Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 01:59 PM EDT

PDB ID	:	2ZBK
Title	:	Crystal structure of an intact type II DNA topoisomerase: insights into DNA transfer mechanisms
Authors	:	Graille, M.; Cladiere, L.; Durand, D.; Lecointe, F.; Forterre, P.; van Tilbeurgh, H.; Paris-Sud Yeast Structural Genomics (YSG)
Deposited on	:	2007-10-22
Resolution	:	3.56 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:

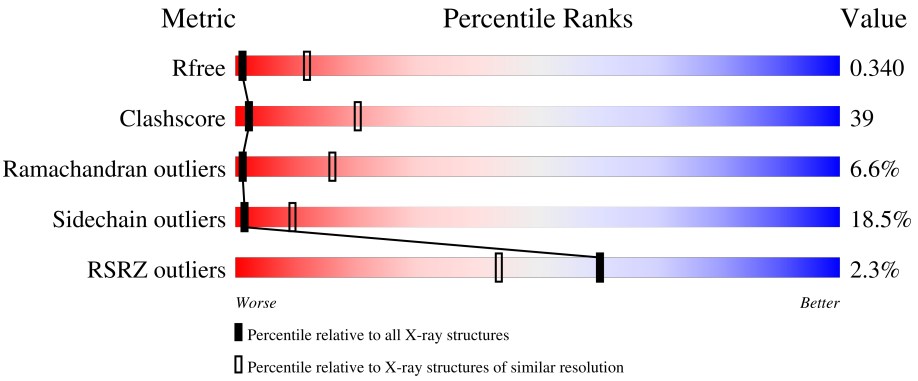
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.56 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}	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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	389	24% 44% 20% • 11%
1	C	389	23% 44% 19% • 11%
1	E	389	25% 42% 19% • 11%
1	G	389	25% 43% 19% • 11%

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Mol	Chain	Length	Quality of chain
2	B	530	2% 50% 36% 8% • 5%
2	D	530	2% 52% 36% 7% • 5%
2	F	530	2% 52% 36% 7% 5%
2	H	530	4% 52% 37% 7% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27776 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.

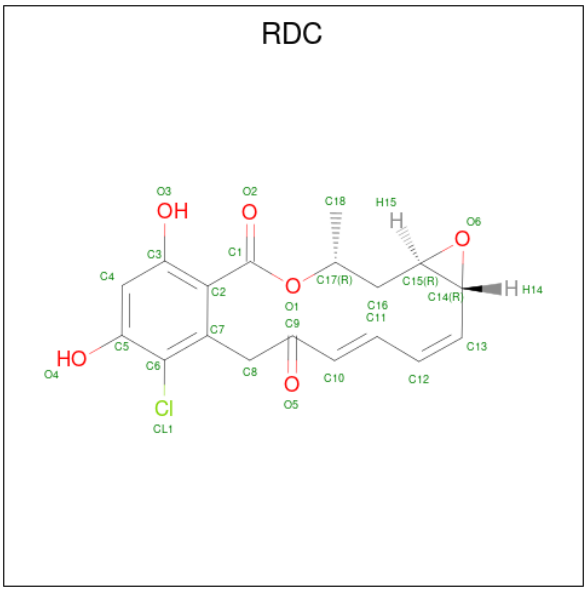
- Molecule 1 is a protein called Type II DNA topoisomerase VI subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2842	1828	483	524	7			
1	C	347	Total	C	N	O	S	0	0	0
			2842	1828	483	524	7			
1	E	347	Total	C	N	O	S	0	0	0
			2842	1828	483	524	7			
1	G	347	Total	C	N	O	S	0	0	0
			2842	1828	483	524	7			

- Molecule 2 is a protein called Type 2 DNA topoisomerase 6 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	506	Total	C	N	O	S	0	0	0
			4077	2625	683	763	6			
2	D	506	Total	C	N	O	S	0	0	0
			4077	2625	683	763	6			
2	F	506	Total	C	N	O	S	0	0	0
			4077	2625	683	763	6			
2	H	506	Total	C	N	O	S	0	0	0
			4077	2625	683	763	6			

- Molecule 3 is RADICICOL (three-letter code: RDC) (formula: $C_{18}H_{17}ClO_6$).



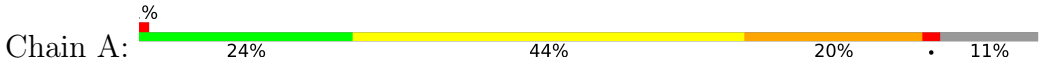
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	Cl	O	0	0
			25	18	1	6		
3	D	1	Total	C	Cl	O	0	0
			25	18	1	6		
3	F	1	Total	C	Cl	O	0	0
			25	18	1	6		
3	H	1	Total	C	Cl	O	0	0
			25	18	1	6		

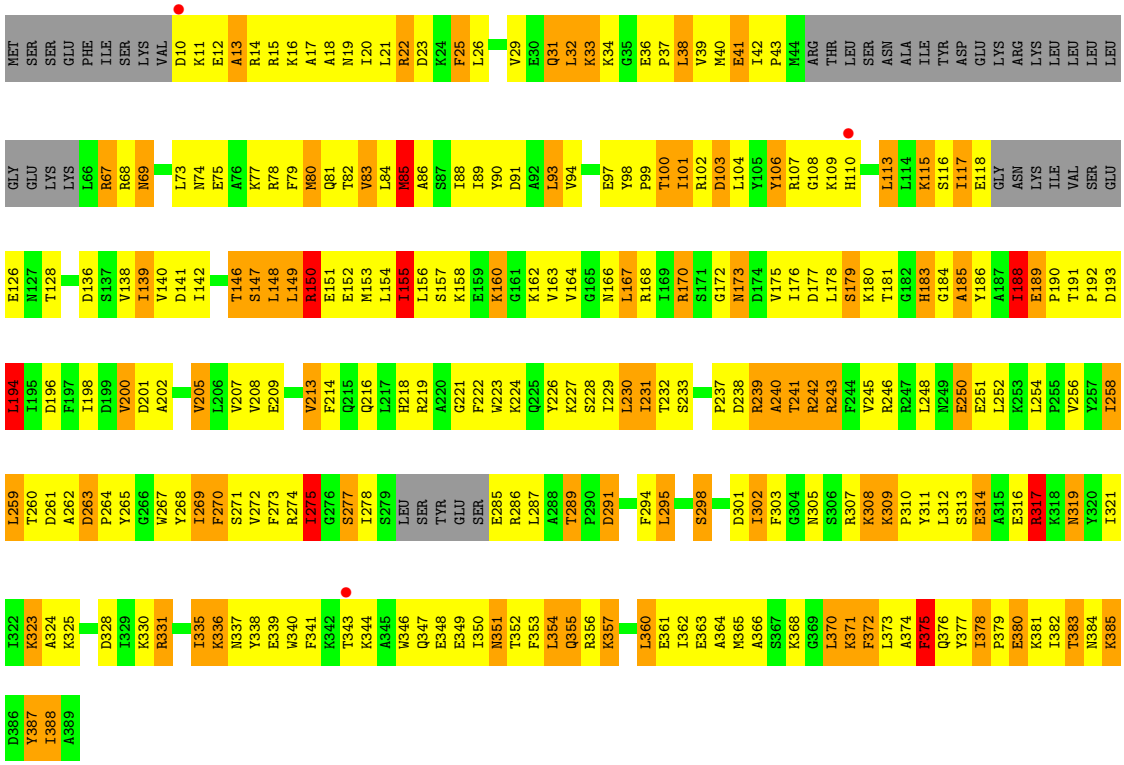
3 Residue-property plots (i)

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: Type II DNA topoisomerase VI subunit A

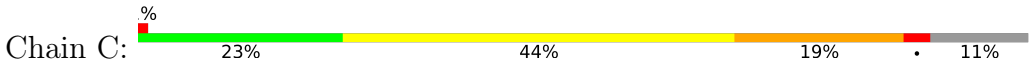
Chain A:

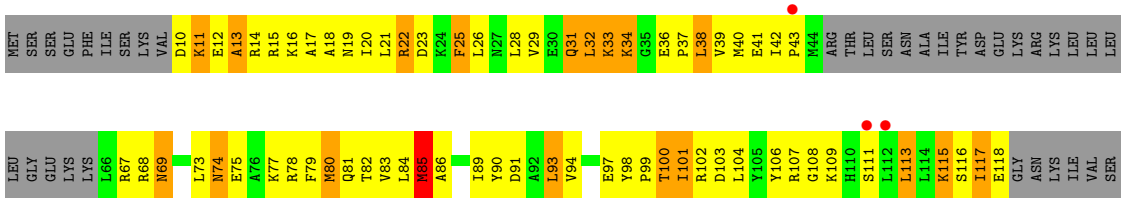


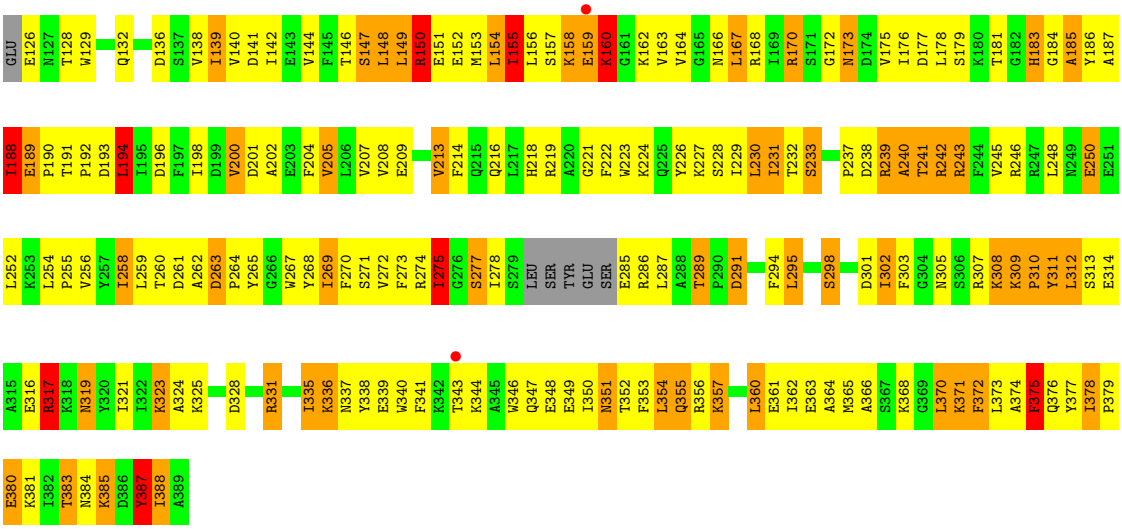


• Molecule 1: Type II DNA topoisomerase VI subunit A

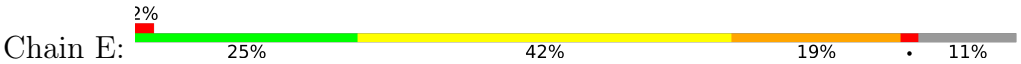
Chain C:

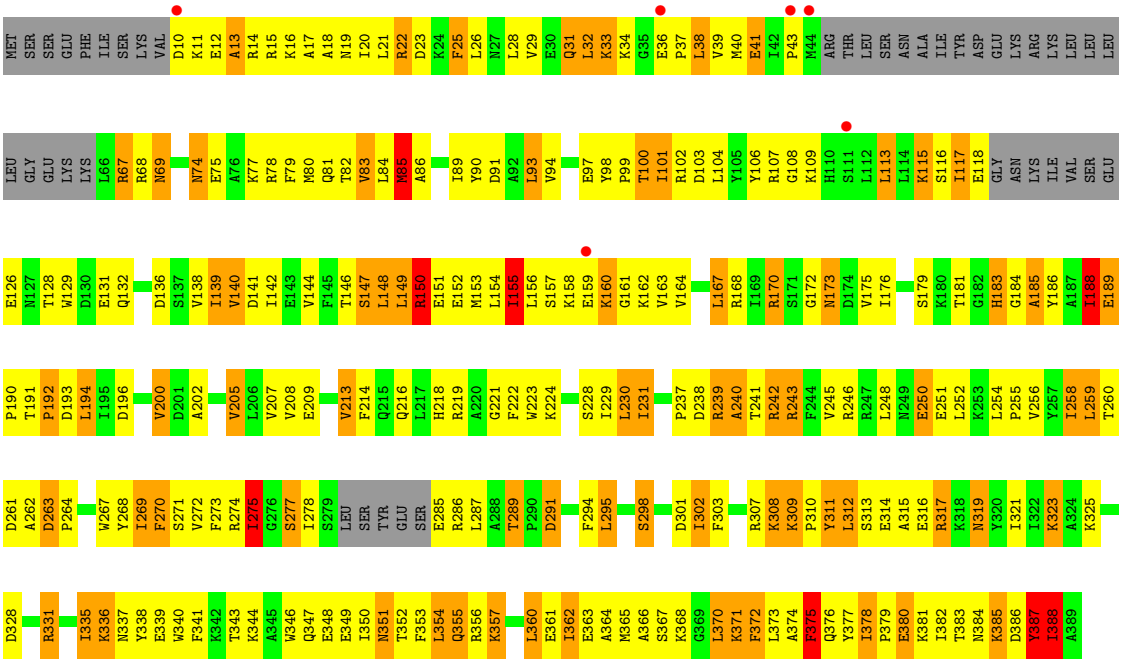




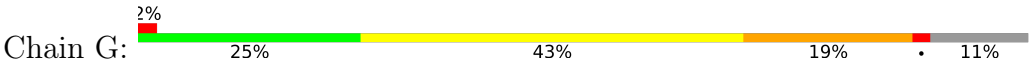


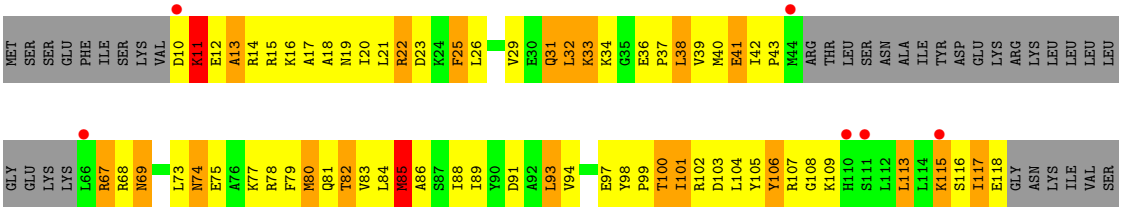
• Molecule 1: Type II DNA topoisomerase VI subunit A

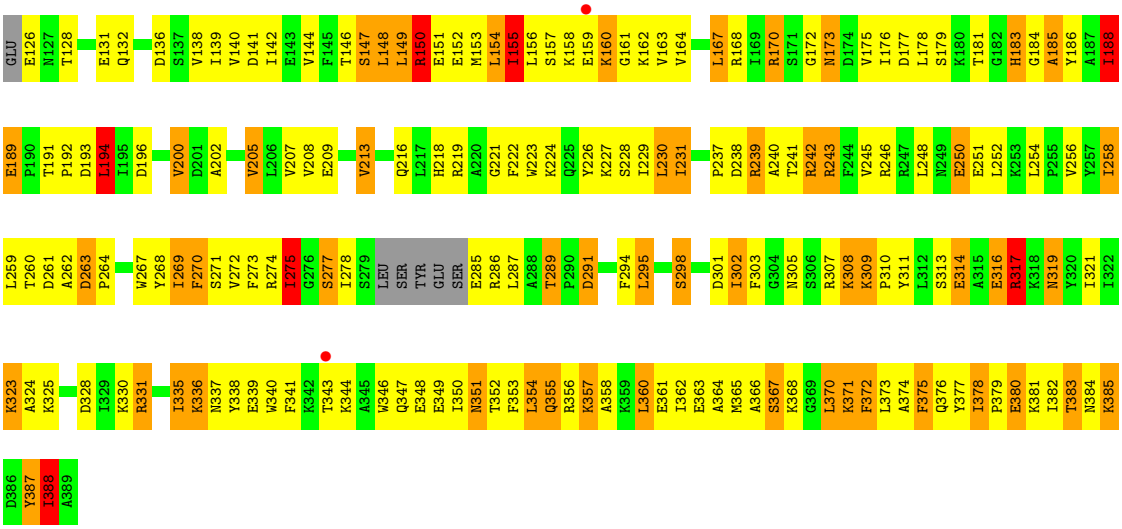




• Molecule 1: Type II DNA topoisomerase VI subunit A

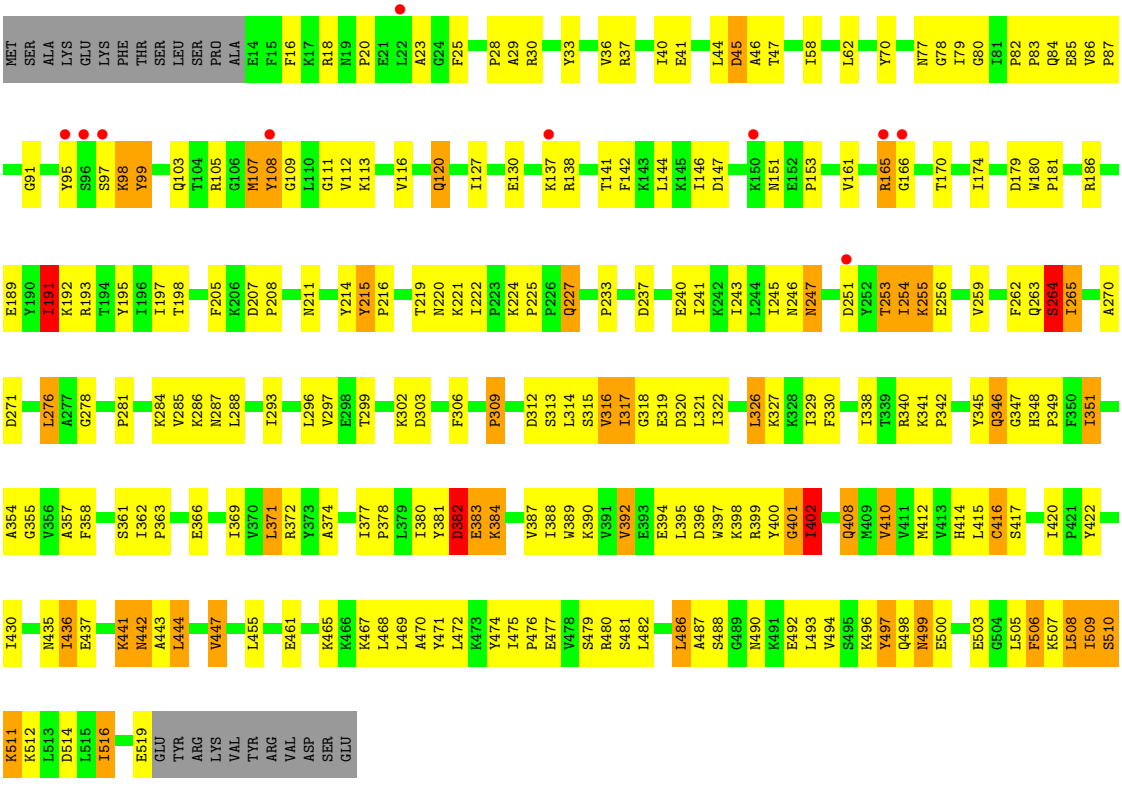






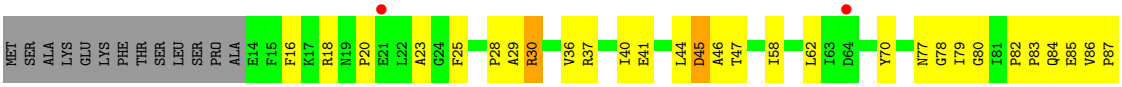
• Molecule 2: Type 2 DNA topoisomerase 6 subunit B

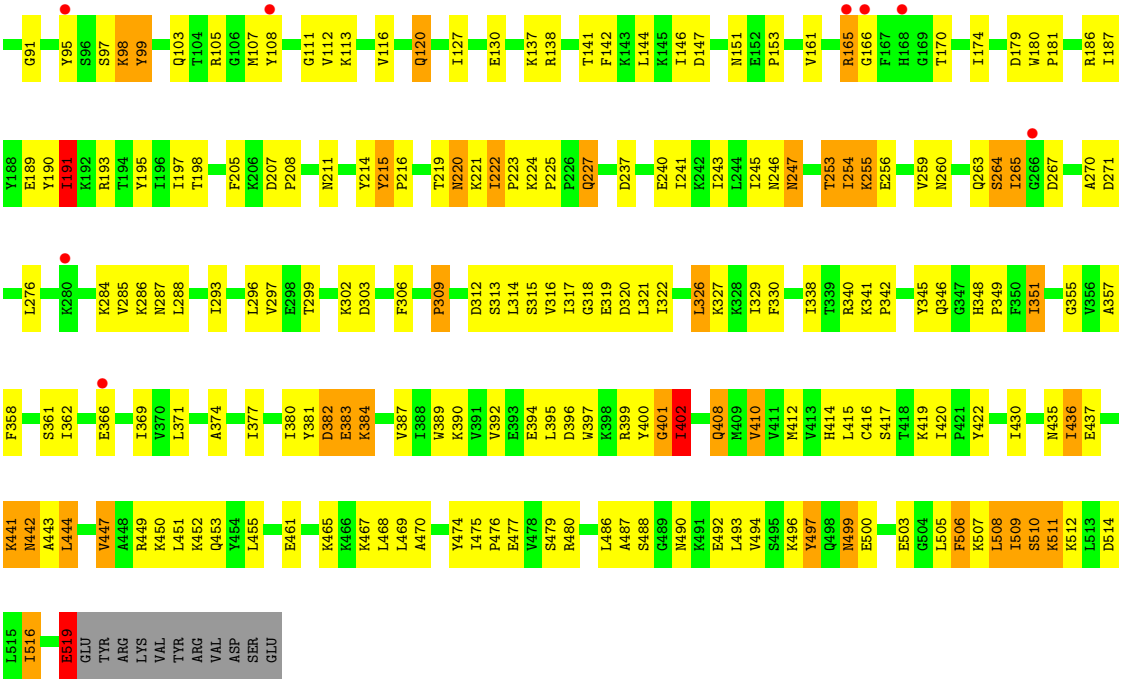
Chain B:



• Molecule 2: Type 2 DNA topoisomerase 6 subunit B

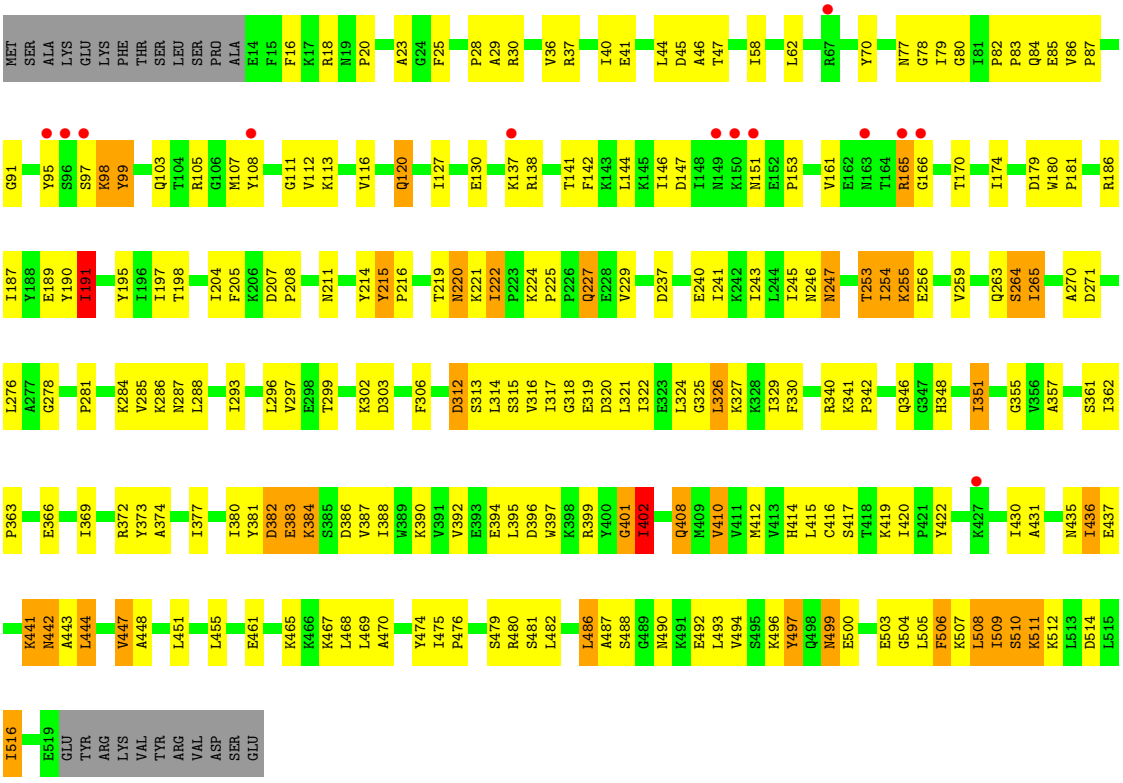
Chain D:





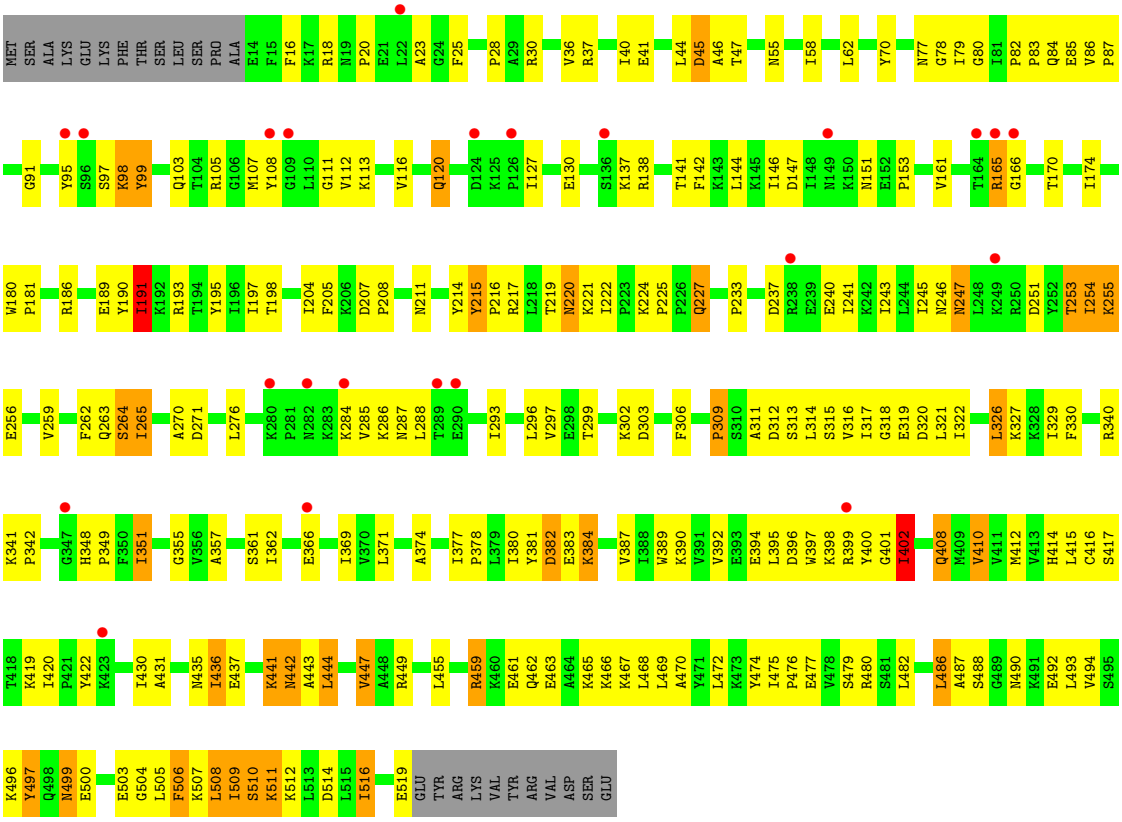
• Molecule 2: Type 2 DNA topoisomerase 6 subunit B

Chain F:



• Molecule 2: Type 2 DNA topoisomerase 6 subunit B

Chain H:


MET SER ALA LYS GLU LYS PHE THR SER LEU SER PRO ALA E14 F15 F16 K17 R18 N19 P20 E21 L22 A23 G24 F25 P28 A29 R30 V36 R37 I40 E41 L44 D45 A46 T47 N55 I58 L62 Y70 N77 G78 I79 G80 I81 P82 P83 Q84 E85 V86 P87
G91 Y95 S96 S97 K98 Y99 Q103 T104 R105 G106 M107 Y108 G109 L110 G111 V112 K113 V116 Q120 D124 K125 P126 I127 E130 S136 K137 R138 T141 F142 K143 L144 K145 I146 D147 I148 N149 K150 N151 E152 P153 V161 T164 R165 G166 T170 I174
W180 P181 R186 E189 Y190 T191 K192 R193 T194 Y195 I196 I197 T198 I204 F205 K206 D207 P208 N211 Y214 Y215 P216 R217 L218 T219 N220 K221 I222 P223 K224 P225 P226 Q227 P233 D237 R238 E239 E240 I241 K242 I243 L244 I245 N246 N247 L248 K249 R250 D251 Y252 T253 I254 K255
E256 V259 F262 Q263 S264 I265 A270 D271 L276 K280 P281 N282 K283 K284 V285 K286 N287 L288 T289 E290 I293 L296 V297 E298 T299 K302 D303 F306 P309 S310 A311 D312 S313 L314 S315 V316 I317 G318 E319 D320 L321 I322 L326 K327 K328 I329 F330 R340
K341 P342 G347 H348 P349 F350 I351 G355 V356 A357 S361 I362 E366 I369 V370 L371 A374 I377 P378 L379 I380 Y381 D382 E383 K384 V387 I388 W389 K390 V391 V392 E393 E394 L395 D396 W397 K398 R399 Y400 G401 I402 Q408 N409 V410 V411 M412 V413 H414 L415 C416 S417
T418 K419 I420 P421 Y422 K423 I430 A431 N435 I436 E437 K441 N442 A443 L444 V447 A448 R449 L455 R459 K460 E461 Q462 E463 A464 K465 K466 K467 L468 L469 A470 Y471 L472 K473 Y474 I475 P476 E477 V478 S479 R480 S481 L482 L486 A487 S488 G489 N490 K491 E492 L493 V494 S495
K496 Y497 Q498 N499 E500 E503 G504 L505 F506 K507 L508 I509 S510 K511 K512 L513 D514 L515 I516 E519 GLU TYR ARG LYS VAL TYR ARG VAL ASP SER GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.96Å 200.53Å 329.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.56 19.99 – 3.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-3.56) 97.7 (19.99-3.56)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.312 , 0.333 0.336 , 0.340	Depositor DCC
R_{free} test set	4435 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	96.3	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	27776	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.73% 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

5.1 Standard geometry

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

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	0.76	2/2893 (0.1%)	0.84	2/3890 (0.1%)
1	C	0.78	3/2893 (0.1%)	0.99	5/3890 (0.1%)
1	E	0.73	3/2893 (0.1%)	0.84	4/3890 (0.1%)
1	G	0.70	0/2893	0.80	3/3890 (0.1%)
2	B	0.51	1/4161 (0.0%)	0.58	0/5623
2	D	0.62	3/4161 (0.1%)	0.55	1/5623 (0.0%)
2	F	0.44	0/4161	0.55	0/5623
2	H	0.40	0/4161	0.55	1/5623 (0.0%)
All	All	0.61	12/28216 (0.0%)	0.70	16/38052 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	2
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	519	GLU	C-O	29.59	1.79	1.23
1	C	158	LYS	C-N	8.86	1.54	1.34
1	A	317	ARG	C-N	8.32	1.53	1.34
1	C	375	PHE	CE2-CZ	6.33	1.49	1.37
1	E	375	PHE	CE2-CZ	6.19	1.49	1.37
1	C	310	PRO	C-N	6.04	1.48	1.34
1	A	375	PHE	CE2-CZ	5.88	1.48	1.37
2	D	519	GLU	CA-CB	5.55	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	311	TYR	C-N	-5.40	1.21	1.34
1	E	317	ARG	C-N	5.17	1.46	1.34
2	B	416	CYS	CB-SG	-5.08	1.73	1.81
2	D	519	GLU	CG-CD	5.07	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	LYS	O-C-N	-24.65	81.30	123.20
1	C	160	LYS	CA-C-N	19.50	155.20	116.20
1	E	311	TYR	O-C-N	-14.86	98.93	122.70
1	C	160	LYS	C-N-CA	13.11	149.82	122.30
1	E	311	TYR	CA-C-N	9.53	138.16	117.20
2	D	519	GLU	CA-C-O	-7.76	103.80	120.10
1	G	317	ARG	NE-CZ-NH2	7.23	123.92	120.30
2	H	459	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	E	194	LEU	CA-CB-CG	6.70	130.70	115.30
1	C	317	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	194	LEU	CA-CB-CG	6.37	129.95	115.30
1	A	317	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	G	194	LEU	CA-CB-CG	6.11	129.35	115.30
1	C	194	LEU	CA-CB-CG	6.00	129.09	115.30
1	E	388	ILE	CG1-CB-CG2	-5.74	98.77	111.40
1	G	388	ILE	CG1-CB-CG2	-5.26	99.84	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	160	LYS	Peptide,Mainchain
1	E	311	TYR	Mainchain
1	E	315	ALA	Mainchain

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	2842	0	2894	388	0
1	C	2842	0	2894	400	0
1	E	2842	0	2895	365	0
1	G	2842	0	2895	366	0
2	B	4077	0	4181	198	0
2	D	4077	0	4181	190	0
2	F	4077	0	4181	189	0
2	H	4077	0	4181	202	0
3	B	25	0	15	5	0
3	D	25	0	15	7	0
3	F	25	0	15	5	0
3	H	25	0	17	4	0
All	All	27776	0	28364	2200	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 39.

All (2200) 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:E:302:ILE:CG2	1:E:312:LEU:HD11	1.58	1.32
1:C:312:LEU:CD2	1:C:317:ARG:HD3	1.63	1.28
1:C:106:TYR:O	1:C:107:ARG:HD3	1.41	1.20
2:H:455:LEU:CD1	2:H:459:ARG:HH12	1.54	1.20
2:D:519:GLU:C	2:D:519:GLU:O	1.79	1.18
1:G:106:TYR:O	1:G:107:ARG:HD3	1.44	1.16
1:A:106:TYR:O	1:A:107:ARG:HD3	1.45	1.16
1:C:160:LYS:O	1:C:160:LYS:HG2	1.33	1.15
1:C:22:ARG:HG3	1:C:23:ASP:H	1.11	1.15
1:E:22:ARG:HG3	1:E:23:ASP:H	1.12	1.13
1:C:155:ILE:H	1:C:155:ILE:HD12	1.13	1.13
1:C:312:LEU:CD1	1:C:312:LEU:H	1.61	1.13
1:A:22:ARG:HG3	1:A:23:ASP:H	1.10	1.11
1:E:106:TYR:O	1:E:107:ARG:HD3	1.47	1.11
1:G:22:ARG:HG3	1:G:23:ASP:H	1.10	1.11
1:C:302:ILE:HG22	1:C:312:LEU:HD21	1.27	1.10
2:F:401:GLY:HA3	2:F:455:LEU:HD21	1.16	1.10
2:D:400:TYR:HA	2:D:452:LYS:HE2	1.34	1.09
1:E:155:ILE:HD12	1:E:155:ILE:H	1.15	1.09
1:E:302:ILE:HG22	1:E:312:LEU:HD11	1.30	1.09
1:A:155:ILE:H	1:A:155:ILE:HD12	1.14	1.09
1:A:307:ARG:HD2	1:A:308:LYS:HZ3	0.99	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ILE:HD11	1:G:176:ILE:HD11	1.11	1.09
1:A:176:ILE:HD11	1:C:176:ILE:HD11	1.11	1.08
1:E:238:ASP:OD1	1:E:241:THR:HB	1.54	1.08
1:E:307:ARG:HD2	1:E:308:LYS:NZ	1.69	1.07
1:E:302:ILE:HG23	1:E:312:LEU:HD11	1.35	1.07
1:A:238:ASP:OD1	1:A:241:THR:HB	1.54	1.07
1:A:298:SER:O	1:A:301:ASP:HB2	1.53	1.07
1:C:307:ARG:HD2	1:C:308:LYS:NZ	1.70	1.06
1:G:307:ARG:HD2	1:G:308:LYS:NZ	1.70	1.06
1:C:312:LEU:HD22	1:C:317:ARG:HD3	1.30	1.05
1:E:307:ARG:HD2	1:E:308:LYS:HZ3	0.93	1.05
1:G:298:SER:O	1:G:301:ASP:HB2	1.55	1.05
1:C:307:ARG:HD2	1:C:308:LYS:HZ3	1.00	1.05
1:E:176:ILE:HD11	1:G:176:ILE:CD1	1.87	1.05
1:A:176:ILE:HD11	1:C:176:ILE:CD1	1.87	1.03
1:G:307:ARG:HD2	1:G:308:LYS:HZ3	0.87	1.03
1:A:176:ILE:CD1	1:C:176:ILE:HD11	1.89	1.03
1:C:238:ASP:OD1	1:C:241:THR:HB	1.56	1.03
1:E:298:SER:O	1:E:301:ASP:HB2	1.55	1.03
1:C:312:LEU:H	1:C:312:LEU:HD12	1.17	1.03
1:G:238:ASP:OD1	1:G:241:THR:HB	1.58	1.03
2:H:455:LEU:HD13	2:H:459:ARG:HH12	1.22	1.03
1:C:312:LEU:CD2	1:C:317:ARG:CD	2.36	1.02
1:A:14:ARG:NH2	1:C:183:HIS:CG	2.25	1.02
1:E:176:ILE:CD1	1:G:176:ILE:HD11	1.89	1.01
1:C:312:LEU:HD12	1:C:312:LEU:N	1.72	1.01
1:G:155:ILE:H	1:G:155:ILE:HD12	1.22	1.00
1:A:14:ARG:NH2	1:C:183:HIS:CD2	2.30	0.98
1:C:302:ILE:HA	1:C:312:LEU:HD11	1.43	0.98
1:C:298:SER:O	1:C:301:ASP:HB2	1.62	0.98
1:A:316:GLU:O	1:A:319:ASN:ND2	1.95	0.98
1:C:335:ILE:HG22	1:C:338:TYR:CE1	1.98	0.98
2:D:480:ARG:HB2	2:D:497:TYR:HE1	1.28	0.98
1:G:314:GLU:HG3	1:G:317:ARG:HH12	1.29	0.97
1:G:160:LYS:O	1:G:188:ILE:HD11	1.62	0.97
1:E:14:ARG:NH2	1:G:183:HIS:CG	2.32	0.97
1:A:31:GLN:HG3	1:A:38:LEU:HD13	1.46	0.96
2:F:401:GLY:HA3	2:F:455:LEU:CD2	1.94	0.96
2:H:79:ILE:HG13	2:H:80:GLY:H	1.31	0.96
1:G:160:LYS:NZ	1:G:160:LYS:CB	2.28	0.95
1:A:22:ARG:HG3	1:A:23:ASP:N	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:O	1:A:33:LYS:N	1.99	0.95
1:G:314:GLU:HG3	1:G:317:ARG:NH1	1.81	0.95
1:C:312:LEU:HD21	1:C:317:ARG:CD	1.96	0.95
1:E:31:GLN:O	1:E:33:LYS:N	1.99	0.95
1:E:224:LYS:O	1:E:224:LYS:HD2	1.64	0.94
1:A:218:HIS:HD2	1:A:223:TRP:HE1	1.13	0.94
1:E:335:ILE:HG22	1:E:338:TYR:CE1	2.02	0.94
1:A:307:ARG:HD2	1:A:308:LYS:NZ	1.83	0.94
1:E:183:HIS:CG	1:G:14:ARG:NH2	2.36	0.93
1:E:160:LYS:CB	1:E:160:LYS:NZ	2.31	0.93
1:A:155:ILE:H	1:A:155:ILE:CD1	1.82	0.93
2:B:480:ARG:HB2	2:B:497:TYR:HE1	1.31	0.93
1:G:31:GLN:O	1:G:33:LYS:N	2.01	0.93
1:A:224:LYS:HD2	1:A:224:LYS:O	1.68	0.93
1:E:150:ARG:HB2	1:E:150:ARG:HH21	1.34	0.92
1:C:31:GLN:O	1:C:33:LYS:N	2.01	0.92
1:E:218:HIS:HD2	1:E:223:TRP:HE1	1.09	0.92
1:G:218:HIS:HD2	1:G:223:TRP:HE1	1.12	0.92
1:E:370:LEU:HD23	1:E:370:LEU:H	1.33	0.92
2:F:480:ARG:HB2	2:F:497:TYR:HE1	1.34	0.92
1:G:224:LYS:HD2	1:G:224:LYS:O	1.69	0.92
2:H:455:LEU:CD1	2:H:459:ARG:NH1	2.32	0.92
1:A:335:ILE:HG22	1:A:338:TYR:CE1	2.04	0.92
1:G:22:ARG:HG3	1:G:23:ASP:N	1.84	0.92
1:C:150:ARG:HH21	1:C:150:ARG:HB2	1.35	0.91
2:B:383:GLU:HG3	2:B:384:LYS:HD3	1.50	0.91
2:H:480:ARG:HB2	2:H:497:TYR:HE1	1.34	0.91
1:A:160:LYS:HB2	1:A:160:LYS:NZ	1.86	0.91
1:A:183:HIS:CG	1:C:14:ARG:NH2	2.37	0.91
1:E:155:ILE:H	1:E:155:ILE:CD1	1.81	0.91
1:A:32:LEU:HD11	2:B:486:LEU:HD11	1.50	0.91
1:C:316:GLU:O	1:C:319:ASN:ND2	2.04	0.91
1:C:218:HIS:HD2	1:C:223:TRP:HE1	1.13	0.91
2:H:455:LEU:HD12	2:H:459:ARG:HH12	1.33	0.91
1:C:31:GLN:HG3	1:C:38:LEU:HD13	1.52	0.90
1:C:155:ILE:H	1:C:155:ILE:CD1	1.82	0.90
1:G:335:ILE:HG22	1:G:338:TYR:CE1	2.05	0.90
1:C:155:ILE:HD12	1:C:155:ILE:N	1.87	0.90
1:C:22:ARG:HG3	1:C:23:ASP:N	1.84	0.90
1:E:22:ARG:HG3	1:E:23:ASP:N	1.83	0.90
2:D:500:GLU:HA	2:D:503:GLU:HB3	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:79:ILE:HG13	2:F:80:GLY:H	1.34	0.90
2:B:500:GLU:HA	2:B:503:GLU:HB3	1.54	0.90
2:H:198:THR:O	2:H:198:THR:HG22	1.71	0.90
1:A:150:ARG:HH21	1:A:150:ARG:HB2	1.36	0.89
2:F:198:THR:O	2:F:198:THR:HG22	1.71	0.89
1:E:155:ILE:HD12	1:E:155:ILE:N	1.88	0.89
2:H:500:GLU:HA	2:H:503:GLU:HB3	1.53	0.89
1:E:319:ASN:H	1:E:319:ASN:HD22	1.18	0.88
2:B:198:THR:HG22	2:B:198:THR:O	1.73	0.88
1:G:150:ARG:HH21	1:G:150:ARG:HB2	1.37	0.88
1:C:181:THR:HG22	1:C:181:THR:O	1.72	0.88
2:D:79:ILE:HG13	2:D:80:GLY:H	1.38	0.88
2:F:516:ILE:HD13	2:F:516:ILE:H	1.38	0.88
1:A:368:LYS:HD3	1:A:372:PHE:HE2	1.37	0.88
1:C:224:LYS:O	1:C:224:LYS:HD2	1.74	0.88
1:C:335:ILE:HG22	1:C:338:TYR:CD1	2.09	0.88
2:D:383:GLU:HG3	2:D:384:LYS:HD3	1.56	0.88
1:E:307:ARG:CD	1:E:308:LYS:HZ3	1.85	0.88
1:E:261:ASP:OD1	1:E:361:GLU:HA	1.72	0.88
2:B:138:ARG:HB3	2:B:161:VAL:O	1.74	0.88
1:G:31:GLN:HG3	1:G:38:LEU:HD13	1.54	0.87
2:H:383:GLU:HG3	2:H:384:LYS:HD3	1.57	0.87
1:C:302:ILE:HG22	1:C:317:ARG:HD2	1.57	0.87
1:C:312:LEU:CD1	1:C:312:LEU:N	2.26	0.87
1:A:160:LYS:HB2	1:A:160:LYS:HZ3	1.37	0.87
1:C:319:ASN:HD22	1:C:319:ASN:H	1.19	0.87
1:E:368:LYS:HD3	1:E:372:PHE:HE2	1.38	0.87
2:F:500:GLU:HA	2:F:503:GLU:HB3	1.55	0.87
1:A:370:LEU:HD23	1:A:370:LEU:H	1.40	0.87
1:E:150:ARG:HH21	1:E:150:ARG:CB	1.88	0.87
1:G:155:ILE:H	1:G:155:ILE:CD1	1.88	0.87
2:D:414:HIS:HD2	2:D:415:LEU:N	1.72	0.86
1:C:101:ILE:HD12	1:C:101:ILE:N	1.91	0.86
2:B:41:GLU:OE1	2:B:105:ARG:HB3	1.75	0.86
1:E:31:GLN:HG3	1:E:38:LEU:HD13	1.56	0.86
1:A:150:ARG:HH21	1:A:150:ARG:CB	1.87	0.86
1:E:368:LYS:HD3	1:E:372:PHE:CE2	2.10	0.86
1:G:261:ASP:OD1	1:G:361:GLU:HA	1.75	0.86
1:A:160:LYS:O	1:A:238:ASP:OD2	1.94	0.86
1:G:153:MET:O	1:G:154:LEU:HB2	1.76	0.86
2:B:414:HIS:HD2	2:B:415:LEU:N	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:LYS:CB	1:E:160:LYS:HZ3	1.87	0.85
2:H:219:THR:HG23	2:H:220:ASN:N	1.90	0.85
2:D:219:THR:HG23	2:D:220:ASN:N	1.90	0.85
1:A:155:ILE:HD12	1:A:155:ILE:N	1.89	0.85
1:A:261:ASP:OD1	1:A:361:GLU:HA	1.77	0.85
1:E:101:ILE:HD12	1:E:101:ILE:N	1.92	0.85
1:A:319:ASN:HD22	1:A:319:ASN:H	1.20	0.85
1:A:368:LYS:HD3	1:A:372:PHE:CE2	2.11	0.85
1:E:181:THR:O	1:E:181:THR:HG22	1.76	0.84
2:H:138:ARG:HB3	2:H:161:VAL:O	1.77	0.84
2:B:79:ILE:HG13	2:B:80:GLY:H	1.40	0.84
1:C:368:LYS:HD3	1:C:372:PHE:HE2	1.42	0.84
2:B:506:PHE:O	2:B:509:ILE:HG13	1.77	0.84
2:F:41:GLU:OE1	2:F:105:ARG:HB3	1.77	0.84
1:A:31:GLN:HB2	1:A:38:LEU:HD22	1.59	0.84
2:F:138:ARG:HB3	2:F:161:VAL:O	1.76	0.84
2:F:221:LYS:HD2	2:F:321:LEU:HD21	1.59	0.84
1:G:307:ARG:CD	1:G:308:LYS:HZ3	1.83	0.84
2:D:198:THR:HG22	2:D:198:THR:O	1.75	0.84
1:E:218:HIS:CD2	1:E:223:TRP:HE1	1.96	0.84
2:F:383:GLU:HG3	2:F:384:LYS:HD3	1.59	0.84
1:G:146:THR:O	1:G:147:SER:HB2	1.78	0.84
2:D:516:ILE:HD13	2:D:516:ILE:H	1.42	0.83
2:B:516:ILE:HD13	2:B:516:ILE:H	1.41	0.83
1:E:316:GLU:O	1:E:319:ASN:ND2	2.11	0.83
2:F:219:THR:HG23	2:F:220:ASN:N	1.92	0.83
1:C:22:ARG:CG	1:C:23:ASP:H	1.91	0.83
1:A:376:GLN:O	1:A:380:GLU:HB2	1.78	0.83
1:E:159:GLU:OE1	1:E:240:ALA:HB3	1.78	0.83
1:E:153:MET:O	1:E:154:LEU:HB2	1.78	0.83
1:C:377:TYR:CE2	1:C:381:LYS:HD2	2.14	0.83
1:G:150:ARG:HH21	1:G:150:ARG:CB	1.91	0.83
1:G:160:LYS:CB	1:G:160:LYS:HZ3	1.91	0.83
1:G:181:THR:O	1:G:181:THR:HG22	1.76	0.83
2:D:506:PHE:O	2:D:509:ILE:HG13	1.79	0.83
2:H:516:ILE:H	2:H:516:ILE:HD13	1.41	0.83
1:A:219:ARG:CZ	1:C:14:ARG:HH21	1.92	0.83
1:C:312:LEU:HD21	1:C:317:ARG:HD2	1.61	0.83
1:C:370:LEU:HD23	1:C:370:LEU:H	1.44	0.83
1:C:153:MET:O	1:C:154:LEU:HB2	1.76	0.82
1:C:376:GLN:O	1:C:380:GLU:HB2	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:HIS:CD2	1:G:223:TRP:HE1	1.96	0.82
1:C:99:PRO:HB2	1:C:104:LEU:HD11	1.62	0.82
1:C:150:ARG:HH21	1:C:150:ARG:CB	1.92	0.82
1:E:374:ALA:HB1	1:E:375:PHE:CE1	2.14	0.82
2:H:455:LEU:HD13	2:H:459:ARG:NH1	1.92	0.82
2:B:340:ARG:NH2	2:B:442:ASN:HB2	1.92	0.82
1:G:335:ILE:HG22	1:G:338:TYR:CD1	2.13	0.82
1:C:302:ILE:O	1:C:317:ARG:CZ	2.28	0.82
1:A:377:TYR:CE2	1:A:381:LYS:HD2	2.14	0.82
2:F:475:ILE:O	2:F:479:SER:OG	1.97	0.82
1:G:155:ILE:HD12	1:G:155:ILE:N	1.92	0.82
1:G:319:ASN:H	1:G:319:ASN:HD22	1.24	0.82
1:A:84:LEU:O	1:A:86:ALA:N	2.13	0.82
1:A:181:THR:HG22	1:A:181:THR:O	1.79	0.82
1:E:85:MET:HE3	1:E:104:LEU:HB3	1.61	0.82
1:C:146:THR:O	1:C:147:SER:HB2	1.78	0.82
2:F:516:ILE:HD13	2:F:516:ILE:N	1.95	0.82
2:D:41:GLU:OE1	2:D:105:ARG:HB3	1.80	0.82
1:E:84:LEU:O	1:E:86:ALA:N	2.13	0.82
2:D:138:ARG:HB3	2:D:161:VAL:O	1.79	0.81
1:E:22:ARG:CG	1:E:23:ASP:H	1.93	0.81
1:G:160:LYS:NZ	1:G:160:LYS:HB2	1.94	0.81
2:D:224:LYS:HG3	2:D:225:PRO:HD2	1.63	0.81
2:F:224:LYS:HG3	2:F:225:PRO:HD2	1.62	0.81
1:G:22:ARG:CG	1:G:23:ASP:H	1.92	0.81
1:G:149:LEU:HD12	1:G:149:LEU:H	1.43	0.81
1:C:160:LYS:O	1:C:160:LYS:CG	2.20	0.81
1:E:160:LYS:O	1:E:188:ILE:HD11	1.79	0.81
2:B:475:ILE:O	2:B:479:SER:OG	1.95	0.81
1:C:218:HIS:CD2	1:C:223:TRP:HE1	1.98	0.81
1:C:39:VAL:HG13	1:C:68:ARG:O	1.81	0.81
1:G:376:GLN:O	1:G:380:GLU:HB2	1.80	0.81
2:H:414:HIS:HD2	2:H:415:LEU:N	1.78	0.81
1:C:374:ALA:HB1	1:C:375:PHE:CE1	2.16	0.81
1:A:22:ARG:CG	1:A:23:ASP:H	1.92	0.80
1:E:377:TYR:CE2	1:E:381:LYS:HD2	2.15	0.80
1:G:377:TYR:CE2	1:G:381:LYS:HD2	2.15	0.80
1:A:374:ALA:C	1:A:375:PHE:HD1	1.82	0.80
1:A:374:ALA:HB1	1:A:375:PHE:CE1	2.16	0.80
1:E:335:ILE:HG22	1:E:338:TYR:CD1	2.15	0.80
2:B:265:ILE:HG22	2:B:270:ALA:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:455:LEU:HD12	2:H:459:ARG:NH1	1.95	0.80
1:A:14:ARG:HH21	1:C:219:ARG:CZ	1.95	0.80
1:C:307:ARG:CD	1:C:308:LYS:HZ3	1.90	0.80
2:H:475:ILE:O	2:H:479:SER:OG	1.99	0.80
2:H:506:PHE:O	2:H:509:ILE:HG13	1.81	0.80
1:A:153:MET:O	1:A:154:LEU:HB2	1.81	0.80
2:B:219:THR:HG23	2:B:220:ASN:N	1.97	0.80
2:D:475:ILE:O	2:D:479:SER:OG	1.98	0.80
2:D:516:ILE:HD13	2:D:516:ILE:N	1.97	0.80
1:A:218:HIS:CD2	1:A:223:TRP:HE1	2.00	0.80
1:G:368:LYS:HD3	1:G:372:PHE:CE2	2.17	0.80
1:G:243:ARG:NH2	1:G:287:LEU:HD22	1.97	0.80
2:H:79:ILE:HG13	2:H:80:GLY:N	1.97	0.80
1:A:101:ILE:N	1:A:101:ILE:HD12	1.96	0.80
1:A:314:GLU:HA	1:A:317:ARG:HH11	1.47	0.80
1:C:31:GLN:HB2	1:C:38:LEU:HD22	1.62	0.80
1:G:368:LYS:HD3	1:G:372:PHE:HE2	1.47	0.80
2:H:41:GLU:OE1	2:H:105:ARG:HB3	1.82	0.80
1:E:17:ALA:HA	1:E:20:ILE:HG22	1.64	0.79
1:A:335:ILE:HG22	1:A:338:TYR:CD1	2.16	0.79
1:C:368:LYS:HD3	1:C:372:PHE:CE2	2.18	0.79
1:E:370:LEU:HD23	1:E:370:LEU:N	1.97	0.79
2:H:516:ILE:HD13	2:H:516:ILE:N	1.97	0.79
2:F:506:PHE:O	2:F:509:ILE:HG13	1.81	0.79
1:E:14:ARG:NH2	1:G:183:HIS:CD2	2.51	0.79
2:D:480:ARG:HB2	2:D:497:TYR:CE1	2.16	0.79
1:A:99:PRO:HB2	1:A:104:LEU:HD11	1.63	0.79
2:H:197:ILE:HB	2:H:317:ILE:HD12	1.63	0.79
2:B:516:ILE:HD13	2:B:516:ILE:N	1.98	0.79
1:C:261:ASP:OD1	1:C:361:GLU:HA	1.83	0.79
1:A:160:LYS:HZ3	1:A:160:LYS:CB	1.94	0.78
1:C:302:ILE:CG2	1:C:312:LEU:HD21	2.12	0.78
1:E:160:LYS:NZ	1:E:160:LYS:HB2	1.97	0.78
1:G:73:LEU:HD21	2:H:467:LYS:HE3	1.63	0.78
1:C:378:ILE:HD13	1:C:378:ILE:H	1.48	0.78
1:E:335:ILE:O	1:E:337:ASN:N	2.16	0.78
2:F:480:ARG:HB2	2:F:497:TYR:CE1	2.19	0.78
2:F:414:HIS:HD2	2:F:415:LEU:N	1.81	0.78
2:B:116:VAL:O	2:B:120:GLN:NE2	2.16	0.78
1:G:101:ILE:HD12	1:G:101:ILE:N	1.98	0.78
1:A:335:ILE:O	1:A:337:ASN:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480:ARG:HB2	2:B:497:TYR:CE1	2.18	0.78
1:C:84:LEU:O	1:C:86:ALA:N	2.17	0.78
1:C:243:ARG:NH2	1:C:287:LEU:HD22	1.97	0.78
1:A:160:LYS:NZ	1:A:160:LYS:CB	2.37	0.78
1:E:146:THR:O	1:E:147:SER:HB2	1.83	0.78
1:A:102:ARG:HD2	1:C:363:GLU:HG3	1.66	0.77
2:F:340:ARG:NH2	2:F:442:ASN:HB2	1.98	0.77
1:E:375:PHE:N	1:E:375:PHE:HD1	1.82	0.77
1:E:374:ALA:C	1:E:375:PHE:HD1	1.88	0.77
1:E:97:GLU:OE1	1:G:370:LEU:HG	1.85	0.77
1:C:378:ILE:HD13	1:C:378:ILE:N	1.98	0.77
1:C:39:VAL:HG22	1:C:69:ASN:HA	1.66	0.77
1:E:85:MET:HE1	1:E:104:LEU:HD23	1.67	0.77
1:E:302:ILE:HG22	1:E:312:LEU:CD1	2.14	0.77
2:H:265:ILE:HG22	2:H:270:ALA:HB2	1.67	0.77
1:A:149:LEU:H	1:A:149:LEU:HD12	1.46	0.77
1:A:13:ALA:HA	1:A:16:LYS:HG3	1.67	0.77
1:C:335:ILE:O	1:C:337:ASN:N	2.17	0.77
1:A:146:THR:O	1:A:147:SER:HB2	1.85	0.76
1:E:183:HIS:CD2	1:G:14:ARG:NH2	2.53	0.76
2:H:455:LEU:O	2:H:459:ARG:NH1	2.18	0.76
2:H:103:GLN:NE2	2:H:315:SER:H	1.84	0.76
2:F:79:ILE:HG13	2:F:80:GLY:N	2.01	0.76
1:G:335:ILE:O	1:G:337:ASN:N	2.18	0.76
1:A:375:PHE:HD1	1:A:375:PHE:N	1.84	0.76
1:E:31:GLN:HB2	1:E:38:LEU:HD22	1.65	0.76
2:H:493:LEU:HG	2:H:494:VAL:HG13	1.67	0.76
1:A:14:ARG:CZ	1:C:183:HIS:CE1	2.69	0.76
2:B:91:GLY:HA3	2:B:153:PRO:HB3	1.68	0.76
1:G:370:LEU:HD23	1:G:370:LEU:H	1.51	0.76
1:C:312:LEU:H	1:C:312:LEU:HD13	1.49	0.76
2:B:340:ARG:HH22	2:B:442:ASN:CB	1.99	0.76
1:C:149:LEU:H	1:C:149:LEU:HD12	1.49	0.76
1:G:160:LYS:HZ3	1:G:160:LYS:HB3	1.49	0.76
1:A:68:ARG:NH2	1:A:141:ASP:OD1	2.19	0.75
1:A:243:ARG:NH2	1:A:287:LEU:HD22	2.01	0.75
1:E:99:PRO:HB2	1:E:104:LEU:HD11	1.66	0.75
1:A:14:ARG:HH22	1:C:183:HIS:CG	2.04	0.75
2:F:37:ARG:O	2:F:41:GLU:HG3	1.86	0.75
1:G:17:ALA:HA	1:G:20:ILE:HG22	1.68	0.75
2:D:36:VAL:O	2:D:40:ILE:HD12	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:265:ILE:HG22	2:D:270:ALA:HB2	1.68	0.75
2:H:37:ARG:O	2:H:41:GLU:HG3	1.87	0.75
2:H:480:ARG:HB2	2:H:497:TYR:CE1	2.20	0.75
1:E:149:LEU:H	1:E:149:LEU:HD12	1.49	0.75
1:E:160:LYS:HZ3	1:E:160:LYS:HB3	1.51	0.75
2:B:116:VAL:HG13	2:B:127:ILE:HG13	1.69	0.75
2:H:193:ARG:HD3	2:H:371:LEU:HD23	1.69	0.75
1:E:32:LEU:HD11	2:F:486:LEU:HD11	1.69	0.75
1:G:374:ALA:HB1	1:G:375:PHE:CE1	2.21	0.75
2:H:116:VAL:O	2:H:120:GLN:NE2	2.19	0.75
1:A:183:HIS:CD2	1:C:14:ARG:NH2	2.55	0.74
2:B:493:LEU:HG	2:B:494:VAL:HG13	1.68	0.74
1:E:335:ILE:C	1:E:337:ASN:H	1.86	0.74
1:C:101:ILE:HD12	1:C:101:ILE:H	1.52	0.74
1:C:374:ALA:HB1	1:C:375:PHE:CD1	2.22	0.74
1:G:319:ASN:H	1:G:319:ASN:ND2	1.86	0.74
1:A:335:ILE:C	1:A:337:ASN:H	1.88	0.74
1:E:68:ARG:NH2	1:E:141:ASP:OD1	2.21	0.74
1:G:378:ILE:HD13	1:G:378:ILE:N	2.03	0.74
2:B:414:HIS:CD2	2:B:415:LEU:N	2.56	0.74
1:G:31:GLN:HB2	1:G:38:LEU:HD22	1.67	0.74
2:D:79:ILE:HG13	2:D:80:GLY:N	2.01	0.74
1:E:77:LYS:NZ	1:E:126:GLU:OE1	2.20	0.74
1:A:295:LEU:O	1:A:295:LEU:HD22	1.88	0.73
1:C:335:ILE:C	1:C:337:ASN:H	1.89	0.73
2:D:414:HIS:CD2	2:D:415:LEU:N	2.55	0.73
1:A:319:ASN:ND2	1:A:319:ASN:H	1.87	0.73
1:E:13:ALA:HA	1:E:16:LYS:HG3	1.70	0.73
1:G:374:ALA:C	1:G:375:PHE:HD1	1.91	0.73
2:F:340:ARG:HH22	2:F:442:ASN:CB	2.01	0.73
1:G:202:ALA:HB1	1:G:228:SER:HA	1.69	0.73
2:H:103:GLN:NE2	2:H:315:SER:N	2.36	0.73
1:A:17:ALA:HA	1:A:20:ILE:HG22	1.68	0.73
1:A:372:PHE:CD1	1:A:372:PHE:C	2.60	0.73
1:C:374:ALA:C	1:C:375:PHE:HD1	1.92	0.73
1:C:378:ILE:N	1:C:378:ILE:CD1	2.49	0.73
1:G:85:MET:HE3	1:G:104:LEU:HB3	1.68	0.73
1:C:319:ASN:ND2	1:C:319:ASN:H	1.85	0.73
2:D:37:ARG:O	2:D:41:GLU:HG3	1.87	0.73
1:A:353:PHE:C	1:A:355:GLN:H	1.90	0.73
1:G:99:PRO:HB2	1:G:104:LEU:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:378:ILE:HD13	1:G:378:ILE:H	1.54	0.73
1:E:319:ASN:H	1:E:319:ASN:ND2	1.85	0.73
2:F:36:VAL:O	2:F:40:ILE:HD12	1.89	0.73
1:C:374:ALA:CB	1:C:375:PHE:CD1	2.72	0.73
2:H:340:ARG:NH2	2:H:442:ASN:HB2	2.03	0.72
2:B:37:ARG:O	2:B:41:GLU:HG3	1.89	0.72
1:C:202:ALA:HB1	1:C:228:SER:HA	1.71	0.72
1:E:374:ALA:HB1	1:E:375:PHE:CD1	2.24	0.72
1:C:335:ILE:CG2	1:C:338:TYR:CE1	2.71	0.72
2:H:116:VAL:HG13	2:H:127:ILE:HG13	1.72	0.72
2:D:91:GLY:HA3	2:D:153:PRO:HB3	1.71	0.72
2:F:91:GLY:HA3	2:F:153:PRO:HB3	1.70	0.72
1:G:200:VAL:HG11	1:G:252:LEU:HD23	1.71	0.72
1:C:380:GLU:O	1:C:384:ASN:HB2	1.89	0.72
1:E:375:PHE:N	1:E:375:PHE:CD1	2.55	0.72
1:G:84:LEU:O	1:G:86:ALA:N	2.23	0.72
2:H:91:GLY:HA3	2:H:153:PRO:HB3	1.70	0.72
1:C:353:PHE:C	1:C:355:GLN:H	1.91	0.72
1:C:17:ALA:HA	1:C:20:ILE:HG22	1.71	0.72
1:C:85:MET:HE1	1:C:104:LEU:HD23	1.72	0.72
1:C:372:PHE:CD1	1:C:372:PHE:C	2.60	0.72
2:D:116:VAL:O	2:D:120:GLN:NE2	2.22	0.72
1:A:370:LEU:HD23	1:A:370:LEU:N	2.05	0.71
1:A:374:ALA:HB1	1:A:375:PHE:CD1	2.24	0.71
1:E:202:ALA:HB1	1:E:228:SER:HA	1.72	0.71
1:G:68:ARG:NH2	1:G:141:ASP:OD1	2.23	0.71
1:C:302:ILE:CA	1:C:312:LEU:HD11	2.20	0.71
1:E:353:PHE:C	1:E:355:GLN:H	1.92	0.71
2:F:116:VAL:O	2:F:120:GLN:NE2	2.23	0.71
1:A:375:PHE:N	1:A:375:PHE:CD1	2.55	0.71
2:B:193:ARG:HD3	2:B:371:LEU:HD23	1.72	0.71
2:B:224:LYS:HG3	2:B:225:PRO:HD2	1.72	0.71
1:G:271:SER:HB3	1:G:340:TRP:CH2	2.25	0.71
1:E:219:ARG:CZ	1:G:14:ARG:HH21	2.04	0.71
1:E:376:GLN:O	1:E:380:GLU:HB2	1.90	0.71
1:G:353:PHE:C	1:G:355:GLN:H	1.93	0.71
2:B:79:ILE:HG13	2:B:80:GLY:N	2.06	0.71
1:E:101:ILE:HD12	1:E:101:ILE:H	1.55	0.71
1:G:335:ILE:C	1:G:337:ASN:H	1.91	0.71
1:A:85:MET:HE3	1:A:104:LEU:HB3	1.71	0.71
2:F:116:VAL:HG13	2:F:127:ILE:HG13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:265:ILE:HG22	2:F:270:ALA:HB2	1.71	0.71
1:C:13:ALA:HA	1:C:16:LYS:HG3	1.73	0.71
1:C:271:SER:HB3	1:C:340:TRP:CH2	2.26	0.71
2:F:86:VAL:HB	2:F:87:PRO:HD3	1.72	0.71
1:G:246:ARG:HG2	1:G:246:ARG:O	1.89	0.71
1:E:243:ARG:NH2	1:E:287:LEU:HD22	2.05	0.71
1:E:200:VAL:HG11	1:E:252:LEU:HD23	1.73	0.71
1:E:264:PRO:HA	1:E:267:TRP:CE3	2.26	0.71
2:D:400:TYR:HA	2:D:452:LYS:CE	2.16	0.71
1:E:370:LEU:HG	1:G:97:GLU:OE1	1.91	0.71
1:G:160:LYS:HB2	1:G:160:LYS:HZ2	1.55	0.71
1:E:319:ASN:HD22	1:E:319:ASN:N	1.86	0.70
1:C:264:PRO:HA	1:C:267:TRP:CE3	2.26	0.70
1:E:378:ILE:HD13	1:E:378:ILE:N	2.06	0.70
1:C:77:LYS:NZ	1:C:126:GLU:OE1	2.24	0.70
1:C:307:ARG:C	1:C:308:LYS:HD3	2.10	0.70
1:E:351:ASN:HA	1:E:354:LEU:HB2	1.73	0.70
2:D:116:VAL:HG13	2:D:127:ILE:HG13	1.73	0.70
1:G:73:LEU:CD2	2:H:467:LYS:HG2	2.22	0.70
1:A:291:ASP:OD1	1:A:291:ASP:O	2.10	0.70
1:E:271:SER:HB3	1:E:340:TRP:CH2	2.27	0.70
2:H:86:VAL:HB	2:H:87:PRO:HD3	1.72	0.70
1:A:77:LYS:NZ	1:A:126:GLU:OE1	2.23	0.70
1:A:246:ARG:O	1:A:246:ARG:HG2	1.91	0.70
1:C:68:ARG:NH2	1:C:141:ASP:OD1	2.25	0.70
2:H:224:LYS:HG3	2:H:225:PRO:HD2	1.74	0.70
1:A:85:MET:HE1	1:A:104:LEU:HD23	1.74	0.70
1:C:181:THR:HG21	1:C:185:ALA:HA	1.73	0.70
2:D:493:LEU:HG	2:D:494:VAL:HG13	1.71	0.70
1:G:378:ILE:N	1:G:378:ILE:CD1	2.55	0.70
1:C:85:MET:HE3	1:C:104:LEU:HB3	1.74	0.70
1:C:181:THR:O	1:C:181:THR:CG2	2.38	0.70
1:A:238:ASP:OD1	1:A:241:THR:CB	2.38	0.69
2:B:36:VAL:O	2:B:40:ILE:HD12	1.92	0.69
1:E:291:ASP:O	1:E:291:ASP:OD1	2.09	0.69
2:F:493:LEU:HG	2:F:494:VAL:HG13	1.73	0.69
1:C:375:PHE:HD1	1:C:375:PHE:N	1.90	0.69
1:E:21:LEU:HD21	1:E:153:MET:HA	1.74	0.69
1:A:31:GLN:HG3	1:A:38:LEU:CD1	2.22	0.69
1:A:380:GLU:O	1:A:384:ASN:HB2	1.92	0.69
1:A:246:ARG:O	1:A:250:GLU:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ILE:HB	1:C:303:PHE:CD2	2.27	0.69
1:A:115:LYS:NZ	1:A:115:LYS:HB3	2.07	0.69
1:E:372:PHE:HA	1:E:376:GLN:OE1	1.92	0.69
2:H:103:GLN:HE22	2:H:315:SER:H	1.38	0.69
1:E:363:GLU:HG3	1:G:102:ARG:HD2	1.73	0.69
1:G:209:GLU:HB3	1:G:260:THR:HG22	1.75	0.69
1:E:335:ILE:CG2	1:E:338:TYR:CE1	2.76	0.69
2:F:475:ILE:N	2:F:476:PRO:HD2	2.06	0.69
1:A:370:LEU:HG	1:C:97:GLU:OE1	1.92	0.69
2:B:197:ILE:HB	2:B:317:ILE:HD12	1.74	0.69
1:C:374:ALA:CB	1:C:375:PHE:HD1	2.06	0.69
2:B:500:GLU:HA	2:B:503:GLU:CB	2.23	0.69
1:C:21:LEU:HD21	1:C:153:MET:HA	1.75	0.69
1:A:25:PHE:HD1	1:A:25:PHE:C	1.96	0.68
1:A:172:GLY:CA	1:C:183:HIS:HE1	2.06	0.68
1:C:84:LEU:C	1:C:86:ALA:H	1.95	0.68
1:E:238:ASP:OD1	1:E:241:THR:CB	2.37	0.68
1:A:202:ALA:HB1	1:A:228:SER:HA	1.75	0.68
2:D:340:ARG:NH2	2:D:442:ASN:HB2	2.07	0.68
1:A:374:ALA:CB	1:A:375:PHE:CD1	2.76	0.68
2:B:99:TYR:HH	2:B:348:HIS:HE2	1.40	0.68
1:E:246:ARG:O	1:E:250:GLU:HB2	1.93	0.68
1:E:374:ALA:CB	1:E:375:PHE:CD1	2.75	0.68
1:G:181:THR:O	1:G:181:THR:CG2	2.42	0.68
1:A:335:ILE:C	1:A:337:ASN:N	2.46	0.68
1:A:351:ASN:O	1:A:355:GLN:HB2	1.93	0.68
1:C:370:LEU:HD23	1:C:370:LEU:N	2.08	0.68
2:D:99:TYR:HH	2:D:348:HIS:HE2	1.40	0.68
1:E:84:LEU:C	1:E:86:ALA:H	1.97	0.68
1:G:335:ILE:CG2	1:G:338:TYR:CE1	2.77	0.68
2:H:322:ILE:HD13	2:H:412:MET:HE1	1.75	0.68
1:A:363:GLU:HG3	1:C:102:ARG:HD2	1.76	0.68
2:B:475:ILE:N	2:B:476:PRO:HD2	2.09	0.68
2:F:499:ASN:C	2:F:499:ASN:HD22	1.97	0.68
1:A:302:ILE:HB	1:A:303:PHE:CD2	2.29	0.68
1:A:385:LYS:HG3	1:A:387:TYR:HE2	1.58	0.68
1:E:208:VAL:HG21	1:E:213:VAL:CG1	2.24	0.68
1:E:303:PHE:CE1	1:E:356:ARG:HD2	2.28	0.68
1:E:335:ILE:C	1:E:337:ASN:N	2.44	0.68
1:G:115:LYS:HB3	1:G:115:LYS:NZ	2.09	0.68
1:G:264:PRO:HA	1:G:267:TRP:CE3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:VAL:O	2:H:40:ILE:HD12	1.94	0.68
1:A:351:ASN:HA	1:A:354:LEU:HB2	1.76	0.68
1:C:246:ARG:O	1:C:246:ARG:HG2	1.93	0.68
2:B:340:ARG:NH2	2:B:442:ASN:CB	2.56	0.68
1:C:200:VAL:HG11	1:C:252:LEU:HD23	1.75	0.68
2:D:86:VAL:HB	2:D:87:PRO:HD3	1.75	0.68
2:D:500:GLU:HA	2:D:503:GLU:CB	2.24	0.68
2:H:414:HIS:CD2	2:H:415:LEU:N	2.61	0.68
1:A:335:ILE:CG2	1:A:338:TYR:CE1	2.77	0.67
2:B:86:VAL:HB	2:B:87:PRO:HD3	1.75	0.67
2:B:499:ASN:C	2:B:499:ASN:HD22	1.98	0.67
2:D:322:ILE:HD13	2:D:412:MET:HE1	1.75	0.67
1:G:146:THR:O	1:G:147:SER:CB	2.43	0.67
1:G:317:ARG:O	1:G:321:ILE:HG13	1.94	0.67
1:A:271:SER:HB3	1:A:340:TRP:CH2	2.28	0.67
1:A:340:TRP:HZ3	1:A:341:PHE:CZ	2.13	0.67
1:C:146:THR:O	1:C:147:SER:CB	2.43	0.67
1:E:351:ASN:O	1:E:355:GLN:HB2	1.93	0.67
1:G:160:LYS:NZ	1:G:160:LYS:HB3	2.08	0.67
1:G:291:ASP:OD1	1:G:291:ASP:O	2.12	0.67
1:G:375:PHE:HD1	1:G:375:PHE:N	1.91	0.67
1:A:84:LEU:C	1:A:86:ALA:H	1.98	0.67
1:C:291:ASP:OD1	1:C:291:ASP:O	2.12	0.67
1:A:370:LEU:O	1:A:374:ALA:N	2.25	0.67
2:F:322:ILE:HD13	2:F:412:MET:HE1	1.74	0.67
2:F:500:GLU:HA	2:F:503:GLU:CB	2.24	0.67
1:G:335:ILE:C	1:G:337:ASN:N	2.47	0.67
1:G:351:ASN:O	1:G:355:GLN:HB2	1.95	0.67
1:A:12:GLU:C	1:A:14:ARG:H	1.98	0.67
2:D:475:ILE:N	2:D:476:PRO:HD2	2.10	0.67
1:G:73:LEU:HD21	2:H:467:LYS:HG2	1.75	0.67
1:A:377:TYR:HE2	1:A:381:LYS:HD2	1.57	0.67
2:F:390:LYS:HG2	2:F:394:GLU:HG3	1.77	0.67
1:C:85:MET:CE	1:C:104:LEU:HB3	2.25	0.67
2:D:197:ILE:HB	2:D:317:ILE:HD12	1.75	0.67
2:H:455:LEU:HD12	2:H:455:LEU:O	1.94	0.67
2:H:475:ILE:N	2:H:476:PRO:HD2	2.09	0.67
1:G:25:PHE:HD1	1:G:25:PHE:C	1.97	0.67
1:G:13:ALA:HA	1:G:16:LYS:HG3	1.76	0.66
1:A:175:VAL:HG23	1:A:175:VAL:O	1.96	0.66
1:C:25:PHE:C	1:C:25:PHE:HD1	1.97	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:HIS:HB2	1:G:189:GLU:HB3	1.77	0.66
1:G:246:ARG:O	1:G:246:ARG:CG	2.43	0.66
1:A:264:PRO:HA	1:A:267:TRP:CE3	2.29	0.66
2:B:221:LYS:HD2	2:B:321:LEU:HD21	1.76	0.66
1:E:21:LEU:HD12	1:E:93:LEU:CD1	2.24	0.66
1:C:351:ASN:HA	1:C:354:LEU:HB2	1.78	0.66
2:D:496:LYS:O	2:D:499:ASN:ND2	2.28	0.66
1:G:181:THR:HG21	1:G:185:ALA:HA	1.77	0.66
2:H:390:LYS:HG2	2:H:394:GLU:HG3	1.78	0.66
3:H:531:RDC:O1	3:H:531:RDC:H81	1.95	0.66
2:B:322:ILE:HD13	2:B:412:MET:HE1	1.78	0.66
1:C:101:ILE:H	1:C:101:ILE:CD1	2.07	0.66
1:E:181:THR:O	1:E:181:THR:CG2	2.42	0.66
1:E:370:LEU:O	1:E:374:ALA:N	2.21	0.66
2:H:499:ASN:C	2:H:499:ASN:HD22	1.99	0.66
1:C:375:PHE:CD1	1:C:375:PHE:N	2.62	0.66
1:G:237:PRO:O	1:G:242:ARG:NH2	2.27	0.66
1:E:302:ILE:HG23	1:E:312:LEU:CD1	2.21	0.66
1:C:115:LYS:NZ	1:C:115:LYS:HB3	2.10	0.66
1:C:208:VAL:HG21	1:C:213:VAL:CG1	2.26	0.66
1:C:335:ILE:C	1:C:337:ASN:N	2.46	0.66
2:D:390:LYS:HG2	2:D:394:GLU:HG3	1.78	0.66
1:E:246:ARG:O	1:E:246:ARG:HG2	1.95	0.66
1:A:303:PHE:CE1	1:A:356:ARG:HD2	2.31	0.66
1:E:13:ALA:HB1	1:E:16:LYS:HE2	1.78	0.66
2:F:165:ARG:HG2	2:F:166:GLY:H	1.61	0.66
2:H:500:GLU:HA	2:H:503:GLU:CB	2.22	0.66
2:D:499:ASN:HD22	2:D:499:ASN:C	1.99	0.65
1:E:149:LEU:HD13	1:E:152:GLU:HG3	1.77	0.65
1:E:181:THR:HG21	1:E:185:ALA:HA	1.77	0.65
1:G:374:ALA:HB1	1:G:375:PHE:CD1	2.31	0.65
2:H:259:VAL:HG13	2:H:265:ILE:O	1.96	0.65
2:B:444:LEU:O	2:B:447:VAL:HG23	1.96	0.65
1:C:351:ASN:O	1:C:355:GLN:HB2	1.95	0.65
1:G:340:TRP:HZ3	1:G:341:PHE:CZ	2.13	0.65
1:G:377:TYR:HE2	1:G:381:LYS:HD2	1.60	0.65
1:A:181:THR:O	1:A:181:THR:CG2	2.45	0.65
1:E:85:MET:CE	1:E:104:LEU:HB3	2.26	0.65
2:H:340:ARG:HH22	2:H:442:ASN:CB	2.09	0.65
1:A:172:GLY:N	1:C:183:HIS:HE1	1.93	0.65
1:A:183:HIS:CE1	1:C:14:ARG:CZ	2.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:LEU:C	1:E:86:ALA:N	2.50	0.65
1:A:25:PHE:C	1:A:25:PHE:CD1	2.69	0.65
1:A:85:MET:CE	1:A:104:LEU:HB3	2.27	0.65
1:G:77:LYS:NZ	1:G:126:GLU:OE1	2.26	0.65
1:G:149:LEU:O	1:G:150:ARG:C	2.32	0.65
1:A:319:ASN:HD22	1:A:319:ASN:N	1.87	0.65
1:A:372:PHE:HA	1:A:376:GLN:OE1	1.96	0.65
1:E:372:PHE:C	1:E:372:PHE:CD1	2.67	0.65
1:G:101:ILE:HD12	1:G:101:ILE:H	1.60	0.65
1:A:270:PHE:CE2	1:A:294:PHE:HB2	2.31	0.65
2:F:496:LYS:O	2:F:499:ASN:ND2	2.30	0.65
1:G:270:PHE:CE2	1:G:294:PHE:HB2	2.31	0.65
1:A:14:ARG:NH2	1:C:219:ARG:CZ	2.59	0.65
1:C:246:ARG:O	1:C:250:GLU:HB2	1.97	0.65
1:E:25:PHE:C	1:E:25:PHE:HD1	2.00	0.65
1:G:351:ASN:HA	1:G:354:LEU:HB2	1.77	0.65
1:A:68:ARG:NH1	1:A:78:ARG:HB3	2.11	0.65
1:A:101:ILE:HD12	1:A:101:ILE:H	1.59	0.65
1:C:39:VAL:HG13	1:C:68:ARG:C	2.17	0.65
2:D:415:LEU:HD23	2:D:430:ILE:HD13	1.78	0.65
1:E:209:GLU:HB3	1:E:260:THR:HG22	1.78	0.65
2:D:165:ARG:HG2	2:D:166:GLY:N	2.12	0.65
1:E:146:THR:O	1:E:147:SER:CB	2.46	0.65
1:E:188:ILE:HD12	1:E:188:ILE:O	1.97	0.65
1:E:237:PRO:O	1:E:242:ARG:NH2	2.29	0.65
1:E:380:GLU:O	1:E:384:ASN:HB2	1.96	0.65
1:G:25:PHE:C	1:G:25:PHE:CD1	2.70	0.65
1:C:25:PHE:C	1:C:25:PHE:CD1	2.70	0.64
2:F:264:SER:C	2:F:265:ILE:HG12	2.17	0.64
1:G:149:LEU:HD13	1:G:152:GLU:HG3	1.78	0.64
1:C:246:ARG:O	1:C:246:ARG:CG	2.45	0.64
1:C:372:PHE:HA	1:C:376:GLN:OE1	1.97	0.64
2:D:165:ARG:HG2	2:D:166:GLY:H	1.63	0.64
1:A:353:PHE:C	1:A:355:GLN:N	2.51	0.64
2:F:455:LEU:HD12	2:F:455:LEU:O	1.97	0.64
1:A:97:GLU:OE1	1:C:370:LEU:HG	1.96	0.64
1:A:150:ARG:CB	1:A:150:ARG:NH2	2.60	0.64
1:A:200:VAL:HG11	1:A:252:LEU:HD23	1.79	0.64
1:C:175:VAL:O	1:C:175:VAL:HG23	1.97	0.64
1:G:13:ALA:O	1:G:16:LYS:HB2	1.96	0.64
1:C:21:LEU:CD2	1:C:153:MET:HA	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:475:ILE:N	2:F:476:PRO:CD	2.61	0.64
1:G:85:MET:CE	1:G:104:LEU:HB3	2.28	0.64
1:G:302:ILE:HB	1:G:303:PHE:CD2	2.33	0.64
1:G:208:VAL:HG21	1:G:213:VAL:CG1	2.27	0.64
2:B:455:LEU:HD12	2:B:455:LEU:O	1.98	0.63
1:C:31:GLN:HG3	1:C:38:LEU:CD1	2.28	0.63
2:D:444:LEU:O	2:D:447:VAL:HG23	1.98	0.63
1:E:150:ARG:CB	1:E:150:ARG:NH2	2.60	0.63
1:G:85:MET:HE1	1:G:104:LEU:HD23	1.81	0.63
1:A:307:ARG:C	1:A:308:LYS:HD3	2.18	0.63
1:C:209:GLU:HB3	1:C:260:THR:HG22	1.78	0.63
1:C:370:LEU:O	1:C:374:ALA:N	2.29	0.63
2:F:165:ARG:HG2	2:F:166:GLY:N	2.12	0.63
1:A:73:LEU:HD21	2:B:467:LYS:HE3	1.78	0.63
1:C:84:LEU:C	1:C:86:ALA:N	2.51	0.63
1:C:353:PHE:C	1:C:355:GLN:N	2.52	0.63
1:E:39:VAL:HG13	1:E:68:ARG:O	1.98	0.63
1:E:307:ARG:C	1:E:308:LYS:HD3	2.18	0.63
2:F:340:ARG:NH2	2:F:442:ASN:CB	2.60	0.63
2:F:508:LEU:C	2:F:510:SER:H	2.02	0.63
1:G:150:ARG:O	1:G:152:GLU:N	2.31	0.63
1:A:189:GLU:HB3	1:C:183:HIS:HB2	1.81	0.63
1:E:85:MET:CE	1:E:104:LEU:HD23	2.28	0.63
2:F:414:HIS:CD2	2:F:415:LEU:N	2.63	0.63
3:F:531:RDC:H81	3:F:531:RDC:O1	1.97	0.63
1:A:188:ILE:HD12	1:A:188:ILE:O	1.98	0.63
2:B:496:LYS:O	2:B:499:ASN:ND2	2.31	0.63
1:E:189:GLU:HB3	1:G:183:HIS:HB2	1.81	0.63
1:G:246:ARG:O	1:G:250:GLU:HB2	1.98	0.63
1:C:100:THR:OG1	1:C:101:ILE:HD12	1.98	0.63
1:A:181:THR:HG21	1:A:185:ALA:HA	1.80	0.63
2:B:259:VAL:HG13	2:B:265:ILE:O	1.99	0.63
1:E:302:ILE:HB	1:E:303:PHE:CD2	2.34	0.63
1:G:39:VAL:HG13	1:G:68:ARG:O	1.99	0.63
2:H:444:LEU:O	2:H:447:VAL:HG23	1.98	0.63
1:A:314:GLU:HA	1:A:317:ARG:NH1	2.13	0.63
1:E:270:PHE:CE2	1:E:294:PHE:HB2	2.34	0.63
1:E:374:ALA:CB	1:E:375:PHE:HD1	2.11	0.63
1:G:31:GLN:HG3	1:G:38:LEU:CD1	2.27	0.63
1:G:370:LEU:HD23	1:G:370:LEU:N	2.14	0.63
1:G:374:ALA:CB	1:G:375:PHE:CD1	2.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:TYR:O	2:B:382:ASP:HB2	1.97	0.62
2:B:390:LYS:HG2	2:B:394:GLU:HG3	1.80	0.62
1:A:21:LEU:HD21	1:A:153:MET:HA	1.80	0.62
1:A:183:HIS:HB2	1:C:189:GLU:HB3	1.79	0.62
2:F:198:THR:O	2:F:198:THR:CG2	2.45	0.62
1:C:21:LEU:HD21	1:C:153:MET:HG2	1.81	0.62
1:G:12:GLU:C	1:G:14:ARG:H	2.03	0.62
2:H:191:ILE:H	2:H:191:ILE:HD13	1.64	0.62
1:A:14:ARG:HH21	1:C:183:HIS:CD2	2.15	0.62
2:B:480:ARG:CB	2:B:497:TYR:HE1	2.10	0.62
1:C:149:LEU:O	1:C:150:ARG:C	2.37	0.62
1:E:14:ARG:CZ	1:G:183:HIS:CE1	2.82	0.62
1:E:14:ARG:HH21	1:G:219:ARG:CZ	2.11	0.62
1:E:101:ILE:H	1:E:101:ILE:CD1	2.10	0.62
1:E:183:HIS:CE1	1:G:14:ARG:CZ	2.81	0.62
2:F:381:TYR:O	2:F:382:ASP:HB2	2.00	0.62
1:E:102:ARG:HD2	1:G:363:GLU:HG3	1.80	0.62
1:E:150:ARG:HH12	1:E:157:SER:HB3	1.64	0.62
1:G:149:LEU:H	1:G:149:LEU:CD1	2.12	0.62
1:G:160:LYS:CB	1:G:160:LYS:HZ2	2.11	0.62
2:H:496:LYS:O	2:H:499:ASN:ND2	2.32	0.62
1:C:22:ARG:O	1:C:25:PHE:HB3	2.00	0.62
1:E:378:ILE:N	1:E:378:ILE:CD1	2.62	0.62
2:H:493:LEU:HG	2:H:494:VAL:N	2.14	0.62
1:A:146:THR:O	1:A:147:SER:CB	2.48	0.62
3:F:531:RDC:CL1	3:F:531:RDC:O5	2.55	0.62
1:G:84:LEU:C	1:G:86:ALA:H	2.02	0.62
2:H:401:GLY:HA3	2:H:455:LEU:HD21	1.80	0.62
1:A:84:LEU:C	1:A:86:ALA:N	2.51	0.62
2:B:318:GLY:O	2:B:320:ASP:N	2.33	0.62
1:C:149:LEU:HD12	1:C:149:LEU:N	2.15	0.62
2:D:480:ARG:CB	2:D:497:TYR:HE1	2.09	0.62
3:D:531:RDC:H81	3:D:531:RDC:O1	1.99	0.62
1:G:372:PHE:CD1	1:G:372:PHE:C	2.69	0.62
1:G:375:PHE:N	1:G:375:PHE:CD1	2.64	0.62
2:H:511:LYS:HB2	2:H:512:LYS:HD2	1.82	0.62
1:A:374:ALA:C	1:A:375:PHE:CD1	2.70	0.62
1:E:183:HIS:ND1	1:E:183:HIS:N	2.48	0.62
1:A:149:LEU:HD12	1:A:149:LEU:N	2.15	0.61
2:D:191:ILE:HD13	2:D:191:ILE:H	1.64	0.61
1:E:378:ILE:HD13	1:E:378:ILE:H	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:353:PHE:C	1:G:355:GLN:N	2.53	0.61
3:B:531:RDC:O1	3:B:531:RDC:H81	1.99	0.61
2:D:259:VAL:HG13	2:D:265:ILE:O	2.00	0.61
1:G:13:ALA:HB1	1:G:16:LYS:HE2	1.82	0.61
1:A:229:ILE:HD11	1:A:248:LEU:HD13	1.83	0.61
1:A:237:PRO:O	1:A:242:ARG:NH2	2.33	0.61
2:D:112:VAL:HG11	3:D:531:RDC:CL1	2.37	0.61
1:G:22:ARG:O	1:G:25:PHE:HB3	1.99	0.61
2:B:475:ILE:N	2:B:476:PRO:CD	2.64	0.61
1:C:42:ILE:HD11	1:C:68:ARG:HG3	1.83	0.61
1:E:353:PHE:C	1:E:355:GLN:N	2.52	0.61
1:A:136:ASP:O	1:A:139:ILE:HB	2.00	0.61
2:B:508:LEU:C	2:B:510:SER:H	2.02	0.61
2:D:511:LYS:HB2	2:D:512:LYS:HD2	1.82	0.61
1:E:13:ALA:O	1:E:16:LYS:HB2	2.01	0.61
1:E:377:TYR:HE2	1:E:381:LYS:HD2	1.66	0.61
1:A:99:PRO:CB	1:A:104:LEU:HD11	2.31	0.61
1:A:246:ARG:O	1:A:246:ARG:CG	2.49	0.61
2:B:241:ILE:O	2:B:245:ILE:HG13	2.00	0.61
1:E:115:LYS:NZ	1:E:115:LYS:HB3	2.14	0.61
2:H:480:ARG:CB	2:H:497:TYR:HE1	2.12	0.61
2:D:340:ARG:HH22	2:D:442:ASN:CB	2.14	0.61
1:E:12:GLU:C	1:E:14:ARG:H	2.04	0.61
1:G:163:VAL:HG23	1:G:231:ILE:HB	1.82	0.61
1:A:101:ILE:H	1:A:101:ILE:CD1	2.12	0.61
2:B:493:LEU:HG	2:B:494:VAL:N	2.15	0.61
2:B:511:LYS:HB2	2:B:512:LYS:HD2	1.83	0.61
2:D:381:TYR:O	2:D:382:ASP:HB2	2.01	0.61
1:G:230:LEU:CD2	1:G:230:LEU:C	2.69	0.61
1:E:149:LEU:O	1:E:150:ARG:C	2.40	0.61
1:E:172:GLY:CA	1:G:183:HIS:HE1	2.13	0.61
1:G:21:LEU:HD21	1:G:153:MET:HA	1.83	0.61
2:H:475:ILE:N	2:H:476:PRO:CD	2.63	0.61
1:A:21:LEU:HD12	1:A:93:LEU:HG	1.83	0.61
1:E:25:PHE:C	1:E:25:PHE:CD1	2.72	0.61
1:E:208:VAL:HG21	1:E:213:VAL:HG11	1.83	0.61
2:F:493:LEU:HG	2:F:494:VAL:N	2.15	0.61
1:A:298:SER:O	1:A:301:ASP:CB	2.40	0.60
1:E:160:LYS:HZ3	1:E:160:LYS:HB2	1.59	0.60
1:A:303:PHE:HA	1:A:317:ARG:HH21	1.65	0.60
1:E:21:LEU:CD2	1:E:153:MET:HA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:243:ILE:O	2:F:247:ASN:HB2	2.00	0.60
2:F:511:LYS:HB2	2:F:512:LYS:HD2	1.84	0.60
3:H:531:RDC:CL1	3:H:531:RDC:O5	2.55	0.60
1:A:149:LEU:HD13	1:A:152:GLU:HG3	1.82	0.60
1:A:209:GLU:HB3	1:A:260:THR:HG22	1.84	0.60
2:B:263:GLN:O	2:B:264:SER:CB	2.49	0.60
1:E:14:ARG:HH21	1:G:183:HIS:CD2	2.19	0.60
1:C:150:ARG:O	1:C:152:GLU:N	2.35	0.60
1:C:319:ASN:HD22	1:C:319:ASN:N	1.86	0.60
1:A:353:PHE:O	1:A:355:GLN:N	2.34	0.60
1:A:374:ALA:CB	1:A:375:PHE:HD1	2.13	0.60
1:C:238:ASP:OD1	1:C:241:THR:CB	2.41	0.60
1:C:303:PHE:CE1	1:C:356:ARG:HD2	2.35	0.60
2:D:493:LEU:HG	2:D:494:VAL:N	2.17	0.60
2:D:508:LEU:C	2:D:510:SER:H	2.04	0.60
1:E:22:ARG:O	1:E:25:PHE:HB3	2.01	0.60
2:F:318:GLY:O	2:F:320:ASP:N	2.34	0.60
1:G:230:LEU:C	1:G:230:LEU:HD23	2.21	0.60
2:B:191:ILE:H	2:B:191:ILE:HD13	1.66	0.60
2:D:243:ILE:O	2:D:247:ASN:HB2	2.01	0.60
2:F:516:ILE:N	2:F:516:ILE:CD1	2.63	0.60
1:A:208:VAL:HG21	1:A:213:VAL:CG1	2.31	0.60
1:E:224:LYS:HD2	1:E:224:LYS:C	2.22	0.60
1:A:13:ALA:O	1:A:16:LYS:HB2	2.02	0.60
1:C:353:PHE:O	1:C:355:GLN:N	2.34	0.60
2:D:475:ILE:N	2:D:476:PRO:CD	2.65	0.60
1:E:374:ALA:C	1:E:375:PHE:CD1	2.75	0.60
1:G:21:LEU:HD12	1:G:93:LEU:HG	1.84	0.60
2:H:381:TYR:O	2:H:382:ASP:HB2	2.01	0.60
2:B:243:ILE:O	2:B:247:ASN:HB2	2.02	0.60
1:C:385:LYS:HG3	1:C:387:TYR:HE2	1.66	0.60
2:F:444:LEU:O	2:F:447:VAL:HG23	2.01	0.60
1:G:238:ASP:OD1	1:G:238:ASP:N	2.35	0.60
1:C:245:VAL:HG12	1:C:246:ARG:N	2.17	0.60
2:H:508:LEU:C	2:H:510:SER:H	2.05	0.60
1:A:13:ALA:HB1	1:A:16:LYS:HE2	1.83	0.59
1:A:219:ARG:CZ	1:C:14:ARG:NH2	2.65	0.59
1:C:39:VAL:HG12	1:C:40:MET:N	2.17	0.59
1:E:268:TYR:O	1:E:269:ILE:C	2.39	0.59
2:D:18:ARG:O	2:D:20:PRO:HD3	2.02	0.59
1:E:374:ALA:HB1	1:E:375:PHE:HE1	1.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:18:ARG:O	2:F:20:PRO:HD3	2.03	0.59
1:G:150:ARG:CB	1:G:150:ARG:NH2	2.64	0.59
1:A:31:GLN:HE21	2:B:482:LEU:HD21	1.67	0.59
1:C:99:PRO:CB	1:C:104:LEU:HD11	2.32	0.59
2:D:267:ASP:HB2	2:H:204:ILE:HD13	1.84	0.59
1:E:175:VAL:HG23	1:E:175:VAL:O	2.01	0.59
1:E:172:GLY:N	1:G:183:HIS:HE1	2.01	0.59
1:G:372:PHE:HA	1:G:376:GLN:OE1	2.03	0.59
2:B:322:ILE:HG22	2:B:326:LEU:HD21	1.84	0.59
2:B:492:GLU:HB3	2:B:496:LYS:HG2	1.85	0.59
1:E:239:ARG:HH22	1:E:277:SER:HB3	1.67	0.59
1:E:246:ARG:O	1:E:246:ARG:CG	2.50	0.59
1:A:149:LEU:H	1:A:149:LEU:CD1	2.15	0.59
1:A:149:LEU:O	1:A:150:ARG:C	2.40	0.59
2:B:18:ARG:O	2:B:20:PRO:HD3	2.02	0.59
1:C:150:ARG:CB	1:C:150:ARG:NH2	2.64	0.59
2:F:180:TRP:HB3	2:F:181:PRO:HD3	1.85	0.59
1:C:163:VAL:HG22	1:C:164:VAL:H	1.66	0.59
2:H:415:LEU:HD23	2:H:430:ILE:HD13	1.84	0.59
1:C:237:PRO:HG2	1:C:272:VAL:HG11	1.83	0.59
2:D:46:ALA:HB2	3:D:531:RDC:H162	1.84	0.59
2:F:293:ILE:O	2:F:296:LEU:HB3	2.03	0.59
2:F:303:ASP:HB3	2:F:306:PHE:HE2	1.67	0.59
1:G:84:LEU:C	1:G:86:ALA:N	2.56	0.59
2:H:243:ILE:O	2:H:247:ASN:HB2	2.02	0.59
2:H:342:PRO:HA	2:H:351:ILE:HG23	1.85	0.59
2:H:516:ILE:N	2:H:516:ILE:CD1	2.65	0.59
1:C:356:ARG:O	1:C:357:LYS:C	2.40	0.59
1:E:113:LEU:HD22	1:E:115:LYS:O	2.03	0.59
2:D:455:LEU:HD12	2:D:455:LEU:O	2.03	0.59
2:H:303:ASP:HB3	2:H:306:PHE:HE2	1.68	0.59
1:A:150:ARG:HH12	1:A:157:SER:HB3	1.67	0.58
1:A:309:LYS:HB2	1:A:309:LYS:NZ	2.17	0.58
1:C:150:ARG:HH12	1:C:157:SER:HB3	1.68	0.58
2:F:259:VAL:HG13	2:F:265:ILE:O	2.02	0.58
2:F:263:GLN:O	2:F:264:SER:CB	2.50	0.58
2:B:516:ILE:N	2:B:516:ILE:CD1	2.66	0.58
1:E:31:GLN:HG3	1:E:38:LEU:CD1	2.32	0.58
2:F:448:ALA:O	2:F:451:LEU:HB3	2.03	0.58
2:D:303:ASP:HB3	2:D:306:PHE:HE2	1.69	0.58
1:E:160:LYS:HB2	1:E:160:LYS:HZ2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LEU:HD22	1:C:317:ARG:HH11	1.67	0.58
1:C:340:TRP:HZ3	1:C:341:PHE:CZ	2.21	0.58
1:A:21:LEU:HD12	1:A:93:LEU:CD1	2.33	0.58
1:G:149:LEU:HD12	1:G:149:LEU:N	2.15	0.58
1:G:163:VAL:HG22	1:G:164:VAL:H	1.69	0.58
1:A:12:GLU:C	1:A:14:ARG:N	2.57	0.58
1:A:183:HIS:ND1	1:A:183:HIS:N	2.52	0.58
2:B:264:SER:C	2:B:265:ILE:HG12	2.22	0.58
2:B:441:LYS:O	2:B:443:ALA:N	2.35	0.58
1:G:268:TYR:O	1:G:269:ILE:C	2.40	0.58
1:C:351:ASN:OD1	1:C:351:ASN:N	2.29	0.58
1:E:21:LEU:HD12	1:E:93:LEU:HG	1.84	0.58
1:E:31:GLN:O	1:E:32:LEU:C	2.42	0.58
1:E:230:LEU:HD23	1:E:230:LEU:C	2.24	0.58
1:A:268:TYR:O	1:A:269:ILE:C	2.41	0.58
1:G:183:HIS:ND1	1:G:183:HIS:N	2.51	0.58
1:G:353:PHE:O	1:G:355:GLN:N	2.37	0.58
2:D:241:ILE:O	2:D:245:ILE:HG13	2.04	0.58
1:E:31:GLN:HE21	2:F:482:LEU:HD21	1.69	0.58
1:G:73:LEU:HD21	2:H:467:LYS:CE	2.34	0.58
2:H:103:GLN:HE22	2:H:315:SER:N	2.01	0.58
1:A:230:LEU:HD23	1:A:230:LEU:C	2.24	0.58
3:B:531:RDC:O5	3:B:531:RDC:CL1	2.58	0.58
3:D:531:RDC:CL1	3:D:531:RDC:O5	2.59	0.58
1:E:39:VAL:HG12	1:E:40:MET:N	2.18	0.58
1:G:189:GLU:O	1:G:191:THR:N	2.36	0.58
1:A:239:ARG:HH22	1:A:277:SER:HB3	1.69	0.57
2:F:197:ILE:HB	2:F:317:ILE:HD12	1.85	0.57
1:G:307:ARG:C	1:G:308:LYS:HD3	2.24	0.57
1:A:230:LEU:C	1:A:230:LEU:CD2	2.72	0.57
1:A:374:ALA:HB1	1:A:375:PHE:HE1	1.69	0.57
2:D:400:TYR:CA	2:D:452:LYS:HE2	2.23	0.57
2:D:516:ILE:N	2:D:516:ILE:CD1	2.65	0.57
2:F:480:ARG:CB	2:F:497:TYR:HE1	2.12	0.57
2:H:263:GLN:O	2:H:264:SER:CB	2.51	0.57
1:A:21:LEU:CD2	1:A:153:MET:HA	2.35	0.57
1:A:183:HIS:HE1	1:C:172:GLY:CA	2.16	0.57
1:C:303:PHE:HA	1:C:317:ARG:NH2	2.19	0.57
2:D:263:GLN:O	2:D:264:SER:CB	2.51	0.57
2:D:264:SER:C	2:D:265:ILE:HG12	2.24	0.57
1:E:170:ARG:HG3	1:E:196:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HG13	1:A:68:ARG:O	2.05	0.57
1:A:163:VAL:HG22	1:A:164:VAL:H	1.70	0.57
1:E:12:GLU:C	1:E:14:ARG:N	2.56	0.57
1:E:149:LEU:H	1:E:149:LEU:CD1	2.17	0.57
1:E:325:LYS:O	1:E:328:ASP:HB2	2.04	0.57
1:C:80:MET:CE	2:D:477:GLU:HB3	2.34	0.57
2:D:46:ALA:CB	3:D:531:RDC:H162	2.35	0.57
1:E:138:VAL:O	1:E:142:ILE:HG13	2.04	0.57
1:E:385:LYS:HG3	1:E:387:TYR:HE2	1.70	0.57
2:F:415:LEU:HD23	2:F:430:ILE:HD13	1.85	0.57
1:G:150:ARG:HH12	1:G:157:SER:HB3	1.68	0.57
1:E:340:TRP:HZ3	1:E:341:PHE:CZ	2.22	0.57
2:H:487:ALA:HB3	2:H:492:GLU:HB2	1.85	0.57
1:A:31:GLN:O	1:A:32:LEU:C	2.43	0.57
1:C:295:LEU:O	1:C:295:LEU:HD22	2.05	0.57
1:E:353:PHE:O	1:E:355:GLN:N	2.37	0.57
2:F:492:GLU:HB3	2:F:496:LYS:HG2	1.85	0.57
1:G:13:ALA:CB	1:G:16:LYS:HE2	2.35	0.57
2:H:180:TRP:HB3	2:H:181:PRO:HD3	1.85	0.57
2:H:340:ARG:HH22	2:H:442:ASN:HB2	1.69	0.57
2:B:401:GLY:HA3	2:B:455:LEU:HD21	1.87	0.57
2:B:441:LYS:O	2:B:442:ASN:C	2.43	0.57
1:C:69:ASN:N	1:C:69:ASN:OD1	2.38	0.57
1:C:149:LEU:HD13	1:C:152:GLU:HG3	1.86	0.57
1:E:13:ALA:CB	1:E:16:LYS:HE2	2.34	0.57
1:G:303:PHE:CE1	1:G:356:ARG:HD2	2.40	0.57
1:A:22:ARG:O	1:A:25:PHE:HB3	2.04	0.57
1:A:36:GLU:HB3	1:A:37:PRO:HD2	1.87	0.57
1:A:85:MET:CE	1:A:104:LEU:HD23	2.35	0.57
2:B:112:VAL:HG21	3:B:531:RDC:CL1	2.42	0.57
2:B:340:ARG:HH22	2:B:442:ASN:HB3	1.70	0.57
2:B:420:ILE:HB	2:B:422:TYR:HE2	1.70	0.57
1:C:13:ALA:O	1:C:16:LYS:HB2	2.05	0.57
1:E:99:PRO:CB	1:E:104:LEU:HD11	2.33	0.57
1:E:238:ASP:O	1:E:242:ARG:NH2	2.38	0.57
1:G:21:LEU:HD12	1:G:93:LEU:CD1	2.34	0.57
1:E:262:ALA:HB2	1:E:360:LEU:HD12	1.86	0.57
1:A:307:ARG:CD	1:A:308:LYS:HZ3	1.94	0.56
1:C:17:ALA:O	1:C:19:ASN:N	2.38	0.56
1:E:100:THR:OG1	1:E:101:ILE:HD12	2.05	0.56
2:F:401:GLY:CA	2:F:455:LEU:HD21	2.11	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:ARG:HH22	1:G:277:SER:HB3	1.70	0.56
1:G:374:ALA:CB	1:G:375:PHE:HD1	2.18	0.56
2:H:455:LEU:HD13	2:H:459:ARG:HH22	1.70	0.56
1:C:39:VAL:CG2	1:C:69:ASN:HA	2.35	0.56
1:C:246:ARG:HB2	1:C:289:THR:HG22	1.87	0.56
1:E:298:SER:O	1:E:301:ASP:CB	2.44	0.56
1:A:13:ALA:CB	1:A:16:LYS:HE2	2.36	0.56
1:C:183:HIS:N	1:C:183:HIS:ND1	2.53	0.56
1:E:69:ASN:N	1:E:69:ASN:OD1	2.38	0.56
1:E:98:TYR:HB3	1:E:156:LEU:CD2	2.35	0.56
1:E:183:HIS:HE1	1:G:172:GLY:CA	2.18	0.56
1:E:319:ASN:ND2	1:E:319:ASN:N	2.47	0.56
2:F:142:PHE:HB3	2:F:144:LEU:CD1	2.36	0.56
1:G:99:PRO:CB	1:G:104:LEU:HD11	2.35	0.56
1:G:270:PHE:HE2	1:G:294:PHE:HB2	1.71	0.56
1:A:274:ARG:O	1:A:275:ILE:HG23	2.05	0.56
1:C:262:ALA:HB2	1:C:360:LEU:HD12	1.88	0.56
1:C:268:TYR:O	1:C:269:ILE:C	2.43	0.56
1:E:246:ARG:HB2	1:E:289:THR:HG22	1.86	0.56
2:F:318:GLY:C	2:F:320:ASP:H	2.09	0.56
1:G:272:VAL:HG13	1:G:277:SER:H	1.69	0.56
1:G:309:LYS:HG3	1:G:310:PRO:HD2	1.87	0.56
2:H:264:SER:C	2:H:265:ILE:HG12	2.24	0.56
1:A:331:ARG:O	1:A:335:ILE:HG12	2.05	0.56
1:C:237:PRO:O	1:C:242:ARG:NH2	2.39	0.56
1:C:270:PHE:CE2	1:C:294:PHE:HB2	2.41	0.56
2:D:112:VAL:HG21	3:D:531:RDC:CL1	2.43	0.56
2:D:342:PRO:HA	2:D:351:ILE:HG23	1.88	0.56
1:E:183:HIS:HE1	1:G:172:GLY:N	2.03	0.56
2:F:467:LYS:O	2:F:469:LEU:N	2.39	0.56
1:A:113:LEU:HD22	1:A:115:LYS:O	2.05	0.56
1:C:113:LEU:HD22	1:C:115:LYS:O	2.06	0.56
1:E:21:LEU:HB3	1:E:93:LEU:HD11	1.87	0.56
1:G:12:GLU:C	1:G:14:ARG:N	2.58	0.56
1:G:36:GLU:HB3	1:G:37:PRO:HD2	1.88	0.56
1:G:68:ARG:NH1	1:G:78:ARG:HB3	2.20	0.56
1:A:262:ALA:HB2	1:A:360:LEU:HD12	1.88	0.56
2:D:180:TRP:HB3	2:D:181:PRO:HD3	1.87	0.56
2:D:221:LYS:HD2	2:D:321:LEU:HD21	1.87	0.56
1:G:100:THR:OG1	1:G:101:ILE:HD12	2.05	0.56
1:A:14:ARG:CZ	1:C:183:HIS:CD2	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:C	1:A:275:ILE:HG12	2.26	0.56
2:B:255:LYS:O	2:B:256:GLU:C	2.44	0.56
1:C:142:ILE:O	1:C:146:THR:HG23	2.05	0.56
1:G:208:VAL:HG21	1:G:213:VAL:HG11	1.88	0.56
2:B:345:TYR:O	2:B:346:GLN:C	2.44	0.56
1:C:12:GLU:C	1:C:14:ARG:H	2.09	0.56
1:C:31:GLN:O	1:C:32:LEU:C	2.44	0.56
1:C:319:ASN:ND2	1:C:319:ASN:N	2.46	0.56
1:C:377:TYR:HE2	1:C:381:LYS:HD2	1.69	0.56
1:E:230:LEU:C	1:E:230:LEU:CD2	2.74	0.56
1:E:351:ASN:OD1	1:E:351:ASN:N	2.34	0.56
1:G:31:GLN:O	1:G:32:LEU:C	2.43	0.56
1:G:192:PRO:HG3	1:G:240:ALA:HB1	1.87	0.56
2:H:420:ILE:HB	2:H:422:TYR:HE2	1.71	0.56
1:A:191:THR:O	1:A:191:THR:OG1	2.24	0.55
1:C:374:ALA:HB1	1:C:375:PHE:HE1	1.68	0.55
2:F:285:VAL:HG13	2:F:286:LYS:N	2.21	0.55
2:B:318:GLY:C	2:B:320:ASP:H	2.09	0.55
1:C:208:VAL:HG21	1:C:213:VAL:HG11	1.88	0.55
2:D:492:GLU:HB3	2:D:496:LYS:HG2	1.88	0.55
1:E:136:ASP:O	1:E:139:ILE:HB	2.06	0.55
1:E:150:ARG:O	1:E:152:GLU:N	2.39	0.55
1:A:101:ILE:N	1:A:101:ILE:CD1	2.63	0.55
1:C:17:ALA:C	1:C:19:ASN:H	2.10	0.55
1:C:149:LEU:H	1:C:149:LEU:CD1	2.18	0.55
1:C:163:VAL:HG23	1:C:231:ILE:HB	1.88	0.55
1:C:191:THR:OG1	1:C:194:LEU:HD21	2.06	0.55
1:E:17:ALA:C	1:E:19:ASN:H	2.10	0.55
1:G:242:ARG:O	1:G:243:ARG:C	2.43	0.55
2:H:112:VAL:HG21	3:H:531:RDC:CL1	2.43	0.55
1:A:21:LEU:HD21	1:A:153:MET:HG2	1.88	0.55
1:A:356:ARG:O	1:A:357:LYS:C	2.43	0.55
2:D:142:PHE:HB3	2:D:144:LEU:CD1	2.36	0.55
2:D:191:ILE:H	2:D:191:ILE:CD1	2.16	0.55
1:E:163:VAL:HG23	1:E:231:ILE:HB	1.88	0.55
2:F:342:PRO:HA	2:F:351:ILE:HG23	1.88	0.55
1:G:295:LEU:O	1:G:295:LEU:HD22	2.06	0.55
2:H:293:ILE:O	2:H:296:LEU:HB3	2.06	0.55
1:A:82:THR:HA	1:A:138:VAL:CG1	2.37	0.55
1:A:142:ILE:O	1:A:146:THR:HG23	2.07	0.55
1:C:136:ASP:O	1:C:139:ILE:HB	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:GLN:O	2:D:313:SER:HA	2.06	0.55
1:G:113:LEU:HD22	1:G:115:LYS:O	2.06	0.55
1:G:238:ASP:OD1	1:G:241:THR:CB	2.45	0.55
1:C:13:ALA:HB1	1:C:16:LYS:HE2	1.89	0.55
1:C:21:LEU:HB3	1:C:93:LEU:HD11	1.88	0.55
1:C:36:GLU:HB3	1:C:37:PRO:HD2	1.88	0.55
1:C:170:ARG:CG	1:C:196:ASP:HB2	2.36	0.55
1:C:261:ASP:OD1	1:C:362:ILE:N	2.39	0.55
1:E:142:ILE:O	1:E:146:THR:HG23	2.07	0.55
1:E:149:LEU:HD12	1:E:149:LEU:N	2.18	0.55
1:E:163:VAL:HG22	1:E:164:VAL:H	1.71	0.55
1:A:42:ILE:HD11	1:A:68:ARG:HG3	1.88	0.55
1:C:73:LEU:HD21	2:D:467:LYS:HG2	1.88	0.55
1:C:101:ILE:N	1:C:101:ILE:CD1	2.59	0.55
1:A:339:GLU:HG3	1:A:339:GLU:O	2.07	0.55
2:B:342:PRO:HA	2:B:351:ILE:HG23	1.89	0.55
2:D:420:ILE:HB	2:D:422:TYR:HE2	1.71	0.55
2:D:487:ALA:HB3	2:D:492:GLU:HB2	1.88	0.55
1:C:85:MET:CE	1:C:104:LEU:HD23	2.36	0.55
1:A:224:LYS:HD2	1:A:224:LYS:C	2.27	0.55
2:B:227:GLN:O	2:B:313:SER:HA	2.07	0.55
1:G:183:HIS:N	1:G:183:HIS:HD1	2.04	0.55
1:A:39:VAL:HG22	1:A:69:ASN:HA	1.88	0.54
1:C:138:VAL:O	1:C:142:ILE:HG13	2.07	0.54
1:C:374:ALA:C	1:C:375:PHE:CD1	2.78	0.54
2:D:293:ILE:O	2:D:296:LEU:HB3	2.07	0.54
2:D:318:GLY:O	2:D:320:ASP:N	2.40	0.54
2:D:355:GLY:N	2:D:412:MET:HE3	2.22	0.54
2:D:401:GLY:HA3	2:D:455:LEU:HD11	1.88	0.54
1:G:32:LEU:HD11	2:H:486:LEU:HD11	1.88	0.54
1:A:21:LEU:HB3	1:A:93:LEU:HD11	1.88	0.54
1:A:69:ASN:OD1	1:A:69:ASN:N	2.39	0.54
2:B:180:TRP:HB3	2:B:181:PRO:HD3	1.88	0.54
2:B:198:THR:O	2:B:198:THR:CG2	2.47	0.54
2:B:293:ILE:O	2:B:296:LEU:HB3	2.08	0.54
1:C:274:ARG:C	1:C:275:ILE:HG12	2.27	0.54
2:B:285:VAL:O	2:B:288:LEU:HG	2.07	0.54
1:C:148:LEU:HD12	1:C:148:LEU:N	2.22	0.54
2:D:215:TYR:CD2	2:D:215:TYR:N	2.74	0.54
1:G:85:MET:CE	1:G:104:LEU:HD23	2.37	0.54
1:G:229:ILE:HD11	1:G:248:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PHE:HE2	1:A:294:PHE:HB2	1.73	0.54
2:B:330:PHE:O	2:B:361:SER:HB2	2.08	0.54
1:C:230:LEU:C	1:C:230:LEU:CD2	2.76	0.54
1:E:176:ILE:CD1	1:G:176:ILE:CD1	2.67	0.54
1:E:356:ARG:O	1:E:357:LYS:C	2.45	0.54
2:F:215:TYR:N	2:F:215:TYR:CD2	2.75	0.54
1:G:69:ASN:OD1	1:G:69:ASN:N	2.39	0.54
1:G:175:VAL:HG23	1:G:175:VAL:O	2.06	0.54
1:A:17:ALA:C	1:A:19:ASN:H	2.10	0.54
1:A:86:ALA:O	1:A:89:ILE:HB	2.08	0.54
1:C:229:ILE:HD11	1:C:248:LEU:HD13	1.88	0.54
1:E:36:GLU:HB3	1:E:37:PRO:HD2	1.89	0.54
2:F:326:LEU:HD12	2:F:357:ALA:HB2	1.89	0.54
1:G:274:ARG:C	1:G:275:ILE:HG12	2.26	0.54
2:H:492:GLU:HB3	2:H:496:LYS:HG2	1.90	0.54
1:A:100:THR:OG1	1:A:101:ILE:HD12	2.08	0.54
1:G:191:THR:O	1:G:191:THR:OG1	2.17	0.54
2:B:396:ASP:HB3	2:B:399:ARG:HH11	1.73	0.54
1:C:21:LEU:HD12	1:C:93:LEU:HG	1.90	0.54
1:E:309:LYS:HG3	1:E:310:PRO:HD2	1.89	0.54
2:F:255:LYS:O	2:F:256:GLU:C	2.45	0.54
1:G:43:PRO:O	1:G:144:VAL:HG11	2.08	0.54
1:G:245:VAL:HG12	1:G:246:ARG:N	2.22	0.54
1:G:261:ASP:OD1	1:G:362:ILE:N	2.40	0.54
1:G:374:ALA:C	1:G:375:PHE:CD1	2.77	0.54
1:A:189:GLU:O	1:A:191:THR:N	2.40	0.54
2:B:303:ASP:HB3	2:B:306:PHE:HE2	1.72	0.54
1:C:309:LYS:HG3	1:C:310:PRO:HD2	1.90	0.54
1:G:339:GLU:O	1:G:339:GLU:HG3	2.07	0.54
2:H:191:ILE:H	2:H:191:ILE:CD1	2.21	0.54
1:A:309:LYS:HG3	1:A:310:PRO:HD2	1.90	0.54
2:B:362:ILE:HG22	2:B:408:GLN:HB3	1.90	0.54
2:H:18:ARG:O	2:H:20:PRO:HD3	2.08	0.54
1:A:176:ILE:CD1	1:C:176:ILE:CD1	2.67	0.53
2:B:415:LEU:HD23	2:B:430:ILE:HD13	1.90	0.53
2:F:330:PHE:O	2:F:361:SER:HB2	2.07	0.53
2:H:285:VAL:O	2:H:288:LEU:HG	2.08	0.53
2:B:467:LYS:O	2:B:470:ALA:N	2.41	0.53
1:C:12:GLU:CG	1:C:13:ALA:N	2.70	0.53
2:F:369:ILE:HB	2:F:410:VAL:HG13	1.90	0.53
2:H:322:ILE:HG22	2:H:326:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:O	1:A:188:ILE:CD1	2.56	0.53
2:B:142:PHE:HB3	2:B:144:LEU:CD1	2.37	0.53
1:C:12:GLU:C	1:C:14:ARG:N	2.60	0.53
1:C:148:LEU:N	1:C:148:LEU:CD1	2.71	0.53
1:E:68:ARG:NH1	1:E:78:ARG:HB3	2.24	0.53
2:F:395:LEU:HD12	2:F:396:ASP:H	1.72	0.53
1:G:86:ALA:O	1:G:89:ILE:HB	2.08	0.53
1:G:262:ALA:HB2	1:G:360:LEU:HD12	1.89	0.53
1:G:270:PHE:CD1	1:G:270:PHE:C	2.81	0.53
1:C:230:LEU:C	1:C:230:LEU:HD23	2.28	0.53
1:E:170:ARG:CG	1:E:196:ASP:HB2	2.38	0.53
1:A:183:HIS:HE1	1:C:172:GLY:N	2.06	0.53
1:A:184:GLY:O	1:A:185:ALA:HB2	2.09	0.53
1:A:237:PRO:HG2	1:A:272:VAL:HG11	1.89	0.53
3:B:531:RDC:CL1	3:B:531:RDC:C9	2.94	0.53
1:C:80:MET:CE	2:D:477:GLU:CB	2.86	0.53
1:C:268:TYR:O	1:C:271:SER:N	2.41	0.53
2:D:285:VAL:O	2:D:288:LEU:HG	2.08	0.53
1:E:188:ILE:O	1:E:188:ILE:CD1	2.56	0.53
2:F:18:ARG:C	2:F:20:PRO:HD3	2.29	0.53
1:G:101:ILE:H	1:G:101:ILE:CD1	2.14	0.53
1:G:356:ARG:O	1:G:357:LYS:C	2.45	0.53
2:H:318:GLY:O	2:H:320:ASP:N	2.39	0.53
1:A:138:VAL:O	1:A:142:ILE:HG13	2.09	0.53
1:C:224:LYS:HD2	1:C:224:LYS:C	2.29	0.53
1:E:39:VAL:HG22	1:E:69:ASN:HA	1.90	0.53
1:E:295:LEU:O	1:E:295:LEU:HD22	2.09	0.53
1:G:21:LEU:CD2	1:G:153:MET:HA	2.38	0.53
2:H:45:ASP:OD1	2:H:105:ARG:HD2	2.09	0.53
1:A:32:LEU:O	1:A:33:LYS:C	2.46	0.53
1:C:42:ILE:CD1	1:C:68:ARG:HG3	2.38	0.53
1:E:339:GLU:HG3	1:E:339:GLU:O	2.08	0.53
1:G:243:ARG:HH22	1:G:287:LEU:HD22	1.73	0.53
1:A:106:TYR:C	1:A:107:ARG:HD3	2.24	0.53
1:E:245:VAL:HG12	1:E:246:ARG:N	2.24	0.53
2:F:47:THR:HG22	2:F:78:GLY:HA2	1.91	0.53
2:H:142:PHE:HB3	2:H:144:LEU:CD1	2.39	0.53
1:A:172:GLY:N	1:C:183:HIS:CE1	2.76	0.53
2:B:467:LYS:O	2:B:469:LEU:N	2.42	0.53
1:C:32:LEU:O	1:C:33:LYS:C	2.46	0.53
1:C:163:VAL:HG22	1:C:164:VAL:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:ALA:O	1:E:19:ASN:N	2.42	0.53
1:G:39:VAL:HG12	1:G:40:MET:N	2.23	0.53
2:B:47:THR:HG22	2:B:78:GLY:HA2	1.91	0.53
2:D:322:ILE:HG22	2:D:326:LEU:HD21	1.91	0.53
2:H:165:ARG:HG2	2:H:166:GLY:H	1.73	0.53
1:A:246:ARG:HB2	1:A:289:THR:HG22	1.91	0.52
1:A:259:LEU:CD1	1:A:259:LEU:O	2.57	0.52
1:C:89:ILE:HD13	1:C:104:LEU:HD21	1.92	0.52
1:C:98:TYR:HB3	1:C:156:LEU:CD2	2.39	0.52
1:C:302:ILE:HG22	1:C:312:LEU:CD2	2.19	0.52
1:G:270:PHE:CD2	1:G:294:PHE:HD1	2.27	0.52
1:G:370:LEU:O	1:G:374:ALA:N	2.33	0.52
1:A:12:GLU:O	1:A:14:ARG:N	2.41	0.52
1:A:170:ARG:CG	1:A:196:ASP:HB2	2.39	0.52
1:A:385:LYS:HG3	1:A:387:TYR:CE2	2.42	0.52
2:D:18:ARG:C	2:D:20:PRO:HD3	2.29	0.52
2:D:326:LEU:HD12	2:D:357:ALA:HB2	1.90	0.52
2:D:402:ILE:O	2:D:402:ILE:HG22	2.10	0.52
2:D:467:LYS:O	2:D:469:LEU:N	2.43	0.52
2:F:191:ILE:HD13	2:F:191:ILE:H	1.73	0.52
1:G:37:PRO:HD3	2:H:507:LYS:NZ	2.23	0.52
2:H:165:ARG:HG2	2:H:166:GLY:N	2.24	0.52
2:H:340:ARG:NH2	2:H:442:ASN:CB	2.67	0.52
1:A:163:VAL:HG23	1:A:231:ILE:HB	1.91	0.52
1:A:379:PRO:O	1:A:383:THR:HG22	2.09	0.52
2:B:165:ARG:HG2	2:B:166:GLY:N	2.23	0.52
1:E:378:ILE:HB	1:E:379:PRO:CD	2.40	0.52
2:F:322:ILE:HG22	2:F:326:LEU:HD21	1.91	0.52
1:G:224:LYS:HD2	1:G:224:LYS:C	2.28	0.52
1:A:39:VAL:HG12	1:A:40:MET:N	2.23	0.52
1:A:325:LYS:O	1:A:328:ASP:HB2	2.09	0.52
2:B:487:ALA:HB3	2:B:492:GLU:HB2	1.90	0.52
2:F:286:LYS:HG3	2:F:287:ASN:HD22	1.74	0.52
1:G:142:ILE:O	1:G:146:THR:HG23	2.10	0.52
1:G:374:ALA:HB1	1:G:375:PHE:HE1	1.70	0.52
2:H:215:TYR:N	2:H:215:TYR:CD2	2.77	0.52
2:H:241:ILE:O	2:H:245:ILE:HG13	2.09	0.52
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.09	0.52
2:B:18:ARG:C	2:B:20:PRO:HD3	2.30	0.52
1:C:12:GLU:HG3	1:C:13:ALA:N	2.25	0.52
1:C:68:ARG:NH1	1:C:78:ARG:HB3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:MET:HE3	2:D:477:GLU:CB	2.39	0.52
2:D:193:ARG:HD3	2:D:371:LEU:HD23	1.91	0.52
2:D:340:ARG:NH2	2:D:442:ASN:CB	2.71	0.52
2:D:340:ARG:HH22	2:D:442:ASN:HB2	1.75	0.52
1:E:184:GLY:O	1:E:185:ALA:HB2	2.09	0.52
1:G:136:ASP:O	1:G:139:ILE:HB	2.10	0.52
2:H:402:ILE:O	2:H:402:ILE:HG22	2.09	0.52
2:B:326:LEU:HD12	2:B:357:ALA:HB2	1.90	0.52
2:B:437:GLU:HG3	2:B:437:GLU:O	2.10	0.52
1:E:159:GLU:HG2	1:E:238:ASP:HB2	1.90	0.52
1:G:17:ALA:C	1:G:19:ASN:H	2.12	0.52
1:A:191:THR:OG1	1:A:194:LEU:HD21	2.10	0.52
1:E:17:ALA:C	1:E:19:ASN:N	2.63	0.52
1:G:177:ASP:C	1:G:177:ASP:OD1	2.47	0.52
1:G:307:ARG:HG3	1:G:308:LYS:N	2.24	0.52
2:H:318:GLY:C	2:H:320:ASP:H	2.12	0.52
1:A:14:ARG:CZ	1:C:183:HIS:NE2	2.73	0.52
2:B:253:THR:OG1	2:B:254:ILE:N	2.42	0.52
1:C:98:TYR:HB3	1:C:156:LEU:HD21	1.91	0.52
1:C:216:GLN:HG2	1:C:370:LEU:HD11	1.92	0.52
1:E:312:LEU:N	1:E:312:LEU:HD23	2.24	0.52
2:F:340:ARG:HH22	2:F:442:ASN:HB3	1.72	0.52
1:G:331:ARG:O	1:G:335:ILE:HG12	2.10	0.52
1:G:385:LYS:HG3	1:G:387:TYR:HE2	1.75	0.52
1:A:17:ALA:C	1:A:19:ASN:N	2.63	0.52
1:A:270:PHE:CD2	1:A:294:PHE:HD1	2.28	0.52
3:D:531:RDC:CL1	3:D:531:RDC:C9	2.95	0.52
1:E:270:PHE:C	1:E:270:PHE:CD1	2.82	0.52
2:F:362:ILE:HG22	2:F:408:GLN:HB3	1.92	0.52
2:H:396:ASP:HB3	2:H:399:ARG:HH11	1.75	0.52
1:C:307:ARG:O	1:C:308:LYS:HD2	2.10	0.52
2:D:224:LYS:CG	2:D:225:PRO:HD2	2.38	0.52
2:D:286:LYS:HG3	2:D:287:ASN:HD22	1.75	0.52
1:E:274:ARG:C	1:E:275:ILE:HG12	2.29	0.52
2:F:467:LYS:O	2:F:470:ALA:N	2.43	0.52
1:C:302:ILE:HB	1:C:303:PHE:HD2	1.72	0.51
1:C:325:LYS:O	1:C:328:ASP:HB2	2.10	0.51
2:D:255:LYS:O	2:D:256:GLU:C	2.47	0.51
2:D:505:LEU:O	2:D:508:LEU:HB2	2.10	0.51
1:E:219:ARG:CZ	1:G:14:ARG:NH2	2.72	0.51
3:H:531:RDC:CL1	3:H:531:RDC:C9	2.95	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ASP:OD1	1:C:238:ASP:N	2.42	0.51
1:E:101:ILE:N	1:E:101:ILE:CD1	2.60	0.51
1:E:331:ARG:O	1:E:335:ILE:HG12	2.09	0.51
2:H:286:LYS:HG3	2:H:287:ASN:HD22	1.74	0.51
1:A:89:ILE:O	1:A:93:LEU:HB2	2.10	0.51
1:A:221:GLY:O	1:A:222:PHE:C	2.47	0.51
1:C:270:PHE:CD2	1:C:294:PHE:HD1	2.29	0.51
2:D:207:ASP:HB2	2:D:208:PRO:CD	2.40	0.51
2:D:318:GLY:C	2:D:320:ASP:H	2.13	0.51
2:F:219:THR:CG2	2:F:220:ASN:N	2.62	0.51
1:E:118:GLU:OE1	1:E:118:GLU:HA	2.10	0.51
2:F:44:LEU:C	2:F:46:ALA:H	2.14	0.51
2:F:441:LYS:O	2:F:442:ASN:C	2.49	0.51
1:G:351:ASN:N	1:G:351:ASN:OD1	2.38	0.51
2:H:395:LEU:HD12	2:H:396:ASP:H	1.75	0.51
1:C:239:ARG:HH22	1:C:277:SER:HB3	1.76	0.51
1:C:261:ASP:OD1	1:C:362:ILE:HG13	2.10	0.51
2:D:362:ILE:HG22	2:D:408:GLN:HB3	1.92	0.51
1:G:32:LEU:O	1:G:33:LYS:C	2.48	0.51
1:G:263:ASP:HB2	1:G:264:PRO:HD2	1.92	0.51
1:A:268:TYR:O	1:A:271:SER:N	2.44	0.51
2:B:395:LEU:HD12	2:B:396:ASP:H	1.75	0.51
1:E:270:PHE:CD2	1:E:294:PHE:HD1	2.29	0.51
2:F:103:GLN:NE2	2:F:315:SER:H	2.08	0.51
3:F:531:RDC:CL1	3:F:531:RDC:C9	2.95	0.51
1:A:80:MET:CE	2:B:477:GLU:HB3	2.41	0.51
2:B:240:GLU:O	2:B:243:ILE:HG12	2.11	0.51
2:B:414:HIS:CD2	2:B:414:HIS:C	2.84	0.51
2:D:219:THR:HG23	2:D:220:ASN:H	1.73	0.51
2:D:441:LYS:O	2:D:443:ALA:N	2.43	0.51
1:E:89:ILE:O	1:E:93:LEU:HB2	2.11	0.51
1:E:229:ILE:HD11	1:E:248:LEU:HD13	1.93	0.51
1:G:31:GLN:HE21	2:H:482:LEU:HD21	1.76	0.51
1:G:319:ASN:ND2	1:G:319:ASN:N	2.52	0.51
1:A:160:LYS:HB2	1:A:160:LYS:HZ2	1.72	0.51
1:C:106:TYR:C	1:C:107:ARG:HD3	2.26	0.51
1:C:378:ILE:O	1:C:379:PRO:C	2.49	0.51
1:E:192:PRO:HG3	1:E:240:ALA:HB1	1.92	0.51
1:G:118:GLU:OE1	1:G:118:GLU:HA	2.10	0.51
2:H:362:ILE:HG22	2:H:408:GLN:HB3	1.93	0.51
1:C:17:ALA:C	1:C:19:ASN:N	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ARG:HG3	1:C:196:ASP:HB2	1.92	0.51
2:D:467:LYS:O	2:D:470:ALA:N	2.44	0.51
1:E:309:LYS:NZ	1:E:309:LYS:HB2	2.26	0.51
2:F:99:TYR:HH	2:F:348:HIS:HE2	1.57	0.51
1:G:159:GLU:CG	1:G:238:ASP:HB2	2.40	0.51
1:G:271:SER:HB3	1:G:340:TRP:HH2	1.75	0.51
2:H:505:LEU:O	2:H:508:LEU:HB2	2.11	0.51
1:A:295:LEU:HD23	1:A:387:TYR:HB3	1.92	0.51
1:C:294:PHE:HB3	1:C:388:ILE:HG13	1.92	0.51
2:D:441:LYS:O	2:D:442:ASN:C	2.49	0.51
1:E:89:ILE:HD13	1:E:104:LEU:HD21	1.93	0.51
1:G:98:TYR:HB3	1:G:156:LEU:HD21	1.93	0.51
1:A:208:VAL:HG22	1:A:209:GLU:N	2.26	0.50
1:A:238:ASP:O	1:A:242:ARG:NH2	2.44	0.50
1:A:243:ARG:HH22	1:A:287:LEU:HD22	1.75	0.50
1:E:21:LEU:HD21	1:E:153:MET:HG2	1.93	0.50
1:A:89:ILE:HD13	1:A:104:LEU:HD21	1.93	0.50
1:A:205:VAL:CG1	1:A:256:VAL:HG22	2.41	0.50
1:A:317:ARG:O	1:A:321:ILE:HG13	2.11	0.50
2:B:58:ILE:O	2:B:205:PHE:HA	2.10	0.50
1:C:274:ARG:O	1:C:275:ILE:HG23	2.11	0.50
2:D:84:GLN:HE21	2:D:85:GLU:HG3	1.76	0.50
1:E:154:LEU:O	1:E:156:LEU:N	2.44	0.50
1:E:294:PHE:HB3	1:E:388:ILE:HG13	1.92	0.50
2:F:99:TYR:HE2	2:F:348:HIS:CE1	2.29	0.50
2:F:355:GLY:N	2:F:412:MET:HE3	2.26	0.50
2:B:286:LYS:HG3	2:B:287:ASN:HD22	1.76	0.50
1:C:13:ALA:CB	1:C:16:LYS:HE2	2.40	0.50
1:C:118:GLU:OE1	1:C:118:GLU:HA	2.11	0.50
1:C:154:LEU:O	1:C:156:LEU:N	2.44	0.50
2:D:348:HIS:ND1	2:D:419:LYS:HB2	2.27	0.50
1:E:183:HIS:CD2	1:G:14:ARG:HH21	2.28	0.50
1:E:336:LYS:O	1:E:336:LYS:HG2	2.12	0.50
1:G:316:GLU:O	1:G:319:ASN:ND2	2.44	0.50
1:G:368:LYS:CB	1:G:372:PHE:HD2	2.24	0.50
1:A:17:ALA:O	1:A:19:ASN:N	2.45	0.50
2:B:192:LYS:O	2:B:195:TYR:HB3	2.11	0.50
2:B:369:ILE:HB	2:B:410:VAL:HG13	1.93	0.50
2:F:395:LEU:HD12	2:F:396:ASP:N	2.26	0.50
1:A:150:ARG:O	1:A:152:GLU:N	2.44	0.50
1:A:238:ASP:OD1	1:A:238:ASP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:GLN:HE21	2:B:85:GLU:HG3	1.77	0.50
1:C:366:ALA:C	1:C:368:LYS:N	2.63	0.50
2:D:255:LYS:HG2	2:H:214:TYR:CE2	2.46	0.50
2:F:103:GLN:NE2	2:F:315:SER:N	2.60	0.50
1:G:21:LEU:HD21	1:G:153:MET:HG2	1.94	0.50
2:H:441:LYS:O	2:H:442:ASN:C	2.50	0.50
2:H:492:GLU:O	2:H:493:LEU:C	2.50	0.50
1:G:17:ALA:C	1:G:19:ASN:N	2.65	0.50
1:G:17:ALA:O	1:G:19:ASN:N	2.45	0.50
2:H:467:LYS:O	2:H:469:LEU:N	2.45	0.50
1:C:205:VAL:CG1	1:C:256:VAL:HG22	2.42	0.50
1:E:98:TYR:HB3	1:E:156:LEU:HD21	1.92	0.50
1:G:80:MET:CE	2:H:477:GLU:HB3	2.41	0.50
1:G:80:MET:CE	2:H:477:GLU:CB	2.89	0.50
1:G:163:VAL:HG22	1:G:164:VAL:N	2.26	0.50
2:H:255:LYS:O	2:H:256:GLU:C	2.50	0.50
2:B:402:ILE:HG22	2:B:402:ILE:O	2.10	0.50
2:D:44:LEU:O	2:D:46:ALA:N	2.45	0.50
1:E:160:LYS:CB	1:E:160:LYS:HZ2	2.21	0.50
2:F:508:LEU:C	2:F:510:SER:N	2.65	0.50
1:G:148:LEU:N	1:G:148:LEU:HD12	2.26	0.50
1:G:294:PHE:HB3	1:G:388:ILE:HG13	1.93	0.50
1:C:243:ARG:HH21	1:C:287:LEU:HD22	1.74	0.50
2:D:198:THR:O	2:D:198:THR:CG2	2.48	0.50
1:G:323:LYS:H	1:G:323:LYS:HD3	1.77	0.50
2:H:309:PRO:O	2:H:349:PRO:HB3	2.12	0.50
1:A:200:VAL:HG11	1:A:252:LEU:CD2	2.42	0.49
1:A:222:PHE:CZ	1:A:378:ILE:HG21	2.47	0.49
1:A:261:ASP:OD1	1:A:362:ILE:N	2.44	0.49
2:B:130:GLU:HG2	2:B:141:THR:HG22	1.94	0.49
2:B:215:TYR:CD2	2:B:215:TYR:N	2.79	0.49
1:C:39:VAL:CG1	1:C:40:MET:N	2.75	0.49
1:C:221:GLY:O	1:C:222:PHE:C	2.51	0.49
1:C:272:VAL:HG13	1:C:277:SER:H	1.77	0.49
1:C:307:ARG:C	1:C:308:LYS:CD	2.80	0.49
1:E:82:THR:HA	1:E:138:VAL:CG1	2.41	0.49
1:E:183:HIS:CG	1:G:14:ARG:HH22	2.24	0.49
1:E:237:PRO:HG2	1:E:272:VAL:HG11	1.93	0.49
1:G:148:LEU:N	1:G:148:LEU:CD1	2.74	0.49
2:H:326:LEU:HD12	2:H:357:ALA:HB2	1.93	0.49
2:H:500:GLU:CA	2:H:503:GLU:HB3	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:HIS:CG	1:C:14:ARG:HH22	2.22	0.49
1:C:189:GLU:O	1:C:191:THR:N	2.45	0.49
2:D:285:VAL:HG13	2:D:286:LYS:N	2.27	0.49
1:E:221:GLY:O	1:E:222:PHE:C	2.50	0.49
1:E:238:ASP:OD1	1:E:238:ASP:N	2.44	0.49
1:E:366:ALA:C	1:E:368:LYS:N	2.65	0.49
2:F:44:LEU:O	2:F:46:ALA:N	2.45	0.49
2:F:285:VAL:O	2:F:288:LEU:HG	2.11	0.49
1:G:98:TYR:HB3	1:G:156:LEU:CD2	2.41	0.49
1:G:177:ASP:OD1	1:G:178:LEU:N	2.46	0.49
1:A:175:VAL:O	1:A:175:VAL:CG2	2.59	0.49
1:A:230:LEU:HD23	1:A:231:ILE:N	2.26	0.49
2:B:191:ILE:H	2:B:191:ILE:CD1	2.22	0.49
2:D:414:HIS:CD2	2:D:414:HIS:C	2.85	0.49
1:G:154:LEU:O	1:G:156:LEU:N	2.45	0.49
1:G:246:ARG:HB2	1:G:289:THR:HG22	1.94	0.49
1:A:263:ASP:HB2	1:A:264:PRO:HD2	1.95	0.49
2:B:508:LEU:C	2:B:510:SER:N	2.65	0.49
1:C:271:SER:HB3	1:C:340:TRP:HH2	1.75	0.49
1:C:370:LEU:H	1:C:370:LEU:CD2	2.19	0.49
2:D:58:ILE:O	2:D:205:PHE:HA	2.12	0.49
1:E:14:ARG:HH22	1:G:183:HIS:CG	2.27	0.49
1:E:148:LEU:N	1:E:148:LEU:CD1	2.75	0.49
2:F:240:GLU:O	2:F:243:ILE:N	2.46	0.49
2:F:240:GLU:O	2:F:243:ILE:HG12	2.12	0.49
2:F:253:THR:OG1	2:F:254:ILE:N	2.45	0.49
2:F:372:ARG:HH21	2:F:383:GLU:HB3	1.78	0.49
1:G:238:ASP:O	1:G:242:ARG:NH2	2.45	0.49
1:A:42:ILE:CD1	1:A:68:ARG:HG3	2.43	0.49
1:A:270:PHE:CD1	1:A:270:PHE:C	2.85	0.49
2:B:44:LEU:C	2:B:46:ALA:H	2.15	0.49
2:B:436:ILE:HG22	2:B:437:GLU:N	2.28	0.49
1:C:209:GLU:CB	1:C:260:THR:HG22	2.42	0.49
1:C:242:ARG:O	1:C:243:ARG:C	2.49	0.49
2:F:314:LEU:HD21	2:F:417:SER:HA	1.94	0.49
2:F:382:ASP:C	2:F:384:LYS:H	2.16	0.49
1:G:31:GLN:HG2	1:G:32:LEU:N	2.27	0.49
1:C:323:LYS:H	1:C:323:LYS:HD3	1.77	0.49
2:F:240:GLU:O	2:F:241:ILE:C	2.51	0.49
1:G:295:LEU:HD23	1:G:387:TYR:HB3	1.93	0.49
2:H:47:THR:HG22	2:H:78:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:O	2:B:481:SER:HB3	2.13	0.49
1:A:163:VAL:HG22	1:A:164:VAL:N	2.27	0.49
1:A:272:VAL:HG13	1:A:277:SER:H	1.77	0.49
1:C:86:ALA:O	1:C:89:ILE:HB	2.12	0.49
1:C:108:GLY:O	1:C:109:LYS:HB2	2.13	0.49
2:D:47:THR:HG22	2:D:78:GLY:HA2	1.94	0.49
2:D:103:GLN:NE2	2:D:315:SER:H	2.10	0.49
2:D:127:ILE:HG23	2:D:174:ILE:HG12	1.93	0.49
1:E:32:LEU:O	1:E:33:LYS:C	2.50	0.49
2:H:44:LEU:C	2:H:46:ALA:H	2.16	0.49
2:H:369:ILE:HB	2:H:410:VAL:HG13	1.95	0.49
1:G:325:LYS:O	1:G:328:ASP:HB2	2.12	0.49
1:G:366:ALA:C	1:G:368:LYS:N	2.65	0.49
1:G:371:LYS:H	1:G:371:LYS:CD	2.25	0.49
2:B:165:ARG:HG2	2:B:166:GLY:H	1.76	0.49
1:C:175:VAL:O	1:C:175:VAL:CG2	2.61	0.49
1:C:214:PHE:CE1	1:C:230:LEU:HD22	2.48	0.49
1:E:148:LEU:N	1:E:148:LEU:HD12	2.27	0.49
1:A:154:LEU:O	1:A:156:LEU:N	2.46	0.49
1:A:208:VAL:HG21	1:A:213:VAL:HG11	1.93	0.49
1:A:378:ILE:HD13	1:A:378:ILE:N	2.27	0.49
2:D:44:LEU:C	2:D:46:ALA:H	2.16	0.49
1:E:216:GLN:HG2	1:E:370:LEU:HD11	1.94	0.49
1:G:82:THR:HA	1:G:138:VAL:CG1	2.43	0.49
1:G:85:MET:SD	1:G:104:LEU:HD23	2.53	0.49
1:G:188:ILE:HD12	1:G:188:ILE:O	2.13	0.49
1:G:379:PRO:O	1:G:383:THR:HG22	2.13	0.49
2:H:311:ALA:O	2:H:314:LEU:HB2	2.11	0.49
1:A:291:ASP:OD1	1:A:291:ASP:C	2.52	0.48
2:B:127:ILE:HG23	2:B:174:ILE:HG12	1.95	0.48
1:C:89:ILE:O	1:C:93:LEU:HB2	2.12	0.48
1:E:21:LEU:HD12	1:E:93:LEU:CG	2.42	0.48
1:E:68:ARG:NH1	1:E:78:ARG:O	2.46	0.48
2:F:222:ILE:H	2:F:222:ILE:HG13	1.46	0.48
2:F:487:ALA:HB3	2:F:492:GLU:HB2	1.93	0.48
1:G:380:GLU:O	1:G:384:ASN:HB2	2.13	0.48
2:H:18:ARG:C	2:H:20:PRO:HD3	2.33	0.48
2:H:441:LYS:O	2:H:444:LEU:N	2.45	0.48
2:H:467:LYS:O	2:H:470:ALA:N	2.45	0.48
1:C:243:ARG:HH22	1:C:287:LEU:HD22	1.76	0.48
1:E:295:LEU:HD23	1:E:387:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:492:GLU:O	2:F:493:LEU:C	2.51	0.48
1:A:12:GLU:CG	1:A:13:ALA:N	2.76	0.48
1:C:285:GLU:HB3	1:C:286:ARG:H	1.47	0.48
1:C:295:LEU:HD23	1:C:387:TYR:HB3	1.96	0.48
2:D:253:THR:OG1	2:D:254:ILE:N	2.46	0.48
2:D:474:TYR:N	2:D:474:TYR:HD1	2.12	0.48
1:E:39:VAL:CG1	1:E:40:MET:N	2.76	0.48
1:E:262:ALA:CB	1:E:360:LEU:H	2.26	0.48
1:E:268:TYR:O	1:E:271:SER:N	2.47	0.48
2:F:302:LYS:O	2:F:303:ASP:C	2.51	0.48
1:G:89:ILE:O	1:G:93:LEU:HB2	2.14	0.48
2:H:127:ILE:HG23	2:H:174:ILE:HG12	1.95	0.48
2:H:285:VAL:HG13	2:H:286:LYS:N	2.29	0.48
1:A:14:ARG:NH1	1:C:183:HIS:CE1	2.81	0.48
1:E:200:VAL:HG11	1:E:252:LEU:CD2	2.41	0.48
1:E:347:GLN:O	1:E:348:GLU:C	2.52	0.48
2:F:441:LYS:O	2:F:443:ALA:N	2.45	0.48
1:G:274:ARG:O	1:G:275:ILE:HG23	2.14	0.48
2:H:237:ASP:HA	2:H:297:VAL:HG21	1.95	0.48
2:H:253:THR:OG1	2:H:254:ILE:N	2.47	0.48
2:H:348:HIS:ND1	2:H:419:LYS:HB2	2.29	0.48
1:A:98:TYR:HB3	1:A:156:LEU:HD21	1.96	0.48
1:A:294:PHE:HB3	1:A:388:ILE:HG13	1.95	0.48
1:C:21:LEU:HD12	1:C:93:LEU:CD1	2.42	0.48
1:C:214:PHE:CD1	1:C:230:LEU:HD21	2.48	0.48
1:C:336:LYS:HG2	1:C:336:LYS:O	2.14	0.48
2:D:240:GLU:O	2:D:243:ILE:HG12	2.14	0.48
2:F:237:ASP:HA	2:F:297:VAL:HG21	1.95	0.48
2:F:505:LEU:O	2:F:508:LEU:HB2	2.14	0.48
2:H:455:LEU:HD13	2:H:459:ARG:NH2	2.27	0.48
1:C:302:ILE:HA	1:C:312:LEU:CD1	2.31	0.48
1:C:307:ARG:O	1:C:308:LYS:CD	2.61	0.48
1:E:242:ARG:O	1:E:243:ARG:C	2.50	0.48
1:E:307:ARG:HG3	1:E:308:LYS:N	2.27	0.48
2:F:276:LEU:HB3	2:F:299:THR:HG21	1.96	0.48
2:F:402:ILE:O	2:F:402:ILE:HG22	2.12	0.48
1:G:21:LEU:HB3	1:G:93:LEU:HD11	1.95	0.48
1:G:68:ARG:NH1	1:G:78:ARG:O	2.46	0.48
2:H:240:GLU:O	2:H:243:ILE:HG12	2.13	0.48
2:H:496:LYS:O	2:H:500:GLU:HG3	2.14	0.48
2:B:237:ASP:HA	2:B:297:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:VAL:HG13	2:B:286:LYS:N	2.29	0.48
2:D:474:TYR:N	2:D:474:TYR:CD1	2.81	0.48
2:D:492:GLU:O	2:D:493:LEU:C	2.50	0.48
1:E:108:GLY:O	1:E:109:LYS:HB2	2.13	0.48
1:E:163:VAL:HG22	1:E:164:VAL:N	2.29	0.48
1:E:271:SER:HB3	1:E:340:TRP:HH2	1.78	0.48
1:E:291:ASP:OD1	1:E:291:ASP:C	2.51	0.48
2:F:414:HIS:CD2	2:F:414:HIS:C	2.87	0.48
2:H:322:ILE:CG2	2:H:412:MET:HE2	2.44	0.48
2:H:474:TYR:N	2:H:474:TYR:CD1	2.80	0.48
1:E:103:ASP:O	1:G:367:SER:HB2	2.13	0.48
1:E:366:ALA:C	1:E:368:LYS:H	2.17	0.48
2:F:146:ILE:HG12	2:F:147:ASP:N	2.29	0.48
2:F:241:ILE:O	2:F:245:ILE:HG13	2.13	0.48
1:A:378:ILE:N	1:A:379:PRO:HD2	2.29	0.48
2:D:130:GLU:HG2	2:D:141:THR:HG22	1.96	0.48
1:E:214:PHE:CE1	1:E:230:LEU:HD22	2.49	0.48
2:F:127:ILE:HG23	2:F:174:ILE:HG12	1.95	0.48
1:G:191:THR:OG1	1:G:194:LEU:HD21	2.14	0.48
2:H:374:ALA:O	2:H:377:ILE:HG13	2.14	0.48
1:A:177:ASP:C	1:A:177:ASP:OD1	2.52	0.48
2:B:496:LYS:O	2:B:500:GLU:HG3	2.13	0.48
1:E:43:PRO:O	1:E:144:VAL:HG11	2.14	0.48
2:F:396:ASP:HB3	2:F:399:ARG:HH11	1.78	0.48
1:G:221:GLY:O	1:G:222:PHE:C	2.51	0.48
2:H:77:ASN:OD1	2:H:77:ASN:N	2.46	0.48
1:C:200:VAL:HG11	1:C:252:LEU:CD2	2.43	0.47
1:C:372:PHE:CD1	1:C:372:PHE:O	2.67	0.47
2:D:77:ASN:OD1	2:D:77:ASN:N	2.47	0.47
2:F:16:PHE:CE1	2:F:23:ALA:HB3	2.49	0.47
1:G:39:VAL:HG22	1:G:69:ASN:HA	1.97	0.47
2:H:58:ILE:O	2:H:205:PHE:HA	2.13	0.47
2:H:82:PRO:HA	2:H:83:PRO:HD2	1.73	0.47
1:A:98:TYR:HB3	1:A:156:LEU:CD2	2.43	0.47
2:B:40:ILE:O	2:B:41:GLU:C	2.52	0.47
2:B:322:ILE:CG2	2:B:412:MET:HE2	2.44	0.47
1:E:153:MET:HB2	1:E:155:ILE:HD13	1.96	0.47
1:E:323:LYS:HD3	1:E:323:LYS:H	1.78	0.47
2:F:474:TYR:N	2:F:474:TYR:HD1	2.13	0.47
1:G:89:ILE:HD13	1:G:104:LEU:HD21	1.96	0.47
1:A:261:ASP:OD1	1:A:361:GLU:CA	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:VAL:HB	1:C:258:ILE:HB	1.97	0.47
1:C:302:ILE:O	1:C:317:ARG:NE	2.47	0.47
1:C:339:GLU:HG3	1:C:339:GLU:O	2.14	0.47
1:G:170:ARG:CG	1:G:196:ASP:HB2	2.44	0.47
2:H:474:TYR:N	2:H:474:TYR:HD1	2.11	0.47
1:A:179:SER:OG	1:A:180:LYS:N	2.46	0.47
2:B:302:LYS:O	2:B:303:ASP:C	2.52	0.47
2:B:414:HIS:NE2	2:B:416:CYS:HB3	2.29	0.47
1:C:331:ARG:O	1:C:335:ILE:HG12	2.15	0.47
1:C:370:LEU:N	1:C:370:LEU:CD2	2.77	0.47
2:D:436:ILE:HG22	2:D:437:GLU:N	2.29	0.47
2:D:508:LEU:C	2:D:510:SER:N	2.67	0.47
1:E:350:ILE:O	1:E:353:PHE:HB3	2.15	0.47
1:G:263:ASP:HB2	1:G:264:PRO:CD	2.45	0.47
1:A:37:PRO:HD3	2:B:507:LYS:NZ	2.30	0.47
1:A:85:MET:SD	1:A:104:LEU:HD23	2.55	0.47
1:A:148:LEU:CD1	1:A:148:LEU:N	2.78	0.47
1:A:177:ASP:OD1	1:A:178:LEU:N	2.48	0.47
2:B:397:TRP:O	2:B:402:ILE:HB	2.14	0.47
2:D:302:LYS:O	2:D:303:ASP:C	2.53	0.47
1:G:268:TYR:O	1:G:271:SER:N	2.48	0.47
1:A:148:LEU:N	1:A:148:LEU:HD12	2.29	0.47
1:A:176:ILE:HG21	1:A:186:TYR:CE1	2.50	0.47
1:A:336:LYS:HG2	1:A:336:LYS:O	2.14	0.47
2:B:372:ARG:HH21	2:B:383:GLU:HB3	1.78	0.47
1:C:263:ASP:HB2	1:C:264:PRO:HD2	1.96	0.47
1:C:294:PHE:O	1:C:387:TYR:HB2	2.14	0.47
1:E:14:ARG:NH2	1:G:219:ARG:CZ	2.77	0.47
1:E:183:HIS:CD2	1:G:189:GLU:OE2	2.67	0.47
1:E:370:LEU:N	1:E:370:LEU:CD2	2.70	0.47
1:E:378:ILE:HB	1:E:379:PRO:HD3	1.96	0.47
1:G:387:TYR:N	1:G:387:TYR:CD2	2.82	0.47
1:A:319:ASN:ND2	1:A:319:ASN:N	2.48	0.47
1:A:340:TRP:HZ3	1:A:341:PHE:CE1	2.33	0.47
2:B:383:GLU:CG	2:B:384:LYS:HD3	2.32	0.47
2:B:492:GLU:O	2:B:493:LEU:C	2.52	0.47
2:B:505:LEU:O	2:B:508:LEU:HB2	2.14	0.47
2:D:237:ASP:HA	2:D:297:VAL:HG21	1.97	0.47
1:E:175:VAL:O	1:E:175:VAL:CG2	2.63	0.47
1:E:261:ASP:OD1	1:E:362:ILE:N	2.47	0.47
1:E:272:VAL:HG13	1:E:277:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:ILE:HB	1:E:303:PHE:HD2	1.77	0.47
2:F:112:VAL:HG11	3:F:531:RDC:O5	2.13	0.47
2:F:348:HIS:ND1	2:F:419:LYS:HB2	2.30	0.47
2:F:441:LYS:O	2:F:444:LEU:N	2.45	0.47
1:G:160:LYS:HZ3	1:G:160:LYS:HB2	1.67	0.47
1:A:166:ASN:HB3	1:A:201:ASP:HB3	1.96	0.47
1:A:323:LYS:H	1:A:323:LYS:HD3	1.80	0.47
2:B:362:ILE:O	2:B:408:GLN:HG2	2.15	0.47
1:C:73:LEU:CD2	2:D:467:LYS:HG2	2.44	0.47
1:G:274:ARG:HE	1:G:274:ARG:HB2	1.55	0.47
1:G:378:ILE:O	1:G:379:PRO:C	2.52	0.47
2:H:207:ASP:HB2	2:H:208:PRO:CD	2.44	0.47
2:B:33:TYR:CZ	2:B:37:ARG:HD3	2.49	0.47
2:B:387:VAL:HG12	2:B:430:ILE:HB	1.97	0.47
2:D:441:LYS:O	2:D:444:LEU:N	2.45	0.47
1:E:100:THR:O	1:E:103:ASP:HB2	2.15	0.47
1:E:230:LEU:HD23	1:E:231:ILE:N	2.29	0.47
1:G:42:ILE:CD1	1:G:68:ARG:HG3	2.45	0.47
1:G:209:GLU:CB	1:G:260:THR:HG22	2.44	0.47
1:G:237:PRO:HG2	1:G:272:VAL:HG11	1.95	0.47
1:G:372:PHE:HD1	1:G:376:GLN:HB2	1.80	0.47
1:A:242:ARG:O	1:A:243:ARG:C	2.53	0.47
1:C:173:ASN:HD22	1:C:173:ASN:HA	1.57	0.47
1:E:160:LYS:NZ	1:E:160:LYS:HB3	2.14	0.47
1:G:12:GLU:C	1:G:12:GLU:CD	2.74	0.47
2:B:16:PHE:HZ	2:B:25:PHE:CD2	2.33	0.46
2:B:103:GLN:NE2	2:B:315:SER:N	2.63	0.46
1:C:204:PHE:HA	1:C:255:PRO:HD2	1.97	0.46
1:C:262:ALA:HB3	1:C:360:LEU:H	1.79	0.46
1:C:305:ASN:ND2	1:C:307:ARG:HE	2.13	0.46
1:E:270:PHE:HE2	1:E:294:PHE:HB2	1.75	0.46
1:E:366:ALA:O	1:E:368:LYS:N	2.48	0.46
1:G:243:ARG:HH21	1:G:287:LEU:HD22	1.76	0.46
1:G:387:TYR:N	1:G:387:TYR:HD2	2.13	0.46
2:H:240:GLU:O	2:H:241:ILE:C	2.54	0.46
2:H:506:PHE:CD2	2:H:507:LYS:N	2.83	0.46
2:B:146:ILE:HG12	2:B:147:ASP:N	2.29	0.46
1:C:192:PRO:HG3	1:C:240:ALA:HB1	1.97	0.46
1:C:291:ASP:OD1	1:C:291:ASP:C	2.53	0.46
2:D:500:GLU:CA	2:D:503:GLU:HB3	2.36	0.46
1:E:209:GLU:CB	1:E:260:THR:HG22	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:ASP:HB2	1:E:264:PRO:HD2	1.96	0.46
2:F:127:ILE:HD12	2:F:174:ILE:HG23	1.97	0.46
2:F:474:TYR:N	2:F:474:TYR:CD1	2.82	0.46
1:A:245:VAL:HG12	1:A:246:ARG:N	2.30	0.46
1:A:371:LYS:CD	1:A:371:LYS:H	2.27	0.46
1:C:85:MET:SD	1:C:104:LEU:HD23	2.55	0.46
1:E:245:VAL:HG12	1:E:289:THR:HG21	1.96	0.46
2:F:219:THR:HG23	2:F:220:ASN:H	1.78	0.46
2:F:397:TRP:O	2:F:402:ILE:HB	2.16	0.46
1:G:138:VAL:O	1:G:142:ILE:HG13	2.15	0.46
1:G:379:PRO:O	1:G:383:THR:CG2	2.63	0.46
2:H:16:PHE:CE1	2:H:23:ALA:HB3	2.51	0.46
1:A:150:ARG:NH2	1:A:150:ARG:HB3	2.29	0.46
2:B:276:LEU:HB3	2:B:299:THR:HG21	1.97	0.46
1:C:309:LYS:HB2	1:C:309:LYS:NZ	2.30	0.46
2:D:45:ASP:OD1	2:D:105:ARG:HD2	2.15	0.46
1:E:150:ARG:NH2	1:E:150:ARG:HB3	2.30	0.46
1:E:368:LYS:CB	1:E:372:PHE:HD2	2.28	0.46
2:F:130:GLU:HG2	2:F:141:THR:HG22	1.97	0.46
1:A:21:LEU:HD12	1:A:93:LEU:CG	2.45	0.46
1:A:100:THR:O	1:A:103:ASP:HB2	2.16	0.46
1:A:170:ARG:HG3	1:A:196:ASP:HB2	1.97	0.46
2:B:314:LEU:HD21	2:B:417:SER:HA	1.98	0.46
2:B:384:LYS:HD3	2:B:384:LYS:N	2.31	0.46
1:C:73:LEU:HD21	2:D:467:LYS:HE3	1.97	0.46
2:D:314:LEU:HD21	2:D:417:SER:HA	1.97	0.46
1:E:371:LYS:H	1:E:371:LYS:CD	2.28	0.46
1:G:200:VAL:HG11	1:G:252:LEU:CD2	2.43	0.46
1:G:208:VAL:HG22	1:G:209:GLU:N	2.29	0.46
1:G:350:ILE:O	1:G:353:PHE:HB3	2.16	0.46
1:G:368:LYS:HB3	1:G:372:PHE:HD2	1.81	0.46
1:A:153:MET:HB2	1:A:155:ILE:HD13	1.97	0.46
1:A:183:HIS:CD2	1:C:189:GLU:OE2	2.69	0.46
1:A:347:GLN:O	1:A:348:GLU:C	2.52	0.46
1:A:350:ILE:O	1:A:353:PHE:HB3	2.15	0.46
2:B:103:GLN:NE2	2:B:315:SER:H	2.13	0.46
1:C:12:GLU:HG3	1:C:13:ALA:H	1.80	0.46
2:F:285:VAL:CG1	2:F:286:LYS:N	2.78	0.46
1:G:12:GLU:CG	1:G:13:ALA:N	2.79	0.46
2:H:414:HIS:CD2	2:H:414:HIS:C	2.88	0.46
2:H:455:LEU:HD13	2:H:459:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:GLN:O	2:B:264:SER:HB2	2.15	0.46
2:B:400:TYR:O	2:B:402:ILE:N	2.48	0.46
2:B:506:PHE:CD2	2:B:507:LYS:N	2.83	0.46
1:C:238:ASP:O	1:C:242:ARG:NH2	2.49	0.46
2:D:330:PHE:O	2:D:361:SER:HB2	2.15	0.46
2:D:382:ASP:C	2:D:384:LYS:H	2.19	0.46
2:D:496:LYS:O	2:D:500:GLU:HG3	2.15	0.46
1:E:378:ILE:O	1:E:379:PRO:C	2.49	0.46
1:G:41:GLU:O	1:G:43:PRO:HD3	2.16	0.46
1:A:216:GLN:HG2	1:A:370:LEU:HD11	1.97	0.46
2:B:240:GLU:O	2:B:243:ILE:N	2.49	0.46
1:C:335:ILE:O	1:C:338:TYR:N	2.41	0.46
1:E:317:ARG:O	1:E:321:ILE:HG13	2.16	0.46
2:F:401:GLY:O	2:F:402:ILE:C	2.54	0.46
1:G:115:LYS:HB3	1:G:115:LYS:HZ3	1.79	0.46
2:H:44:LEU:O	2:H:46:ALA:N	2.49	0.46
2:H:276:LEU:HB3	2:H:299:THR:HG21	1.98	0.46
2:H:508:LEU:C	2:H:510:SER:N	2.68	0.46
1:A:14:ARG:CZ	1:C:183:HIS:CG	2.96	0.46
2:B:500:GLU:CA	2:B:503:GLU:HB3	2.37	0.46
1:E:274:ARG:O	1:E:275:ILE:HG23	2.15	0.46
2:F:86:VAL:CB	2:F:87:PRO:HD3	2.45	0.46
2:F:197:ILE:HG12	2:F:373:TYR:CE1	2.51	0.46
2:F:207:ASP:HB2	2:F:208:PRO:CD	2.45	0.46
1:G:79:PHE:O	1:G:82:THR:N	2.49	0.46
1:G:363:GLU:O	1:G:364:ALA:C	2.52	0.46
2:H:198:THR:O	2:H:198:THR:CG2	2.44	0.46
1:A:68:ARG:NH1	1:A:78:ARG:O	2.49	0.46
1:C:374:ALA:HB3	1:C:375:PHE:CD1	2.50	0.46
2:F:420:ILE:HB	2:F:422:TYR:HE2	1.80	0.46
1:G:21:LEU:HD12	1:G:93:LEU:CG	2.45	0.46
1:G:73:LEU:HD21	2:H:467:LYS:CG	2.45	0.46
2:H:302:LYS:O	2:H:303:ASP:C	2.54	0.46
1:A:108:GLY:O	1:A:109:LYS:HB2	2.16	0.45
1:A:370:LEU:N	1:A:370:LEU:CD2	2.76	0.45
2:B:77:ASN:N	2:B:77:ASN:OD1	2.49	0.45
1:C:153:MET:HB2	1:C:155:ILE:HD13	1.98	0.45
1:C:188:ILE:O	1:C:188:ILE:HD12	2.16	0.45
2:D:240:GLU:O	2:D:241:ILE:C	2.53	0.45
1:E:83:VAL:O	2:F:481:SER:HB3	2.15	0.45
2:F:77:ASN:OD1	2:F:77:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:195:TYR:CE2	2:F:215:TYR:HB3	2.51	0.45
1:G:348:GLU:O	1:G:352:THR:HG23	2.16	0.45
1:G:366:ALA:C	1:G:368:LYS:H	2.19	0.45
2:H:395:LEU:HD12	2:H:396:ASP:N	2.30	0.45
1:A:259:LEU:O	1:A:259:LEU:HD13	2.15	0.45
1:C:317:ARG:O	1:C:321:ILE:HG13	2.17	0.45
1:E:74:ASN:OD1	1:E:74:ASN:N	2.49	0.45
1:E:207:VAL:HB	1:E:258:ILE:HB	1.98	0.45
1:E:262:ALA:HB3	1:E:360:LEU:H	1.81	0.45
1:E:363:GLU:O	1:E:364:ALA:C	2.53	0.45
1:A:309:LYS:HB2	1:A:309:LYS:HZ2	1.80	0.45
1:A:368:LYS:CB	1:A:372:PHE:HD2	2.29	0.45
1:C:74:ASN:OD1	1:C:74:ASN:N	2.49	0.45
1:C:347:GLN:O	1:C:348:GLU:C	2.53	0.45
2:D:276:LEU:HB3	2:D:299:THR:HG21	1.99	0.45
2:D:369:ILE:HB	2:D:410:VAL:HG13	1.99	0.45
1:E:189:GLU:OE2	1:G:183:HIS:CD2	2.69	0.45
1:E:259:LEU:HD12	1:E:259:LEU:O	2.16	0.45
1:G:285:GLU:HB3	1:G:286:ARG:H	1.56	0.45
1:G:309:LYS:HB2	1:G:309:LYS:NZ	2.31	0.45
1:A:192:PRO:HG3	1:A:240:ALA:HB1	1.99	0.45
2:B:29:ALA:HB2	2:B:179:ASP:HB3	1.97	0.45
2:B:355:GLY:N	2:B:412:MET:HE3	2.31	0.45
1:C:159:GLU:HG2	1:C:240:ALA:HB3	1.98	0.45
1:C:366:ALA:C	1:C:368:LYS:H	2.20	0.45
1:E:381:LYS:HE2	1:E:386:ASP:CG	2.37	0.45
2:F:506:PHE:CD2	2:F:507:LYS:N	2.84	0.45
1:G:305:ASN:ND2	1:G:307:ARG:HE	2.15	0.45
1:A:115:LYS:HB3	1:A:115:LYS:HZ3	1.80	0.45
1:C:177:ASP:C	1:C:177:ASP:OD1	2.54	0.45
2:D:506:PHE:CD2	2:D:507:LYS:N	2.85	0.45
2:F:496:LYS:O	2:F:500:GLU:HG3	2.16	0.45
1:G:222:PHE:CZ	1:G:378:ILE:HG21	2.51	0.45
2:H:314:LEU:HD21	2:H:417:SER:HA	1.98	0.45
1:A:245:VAL:HG12	1:A:289:THR:HG21	1.99	0.45
2:B:441:LYS:O	2:B:444:LEU:N	2.45	0.45
1:C:31:GLN:HG2	1:C:32:LEU:N	2.31	0.45
1:C:90:TYR:CD2	1:C:90:TYR:C	2.90	0.45
2:D:40:ILE:O	2:D:41:GLU:C	2.54	0.45
1:E:12:GLU:O	1:E:14:ARG:N	2.50	0.45
1:G:39:VAL:CG1	1:G:40:MET:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:LYS:O	1:G:336:LYS:HG2	2.15	0.45
2:H:84:GLN:HE21	2:H:85:GLU:HG3	1.82	0.45
1:A:67:ARG:H	1:A:67:ARG:HG2	1.59	0.45
1:A:294:PHE:O	1:A:387:TYR:HB2	2.17	0.45
1:A:335:ILE:O	1:A:338:TYR:N	2.43	0.45
1:C:82:THR:HA	1:C:138:VAL:CG1	2.46	0.45
1:C:102:ARG:C	1:C:104:LEU:N	2.68	0.45
1:C:102:ARG:O	1:C:103:ASP:C	2.54	0.45
1:C:270:PHE:HD2	1:C:294:PHE:HD1	1.65	0.45
2:D:214:TYR:CE2	2:D:216:PRO:HB3	2.51	0.45
2:D:345:TYR:O	2:D:346:GLN:C	2.55	0.45
1:E:86:ALA:O	1:E:89:ILE:HB	2.17	0.45
1:E:242:ARG:O	1:E:245:VAL:N	2.49	0.45
2:F:436:ILE:HG22	2:F:437:GLU:N	2.31	0.45
1:G:150:ARG:O	1:G:153:MET:N	2.45	0.45
1:G:153:MET:HB2	1:G:155:ILE:HD13	1.99	0.45
1:G:270:PHE:HD2	1:G:294:PHE:HD1	1.65	0.45
1:A:243:ARG:HD2	1:A:243:ARG:HA	1.65	0.45
2:B:44:LEU:O	2:B:46:ALA:N	2.50	0.45
2:B:398:LYS:C	2:B:400:TYR:N	2.70	0.45
2:B:465:LYS:NZ	2:B:465:LYS:HB3	2.32	0.45
2:B:497:TYR:HB3	2:B:498:GLN:H	1.68	0.45
1:C:26:LEU:HD23	1:C:26:LEU:C	2.38	0.45
1:C:34:LYS:HD2	1:C:34:LYS:HA	1.86	0.45
1:C:85:MET:HG2	1:C:129:TRP:CH2	2.51	0.45
1:C:208:VAL:HG22	1:C:209:GLU:N	2.32	0.45
1:C:260:THR:HB	1:C:261:ASP:H	1.53	0.45
1:G:108:GLY:O	1:G:109:LYS:HB2	2.17	0.45
1:G:184:GLY:O	1:G:185:ALA:HB2	2.17	0.45
1:G:347:GLN:O	1:G:348:GLU:C	2.54	0.45
2:H:355:GLY:N	2:H:412:MET:HE3	2.32	0.45
1:A:219:ARG:NE	1:C:14:ARG:NH2	2.64	0.45
1:A:379:PRO:O	1:A:383:THR:CG2	2.63	0.45
2:B:240:GLU:O	2:B:241:ILE:C	2.54	0.45
2:B:362:ILE:HA	2:B:363:PRO:HD3	1.79	0.45
2:B:401:GLY:O	2:B:402:ILE:C	2.55	0.45
1:C:21:LEU:HD22	1:C:21:LEU:HA	1.67	0.45
1:C:176:ILE:HG21	1:C:186:TYR:CE1	2.52	0.45
2:D:374:ALA:O	2:D:377:ILE:HG13	2.17	0.45
2:D:444:LEU:O	2:D:447:VAL:CG2	2.65	0.45
1:E:263:ASP:HB2	1:E:264:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:ASP:O	1:E:387:TYR:HB3	2.17	0.45
2:F:362:ILE:O	2:F:408:GLN:HG2	2.17	0.45
1:G:159:GLU:HG2	1:G:238:ASP:HB2	1.98	0.45
2:H:240:GLU:O	2:H:243:ILE:N	2.50	0.45
1:A:232:THR:OG1	1:A:233:SER:O	2.21	0.45
2:B:45:ASP:OD1	2:B:105:ARG:HD2	2.17	0.45
2:B:474:TYR:N	2:B:474:TYR:CD1	2.84	0.45
1:C:12:GLU:O	1:C:14:ARG:N	2.50	0.45
1:C:302:ILE:HG22	1:C:317:ARG:CD	2.38	0.45
2:D:401:GLY:O	2:D:402:ILE:C	2.55	0.45
1:E:214:PHE:CD1	1:E:230:LEU:HD21	2.52	0.45
2:F:382:ASP:O	2:F:384:LYS:N	2.50	0.45
1:A:154:LEU:HD13	1:A:154:LEU:HA	1.76	0.44
1:C:33:LYS:HA	1:C:33:LYS:HD2	1.80	0.44
1:C:214:PHE:CE1	1:C:230:LEU:CD2	3.00	0.44
1:C:387:TYR:CD2	1:C:387:TYR:N	2.85	0.44
1:E:19:ASN:C	1:E:21:LEU:N	2.71	0.44
1:E:252:LEU:HD12	1:E:252:LEU:N	2.31	0.44
1:E:285:GLU:HB3	1:E:286:ARG:H	1.51	0.44
2:F:312:ASP:OD2	2:F:312:ASP:N	2.50	0.44
1:G:170:ARG:HG3	1:G:196:ASP:HB2	1.99	0.44
2:H:103:GLN:HE21	2:H:315:SER:N	2.15	0.44
1:A:14:ARG:CZ	1:C:183:HIS:ND1	2.81	0.44
1:C:191:THR:OG1	1:C:191:THR:O	2.27	0.44
1:C:372:PHE:O	1:C:372:PHE:HD1	2.00	0.44
2:D:16:PHE:HZ	2:D:25:PHE:CD2	2.35	0.44
2:D:219:THR:CG2	2:D:220:ASN:N	2.60	0.44
2:D:240:GLU:O	2:D:243:ILE:N	2.50	0.44
2:D:506:PHE:C	2:D:508:LEU:H	2.21	0.44
1:E:259:LEU:O	1:E:259:LEU:CD1	2.65	0.44
1:E:307:ARG:HH11	1:E:308:LYS:NZ	2.15	0.44
1:G:261:ASP:OD1	1:G:361:GLU:CA	2.57	0.44
2:H:382:ASP:C	2:H:384:LYS:H	2.21	0.44
1:A:39:VAL:CG1	1:A:40:MET:N	2.80	0.44
2:B:382:ASP:C	2:B:384:LYS:H	2.21	0.44
2:B:474:TYR:N	2:B:474:TYR:HD1	2.15	0.44
1:E:106:TYR:C	1:E:107:ARG:HD3	2.31	0.44
1:E:160:LYS:H	1:E:160:LYS:HG2	1.59	0.44
1:E:176:ILE:HG21	1:E:186:TYR:CE1	2.52	0.44
1:E:208:VAL:HG22	1:E:209:GLU:N	2.32	0.44
1:E:261:ASP:OD1	1:E:361:GLU:CA	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:44:LEU:C	2:F:46:ALA:N	2.71	0.44
2:H:219:THR:HG23	2:H:220:ASN:H	1.77	0.44
1:A:14:ARG:HH22	1:C:183:HIS:CB	2.30	0.44
1:A:84:LEU:O	1:A:85:MET:C	2.56	0.44
2:B:472:LEU:HD23	2:B:472:LEU:HA	1.64	0.44
1:C:111:SER:HB2	2:D:480:ARG:HH22	1.83	0.44
1:C:335:ILE:HG12	1:C:335:ILE:H	1.61	0.44
1:E:251:GLU:C	1:E:252:LEU:HD12	2.36	0.44
1:E:372:PHE:HD1	1:E:376:GLN:HB2	1.82	0.44
2:F:190:TYR:O	2:F:191:ILE:C	2.56	0.44
2:F:229:VAL:HG12	2:F:313:SER:HB3	2.00	0.44
1:G:189:GLU:C	1:G:191:THR:N	2.71	0.44
1:A:14:ARG:HH22	1:C:183:HIS:HB3	1.83	0.44
1:A:372:PHE:CD1	1:A:372:PHE:O	2.70	0.44
1:C:150:ARG:O	1:C:153:MET:N	2.47	0.44
1:C:226:TYR:O	1:C:227:LYS:C	2.55	0.44
1:C:336:LYS:HB2	1:C:350:ILE:HG21	2.00	0.44
1:C:379:PRO:O	1:C:383:THR:HG22	2.18	0.44
2:D:127:ILE:HD12	2:D:174:ILE:HG23	1.97	0.44
2:D:142:PHE:HB3	2:D:144:LEU:HD13	1.99	0.44
2:D:146:ILE:HG12	2:D:147:ASP:N	2.33	0.44
2:D:395:LEU:HD12	2:D:396:ASP:H	1.81	0.44
1:E:91:ASP:C	1:E:93:LEU:N	2.71	0.44
2:F:83:PRO:O	2:F:86:VAL:HG23	2.18	0.44
2:F:465:LYS:NZ	2:F:465:LYS:HB3	2.33	0.44
2:F:508:LEU:HD13	2:F:508:LEU:HA	1.71	0.44
1:G:67:ARG:H	1:G:67:ARG:HG2	1.56	0.44
1:G:336:LYS:HB2	1:G:350:ILE:HG21	1.99	0.44
2:B:97:SER:OG	2:B:109:GLY:HA3	2.18	0.44
2:D:16:PHE:CE1	2:D:23:ALA:HB3	2.53	0.44
1:E:362:ILE:H	1:E:362:ILE:HG13	1.64	0.44
2:F:191:ILE:H	2:F:191:ILE:CD1	2.24	0.44
1:G:12:GLU:O	1:G:14:ARG:N	2.50	0.44
1:A:363:GLU:O	1:A:364:ALA:C	2.54	0.44
1:A:372:PHE:O	1:A:376:GLN:HB2	2.18	0.44
1:C:262:ALA:CB	1:C:360:LEU:H	2.30	0.44
2:D:276:LEU:HD23	2:D:276:LEU:HA	1.84	0.44
1:E:173:ASN:HD22	1:E:173:ASN:HA	1.54	0.44
2:F:40:ILE:O	2:F:41:GLU:C	2.56	0.44
2:F:499:ASN:C	2:F:499:ASN:ND2	2.69	0.44
1:G:21:LEU:HD22	1:G:21:LEU:HA	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ILE:HD11	1:G:68:ARG:HG3	2.00	0.44
1:G:167:LEU:HG	1:G:168:ARG:N	2.32	0.44
1:G:340:TRP:HZ3	1:G:341:PHE:CE1	2.35	0.44
2:H:130:GLU:HG2	2:H:141:THR:HG22	2.00	0.44
1:A:97:GLU:O	1:A:98:TYR:CD1	2.71	0.44
2:B:338:ILE:HG23	2:B:338:ILE:O	2.18	0.44
1:C:91:ASP:C	1:C:93:LEU:N	2.70	0.44
1:C:270:PHE:CD1	1:C:270:PHE:C	2.90	0.44
2:D:97:SER:O	2:D:98:LYS:C	2.56	0.44
2:D:103:GLN:HE22	2:D:315:SER:H	1.66	0.44
2:F:58:ILE:O	2:F:205:PHE:HA	2.17	0.44
2:F:221:LYS:O	2:F:221:LYS:HD3	2.17	0.44
2:F:506:PHE:C	2:F:508:LEU:H	2.21	0.44
1:G:100:THR:O	1:G:103:ASP:HB2	2.18	0.44
2:H:330:PHE:O	2:H:361:SER:HB2	2.18	0.44
2:H:441:LYS:O	2:H:443:ALA:N	2.50	0.44
1:A:21:LEU:HD22	1:A:21:LEU:HA	1.70	0.44
1:C:263:ASP:HB2	1:C:264:PRO:CD	2.47	0.44
2:D:30:ARG:HE	2:D:30:ARG:HB3	1.42	0.44
1:G:216:GLN:HG2	1:G:370:LEU:HD11	2.00	0.44
1:G:230:LEU:HD23	1:G:231:ILE:N	2.32	0.44
1:G:291:ASP:OD1	1:G:291:ASP:C	2.56	0.44
2:H:127:ILE:HD12	2:H:174:ILE:HG23	1.99	0.44
2:H:195:TYR:CE2	2:H:215:TYR:HB3	2.53	0.44
2:H:506:PHE:C	2:H:508:LEU:H	2.20	0.44
1:A:262:ALA:HB3	1:A:360:LEU:H	1.83	0.43
1:A:340:TRP:CZ3	1:A:341:PHE:CZ	2.99	0.43
2:B:127:ILE:HD12	2:B:174:ILE:HG23	1.99	0.43
2:D:103:GLN:NE2	2:D:315:SER:N	2.66	0.43
1:E:286:ARG:C	1:E:287:LEU:HG	2.39	0.43
1:G:39:VAL:HG12	1:G:40:MET:O	2.18	0.43
1:A:31:GLN:HG2	1:A:32:LEU:N	2.33	0.43
1:A:368:LYS:HB3	1:A:372:PHE:HD2	1.83	0.43
2:B:358:PHE:HD1	2:B:408:GLN:O	2.01	0.43
1:C:79:PHE:O	1:C:82:THR:N	2.51	0.43
1:C:254:LEU:HA	1:C:255:PRO:HD3	1.78	0.43
2:D:322:ILE:CG2	2:D:412:MET:HE2	2.49	0.43
2:D:396:ASP:HB3	2:D:399:ARG:HH11	1.82	0.43
1:E:25:PHE:O	1:E:26:LEU:C	2.55	0.43
1:E:31:GLN:HG2	1:E:32:LEU:N	2.32	0.43
1:E:154:LEU:HA	1:E:154:LEU:HD13	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:ARG:HH22	1:E:287:LEU:HD22	1.81	0.43
1:G:74:ASN:N	1:G:74:ASN:OD1	2.50	0.43
1:G:88:ILE:H	1:G:88:ILE:HG12	1.69	0.43
1:G:378:ILE:HB	1:G:379:PRO:CD	2.48	0.43
2:H:401:GLY:O	2:H:402:ILE:C	2.56	0.43
1:A:160:LYS:CB	1:A:160:LYS:HZ2	2.29	0.43
1:A:263:ASP:HB2	1:A:264:PRO:CD	2.48	0.43
1:A:302:ILE:H	1:A:302:ILE:HG13	1.69	0.43
2:B:374:ALA:O	2:B:377:ILE:HG13	2.18	0.43
2:B:467:LYS:C	2:B:469:LEU:N	2.72	0.43
2:D:309:PRO:O	2:D:349:PRO:HB3	2.18	0.43
1:E:159:GLU:CD	1:E:240:ALA:HB3	2.38	0.43
1:E:189:GLU:O	1:E:191:THR:N	2.52	0.43
1:A:91:ASP:C	1:A:93:LEU:N	2.71	0.43
2:B:44:LEU:C	2:B:46:ALA:N	2.72	0.43
2:B:47:THR:HG22	2:B:78:GLY:CA	2.48	0.43
1:C:100:THR:O	1:C:103:ASP:HB2	2.18	0.43
2:D:362:ILE:O	2:D:408:GLN:HG2	2.18	0.43
2:D:387:VAL:HG12	2:D:430:ILE:HB	1.99	0.43
2:F:324:LEU:O	2:F:325:GLY:C	2.56	0.43
1:A:176:ILE:HG21	1:A:186:TYR:HE1	1.83	0.43
1:A:189:GLU:C	1:A:191:THR:N	2.71	0.43
2:D:508:LEU:HA	2:D:508:LEU:HD13	1.70	0.43
1:E:131:GLU:O	1:E:132:GLN:C	2.55	0.43
1:E:260:THR:HB	1:E:261:ASP:H	1.55	0.43
1:E:335:ILE:HG12	1:E:335:ILE:H	1.62	0.43
1:E:355:GLN:HE21	1:E:355:GLN:HB3	1.63	0.43
2:F:382:ASP:C	2:F:384:LYS:N	2.71	0.43
1:G:154:LEU:HD13	1:G:154:LEU:HA	1.76	0.43
1:G:294:PHE:O	1:G:387:TYR:HB2	2.18	0.43
2:H:97:SER:O	2:H:98:LYS:C	2.57	0.43
1:C:177:ASP:OD1	1:C:178:LEU:N	2.51	0.43
1:C:371:LYS:CD	1:C:371:LYS:H	2.29	0.43
1:E:33:LYS:HA	1:E:33:LYS:HD2	1.78	0.43
1:E:39:VAL:HG12	1:E:40:MET:O	2.18	0.43
1:E:98:TYR:HB3	1:E:156:LEU:HD23	2.01	0.43
2:F:467:LYS:C	2:F:469:LEU:N	2.71	0.43
2:F:504:GLY:O	2:F:505:LEU:C	2.57	0.43
1:G:79:PHE:O	1:G:81:GLN:N	2.51	0.43
2:H:465:LYS:HB3	2:H:465:LYS:NZ	2.34	0.43
1:A:80:MET:HE3	2:B:477:GLU:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HG	1:A:168:ARG:N	2.33	0.43
1:A:188:ILE:CD1	1:A:188:ILE:C	2.87	0.43
1:A:252:LEU:O	1:A:254:LEU:HD12	2.18	0.43
1:A:387:TYR:N	1:A:387:TYR:HD2	2.17	0.43
1:C:28:LEU:HD23	1:C:28:LEU:HA	1.90	0.43
1:C:372:PHE:HD1	1:C:376:GLN:HB2	1.83	0.43
2:D:465:LYS:NZ	2:D:465:LYS:HB3	2.34	0.43
1:E:85:MET:SD	1:E:104:LEU:HD23	2.58	0.43
1:E:172:GLY:N	1:G:183:HIS:CE1	2.85	0.43
1:E:188:ILE:CD1	1:E:188:ILE:C	2.87	0.43
2:F:430:ILE:HG22	2:F:431:ALA:N	2.33	0.43
1:G:261:ASP:OD1	1:G:362:ILE:HG13	2.19	0.43
1:A:189:GLU:OE2	1:C:183:HIS:CD2	2.72	0.43
1:A:270:PHE:HD2	1:A:294:PHE:HD1	1.67	0.43
1:A:378:ILE:N	1:A:378:ILE:CD1	2.82	0.43
2:B:207:ASP:HB2	2:B:208:PRO:CD	2.48	0.43
2:B:382:ASP:O	2:B:384:LYS:N	2.52	0.43
2:B:396:ASP:HB3	2:B:399:ARG:NH1	2.34	0.43
1:C:80:MET:HE3	2:D:477:GLU:HB2	2.00	0.43
1:C:159:GLU:CG	1:C:240:ALA:HB3	2.49	0.43
1:C:307:ARG:HG3	1:C:308:LYS:N	2.33	0.43
1:C:350:ILE:O	1:C:353:PHE:HB3	2.19	0.43
1:E:254:LEU:HA	1:E:255:PRO:HD3	1.74	0.43
1:E:270:PHE:O	1:E:271:SER:C	2.56	0.43
2:F:16:PHE:HZ	2:F:25:PHE:CD2	2.37	0.43
2:F:142:PHE:HB3	2:F:144:LEU:HD13	2.01	0.43
2:F:204:ILE:HG12	2:F:214:TYR:HD1	1.83	0.43
1:G:19:ASN:C	1:G:21:LEU:N	2.72	0.43
1:G:80:MET:HE3	2:H:477:GLU:CB	2.48	0.43
1:G:262:ALA:HB3	1:G:360:LEU:H	1.84	0.43
2:H:40:ILE:O	2:H:41:GLU:C	2.57	0.43
2:H:219:THR:CG2	2:H:220:ASN:N	2.60	0.43
2:H:340:ARG:HH22	2:H:442:ASN:HB3	1.82	0.43
1:A:80:MET:CE	2:B:477:GLU:CB	2.97	0.43
2:D:44:LEU:C	2:D:46:ALA:N	2.72	0.43
2:F:506:PHE:C	2:F:508:LEU:N	2.72	0.43
1:G:80:MET:HE3	2:H:477:GLU:HB2	2.01	0.43
1:G:175:VAL:O	1:G:175:VAL:CG2	2.65	0.43
2:H:99:TYR:HE2	2:H:348:HIS:CE1	2.37	0.43
1:A:39:VAL:HG12	1:A:40:MET:O	2.19	0.43
1:A:88:ILE:H	1:A:88:ILE:HG12	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:PHE:CD1	1:A:230:LEU:HD21	2.54	0.43
1:A:219:ARG:NH2	1:C:14:ARG:HH21	2.16	0.43
2:B:62:LEU:HD13	2:B:70:TYR:CE1	2.54	0.43
1:C:79:PHE:O	1:C:81:GLN:N	2.52	0.43
1:C:243:ARG:NH2	1:C:287:LEU:CD2	2.77	0.43
1:C:307:ARG:CB	1:C:308:LYS:HD3	2.49	0.43
2:D:506:PHE:C	2:D:508:LEU:N	2.72	0.43
1:E:21:LEU:HD22	1:E:21:LEU:HA	1.71	0.43
1:G:26:LEU:HD23	1:G:26:LEU:C	2.40	0.43
2:H:190:TYR:O	2:H:191:ILE:C	2.57	0.43
2:H:506:PHE:C	2:H:508:LEU:N	2.71	0.43
1:A:305:ASN:ND2	1:A:307:ARG:HE	2.17	0.42
2:B:197:ILE:HB	2:B:317:ILE:CD1	2.47	0.42
2:B:420:ILE:HB	2:B:422:TYR:CE2	2.51	0.42
1:C:68:ARG:NH1	1:C:78:ARG:O	2.52	0.42
1:C:372:PHE:CE1	1:C:377:TYR:HB2	2.54	0.42
1:E:28:LEU:HD23	1:E:28:LEU:HA	1.92	0.42
2:F:195:TYR:OH	2:F:216:PRO:HD2	2.18	0.42
2:F:263:GLN:O	2:F:264:SER:HB3	2.19	0.42
1:A:335:ILE:HG12	1:A:335:ILE:H	1.54	0.42
1:C:189:GLU:C	1:C:191:THR:N	2.71	0.42
1:C:379:PRO:O	1:C:383:THR:CG2	2.67	0.42
2:D:383:GLU:O	2:D:389:TRP:HB2	2.20	0.42
1:E:102:ARG:C	1:E:104:LEU:N	2.72	0.42
1:G:226:TYR:O	1:G:227:LYS:C	2.58	0.42
2:H:472:LEU:HD23	2:H:472:LEU:HA	1.64	0.42
1:A:21:LEU:O	1:A:22:ARG:O	2.37	0.42
1:A:302:ILE:HB	1:A:303:PHE:HD2	1.77	0.42
1:A:366:ALA:C	1:A:368:LYS:N	2.72	0.42
1:A:387:TYR:N	1:A:387:TYR:CD2	2.87	0.42
2:B:395:LEU:HD12	2:B:396:ASP:N	2.33	0.42
2:D:29:ALA:HB2	2:D:179:ASP:HB3	2.01	0.42
2:D:82:PRO:HA	2:D:83:PRO:HD2	1.72	0.42
2:D:260:ASN:HD21	2:H:214:TYR:H	1.68	0.42
2:D:382:ASP:O	2:D:384:LYS:N	2.52	0.42
1:E:98:TYR:HA	1:E:99:PRO:HD3	1.76	0.42
1:E:381:LYS:HE2	1:E:386:ASP:HB3	2.00	0.42
2:F:187:ILE:O	2:F:190:TYR:N	2.52	0.42
2:F:414:HIS:NE2	2:F:416:CYS:HB3	2.34	0.42
2:H:214:TYR:CE2	2:H:216:PRO:HB3	2.54	0.42
2:H:420:ILE:HB	2:H:422:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:PRO:O	2:B:349:PRO:HB3	2.19	0.42
2:B:318:GLY:C	2:B:320:ASP:N	2.72	0.42
1:C:39:VAL:HG12	1:C:40:MET:O	2.19	0.42
1:C:43:PRO:O	1:C:144:VAL:HG11	2.19	0.42
1:C:270:PHE:HE2	1:C:294:PHE:HB2	1.82	0.42
1:E:41:GLU:O	1:E:43:PRO:HD3	2.20	0.42
1:E:243:ARG:HH21	1:E:287:LEU:HD22	1.81	0.42
2:F:44:LEU:HD23	2:F:44:LEU:HA	1.87	0.42
1:G:77:LYS:HA	2:H:474:TYR:CE2	2.54	0.42
1:G:370:LEU:N	1:G:370:LEU:CD2	2.83	0.42
1:A:90:TYR:CD2	1:A:90:TYR:C	2.93	0.42
1:A:102:ARG:HD2	1:C:363:GLU:CG	2.45	0.42
1:C:187:ALA:O	1:C:188:ILE:O	2.37	0.42
1:C:302:ILE:HB	1:C:303:PHE:CE2	2.55	0.42
1:C:366:ALA:O	1:C:368:LYS:N	2.52	0.42
2:D:450:LYS:O	2:D:453:GLN:HB3	2.19	0.42
2:D:499:ASN:ND2	2:D:499:ASN:C	2.70	0.42
1:E:26:LEU:C	1:E:26:LEU:HD23	2.40	0.42
1:G:324:ALA:HB3	1:G:357:LYS:HB3	2.01	0.42
1:A:251:GLU:C	1:A:252:LEU:HD12	2.40	0.42
2:B:97:SER:O	2:B:98:LYS:C	2.58	0.42
2:B:221:LYS:O	2:B:221:LYS:HD3	2.20	0.42
1:C:363:GLU:O	1:C:364:ALA:C	2.57	0.42
1:E:79:PHE:O	1:E:81:GLN:N	2.53	0.42
2:F:227:GLN:O	2:F:313:SER:HA	2.20	0.42
1:G:208:VAL:CG2	1:G:209:GLU:N	2.82	0.42
1:G:286:ARG:C	1:G:287:LEU:HG	2.39	0.42
2:H:142:PHE:HB3	2:H:144:LEU:HD13	2.01	0.42
2:H:221:LYS:HD2	2:H:321:LEU:HD21	2.01	0.42
2:H:387:VAL:HG12	2:H:430:ILE:HB	2.01	0.42
1:A:25:PHE:O	1:A:26:LEU:C	2.57	0.42
1:A:214:PHE:CE1	1:A:230:LEU:HD22	2.54	0.42
1:A:307:ARG:HG3	1:A:308:LYS:N	2.35	0.42
1:A:372:PHE:O	1:A:372:PHE:HD1	2.02	0.42
1:A:378:ILE:O	1:A:379:PRO:C	2.57	0.42
2:D:467:LYS:C	2:D:469:LEU:N	2.72	0.42
1:E:21:LEU:CD1	1:E:93:LEU:HG	2.50	0.42
2:F:29:ALA:HB2	2:F:179:ASP:HB3	2.02	0.42
2:F:47:THR:HG22	2:F:78:GLY:CA	2.49	0.42
2:H:362:ILE:O	2:H:408:GLN:HG2	2.20	0.42
2:H:414:HIS:NE2	2:H:416:CYS:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HH21	1:C:219:ARG:NH2	2.15	0.42
1:A:271:SER:HB3	1:A:340:TRP:HH2	1.78	0.42
2:B:233:PRO:HD3	2:B:262:PHE:HB3	2.01	0.42
1:C:19:ASN:C	1:C:21:LEU:N	2.73	0.42
1:C:132:GLN:HE21	1:C:132:GLN:HB2	1.62	0.42
1:C:316:GLU:HA	1:C:319:ASN:HD21	1.85	0.42
1:E:67:ARG:H	1:E:67:ARG:HG2	1.56	0.42
2:F:276:LEU:C	2:F:278:GLY:N	2.72	0.42
1:G:91:ASP:C	1:G:93:LEU:N	2.72	0.42
1:G:106:TYR:C	1:G:107:ARG:HD3	2.27	0.42
1:G:159:GLU:HG3	1:G:238:ASP:HB2	2.00	0.42
2:H:233:PRO:HD3	2:H:262:PHE:HB3	2.01	0.42
2:H:397:TRP:O	2:H:402:ILE:HB	2.18	0.42
2:H:467:LYS:C	2:H:469:LEU:N	2.73	0.42
1:C:378:ILE:HB	1:C:379:PRO:CD	2.50	0.42
1:E:21:LEU:HD12	1:E:93:LEU:HD11	2.02	0.42
1:E:159:GLU:OE1	1:E:190:PRO:HA	2.20	0.42
1:E:214:PHE:CE1	1:E:230:LEU:CD2	3.03	0.42
2:F:82:PRO:HA	2:F:83:PRO:HD2	1.71	0.42
2:F:386:ASP:OD1	2:F:388:ILE:HB	2.19	0.42
1:G:321:ILE:HG21	1:G:358:ALA:HB1	2.02	0.42
2:H:398:LYS:C	2:H:400:TYR:N	2.73	0.42
2:H:436:ILE:HG22	2:H:437:GLU:N	2.35	0.42
1:A:259:LEU:O	1:A:259:LEU:HD12	2.19	0.42
1:A:302:ILE:HB	1:A:303:PHE:CE2	2.54	0.42
2:B:16:PHE:CE1	2:B:23:ALA:HB3	2.55	0.42
2:B:506:PHE:C	2:B:508:LEU:N	2.73	0.42
3:B:531:RDC:H182	3:B:531:RDC:H15	1.96	0.42
2:D:382:ASP:C	2:D:384:LYS:N	2.73	0.42
1:E:85:MET:HG2	1:E:129:TRP:CH2	2.55	0.42
1:E:113:LEU:CD2	1:E:115:LYS:O	2.68	0.42
2:F:97:SER:O	2:F:98:LYS:C	2.57	0.42
2:F:322:ILE:CG2	2:F:412:MET:HE2	2.49	0.42
2:H:430:ILE:HG22	2:H:431:ALA:N	2.35	0.42
2:H:459:ARG:O	2:H:463:GLU:HB2	2.20	0.42
1:A:274:ARG:HE	1:A:274:ARG:HB2	1.46	0.41
1:C:11:LYS:H	1:C:11:LYS:HG2	1.58	0.41
1:C:167:LEU:HG	1:C:168:ARG:N	2.34	0.41
1:E:218:HIS:CD2	1:E:223:TRP:NE1	2.78	0.41
2:H:86:VAL:CB	2:H:87:PRO:HD3	2.46	0.41
1:A:79:PHE:O	1:A:81:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:HB3	1:A:175:VAL:HG12	2.02	0.41
1:A:252:LEU:HB3	1:A:254:LEU:HD13	2.02	0.41
1:A:316:GLU:HA	1:A:319:ASN:HD21	1.84	0.41
1:C:216:GLN:HE21	1:C:216:GLN:HB2	1.60	0.41
1:G:79:PHE:C	1:G:81:GLN:N	2.74	0.41
1:G:150:ARG:NH2	1:G:150:ARG:HB3	2.34	0.41
1:G:262:ALA:CB	1:G:360:LEU:H	2.33	0.41
2:H:146:ILE:HG12	2:H:147:ASP:N	2.34	0.41
1:A:13:ALA:HA	1:A:16:LYS:HZ3	1.84	0.41
1:A:173:ASN:HD22	1:A:173:ASN:HA	1.54	0.41
1:A:183:HIS:ND1	1:C:14:ARG:CZ	2.84	0.41
1:A:324:ALA:HB3	1:A:357:LYS:HB3	2.02	0.41
1:C:166:ASN:HB3	1:C:201:ASP:HB3	2.02	0.41
1:C:184:GLY:O	1:C:185:ALA:HB2	2.20	0.41
1:E:21:LEU:O	1:E:22:ARG:O	2.37	0.41
1:E:90:TYR:CD2	1:E:90:TYR:C	2.92	0.41
1:E:205:VAL:CG1	1:E:256:VAL:HG22	2.50	0.41
2:F:103:GLN:HE22	2:F:315:SER:H	1.67	0.41
2:F:374:ALA:O	2:F:377:ILE:HG13	2.21	0.41
1:G:21:LEU:C	1:G:21:LEU:HD13	2.40	0.41
1:G:188:ILE:O	1:G:188:ILE:CD1	2.68	0.41
2:H:16:PHE:HZ	2:H:25:PHE:CD2	2.38	0.41
1:A:12:GLU:C	1:A:12:GLU:CD	2.79	0.41
1:A:79:PHE:C	1:A:81:GLN:N	2.74	0.41
1:A:238:ASP:C	1:A:242:ARG:NH2	2.73	0.41
2:B:86:VAL:CB	2:B:87:PRO:HD3	2.47	0.41
2:B:377:ILE:HA	2:B:378:PRO:HD3	1.94	0.41
2:B:508:LEU:O	2:B:510:SER:N	2.53	0.41
1:C:12:GLU:C	1:C:12:GLU:CD	2.78	0.41
2:D:195:TYR:OH	2:D:216:PRO:HD2	2.21	0.41
2:D:222:ILE:HA	2:D:223:PRO:HD3	1.91	0.41
2:F:500:GLU:CA	2:F:503:GLU:HB3	2.37	0.41
1:G:131:GLU:O	1:G:132:GLN:C	2.59	0.41
1:G:150:ARG:C	1:G:152:GLU:H	2.23	0.41
1:G:335:ILE:O	1:G:338:TYR:N	2.46	0.41
1:A:19:ASN:C	1:A:21:LEU:N	2.73	0.41
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.75	0.41
2:B:476:PRO:O	2:B:479:SER:HB2	2.20	0.41
1:C:265:TYR:O	1:C:268:TYR:HB3	2.19	0.41
2:D:397:TRP:O	2:D:402:ILE:HB	2.19	0.41
1:E:84:LEU:O	1:E:85:MET:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:ARG:C	1:E:308:LYS:CD	2.87	0.41
2:F:84:GLN:HE21	2:F:85:GLU:HG3	1.85	0.41
2:F:497:TYR:O	2:F:500:GLU:OE2	2.38	0.41
2:H:55:ASN:OD1	2:H:217:ARG:NH2	2.54	0.41
2:H:462:GLN:O	2:H:466:LYS:HB2	2.21	0.41
1:A:12:GLU:HG3	1:A:13:ALA:N	2.35	0.41
1:A:102:ARG:C	1:A:104:LEU:N	2.72	0.41
1:A:226:TYR:O	1:A:227:LYS:C	2.58	0.41
2:B:82:PRO:HA	2:B:83:PRO:HD2	1.73	0.41
2:B:499:ASN:C	2:B:499:ASN:ND2	2.70	0.41
1:C:21:LEU:O	1:C:22:ARG:O	2.39	0.41
2:D:62:LEU:HD13	2:D:70:TYR:CE1	2.56	0.41
1:G:252:LEU:HB3	1:G:254:LEU:HD13	2.02	0.41
1:G:319:ASN:HD22	1:G:319:ASN:N	1.94	0.41
1:A:208:VAL:CG2	1:A:209:GLU:N	2.83	0.41
1:A:285:GLU:HB3	1:A:286:ARG:H	1.53	0.41
1:C:232:THR:OG1	1:C:233:SER:O	2.33	0.41
1:C:240:ALA:C	1:C:242:ARG:N	2.70	0.41
2:D:340:ARG:HH22	2:D:442:ASN:HB3	1.85	0.41
1:E:12:GLU:CG	1:E:13:ALA:N	2.83	0.41
1:G:251:GLU:C	1:G:252:LEU:HD12	2.40	0.41
1:A:110:HIS:HD2	2:B:480:ARG:NH1	2.19	0.41
2:B:142:PHE:HB3	2:B:144:LEU:HD13	2.02	0.41
2:B:276:LEU:C	2:B:278:GLY:N	2.74	0.41
1:C:79:PHE:C	1:C:81:GLN:N	2.74	0.41
1:C:245:VAL:HG12	1:C:289:THR:HG21	2.02	0.41
2:D:358:PHE:CB	2:D:451:LEU:HD11	2.51	0.41
1:E:21:LEU:O	1:E:22:ARG:C	2.58	0.41
1:E:167:LEU:HG	1:E:168:ARG:N	2.35	0.41
2:F:62:LEU:HD13	2:F:70:TYR:CE1	2.56	0.41
1:G:245:VAL:HG12	1:G:289:THR:HG21	2.03	0.41
1:G:307:ARG:CG	1:G:308:LYS:HD3	2.50	0.41
2:H:322:ILE:HG23	2:H:412:MET:HE2	2.03	0.41
2:H:382:ASP:C	2:H:384:LYS:N	2.74	0.41
2:H:497:TYR:O	2:H:500:GLU:OE2	2.38	0.41
1:A:189:GLU:C	1:A:191:THR:H	2.24	0.41
2:B:506:PHE:C	2:B:508:LEU:H	2.22	0.41
1:C:91:ASP:C	1:C:93:LEU:H	2.23	0.41
2:D:285:VAL:CG1	2:D:286:LYS:N	2.83	0.41
2:D:414:HIS:NE2	2:D:416:CYS:HB3	2.36	0.41
1:E:102:ARG:HD3	1:G:361:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:ASN:O	1:E:352:THR:C	2.59	0.41
1:E:378:ILE:N	1:E:379:PRO:HD2	2.36	0.41
1:E:387:TYR:N	1:E:387:TYR:CD2	2.89	0.41
3:F:531:RDC:H182	3:F:531:RDC:H15	2.00	0.41
1:G:11:LYS:H	1:G:11:LYS:HG2	1.60	0.41
1:G:102:ARG:O	1:G:103:ASP:C	2.60	0.41
1:G:189:GLU:C	1:G:191:THR:H	2.23	0.41
1:G:207:VAL:HB	1:G:258:ILE:HB	2.03	0.41
1:G:252:LEU:HD12	1:G:252:LEU:N	2.35	0.41
1:G:330:LYS:O	1:G:331:ARG:C	2.59	0.41
2:H:383:GLU:O	2:H:389:TRP:HB2	2.21	0.41
2:H:504:GLY:O	2:H:505:LEU:C	2.59	0.41
1:A:260:THR:HB	1:A:261:ASP:H	1.49	0.41
1:A:372:PHE:HD1	1:A:376:GLN:HB2	1.86	0.41
2:B:214:TYR:CE2	2:B:216:PRO:HB3	2.56	0.41
1:C:324:ALA:HB3	1:C:357:LYS:HB3	2.02	0.41
1:C:355:GLN:HE21	1:C:355:GLN:HB3	1.60	0.41
1:C:372:PHE:C	1:C:372:PHE:HD1	2.20	0.41
2:D:374:ALA:O	2:D:377:ILE:CG1	2.69	0.41
1:E:270:PHE:HD2	1:E:294:PHE:HD1	1.67	0.41
1:E:335:ILE:O	1:E:338:TYR:N	2.46	0.41
1:E:385:LYS:HA	1:E:387:TYR:CE2	2.56	0.41
2:F:362:ILE:HA	2:F:363:PRO:HD3	1.82	0.41
2:F:508:LEU:O	2:F:510:SER:N	2.54	0.41
1:G:362:ILE:HG13	1:G:362:ILE:H	1.66	0.41
2:B:471:TYR:HB3	2:B:475:ILE:HD11	2.03	0.40
2:D:338:ILE:O	2:D:338:ILE:HG23	2.20	0.40
2:F:224:LYS:CG	2:F:225:PRO:HD2	2.42	0.40
2:H:44:LEU:C	2:H:46:ALA:N	2.74	0.40
2:H:251:ASP:OD2	2:H:251:ASP:N	2.53	0.40
2:H:374:ALA:O	2:H:377:ILE:CG1	2.69	0.40
2:H:377:ILE:HA	2:H:378:PRO:HD3	1.95	0.40
1:A:31:GLN:O	1:A:33:LYS:HB2	2.20	0.40
1:A:265:TYR:O	1:A:268:TYR:HB3	2.20	0.40
1:A:307:ARG:HH11	1:A:308:LYS:NZ	2.20	0.40
2:B:316:VAL:HG13	2:B:351:ILE:HD12	2.04	0.40
2:B:497:TYR:O	2:B:500:GLU:OE2	2.39	0.40
1:E:102:ARG:O	1:E:103:ASP:C	2.59	0.40
2:F:387:VAL:HG12	2:F:430:ILE:HB	2.02	0.40
1:G:102:ARG:C	1:G:104:LEU:N	2.73	0.40
1:G:176:ILE:HG21	1:G:186:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:VAL:CG1	1:G:256:VAL:HG22	2.51	0.40
2:H:99:TYR:HH	2:H:348:HIS:HE2	1.69	0.40
2:H:227:GLN:O	2:H:313:SER:HA	2.21	0.40
1:A:41:GLU:O	1:A:43:PRO:HD3	2.21	0.40
1:A:207:VAL:HB	1:A:258:ILE:HB	2.04	0.40
1:A:261:ASP:OD1	1:A:362:ILE:HG13	2.22	0.40
2:B:83:PRO:O	2:B:86:VAL:HG23	2.21	0.40
2:B:382:ASP:C	2:B:384:LYS:N	2.74	0.40
2:B:388:ILE:O	2:B:392:VAL:HG13	2.22	0.40
1:C:150:ARG:NH2	1:C:150:ARG:HB3	2.36	0.40
1:C:154:LEU:O	1:C:155:ILE:C	2.59	0.40
1:C:286:ARG:C	1:C:287:LEU:HG	2.41	0.40
1:C:387:TYR:N	1:C:387:TYR:HD2	2.18	0.40
1:E:270:PHE:C	1:E:270:PHE:HD1	2.25	0.40
1:E:374:ALA:HB3	1:E:375:PHE:CD1	2.56	0.40
2:F:318:GLY:C	2:F:320:ASP:N	2.73	0.40
1:G:252:LEU:O	1:G:254:LEU:HD12	2.20	0.40
2:H:62:LEU:HD13	2:H:70:TYR:CE1	2.57	0.40
1:A:102:ARG:O	1:A:103:ASP:C	2.57	0.40
1:A:189:GLU:HA	1:A:190:PRO:HD3	1.97	0.40
1:A:262:ALA:CB	1:A:360:LEU:H	2.34	0.40
2:B:107:MET:O	2:B:108:TYR:O	2.38	0.40
2:B:251:ASP:OD2	2:B:251:ASP:N	2.53	0.40
2:B:354:ALA:HA	2:B:412:MET:O	2.21	0.40
1:C:153:MET:O	1:C:154:LEU:CB	2.56	0.40
1:C:348:GLU:O	1:C:352:THR:HG23	2.21	0.40
2:D:187:ILE:O	2:D:190:TYR:N	2.50	0.40
1:E:336:LYS:HB2	1:E:350:ILE:HG21	2.04	0.40
2:F:437:GLU:O	2:F:437:GLU:HG3	2.22	0.40
2:F:496:LYS:O	2:F:497:TYR:C	2.60	0.40
1:G:173:ASN:HD22	1:G:173:ASN:HA	1.54	0.40
1:G:178:LEU:HD23	1:G:178:LEU:HA	1.79	0.40
1:A:170:ARG:HG2	1:A:196:ASP:HB2	2.03	0.40
1:A:183:HIS:CE1	1:C:172:GLY:N	2.89	0.40
1:A:209:GLU:CB	1:A:260:THR:HG22	2.50	0.40
1:A:286:ARG:C	1:A:287:LEU:HG	2.42	0.40
1:A:330:LYS:O	1:A:331:ARG:C	2.60	0.40
1:A:348:GLU:O	1:A:352:THR:HG23	2.21	0.40
1:A:370:LEU:H	1:A:370:LEU:CD2	2.17	0.40
2:B:383:GLU:O	2:B:389:TRP:HB2	2.21	0.40
1:C:159:GLU:HB2	1:C:190:PRO:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ILE:H	1:C:302:ILE:HG13	1.71	0.40
1:C:311:TYR:CE1	1:C:377:TYR:CD2	3.10	0.40
2:D:190:TYR:O	2:D:191:ILE:C	2.59	0.40
1:E:140:VAL:CG1	1:E:141:ASP:N	2.84	0.40
1:G:31:GLN:O	1:G:33:LYS:HB2	2.21	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	339/389 (87%)	235 (69%)	76 (22%)	28 (8%)	1	10
1	C	339/389 (87%)	238 (70%)	73 (22%)	28 (8%)	1	10
1	E	339/389 (87%)	232 (68%)	78 (23%)	29 (9%)	1	10
1	G	339/389 (87%)	235 (69%)	76 (22%)	28 (8%)	1	10
2	B	504/530 (95%)	385 (76%)	88 (18%)	31 (6%)	1	17
2	D	504/530 (95%)	391 (78%)	87 (17%)	26 (5%)	2	20
2	F	504/530 (95%)	387 (77%)	90 (18%)	27 (5%)	2	19
2	H	504/530 (95%)	389 (77%)	91 (18%)	24 (5%)	2	22
All	All	3372/3676 (92%)	2492 (74%)	659 (20%)	221 (7%)	1	16

All (221) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	32	LEU
1	A	151	GLU
1	A	188	ILE
1	A	275	ILE

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Mol	Chain	Res	Type
1	A	277	SER
2	B	107	MET
2	B	108	TYR
2	B	165	ARG
2	B	264	SER
2	B	319	GLU
2	B	441	LYS
2	B	442	ASN
2	B	486	LEU
2	B	497	TYR
1	C	22	ARG
1	C	32	LEU
1	C	151	GLU
1	C	188	ILE
1	C	275	ILE
1	C	277	SER
2	D	107	MET
2	D	108	TYR
2	D	165	ARG
2	D	264	SER
2	D	319	GLU
2	D	442	ASN
2	D	486	LEU
2	D	497	TYR
1	E	22	ARG
1	E	32	LEU
1	E	151	GLU
1	E	188	ILE
1	E	275	ILE
1	E	277	SER
2	F	107	MET
2	F	108	TYR
2	F	165	ARG
2	F	264	SER
2	F	319	GLU
2	F	441	LYS
2	F	442	ASN
2	F	486	LEU
2	F	497	TYR
1	G	22	ARG
1	G	32	LEU
1	G	151	GLU

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Mol	Chain	Res	Type
1	G	188	ILE
1	G	275	ILE
1	G	277	SER
2	H	107	MET
2	H	108	TYR
2	H	165	ARG
2	H	264	SER
2	H	319	GLU
2	H	486	LEU
2	H	497	TYR
1	A	13	ALA
1	A	33	LYS
1	A	85	MET
1	A	155	ILE
1	A	336	LYS
1	A	354	LEU
1	A	370	LEU
2	B	255	LYS
2	B	346	GLN
2	B	402	ILE
2	B	468	LEU
2	B	509	ILE
1	C	13	ALA
1	C	18	ALA
1	C	33	LYS
1	C	85	MET
1	C	155	ILE
1	C	336	LYS
1	C	354	LEU
2	D	45	ASP
2	D	255	LYS
2	D	402	ILE
2	D	441	LYS
2	D	468	LEU
2	D	509	ILE
1	E	33	LYS
1	E	85	MET
1	E	147	SER
1	E	155	ILE
1	E	336	LYS
1	E	354	LEU
1	E	370	LEU

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Mol	Chain	Res	Type
2	F	45	ASP
2	F	255	LYS
2	F	402	ILE
2	F	468	LEU
2	F	509	ILE
1	G	33	LYS
1	G	85	MET
1	G	155	ILE
1	G	336	LYS
1	G	354	LEU
2	H	45	ASP
2	H	255	LYS
2	H	402	ILE
2	H	441	LYS
2	H	442	ASN
2	H	468	LEU
2	H	509	ILE
1	A	18	ALA
1	A	117	ILE
1	A	147	SER
1	A	150	ARG
1	A	357	LYS
2	B	45	ASP
2	B	98	LYS
2	B	99	TYR
2	B	151	ASN
2	B	401	GLY
1	C	147	SER
1	C	150	ARG
1	C	357	LYS
1	C	370	LEU
2	D	98	LYS
2	D	99	TYR
2	D	151	ASN
2	D	220	ASN
1	E	18	ALA
1	E	117	ILE
1	E	150	ARG
1	E	357	LYS
1	E	367	SER
1	E	387	TYR
2	F	98	LYS

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Mol	Chain	Res	Type
2	F	99	TYR
2	F	220	ASN
1	G	117	ILE
1	G	147	SER
1	G	150	ARG
1	G	357	LYS
1	G	370	LEU
2	H	98	LYS
2	H	99	TYR
2	H	151	ASN
2	H	220	ASN
1	A	185	ALA
2	B	95	TYR
2	B	191	ILE
2	B	347	GLY
2	B	383	GLU
1	C	117	ILE
1	C	240	ALA
1	E	13	ALA
1	E	185	ALA
2	F	95	TYR
2	F	111	GLY
2	F	151	ASN
2	F	383	GLU
1	G	13	ALA
1	G	18	ALA
1	G	161	GLY
1	G	382	ILE
1	A	103	ASP
1	A	263	ASP
1	A	278	ILE
2	B	276	LEU
1	C	154	LEU
1	C	185	ALA
1	C	278	ILE
2	D	95	TYR
2	D	111	GLY
2	D	383	GLU
1	E	263	ASP
1	E	278	ILE
2	F	346	GLN
1	G	11	LYS

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Mol	Chain	Res	Type
1	G	106	TYR
1	G	263	ASP
1	G	278	ILE
1	G	367	SER
2	H	95	TYR
1	A	106	TYR
1	A	139	ILE
1	A	240	ALA
2	B	329	ILE
2	B	382	ASP
1	C	233	SER
1	C	263	ASP
1	C	387	TYR
1	E	240	ALA
1	G	154	LEU
1	G	185	ALA
1	A	269	ILE
2	B	28	PRO
2	B	111	GLY
2	D	191	ILE
2	D	329	ILE
1	E	139	ILE
2	F	28	PRO
2	F	191	ILE
2	F	329	ILE
2	F	401	GLY
1	G	269	ILE
2	H	28	PRO
2	H	111	GLY
2	H	191	ILE
2	H	329	ILE
1	C	139	ILE
1	C	269	ILE
2	D	28	PRO
2	D	401	GLY
1	E	269	ILE
2	D	309	PRO
1	E	161	GLY
1	E	382	ILE
2	H	309	PRO
1	A	198	ILE
1	A	382	ILE

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Mol	Chain	Res	Type
2	B	317	ILE
1	E	192	PRO
2	B	281	PRO
2	B	309	PRO
1	C	198	ILE
2	F	281	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	306/345 (89%)	214 (70%)	92 (30%)	0 3
1	C	306/345 (89%)	215 (70%)	91 (30%)	0 3
1	E	306/345 (89%)	217 (71%)	89 (29%)	0 3
1	G	306/345 (89%)	214 (70%)	92 (30%)	0 3
2	B	451/473 (95%)	401 (89%)	50 (11%)	6 31
2	D	451/473 (95%)	402 (89%)	49 (11%)	6 31
2	F	451/473 (95%)	404 (90%)	47 (10%)	7 33
2	H	451/473 (95%)	402 (89%)	49 (11%)	6 31
All	All	3028/3272 (92%)	2469 (82%)	559 (18%)	1 9

All (559) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	11	LYS
1	A	15	ARG
1	A	25	PHE
1	A	29	VAL
1	A	31	GLN
1	A	34	LYS
1	A	38	LEU
1	A	41	GLU

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Mol	Chain	Res	Type
1	A	67	ARG
1	A	69	ASN
1	A	74	ASN
1	A	75	GLU
1	A	80	MET
1	A	83	VAL
1	A	85	MET
1	A	93	LEU
1	A	94	VAL
1	A	100	THR
1	A	101	ILE
1	A	113	LEU
1	A	115	LYS
1	A	116	SER
1	A	117	ILE
1	A	128	THR
1	A	140	VAL
1	A	146	THR
1	A	148	LEU
1	A	149	LEU
1	A	150	ARG
1	A	155	ILE
1	A	158	LYS
1	A	160	LYS
1	A	162	LYS
1	A	167	LEU
1	A	170	ARG
1	A	173	ASN
1	A	179	SER
1	A	183	HIS
1	A	188	ILE
1	A	189	GLU
1	A	193	ASP
1	A	194	LEU
1	A	200	VAL
1	A	205	VAL
1	A	213	VAL
1	A	230	LEU
1	A	231	ILE
1	A	239	ARG
1	A	241	THR
1	A	242	ARG

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Mol	Chain	Res	Type
1	A	243	ARG
1	A	250	GLU
1	A	258	ILE
1	A	259	LEU
1	A	270	PHE
1	A	273	PHE
1	A	275	ILE
1	A	289	THR
1	A	291	ASP
1	A	295	LEU
1	A	298	SER
1	A	302	ILE
1	A	308	LYS
1	A	309	LYS
1	A	311	TYR
1	A	312	LEU
1	A	313	SER
1	A	314	GLU
1	A	317	ARG
1	A	319	ASN
1	A	323	LYS
1	A	331	ARG
1	A	335	ILE
1	A	343	THR
1	A	344	LYS
1	A	346	TRP
1	A	349	GLU
1	A	351	ASN
1	A	355	GLN
1	A	360	LEU
1	A	365	MET
1	A	371	LYS
1	A	372	PHE
1	A	373	LEU
1	A	375	PHE
1	A	378	ILE
1	A	380	GLU
1	A	383	THR
1	A	385	LYS
1	A	387	TYR
1	A	388	ILE
2	B	30	ARG

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Mol	Chain	Res	Type
2	B	113	LYS
2	B	120	GLN
2	B	137	LYS
2	B	170	THR
2	B	186	ARG
2	B	189	GLU
2	B	191	ILE
2	B	211	ASN
2	B	215	TYR
2	B	222	ILE
2	B	227	GLN
2	B	246	ASN
2	B	247	ASN
2	B	253	THR
2	B	254	ILE
2	B	264	SER
2	B	265	ILE
2	B	271	ASP
2	B	284	LYS
2	B	312	ASP
2	B	316	VAL
2	B	326	LEU
2	B	327	LYS
2	B	341	LYS
2	B	351	ILE
2	B	366	GLU
2	B	371	LEU
2	B	380	ILE
2	B	382	ASP
2	B	384	LYS
2	B	392	VAL
2	B	402	ILE
2	B	408	GLN
2	B	410	VAL
2	B	435	ASN
2	B	436	ILE
2	B	444	LEU
2	B	447	VAL
2	B	461	GLU
2	B	488	SER
2	B	490	ASN
2	B	499	ASN

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Mol	Chain	Res	Type
2	B	506	PHE
2	B	508	LEU
2	B	510	SER
2	B	511	LYS
2	B	514	ASP
2	B	516	ILE
2	B	519	GLU
1	C	10	ASP
1	C	11	LYS
1	C	15	ARG
1	C	25	PHE
1	C	29	VAL
1	C	31	GLN
1	C	34	LYS
1	C	38	LEU
1	C	41	GLU
1	C	67	ARG
1	C	69	ASN
1	C	74	ASN
1	C	75	GLU
1	C	80	MET
1	C	83	VAL
1	C	85	MET
1	C	93	LEU
1	C	94	VAL
1	C	100	THR
1	C	101	ILE
1	C	113	LEU
1	C	115	LYS
1	C	116	SER
1	C	117	ILE
1	C	128	THR
1	C	140	VAL
1	C	148	LEU
1	C	149	LEU
1	C	150	ARG
1	C	155	ILE
1	C	158	LYS
1	C	159	GLU
1	C	160	LYS
1	C	162	LYS
1	C	167	LEU

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Mol	Chain	Res	Type
1	C	170	ARG
1	C	173	ASN
1	C	179	SER
1	C	183	HIS
1	C	188	ILE
1	C	189	GLU
1	C	193	ASP
1	C	194	LEU
1	C	200	VAL
1	C	205	VAL
1	C	213	VAL
1	C	230	LEU
1	C	231	ILE
1	C	239	ARG
1	C	241	THR
1	C	242	ARG
1	C	243	ARG
1	C	250	GLU
1	C	258	ILE
1	C	259	LEU
1	C	273	PHE
1	C	275	ILE
1	C	289	THR
1	C	291	ASP
1	C	295	LEU
1	C	298	SER
1	C	302	ILE
1	C	308	LYS
1	C	309	LYS
1	C	311	TYR
1	C	312	LEU
1	C	313	SER
1	C	314	GLU
1	C	317	ARG
1	C	319	ASN
1	C	323	LYS
1	C	331	ARG
1	C	335	ILE
1	C	343	THR
1	C	344	LYS
1	C	346	TRP
1	C	349	GLU

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Mol	Chain	Res	Type
1	C	351	ASN
1	C	355	GLN
1	C	360	LEU
1	C	365	MET
1	C	371	LYS
1	C	372	PHE
1	C	373	LEU
1	C	375	PHE
1	C	378	ILE
1	C	380	GLU
1	C	383	THR
1	C	385	LYS
1	C	387	TYR
1	C	388	ILE
2	D	30	ARG
2	D	113	LYS
2	D	120	GLN
2	D	137	LYS
2	D	170	THR
2	D	186	ARG
2	D	189	GLU
2	D	191	ILE
2	D	211	ASN
2	D	215	TYR
2	D	222	ILE
2	D	227	GLN
2	D	246	ASN
2	D	247	ASN
2	D	253	THR
2	D	254	ILE
2	D	265	ILE
2	D	271	ASP
2	D	284	LYS
2	D	312	ASP
2	D	316	VAL
2	D	326	LEU
2	D	327	LYS
2	D	341	LYS
2	D	351	ILE
2	D	366	GLU
2	D	380	ILE
2	D	382	ASP

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Mol	Chain	Res	Type
2	D	384	LYS
2	D	392	VAL
2	D	402	ILE
2	D	408	GLN
2	D	410	VAL
2	D	435	ASN
2	D	436	ILE
2	D	444	LEU
2	D	447	VAL
2	D	449	ARG
2	D	461	GLU
2	D	488	SER
2	D	490	ASN
2	D	499	ASN
2	D	506	PHE
2	D	508	LEU
2	D	510	SER
2	D	511	LYS
2	D	514	ASP
2	D	516	ILE
2	D	519	GLU
1	E	10	ASP
1	E	11	LYS
1	E	15	ARG
1	E	25	PHE
1	E	29	VAL
1	E	31	GLN
1	E	34	LYS
1	E	38	LEU
1	E	41	GLU
1	E	67	ARG
1	E	69	ASN
1	E	74	ASN
1	E	75	GLU
1	E	80	MET
1	E	83	VAL
1	E	85	MET
1	E	93	LEU
1	E	94	VAL
1	E	100	THR
1	E	101	ILE
1	E	113	LEU

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Mol	Chain	Res	Type
1	E	115	LYS
1	E	116	SER
1	E	117	ILE
1	E	128	THR
1	E	140	VAL
1	E	148	LEU
1	E	149	LEU
1	E	150	ARG
1	E	155	ILE
1	E	158	LYS
1	E	160	LYS
1	E	162	LYS
1	E	167	LEU
1	E	170	ARG
1	E	173	ASN
1	E	179	SER
1	E	183	HIS
1	E	188	ILE
1	E	189	GLU
1	E	193	ASP
1	E	194	LEU
1	E	200	VAL
1	E	205	VAL
1	E	213	VAL
1	E	230	LEU
1	E	231	ILE
1	E	239	ARG
1	E	242	ARG
1	E	243	ARG
1	E	250	GLU
1	E	258	ILE
1	E	259	LEU
1	E	270	PHE
1	E	273	PHE
1	E	275	ILE
1	E	289	THR
1	E	291	ASP
1	E	295	LEU
1	E	298	SER
1	E	302	ILE
1	E	308	LYS
1	E	309	LYS

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Mol	Chain	Res	Type
1	E	312	LEU
1	E	313	SER
1	E	314	GLU
1	E	319	ASN
1	E	323	LYS
1	E	331	ARG
1	E	335	ILE
1	E	343	THR
1	E	344	LYS
1	E	346	TRP
1	E	349	GLU
1	E	351	ASN
1	E	355	GLN
1	E	360	LEU
1	E	362	ILE
1	E	365	MET
1	E	371	LYS
1	E	372	PHE
1	E	373	LEU
1	E	375	PHE
1	E	378	ILE
1	E	380	GLU
1	E	383	THR
1	E	385	LYS
1	E	387	TYR
1	E	388	ILE
2	F	30	ARG
2	F	113	LYS
2	F	120	GLN
2	F	137	LYS
2	F	170	THR
2	F	186	ARG
2	F	189	GLU
2	F	191	ILE
2	F	211	ASN
2	F	215	TYR
2	F	222	ILE
2	F	227	GLN
2	F	246	ASN
2	F	247	ASN
2	F	253	THR
2	F	254	ILE

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Mol	Chain	Res	Type
2	F	265	ILE
2	F	271	ASP
2	F	284	LYS
2	F	312	ASP
2	F	316	VAL
2	F	326	LEU
2	F	327	LYS
2	F	341	LYS
2	F	351	ILE
2	F	366	GLU
2	F	380	ILE
2	F	382	ASP
2	F	384	LYS
2	F	392	VAL
2	F	402	ILE
2	F	408	GLN
2	F	410	VAL
2	F	435	ASN
2	F	436	ILE
2	F	444	LEU
2	F	447	VAL
2	F	461	GLU
2	F	488	SER
2	F	490	ASN
2	F	499	ASN
2	F	506	PHE
2	F	508	LEU
2	F	510	SER
2	F	511	LYS
2	F	514	ASP
2	F	516	ILE
1	G	10	ASP
1	G	11	LYS
1	G	15	ARG
1	G	25	PHE
1	G	29	VAL
1	G	31	GLN
1	G	34	LYS
1	G	38	LEU
1	G	41	GLU
1	G	67	ARG
1	G	69	ASN

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Mol	Chain	Res	Type
1	G	74	ASN
1	G	75	GLU
1	G	80	MET
1	G	82	THR
1	G	83	VAL
1	G	85	MET
1	G	93	LEU
1	G	94	VAL
1	G	100	THR
1	G	101	ILE
1	G	105	TYR
1	G	113	LEU
1	G	115	LYS
1	G	116	SER
1	G	117	ILE
1	G	128	THR
1	G	140	VAL
1	G	148	LEU
1	G	149	LEU
1	G	150	ARG
1	G	155	ILE
1	G	158	LYS
1	G	160	LYS
1	G	162	LYS
1	G	167	LEU
1	G	170	ARG
1	G	173	ASN
1	G	179	SER
1	G	183	HIS
1	G	188	ILE
1	G	189	GLU
1	G	193	ASP
1	G	194	LEU
1	G	200	VAL
1	G	205	VAL
1	G	213	VAL
1	G	230	LEU
1	G	231	ILE
1	G	239	ARG
1	G	242	ARG
1	G	243	ARG
1	G	250	GLU

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Mol	Chain	Res	Type
1	G	258	ILE
1	G	259	LEU
1	G	270	PHE
1	G	273	PHE
1	G	275	ILE
1	G	289	THR
1	G	291	ASP
1	G	295	LEU
1	G	298	SER
1	G	302	ILE
1	G	308	LYS
1	G	309	LYS
1	G	311	TYR
1	G	313	SER
1	G	314	GLU
1	G	316	GLU
1	G	317	ARG
1	G	319	ASN
1	G	323	LYS
1	G	331	ARG
1	G	335	ILE
1	G	343	THR
1	G	344	LYS
1	G	346	TRP
1	G	349	GLU
1	G	351	ASN
1	G	355	GLN
1	G	360	LEU
1	G	365	MET
1	G	371	LYS
1	G	372	PHE
1	G	373	LEU
1	G	375	PHE
1	G	378	ILE
1	G	380	GLU
1	G	383	THR
1	G	385	LYS
1	G	387	TYR
1	G	388	ILE
2	H	30	ARG
2	H	113	LYS
2	H	120	GLN

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Mol	Chain	Res	Type
2	H	137	LYS
2	H	170	THR
2	H	186	ARG
2	H	189	GLU
2	H	191	ILE
2	H	211	ASN
2	H	215	TYR
2	H	222	ILE
2	H	227	GLN
2	H	246	ASN
2	H	247	ASN
2	H	253	THR
2	H	254	ILE
2	H	265	ILE
2	H	271	ASP
2	H	284	LYS
2	H	312	ASP
2	H	316	VAL
2	H	326	LEU
2	H	327	LYS
2	H	341	LYS
2	H	351	ILE
2	H	366	GLU
2	H	380	ILE
2	H	382	ASP
2	H	384	LYS
2	H	392	VAL
2	H	402	ILE
2	H	408	GLN
2	H	410	VAL
2	H	435	ASN
2	H	436	ILE
2	H	444	LEU
2	H	447	VAL
2	H	449	ARG
2	H	461	GLU
2	H	488	SER
2	H	490	ASN
2	H	499	ASN
2	H	506	PHE
2	H	508	LEU
2	H	510	SER

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Mol	Chain	Res	Type
2	H	511	LYS
2	H	514	ASP
2	H	516	ILE
2	H	519	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	81	GLN
1	A	110	HIS
1	A	132	GLN
1	A	173	ASN
1	A	183	HIS
1	A	215	GLN
1	A	216	GLN
1	A	218	HIS
1	A	225	GLN
1	A	236	GLN
1	A	305	ASN
1	A	319	ASN
1	A	355	GLN
2	B	84	GLN
2	B	103	GLN
2	B	149	ASN
2	B	227	GLN
2	B	246	ASN
2	B	247	ASN
2	B	287	ASN
2	B	414	HIS
2	B	435	ASN
2	B	442	ASN
2	B	499	ASN
1	C	31	GLN
1	C	81	GLN
1	C	110	HIS
1	C	132	GLN
1	C	173	ASN
1	C	183	HIS
1	C	215	GLN
1	C	216	GLN
1	C	218	HIS

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Mol	Chain	Res	Type
1	C	225	GLN
1	C	236	GLN
1	C	305	ASN
1	C	319	ASN
1	C	355	GLN
2	D	84	GLN
2	D	103	GLN
2	D	149	ASN
2	D	227	GLN
2	D	246	ASN
2	D	247	ASN
2	D	287	ASN
2	D	414	HIS
2	D	435	ASN
2	D	442	ASN
2	D	499	ASN
1	E	31	GLN
1	E	81	GLN
1	E	110	HIS
1	E	132	GLN
1	E	173	ASN
1	E	183	HIS
1	E	215	GLN
1	E	216	GLN
1	E	218	HIS
1	E	225	GLN
1	E	236	GLN
1	E	305	ASN
1	E	319	ASN
1	E	355	GLN
2	F	84	GLN
2	F	103	GLN
2	F	149	ASN
2	F	227	GLN
2	F	246	ASN
2	F	247	ASN
2	F	287	ASN
2	F	414	HIS
2	F	435	ASN
2	F	442	ASN
2	F	499	ASN
1	G	31	GLN

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Mol	Chain	Res	Type
1	G	81	GLN
1	G	110	HIS
1	G	132	GLN
1	G	173	ASN
1	G	183	HIS
1	G	215	GLN
1	G	216	GLN
1	G	218	HIS
1	G	225	GLN
1	G	236	GLN
1	G	305	ASN
1	G	319	ASN
1	G	355	GLN
2	H	84	GLN
2	H	103	GLN
2	H	149	ASN
2	H	227	GLN
2	H	246	ASN
2	H	247	ASN
2	H	287	ASN
2	H	414	HIS
2	H	435	ASN
2	H	442	ASN
2	H	499	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
3	RDC	B	531	-	26,27,27	3.10	7 (26%)	30,39,39	1.73	8 (26%)
3	RDC	H	531	-	26,27,27	3.21	7 (26%)	30,39,39	1.70	8 (26%)
3	RDC	D	531	-	26,27,27	3.04	7 (26%)	30,39,39	1.67	9 (30%)
3	RDC	F	531	-	26,27,27	3.14	6 (23%)	30,39,39	1.65	8 (26%)

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	RDC	B	531	-	-	6/23/28/28	0/2/3/3
3	RDC	H	531	-	-	5/23/28/28	0/2/3/3
3	RDC	D	531	-	-	6/23/28/28	0/2/3/3
3	RDC	F	531	-	-	5/23/28/28	0/2/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	531	RDC	C6-CL1	-10.35	1.50	1.72
3	B	531	RDC	C6-CL1	-10.22	1.50	1.72
3	H	531	RDC	C6-CL1	-10.16	1.51	1.72
3	F	531	RDC	C6-CL1	-9.99	1.51	1.72
3	H	531	RDC	C5-C6	7.98	1.49	1.40
3	F	531	RDC	C5-C6	7.80	1.49	1.40
3	B	531	RDC	C5-C6	7.44	1.49	1.40
3	D	531	RDC	C5-C6	6.58	1.47	1.40
3	F	531	RDC	O1-C1	5.82	1.46	1.34
3	H	531	RDC	O1-C1	5.58	1.45	1.34
3	B	531	RDC	O1-C1	5.52	1.45	1.34
3	D	531	RDC	O1-C1	5.40	1.45	1.34
3	H	531	RDC	C2-C3	4.84	1.49	1.41
3	D	531	RDC	C2-C3	4.58	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	531	RDC	C2-C3	4.55	1.48	1.41
3	B	531	RDC	C2-C3	4.50	1.48	1.41
3	F	531	RDC	C2-C7	4.47	1.48	1.40
3	H	531	RDC	C2-C7	4.43	1.48	1.40
3	D	531	RDC	C2-C7	4.35	1.48	1.40
3	B	531	RDC	C2-C7	4.24	1.48	1.40
3	H	531	RDC	C6-C7	3.94	1.50	1.40
3	F	531	RDC	C6-C7	3.68	1.49	1.40
3	B	531	RDC	C6-C7	3.60	1.49	1.40
3	D	531	RDC	C6-C7	3.56	1.49	1.40
3	H	531	RDC	O1-C17	-2.25	1.43	1.47
3	D	531	RDC	O1-C17	-2.17	1.43	1.47
3	B	531	RDC	O1-C17	-2.16	1.43	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	531	RDC	C15-C14-C13	-3.68	111.39	122.47
3	B	531	RDC	C15-C14-C13	-3.67	111.42	122.47
3	B	531	RDC	O6-C15-C16	-3.62	108.69	116.33
3	H	531	RDC	C17-O1-C1	-3.61	111.33	117.61
3	F	531	RDC	C15-C14-C13	-3.51	111.90	122.47
3	B	531	RDC	C17-O1-C1	-3.45	111.61	117.61
3	D	531	RDC	C15-C14-C13	-3.37	112.31	122.47
3	D	531	RDC	C17-O1-C1	-3.24	111.97	117.61
3	F	531	RDC	O6-C15-C16	-3.08	109.82	116.33
3	H	531	RDC	C12-C11-C10	-3.06	117.04	124.67
3	B	531	RDC	C12-C11-C10	-3.04	117.09	124.67
3	D	531	RDC	O6-C15-C16	-3.03	109.92	116.33
3	F	531	RDC	C4-C5-C6	3.02	121.82	119.20
3	D	531	RDC	C12-C11-C10	-3.01	117.16	124.67
3	H	531	RDC	O1-C1-C2	2.93	120.80	113.33
3	F	531	RDC	C17-O1-C1	-2.93	112.51	117.61
3	F	531	RDC	C12-C11-C10	-2.88	117.48	124.67
3	D	531	RDC	O1-C1-O2	-2.82	118.93	123.53
3	H	531	RDC	O6-C15-C16	-2.77	110.49	116.33
3	H	531	RDC	O6-C14-C13	-2.62	108.86	115.37
3	B	531	RDC	O1-C1-O2	-2.62	119.25	123.53
3	B	531	RDC	O1-C1-C2	2.61	119.97	113.33
3	F	531	RDC	O6-C14-C13	-2.58	108.97	115.37
3	B	531	RDC	O6-C14-C13	-2.57	108.99	115.37
3	F	531	RDC	O1-C1-C2	2.56	119.84	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	531	RDC	O6-C14-C13	-2.53	109.10	115.37
3	D	531	RDC	O1-C1-C2	2.50	119.69	113.33
3	B	531	RDC	C4-C5-C6	2.47	121.34	119.20
3	H	531	RDC	C4-C5-C6	2.45	121.32	119.20
3	H	531	RDC	O1-C1-O2	-2.44	119.55	123.53
3	D	531	RDC	C4-C5-C6	2.35	121.24	119.20
3	D	531	RDC	C5-C4-C3	2.16	122.28	120.14
3	F	531	RDC	O1-C1-O2	-2.06	120.18	123.53

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	531	RDC	C6-C7-C8-C9
3	D	531	RDC	C6-C7-C8-C9
3	F	531	RDC	C6-C7-C8-C9
3	H	531	RDC	C6-C7-C8-C9
3	B	531	RDC	C2-C7-C8-C9
3	D	531	RDC	C2-C7-C8-C9
3	F	531	RDC	C2-C7-C8-C9
3	H	531	RDC	C2-C7-C8-C9
3	F	531	RDC	O2-C1-C2-C3
3	B	531	RDC	O2-C1-C2-C3
3	D	531	RDC	O2-C1-C2-C3
3	H	531	RDC	O2-C1-C2-C7
3	D	531	RDC	O2-C1-C2-C7
3	H	531	RDC	O2-C1-C2-C3
3	B	531	RDC	O2-C1-C2-C7
3	F	531	RDC	O2-C1-C2-C7
3	H	531	RDC	O1-C1-C2-C7
3	F	531	RDC	O1-C1-C2-C3
3	B	531	RDC	O1-C1-C2-C3
3	D	531	RDC	O1-C1-C2-C3
3	B	531	RDC	O1-C1-C2-C7
3	D	531	RDC	O1-C1-C2-C7

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	531	RDC	5	0

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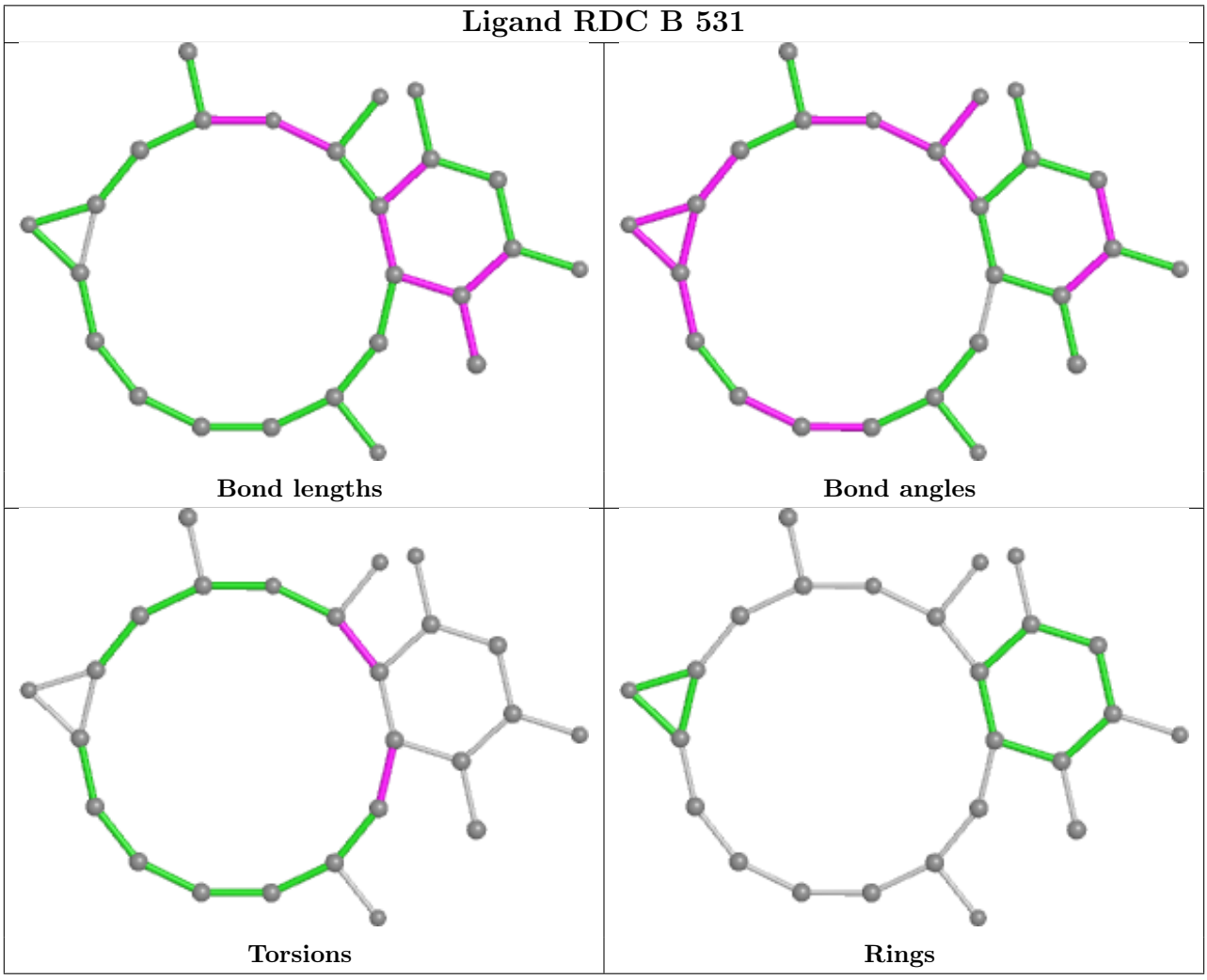
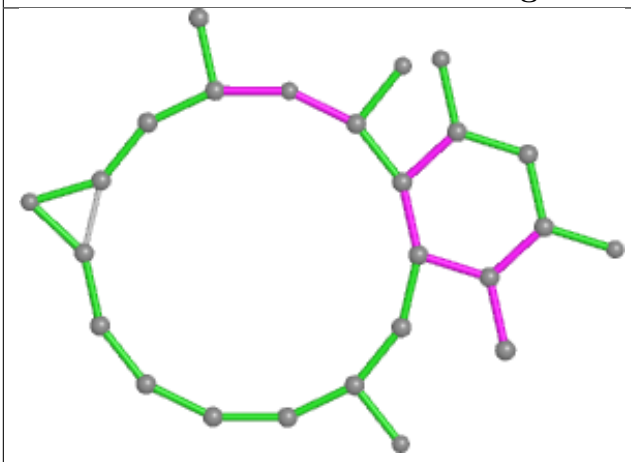
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	531	RDC	4	0
3	D	531	RDC	7	0
3	F	531	RDC	5	0

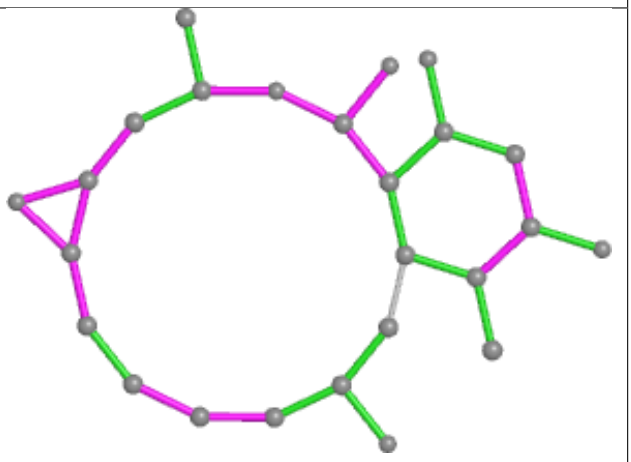
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



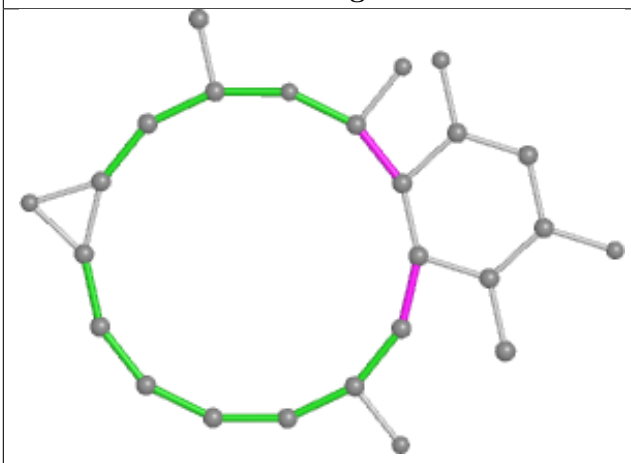
Ligand RDC H 531



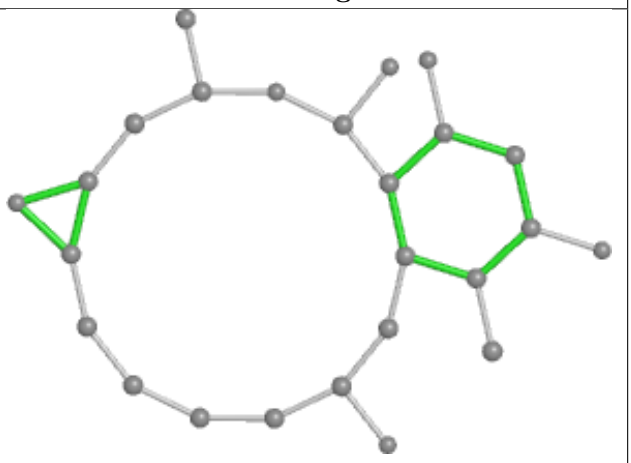
Bond lengths



Bond angles

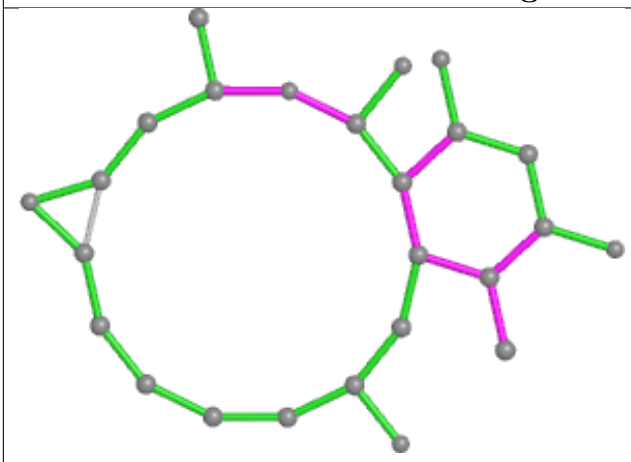


Torsions

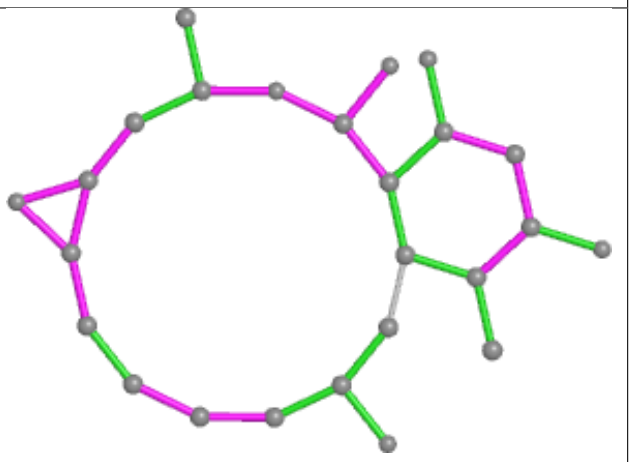


Rings

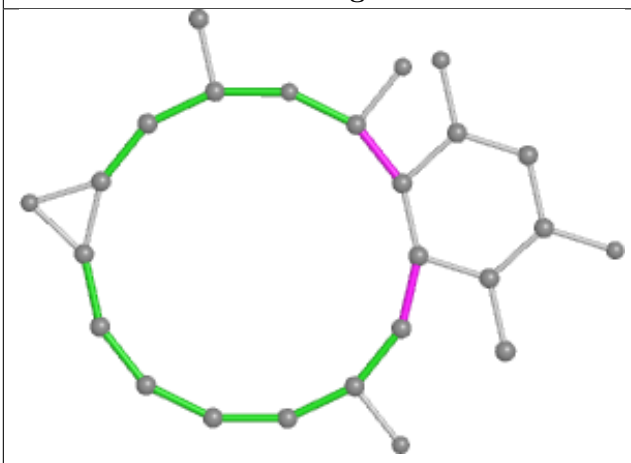
Ligand RDC D 531



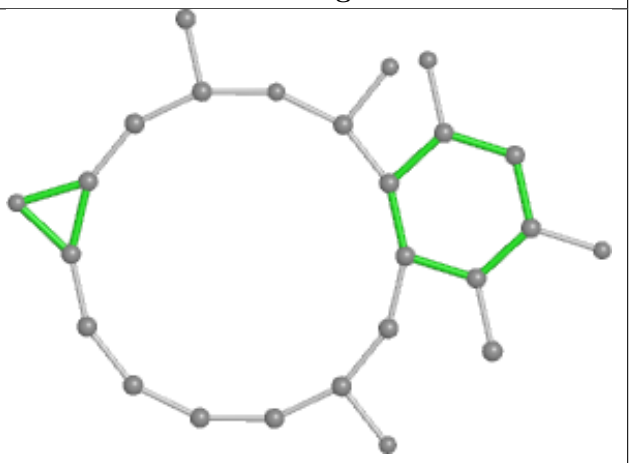
Bond lengths



Bond angles

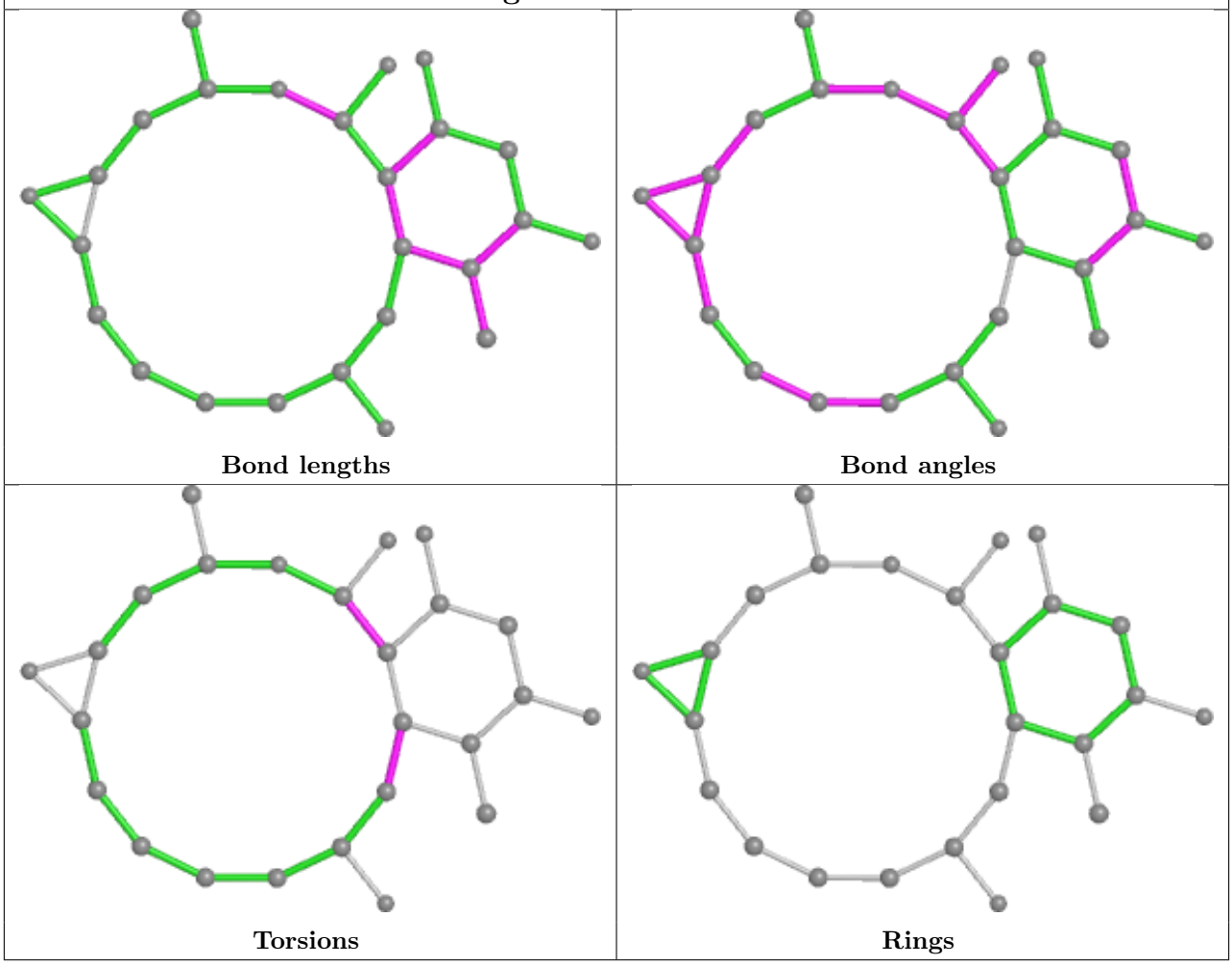


Torsions



Rings

Ligand RDC F 531



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	347/389 (89%)	-0.23	3 (0%)	84	72	20, 72, 83, 85	0
1	C	347/389 (89%)	-0.19	5 (1%)	75	60	20, 72, 83, 85	0
1	E	347/389 (89%)	-0.22	6 (1%)	70	55	20, 72, 83, 85	0
1	G	347/389 (89%)	-0.20	8 (2%)	60	43	20, 72, 83, 85	0
2	B	506/530 (95%)	-0.15	10 (1%)	65	49	23, 71, 78, 86	0
2	D	506/530 (95%)	-0.07	10 (1%)	65	49	23, 71, 78, 87	0
2	F	506/530 (95%)	-0.12	13 (2%)	56	39	23, 71, 78, 90	0
2	H	506/530 (95%)	0.11	23 (4%)	33	21	23, 71, 78, 86	0
All	All	3412/3676 (92%)	-0.12	78 (2%)	60	43	20, 71, 80, 90	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	166	GLY	5.0
2	F	166	GLY	4.9
2	F	95	TYR	4.4
2	B	95	TYR	4.1
2	D	95	TYR	4.1
2	D	165	ARG	4.0
2	H	249	LYS	4.0
2	B	96	SER	3.9
2	H	95	TYR	3.8
2	H	366	GLU	3.7
2	H	165	ARG	3.6
2	H	166	GLY	3.4
2	H	282	ASN	3.4
2	B	166	GLY	3.2
1	G	110	HIS	3.1
2	B	165	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	43	PRO	3.0
2	F	137	LYS	3.0
2	F	108	TYR	3.0
2	F	165	ARG	2.9
2	H	149	ASN	2.9
2	F	427	LYS	2.9
2	D	108	TYR	2.9
1	G	111	SER	2.8
1	G	343	THR	2.8
2	B	137	LYS	2.8
1	G	44	MET	2.8
1	C	111	SER	2.7
2	F	96	SER	2.7
2	H	290	GLU	2.7
2	B	108	TYR	2.7
2	D	280	LYS	2.6
2	F	149	ASN	2.6
2	B	97	SER	2.5
2	D	21	GLU	2.5
2	D	366	GLU	2.5
2	H	399	ARG	2.5
2	H	289	THR	2.5
1	G	159	GLU	2.4
1	E	111	SER	2.4
2	B	251	ASP	2.4
1	G	66	LEU	2.4
2	D	64	ASP	2.4
1	E	10	ASP	2.4
2	D	266	GLY	2.4
1	C	343	THR	2.4
2	B	22	LEU	2.3
2	H	238	ARG	2.3
2	H	126	PRO	2.3
2	H	280	LYS	2.3
2	H	109	GLY	2.3
2	H	164	THR	2.3
1	A	10	ASP	2.3
2	H	347	GLY	2.2
1	A	343	THR	2.2
2	H	22	LEU	2.2
1	E	159	GLU	2.2
2	F	97	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	423	LYS	2.2
1	G	10	ASP	2.2
2	D	168	HIS	2.2
2	F	151	ASN	2.2
2	H	124	ASP	2.2
1	C	112	LEU	2.1
2	H	108	TYR	2.1
2	H	96	SER	2.1
2	F	150	LYS	2.1
1	A	110	HIS	2.1
1	E	36	GLU	2.1
1	G	115	LYS	2.1
1	E	44	MET	2.1
2	H	284	LYS	2.1
1	C	159	GLU	2.1
2	B	150	LYS	2.0
2	F	67	ARG	2.0
2	H	136	SER	2.0
1	C	43	PRO	2.0
2	F	163	ASN	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RDC	D	531	25/25	0.74	0.40	92,93,94,94	0
3	RDC	B	531	25/25	0.80	0.37	92,93,94,94	0
3	RDC	H	531	25/25	0.80	0.31	92,93,94,94	0

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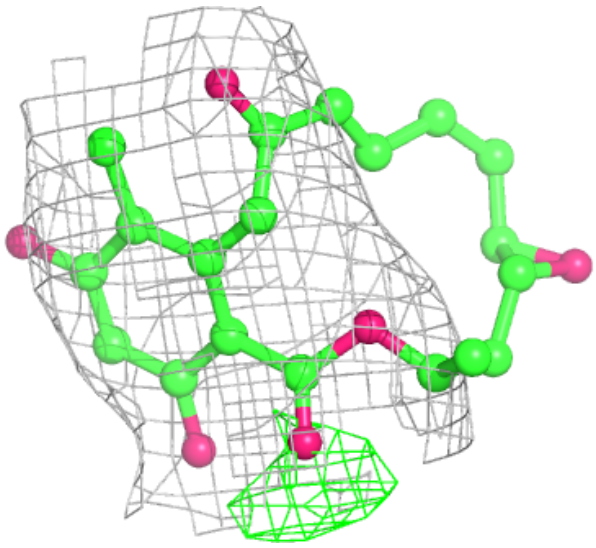
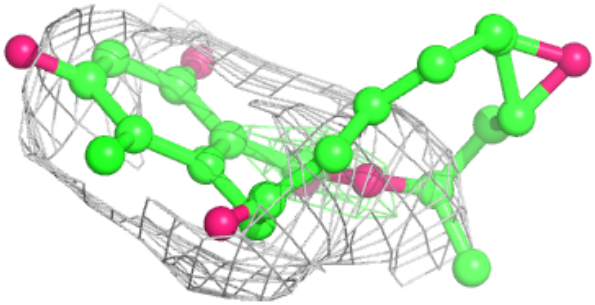
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RDC	F	531	25/25	0.85	0.29	92,93,94,94	0

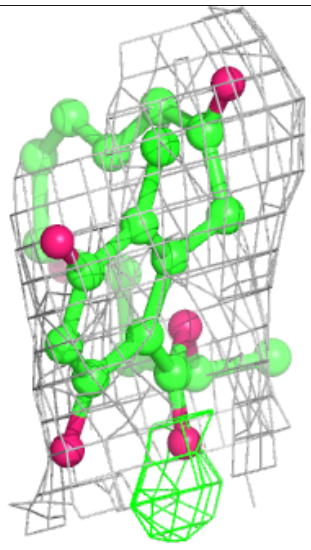
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RDC D 531:

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

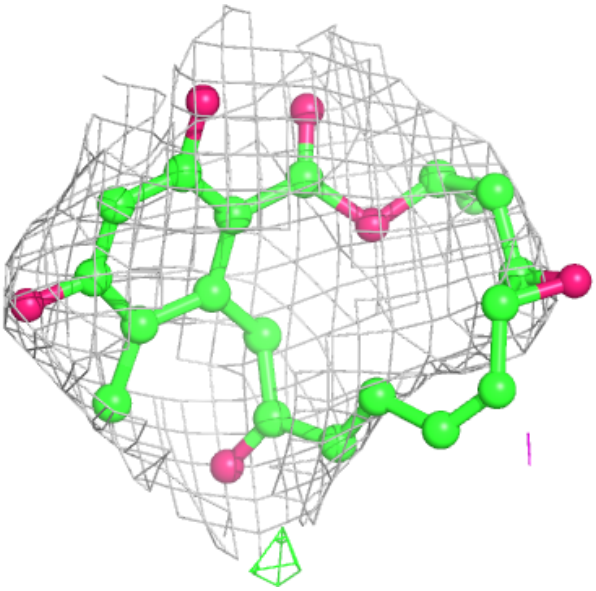


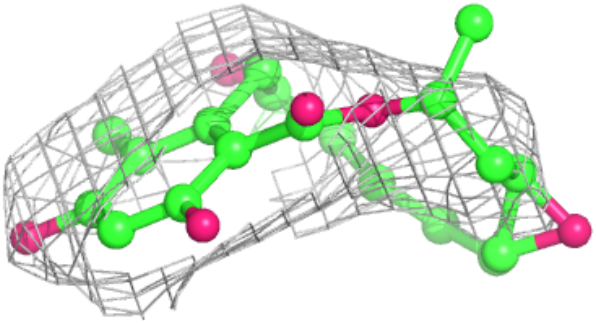


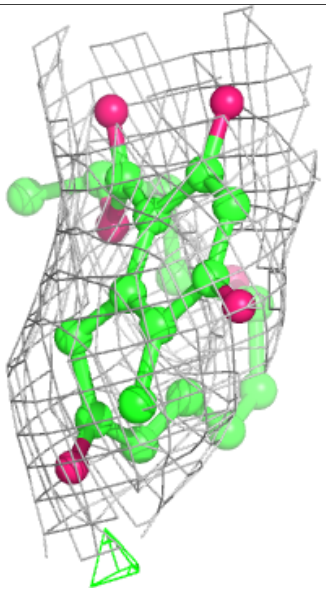


Electron density around RDC B 531:

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

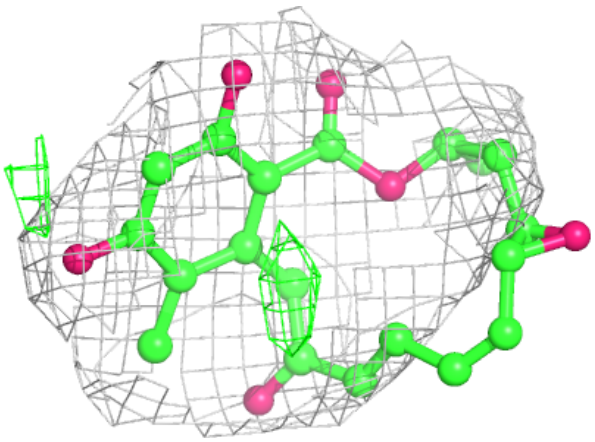


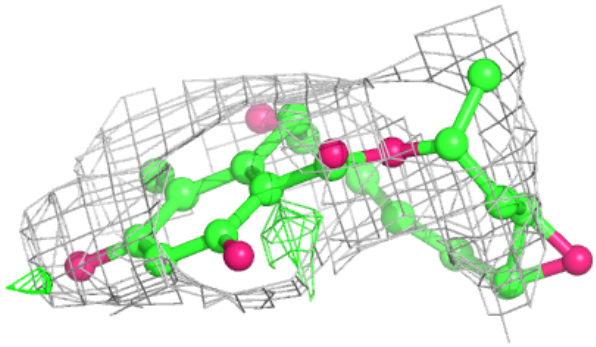


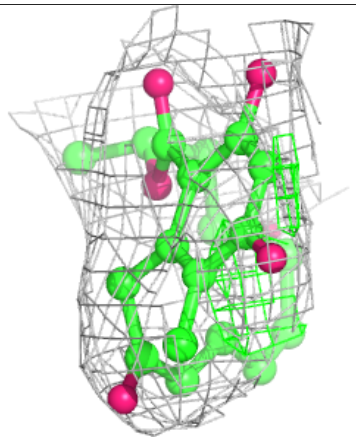


Electron density around RDC H 531:

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

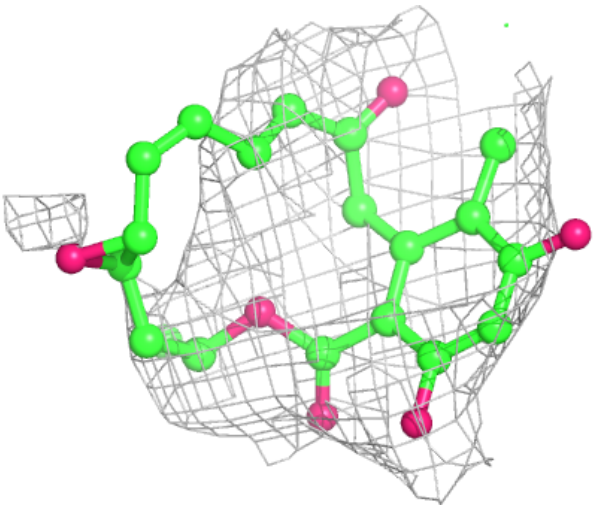


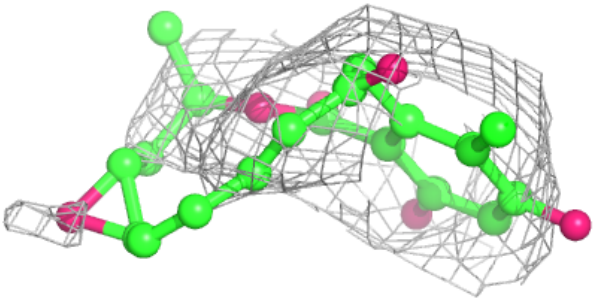


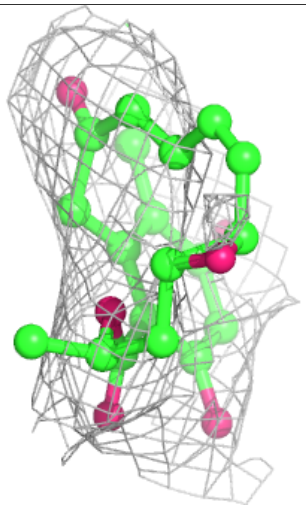


Electron density around RDC F 531:

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







6.5 Other polymers

There are no such residues in this entry.