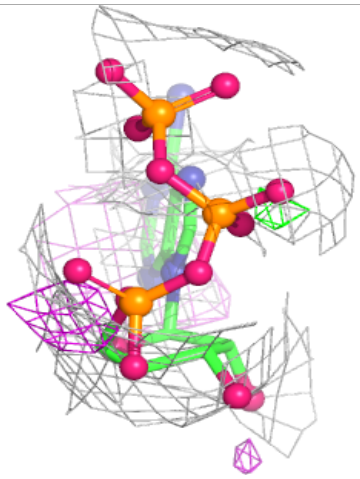
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 801:

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

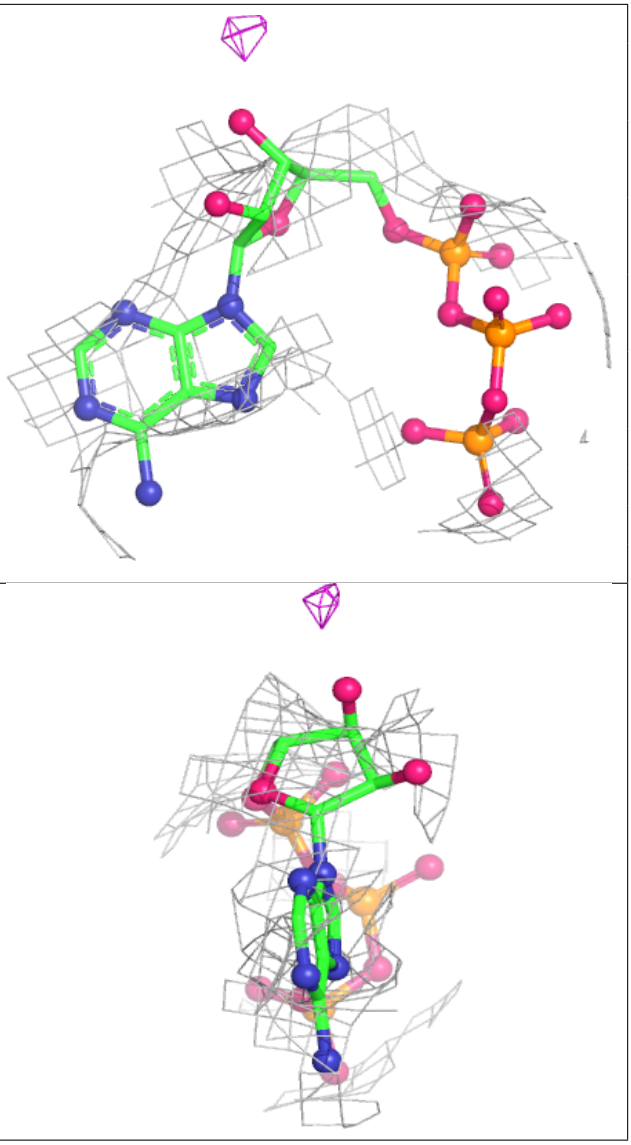






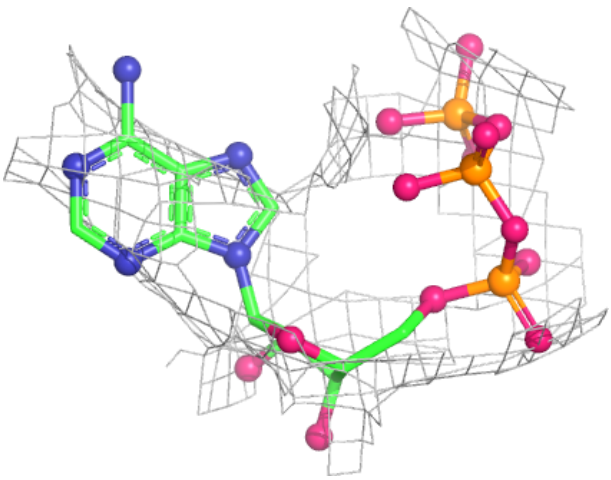
Electron density around ATP D 801:

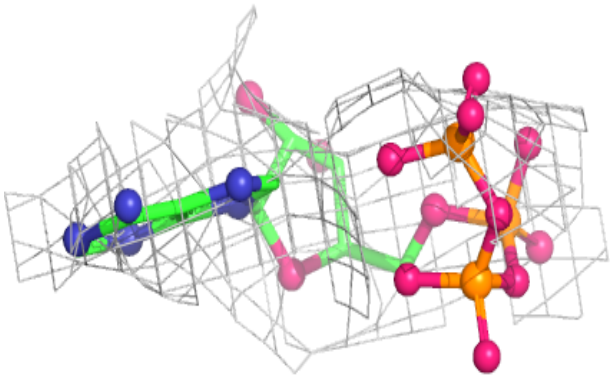
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

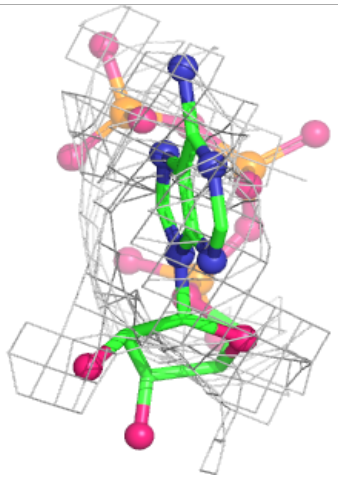


Electron density around ATP B 801:

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

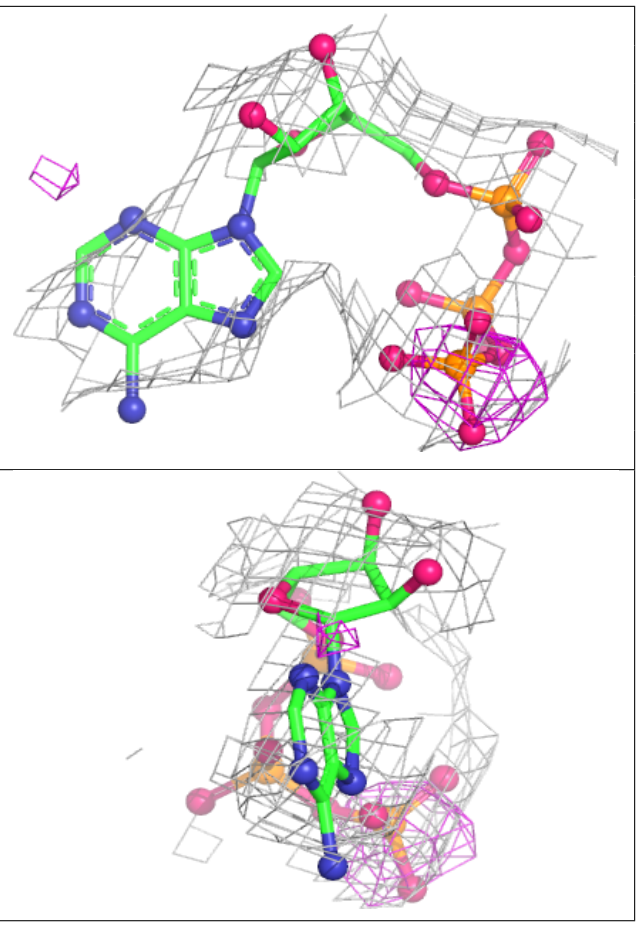






Electron density around ATP A 801:

$2mF_o$-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 (i)

There are no such residues in this entry.