Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID	:	3K6S
Title	:	Structure of integrin alphaXbeta2 ectodomain
Authors	:	Xie, C.; Zhu, J.; Chen, X.; Mi, L.; Nishida, N.; Springer, T.A.
Deposited on	:	2009-10-09
Resolution	:	3.50 Å(reported)

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

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

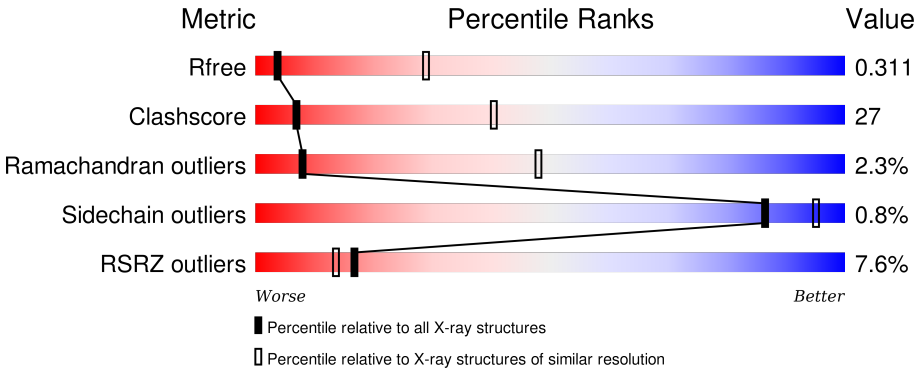
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	1095	2% 56% 40%
1	C	1095	5% 43% 35% 19%
1	E	1095	3% 43% 35% 19%
1	G	1095	3% 43% 35% 19%
2	B	687	7% 64% 33%

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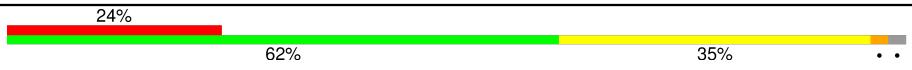
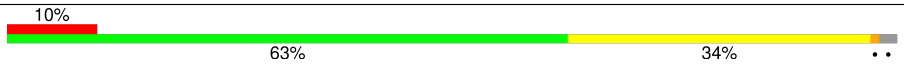
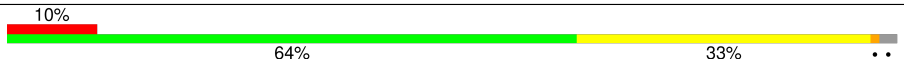
Mol	Chain	Length	Quality of chain
2	D	687	
2	F	687	
2	H	687	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	3373	X	-	-	-
4	NAG	A	3373	X	-	-	-
4	MAN	A	3375	X	-	-	-
9	NAG	E	3373	X	-	-	-
9	MAN	E	3375	X	-	-	-
9	NAG	G	3373	X	-	-	-
9	MAN	G	3375	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 50187 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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1082	Total	C	N	O	S	0	0	0
			8392	5304	1454	1596	38			
1	C	885	Total	C	N	O	S	0	0	0
			6825	4311	1182	1298	34			
1	E	884	Total	C	N	O	S	0	0	0
			6819	4308	1181	1296	34			
1	G	885	Total	C	N	O	S	0	0	0
			6825	4311	1182	1298	34			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	EXPRESSION TAG	UNP P20702
A	1086	CYS	-	EXPRESSION TAG	UNP P20702
A	1087	GLY	-	EXPRESSION TAG	UNP P20702
A	1088	GLY	-	EXPRESSION TAG	UNP P20702
A	1089	LEU	-	EXPRESSION TAG	UNP P20702
A	1090	GLU	-	EXPRESSION TAG	UNP P20702
A	1091	ASN	-	EXPRESSION TAG	UNP P20702
A	1092	LEU	-	EXPRESSION TAG	UNP P20702
A	1093	TYR	-	EXPRESSION TAG	UNP P20702
A	1094	PHE	-	EXPRESSION TAG	UNP P20702
A	1095	GLN	-	EXPRESSION TAG	UNP P20702
C	1085	GLY	-	EXPRESSION TAG	UNP P20702
C	1086	CYS	-	EXPRESSION TAG	UNP P20702
C	1087	GLY	-	EXPRESSION TAG	UNP P20702
C	1088	GLY	-	EXPRESSION TAG	UNP P20702
C	1089	LEU	-	EXPRESSION TAG	UNP P20702
C	1090	GLU	-	EXPRESSION TAG	UNP P20702
C	1091	ASN	-	EXPRESSION TAG	UNP P20702
C	1092	LEU	-	EXPRESSION TAG	UNP P20702
C	1093	TYR	-	EXPRESSION TAG	UNP P20702
C	1094	PHE	-	EXPRESSION TAG	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1095	GLN	-	EXPRESSION TAG	UNP P20702
E	1085	GLY	-	EXPRESSION TAG	UNP P20702
E	1086	CYS	-	EXPRESSION TAG	UNP P20702
E	1087	GLY	-	EXPRESSION TAG	UNP P20702
E	1088	GLY	-	EXPRESSION TAG	UNP P20702
E	1089	LEU	-	EXPRESSION TAG	UNP P20702
E	1090	GLU	-	EXPRESSION TAG	UNP P20702
E	1091	ASN	-	EXPRESSION TAG	UNP P20702
E	1092	LEU	-	EXPRESSION TAG	UNP P20702
E	1093	TYR	-	EXPRESSION TAG	UNP P20702
E	1094	PHE	-	EXPRESSION TAG	UNP P20702
E	1095	GLN	-	EXPRESSION TAG	UNP P20702
G	1085	GLY	-	EXPRESSION TAG	UNP P20702
G	1086	CYS	-	EXPRESSION TAG	UNP P20702
G	1087	GLY	-	EXPRESSION TAG	UNP P20702
G	1088	GLY	-	EXPRESSION TAG	UNP P20702
G	1089	LEU	-	EXPRESSION TAG	UNP P20702
G	1090	GLU	-	EXPRESSION TAG	UNP P20702
G	1091	ASN	-	EXPRESSION TAG	UNP P20702
G	1092	LEU	-	EXPRESSION TAG	UNP P20702
G	1093	TYR	-	EXPRESSION TAG	UNP P20702
G	1094	PHE	-	EXPRESSION TAG	UNP P20702
G	1095	GLN	-	EXPRESSION TAG	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	D	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	F	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	H	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	EXPRESSION TAG	UNP P05107
B	679	GLY	-	EXPRESSION TAG	UNP P05107
B	680	CYS	-	EXPRESSION TAG	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	GLY	-	EXPRESSION TAG	UNP P05107
B	682	GLU	-	EXPRESSION TAG	UNP P05107
B	684	LEU	-	EXPRESSION TAG	UNP P05107
B	685	TYR	-	EXPRESSION TAG	UNP P05107
B	686	PHE	-	EXPRESSION TAG	UNP P05107
B	687	GLN	-	EXPRESSION TAG	UNP P05107
D	678	ASP	-	EXPRESSION TAG	UNP P05107
D	679	GLY	-	EXPRESSION TAG	UNP P05107
D	680	CYS	-	EXPRESSION TAG	UNP P05107
D	681	GLY	-	EXPRESSION TAG	UNP P05107
D	682	GLU	-	EXPRESSION TAG	UNP P05107
D	684	LEU	-	EXPRESSION TAG	UNP P05107
D	685	TYR	-	EXPRESSION TAG	UNP P05107
D	686	PHE	-	EXPRESSION TAG	UNP P05107
D	687	GLN	-	EXPRESSION TAG	UNP P05107
F	678	ASP	-	EXPRESSION TAG	UNP P05107
F	679	GLY	-	EXPRESSION TAG	UNP P05107
F	680	CYS	-	EXPRESSION TAG	UNP P05107
F	681	GLY	-	EXPRESSION TAG	UNP P05107
F	682	GLU	-	EXPRESSION TAG	UNP P05107
F	684	LEU	-	EXPRESSION TAG	UNP P05107
F	685	TYR	-	EXPRESSION TAG	UNP P05107
F	686	PHE	-	EXPRESSION TAG	UNP P05107
F	687	GLN	-	EXPRESSION TAG	UNP P05107
H	678	ASP	-	EXPRESSION TAG	UNP P05107
H	679	GLY	-	EXPRESSION TAG	UNP P05107
H	680	CYS	-	EXPRESSION TAG	UNP P05107
H	681	GLY	-	EXPRESSION TAG	UNP P05107
H	682	GLU	-	EXPRESSION TAG	UNP P05107
H	684	LEU	-	EXPRESSION TAG	UNP P05107
H	685	TYR	-	EXPRESSION TAG	UNP P05107
H	686	PHE	-	EXPRESSION TAG	UNP P05107
H	687	GLN	-	EXPRESSION TAG	UNP P05107

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

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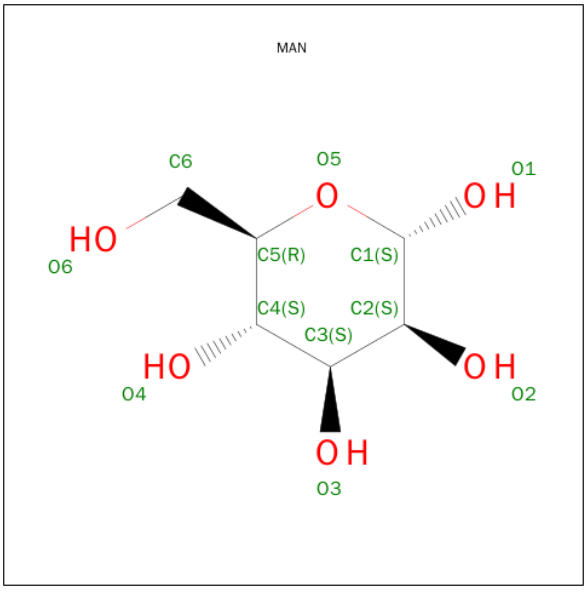
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		

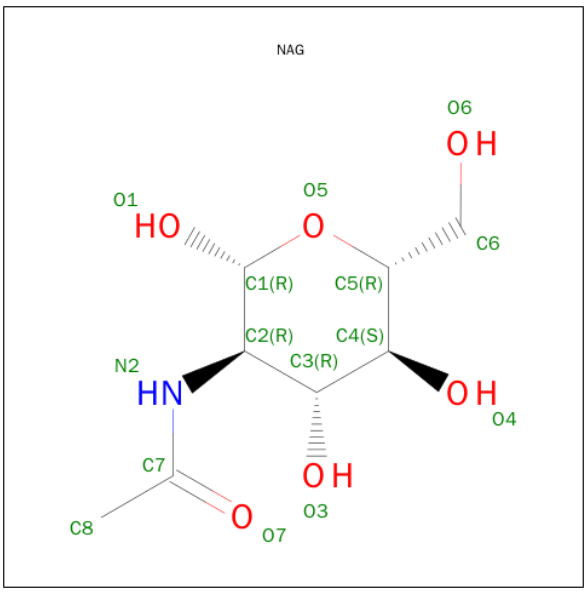
- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	H	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	3	Total Ca 3 3	0	0
7	D	1	Total Ca 1 1	0	0
7	E	3	Total Ca 3 3	0	0
7	H	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	3	Total Ca 3 3	0	0
7	A	3	Total Ca 3 3	0	0
7	F	1	Total Ca 1 1	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mg 1 1	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	3	Total C N O 39 22 2 15	0	0
9	G	3	Total C N O 39 22 2 15	0	0

- Molecule 10 is water.

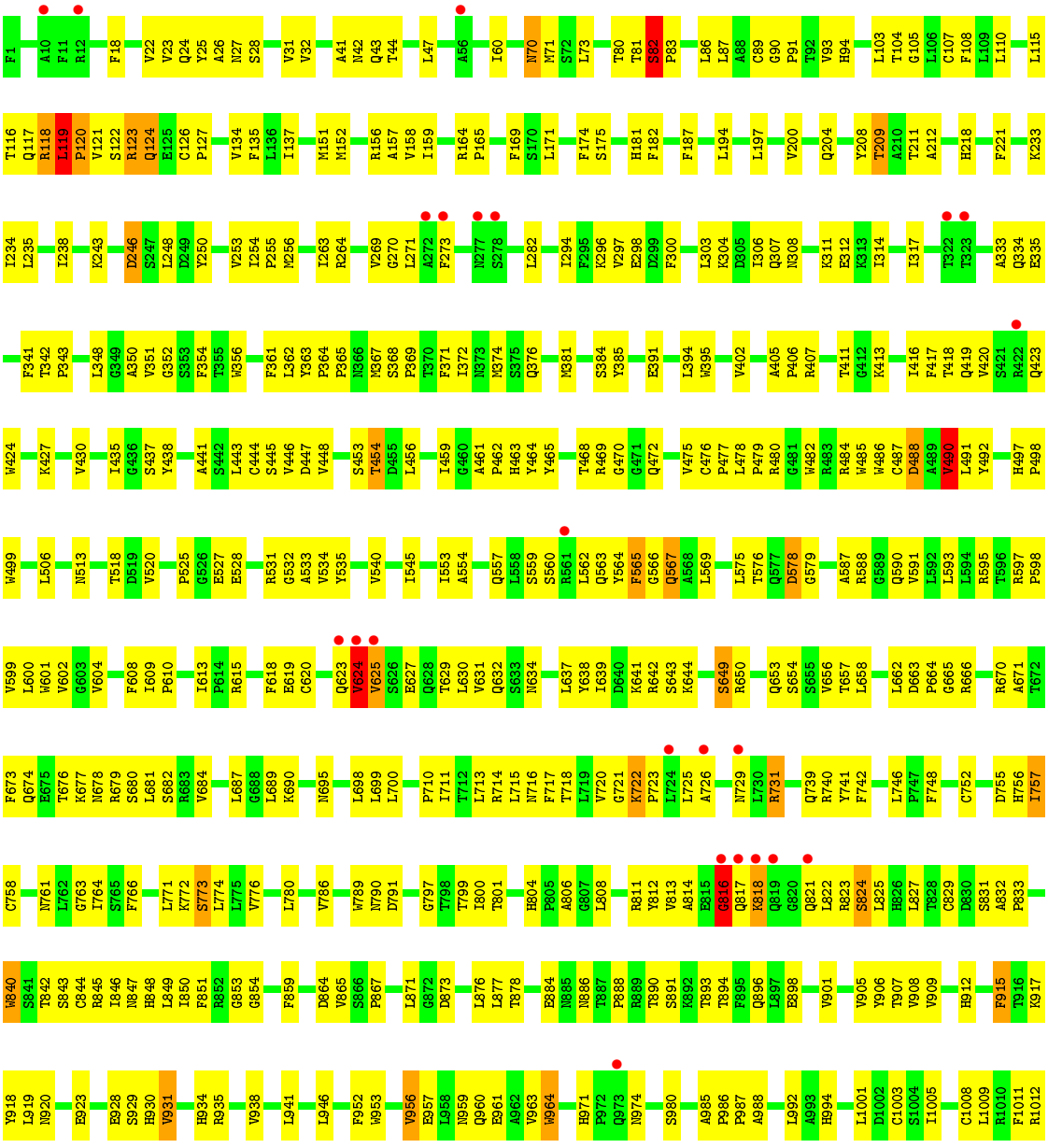
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total O 3 3	0	0

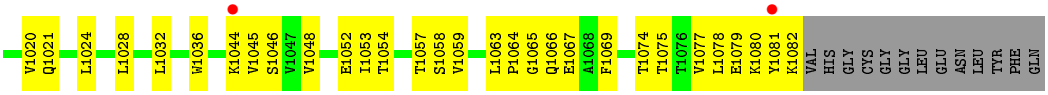
3 Residue-property plots (i)

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

- Molecule 1: Integrin alpha-X

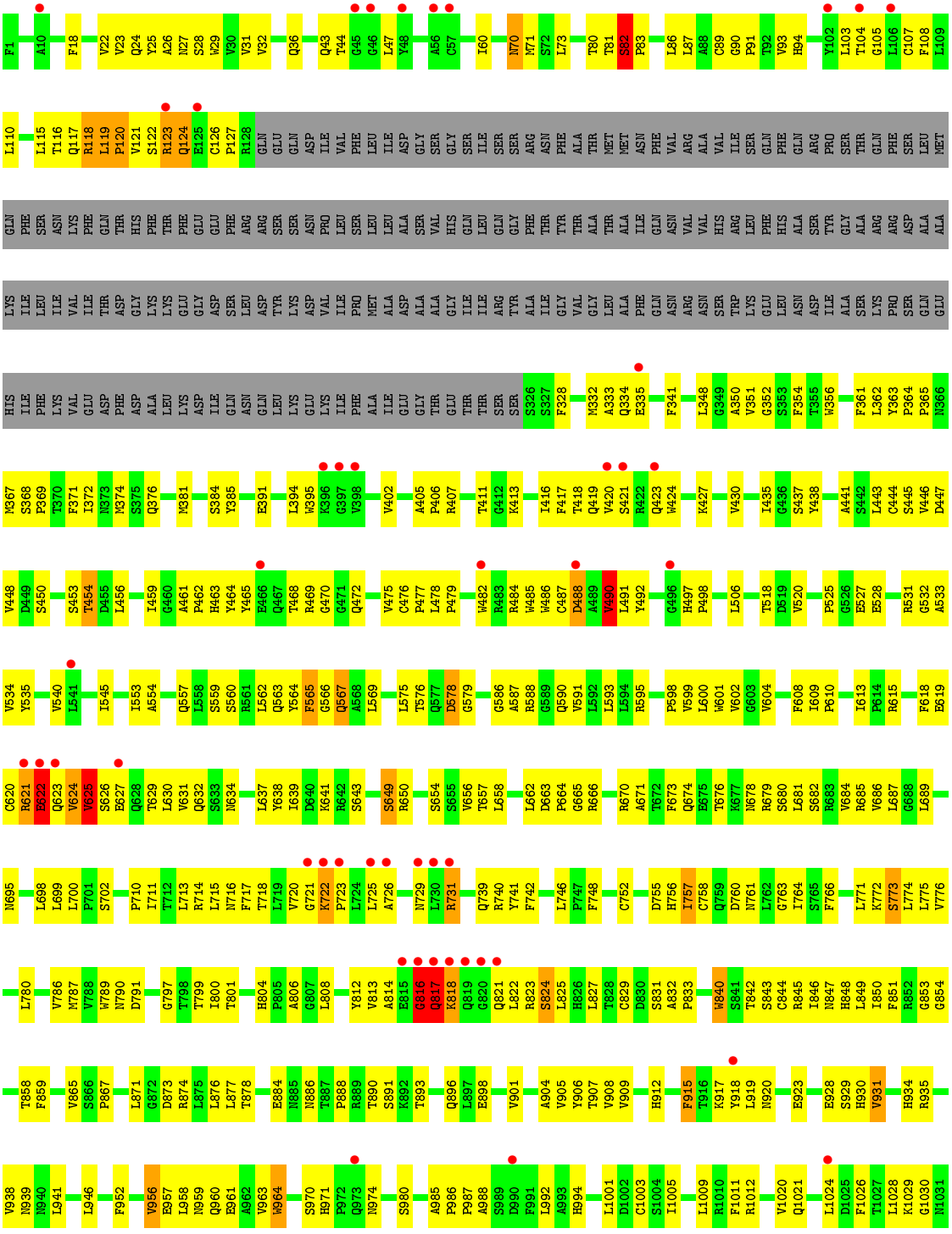
Chain A:

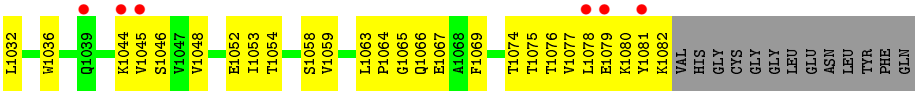




- Molecule 1: Integrin alpha-X

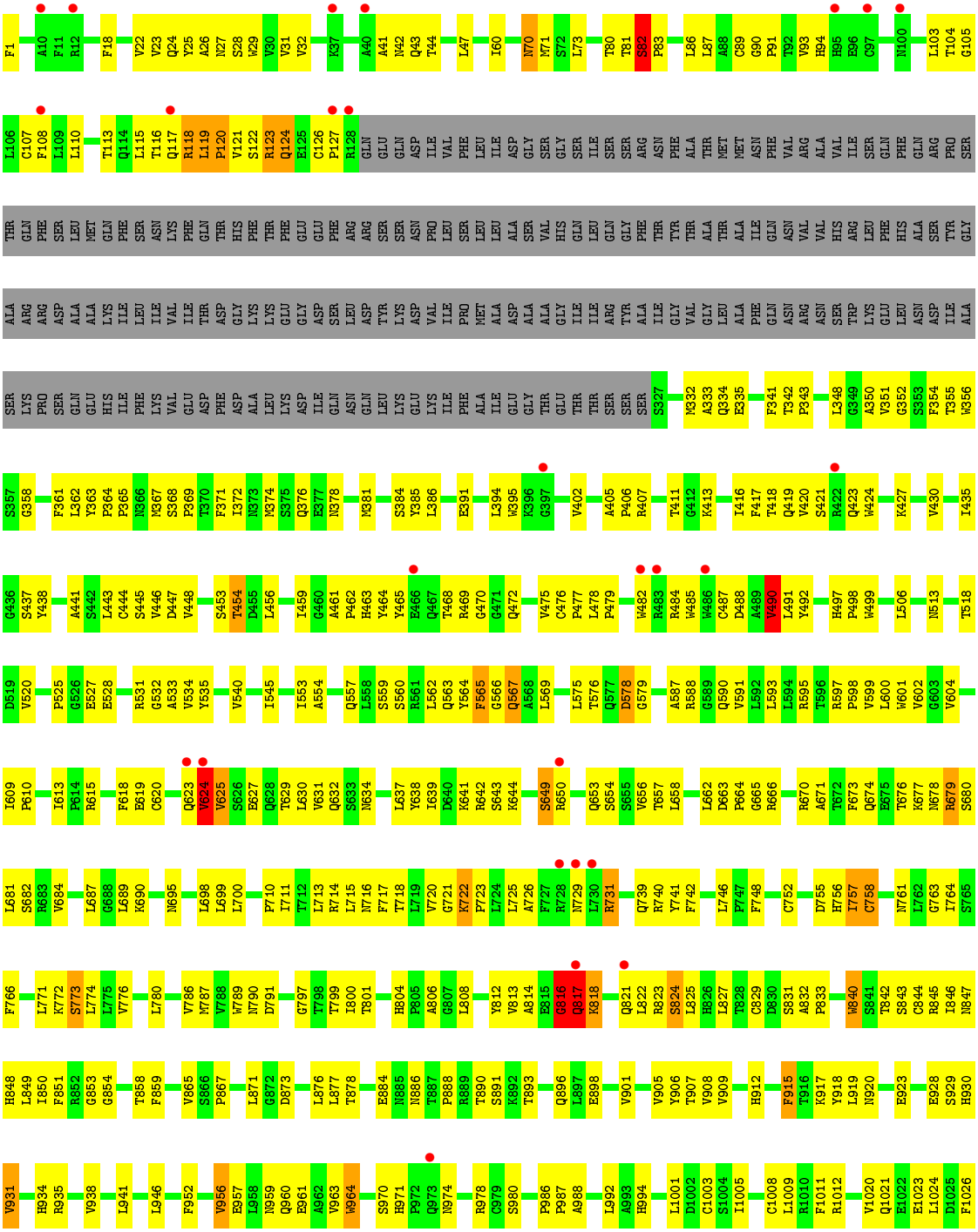
Chain C:

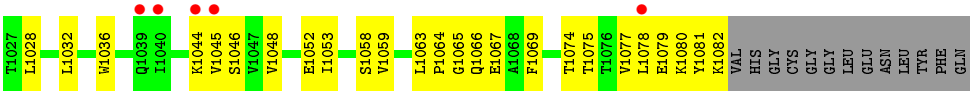




• Molecule 1: Integrin alpha-X

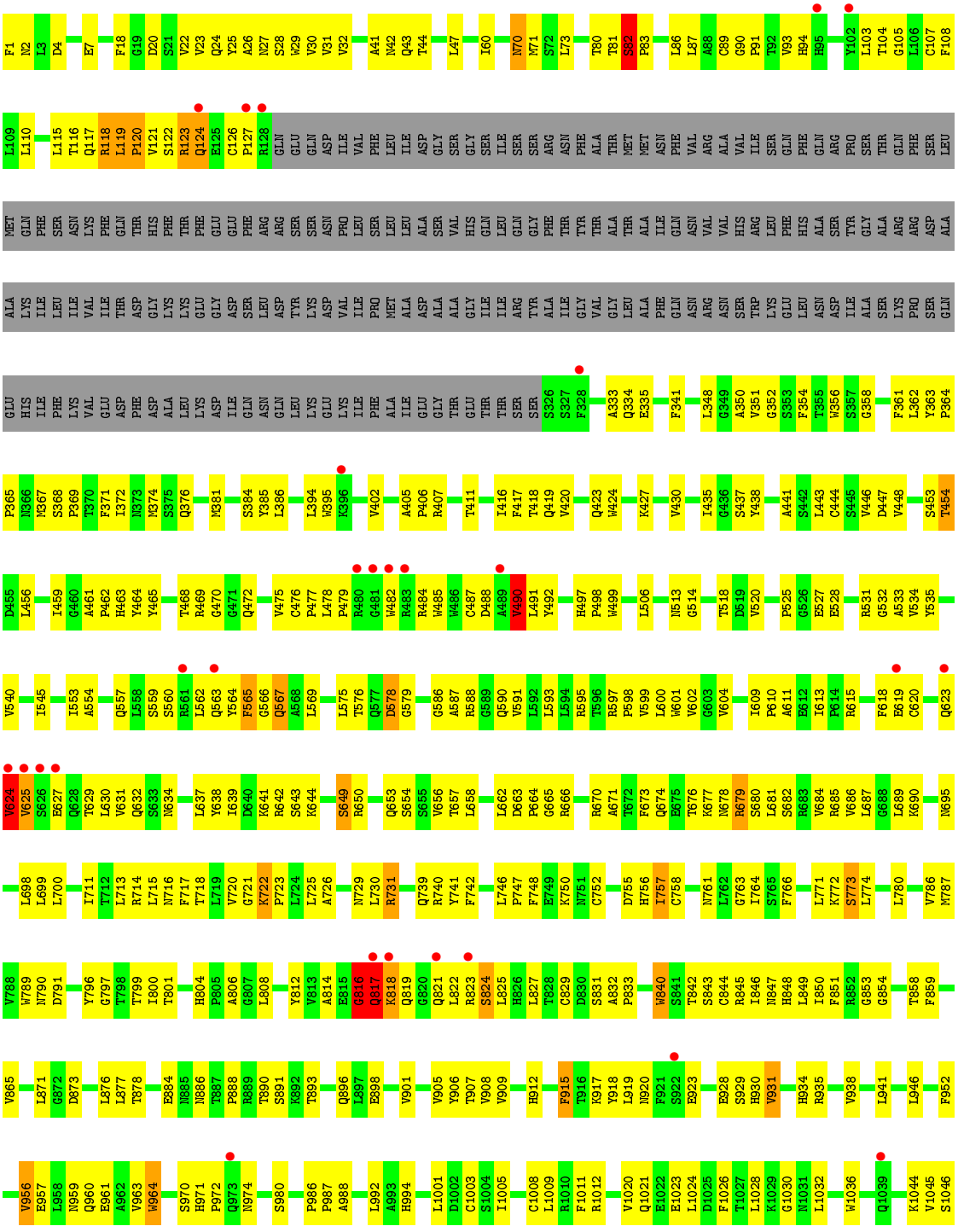
Chain E:

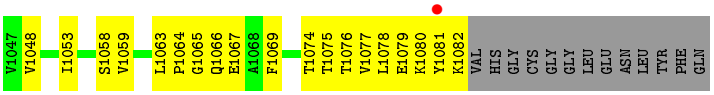




• Molecule 1: Integrin alpha-X

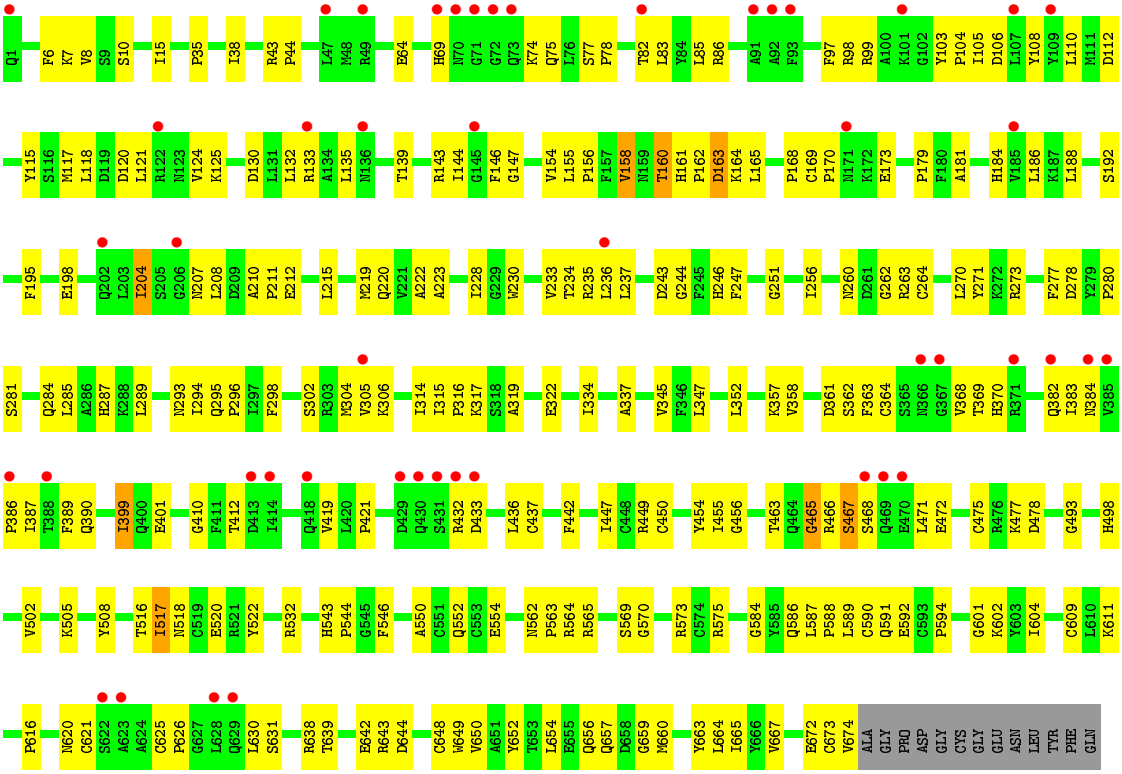
Chain G:





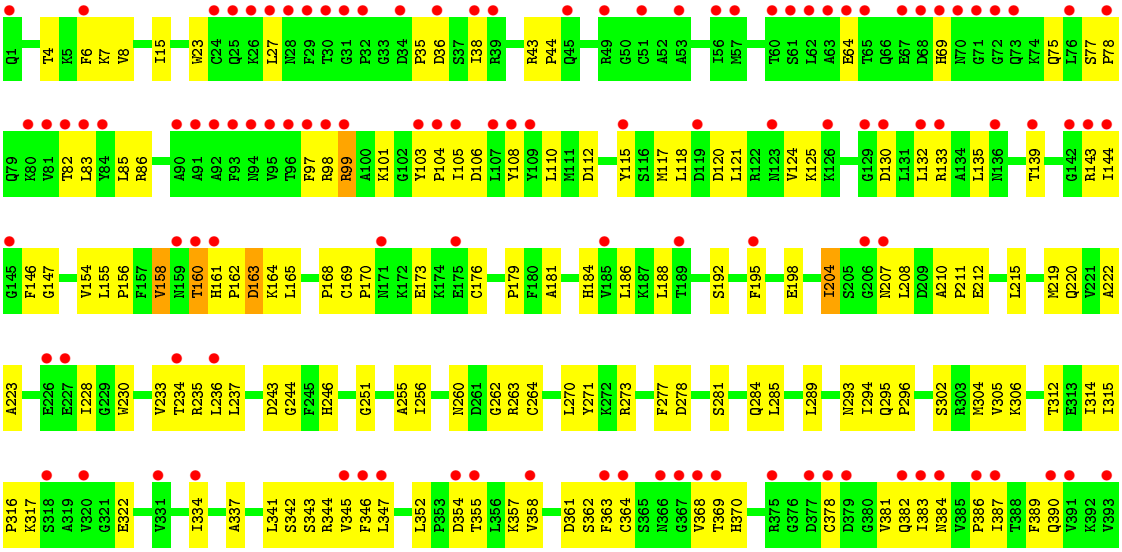
• Molecule 2: Integrin beta-2

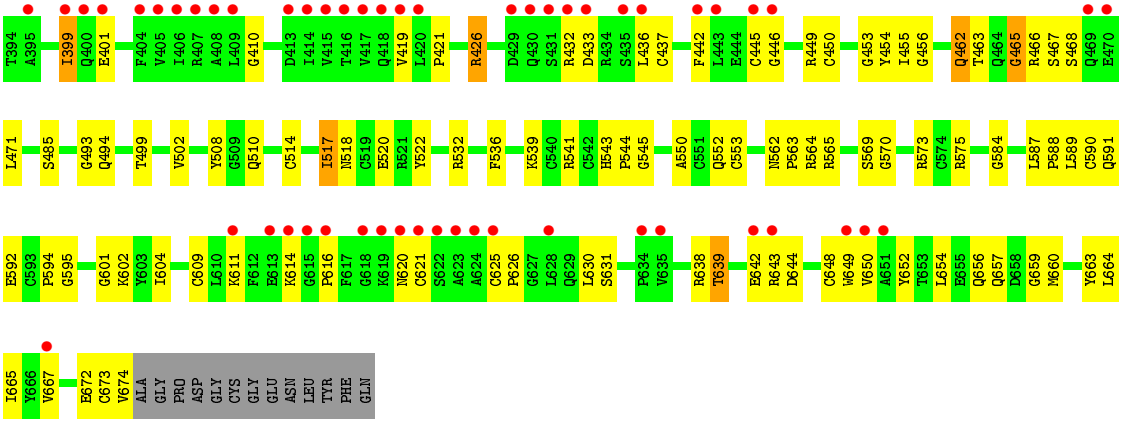
Chain B:



• Molecule 2: Integrin beta-2

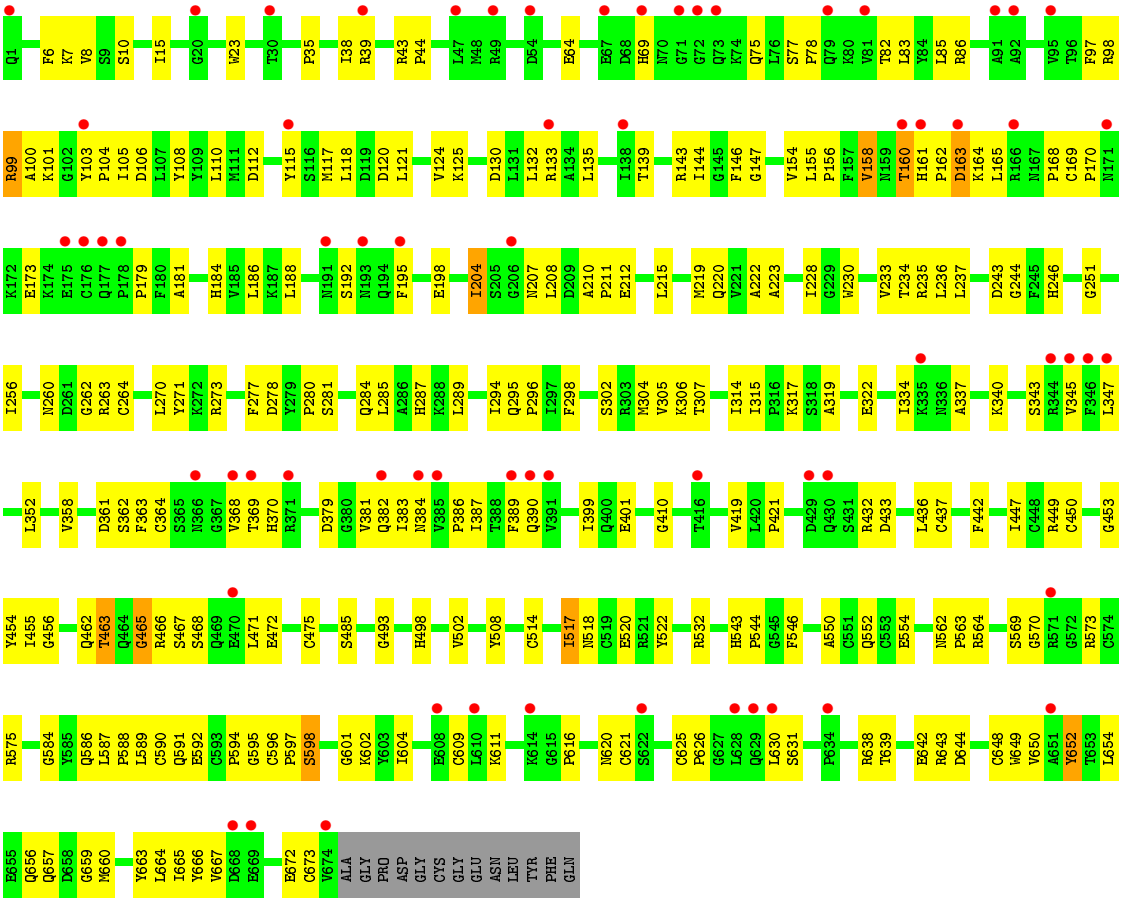
Chain D:





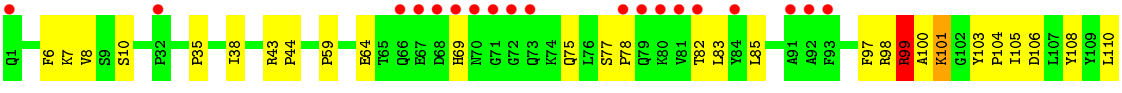
• Molecule 2: Integrin beta-2

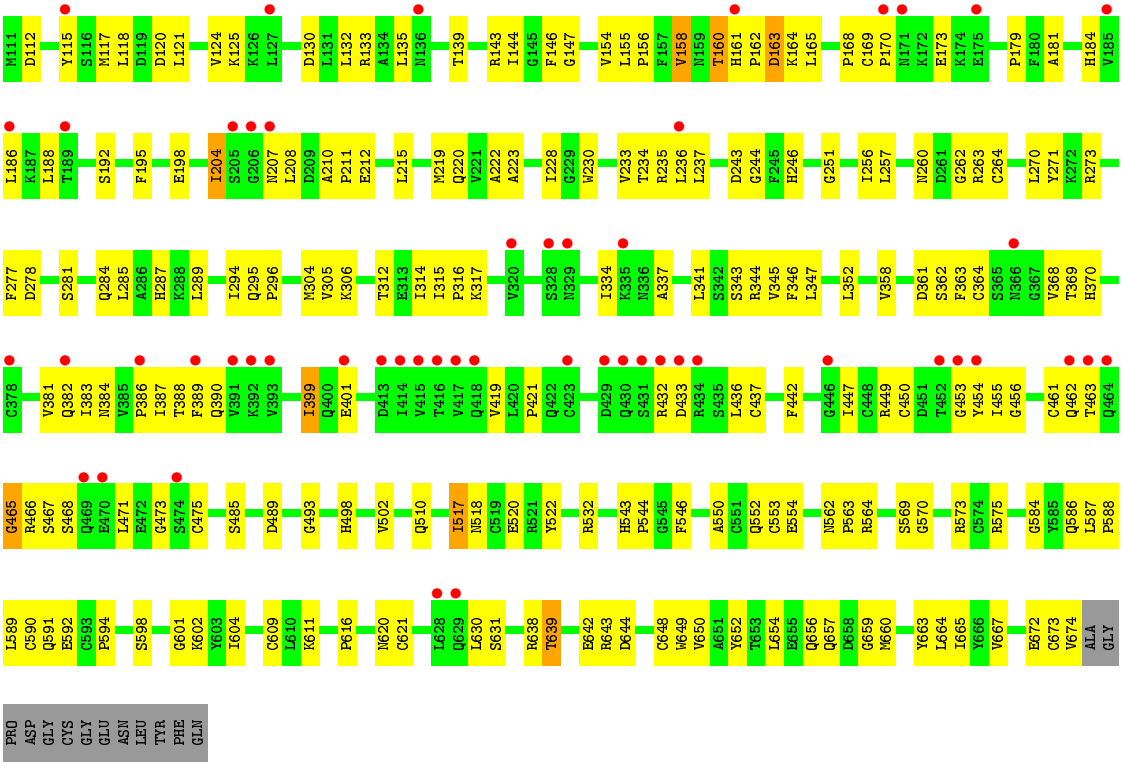
Chain F:



• Molecule 2: Integrin beta-2

Chain H:




M111 D112 Y115 S116 M117 L118 D119 D120 L121 V124 K125 K126 L127 D130 L131 L132 R133 A134 L135 N136 T139 R143 I144 G145 F146 G147 V154 L155 P156 F157 V158 N159 T160 H161 P162 D163 K164 L165 P168 C169 P170 N171 K172 E173 K174 E175 P179 F180 A181 H184 V185
L186 K187 L188 T189 S192 F195 E198 I204 S205 G206 N207 L208 D209 A210 P211 E212 L215 M219 Q220 V221 A222 A223 I228 G229 W230 V233 T234 R235 L236 L237 D243 G244 F245 H246 G251 I256 L257 N260 D261 G262 R263 C264 L270 Y271 K272 R273
F277 D278 S281 Q284 L285 A286 H287 K288 L289 I294 Q295 P296 M304 V305 K306 T312 E313 I314 I315 P316 K317 V320 S328 N329 I334 K335 N336 A337 L341 S342 S343 R344 V345 F346 L347 L352 V358 D361 S362 F363 C364 S365 N366 G367 V368 T369 H370
C378 V381 Q382 I383 N384 V385 P386 I387 T388 F389 Q390 V391 K392 V393 I399 Q400 E401 D413 I414 V415 T416 V417 Q418 V419 L420 P421 Q422 C423 D429 Q430 S431 R432 D433 R434 S435 L436 C437 F442 G446 I447 C448 R449 C450 D451 T452 G453 Y454 I455 G456 C461 Q462 T463 Q464
G465 R466 S467 S468 Q469 E470 L471 E472 G473 S474 C475 S485 D489 G493 H498 V502 Q510 I517 N518 C519 E520 R521 Y522 R532 H543 P544 G545 F546 A550 C551 Q552 C553 E554 N562 P563 R564 S569 G570 R573 C574 R575 G584 Y585 Q586 L587 P588
L589 C590 Q591 E592 C593 P594 S598 G601 K602 Y603 I604 C609 L610 K611 P616 N620 C621 L628 Q629 L630 S631 R638 T639 E642 R643 D644 C648 W649 V650 A651 Y652 T653 L654 E655 Q656 Q657 D658 G659 M660 Y663 L664 I665 Y666 V667 E672 C673 V674 ALA GLY
PRO ASP GLY CYS GLY GLU ASN LEU TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.09Å 163.56Å 536.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.50 48.61 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.61-3.50) 100.0 (48.61-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.297 , 0.335 0.280 , 0.311	Depositor DCC
R_{free} test set	1531 reflections (1.04%)	DCC
Wilson B-factor (Å^2)	80.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 177.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 147305 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	50187	wwPDB-VP
Average B, all atoms (Å^2)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MAN, CA, NAG

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	0.23	0/8579	0.44	1/11652 (0.0%)
1	C	0.24	0/6980	0.46	0/9494
1	E	0.23	0/6974	0.45	0/9486
1	G	0.24	0/6980	0.45	0/9494
2	B	0.22	0/5280	0.41	0/7129
2	D	0.24	0/5280	0.43	0/7129
2	F	0.23	0/5280	0.42	0/7129
2	H	0.23	0/5280	0.42	0/7129
All	All	0.23	0/50633	0.44	1/68642 (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	A	0	10
1	C	0	11
1	E	0	10
1	G	0	11
2	B	0	2
2	D	0	3
2	F	0	2
2	H	0	3
3	C	1	0
4	A	2	0
9	E	2	0
9	G	2	0
All	All	7	52

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	LEU	C-N-CD	-5.77	107.90	120.60

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3373	NAG	C1
4	A	3375	MAN	C1
3	C	3373	NAG	C1
9	E	3373	NAG	C1
9	E	3375	MAN	C1
9	G	3373	NAG	C1
9	G	3375	MAN	C1

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Peptide
1	A	119	LEU	Peptide
1	A	488	ASP	Peptide
1	A	490	VAL	Peptide
1	A	624	VAL	Peptide
1	A	625	VAL	Peptide
1	A	816	GLY	Peptide
1	A	82	SER	Peptide
1	A	821	GLN	Peptide
1	A	824	SER	Peptide
2	B	160	THR	Peptide
2	B	163	ASP	Peptide
1	C	118	ARG	Peptide
1	C	488	ASP	Peptide
1	C	490	VAL	Peptide
1	C	621	ARG	Peptide
1	C	622	GLU	Peptide
1	C	625	VAL	Peptide
1	C	816	GLY	Peptide
1	C	817	GLN	Peptide
1	C	82	SER	Peptide
1	C	821	GLN	Peptide
1	C	824	SER	Peptide
2	D	160	THR	Peptide
2	D	163	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	D	462	GLN	Peptide
1	E	118	ARG	Peptide
1	E	488	ASP	Peptide
1	E	490	VAL	Peptide
1	E	624	VAL	Peptide
1	E	625	VAL	Peptide
1	E	816	GLY	Peptide
1	E	817	GLN	Peptide
1	E	82	SER	Peptide
1	E	821	GLN	Peptide
1	E	824	SER	Peptide
2	F	160	THR	Peptide
2	F	163	ASP	Peptide
1	G	118	ARG	Peptide
1	G	488	ASP	Peptide
1	G	490	VAL	Peptide
1	G	624	VAL	Peptide
1	G	625	VAL	Peptide
1	G	816	GLY	Peptide
1	G	817	GLN	Peptide
1	G	819	GLN	Peptide
1	G	82	SER	Peptide
1	G	821	GLN	Peptide
1	G	824	SER	Peptide
2	H	160	THR	Peptide
2	H	163	ASP	Peptide
2	H	99	ARG	Peptide

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	8392	0	8227	495	0
1	C	6825	0	6685	457	0
1	E	6819	0	6680	428	0
1	G	6825	0	6685	438	0
2	B	5184	0	4975	218	0
2	D	5184	0	4975	255	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	5184	0	4975	228	0
2	H	5184	0	4975	216	0
3	A	56	0	50	0	0
3	C	84	0	75	4	0
3	E	56	0	50	1	0
3	G	56	0	50	1	0
4	A	61	0	52	10	0
5	A	11	0	10	4	0
6	A	28	0	25	0	0
6	B	14	0	13	0	0
6	C	28	0	25	1	0
6	D	14	0	13	0	0
6	E	28	0	25	0	0
6	F	14	0	13	0	0
6	G	28	0	24	1	0
6	H	14	0	13	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
7	E	3	0	0	0	0
7	F	1	0	0	0	0
7	G	3	0	0	0	0
7	H	1	0	0	0	0
8	A	1	0	0	0	0
9	E	39	0	34	6	0
9	G	39	0	34	7	0
10	A	3	0	0	0	0
All	All	50187	0	48683	2634	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 27.

All (2634) 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:A:985:ALA:CB	1:C:621:ARG:HB2	1.81	1.11
1:A:985:ALA:HB2	1:C:621:ARG:CB	1.90	1.01
1:A:985:ALA:HB2	1:C:621:ARG:CD	1.91	1.00
1:C:484:ARG:NH2	1:C:1021:GLN:HA	1.81	0.95
1:A:985:ALA:HB2	1:C:621:ARG:HB2	1.42	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:GLU:CB	1:C:621:ARG:HH22	1.81	0.93
1:E:923:GLU:HB2	1:E:1080:LYS:HB3	1.51	0.93
1:G:923:GLU:HB2	1:G:1080:LYS:HB3	1.51	0.92
1:A:484:ARG:HD2	2:B:586:GLN:HG3	1.52	0.91
1:C:923:GLU:HB2	1:C:1080:LYS:HB3	1.51	0.90
1:A:480:ARG:HG2	1:A:1021:GLN:HB3	1.54	0.89
1:A:923:GLU:HB2	1:A:1080:LYS:HB3	1.51	0.89
2:D:455:ILE:CG2	2:D:494:GLN:NE2	2.36	0.89
4:A:3377:MAN:H4	5:A:3378:MAN:C1	2.02	0.88
1:A:491:LEU:HD11	1:A:545:ILE:HG12	1.56	0.88
1:C:491:LEU:HD11	1:C:545:ILE:HG12	1.55	0.88
1:A:625:VAL:HG21	1:A:627:GLU:HG3	1.54	0.88
1:G:491:LEU:HD11	1:G:545:ILE:HG12	1.55	0.88
1:C:822:LEU:HG	1:C:823:ARG:H	1.37	0.87
2:D:570:GLY:HA2	2:D:659:GLY:HA2	1.57	0.87
1:E:491:LEU:HD11	1:E:545:ILE:HG12	1.56	0.86
1:C:650:ARG:HD3	1:C:729:ASN:HB3	1.58	0.85
1:G:119:LEU:N	1:G:120:PRO:HA	1.91	0.85
1:E:119:LEU:N	1:E:120:PRO:HA	1.91	0.85
1:C:119:LEU:N	1:C:120:PRO:HA	1.92	0.85
1:C:486:TRP:HH2	1:C:1021:GLN:HG2	1.42	0.85
1:E:650:ARG:HD3	1:E:729:ASN:HB3	1.59	0.84
1:E:822:LEU:HG	1:E:823:ARG:H	1.42	0.84
1:A:650:ARG:HD3	1:A:729:ASN:HB3	1.58	0.84
1:C:630:LEU:HD21	1:G:653:GLN:HB2	1.60	0.83
1:G:650:ARG:HD3	1:G:729:ASN:HB3	1.61	0.82
1:G:816:GLY:O	1:G:818:LYS:N	2.13	0.82
1:A:985:ALA:CB	1:C:621:ARG:CD	2.57	0.82
2:D:455:ILE:HG22	2:D:494:GLN:NE2	1.94	0.82
9:G:3374:NAG:O3	9:G:3375:MAN:H2	1.79	0.82
1:E:816:GLY:O	1:E:818:LYS:N	2.12	0.82
1:A:822:LEU:HG	1:A:823:ARG:H	1.43	0.82
9:E:3374:NAG:O3	9:E:3375:MAN:H2	1.80	0.82
1:A:985:ALA:CB	1:C:621:ARG:HD2	2.10	0.81
2:D:160:THR:O	2:D:165:LEU:HD22	1.80	0.81
2:F:160:THR:O	2:F:165:LEU:HD22	1.80	0.81
2:H:160:THR:O	2:H:165:LEU:HD22	1.80	0.81
1:C:908:VAL:HG11	2:D:595:GLY:HA3	1.62	0.81
1:E:789:TRP:CZ2	1:G:772:LYS:HA	2.16	0.81
2:B:160:THR:O	2:B:165:LEU:HD22	1.80	0.80
1:A:119:LEU:O	1:A:363:TYR:CE1	2.35	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:455:ILE:CG2	2:D:494:GLN:HE22	1.94	0.79
1:A:985:ALA:HB2	1:C:621:ARG:HD3	1.64	0.79
2:B:210:ALA:HB3	2:B:211:PRO:HD3	1.65	0.79
4:A:3374:NAG:O3	4:A:3375:MAN:H2	1.81	0.79
1:G:597:ARG:HB3	1:G:731:ARG:O	1.83	0.79
2:F:210:ALA:HB3	2:F:211:PRO:HD3	1.65	0.79
1:A:194:LEU:HD22	1:A:197:LEU:HD12	1.66	0.78
1:C:491:LEU:HD11	1:C:545:ILE:CG1	2.14	0.78
2:D:317:LYS:HA	2:D:344:ARG:HD2	1.66	0.77
1:G:491:LEU:HD11	1:G:545:ILE:CG1	2.14	0.77
1:C:484:ARG:NH1	1:C:939:ASN:HB2	1.99	0.77
1:A:480:ARG:CG	1:A:1021:GLN:HB3	2.14	0.77
1:E:491:LEU:HD11	1:E:545:ILE:CG1	2.14	0.77
2:H:210:ALA:HB3	2:H:211:PRO:HD3	1.65	0.77
1:A:118:ARG:HA	1:A:120:PRO:HA	1.67	0.77
2:D:210:ALA:HB3	2:D:211:PRO:HD3	1.65	0.77
1:A:491:LEU:HD11	1:A:545:ILE:CG1	2.14	0.76
1:G:597:ARG:HD2	1:G:731:ARG:O	1.86	0.76
1:C:486:TRP:CH2	1:C:1021:GLN:HG2	2.20	0.76
1:A:484:ARG:HD3	2:B:594:PRO:HG2	1.67	0.76
1:C:1032:LEU:HD21	1:C:1078:LEU:HD21	1.68	0.76
1:A:484:ARG:CD	2:B:594:PRO:HG2	2.15	0.76
1:A:957:GLU:HB3	1:C:621:ARG:HH22	1.51	0.76
1:A:1063:LEU:HD12	1:A:1064:PRO:N	2.01	0.76
1:A:1032:LEU:HD21	1:A:1078:LEU:HD21	1.68	0.76
1:E:1032:LEU:HD21	1:E:1078:LEU:HD21	1.68	0.76
1:A:119:LEU:N	1:A:120:PRO:HA	2.01	0.75
1:G:822:LEU:HG	1:G:823:ARG:H	1.51	0.75
1:A:623:GLN:O	1:A:624:VAL:HG22	1.86	0.75
1:G:597:ARG:HG3	1:G:731:ARG:HG2	1.68	0.75
1:E:1063:LEU:HD12	1:E:1064:PRO:N	2.02	0.75
1:G:1032:LEU:HD21	1:G:1078:LEU:HD21	1.68	0.75
1:A:957:GLU:CB	1:C:621:ARG:NH2	2.50	0.75
1:G:625:VAL:HG21	1:G:627:GLU:HG3	1.67	0.75
1:C:490:VAL:HG12	1:C:491:LEU:CA	2.17	0.75
1:E:625:VAL:HG21	1:E:627:GLU:HG3	1.68	0.75
1:E:490:VAL:HG12	1:E:491:LEU:N	2.02	0.75
1:A:490:VAL:HG12	1:A:491:LEU:CA	2.17	0.75
1:E:490:VAL:HG12	1:E:491:LEU:CA	2.17	0.75
1:C:848:HIS:HB2	2:D:485:SER:HB3	1.69	0.75
1:G:490:VAL:HG12	1:G:491:LEU:CA	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1063:LEU:HD12	1:C:1064:PRO:N	2.02	0.74
1:G:490:VAL:HG12	1:G:491:LEU:N	2.02	0.74
1:C:119:LEU:H	1:C:120:PRO:HA	1.53	0.74
1:A:816:GLY:O	1:A:818:LYS:N	2.20	0.74
1:G:1063:LEU:HD12	1:G:1064:PRO:N	2.02	0.74
2:F:455:ILE:HG13	2:F:463:THR:CG2	2.16	0.74
1:G:623:GLN:O	1:G:624:VAL:HG22	1.87	0.74
2:F:570:GLY:HA2	2:F:659:GLY:HA2	1.70	0.74
1:C:490:VAL:HG12	1:C:491:LEU:N	2.02	0.74
1:E:623:GLN:O	1:E:624:VAL:HG22	1.88	0.73
1:E:908:VAL:HG11	2:F:595:GLY:HA3	1.69	0.73
1:A:164:ARG:HB2	1:A:165:PRO:HA	1.70	0.73
1:E:731:ARG:HG3	1:E:731:ARG:O	1.88	0.73
2:B:317:LYS:HE3	2:B:410:GLY:HA3	1.70	0.73
1:G:721:GLY:C	1:G:723:PRO:HD3	2.09	0.73
1:A:395:TRP:CZ2	1:A:1021:GLN:OE1	2.42	0.73
1:E:721:GLY:C	1:E:723:PRO:HD3	2.09	0.73
1:G:119:LEU:O	1:G:363:TYR:CE1	2.41	0.73
1:G:731:ARG:O	1:G:731:ARG:HG3	1.89	0.73
1:A:490:VAL:HG12	1:A:491:LEU:N	2.02	0.73
1:E:119:LEU:O	1:E:363:TYR:CE1	2.41	0.73
1:C:119:LEU:O	1:C:363:TYR:CE1	2.41	0.72
1:C:721:GLY:C	1:C:723:PRO:HD3	2.09	0.72
1:C:731:ARG:O	1:C:731:ARG:HG3	1.89	0.72
1:A:721:GLY:C	1:A:723:PRO:HD3	2.09	0.72
4:A:3377:MAN:C4	5:A:3378:MAN:C1	2.67	0.72
1:E:121:VAL:O	1:E:121:VAL:HG12	1.90	0.72
1:A:731:ARG:O	1:A:731:ARG:HG3	1.88	0.72
2:F:455:ILE:CG1	2:F:463:THR:HG23	2.19	0.72
2:H:100:ALA:O	2:H:101:LYS:HB2	1.90	0.72
1:E:119:LEU:H	1:E:120:PRO:HA	1.52	0.72
1:A:957:GLU:HB2	1:C:621:ARG:HH22	1.53	0.71
2:F:455:ILE:HG12	2:F:463:THR:HG23	1.72	0.71
1:C:121:VAL:HG12	1:C:121:VAL:O	1.90	0.71
1:G:119:LEU:H	1:G:120:PRO:HA	1.52	0.71
1:A:194:LEU:CD2	1:A:197:LEU:HD12	2.20	0.71
1:A:121:VAL:O	1:A:121:VAL:HG12	1.90	0.71
1:G:121:VAL:HG12	1:G:121:VAL:O	1.90	0.71
1:A:772:LYS:HA	1:C:789:TRP:CZ2	2.26	0.71
1:G:928:GLU:HG3	1:G:929:SER:N	2.07	0.70
1:G:598:PRO:CG	1:G:650:ARG:NH1	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:928:GLU:HG3	1:E:929:SER:N	2.06	0.70
2:H:532:ARG:HD3	2:H:554:GLU:CD	2.12	0.70
1:E:772:LYS:HA	1:G:789:TRP:CZ2	2.25	0.70
1:C:928:GLU:HG3	1:C:929:SER:N	2.07	0.70
2:H:99:ARG:HG2	2:H:100:ALA:H	1.55	0.70
1:A:953:TRP:CH2	1:C:755:ASP:HA	2.26	0.70
1:A:662:LEU:HD11	1:A:673:PHE:CZ	2.27	0.70
1:C:662:LEU:HD11	1:C:673:PHE:CZ	2.27	0.69
1:A:928:GLU:HG3	1:A:929:SER:N	2.07	0.69
1:G:662:LEU:HD11	1:G:673:PHE:CZ	2.27	0.69
1:E:662:LEU:HD11	1:E:673:PHE:CZ	2.27	0.69
1:C:630:LEU:HD21	1:G:653:GLN:CB	2.22	0.69
2:F:472:GLU:HA	2:F:475:CYS:CB	2.23	0.69
2:F:472:GLU:HA	2:F:475:CYS:HB3	1.74	0.69
2:D:316:PRO:HB3	2:D:346:PHE:CZ	2.27	0.68
2:F:15:ILE:HG23	2:F:86:ARG:CZ	2.23	0.68
1:A:1064:PRO:HG3	1:A:1067:GLU:HG3	1.76	0.68
1:E:871:LEU:HD11	1:E:901:VAL:HG21	1.76	0.68
1:A:957:GLU:HB3	1:C:621:ARG:NH2	2.07	0.68
1:G:1064:PRO:HG3	1:G:1067:GLU:CD	2.14	0.68
1:G:1064:PRO:HG3	1:G:1067:GLU:HG3	1.75	0.68
1:G:657:THR:HG23	1:G:720:VAL:HB	1.76	0.68
1:E:756:HIS:O	1:E:757:ILE:HG22	1.94	0.68
1:A:871:LEU:HD11	1:A:901:VAL:HG21	1.76	0.68
1:A:395:TRP:HZ2	1:A:1021:GLN:OE1	1.76	0.67
1:A:1064:PRO:HG3	1:A:1067:GLU:CD	2.14	0.67
1:C:1064:PRO:HG3	1:C:1067:GLU:CD	2.14	0.67
1:A:953:TRP:CZ2	1:C:755:ASP:HA	2.29	0.67
1:C:871:LEU:HD11	1:C:901:VAL:HG21	1.76	0.67
1:E:657:THR:HG23	1:E:720:VAL:HB	1.76	0.67
1:A:957:GLU:HB2	1:C:621:ARG:NH2	2.09	0.67
1:E:1064:PRO:HG3	1:E:1067:GLU:HG3	1.76	0.67
1:C:657:THR:HG23	1:C:720:VAL:HB	1.76	0.67
1:A:657:THR:HG23	1:A:720:VAL:HB	1.76	0.67
1:E:812:TYR:CD2	1:E:814:ALA:HB2	2.30	0.67
1:A:919:LEU:HB2	1:A:1079:GLU:HB3	1.76	0.67
1:G:362:LEU:HD23	1:G:363:TYR:N	2.10	0.67
1:G:673:PHE:CG	1:G:681:LEU:HD23	2.30	0.67
1:A:789:TRP:CZ2	1:C:772:LYS:HA	2.29	0.67
1:G:871:LEU:HD11	1:G:901:VAL:HG21	1.76	0.67
1:C:816:GLY:O	1:C:818:LYS:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:LEU:HD23	1:E:363:TYR:N	2.10	0.67
1:C:919:LEU:HB2	1:C:1079:GLU:HB3	1.76	0.67
1:G:919:LEU:HB2	1:G:1079:GLU:HB3	1.76	0.67
1:C:1064:PRO:HG3	1:C:1067:GLU:HG3	1.76	0.67
1:A:650:ARG:HD3	1:A:729:ASN:CB	2.25	0.66
1:E:812:TYR:CE2	1:E:814:ALA:HB2	2.29	0.66
1:A:362:LEU:HD23	1:A:363:TYR:N	2.10	0.66
1:G:650:ARG:HD3	1:G:729:ASN:CB	2.26	0.66
1:E:1064:PRO:HG3	1:E:1067:GLU:CD	2.15	0.66
1:E:673:PHE:CG	1:E:681:LEU:HD23	2.31	0.66
1:E:919:LEU:HB2	1:E:1079:GLU:HB3	1.76	0.66
1:C:650:ARG:HD3	1:C:729:ASN:CB	2.24	0.66
1:E:650:ARG:HD3	1:E:729:ASN:CB	2.26	0.66
2:F:10:SER:HB3	2:F:449:ARG:CZ	2.25	0.66
1:G:118:ARG:HA	1:G:120:PRO:HA	1.78	0.66
1:A:673:PHE:CG	1:A:681:LEU:HD23	2.31	0.66
1:C:673:PHE:CG	1:C:681:LEU:HD23	2.30	0.66
1:A:311:LYS:HG3	1:A:312:GLU:N	2.10	0.66
1:C:118:ARG:HA	1:C:120:PRO:HA	1.78	0.66
1:C:362:LEU:HD23	1:C:363:TYR:N	2.10	0.66
2:H:455:ILE:HG12	2:H:463:THR:HG23	1.76	0.66
1:G:756:HIS:O	1:G:757:ILE:HG22	1.96	0.66
2:D:471:LEU:O	2:D:493:GLY:HA2	1.96	0.65
1:E:118:ARG:HA	1:E:120:PRO:HA	1.78	0.65
1:A:273:PHE:HB2	1:A:296:LYS:HD2	1.78	0.65
2:F:532:ARG:HD3	2:F:554:GLU:CD	2.16	0.65
1:A:812:TYR:CE2	1:A:814:ALA:HB2	2.32	0.65
2:B:532:ARG:HD3	2:B:554:GLU:CD	2.16	0.65
2:B:75:GLN:O	2:B:97:PHE:HA	1.97	0.65
1:C:665:GLY:HA2	2:D:499:THR:O	1.95	0.65
1:C:1063:LEU:HD12	1:C:1064:PRO:CA	2.27	0.65
2:F:587:LEU:HB3	2:F:588:PRO:HA	1.79	0.65
1:A:985:ALA:HB2	1:C:621:ARG:CG	2.27	0.65
1:C:622:GLU:HG3	1:C:623:GLN:HB3	1.79	0.65
1:G:812:TYR:CE2	1:G:814:ALA:HB2	2.31	0.65
1:A:562:LEU:HD11	1:A:590:GLN:HG2	1.79	0.65
1:E:1063:LEU:HD12	1:E:1064:PRO:CA	2.27	0.64
2:F:75:GLN:O	2:F:97:PHE:HA	1.97	0.64
2:H:75:GLN:O	2:H:97:PHE:HA	1.97	0.64
1:A:1063:LEU:HD12	1:A:1064:PRO:CA	2.27	0.64
1:G:1063:LEU:HD12	1:G:1064:PRO:CA	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:562:LEU:HD11	1:G:590:GLN:HG2	1.80	0.64
1:C:622:GLU:C	1:C:623:GLN:HG2	2.18	0.64
2:D:456:GLY:HA2	2:D:494:GLN:OE1	1.97	0.64
1:A:531:ARG:HA	1:A:563:GLN:O	1.98	0.64
1:C:531:ARG:HA	1:C:563:GLN:O	1.98	0.64
1:A:985:ALA:HB1	1:C:621:ARG:HD2	1.79	0.64
1:E:531:ARG:HA	1:E:563:GLN:O	1.98	0.64
1:C:94:HIS:NE2	2:D:155:LEU:HD21	2.12	0.64
2:H:587:LEU:HB3	2:H:588:PRO:HA	1.79	0.64
2:F:161:HIS:HB3	2:F:162:PRO:HA	1.80	0.64
2:B:161:HIS:HB3	2:B:162:PRO:HA	1.80	0.64
2:B:15:ILE:HG23	2:B:86:ARG:CZ	2.28	0.64
2:D:75:GLN:O	2:D:97:PHE:HA	1.97	0.64
2:D:6:PHE:CE1	2:D:541:ARG:HD2	2.33	0.64
1:C:623:GLN:O	1:C:624:VAL:HG22	1.98	0.64
1:E:609:ILE:HB	1:E:610:PRO:HD3	1.80	0.64
2:B:587:LEU:HB3	2:B:588:PRO:HA	1.79	0.64
1:A:174:PHE:CE1	1:A:209:THR:HA	2.32	0.64
1:C:812:TYR:CE2	1:C:814:ALA:HB2	2.32	0.64
1:A:469:ARG:NH2	2:B:287:HIS:HB2	2.13	0.63
2:H:471:LEU:O	2:H:493:GLY:HA2	1.98	0.63
1:E:562:LEU:HD11	1:E:590:GLN:HG2	1.79	0.63
2:D:161:HIS:HB3	2:D:162:PRO:HA	1.80	0.63
2:F:289:LEU:HD21	2:F:296:PRO:CD	2.29	0.63
2:D:587:LEU:HB3	2:D:588:PRO:HA	1.79	0.63
1:A:609:ILE:HB	1:A:610:PRO:HD3	1.80	0.63
1:G:531:ARG:HA	1:G:563:GLN:O	1.98	0.63
2:H:161:HIS:HB3	2:H:162:PRO:HA	1.80	0.63
2:B:289:LEU:HD21	2:B:296:PRO:CD	2.29	0.63
1:A:625:VAL:CG2	1:A:627:GLU:HG3	2.29	0.63
1:A:756:HIS:O	1:A:757:ILE:HG22	1.98	0.63
2:B:468:SER:HB2	2:B:471:LEU:HG	1.81	0.63
1:A:44:THR:HG22	1:A:71:MET:HG2	1.81	0.63
2:F:455:ILE:CG1	2:F:463:THR:CG2	2.76	0.63
1:A:250:TYR:HA	1:A:253:VAL:HG22	1.81	0.63
2:D:468:SER:HB2	2:D:471:LEU:HG	1.81	0.62
1:G:18:PHE:CE2	1:G:32:VAL:HG21	2.34	0.62
1:E:44:THR:HG22	1:E:71:MET:HG2	1.81	0.62
1:G:812:TYR:CD2	1:G:814:ALA:HB2	2.34	0.62
1:G:119:LEU:N	1:G:120:PRO:CA	2.62	0.62
1:G:609:ILE:HB	1:G:610:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:PHE:CE2	1:C:32:VAL:HG21	2.34	0.62
1:A:985:ALA:HB3	1:C:621:ARG:HB2	1.80	0.62
1:C:609:ILE:HB	1:C:610:PRO:HD3	1.80	0.62
2:H:289:LEU:HD21	2:H:296:PRO:CD	2.29	0.62
1:A:953:TRP:CE2	1:C:755:ASP:HB2	2.35	0.62
1:C:756:HIS:O	1:C:757:ILE:HG22	1.99	0.62
1:E:822:LEU:CG	1:E:823:ARG:H	2.10	0.62
1:C:1064:PRO:HG3	1:C:1067:GLU:CG	2.30	0.62
2:D:289:LEU:HD21	2:D:296:PRO:CD	2.29	0.62
1:A:406:PRO:HB3	1:A:438:TYR:CE2	2.35	0.62
1:A:18:PHE:CE2	1:A:32:VAL:HG21	2.34	0.62
1:E:18:PHE:CE2	1:E:32:VAL:HG21	2.34	0.62
1:G:406:PRO:HB3	1:G:438:TYR:CE2	2.35	0.62
2:B:115:TYR:HA	2:B:204:ILE:HD13	1.82	0.62
1:E:406:PRO:HB3	1:E:438:TYR:CE2	2.35	0.62
1:A:1064:PRO:HG3	1:A:1067:GLU:CG	2.30	0.62
2:H:468:SER:HB2	2:H:471:LEU:HG	1.82	0.62
2:D:115:TYR:HA	2:D:204:ILE:HD13	1.82	0.62
2:D:355:THR:HA	2:D:544:PRO:CB	2.29	0.62
1:C:44:THR:HG22	1:C:71:MET:HG2	1.81	0.61
1:G:94:HIS:NE2	2:H:155:LEU:HD21	2.15	0.61
2:F:468:SER:HB2	2:F:471:LEU:HG	1.81	0.61
1:C:406:PRO:HB3	1:C:438:TYR:CE2	2.35	0.61
1:C:562:LEU:HD11	1:C:590:GLN:HG2	1.79	0.61
2:D:562:ASN:HB2	2:D:563:PRO:HD2	1.82	0.61
4:A:3377:MAN:O3	5:A:3378:MAN:C1	2.48	0.61
1:G:44:THR:HG22	1:G:71:MET:HG2	1.81	0.61
9:G:3374:NAG:C3	9:G:3375:MAN:H2	2.30	0.61
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.36	0.61
2:F:115:TYR:HA	2:F:204:ILE:HD13	1.82	0.61
2:D:155:LEU:HB2	2:D:156:PRO:HA	1.83	0.61
1:A:1052:GLU:OE1	1:C:756:HIS:HA	2.00	0.61
1:A:822:LEU:CG	1:A:823:ARG:H	2.10	0.61
1:A:103:LEU:HD11	2:B:155:LEU:HD13	1.82	0.61
1:E:1064:PRO:HG3	1:E:1067:GLU:CG	2.30	0.61
2:D:220:GLN:HA	2:D:264:CYS:HB3	1.83	0.61
2:D:155:LEU:H	2:D:160:THR:HG21	1.66	0.61
1:G:1064:PRO:HG3	1:G:1067:GLU:CG	2.30	0.61
2:F:508:TYR:CZ	2:F:514:CYS:HB3	2.36	0.61
2:H:115:TYR:HA	2:H:204:ILE:HD13	1.82	0.61
1:E:119:LEU:N	1:E:120:PRO:CA	2.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:GLN:HA	2:B:264:CYS:HB3	1.83	0.61
2:F:155:LEU:H	2:F:160:THR:HG21	1.66	0.61
1:A:812:TYR:CD2	1:A:814:ALA:HB2	2.35	0.61
2:D:98:ARG:HG2	2:D:98:ARG:O	2.01	0.61
2:H:220:GLN:HA	2:H:264:CYS:HB3	1.83	0.61
2:H:155:LEU:H	2:H:160:THR:HG21	1.66	0.60
2:B:155:LEU:H	2:B:160:THR:HG21	1.66	0.60
2:H:155:LEU:HB2	2:H:156:PRO:HA	1.83	0.60
2:B:155:LEU:HB2	2:B:156:PRO:HA	1.83	0.60
2:B:562:ASN:HB2	2:B:563:PRO:HD2	1.82	0.60
1:E:599:VAL:HG23	1:E:599:VAL:O	2.01	0.60
1:G:822:LEU:CG	1:G:823:ARG:H	2.15	0.60
2:F:220:GLN:HA	2:F:264:CYS:HB3	1.83	0.60
1:A:630:LEU:HD21	1:E:653:GLN:HB2	1.83	0.60
1:A:825:LEU:HD12	1:A:859:PHE:HB3	1.83	0.60
2:F:98:ARG:O	2:F:98:ARG:HG2	2.02	0.60
2:H:442:PHE:CZ	2:H:449:ARG:HB2	2.36	0.60
2:H:562:ASN:HB2	2:H:563:PRO:HD2	1.83	0.60
1:E:721:GLY:C	1:E:723:PRO:CD	2.70	0.60
2:B:357:LYS:HG3	2:B:544:PRO:HB2	1.83	0.60
2:B:562:ASN:HB3	2:B:589:LEU:HD13	1.84	0.60
2:F:522:TYR:CD1	2:F:552:GLN:HA	2.36	0.60
2:F:562:ASN:HB2	2:F:563:PRO:HD2	1.82	0.60
1:A:181:HIS:CE1	1:A:200:VAL:HG13	2.37	0.60
1:G:825:LEU:HD12	1:G:859:PHE:HB3	1.84	0.60
2:D:27:LEU:CD2	2:D:446:GLY:HA2	2.32	0.60
1:G:721:GLY:C	1:G:723:PRO:CD	2.70	0.60
1:C:721:GLY:C	1:C:723:PRO:CD	2.70	0.60
1:A:721:GLY:C	1:A:723:PRO:CD	2.70	0.60
1:A:715:LEU:HD12	1:A:715:LEU:O	2.02	0.60
1:A:472:GLN:NE2	1:A:492:TYR:HB2	2.17	0.60
2:D:442:PHE:CZ	2:D:449:ARG:HB2	2.36	0.60
1:C:1029:LYS:CE	1:E:113:THR:HG22	2.32	0.60
2:B:442:PHE:CZ	2:B:449:ARG:HB2	2.36	0.60
2:B:364:CYS:HB2	2:B:368:VAL:HB	1.84	0.60
1:A:1020:VAL:HG12	1:A:1021:GLN:HG3	1.84	0.60
2:D:293:ASN:HA	2:D:410:GLY:HA2	1.82	0.60
1:G:715:LEU:O	1:G:715:LEU:HD12	2.02	0.60
2:B:98:ARG:HG2	2:B:98:ARG:O	2.01	0.59
1:E:825:LEU:HD12	1:E:859:PHE:HB3	1.83	0.59
2:D:357:LYS:HE3	2:D:545:GLY:HA2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:986:PRO:CB	1:E:987:PRO:HD2	2.32	0.59
1:C:822:LEU:CG	1:C:823:ARG:H	2.07	0.59
2:F:155:LEU:HB2	2:F:156:PRO:HA	1.83	0.59
1:C:1064:PRO:CG	1:C:1067:GLU:HG3	2.32	0.59
2:F:562:ASN:HB3	2:F:589:LEU:HD13	1.84	0.59
1:G:797:GLY:CA	1:G:884:GLU:HB2	2.32	0.59
1:A:797:GLY:CA	1:A:884:GLU:HB2	2.32	0.59
1:C:986:PRO:CB	1:C:987:PRO:HD2	2.32	0.59
1:C:472:GLN:NE2	1:C:492:TYR:HB2	2.17	0.59
9:E:3374:NAG:C3	9:E:3375:MAN:H2	2.32	0.59
1:A:1064:PRO:CG	1:A:1067:GLU:HG3	2.32	0.59
2:F:364:CYS:HB2	2:F:368:VAL:HB	1.84	0.59
1:G:513:ASN:HA	1:G:599:VAL:HG22	1.83	0.59
1:G:599:VAL:O	1:G:599:VAL:HG23	2.01	0.59
2:D:343:SER:HA	2:D:381:VAL:O	2.03	0.59
1:E:103:LEU:HD11	2:F:155:LEU:HD13	1.82	0.59
2:F:162:PRO:O	2:F:164:LYS:N	2.35	0.59
2:D:162:PRO:O	2:D:164:LYS:N	2.35	0.59
2:F:442:PHE:CZ	2:F:449:ARG:HB2	2.37	0.59
2:B:162:PRO:O	2:B:164:LYS:N	2.35	0.59
1:C:812:TYR:CD2	1:C:814:ALA:HB2	2.36	0.59
1:C:825:LEU:HD12	1:C:859:PHE:HB3	1.85	0.59
1:C:484:ARG:CZ	1:C:1021:GLN:HA	2.31	0.59
1:G:918:TYR:HA	2:H:643:ARG:NH2	2.18	0.59
2:D:27:LEU:HD21	2:D:446:GLY:O	2.03	0.59
1:G:986:PRO:CB	1:G:987:PRO:HD2	2.32	0.59
1:A:986:PRO:CB	1:A:987:PRO:HD2	2.32	0.59
2:H:616:PRO:HB2	2:H:620:ASN:HA	1.84	0.59
2:H:98:ARG:O	2:H:98:ARG:HG2	2.02	0.59
2:D:616:PRO:HB2	2:D:620:ASN:HA	1.85	0.59
2:H:364:CYS:HB2	2:H:368:VAL:HB	1.84	0.59
1:G:1064:PRO:CG	1:G:1067:GLU:HG3	2.31	0.59
2:D:364:CYS:HB2	2:D:368:VAL:HB	1.84	0.59
1:E:1020:VAL:HG12	1:E:1021:GLN:HG3	1.85	0.59
1:G:1020:VAL:HG12	1:G:1021:GLN:HG3	1.85	0.59
1:E:472:GLN:NE2	1:E:492:TYR:HB2	2.17	0.59
1:A:674:GLN:HB2	1:A:699:LEU:HD11	1.85	0.59
1:C:797:GLY:CA	1:C:884:GLU:HB2	2.33	0.59
1:A:604:VAL:HG11	1:A:742:PHE:CD2	2.38	0.59
1:G:472:GLN:NE2	1:G:492:TYR:HB2	2.17	0.58
1:G:722:LYS:N	1:G:723:PRO:CD	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:PHE:HE1	2:D:536:PHE:CB	2.15	0.58
1:A:599:VAL:HG23	1:A:599:VAL:O	2.01	0.58
1:C:374:MET:HG3	1:C:381:MET:SD	2.43	0.58
2:H:103:TYR:HB3	2:H:104:PRO:HD2	1.85	0.58
2:B:616:PRO:HB2	2:B:620:ASN:HA	1.84	0.58
1:E:797:GLY:CA	1:E:884:GLU:HB2	2.32	0.58
1:E:674:GLN:HB2	1:E:699:LEU:HD11	1.84	0.58
2:H:162:PRO:O	2:H:164:LYS:N	2.36	0.58
2:D:562:ASN:HB3	2:D:589:LEU:HD13	1.84	0.58
1:G:604:VAL:HG11	1:G:742:PHE:CD2	2.38	0.58
2:F:135:LEU:HD11	2:F:139:THR:HB	1.85	0.58
1:C:599:VAL:O	1:C:599:VAL:HG23	2.01	0.58
1:A:119:LEU:N	1:A:120:PRO:CA	2.66	0.58
1:E:722:LYS:N	1:E:723:PRO:CD	2.66	0.58
1:C:722:LYS:N	1:C:723:PRO:CD	2.66	0.58
2:B:471:LEU:O	2:B:493:GLY:HA2	2.03	0.58
1:A:430:VAL:HG21	1:A:487:CYS:SG	2.43	0.58
2:H:399:ILE:HG13	2:H:421:PRO:HG3	1.85	0.58
2:F:616:PRO:HB2	2:F:620:ASN:HA	1.85	0.58
1:E:604:VAL:HG11	1:E:742:PHE:CD2	2.39	0.58
1:E:994:HIS:CG	1:E:1005:ILE:HD11	2.38	0.58
1:C:43:GLN:HA	1:C:70:ASN:H	1.68	0.58
1:E:1064:PRO:CG	1:E:1067:GLU:HG3	2.32	0.58
1:G:674:GLN:HB2	1:G:699:LEU:HD11	1.84	0.58
2:H:562:ASN:HB3	2:H:589:LEU:HD13	1.84	0.58
2:B:399:ILE:HG13	2:B:421:PRO:HG3	1.85	0.58
1:C:430:VAL:HG21	1:C:487:CYS:SG	2.43	0.58
2:D:468:SER:HB2	2:D:471:LEU:CG	2.34	0.58
2:B:468:SER:HB2	2:B:471:LEU:CG	2.34	0.58
1:E:715:LEU:HD12	1:E:715:LEU:O	2.03	0.58
1:C:715:LEU:HD12	1:C:715:LEU:O	2.03	0.58
1:C:674:GLN:HB2	1:C:699:LEU:HD11	1.84	0.58
1:C:604:VAL:HG11	1:C:742:PHE:CD2	2.38	0.58
2:F:103:TYR:HB3	2:F:104:PRO:HD2	1.86	0.58
1:G:833:PRO:HA	1:G:840:TRP:CB	2.34	0.58
2:H:468:SER:HB2	2:H:471:LEU:CG	2.34	0.58
2:F:399:ILE:HG13	2:F:421:PRO:HG3	1.85	0.58
1:A:374:MET:HG3	1:A:381:MET:SD	2.44	0.58
2:B:74:LYS:HD3	2:B:103:TYR:OH	2.04	0.58
2:B:135:LEU:HD11	2:B:139:THR:HB	1.85	0.58
1:A:833:PRO:HA	1:A:840:TRP:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1020:VAL:HG12	1:C:1021:GLN:HG3	1.86	0.58
1:A:953:TRP:CE2	1:C:755:ASP:CB	2.87	0.58
1:A:1044:LYS:HA	1:A:1079:GLU:HB2	1.86	0.58
1:A:253:VAL:HG23	1:A:254:ILE:N	2.18	0.58
1:G:994:HIS:CG	1:G:1005:ILE:HD11	2.38	0.58
1:A:490:VAL:HG12	1:A:491:LEU:HB3	1.86	0.58
1:A:43:GLN:HA	1:A:70:ASN:H	1.68	0.58
2:D:316:PRO:HB3	2:D:346:PHE:CE1	2.38	0.58
1:C:964:TRP:CB	1:C:1032:LEU:HA	2.33	0.58
1:C:1044:LYS:HA	1:C:1079:GLU:HB2	1.86	0.58
2:H:295:GLN:HG3	2:H:317:LYS:HE2	1.86	0.58
1:E:833:PRO:HA	1:E:840:TRP:CB	2.34	0.58
1:C:615:ARG:HA	1:C:618:PHE:HB2	1.86	0.58
1:C:833:PRO:HA	1:C:840:TRP:CB	2.34	0.58
2:F:155:LEU:H	2:F:160:THR:CG2	2.17	0.57
1:A:119:LEU:H	1:A:120:PRO:HA	1.68	0.57
1:A:964:TRP:CB	1:A:1032:LEU:HA	2.34	0.57
1:G:964:TRP:CB	1:G:1032:LEU:HA	2.33	0.57
1:A:722:LYS:N	1:A:723:PRO:CD	2.67	0.57
1:E:430:VAL:HG21	1:E:487:CYS:SG	2.44	0.57
1:E:374:MET:HG3	1:E:381:MET:SD	2.44	0.57
2:D:155:LEU:H	2:D:160:THR:CG2	2.18	0.57
1:G:739:GLN:HB2	1:G:742:PHE:CZ	2.39	0.57
2:B:103:TYR:HB3	2:B:104:PRO:HD2	1.84	0.57
1:E:418:THR:HG21	1:E:482:TRP:CZ2	2.39	0.57
2:D:399:ILE:HG13	2:D:421:PRO:HG3	1.85	0.57
2:F:295:GLN:HG3	2:F:317:LYS:HE2	1.86	0.57
2:B:289:LEU:HD21	2:B:296:PRO:HD3	1.86	0.57
2:D:312:THR:CG2	2:D:344:ARG:HH22	2.16	0.57
2:D:36:ASP:H	2:D:510:GLN:NE2	2.02	0.57
2:H:135:LEU:HD11	2:H:139:THR:HB	1.85	0.57
2:D:23:TRP:HE1	2:D:445:CYS:HB3	1.70	0.57
1:A:994:HIS:CG	1:A:1005:ILE:HD11	2.39	0.57
1:C:418:THR:HG21	1:C:482:TRP:CZ2	2.39	0.57
1:G:490:VAL:HG12	1:G:491:LEU:HB3	1.86	0.57
2:H:289:LEU:HD21	2:H:296:PRO:HD3	1.86	0.57
1:E:490:VAL:HG12	1:E:491:LEU:HB3	1.86	0.57
2:B:295:GLN:HG3	2:B:317:LYS:HE2	1.86	0.57
1:E:657:THR:HG22	1:E:684:VAL:HG22	1.87	0.57
1:A:657:THR:HG22	1:A:684:VAL:HG22	1.87	0.57
1:G:430:VAL:HG21	1:G:487:CYS:SG	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1044:LYS:HA	1:G:1079:GLU:HB2	1.86	0.57
1:C:739:GLN:HB2	1:C:742:PHE:CZ	2.39	0.57
1:A:444:CYS:HB2	1:A:506:LEU:CD1	2.35	0.57
1:A:93:VAL:O	1:A:103:LEU:HA	2.05	0.57
2:F:453:GLY:O	2:F:462:GLN:HG3	2.05	0.57
1:G:598:PRO:HG3	1:G:650:ARG:NH1	2.19	0.57
2:H:155:LEU:H	2:H:160:THR:CG2	2.17	0.57
2:B:155:LEU:H	2:B:160:THR:CG2	2.18	0.57
2:D:295:GLN:HG3	2:D:317:LYS:HE2	1.86	0.57
2:D:6:PHE:CE1	2:D:536:PHE:HB3	2.40	0.57
2:D:6:PHE:CE1	2:D:536:PHE:CB	2.88	0.57
2:D:587:LEU:N	2:D:587:LEU:HD12	2.20	0.57
1:A:739:GLN:HB2	1:A:742:PHE:CZ	2.39	0.57
1:G:374:MET:HG3	1:G:381:MET:SD	2.44	0.57
2:B:347:LEU:HD22	2:B:389:PHE:CD1	2.39	0.57
2:H:455:ILE:CG1	2:H:463:THR:HG23	2.34	0.57
2:H:455:ILE:HG13	2:H:463:THR:CG2	2.34	0.57
2:F:468:SER:HB2	2:F:471:LEU:CG	2.34	0.57
1:E:513:ASN:HA	1:E:599:VAL:CG2	2.35	0.57
2:H:312:THR:CG2	2:H:344:ARG:HH22	2.18	0.57
1:E:444:CYS:HB2	1:E:506:LEU:CD1	2.35	0.57
1:C:490:VAL:HG12	1:C:491:LEU:HB3	1.86	0.57
1:C:119:LEU:N	1:C:120:PRO:CA	2.63	0.57
1:A:418:THR:HG21	1:A:482:TRP:CZ2	2.39	0.57
1:E:739:GLN:HB2	1:E:742:PHE:CZ	2.39	0.57
1:E:848:HIS:HB2	2:F:485:SER:HB3	1.86	0.57
2:B:454:TYR:O	2:B:455:ILE:HD13	2.05	0.57
1:E:964:TRP:CB	1:E:1032:LEU:HA	2.34	0.57
1:E:117:GLN:HB3	1:E:121:VAL:HG21	1.86	0.57
1:E:1044:LYS:HA	1:E:1079:GLU:HB2	1.86	0.57
1:A:756:HIS:HA	1:C:1052:GLU:OE1	2.04	0.57
1:G:597:ARG:NH2	1:G:730:LEU:HD12	2.18	0.56
1:A:1054:THR:HG21	1:C:757:ILE:HG21	1.87	0.56
1:G:418:THR:HG21	1:G:482:TRP:CZ2	2.39	0.56
1:G:117:GLN:HB3	1:G:121:VAL:HG21	1.86	0.56
2:F:10:SER:HA	2:F:447:ILE:HD11	1.87	0.56
2:F:587:LEU:HD12	2:F:587:LEU:N	2.20	0.56
1:E:468:THR:HG23	1:E:498:PRO:HG3	1.87	0.56
1:C:93:VAL:O	1:C:103:LEU:HA	2.05	0.56
1:G:94:HIS:CD2	2:H:155:LEU:HD21	2.40	0.56
1:E:43:GLN:HA	1:E:70:ASN:H	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:VAL:O	1:E:103:LEU:HA	2.05	0.56
1:E:789:TRP:NE1	1:G:772:LYS:HB3	2.20	0.56
1:C:117:GLN:HB3	1:C:121:VAL:HG21	1.86	0.56
1:C:755:ASP:O	1:C:756:HIS:HB3	2.05	0.56
2:D:355:THR:HG22	2:D:544:PRO:HG2	1.86	0.56
2:B:10:SER:HB3	2:B:449:ARG:CZ	2.35	0.56
1:G:1:PHE:CE2	1:G:599:VAL:HG11	2.40	0.56
1:C:620:CYS:HB3	1:C:702:SER:C	2.26	0.56
2:D:103:TYR:HB3	2:D:104:PRO:HD2	1.86	0.56
1:C:468:THR:HG23	1:C:498:PRO:HG3	1.87	0.56
1:G:444:CYS:HB2	1:G:506:LEU:CD1	2.35	0.56
1:C:444:CYS:HB2	1:C:506:LEU:CD1	2.35	0.56
1:E:364:PRO:CB	1:E:365:PRO:HD2	2.36	0.56
1:A:117:GLN:HB3	1:A:121:VAL:HG21	1.86	0.56
2:H:587:LEU:HD12	2:H:587:LEU:N	2.20	0.56
2:B:587:LEU:N	2:B:587:LEU:HD12	2.20	0.56
1:G:747:PRO:HB3	1:G:884:GLU:HG2	1.87	0.56
2:D:135:LEU:HD11	2:D:139:THR:HB	1.85	0.56
1:C:491:LEU:HD12	1:C:491:LEU:C	2.26	0.56
1:E:598:PRO:HB3	1:E:650:ARG:NH1	2.20	0.56
2:F:23:TRP:CH2	2:F:447:ILE:HD13	2.41	0.56
1:C:394:LEU:HD23	1:C:395:TRP:N	2.20	0.56
2:F:289:LEU:HD21	2:F:296:PRO:HD3	1.86	0.56
1:E:394:LEU:HD23	1:E:395:TRP:N	2.21	0.56
1:G:468:THR:HG23	1:G:498:PRO:HG3	1.87	0.56
1:E:963:VAL:HA	1:E:1036:TRP:CD1	2.41	0.56
1:G:394:LEU:HD23	1:G:395:TRP:N	2.21	0.56
2:D:456:GLY:CA	2:D:494:GLN:OE1	2.53	0.56
1:G:598:PRO:HB3	1:G:650:ARG:NH1	2.21	0.56
2:H:295:GLN:CG	2:H:317:LYS:HE2	2.36	0.56
1:E:741:TYR:CD2	2:F:502:VAL:HG22	2.41	0.56
1:G:364:PRO:CB	1:G:365:PRO:HD2	2.36	0.56
1:C:908:VAL:O	1:C:938:VAL:HG23	2.06	0.56
1:A:156:ARG:HB3	1:A:197:LEU:HD13	1.87	0.56
2:F:10:SER:HB3	2:F:449:ARG:NE	2.21	0.56
1:E:32:VAL:HG11	1:E:591:VAL:HG11	1.88	0.56
1:G:833:PRO:HA	1:G:840:TRP:HB2	1.88	0.56
1:G:908:VAL:O	1:G:938:VAL:HG23	2.06	0.56
1:C:941:LEU:HD12	1:C:941:LEU:N	2.21	0.56
1:A:394:LEU:HD23	1:A:395:TRP:N	2.21	0.56
1:E:491:LEU:HD12	1:E:491:LEU:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:GLN:HA	1:G:70:ASN:H	1.68	0.56
2:F:454:TYR:O	2:F:455:ILE:HD13	2.06	0.56
1:E:919:LEU:O	2:F:643:ARG:NH1	2.35	0.56
2:D:289:LEU:HD21	2:D:296:PRO:HD3	1.86	0.56
1:A:963:VAL:HA	1:A:1036:TRP:CD1	2.41	0.56
1:G:491:LEU:HD12	1:G:491:LEU:C	2.26	0.56
1:G:93:VAL:O	1:G:103:LEU:HA	2.06	0.56
1:G:657:THR:HG22	1:G:684:VAL:HG22	1.87	0.56
1:A:32:VAL:HG11	1:A:591:VAL:HG11	1.88	0.56
2:B:146:PHE:HB2	2:B:195:PHE:CZ	2.41	0.56
1:C:332:MET:SD	2:D:208:LEU:HD13	2.45	0.56
1:C:994:HIS:CG	1:C:1005:ILE:HD11	2.41	0.56
1:G:578:ASP:OD2	1:G:595:ARG:HD2	2.06	0.56
1:G:597:ARG:HG3	1:G:731:ARG:CG	2.36	0.55
1:G:333:ALA:HB1	1:G:350:ALA:HB1	1.89	0.55
1:C:578:ASP:OD2	1:C:595:ARG:HD2	2.06	0.55
1:E:575:LEU:HD12	1:E:576:THR:N	2.22	0.55
1:G:941:LEU:HD12	1:G:941:LEU:N	2.21	0.55
1:E:363:TYR:CD1	1:E:369:PRO:HB3	2.41	0.55
1:E:824:SER:H	1:E:825:LEU:HG	1.72	0.55
2:F:260:ASN:HA	2:F:277:PHE:CE2	2.42	0.55
2:H:146:PHE:HB2	2:H:195:PHE:CZ	2.41	0.55
1:C:364:PRO:CB	1:C:365:PRO:HD2	2.36	0.55
2:H:10:SER:HB3	2:H:449:ARG:CZ	2.36	0.55
1:E:416:ILE:HD11	1:E:485:TRP:CZ2	2.42	0.55
1:E:578:ASP:OD2	1:E:595:ARG:HD2	2.06	0.55
1:C:479:PRO:HD2	1:C:485:TRP:CD1	2.42	0.55
1:C:32:VAL:HG11	1:C:591:VAL:HG11	1.88	0.55
1:G:963:VAL:HA	1:G:1036:TRP:CD1	2.41	0.55
1:E:446:VAL:HG21	1:E:520:VAL:CG1	2.37	0.55
1:A:169:PHE:HB2	1:A:187:PHE:CE1	2.41	0.55
1:E:941:LEU:N	1:E:941:LEU:HD12	2.21	0.55
1:E:908:VAL:O	1:E:938:VAL:HG23	2.05	0.55
1:G:32:VAL:HG11	1:G:591:VAL:HG11	1.88	0.55
1:C:1029:LYS:HE2	1:E:113:THR:HG22	1.88	0.55
1:E:786:VAL:HG11	1:E:859:PHE:CZ	2.42	0.55
1:G:513:ASN:HB2	1:G:599:VAL:HG21	1.87	0.55
1:C:786:VAL:HG11	1:C:859:PHE:CZ	2.42	0.55
2:F:295:GLN:CG	2:F:317:LYS:HE2	2.36	0.55
2:D:4:THR:HG21	2:D:539:LYS:NZ	2.21	0.55
1:A:363:TYR:CD1	1:A:369:PRO:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:786:VAL:HG11	1:G:859:PHE:CZ	2.42	0.55
1:A:513:ASN:HA	1:A:599:VAL:HG21	1.89	0.55
2:F:146:PHE:HB2	2:F:195:PHE:CZ	2.41	0.55
1:A:908:VAL:O	1:A:938:VAL:HG23	2.06	0.55
2:H:260:ASN:HA	2:H:277:PHE:CE2	2.42	0.55
1:C:416:ILE:HD11	1:C:485:TRP:CZ2	2.42	0.55
1:G:513:ASN:HA	1:G:599:VAL:CG2	2.36	0.55
1:A:416:ILE:HD11	1:A:485:TRP:CZ2	2.42	0.55
1:E:333:ALA:HB1	1:E:350:ALA:HB1	1.88	0.55
1:A:615:ARG:HA	1:A:618:PHE:HB2	1.88	0.55
1:C:963:VAL:HA	1:C:1036:TRP:CD1	2.41	0.55
1:A:468:THR:HG23	1:A:498:PRO:HG3	1.87	0.55
1:G:575:LEU:HD12	1:G:576:THR:N	2.21	0.55
1:A:575:LEU:HD12	1:A:576:THR:N	2.22	0.55
2:D:347:LEU:HD22	2:D:389:PHE:CD1	2.42	0.55
1:A:491:LEU:HD12	1:A:491:LEU:C	2.26	0.55
2:B:295:GLN:CG	2:B:317:LYS:HE2	2.36	0.55
1:C:657:THR:HG22	1:C:684:VAL:HG22	1.87	0.55
2:D:355:THR:HA	2:D:544:PRO:HB3	1.89	0.55
1:A:786:VAL:HG11	1:A:859:PHE:CZ	2.42	0.55
1:A:618:PHE:CE2	1:A:619:GLU:HG3	2.42	0.55
1:C:446:VAL:HG21	1:C:520:VAL:CG1	2.37	0.55
2:D:260:ASN:HA	2:D:277:PHE:CE2	2.42	0.55
2:D:295:GLN:CG	2:D:317:LYS:HE2	2.36	0.55
1:E:833:PRO:HA	1:E:840:TRP:HB2	1.89	0.55
1:E:479:PRO:HD2	1:E:485:TRP:CD1	2.42	0.55
1:A:941:LEU:HD12	1:A:941:LEU:N	2.21	0.55
1:A:81:THR:O	1:A:82:SER:C	2.45	0.55
1:G:363:TYR:CD1	1:G:369:PRO:HB3	2.41	0.55
1:C:363:TYR:CD1	1:C:369:PRO:HB3	2.41	0.55
1:G:70:ASN:HB3	1:G:94:HIS:ND1	2.22	0.55
1:A:364:PRO:CB	1:A:365:PRO:HD2	2.36	0.55
2:F:347:LEU:HD22	2:F:389:PHE:CD1	2.42	0.55
1:A:917:LYS:HE3	1:A:1077:VAL:CG2	2.37	0.55
2:B:260:ASN:HA	2:B:277:PHE:CE2	2.42	0.55
1:C:70:ASN:HB3	1:C:94:HIS:ND1	2.22	0.54
1:E:681:LEU:HD12	1:E:681:LEU:C	2.28	0.54
2:B:161:HIS:HB3	2:B:162:PRO:CA	2.37	0.54
1:A:479:PRO:HD2	1:A:485:TRP:CD1	2.42	0.54
2:D:146:PHE:HB2	2:D:195:PHE:CZ	2.41	0.54
1:E:615:ARG:HA	1:E:618:PHE:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ASN:HB3	1:E:94:HIS:ND1	2.22	0.54
2:D:161:HIS:HB3	2:D:162:PRO:CA	2.37	0.54
2:F:115:TYR:CD1	2:F:170:PRO:HD2	2.43	0.54
1:C:619:GLU:O	1:C:620:CYS:SG	2.65	0.54
1:E:459:ILE:HD12	1:E:487:CYS:SG	2.47	0.54
1:C:333:ALA:HB1	1:C:350:ALA:HB1	1.88	0.54
2:F:161:HIS:HB3	2:F:162:PRO:CA	2.37	0.54
1:G:528:GLU:HB2	1:G:531:ARG:HB2	1.90	0.54
2:H:161:HIS:HB3	2:H:162:PRO:CA	2.37	0.54
1:A:459:ILE:HD12	1:A:487:CYS:SG	2.48	0.54
1:C:741:TYR:CD2	2:D:502:VAL:HG13	2.42	0.54
1:A:70:ASN:HB3	1:A:94:HIS:ND1	2.22	0.54
2:B:115:TYR:CD1	2:B:170:PRO:HD2	2.43	0.54
1:G:416:ILE:HD11	1:G:485:TRP:CZ2	2.42	0.54
1:G:615:ARG:HA	1:G:618:PHE:HB2	1.89	0.54
2:D:426:ARG:HB3	2:D:426:ARG:CZ	2.37	0.54
1:E:624:VAL:HG23	1:E:625:VAL:H	1.73	0.54
1:C:81:THR:O	1:C:82:SER:C	2.45	0.54
2:H:520:GLU:HB3	2:H:550:ALA:HB2	1.90	0.54
1:G:917:LYS:HE3	1:G:1077:VAL:CG2	2.38	0.54
1:C:917:LYS:HE3	1:C:1077:VAL:CG2	2.37	0.54
2:B:654:LEU:HD13	2:B:665:ILE:HG13	1.90	0.54
2:H:110:LEU:HD11	2:H:237:LEU:HD23	1.90	0.54
1:A:681:LEU:C	1:A:681:LEU:HD12	2.28	0.54
1:C:681:LEU:C	1:C:681:LEU:HD12	2.28	0.54
1:A:986:PRO:CB	1:A:987:PRO:CD	2.86	0.54
1:A:578:ASP:OD2	1:A:595:ARG:HD2	2.07	0.54
1:C:459:ILE:HD12	1:C:487:CYS:SG	2.47	0.54
2:B:592:GLU:O	2:B:594:PRO:HD3	2.08	0.54
1:G:2:ASN:HB2	1:G:597:ARG:O	2.08	0.54
2:H:454:TYR:O	2:H:455:ILE:HD13	2.08	0.54
1:G:459:ILE:HD12	1:G:487:CYS:SG	2.48	0.54
1:G:479:PRO:HD2	1:G:485:TRP:CD1	2.42	0.54
1:E:917:LYS:HE3	1:E:1077:VAL:CG2	2.38	0.54
1:C:575:LEU:HD12	1:C:576:THR:N	2.22	0.54
1:C:650:ARG:CD	1:C:729:ASN:CB	2.86	0.54
1:A:833:PRO:HA	1:A:840:TRP:HB2	1.88	0.54
2:F:520:GLU:HB3	2:F:550:ALA:HB2	1.89	0.54
1:E:491:LEU:HD11	1:E:545:ILE:CD1	2.38	0.54
2:H:455:ILE:CG1	2:H:463:THR:CG2	2.86	0.54
1:E:905:VAL:HG11	1:E:946:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:HIS:HB2	1:A:808:LEU:HD11	1.90	0.54
1:A:333:ALA:HB1	1:A:350:ALA:HB1	1.89	0.54
2:H:347:LEU:HD22	2:H:389:PHE:CD1	2.43	0.54
2:D:520:GLU:HB3	2:D:550:ALA:HB2	1.89	0.54
1:G:816:GLY:O	1:G:818:LYS:CA	2.56	0.54
2:H:115:TYR:CD1	2:H:170:PRO:HD2	2.43	0.54
2:H:562:ASN:HB2	2:H:563:PRO:CD	2.38	0.54
1:C:833:PRO:HA	1:C:840:TRP:HB2	1.89	0.54
1:G:446:VAL:HG21	1:G:520:VAL:CG1	2.37	0.54
2:H:654:LEU:HD13	2:H:665:ILE:HG13	1.90	0.54
4:A:3373:NAG:H3	4:A:3374:NAG:N2	2.22	0.53
1:G:624:VAL:HG23	1:G:625:VAL:H	1.73	0.53
1:G:681:LEU:HD12	1:G:681:LEU:C	2.29	0.53
2:D:115:TYR:CD1	2:D:170:PRO:HD2	2.42	0.53
2:B:562:ASN:HB2	2:B:563:PRO:CD	2.38	0.53
1:C:25:TYR:CE1	1:C:86:LEU:HB2	2.44	0.53
1:A:905:VAL:HG11	1:A:946:LEU:HD21	1.90	0.53
1:E:81:THR:O	1:E:82:SER:C	2.45	0.53
1:A:741:TYR:CD2	2:B:502:VAL:HG22	2.43	0.53
1:E:908:VAL:HG13	1:E:1069:PHE:HB3	1.90	0.53
1:A:513:ASN:HA	1:A:599:VAL:CG2	2.38	0.53
1:G:602:VAL:HG23	1:G:638:TYR:O	2.09	0.53
1:G:80:THR:HB	1:G:341:PHE:CG	2.43	0.53
1:G:81:THR:O	1:G:82:SER:C	2.46	0.53
2:D:454:TYR:CE2	2:D:462:GLN:HG3	2.43	0.53
2:B:110:LEU:HD11	2:B:237:LEU:HD23	1.90	0.53
1:C:908:VAL:HG13	1:C:1069:PHE:HB3	1.90	0.53
1:A:528:GLU:HB2	1:A:531:ARG:HB2	1.90	0.53
1:A:908:VAL:HG13	1:A:1069:PHE:HB3	1.90	0.53
1:A:905:VAL:HG21	1:A:946:LEU:HD22	1.91	0.53
1:E:81:THR:O	1:E:82:SER:O	2.26	0.53
2:H:453:GLY:O	2:H:462:GLN:HG3	2.07	0.53
1:A:484:ARG:HD2	2:B:594:PRO:HG2	1.87	0.53
1:G:597:ARG:CG	1:G:731:ARG:HG2	2.37	0.53
2:D:211:PRO:HB2	2:D:246:HIS:CE1	2.44	0.53
2:D:6:PHE:HE1	2:D:536:PHE:HB2	1.73	0.53
2:D:35:PRO:CB	2:D:510:GLN:HE22	2.21	0.53
1:E:804:HIS:HB2	1:E:808:LEU:HD11	1.90	0.53
1:G:804:HIS:HB2	1:G:808:LEU:HD11	1.90	0.53
1:A:446:VAL:HG21	1:A:520:VAL:CG1	2.37	0.53
1:G:725:LEU:HG	1:G:726:ALA:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:GLU:HB3	2:B:550:ALA:HB2	1.89	0.53
1:A:602:VAL:HG23	1:A:638:TYR:O	2.09	0.53
1:C:725:LEU:HG	1:C:726:ALA:N	2.23	0.53
1:G:905:VAL:HG21	1:G:946:LEU:HD22	1.91	0.53
9:E:3373:NAG:H3	9:E:3374:NAG:N2	2.23	0.53
1:E:618:PHE:CE2	1:E:619:GLU:HG3	2.44	0.53
1:C:780:LEU:O	1:C:865:VAL:HG12	2.09	0.53
1:A:80:THR:HB	1:A:341:PHE:CG	2.43	0.53
1:E:920:ASN:OD1	1:E:1080:LYS:HE2	2.09	0.53
1:C:475:VAL:HG11	1:C:491:LEU:HG	1.90	0.53
1:C:491:LEU:HD11	1:C:545:ILE:CD1	2.38	0.53
1:E:94:HIS:NE2	2:F:155:LEU:HD21	2.24	0.53
1:E:528:GLU:HB2	1:E:531:ARG:HB2	1.90	0.53
1:C:710:PRO:HG3	1:C:884:GLU:OE2	2.09	0.53
1:A:81:THR:O	1:A:82:SER:O	2.27	0.53
1:E:905:VAL:HG21	1:E:946:LEU:HD22	1.91	0.53
1:C:80:THR:HB	1:C:341:PHE:CG	2.43	0.53
1:E:80:THR:HB	1:E:341:PHE:CG	2.43	0.53
2:D:363:PHE:CE2	2:D:369:THR:HG23	2.44	0.53
1:G:600:LEU:O	1:G:600:LEU:HD12	2.09	0.53
1:C:625:VAL:HG23	1:C:626:SER:C	2.29	0.53
1:A:491:LEU:HD11	1:A:545:ILE:CD1	2.38	0.53
1:E:465:TYR:CG	1:E:469:ARG:HG3	2.44	0.53
1:C:528:GLU:HB2	1:C:531:ARG:HB2	1.90	0.53
2:D:562:ASN:HB2	2:D:563:PRO:CD	2.38	0.53
1:A:506:LEU:HA	1:A:569:LEU:HD11	1.91	0.53
2:D:15:ILE:HG23	2:D:86:ARG:CZ	2.39	0.53
2:H:363:PHE:CE2	2:H:369:THR:HG23	2.44	0.53
2:B:363:PHE:CE2	2:B:369:THR:HG23	2.44	0.53
1:G:491:LEU:HD11	1:G:545:ILE:CD1	2.38	0.53
1:C:908:VAL:HG11	2:D:595:GLY:CA	2.36	0.53
1:E:756:HIS:CG	1:E:756:HIS:O	2.61	0.53
2:F:562:ASN:HB2	2:F:563:PRO:CD	2.38	0.53
1:E:506:LEU:HA	1:E:569:LEU:HD11	1.91	0.53
2:F:604:ILE:HD11	2:F:642:GLU:HB2	1.91	0.53
1:E:725:LEU:HG	1:E:726:ALA:N	2.23	0.53
1:C:624:VAL:HG23	1:C:625:VAL:N	2.24	0.53
1:C:476:CYS:CB	1:C:487:CYS:HA	2.39	0.53
2:F:110:LEU:HD11	2:F:237:LEU:HD23	1.90	0.53
1:C:986:PRO:CB	1:C:987:PRO:CD	2.87	0.53
1:G:905:VAL:HG11	1:G:946:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:363:PHE:CE2	2:F:369:THR:HG23	2.44	0.53
1:C:94:HIS:CD2	2:D:155:LEU:HD21	2.44	0.53
2:D:289:LEU:HD23	2:D:315:ILE:HD11	1.91	0.53
1:E:25:TYR:CE1	1:E:86:LEU:HB2	2.43	0.53
2:B:83:LEU:HD13	2:B:85:LEU:HB2	1.91	0.53
1:A:25:TYR:CE1	1:A:86:LEU:HB2	2.43	0.53
1:A:475:VAL:HG11	1:A:491:LEU:HG	1.90	0.52
1:E:789:TRP:CZ2	1:G:771:LEU:O	2.61	0.52
1:G:756:HIS:CG	1:G:756:HIS:O	2.62	0.52
1:E:986:PRO:CB	1:E:987:PRO:CD	2.87	0.52
1:G:506:LEU:HA	1:G:569:LEU:HD11	1.91	0.52
2:F:592:GLU:O	2:F:594:PRO:HD3	2.09	0.52
1:A:465:TYR:CG	1:A:469:ARG:HG3	2.44	0.52
2:B:285:LEU:O	2:B:289:LEU:HB3	2.09	0.52
1:C:465:TYR:CG	1:C:469:ARG:HG3	2.44	0.52
2:B:401:GLU:HA	2:B:421:PRO:HD3	1.92	0.52
2:F:104:PRO:HD2	2:F:233:VAL:HG11	1.91	0.52
2:H:83:LEU:HD13	2:H:85:LEU:HB2	1.91	0.52
1:C:47:LEU:HB2	1:C:60:ILE:HG21	1.91	0.52
2:D:654:LEU:HD13	2:D:665:ILE:HG13	1.90	0.52
1:A:47:LEU:HB2	1:A:60:ILE:HG21	1.91	0.52
1:A:920:ASN:OD1	1:A:1080:LYS:HE2	2.09	0.52
1:G:465:TYR:CG	1:G:469:ARG:HG3	2.44	0.52
1:G:475:VAL:HG11	1:G:491:LEU:HG	1.90	0.52
2:H:285:LEU:O	2:H:289:LEU:HB3	2.10	0.52
2:B:211:PRO:HB2	2:B:246:HIS:CE1	2.44	0.52
2:F:105:ILE:HG12	2:F:106:ASP:N	2.24	0.52
2:B:105:ILE:HG21	2:B:135:LEU:HD13	1.91	0.52
2:B:455:ILE:HG12	2:B:463:THR:HG23	1.91	0.52
2:H:592:GLU:O	2:H:594:PRO:HD3	2.09	0.52
2:H:570:GLY:HA2	2:H:659:GLY:HA2	1.91	0.52
1:C:89:CYS:C	1:C:91:PRO:HD3	2.30	0.52
1:E:47:LEU:HB2	1:E:60:ILE:HG21	1.91	0.52
2:H:43:ARG:HB3	2:H:44:PRO:HD3	1.92	0.52
1:C:602:VAL:HG23	1:C:638:TYR:O	2.09	0.52
1:C:600:LEU:HD12	1:C:600:LEU:O	2.10	0.52
1:A:465:TYR:HB3	1:A:469:ARG:HA	1.91	0.52
1:C:364:PRO:HB3	1:C:365:PRO:HD2	1.92	0.52
2:B:317:LYS:HE3	2:B:410:GLY:CA	2.40	0.52
1:A:824:SER:H	1:A:825:LEU:HG	1.74	0.52
1:E:476:CYS:CB	1:E:487:CYS:HA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:SER:CB	1:E:83:PRO:CD	2.88	0.52
2:F:591:GLN:HG2	2:F:592:GLU:N	2.25	0.52
1:A:89:CYS:C	1:A:91:PRO:HD3	2.30	0.52
2:D:43:ARG:HB3	2:D:44:PRO:HD3	1.91	0.52
2:B:505:LYS:HA	2:B:517:ILE:CG2	2.40	0.52
1:E:671:ALA:HB2	1:E:700:LEU:HD23	1.92	0.52
1:E:780:LEU:O	1:E:865:VAL:HG12	2.10	0.52
1:G:47:LEU:HB2	1:G:60:ILE:HG21	1.91	0.52
1:A:624:VAL:HG23	1:A:625:VAL:H	1.74	0.52
1:G:598:PRO:CB	1:G:650:ARG:NH1	2.73	0.52
2:F:211:PRO:HB2	2:F:246:HIS:CE1	2.44	0.52
2:D:341:LEU:C	2:D:343:SER:H	2.13	0.52
2:D:654:LEU:CD1	2:D:665:ILE:HG13	2.40	0.52
1:G:1065:GLY:C	1:G:1066:GLN:HG3	2.30	0.52
1:C:804:HIS:HB2	1:C:808:LEU:HD11	1.90	0.52
2:B:289:LEU:HD23	2:B:315:ILE:HD11	1.91	0.52
1:G:490:VAL:HG12	1:G:491:LEU:CB	2.39	0.52
1:E:475:VAL:HG11	1:E:491:LEU:HG	1.90	0.52
1:C:928:GLU:HG3	1:C:929:SER:H	1.75	0.52
2:H:104:PRO:HD2	2:H:233:VAL:HG11	1.91	0.52
2:D:35:PRO:HB3	2:D:510:GLN:OE1	2.09	0.52
1:G:908:VAL:HG13	1:G:1069:PHE:HB3	1.90	0.52
1:A:82:SER:CB	1:A:83:PRO:CD	2.88	0.52
1:E:619:GLU:O	1:E:620:CYS:SG	2.68	0.52
1:C:1065:GLY:C	1:C:1066:GLN:HG3	2.30	0.52
2:F:654:LEU:HD13	2:F:665:ILE:HG13	1.90	0.52
1:G:671:ALA:HB2	1:G:700:LEU:HD23	1.92	0.52
1:E:602:VAL:HG23	1:E:638:TYR:O	2.09	0.52
1:C:465:TYR:HB3	1:C:469:ARG:HA	1.91	0.52
1:G:364:PRO:HB3	1:G:365:PRO:HD2	1.92	0.52
1:C:362:LEU:C	1:C:362:LEU:HD23	2.30	0.52
9:G:3373:NAG:H3	9:G:3374:NAG:N2	2.24	0.52
2:D:105:ILE:HG12	2:D:106:ASP:N	2.24	0.52
1:A:333:ALA:HA	1:A:352:GLY:H	1.75	0.52
1:G:484:ARG:HH12	2:H:586:GLN:HG3	1.75	0.52
2:D:592:GLU:O	2:D:594:PRO:HD3	2.09	0.52
1:A:656:VAL:HG21	1:A:687:LEU:CD1	2.40	0.52
1:C:905:VAL:HG21	1:C:946:LEU:HD22	1.91	0.52
2:H:75:GLN:CD	2:H:98:ARG:O	2.48	0.52
2:D:110:LEU:HD11	2:D:237:LEU:HD23	1.90	0.52
2:D:285:LEU:O	2:D:289:LEU:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:ILE:HG12	2:B:106:ASP:N	2.25	0.52
1:C:81:THR:O	1:C:82:SER:O	2.27	0.52
2:D:83:LEU:HD13	2:D:85:LEU:HB2	1.91	0.52
1:C:920:ASN:OD1	1:C:1080:LYS:HE2	2.09	0.52
2:D:450:CYS:HB2	2:D:454:TYR:O	2.10	0.52
1:A:490:VAL:HG12	1:A:491:LEU:CB	2.39	0.52
2:H:289:LEU:HD23	2:H:315:ILE:HD11	1.91	0.52
1:E:465:TYR:HB3	1:E:469:ARG:HA	1.91	0.52
2:F:289:LEU:HD23	2:F:315:ILE:HD11	1.91	0.52
1:E:650:ARG:CD	1:E:729:ASN:HB3	2.36	0.52
1:A:650:ARG:CD	1:A:729:ASN:CB	2.87	0.52
1:G:824:SER:H	1:G:825:LEU:HG	1.74	0.52
1:G:476:CYS:CB	1:G:487:CYS:HA	2.40	0.52
2:D:105:ILE:HG21	2:D:135:LEU:HD13	1.91	0.52
1:G:619:GLU:O	1:G:620:CYS:SG	2.67	0.52
1:C:905:VAL:HG11	1:C:946:LEU:HD21	1.90	0.52
1:E:912:HIS:ND1	1:E:935:ARG:HD2	2.25	0.52
2:B:345:VAL:HG11	2:B:387:ILE:CD1	2.40	0.52
1:C:565:PHE:HB2	1:C:587:ALA:HB2	1.92	0.52
2:H:270:LEU:HD23	2:H:271:TYR:O	2.10	0.52
2:D:270:LEU:HD23	2:D:271:TYR:O	2.10	0.52
2:D:454:TYR:O	2:D:455:ILE:HD13	2.10	0.52
1:C:490:VAL:HG12	1:C:491:LEU:CB	2.39	0.52
2:F:285:LEU:O	2:F:289:LEU:HB3	2.10	0.52
2:D:508:TYR:CZ	2:D:514:CYS:HB3	2.45	0.52
2:B:104:PRO:HD2	2:B:233:VAL:HG11	1.91	0.52
2:D:401:GLU:HA	2:D:421:PRO:HD3	1.92	0.52
1:C:506:LEU:HA	1:C:569:LEU:HD11	1.91	0.52
1:C:333:ALA:HA	1:C:352:GLY:H	1.75	0.52
1:C:82:SER:CB	1:C:83:PRO:CD	2.88	0.52
2:H:654:LEU:CD1	2:H:665:ILE:HG13	2.40	0.52
1:E:82:SER:HB2	1:E:83:PRO:CD	2.40	0.52
2:D:591:GLN:HG2	2:D:592:GLU:N	2.25	0.52
1:A:878:THR:HG22	1:A:896:GLN:HB3	1.92	0.52
1:G:565:PHE:HB2	1:G:587:ALA:HB2	1.92	0.52
2:H:316:PRO:HB3	2:H:346:PHE:CE1	2.44	0.52
2:B:270:LEU:HD23	2:B:271:TYR:O	2.11	0.52
2:D:604:ILE:HD11	2:D:642:GLU:HB2	1.91	0.52
1:A:665:GLY:HA3	2:B:498:HIS:HB3	1.92	0.52
1:A:671:ALA:HB2	1:A:700:LEU:HD23	1.92	0.52
1:E:1065:GLY:C	1:E:1066:GLN:HG3	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LEU:O	1:A:600:LEU:HD12	2.09	0.52
2:B:591:GLN:HG2	2:B:592:GLU:N	2.25	0.51
1:C:364:PRO:CB	1:C:365:PRO:CD	2.89	0.51
1:G:650:ARG:CD	1:G:729:ASN:CB	2.88	0.51
2:H:105:ILE:HG21	2:H:135:LEU:HD13	1.91	0.51
1:A:82:SER:HB2	1:A:83:PRO:CD	2.40	0.51
1:G:780:LEU:O	1:G:865:VAL:HG12	2.09	0.51
1:G:656:VAL:HG21	1:G:687:LEU:CD1	2.40	0.51
1:A:725:LEU:HG	1:A:726:ALA:N	2.25	0.51
1:E:565:PHE:HB2	1:E:587:ALA:HB2	1.92	0.51
1:G:637:LEU:HD11	1:G:658:LEU:HD21	1.92	0.51
1:G:912:HIS:ND1	1:G:935:ARG:HD2	2.25	0.51
2:F:83:LEU:HD13	2:F:85:LEU:HB2	1.91	0.51
1:C:624:VAL:HG23	1:C:625:VAL:H	1.75	0.51
1:A:649:SER:O	1:A:650:ARG:HB3	2.11	0.51
1:A:364:PRO:HB3	1:A:365:PRO:HD2	1.92	0.51
2:H:211:PRO:HB2	2:H:246:HIS:CE1	2.44	0.51
2:F:135:LEU:CD1	2:F:139:THR:HB	2.41	0.51
1:G:333:ALA:HA	1:G:352:GLY:H	1.75	0.51
2:B:654:LEU:CD1	2:B:665:ILE:HG13	2.40	0.51
1:E:89:CYS:C	1:E:91:PRO:HD3	2.30	0.51
2:B:43:ARG:HB3	2:B:44:PRO:HD3	1.92	0.51
1:G:89:CYS:C	1:G:91:PRO:HD3	2.30	0.51
1:G:920:ASN:OD1	1:G:1080:LYS:HE2	2.09	0.51
1:C:491:LEU:HD12	1:C:492:TYR:N	2.26	0.51
1:G:465:TYR:HB3	1:G:469:ARG:HA	1.91	0.51
1:E:469:ARG:NH2	2:F:287:HIS:HB2	2.24	0.51
4:A:3374:NAG:C3	4:A:3375:MAN:H2	2.39	0.51
2:D:75:GLN:CD	2:D:98:ARG:O	2.49	0.51
2:F:508:TYR:CE1	2:F:514:CYS:HB3	2.46	0.51
1:G:986:PRO:CB	1:G:987:PRO:CD	2.87	0.51
1:G:986:PRO:HB3	1:G:987:PRO:HD2	1.93	0.51
2:H:105:ILE:HG12	2:H:106:ASP:N	2.24	0.51
1:E:637:LEU:HD11	1:E:658:LEU:HD21	1.93	0.51
2:F:6:PHE:O	2:F:8:VAL:HG23	2.11	0.51
1:A:780:LEU:O	1:A:865:VAL:HG12	2.09	0.51
1:A:637:LEU:HD11	1:A:658:LEU:HD21	1.93	0.51
2:F:184:HIS:CE1	2:F:228:ILE:HG23	2.46	0.51
1:E:600:LEU:HD12	1:E:600:LEU:O	2.09	0.51
1:C:637:LEU:HD11	1:C:658:LEU:HD21	1.92	0.51
1:E:650:ARG:CD	1:E:729:ASN:CB	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:649:SER:O	1:G:650:ARG:HB3	2.10	0.51
1:C:756:HIS:O	1:C:756:HIS:CG	2.63	0.51
2:B:522:TYR:CE1	2:B:552:GLN:HA	2.45	0.51
2:F:522:TYR:CE1	2:F:552:GLN:HA	2.46	0.51
2:F:105:ILE:HG21	2:F:135:LEU:HD13	1.91	0.51
2:H:591:GLN:HG2	2:H:592:GLU:N	2.25	0.51
1:G:532:GLY:HA3	1:G:565:PHE:HD2	1.76	0.51
2:B:184:HIS:CE1	2:B:228:ILE:HG23	2.46	0.51
2:H:343:SER:HA	2:H:381:VAL:O	2.10	0.51
1:A:532:GLY:HA3	1:A:565:PHE:HD2	1.76	0.51
1:E:362:LEU:HD23	1:E:362:LEU:C	2.30	0.51
1:E:364:PRO:HB3	1:E:365:PRO:HD2	1.92	0.51
1:E:94:HIS:CD2	2:F:155:LEU:HD21	2.45	0.51
2:D:104:PRO:HD2	2:D:233:VAL:HG11	1.92	0.51
2:F:654:LEU:CD1	2:F:665:ILE:HG13	2.40	0.51
2:F:270:LEU:HD23	2:F:271:TYR:O	2.10	0.51
1:A:211:THR:HA	1:A:248:LEU:HD12	1.91	0.51
1:E:649:SER:O	1:E:650:ARG:HB3	2.10	0.51
1:E:986:PRO:HB3	1:E:987:PRO:HD2	1.93	0.51
1:G:25:TYR:CE1	1:G:86:LEU:HB2	2.45	0.51
1:A:912:HIS:ND1	1:A:935:ARG:HD2	2.25	0.51
2:F:121:LEU:O	2:F:125:LYS:HB3	2.11	0.51
1:C:907:THR:CG2	1:C:1053:ILE:HD13	2.41	0.51
1:C:622:GLU:O	1:C:623:GLN:HG2	2.10	0.51
2:B:546:PHE:CE2	2:B:554:GLU:HG2	2.46	0.51
2:D:362:SER:HB2	2:D:370:HIS:HB2	1.93	0.51
1:E:710:PRO:HG3	1:E:884:GLU:OE2	2.10	0.51
2:B:505:LYS:HA	2:B:517:ILE:HG21	1.93	0.51
1:E:532:GLY:HA3	1:E:565:PHE:HD2	1.76	0.51
2:H:604:ILE:HD11	2:H:642:GLU:HB2	1.91	0.51
2:F:43:ARG:HB3	2:F:44:PRO:HD3	1.92	0.51
1:G:907:THR:CG2	1:G:1053:ILE:HD13	2.41	0.51
2:B:604:ILE:HD11	2:B:642:GLU:HB2	1.91	0.51
1:G:362:LEU:HD23	1:G:362:LEU:C	2.30	0.51
1:G:364:PRO:CB	1:G:365:PRO:CD	2.89	0.51
1:A:362:LEU:C	1:A:362:LEU:HD23	2.30	0.51
1:G:928:GLU:HG3	1:G:929:SER:H	1.74	0.51
1:E:725:LEU:HG	1:E:726:ALA:H	1.76	0.51
1:C:685:ARG:CZ	1:G:685:ARG:NH2	2.74	0.51
1:E:907:THR:CG2	1:E:1053:ILE:HD13	2.41	0.51
1:C:649:SER:O	1:C:650:ARG:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:HG3	1:A:157:ALA:N	2.26	0.51
1:E:121:VAL:O	1:E:121:VAL:CG1	2.59	0.51
1:C:919:LEU:CD1	2:D:643:ARG:NH1	2.74	0.51
2:D:354:ASP:O	2:D:544:PRO:HB2	2.11	0.51
1:E:656:VAL:HG21	1:E:687:LEU:CD1	2.40	0.51
2:B:6:PHE:O	2:B:8:VAL:HG23	2.11	0.51
1:E:490:VAL:HG12	1:E:491:LEU:CB	2.39	0.51
1:G:822:LEU:HG	1:G:823:ARG:N	2.23	0.51
1:G:121:VAL:CG1	1:G:121:VAL:O	2.59	0.51
2:H:401:GLU:HA	2:H:421:PRO:HD3	1.92	0.51
1:E:446:VAL:HG22	1:E:447:ASP:H	1.76	0.51
1:G:81:THR:O	1:G:82:SER:O	2.28	0.51
1:G:82:SER:CB	1:G:83:PRO:CD	2.88	0.51
1:A:907:THR:CG2	1:A:1053:ILE:HD13	2.41	0.51
1:C:671:ALA:HB2	1:C:700:LEU:HD23	1.92	0.51
1:A:122:SER:O	1:A:123:ARG:C	2.50	0.51
2:H:184:HIS:CE1	2:H:228:ILE:HG23	2.46	0.51
1:C:656:VAL:HG21	1:C:687:LEU:CD1	2.40	0.51
1:C:623:GLN:O	1:C:624:VAL:CG2	2.58	0.50
1:A:364:PRO:CB	1:A:365:PRO:CD	2.88	0.50
1:G:7:GLU:HB2	1:G:730:LEU:HD13	1.92	0.50
1:A:311:LYS:CG	1:A:312:GLU:N	2.74	0.50
2:B:75:GLN:CD	2:B:98:ARG:O	2.49	0.50
2:D:6:PHE:O	2:D:8:VAL:HG23	2.11	0.50
2:B:135:LEU:CD1	2:B:139:THR:HB	2.41	0.50
1:G:618:PHE:CE2	1:G:619:GLU:HG3	2.46	0.50
1:G:725:LEU:HG	1:G:726:ALA:H	1.77	0.50
2:D:638:ARG:HB2	2:D:654:LEU:O	2.12	0.50
2:H:121:LEU:O	2:H:125:LYS:HB3	2.11	0.50
2:D:121:LEU:O	2:D:125:LYS:HB3	2.11	0.50
1:C:484:ARG:HH11	1:C:939:ASN:HB2	1.73	0.50
1:G:465:TYR:CG	1:G:469:ARG:CG	2.94	0.50
1:A:476:CYS:CB	1:A:487:CYS:HA	2.40	0.50
1:E:333:ALA:HA	1:E:352:GLY:H	1.75	0.50
1:G:446:VAL:HG22	1:G:447:ASP:H	1.76	0.50
1:A:420:VAL:HB	1:A:423:GLN:HB2	1.93	0.50
1:E:1009:LEU:HD22	1:E:1011:PHE:CE1	2.47	0.50
2:D:184:HIS:CE1	2:D:228:ILE:HG23	2.46	0.50
1:E:491:LEU:HD12	1:E:492:TYR:N	2.26	0.50
1:E:817:GLN:O	1:E:818:LYS:HG2	2.12	0.50
2:B:546:PHE:CD2	2:B:554:GLU:O	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:PRO:HB3	1:C:987:PRO:HD2	1.94	0.50
2:H:135:LEU:CD1	2:H:139:THR:HB	2.41	0.50
1:C:82:SER:HB2	1:C:83:PRO:CD	2.40	0.50
2:H:638:ARG:HB2	2:H:654:LEU:O	2.11	0.50
1:C:532:GLY:HA3	1:C:565:PHE:HD2	1.76	0.50
1:A:565:PHE:HB2	1:A:587:ALA:HB2	1.92	0.50
2:B:121:LEU:O	2:B:125:LYS:HB3	2.11	0.50
1:G:886:ASN:O	1:G:888:PRO:HD3	2.12	0.50
1:A:126:CYS:HB3	1:A:127:PRO:CD	2.41	0.50
1:E:122:SER:O	1:E:123:ARG:C	2.50	0.50
1:G:650:ARG:CD	1:G:729:ASN:HB3	2.38	0.50
2:F:210:ALA:HB3	2:F:211:PRO:CD	2.39	0.50
2:F:401:GLU:HA	2:F:421:PRO:HD3	1.92	0.50
2:D:135:LEU:CD1	2:D:139:THR:HB	2.41	0.50
1:C:31:VAL:HG21	1:C:86:LEU:HD13	1.94	0.50
1:G:420:VAL:HB	1:G:423:GLN:HB2	1.93	0.50
1:A:1065:GLY:C	1:A:1066:GLN:HG3	2.30	0.50
1:C:878:THR:HG22	1:C:896:GLN:HB3	1.93	0.50
2:B:631:SER:HB3	2:B:664:LEU:HD11	1.94	0.50
2:F:345:VAL:HG11	2:F:387:ILE:CD1	2.42	0.50
1:C:420:VAL:HB	1:C:423:GLN:HB2	1.93	0.50
1:G:499:TRP:CZ2	2:H:284:GLN:HG3	2.46	0.50
1:A:491:LEU:HD12	1:A:492:TYR:N	2.26	0.50
1:G:491:LEU:HD12	1:G:492:TYR:N	2.26	0.50
1:E:364:PRO:CB	1:E:365:PRO:CD	2.89	0.50
1:A:650:ARG:CD	1:A:729:ASN:HB3	2.35	0.50
1:A:94:HIS:CD2	2:B:155:LEU:HD21	2.47	0.50
1:G:31:VAL:HG21	1:G:86:LEU:HD13	1.94	0.50
1:C:912:HIS:ND1	1:C:935:ARG:HD2	2.25	0.50
1:G:878:THR:HG22	1:G:896:GLN:HB3	1.93	0.50
1:A:1009:LEU:HD22	1:A:1011:PHE:CE1	2.46	0.50
2:H:6:PHE:O	2:H:8:VAL:HG23	2.11	0.50
1:C:716:ASN:C	1:C:716:ASN:OD1	2.50	0.50
1:C:650:ARG:CD	1:C:729:ASN:HB3	2.35	0.50
1:A:987:PRO:O	1:A:988:ALA:HB3	2.10	0.50
2:D:35:PRO:HB3	2:D:510:GLN:HE22	1.76	0.50
3:C:3373:NAG:H3	3:C:3374:NAG:N2	2.27	0.50
1:E:716:ASN:OD1	1:E:716:ASN:C	2.50	0.50
1:E:465:TYR:CG	1:E:469:ARG:CG	2.94	0.50
1:A:964:TRP:HB2	1:A:1032:LEU:HA	1.93	0.50
1:A:121:VAL:CG1	1:A:121:VAL:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:LYS:O	1:A:772:LYS:HG3	2.12	0.50
1:A:928:GLU:HG3	1:A:929:SER:H	1.75	0.50
2:H:10:SER:HA	2:H:447:ILE:HD11	1.94	0.50
1:G:122:SER:O	1:G:123:ARG:C	2.50	0.50
1:A:304:LYS:O	1:A:307:GLN:HB3	2.11	0.50
1:E:484:ARG:NH1	2:F:586:GLN:HG3	2.26	0.50
1:E:850:ILE:HG22	1:E:851:PHE:N	2.26	0.50
2:H:673:CYS:O	2:H:674:VAL:C	2.50	0.50
1:A:623:GLN:O	1:A:624:VAL:CG2	2.58	0.50
1:C:364:PRO:HD2	1:C:369:PRO:HA	1.93	0.50
1:G:772:LYS:O	1:G:772:LYS:HG3	2.12	0.50
1:C:964:TRP:HB2	1:C:1032:LEU:HA	1.93	0.50
1:G:625:VAL:CG2	1:G:627:GLU:HG3	2.40	0.50
1:A:756:HIS:O	1:A:756:HIS:CG	2.64	0.50
1:A:886:ASN:O	1:A:888:PRO:HD3	2.12	0.50
1:G:952:PHE:HB2	1:G:1011:PHE:HB2	1.94	0.50
1:A:499:TRP:CZ2	2:B:284:GLN:HG3	2.46	0.50
1:C:465:TYR:CG	1:C:469:ARG:CG	2.94	0.50
1:E:772:LYS:HG3	1:E:772:LYS:O	2.12	0.50
2:F:75:GLN:CD	2:F:98:ARG:O	2.49	0.50
2:B:638:ARG:HB2	2:B:654:LEU:O	2.12	0.50
1:A:446:VAL:HG22	1:A:447:ASP:H	1.76	0.50
2:H:181:ALA:HB3	2:H:271:TYR:CZ	2.47	0.50
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	1.94	0.50
2:F:100:ALA:C	2:F:101:LYS:HG3	2.32	0.50
1:C:430:VAL:HG22	1:C:485:TRP:HZ3	1.77	0.49
1:E:364:PRO:HD2	1:E:369:PRO:HA	1.93	0.49
1:C:446:VAL:HG22	1:C:447:ASP:H	1.76	0.49
1:C:725:LEU:HG	1:C:726:ALA:H	1.76	0.49
1:C:685:ARG:NH2	1:G:685:ARG:CZ	2.75	0.49
1:A:110:LEU:HD12	1:A:110:LEU:N	2.27	0.49
1:G:716:ASN:OD1	1:G:716:ASN:C	2.50	0.49
1:A:465:TYR:CG	1:A:469:ARG:CG	2.94	0.49
2:D:317:LYS:HG3	2:D:346:PHE:HE1	1.77	0.49
1:G:446:VAL:HG12	1:G:456:LEU:CD1	2.42	0.49
1:G:82:SER:HB2	1:G:83:PRO:CD	2.40	0.49
1:A:766:PHE:CZ	1:A:877:LEU:CD1	2.95	0.49
1:A:766:PHE:CZ	1:A:877:LEU:HD12	2.47	0.49
1:C:850:ILE:HG22	1:C:851:PHE:N	2.28	0.49
1:C:766:PHE:CZ	1:C:877:LEU:HD12	2.47	0.49
1:E:766:PHE:CZ	1:E:877:LEU:CD1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:766:PHE:CZ	1:E:877:LEU:HD12	2.47	0.49
1:C:876:LEU:HD12	1:C:876:LEU:C	2.32	0.49
1:A:850:ILE:HG22	1:A:851:PHE:N	2.27	0.49
1:C:598:PRO:HB3	1:C:650:ARG:NH1	2.27	0.49
1:A:364:PRO:HD2	1:A:369:PRO:HA	1.94	0.49
2:B:210:ALA:HB3	2:B:211:PRO:CD	2.39	0.49
1:A:174:PHE:CG	1:A:174:PHE:O	2.65	0.49
1:A:243:LYS:HG3	1:A:243:LYS:O	2.12	0.49
2:D:237:LEU:HD13	2:D:294:ILE:HG23	1.94	0.49
1:C:806:ALA:HA	1:C:840:TRP:NE1	2.27	0.49
2:D:35:PRO:CA	2:D:510:GLN:HE22	2.25	0.49
2:F:638:ARG:HB2	2:F:654:LEU:O	2.11	0.49
1:G:1009:LEU:HD22	1:G:1011:PHE:CE1	2.46	0.49
1:G:766:PHE:CZ	1:G:877:LEU:HD12	2.47	0.49
1:A:263:ILE:HD12	1:A:317:ILE:CD1	2.42	0.49
2:D:631:SER:HB3	2:D:664:LEU:HD11	1.93	0.49
1:E:107:CYS:SG	1:E:348:LEU:HD21	2.52	0.49
1:G:469:ARG:NH2	2:H:287:HIS:HB2	2.26	0.49
1:G:964:TRP:HB2	1:G:1032:LEU:HA	1.93	0.49
1:E:771:LEU:HD11	1:E:774:LEU:HB2	1.94	0.49
1:E:430:VAL:HG22	1:E:485:TRP:HZ3	1.78	0.49
1:A:444:CYS:CB	1:A:506:LEU:CD1	2.91	0.49
1:A:456:LEU:HA	1:A:477:PRO:HA	1.94	0.49
1:C:886:ASN:O	1:C:888:PRO:HD3	2.13	0.49
1:E:878:THR:HG22	1:E:896:GLN:HB3	1.93	0.49
1:A:716:ASN:OD1	1:A:716:ASN:C	2.49	0.49
1:G:364:PRO:HD2	1:G:369:PRO:HA	1.94	0.49
1:E:71:MET:HG3	1:E:90:GLY:HA3	1.95	0.49
2:F:472:GLU:HA	2:F:475:CYS:HB2	1.92	0.49
1:A:430:VAL:HG22	1:A:485:TRP:HZ3	1.78	0.49
2:D:426:ARG:CZ	2:D:426:ARG:CB	2.91	0.49
1:E:110:LEU:HD12	1:E:110:LEU:N	2.27	0.49
1:C:1009:LEU:HD22	1:C:1011:PHE:CE1	2.47	0.49
1:G:876:LEU:HD12	1:G:876:LEU:C	2.33	0.49
1:E:420:VAL:HB	1:E:423:GLN:HB2	1.93	0.49
1:A:480:ARG:HB3	1:A:1021:GLN:HG2	1.95	0.49
1:G:71:MET:HG3	1:G:90:GLY:HA3	1.95	0.49
1:G:771:LEU:HD11	1:G:774:LEU:HB2	1.95	0.49
1:E:755:ASP:O	1:E:756:HIS:HB3	2.12	0.49
2:H:455:ILE:HG22	2:H:456:GLY:N	2.27	0.49
2:B:74:LYS:HZ2	2:B:103:TYR:HE2	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:VAL:HG12	1:E:456:LEU:CD1	2.42	0.49
1:C:446:VAL:HG12	1:C:456:LEU:CD1	2.42	0.49
2:F:181:ALA:HB3	2:F:271:TYR:CZ	2.47	0.49
1:E:499:TRP:CZ2	2:F:284:GLN:HG3	2.48	0.49
1:E:886:ASN:O	1:E:888:PRO:HD3	2.12	0.49
1:C:71:MET:HG3	1:C:90:GLY:HA3	1.95	0.49
1:C:121:VAL:O	1:C:121:VAL:CG1	2.59	0.49
2:H:450:CYS:HB2	2:H:454:TYR:O	2.12	0.49
2:B:98:ARG:HB2	2:B:386:PRO:HG3	1.94	0.49
1:G:987:PRO:O	1:G:988:ALA:HB3	2.11	0.49
1:A:31:VAL:HG21	1:A:86:LEU:HD13	1.94	0.49
2:D:181:ALA:HB3	2:D:271:TYR:CZ	2.48	0.49
2:F:212:GLU:HG2	2:F:243:ASP:HB2	1.95	0.49
2:D:465:GLY:O	2:D:466:ARG:HG2	2.13	0.49
1:C:771:LEU:HD11	1:C:774:LEU:HB2	1.94	0.49
1:E:816:GLY:O	1:E:818:LYS:CA	2.61	0.49
1:G:71:MET:CG	1:G:90:GLY:HA3	2.43	0.49
1:G:597:ARG:NH2	1:G:730:LEU:CD1	2.76	0.49
1:G:108:PHE:HD1	1:G:117:GLN:HG2	1.78	0.49
1:C:772:LYS:O	1:C:772:LYS:HG3	2.12	0.49
1:A:986:PRO:HB3	1:A:987:PRO:HD2	1.95	0.49
1:G:1069:PHE:CE2	2:H:584:GLY:HA3	2.47	0.49
1:C:110:LEU:N	1:C:110:LEU:HD12	2.27	0.49
2:B:181:ALA:HB3	2:B:271:TYR:CZ	2.47	0.49
1:C:952:PHE:HB2	1:C:1011:PHE:HB2	1.94	0.49
2:H:212:GLU:HG2	2:H:243:ASP:HB2	1.95	0.49
1:C:126:CYS:HB3	1:C:127:PRO:CD	2.43	0.49
1:A:171:LEU:HB3	1:A:182:PHE:CE1	2.48	0.49
1:E:126:CYS:HB3	1:E:127:PRO:CD	2.42	0.49
1:A:771:LEU:HD11	1:A:774:LEU:HB2	1.94	0.49
2:B:237:LEU:HD13	2:B:294:ILE:HG23	1.94	0.49
1:G:26:ALA:O	1:G:28:SER:N	2.45	0.49
1:G:25:TYR:CD1	1:G:86:LEU:HB2	2.48	0.49
1:E:952:PHE:HB2	1:E:1011:PHE:HB2	1.94	0.49
1:G:107:CYS:SG	1:G:348:LEU:HD21	2.53	0.49
1:G:850:ILE:HG22	1:G:851:PHE:N	2.28	0.49
1:A:470:GLY:HA2	1:A:497:HIS:O	2.13	0.49
1:G:964:TRP:HB3	1:G:1032:LEU:HA	1.95	0.49
1:C:987:PRO:O	1:C:988:ALA:HB3	2.13	0.49
1:G:806:ALA:HA	1:G:840:TRP:NE1	2.27	0.49
1:A:446:VAL:HG12	1:A:456:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:522:TYR:CD1	2:D:552:GLN:HA	2.48	0.49
1:E:470:GLY:HA2	1:E:497:HIS:O	2.13	0.49
2:F:465:GLY:O	2:F:466:ARG:HG2	2.13	0.49
1:E:876:LEU:C	1:E:876:LEU:HD12	2.33	0.49
1:A:269:VAL:HG11	1:A:300:PHE:CE2	2.48	0.49
1:A:94:HIS:NE2	2:B:155:LEU:HD21	2.28	0.48
1:A:159:ILE:HD12	1:A:197:LEU:HD11	1.94	0.48
2:F:98:ARG:HB2	2:F:386:PRO:HG3	1.94	0.48
1:C:1029:LYS:HE3	1:E:113:THR:HG22	1.95	0.48
1:E:31:VAL:HG21	1:E:86:LEU:HD13	1.94	0.48
1:G:110:LEU:N	1:G:110:LEU:HD12	2.27	0.48
1:C:766:PHE:CZ	1:C:877:LEU:CD1	2.95	0.48
1:G:766:PHE:CZ	1:G:877:LEU:CD1	2.95	0.48
1:A:876:LEU:HD12	1:A:876:LEU:C	2.33	0.48
1:E:453:SER:O	1:E:454:THR:C	2.51	0.48
1:C:711:ILE:HD11	1:C:746:LEU:HD13	1.95	0.48
1:C:122:SER:O	1:C:123:ARG:C	2.50	0.48
2:H:522:TYR:CD1	2:H:552:GLN:HA	2.48	0.48
1:E:964:TRP:HB2	1:E:1032:LEU:HA	1.94	0.48
2:D:98:ARG:HB2	2:D:386:PRO:HG3	1.94	0.48
2:D:355:THR:HA	2:D:544:PRO:CG	2.44	0.48
2:B:450:CYS:HB2	2:B:454:TYR:O	2.13	0.48
1:C:26:ALA:O	1:C:28:SER:N	2.46	0.48
1:E:26:ALA:O	1:E:28:SER:N	2.46	0.48
1:A:934:HIS:ND1	1:A:1074:THR:CG2	2.77	0.48
2:B:570:GLY:HA2	2:B:659:GLY:HA2	1.95	0.48
2:H:219:MET:HE2	2:H:262:GLY:HA2	1.95	0.48
2:B:219:MET:HE2	2:B:262:GLY:HA2	1.95	0.48
2:F:471:LEU:O	2:F:493:GLY:HA2	2.13	0.48
1:C:444:CYS:CB	1:C:506:LEU:CD1	2.91	0.48
1:E:456:LEU:HA	1:E:477:PRO:HA	1.94	0.48
1:A:26:ALA:O	1:A:28:SER:N	2.46	0.48
1:G:126:CYS:HB3	1:G:127:PRO:CD	2.43	0.48
1:E:761:ASN:ND2	1:E:791:ASP:HB2	2.28	0.48
1:A:559:SER:O	1:A:560:SER:C	2.52	0.48
1:A:107:CYS:SG	1:A:348:LEU:HD21	2.53	0.48
2:H:237:LEU:HD13	2:H:294:ILE:HG23	1.94	0.48
1:A:354:PHE:CG	4:A:3373:NAG:H62	2.48	0.48
1:C:772:LYS:O	1:C:773:SER:HB3	2.14	0.48
1:A:254:ILE:N	1:A:255:PRO:CD	2.76	0.48
1:A:806:ALA:HA	1:A:840:TRP:NE1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:806:ALA:HA	1:E:840:TRP:NE1	2.27	0.48
1:G:430:VAL:HG22	1:G:485:TRP:HZ3	1.78	0.48
1:C:25:TYR:CD1	1:C:86:LEU:HB2	2.48	0.48
1:C:107:CYS:SG	1:C:348:LEU:HD21	2.53	0.48
2:B:212:GLU:HG2	2:B:243:ASP:HB2	1.95	0.48
2:D:64:GLU:HB3	2:D:82:THR:HB	1.96	0.48
1:C:453:SER:O	1:C:454:THR:C	2.51	0.48
1:A:761:ASN:ND2	1:A:791:ASP:HB2	2.29	0.48
2:D:455:ILE:HG21	2:D:494:GLN:NE2	2.25	0.48
1:G:490:VAL:CG1	1:G:491:LEU:N	2.68	0.48
1:E:964:TRP:HB3	1:E:1032:LEU:HA	1.95	0.48
1:C:816:GLY:O	1:C:818:LYS:HA	2.14	0.48
1:C:609:ILE:CB	1:C:610:PRO:HD3	2.44	0.48
2:F:186:LEU:HD13	2:F:195:PHE:CD1	2.49	0.48
1:C:456:LEU:HA	1:C:477:PRO:HA	1.94	0.48
1:C:351:VAL:HG23	1:C:352:GLY:N	2.29	0.48
1:E:764:ILE:CD1	1:E:800:ILE:HD11	2.44	0.48
1:G:559:SER:O	1:G:560:SER:C	2.52	0.48
1:G:761:ASN:ND2	1:G:791:ASP:HB2	2.28	0.48
2:B:644:ASP:HB3	2:B:650:VAL:HG23	1.96	0.48
2:F:154:VAL:HA	2:F:160:THR:HG22	1.96	0.48
1:G:772:LYS:O	1:G:773:SER:HB3	2.14	0.48
1:G:623:GLN:O	1:G:624:VAL:CG2	2.59	0.48
1:C:848:HIS:O	1:C:849:LEU:HB3	2.14	0.48
1:C:108:PHE:HD1	1:C:117:GLN:HG2	1.78	0.48
1:A:108:PHE:HD1	1:A:117:GLN:HG2	1.78	0.48
1:A:755:ASP:O	1:A:756:HIS:HB3	2.14	0.48
1:G:609:ILE:CB	1:G:610:PRO:HD3	2.44	0.48
2:B:362:SER:HB2	2:B:370:HIS:HB2	1.96	0.48
1:C:824:SER:H	1:C:825:LEU:HG	1.77	0.48
1:A:725:LEU:HG	1:A:726:ALA:H	1.79	0.48
1:G:934:HIS:ND1	1:G:1074:THR:CG2	2.76	0.48
2:H:656:GLN:HG2	2:H:657:GLN:N	2.29	0.48
1:G:470:GLY:HA2	1:G:497:HIS:O	2.13	0.48
1:C:484:ARG:NH2	1:C:1021:GLN:CA	2.67	0.48
2:F:237:LEU:HD13	2:F:294:ILE:HG23	1.95	0.48
2:F:455:ILE:HG22	2:F:456:GLY:N	2.29	0.48
1:A:690:LYS:HB3	1:E:609:ILE:HD11	1.96	0.48
1:G:444:CYS:CB	1:G:506:LEU:CD1	2.91	0.48
1:E:25:TYR:CD1	1:E:86:LEU:HB2	2.48	0.48
1:E:711:ILE:HD11	1:E:746:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:764:ILE:CD1	1:G:800:ILE:HD11	2.44	0.48
1:A:711:ILE:HD11	1:A:746:LEU:HD13	1.95	0.48
1:C:934:HIS:ND1	1:C:1074:THR:CG2	2.76	0.48
2:B:64:GLU:HB3	2:B:82:THR:HB	1.96	0.48
2:D:154:VAL:HA	2:D:160:THR:HG22	1.96	0.48
1:E:71:MET:CG	1:E:90:GLY:HA3	2.43	0.48
1:A:964:TRP:HB3	1:A:1032:LEU:HA	1.95	0.48
1:E:623:GLN:O	1:E:624:VAL:CG2	2.60	0.48
2:F:10:SER:CB	2:F:449:ARG:CZ	2.91	0.48
1:E:513:ASN:HA	1:E:599:VAL:HG22	1.95	0.48
2:D:273:ARG:O	2:D:277:PHE:HB3	2.14	0.48
1:A:351:VAL:HG23	1:A:352:GLY:N	2.29	0.48
1:C:376:GLN:HB2	3:C:3373:NAG:O4	2.14	0.48
2:D:644:ASP:HB3	2:D:650:VAL:HG23	1.95	0.48
1:G:971:HIS:CE1	1:G:974:ASN:HB2	2.49	0.48
2:D:212:GLU:HG2	2:D:243:ASP:HB2	1.95	0.48
1:G:453:SER:O	1:G:454:THR:C	2.51	0.48
2:F:64:GLU:HB3	2:F:82:THR:HB	1.95	0.48
1:C:559:SER:O	1:C:560:SER:C	2.52	0.48
1:C:71:MET:CG	1:C:90:GLY:HA3	2.43	0.48
1:E:108:PHE:HD1	1:E:117:GLN:HG2	1.78	0.48
1:G:662:LEU:HD11	1:G:673:PHE:CE1	2.49	0.48
2:H:98:ARG:HB2	2:H:386:PRO:HG3	1.95	0.48
1:G:456:LEU:HA	1:G:477:PRO:HA	1.95	0.48
1:G:25:TYR:O	1:G:26:ALA:C	2.52	0.48
1:E:559:SER:O	1:E:560:SER:C	2.52	0.48
2:H:465:GLY:O	2:H:466:ARG:HG2	2.13	0.48
1:G:354:PHE:CG	9:G:3373:NAG:H62	2.49	0.48
1:A:1063:LEU:HG	1:A:1064:PRO:HD3	1.96	0.48
2:B:98:ARG:HD2	2:B:384:ASN:OD1	2.14	0.48
2:D:357:LYS:CE	2:D:545:GLY:HA2	2.43	0.48
2:F:362:SER:HB2	2:F:370:HIS:HB2	1.96	0.48
1:E:444:CYS:CB	1:E:506:LEU:CD1	2.91	0.48
1:E:848:HIS:O	1:E:849:LEU:HB3	2.14	0.48
1:A:25:TYR:CD1	1:A:86:LEU:HB2	2.48	0.48
1:C:470:GLY:HA2	1:C:497:HIS:O	2.13	0.48
1:A:971:HIS:CE1	1:A:974:ASN:HB2	2.49	0.48
1:A:1058:SER:O	1:A:1059:VAL:HB	2.14	0.48
1:C:411:THR:HG22	1:C:435:ILE:HA	1.96	0.48
1:A:764:ILE:CD1	1:A:800:ILE:HD11	2.44	0.48
1:E:971:HIS:CE1	1:E:974:ASN:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:490:VAL:CG1	1:E:491:LEU:N	2.68	0.47
1:E:598:PRO:CB	1:E:650:ARG:NH1	2.77	0.47
1:A:71:MET:HG3	1:A:90:GLY:HA3	1.95	0.47
2:D:317:LYS:N	2:D:344:ARG:HH11	2.12	0.47
1:E:928:GLU:HG3	1:E:929:SER:H	1.74	0.47
1:E:772:LYS:O	1:E:773:SER:HB3	2.14	0.47
2:H:118:LEU:HD21	2:H:204:ILE:CD1	2.44	0.47
2:B:455:ILE:HG22	2:B:456:GLY:N	2.29	0.47
1:A:453:SER:O	1:A:454:THR:C	2.52	0.47
1:A:71:MET:CG	1:A:90:GLY:HA3	2.43	0.47
1:A:597:ARG:HG3	1:A:731:ARG:HE	1.79	0.47
1:A:662:LEU:CD1	1:A:673:PHE:CE1	2.97	0.47
1:C:662:LEU:HD11	1:C:673:PHE:CE1	2.49	0.47
2:B:118:LEU:HD21	2:B:204:ILE:CD1	2.44	0.47
2:F:118:LEU:HD21	2:F:204:ILE:CD1	2.44	0.47
2:D:186:LEU:HD13	2:D:195:PHE:CD1	2.49	0.47
1:G:411:THR:HG22	1:G:435:ILE:HA	1.96	0.47
1:E:676:THR:HG23	1:E:678:ASN:H	1.79	0.47
1:E:934:HIS:ND1	1:E:1074:THR:CG2	2.76	0.47
1:E:598:PRO:CG	1:E:650:ARG:NH1	2.77	0.47
1:C:43:GLN:HG2	1:C:44:THR:HG23	1.97	0.47
1:C:964:TRP:HB3	1:C:1032:LEU:HA	1.95	0.47
2:B:295:GLN:CD	2:B:317:LYS:HE2	2.35	0.47
2:F:118:LEU:HD21	2:F:204:ILE:HD13	1.97	0.47
1:A:181:HIS:CE1	1:A:200:VAL:CG1	2.96	0.47
1:C:840:TRP:CD1	1:C:840:TRP:N	2.83	0.47
2:B:212:GLU:HG2	2:B:243:ASP:CB	2.45	0.47
2:D:212:GLU:HG2	2:D:243:ASP:CB	2.45	0.47
1:C:761:ASN:ND2	1:C:791:ASP:HB2	2.28	0.47
1:E:831:SER:CB	1:E:842:THR:HG22	2.45	0.47
1:G:711:ILE:HD11	1:G:746:LEU:HD13	1.95	0.47
2:D:453:GLY:O	2:D:463:THR:HG23	2.13	0.47
1:A:1028:LEU:O	1:A:1028:LEU:HD12	2.14	0.47
1:G:406:PRO:HB3	1:G:438:TYR:CD2	2.50	0.47
2:B:347:LEU:HD22	2:B:389:PHE:CG	2.49	0.47
1:A:221:PHE:CE1	1:A:233:LYS:HD2	2.50	0.47
2:H:64:GLU:HB3	2:H:82:THR:HB	1.96	0.47
1:E:566:GLY:O	1:E:567:GLN:C	2.53	0.47
1:G:831:SER:CB	1:G:842:THR:HG22	2.44	0.47
1:A:713:LEU:HD23	1:A:713:LEU:C	2.35	0.47
1:G:465:TYR:HB3	1:G:469:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:TYR:HB3	1:E:469:ARG:HG2	1.97	0.47
1:E:1063:LEU:HG	1:E:1064:PRO:HD3	1.96	0.47
1:C:906:TYR:CE2	1:C:1067:GLU:OE1	2.68	0.47
1:G:1063:LEU:HG	1:G:1064:PRO:HD3	1.96	0.47
1:G:906:TYR:CE2	1:G:1067:GLU:OE1	2.68	0.47
2:F:260:ASN:ND2	2:F:277:PHE:HZ	2.13	0.47
2:H:273:ARG:O	2:H:277:PHE:HB3	2.14	0.47
1:C:831:SER:CB	1:C:842:THR:HG22	2.45	0.47
1:G:1058:SER:O	1:G:1059:VAL:HB	2.14	0.47
1:C:1058:SER:O	1:C:1059:VAL:HB	2.14	0.47
2:F:644:ASP:HB3	2:F:650:VAL:HG23	1.95	0.47
1:E:1028:LEU:O	1:E:1028:LEU:HD12	2.15	0.47
1:G:1028:LEU:O	1:G:1028:LEU:HD12	2.14	0.47
1:C:465:TYR:HB3	1:C:469:ARG:HG2	1.97	0.47
1:A:906:TYR:CE2	1:A:1067:GLU:OE1	2.68	0.47
1:G:662:LEU:CD1	1:G:673:PHE:CE1	2.98	0.47
2:D:98:ARG:HD2	2:D:384:ASN:OD1	2.14	0.47
1:E:609:ILE:CB	1:E:610:PRO:HD3	2.44	0.47
2:B:118:LEU:HD21	2:B:204:ILE:HD13	1.97	0.47
2:D:343:SER:O	2:D:378:CYS:O	2.33	0.47
2:D:609:CYS:SG	2:D:616:PRO:HB3	2.55	0.47
2:B:186:LEU:HD13	2:B:195:PHE:CD1	2.49	0.47
1:A:618:PHE:CD2	1:A:619:GLU:N	2.82	0.47
1:G:670:ARG:HG2	1:G:711:ILE:CG2	2.45	0.47
1:C:566:GLY:O	1:C:567:GLN:C	2.53	0.47
2:B:352:LEU:CD2	2:B:358:VAL:HG23	2.45	0.47
1:C:764:ILE:CD1	1:C:800:ILE:HD11	2.44	0.47
2:B:465:GLY:O	2:B:466:ARG:HG2	2.13	0.47
1:C:478:LEU:HA	1:C:485:TRP:HE1	1.80	0.47
1:E:920:ASN:O	1:E:1080:LYS:HG2	2.14	0.47
1:G:920:ASN:O	1:G:1080:LYS:HG2	2.15	0.47
1:A:465:TYR:HB3	1:A:469:ARG:HG2	1.97	0.47
1:A:90:GLY:O	1:A:105:GLY:HA2	2.15	0.47
2:B:154:VAL:HA	2:B:160:THR:HG22	1.96	0.47
1:A:376:GLN:HB2	4:A:3373:NAG:O4	2.15	0.47
1:C:1063:LEU:HG	1:C:1064:PRO:HD3	1.96	0.47
1:E:662:LEU:CD1	1:E:673:PHE:CE1	2.97	0.47
2:H:98:ARG:HD2	2:H:384:ASN:OD1	2.14	0.47
1:A:253:VAL:CG2	1:A:254:ILE:N	2.78	0.47
2:D:118:LEU:HD21	2:D:204:ILE:HD13	1.97	0.47
2:F:609:CYS:SG	2:F:616:PRO:HB3	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:TRP:CD1	1:A:840:TRP:N	2.83	0.47
1:G:351:VAL:HG23	1:G:352:GLY:N	2.29	0.47
1:E:351:VAL:HG23	1:E:352:GLY:N	2.29	0.47
2:B:630:LEU:HD12	2:B:665:ILE:HB	1.97	0.47
1:E:25:TYR:O	1:E:26:ALA:C	2.52	0.47
2:D:43:ARG:N	2:D:44:PRO:CD	2.78	0.47
2:F:630:LEU:HD12	2:F:665:ILE:HB	1.97	0.47
2:F:121:LEU:HD23	2:F:121:LEU:O	2.15	0.47
2:H:234:THR:CG2	2:H:236:LEU:HD13	2.45	0.47
1:C:971:HIS:CE1	1:C:974:ASN:HB2	2.49	0.47
1:A:848:HIS:O	1:A:849:LEU:HB3	2.14	0.47
3:G:3716:NAG:H4	3:G:3717:NAG:H2	1.70	0.47
1:C:980:SER:HB3	1:C:1012:ARG:HB3	1.97	0.47
1:G:980:SER:HB3	1:G:1012:ARG:HB3	1.97	0.47
2:H:644:ASP:HB3	2:H:650:VAL:HG23	1.96	0.47
2:H:154:VAL:HA	2:H:160:THR:HG22	1.96	0.47
1:A:43:GLN:HG2	1:A:44:THR:HG23	1.97	0.47
1:A:772:LYS:O	1:A:773:SER:HB3	2.14	0.47
1:A:953:TRP:NE1	1:C:755:ASP:HB2	2.30	0.47
1:E:662:LEU:HD11	1:E:673:PHE:CE1	2.49	0.47
1:A:609:ILE:CB	1:A:610:PRO:HD3	2.44	0.47
1:G:840:TRP:N	1:G:840:TRP:CD1	2.83	0.47
2:F:273:ARG:O	2:F:277:PHE:HB3	2.14	0.47
2:B:273:ARG:O	2:B:277:PHE:HB3	2.14	0.47
1:A:25:TYR:O	1:A:26:ALA:C	2.52	0.47
1:E:780:LEU:C	1:E:780:LEU:HD23	2.35	0.47
1:A:158:VAL:HG12	1:A:158:VAL:O	2.15	0.47
2:H:352:LEU:CD2	2:H:358:VAL:HG23	2.45	0.47
1:G:741:TYR:CD2	2:H:502:VAL:HG22	2.50	0.47
1:G:848:HIS:O	1:G:849:LEU:HB3	2.14	0.47
1:E:411:THR:HG22	1:E:435:ILE:HA	1.96	0.47
1:C:119:LEU:CD2	1:C:124:GLN:NE2	2.78	0.47
1:E:598:PRO:HB3	1:E:650:ARG:HH12	1.79	0.47
1:E:597:ARG:HB3	1:E:731:ARG:O	2.14	0.47
1:G:376:GLN:HB2	9:G:3373:NAG:O4	2.15	0.47
2:D:295:GLN:CD	2:D:317:LYS:HE2	2.36	0.47
2:F:450:CYS:HB2	2:F:454:TYR:O	2.15	0.47
2:F:98:ARG:HD2	2:F:384:ASN:OD1	2.14	0.47
2:H:609:CYS:SG	2:H:616:PRO:HB3	2.55	0.47
2:F:295:GLN:CD	2:F:317:LYS:HE2	2.35	0.47
2:D:260:ASN:ND2	2:D:277:PHE:HZ	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:630:LEU:HD12	2:H:665:ILE:HB	1.97	0.47
2:H:121:LEU:HD23	2:H:121:LEU:O	2.15	0.47
2:D:522:TYR:CE1	2:D:552:GLN:HA	2.49	0.47
2:H:305:VAL:HG13	2:H:306:LYS:N	2.30	0.47
1:A:411:THR:HG22	1:A:435:ILE:HA	1.96	0.47
1:G:514:GLY:CA	1:G:644:LYS:HD3	2.45	0.47
2:D:234:THR:CG2	2:D:236:LEU:HD13	2.45	0.47
1:E:119:LEU:CD2	1:E:124:GLN:NE2	2.78	0.47
1:C:119:LEU:O	1:C:363:TYR:HE1	1.97	0.47
1:C:662:LEU:CD1	1:C:673:PHE:CE1	2.98	0.47
1:E:840:TRP:CD1	1:E:840:TRP:N	2.83	0.47
2:H:186:LEU:HD13	2:H:195:PHE:CD1	2.49	0.47
2:H:43:ARG:N	2:H:44:PRO:CD	2.78	0.47
2:H:341:LEU:C	2:H:343:SER:H	2.17	0.47
2:H:212:GLU:HG2	2:H:243:ASP:CB	2.45	0.47
1:C:601:TRP:HZ2	1:C:641:LYS:HD3	1.80	0.47
2:H:631:SER:HB3	2:H:664:LEU:HD11	1.97	0.47
2:F:656:GLN:HG2	2:F:657:GLN:N	2.29	0.47
1:A:831:SER:CB	1:A:842:THR:HG22	2.45	0.47
2:B:656:GLN:HG2	2:B:657:GLN:N	2.29	0.47
1:A:676:THR:HG23	1:A:678:ASN:H	1.80	0.47
1:G:465:TYR:CD1	1:G:469:ARG:HG2	2.50	0.46
1:E:376:GLN:HB2	9:E:3373:NAG:O4	2.15	0.46
1:E:90:GLY:O	1:E:105:GLY:HA2	2.15	0.46
1:E:906:TYR:CE2	1:E:1067:GLU:OE1	2.68	0.46
2:B:98:ARG:O	2:B:99:ARG:C	2.53	0.46
1:C:406:PRO:HB3	1:C:438:TYR:CD2	2.50	0.46
1:E:987:PRO:O	1:E:988:ALA:HB3	2.14	0.46
1:G:476:CYS:HB3	1:G:487:CYS:HA	1.97	0.46
1:A:799:THR:HA	1:A:845:ARG:HA	1.98	0.46
2:B:234:THR:CG2	2:B:236:LEU:HD13	2.45	0.46
1:A:566:GLY:O	1:A:567:GLN:C	2.53	0.46
1:E:1058:SER:O	1:E:1059:VAL:HB	2.14	0.46
1:G:676:THR:HG23	1:G:678:ASN:H	1.80	0.46
1:G:713:LEU:C	1:G:713:LEU:HD23	2.35	0.46
1:C:476:CYS:HB3	1:C:487:CYS:HA	1.97	0.46
1:C:920:ASN:O	1:C:1080:LYS:HG2	2.14	0.46
1:E:909:VAL:HG12	1:E:1069:PHE:O	2.15	0.46
1:A:662:LEU:HD11	1:A:673:PHE:CE1	2.49	0.46
1:A:174:PHE:HB2	1:A:212:ALA:HB2	1.96	0.46
1:E:406:PRO:HB3	1:E:438:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:797:GLY:N	1:G:884:GLU:HB2	2.31	0.46
1:A:478:LEU:HA	1:A:485:TRP:HE1	1.80	0.46
2:D:630:LEU:HD12	2:D:665:ILE:HB	1.97	0.46
1:G:831:SER:HA	1:G:842:THR:HG22	1.97	0.46
2:D:352:LEU:CD2	2:D:358:VAL:HG23	2.45	0.46
2:F:340:LYS:HD2	2:F:379:ASP:OD1	2.16	0.46
2:B:334:ILE:HA	2:B:337:ALA:CB	2.45	0.46
1:A:601:TRP:HZ2	1:A:641:LYS:HD3	1.81	0.46
1:C:992:LEU:HD23	1:C:992:LEU:C	2.36	0.46
1:A:920:ASN:O	1:A:1080:LYS:HG2	2.14	0.46
1:G:119:LEU:CD2	1:G:124:GLN:NE2	2.78	0.46
2:H:210:ALA:HB3	2:H:211:PRO:CD	2.39	0.46
2:D:210:ALA:HB3	2:D:211:PRO:CD	2.40	0.46
1:C:698:LEU:N	1:C:698:LEU:HD12	2.30	0.46
2:F:161:HIS:CB	2:F:162:PRO:HA	2.43	0.46
2:D:7:LYS:HD2	2:D:508:TYR:CD1	2.49	0.46
1:A:619:GLU:O	1:A:620:CYS:SG	2.73	0.46
2:F:43:ARG:N	2:F:44:PRO:CD	2.78	0.46
2:B:121:LEU:O	2:B:121:LEU:HD23	2.15	0.46
2:F:465:GLY:O	2:F:466:ARG:CG	2.63	0.46
2:F:158:VAL:HA	2:F:208:LEU:HG	1.97	0.46
1:C:676:THR:HG23	1:C:678:ASN:H	1.80	0.46
1:G:799:THR:HA	1:G:845:ARG:HA	1.97	0.46
1:C:465:TYR:CD1	1:C:469:ARG:HG2	2.50	0.46
1:E:465:TYR:CD1	1:E:469:ARG:HG2	2.50	0.46
1:E:354:PHE:CG	9:E:3373:NAG:H62	2.50	0.46
2:F:643:ARG:NH2	2:F:649:TRP:CZ2	2.84	0.46
2:F:39:ARG:HD2	2:F:447:ILE:CG2	2.45	0.46
1:C:609:ILE:HD11	1:G:690:LYS:HB3	1.97	0.46
2:D:118:LEU:HD21	2:D:204:ILE:CD1	2.44	0.46
2:H:118:LEU:HD21	2:H:204:ILE:HD13	1.97	0.46
2:D:35:PRO:HB3	2:D:510:GLN:NE2	2.29	0.46
2:F:212:GLU:HG2	2:F:243:ASP:CB	2.45	0.46
1:A:670:ARG:HG2	1:A:711:ILE:CG2	2.45	0.46
2:H:461:CYS:SG	2:H:466:ARG:CD	3.04	0.46
2:H:334:ILE:HA	2:H:337:ALA:CB	2.45	0.46
1:E:799:THR:HA	1:E:845:ARG:HA	1.98	0.46
2:D:361:ASP:HB2	2:D:390:GLN:HB3	1.97	0.46
1:E:713:LEU:C	1:E:713:LEU:HD23	2.35	0.46
1:C:964:TRP:HB3	1:C:1032:LEU:HG	1.98	0.46
1:E:698:LEU:N	1:E:698:LEU:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1052:GLU:OE1	1:G:756:HIS:HA	2.16	0.46
2:H:75:GLN:HG3	2:H:98:ARG:O	2.15	0.46
1:C:609:ILE:HB	1:C:610:PRO:CD	2.45	0.46
1:A:406:PRO:HB3	1:A:438:TYR:CD2	2.50	0.46
2:D:562:ASN:OD1	2:D:564:ARG:HB2	2.15	0.46
2:F:562:ASN:OD1	2:F:564:ARG:HB2	2.16	0.46
1:A:797:GLY:N	1:A:884:GLU:HB2	2.31	0.46
1:A:698:LEU:HD12	1:A:698:LEU:N	2.30	0.46
2:D:158:VAL:HA	2:D:208:LEU:HG	1.97	0.46
2:H:260:ASN:ND2	2:H:277:PHE:HZ	2.13	0.46
2:B:305:VAL:HG13	2:B:306:LYS:N	2.31	0.46
2:D:652:TYR:HB3	2:D:667:VAL:HA	1.97	0.46
2:F:305:VAL:HG13	2:F:306:LYS:N	2.31	0.46
2:F:597:PRO:O	2:F:598:SER:CB	2.63	0.46
1:G:119:LEU:H	1:G:120:PRO:CA	2.25	0.46
1:A:598:PRO:HB3	1:A:650:ARG:NH1	2.31	0.46
1:G:90:GLY:O	1:G:105:GLY:HA2	2.15	0.46
1:A:164:ARG:CB	1:A:165:PRO:HA	2.44	0.46
1:C:873:ASP:C	1:C:901:VAL:HG12	2.36	0.46
2:F:75:GLN:HG3	2:F:98:ARG:O	2.16	0.46
2:H:103:TYR:HB3	2:H:233:VAL:HG11	1.98	0.46
1:G:478:LEU:HA	1:G:485:TRP:HE1	1.80	0.46
2:B:260:ASN:ND2	2:B:277:PHE:HZ	2.13	0.46
1:E:618:PHE:CD2	1:E:619:GLU:N	2.84	0.46
1:G:780:LEU:C	1:G:780:LEU:HD23	2.36	0.46
1:C:670:ARG:HG2	1:C:711:ILE:CG2	2.46	0.46
1:A:151:MET:SD	1:A:238:ILE:HG21	2.56	0.46
2:D:130:ASP:HA	2:D:133:ARG:HB3	1.98	0.46
2:F:361:ASP:HB2	2:F:390:GLN:HB3	1.97	0.46
1:C:90:GLY:O	1:C:105:GLY:HA2	2.15	0.46
1:A:119:LEU:CD2	1:A:124:GLN:NE2	2.78	0.46
2:F:39:ARG:CD	2:F:447:ILE:HG23	2.46	0.46
1:A:181:HIS:CG	1:A:200:VAL:HG21	2.50	0.46
2:B:143:ARG:C	2:B:144:ILE:HD12	2.36	0.46
2:F:665:ILE:HD12	2:F:665:ILE:N	2.31	0.46
2:D:121:LEU:O	2:D:121:LEU:HD23	2.15	0.46
1:C:831:SER:HA	1:C:842:THR:HG22	1.98	0.46
1:A:1057:THR:HG21	1:C:760:ASP:O	2.16	0.46
2:H:361:ASP:HB2	2:H:390:GLN:HB3	1.97	0.46
1:G:827:LEU:CD1	1:G:829:CYS:SG	3.04	0.46
1:A:827:LEU:HD13	1:A:829:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:TYR:CE2	1:A:407:ARG:HD3	2.51	0.46
1:E:43:GLN:HG2	1:E:44:THR:HG23	1.97	0.46
1:G:698:LEU:HD12	1:G:698:LEU:N	2.30	0.46
2:D:99:ARG:NH1	2:D:101:LYS:O	2.49	0.46
2:H:362:SER:HB2	2:H:370:HIS:HB2	1.96	0.46
2:B:609:CYS:SG	2:B:616:PRO:HB3	2.55	0.46
1:E:416:ILE:HG22	1:E:427:LYS:HD3	1.98	0.46
1:E:476:CYS:HB3	1:E:487:CYS:HA	1.97	0.46
2:B:43:ARG:N	2:B:44:PRO:CD	2.78	0.46
1:A:300:PHE:O	1:A:303:LEU:HB3	2.15	0.46
1:G:827:LEU:HD13	1:G:829:CYS:SG	2.55	0.46
2:H:130:ASP:HA	2:H:133:ARG:HB3	1.98	0.46
2:F:352:LEU:CD2	2:F:358:VAL:HG23	2.45	0.46
1:E:827:LEU:HD13	1:E:829:CYS:SG	2.56	0.46
1:E:564:TYR:CZ	1:E:588:ARG:HD2	2.51	0.46
1:A:894:THR:O	1:C:874:ARG:NH2	2.48	0.46
2:B:158:VAL:HA	2:B:208:LEU:HG	1.97	0.46
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.97	0.46
2:D:143:ARG:C	2:D:144:ILE:HD12	2.36	0.46
1:C:25:TYR:CG	1:C:26:ALA:N	2.84	0.46
1:A:25:TYR:CG	1:A:26:ALA:N	2.84	0.46
1:C:827:LEU:CD1	1:C:829:CYS:SG	3.04	0.46
2:H:120:ASP:O	2:H:124:VAL:HB	2.16	0.46
2:B:120:ASP:O	2:B:124:VAL:HB	2.16	0.46
1:A:448:VAL:HA	1:A:518:THR:HG22	1.98	0.46
2:H:158:VAL:HA	2:H:208:LEU:HG	1.97	0.46
2:B:293:ASN:OD1	2:B:412:THR:HG22	2.16	0.46
1:C:713:LEU:C	1:C:713:LEU:HD23	2.36	0.46
1:A:465:TYR:CD1	1:A:469:ARG:HG2	2.50	0.46
1:G:119:LEU:O	1:G:363:TYR:HE1	1.96	0.46
1:G:43:GLN:HG2	1:G:44:THR:HG23	1.97	0.46
1:C:909:VAL:HG12	1:C:1069:PHE:O	2.16	0.46
1:E:625:VAL:CG2	1:E:627:GLU:HG3	2.40	0.46
1:G:1063:LEU:N	1:G:1064:PRO:CD	2.79	0.46
2:F:23:TRP:HH2	2:F:447:ILE:HD13	1.81	0.46
1:E:797:GLY:N	1:E:884:GLU:HB2	2.31	0.46
1:A:430:VAL:HG13	1:A:485:TRP:CE3	2.51	0.46
2:H:295:GLN:CD	2:H:317:LYS:HE2	2.35	0.46
2:F:143:ARG:C	2:F:144:ILE:HD12	2.36	0.46
1:A:263:ILE:HD12	1:A:317:ILE:HD12	1.98	0.46
2:D:465:GLY:O	2:D:466:ARG:CG	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:465:GLY:O	2:H:466:ARG:CG	2.64	0.46
1:E:827:LEU:CD1	1:E:829:CYS:SG	3.04	0.46
2:F:334:ILE:HA	2:F:337:ALA:CB	2.46	0.46
1:G:663:ASP:N	1:G:664:PRO:HD3	2.31	0.46
1:A:752:CYS:SG	1:A:758:CYS:N	2.89	0.46
1:G:564:TYR:CZ	1:G:588:ARG:HD2	2.51	0.46
1:C:1028:LEU:HD12	1:C:1028:LEU:O	2.16	0.46
1:A:354:PHE:CE2	4:A:3373:NAG:O5	2.69	0.45
1:C:1063:LEU:N	1:C:1064:PRO:CD	2.79	0.45
1:G:873:ASP:C	1:G:901:VAL:HG12	2.37	0.45
2:H:643:ARG:NH2	2:H:649:TRP:CZ2	2.84	0.45
1:A:308:ASN:O	1:A:311:LYS:HD3	2.17	0.45
1:C:797:GLY:N	1:C:884:GLU:HB2	2.31	0.45
1:G:430:VAL:HG13	1:G:485:TRP:CE3	2.51	0.45
2:H:665:ILE:N	2:H:665:ILE:HD12	2.31	0.45
1:A:827:LEU:CD1	1:A:829:CYS:SG	3.04	0.45
2:B:673:CYS:O	2:B:674:VAL:C	2.54	0.45
1:A:980:SER:HB3	1:A:1012:ARG:HB3	1.97	0.45
1:G:448:VAL:HA	1:G:518:THR:HG22	1.98	0.45
1:A:564:TYR:CZ	1:A:588:ARG:HD2	2.51	0.45
1:E:959:ASN:O	1:E:960:GLN:HB3	2.16	0.45
2:D:334:ILE:HA	2:D:337:ALA:CB	2.45	0.45
1:C:430:VAL:HG13	1:C:485:TRP:CE3	2.51	0.45
1:A:1020:VAL:O	1:A:1021:GLN:HB2	2.16	0.45
1:C:938:VAL:HG12	1:C:1024:LEU:O	2.16	0.45
1:A:873:ASP:C	1:A:901:VAL:HG12	2.37	0.45
2:D:345:VAL:HG11	2:D:387:ILE:CD1	2.46	0.45
1:A:757:ILE:HG21	1:C:1054:THR:HG21	1.97	0.45
2:B:562:ASN:OD1	2:B:564:ARG:HB2	2.16	0.45
1:A:739:GLN:HB2	1:A:742:PHE:CE1	2.51	0.45
1:C:575:LEU:HD12	1:C:576:THR:CG2	2.47	0.45
2:B:465:GLY:O	2:B:466:ARG:CG	2.64	0.45
2:D:219:MET:HE2	2:D:262:GLY:HA2	1.97	0.45
1:A:1048:VAL:HG22	1:A:1075:THR:HB	1.99	0.45
1:G:959:ASN:O	1:G:960:GLN:HB3	2.16	0.45
2:D:305:VAL:HG13	2:D:306:LYS:N	2.31	0.45
2:D:120:ASP:O	2:D:124:VAL:HB	2.16	0.45
2:F:652:TYR:HB3	2:F:667:VAL:HA	1.98	0.45
2:D:601:GLY:O	2:D:602:LYS:HB2	2.16	0.45
1:E:789:TRP:NE1	1:G:772:LYS:CB	2.79	0.45
1:G:964:TRP:HB3	1:G:1032:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:PHE:CD1	1:G:117:GLN:HG2	2.52	0.45
1:E:681:LEU:HD12	1:E:682:SER:N	2.32	0.45
1:C:18:PHE:CZ	1:C:32:VAL:HG21	2.51	0.45
1:A:402:VAL:HG22	1:A:416:ILE:HG23	1.98	0.45
1:A:476:CYS:HB3	1:A:487:CYS:HA	1.97	0.45
1:E:739:GLN:HB2	1:E:742:PHE:CE1	2.52	0.45
1:E:402:VAL:HG22	1:E:416:ILE:HG23	1.98	0.45
2:D:665:ILE:HD12	2:D:665:ILE:N	2.31	0.45
2:D:271:TYR:O	2:D:271:TYR:CG	2.69	0.45
2:F:83:LEU:HD12	2:F:83:LEU:O	2.16	0.45
2:F:271:TYR:O	2:F:271:TYR:CG	2.69	0.45
1:E:670:ARG:HG2	1:E:711:ILE:CG2	2.45	0.45
1:A:959:ASN:O	1:A:960:GLN:HB3	2.16	0.45
1:E:437:SER:HA	1:E:463:HIS:O	2.17	0.45
2:B:601:GLY:O	2:B:602:LYS:HB2	2.17	0.45
2:F:234:THR:CG2	2:F:236:LEU:HD13	2.45	0.45
1:C:613:ILE:HD12	1:C:748:PHE:CD2	2.52	0.45
2:H:35:PRO:HG2	2:H:510:GLN:CD	2.37	0.45
2:B:643:ARG:NH2	2:B:649:TRP:CZ2	2.85	0.45
1:A:663:ASP:N	1:A:664:PRO:HD3	2.31	0.45
1:E:964:TRP:HB3	1:E:1032:LEU:HG	1.98	0.45
1:A:108:PHE:CD1	1:A:117:GLN:HG2	2.52	0.45
1:E:478:LEU:HA	1:E:485:TRP:HE1	1.80	0.45
1:A:909:VAL:HG12	1:A:1069:PHE:O	2.16	0.45
1:E:25:TYR:CG	1:E:26:ALA:N	2.85	0.45
2:D:83:LEU:HD12	2:D:83:LEU:O	2.17	0.45
1:A:565:PHE:O	1:A:565:PHE:CD2	2.69	0.45
1:C:827:LEU:HD13	1:C:829:CYS:SG	2.56	0.45
1:E:448:VAL:HA	1:E:518:THR:HG22	1.98	0.45
2:H:652:TYR:HB3	2:H:667:VAL:HA	1.98	0.45
2:D:656:GLN:HG2	2:D:657:GLN:N	2.29	0.45
1:E:385:TYR:CE2	1:E:407:ARG:HD3	2.51	0.45
1:C:799:THR:HG22	1:C:845:ARG:CB	2.47	0.45
1:C:448:VAL:HA	1:C:518:THR:HG22	1.98	0.45
1:C:775:LEU:CD1	1:C:904:ALA:HB2	2.46	0.45
2:F:130:ASP:HA	2:F:133:ARG:HB3	1.98	0.45
1:G:475:VAL:HG12	1:G:491:LEU:O	2.16	0.45
1:E:491:LEU:HD11	1:E:545:ILE:HD11	1.99	0.45
1:E:822:LEU:HG	1:E:823:ARG:N	2.22	0.45
1:G:103:LEU:HD12	2:H:156:PRO:HB3	1.96	0.45
1:C:816:GLY:O	1:C:818:LYS:CA	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:532:ARG:O	2:F:543:HIS:HB2	2.17	0.45
2:F:382:GLN:HG3	2:F:383:ILE:H	1.81	0.45
1:G:609:ILE:HB	1:G:610:PRO:CD	2.45	0.45
1:A:18:PHE:CZ	1:A:32:VAL:HG21	2.51	0.45
1:G:909:VAL:HG12	1:G:1069:PHE:O	2.15	0.45
1:E:575:LEU:HD12	1:E:576:THR:CG2	2.47	0.45
2:F:186:LEU:HD21	2:F:198:GLU:CB	2.47	0.45
2:D:186:LEU:HD21	2:D:198:GLU:CB	2.47	0.45
2:B:130:ASP:HA	2:B:133:ARG:HB3	1.98	0.45
1:G:1048:VAL:HG22	1:G:1075:THR:HB	1.98	0.45
1:E:663:ASP:N	1:E:664:PRO:HD3	2.31	0.45
2:B:652:TYR:HB3	2:B:667:VAL:HA	1.98	0.45
1:G:437:SER:HA	1:G:463:HIS:O	2.16	0.45
2:F:219:MET:HE2	2:F:262:GLY:HA2	1.97	0.45
1:A:491:LEU:HD11	1:A:545:ILE:HD11	1.99	0.45
1:C:681:LEU:HD12	1:C:682:SER:N	2.32	0.45
2:B:382:GLN:HG3	2:B:383:ILE:H	1.81	0.45
2:B:75:GLN:HG3	2:B:98:ARG:O	2.16	0.45
1:G:18:PHE:CZ	1:G:32:VAL:HG21	2.51	0.45
1:G:797:GLY:H	1:G:884:GLU:HB2	1.81	0.45
1:A:986:PRO:HG3	1:A:1003:CYS:O	2.17	0.45
2:B:616:PRO:HB2	2:B:620:ASN:CA	2.47	0.45
1:G:569:LEU:HD12	1:G:569:LEU:O	2.17	0.45
2:H:143:ARG:C	2:H:144:ILE:HD12	2.36	0.45
1:A:938:VAL:HG12	1:A:1024:LEU:O	2.17	0.45
1:A:1069:PHE:CZ	2:B:584:GLY:HA3	2.52	0.45
1:C:25:TYR:O	1:C:26:ALA:C	2.52	0.45
1:C:780:LEU:C	1:C:780:LEU:HD23	2.36	0.45
1:E:565:PHE:O	1:E:565:PHE:CD2	2.69	0.45
1:A:780:LEU:HD23	1:A:780:LEU:C	2.36	0.45
1:A:831:SER:HA	1:A:842:THR:HG22	1.98	0.45
1:A:799:THR:HG22	1:A:845:ARG:CB	2.47	0.45
1:E:799:THR:HG22	1:E:845:ARG:CB	2.47	0.45
1:C:663:ASP:N	1:C:664:PRO:HD3	2.31	0.45
1:G:601:TRP:HZ2	1:G:641:LYS:HD3	1.81	0.45
1:C:1048:VAL:HG22	1:C:1075:THR:HB	1.98	0.45
1:G:566:GLY:O	1:G:567:GLN:C	2.53	0.45
1:E:629:THR:CG2	1:E:630:LEU:N	2.80	0.45
1:E:1048:VAL:HG22	1:E:1075:THR:HB	1.98	0.45
2:F:120:ASP:O	2:F:124:VAL:HB	2.16	0.45
1:G:491:LEU:HD11	1:G:545:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:938:VAL:HG12	1:E:1024:LEU:O	2.16	0.45
1:E:873:ASP:C	1:E:901:VAL:HG12	2.37	0.45
2:D:75:GLN:HG3	2:D:98:ARG:O	2.16	0.45
1:E:18:PHE:CZ	1:E:32:VAL:HG21	2.51	0.45
2:H:562:ASN:OD1	2:H:564:ARG:HB2	2.16	0.45
1:A:416:ILE:HG22	1:A:427:LYS:HD3	1.98	0.45
1:C:739:GLN:HB2	1:C:742:PHE:CE1	2.52	0.45
1:G:575:LEU:HD12	1:G:576:THR:CG2	2.47	0.45
2:B:665:ILE:HD12	2:B:665:ILE:N	2.31	0.45
2:F:83:LEU:HD11	2:F:419:VAL:HG13	1.99	0.45
1:E:348:LEU:HD12	1:E:348:LEU:N	2.32	0.45
1:C:385:TYR:CE2	1:C:407:ARG:HD3	2.51	0.45
2:B:168:PRO:CG	2:B:179:PRO:HG3	2.47	0.45
2:H:168:PRO:CG	2:H:179:PRO:HG3	2.47	0.45
2:H:382:GLN:HG3	2:H:383:ILE:H	1.81	0.45
1:C:491:LEU:HD11	1:C:545:ILE:HD11	1.99	0.45
2:D:154:VAL:HA	2:D:160:THR:CG2	2.47	0.45
2:H:154:VAL:HA	2:H:160:THR:CG2	2.47	0.45
1:G:681:LEU:HD12	1:G:682:SER:N	2.32	0.45
2:F:546:PHE:CD2	2:F:554:GLU:O	2.69	0.45
1:A:609:ILE:HD12	1:A:632:GLN:OE1	2.17	0.45
1:G:444:CYS:HB2	1:G:506:LEU:HD12	1.99	0.45
1:C:444:CYS:HB2	1:C:506:LEU:HD12	1.99	0.45
2:B:186:LEU:HD21	2:B:198:GLU:CB	2.47	0.45
1:C:961:GLU:HG2	1:C:1036:TRP:HA	1.99	0.45
1:C:354:PHE:CG	3:C:3373:NAG:H62	2.51	0.45
1:E:831:SER:HA	1:E:842:THR:HG22	1.98	0.45
1:C:959:ASN:O	1:C:960:GLN:HB3	2.16	0.45
2:H:601:GLY:O	2:H:602:LYS:HB2	2.17	0.45
2:D:673:CYS:O	2:D:674:VAL:C	2.55	0.45
1:A:527:GLU:HG3	1:A:533:ALA:CB	2.47	0.45
1:G:629:THR:CG2	1:G:630:LEU:N	2.80	0.45
1:G:801:THR:HG22	1:G:843:SER:CB	2.47	0.45
1:C:1069:PHE:CE2	2:D:584:GLY:HA3	2.52	0.45
1:A:1063:LEU:N	1:A:1064:PRO:CD	2.79	0.45
1:E:1063:LEU:N	1:E:1064:PRO:CD	2.79	0.45
2:H:100:ALA:O	2:H:101:LYS:CB	2.62	0.45
2:H:532:ARG:O	2:H:543:HIS:HB2	2.17	0.45
1:A:243:LYS:HB2	1:A:246:ASP:HB2	1.98	0.45
1:E:430:VAL:HG13	1:E:485:TRP:CE3	2.51	0.45
2:D:347:LEU:HD22	2:D:389:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:LEU:HD11	2:H:419:VAL:HG13	1.99	0.45
1:C:565:PHE:CD2	1:C:565:PHE:O	2.69	0.45
1:A:269:VAL:HA	1:A:297:VAL:O	2.17	0.45
2:H:552:GLN:HG3	2:H:553:CYS:H	1.82	0.45
1:G:799:THR:HG22	1:G:845:ARG:CB	2.47	0.45
2:F:188:LEU:HD12	2:F:230:TRP:HA	1.99	0.45
1:A:653:GLN:HB2	1:E:630:LEU:HD21	1.99	0.45
1:G:613:ILE:HD12	1:G:748:PHE:CD2	2.52	0.45
1:A:613:ILE:HD12	1:A:748:PHE:CD2	2.52	0.45
1:G:527:GLU:HG3	1:G:533:ALA:CB	2.47	0.45
1:A:801:THR:HG22	1:A:843:SER:CB	2.47	0.45
1:E:980:SER:HB3	1:E:1012:ARG:HB3	1.97	0.45
1:C:416:ILE:HG22	1:C:427:LYS:HD3	1.98	0.45
1:A:475:VAL:HG12	1:A:491:LEU:O	2.17	0.45
2:F:154:VAL:HA	2:F:160:THR:CG2	2.47	0.45
2:B:154:VAL:HA	2:B:160:THR:CG2	2.47	0.45
1:A:657:THR:HG23	1:A:720:VAL:CB	2.45	0.45
1:A:609:ILE:HB	1:A:610:PRO:CD	2.45	0.45
1:A:629:THR:CG2	1:A:630:LEU:N	2.79	0.45
1:A:418:THR:HB	1:A:427:LYS:CG	2.47	0.45
1:G:25:TYR:CG	1:G:26:ALA:N	2.84	0.45
1:E:764:ILE:HD12	1:E:800:ILE:HD13	1.99	0.45
1:E:801:THR:HG22	1:E:843:SER:CB	2.47	0.45
1:A:137:ILE:HD13	1:A:152:MET:SD	2.57	0.45
1:C:801:THR:HG22	1:C:843:SER:CB	2.47	0.45
1:C:73:LEU:C	1:C:73:LEU:HD12	2.38	0.45
4:A:3377:MAN:C3	5:A:3378:MAN:C1	2.95	0.44
1:A:464:TYR:HD2	1:A:472:GLN:HB2	1.82	0.44
1:C:464:TYR:HD2	1:C:472:GLN:HB2	1.82	0.44
1:A:822:LEU:HG	1:A:823:ARG:N	2.21	0.44
1:C:108:PHE:CD1	1:C:117:GLN:HG2	2.52	0.44
2:B:532:ARG:O	2:B:543:HIS:HB2	2.16	0.44
1:E:797:GLY:H	1:E:884:GLU:HB2	1.82	0.44
2:D:36:ASP:N	2:D:510:GLN:HE22	2.15	0.44
1:E:956:VAL:HG12	1:E:957:GLU:N	2.32	0.44
1:C:956:VAL:HG12	1:C:957:GLU:N	2.32	0.44
1:A:303:LEU:O	1:A:306:ILE:HG12	2.17	0.44
2:D:453:GLY:HA2	2:D:463:THR:HG21	1.99	0.44
1:C:764:ILE:HD12	1:C:800:ILE:HD13	1.99	0.44
2:H:305:VAL:HG13	2:H:306:LYS:HG3	1.99	0.44
2:F:305:VAL:HG13	2:F:306:LYS:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:SER:HA	1:A:463:HIS:O	2.17	0.44
1:G:1001:LEU:HD23	1:G:1001:LEU:O	2.18	0.44
1:G:385:TYR:CE2	1:G:407:ARG:HD3	2.51	0.44
1:C:418:THR:HB	1:C:427:LYS:CG	2.48	0.44
1:G:598:PRO:HG2	1:G:650:ARG:HD2	1.99	0.44
2:D:587:LEU:N	2:D:587:LEU:CD1	2.80	0.44
1:E:986:PRO:HG3	1:E:1003:CYS:O	2.17	0.44
1:A:797:GLY:H	1:A:884:GLU:HB2	1.82	0.44
2:F:616:PRO:HB2	2:F:620:ASN:CA	2.47	0.44
2:B:188:LEU:HD12	2:B:230:TRP:HA	1.99	0.44
2:F:317:LYS:HE3	2:F:410:GLY:HA3	1.99	0.44
1:E:569:LEU:HD12	1:E:569:LEU:O	2.17	0.44
2:B:83:LEU:HD12	2:B:83:LEU:O	2.17	0.44
1:C:534:VAL:HG23	1:C:565:PHE:CE2	2.53	0.44
1:G:89:CYS:O	1:G:91:PRO:HD3	2.18	0.44
1:G:348:LEU:N	1:G:348:LEU:HD12	2.32	0.44
1:A:407:ARG:HG2	2:B:247:PHE:CZ	2.52	0.44
1:E:717:PHE:CE1	1:E:740:ARG:HA	2.52	0.44
1:E:752:CYS:SG	1:E:758:CYS:N	2.90	0.44
2:B:432:ARG:O	2:B:433:ASP:HB2	2.17	0.44
2:B:436:LEU:O	2:B:437:CYS:HB2	2.17	0.44
2:H:188:LEU:HD12	2:H:230:TRP:HA	2.00	0.44
1:E:992:LEU:C	1:E:992:LEU:HD23	2.37	0.44
1:E:73:LEU:C	1:E:73:LEU:HD12	2.38	0.44
1:A:956:VAL:HG12	1:A:957:GLU:N	2.32	0.44
1:C:402:VAL:HG22	1:C:416:ILE:HG23	1.98	0.44
1:C:475:VAL:HG12	1:C:491:LEU:O	2.16	0.44
1:E:475:VAL:HG12	1:E:491:LEU:O	2.17	0.44
1:C:116:THR:HG22	1:C:118:ARG:HG3	1.99	0.44
1:E:108:PHE:CD1	1:E:117:GLN:HG2	2.52	0.44
2:D:643:ARG:NH2	2:D:649:TRP:CZ2	2.85	0.44
1:E:919:LEU:CB	1:E:1079:GLU:HB3	2.46	0.44
2:D:382:GLN:HG3	2:D:383:ILE:H	1.82	0.44
2:D:98:ARG:O	2:D:99:ARG:C	2.56	0.44
1:C:797:GLY:H	1:C:884:GLU:HB2	1.82	0.44
1:G:739:GLN:HB2	1:G:742:PHE:CE1	2.52	0.44
2:F:103:TYR:HB3	2:F:233:VAL:HG11	1.99	0.44
1:G:418:THR:HB	1:G:427:LYS:CG	2.48	0.44
1:G:938:VAL:HG12	1:G:1024:LEU:O	2.17	0.44
1:A:1024:LEU:C	1:A:1024:LEU:HD23	2.38	0.44
1:G:565:PHE:O	1:G:565:PHE:CD2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:LEU:HD12	1:C:348:LEU:N	2.32	0.44
2:F:601:GLY:O	2:F:602:LYS:HB2	2.17	0.44
1:C:564:TYR:CZ	1:C:588:ARG:HD2	2.52	0.44
1:E:601:TRP:HZ2	1:E:641:LYS:HD3	1.81	0.44
2:H:436:LEU:O	2:H:437:CYS:HB2	2.17	0.44
1:C:527:GLU:HG3	1:C:533:ALA:CB	2.47	0.44
1:G:717:PHE:CE1	1:G:740:ARG:HA	2.52	0.44
1:G:598:PRO:HB3	1:G:650:ARG:HH12	1.82	0.44
1:E:354:PHE:CE2	9:E:3373:NAG:O5	2.70	0.44
1:E:1024:LEU:HD23	1:E:1024:LEU:C	2.38	0.44
2:F:75:GLN:CG	2:F:98:ARG:O	2.66	0.44
1:E:609:ILE:HB	1:E:610:PRO:CD	2.45	0.44
1:G:416:ILE:HG22	1:G:427:LYS:HD3	1.98	0.44
2:D:103:TYR:HB3	2:D:233:VAL:HG11	1.99	0.44
2:H:186:LEU:HD21	2:H:198:GLU:CB	2.47	0.44
1:G:956:VAL:HG12	1:G:957:GLU:N	2.32	0.44
2:F:144:ILE:HG22	2:F:195:PHE:CZ	2.53	0.44
2:B:271:TYR:CG	2:B:271:TYR:O	2.70	0.44
2:D:305:VAL:HG13	2:D:306:LYS:HG3	1.99	0.44
2:D:168:PRO:CG	2:D:179:PRO:HG3	2.47	0.44
1:A:717:PHE:CE1	1:A:740:ARG:HA	2.53	0.44
2:D:77:SER:HA	2:D:78:PRO:C	2.37	0.44
2:F:631:SER:HB3	2:F:664:LEU:HD11	1.99	0.44
2:F:112:ASP:O	2:F:117:MET:HG3	2.17	0.44
1:E:116:THR:HG22	1:E:118:ARG:HG3	2.00	0.44
1:C:629:THR:CG2	1:C:630:LEU:N	2.80	0.44
2:D:75:GLN:CG	2:D:98:ARG:O	2.66	0.44
1:A:444:CYS:HB2	1:A:506:LEU:HD12	1.98	0.44
1:A:569:LEU:HD12	1:A:569:LEU:O	2.17	0.44
1:E:444:CYS:HB2	1:E:506:LEU:HD12	1.99	0.44
1:C:569:LEU:HD12	1:C:569:LEU:O	2.17	0.44
1:G:1024:LEU:C	1:G:1024:LEU:HD23	2.38	0.44
2:B:144:ILE:HG22	2:B:195:PHE:CZ	2.53	0.44
1:G:961:GLU:HG2	1:G:1036:TRP:HA	1.99	0.44
1:C:89:CYS:O	1:C:91:PRO:HD3	2.18	0.44
2:H:271:TYR:CG	2:H:271:TYR:O	2.70	0.44
1:G:565:PHE:HB2	1:G:587:ALA:CB	2.48	0.44
1:C:766:PHE:HZ	1:C:877:LEU:HD12	1.83	0.44
2:H:522:TYR:CE1	2:H:552:GLN:HA	2.53	0.44
2:H:158:VAL:HB	2:H:207:ASN:HB2	2.00	0.44
1:A:134:VAL:O	1:A:235:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:436:LEU:O	2:F:437:CYS:HB2	2.17	0.44
1:A:553:ILE:HG23	1:A:557:GLN:HG3	2.00	0.44
1:G:4:ASP:OD2	1:G:597:ARG:NH2	2.51	0.44
1:A:964:TRP:HB3	1:A:1032:LEU:HG	1.99	0.44
2:H:345:VAL:HG11	2:H:387:ILE:CD1	2.47	0.44
2:H:75:GLN:CG	2:H:98:ARG:O	2.65	0.44
1:C:986:PRO:HG3	1:C:1003:CYS:O	2.17	0.44
1:E:418:THR:HB	1:E:427:LYS:CG	2.47	0.44
2:H:83:LEU:O	2:H:83:LEU:HD12	2.16	0.44
1:A:89:CYS:O	1:A:91:PRO:HD3	2.18	0.44
2:B:345:VAL:HG11	2:B:387:ILE:HD11	1.99	0.44
1:E:89:CYS:O	1:E:91:PRO:HD3	2.18	0.44
2:F:158:VAL:HB	2:F:207:ASN:HB2	1.99	0.44
1:C:799:THR:HA	1:C:845:ARG:HA	1.98	0.44
2:D:168:PRO:HG2	2:D:179:PRO:HG3	1.99	0.44
1:E:527:GLU:HG3	1:E:533:ALA:CB	2.47	0.44
2:B:77:SER:HA	2:B:78:PRO:C	2.37	0.44
1:C:717:PHE:CE1	1:C:740:ARG:HA	2.52	0.44
1:A:1001:LEU:O	1:A:1001:LEU:HD23	2.18	0.44
1:C:908:VAL:CG1	2:D:595:GLY:HA3	2.41	0.44
1:A:116:THR:HG22	1:A:118:ARG:HG3	2.00	0.44
1:A:953:TRP:CD2	1:C:755:ASP:HB3	2.52	0.44
1:A:254:ILE:HG23	1:A:264:ARG:NH2	2.32	0.44
2:F:368:VAL:HG11	2:F:370:HIS:CE1	2.53	0.44
1:G:402:VAL:HG22	1:G:416:ILE:HG23	1.98	0.44
1:E:534:VAL:HG23	1:E:565:PHE:CE2	2.53	0.44
1:A:534:VAL:HG12	1:A:535:TYR:N	2.33	0.44
1:A:110:LEU:HG	1:A:115:LEU:CD2	2.48	0.44
2:B:158:VAL:HB	2:B:207:ASN:HB2	1.99	0.44
1:E:119:LEU:O	1:E:363:TYR:HE1	1.97	0.44
1:C:119:LEU:HD23	1:C:124:GLN:HE21	1.83	0.44
1:A:367:MET:HG2	1:A:368:SER:O	2.18	0.44
2:D:317:LYS:HG3	2:D:346:PHE:CE1	2.53	0.44
1:A:816:GLY:O	1:A:818:LYS:CA	2.66	0.44
1:A:270:GLY:O	1:A:271:LEU:HB3	2.18	0.44
1:G:609:ILE:HD12	1:G:632:GLN:OE1	2.18	0.44
2:B:368:VAL:HG11	2:B:370:HIS:CE1	2.53	0.44
1:E:1020:VAL:O	1:E:1021:GLN:HB2	2.18	0.44
2:B:103:TYR:HB3	2:B:233:VAL:HG11	1.98	0.44
1:A:575:LEU:HD12	1:A:576:THR:CG2	2.47	0.44
1:E:565:PHE:HB2	1:E:587:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:553:ILE:HG23	1:E:557:GLN:HG3	2.00	0.44
1:A:1081:TYR:O	1:A:1082:LYS:HB2	2.18	0.44
1:G:20:ASP:OD1	2:H:257:LEU:HD22	2.18	0.44
2:D:436:LEU:O	2:D:437:CYS:HB2	2.17	0.44
2:H:112:ASP:O	2:H:117:MET:HG3	2.17	0.44
1:A:961:GLU:HG2	1:A:1036:TRP:HA	1.99	0.44
2:B:289:LEU:HD12	2:B:294:ILE:HB	2.00	0.44
2:H:289:LEU:HD12	2:H:294:ILE:HB	2.00	0.44
1:G:119:LEU:HD23	1:G:124:GLN:HE21	1.83	0.44
1:G:822:LEU:CG	1:G:823:ARG:N	2.81	0.44
2:B:99:ARG:O	2:B:383:ILE:O	2.36	0.44
2:B:75:GLN:CG	2:B:98:ARG:O	2.66	0.44
2:B:587:LEU:N	2:B:587:LEU:CD1	2.80	0.44
2:D:368:VAL:HG11	2:D:370:HIS:CE1	2.53	0.44
2:D:277:PHE:CE1	2:D:278:ASP:O	2.71	0.44
1:G:525:PRO:HA	1:G:532:GLY:HA2	2.00	0.44
1:G:534:VAL:HG12	1:G:535:TYR:N	2.33	0.44
1:G:534:VAL:HG23	1:G:565:PHE:CE2	2.53	0.44
1:A:565:PHE:HB2	1:A:587:ALA:CB	2.48	0.44
2:B:112:ASP:O	2:B:117:MET:HG3	2.17	0.44
1:E:22:VAL:HG22	1:E:23:VAL:N	2.33	0.44
2:H:108:TYR:CE2	2:H:147:GLY:HA3	2.53	0.44
2:D:112:ASP:O	2:D:117:MET:HG3	2.17	0.44
1:C:22:VAL:HG22	1:C:23:VAL:N	2.33	0.44
1:E:367:MET:HG2	1:E:368:SER:O	2.18	0.43
1:C:367:MET:HG2	1:C:368:SER:O	2.18	0.43
1:C:103:LEU:HD11	2:D:155:LEU:HD13	2.00	0.43
1:A:681:LEU:HD12	1:A:682:SER:N	2.32	0.43
2:F:98:ARG:O	2:F:99:ARG:C	2.57	0.43
1:A:254:ILE:HB	1:A:255:PRO:HD3	2.00	0.43
2:D:532:ARG:O	2:D:543:HIS:HB2	2.17	0.43
2:H:144:ILE:HG22	2:H:195:PHE:CZ	2.53	0.43
1:C:525:PRO:HA	1:C:532:GLY:HA2	2.00	0.43
1:C:565:PHE:HB2	1:C:587:ALA:CB	2.48	0.43
2:H:461:CYS:SG	2:H:466:ARG:NE	2.91	0.43
2:B:305:VAL:HG13	2:B:306:LYS:HG3	1.99	0.43
1:G:22:VAL:HG22	1:G:23:VAL:N	2.33	0.43
1:C:1001:LEU:HD23	1:C:1001:LEU:O	2.18	0.43
1:G:986:PRO:HG3	1:G:1003:CYS:O	2.17	0.43
2:H:277:PHE:CE1	2:H:278:ASP:O	2.71	0.43
2:F:347:LEU:HD22	2:F:389:PHE:CG	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:PHE:CE1	2:B:278:ASP:O	2.71	0.43
1:A:348:LEU:N	1:A:348:LEU:HD12	2.32	0.43
1:A:419:GLN:HA	1:A:424:TRP:HA	2.00	0.43
2:F:168:PRO:CG	2:F:179:PRO:HG3	2.47	0.43
2:B:108:TYR:CE2	2:B:147:GLY:HA3	2.53	0.43
1:G:553:ILE:HG23	1:G:557:GLN:HG3	2.00	0.43
1:E:597:ARG:HA	1:E:598:PRO:HD3	1.88	0.43
1:G:354:PHE:CE2	9:G:3373:NAG:O5	2.71	0.43
1:C:103:LEU:HD12	2:D:156:PRO:HB3	2.00	0.43
1:E:71:MET:SD	1:E:90:GLY:HA3	2.59	0.43
2:D:354:ASP:O	2:D:544:PRO:CB	2.66	0.43
2:H:616:PRO:HB2	2:H:620:ASN:CA	2.47	0.43
2:H:368:VAL:HG11	2:H:370:HIS:CE1	2.53	0.43
2:H:103:TYR:HB3	2:H:104:PRO:CD	2.48	0.43
1:A:915:PHE:CZ	1:A:917:LYS:HB2	2.53	0.43
1:C:917:LYS:HE3	1:C:1077:VAL:HG23	2.00	0.43
2:H:347:LEU:HD22	2:H:389:PHE:CG	2.53	0.43
1:C:110:LEU:HG	1:C:115:LEU:CD2	2.48	0.43
1:C:534:VAL:HG12	1:C:535:TYR:N	2.33	0.43
2:D:552:GLN:HG3	2:D:553:CYS:H	1.83	0.43
1:G:764:ILE:HD12	1:G:800:ILE:HD13	1.99	0.43
1:A:764:ILE:HD12	1:A:800:ILE:HD13	1.99	0.43
1:E:639:ILE:HG13	1:E:689:LEU:HA	2.00	0.43
1:C:437:SER:HA	1:C:463:HIS:O	2.17	0.43
1:C:930:HIS:O	1:C:931:VAL:C	2.57	0.43
1:A:361:PHE:CE2	1:A:371:PHE:CE1	3.06	0.43
1:E:613:ILE:HD12	1:E:748:PHE:CD2	2.52	0.43
2:D:108:TYR:CE2	2:D:147:GLY:HA3	2.53	0.43
1:A:73:LEU:HD12	1:A:73:LEU:C	2.38	0.43
1:G:116:THR:HG22	1:G:118:ARG:HG3	2.00	0.43
2:D:289:LEU:HD12	2:D:294:ILE:HB	2.00	0.43
2:B:10:SER:HA	2:B:447:ILE:HD11	2.01	0.43
2:D:83:LEU:HD11	2:D:419:VAL:HG13	1.99	0.43
2:F:345:VAL:HG11	2:F:387:ILE:HD11	1.99	0.43
1:G:934:HIS:ND1	1:G:1074:THR:HB	2.33	0.43
2:B:466:ARG:O	2:B:467:SER:CB	2.65	0.43
1:A:799:THR:HG22	1:A:845:ARG:HB3	2.00	0.43
1:E:799:THR:HG22	1:E:845:ARG:HB3	2.00	0.43
1:C:553:ILE:HG23	1:C:557:GLN:HG3	2.00	0.43
1:A:634:ASN:HB2	1:A:695:ASN:HB3	2.01	0.43
1:E:665:GLY:HA3	2:F:498:HIS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:289:LEU:HD12	2:F:294:ILE:HB	2.00	0.43
1:E:657:THR:HG23	1:E:720:VAL:CB	2.45	0.43
1:C:919:LEU:CB	1:C:1079:GLU:HB3	2.46	0.43
2:B:616:PRO:HB3	2:B:621:CYS:SG	2.58	0.43
1:G:402:VAL:HG12	1:G:443:LEU:HD22	2.00	0.43
1:E:961:GLU:HG2	1:E:1036:TRP:HA	1.99	0.43
2:D:251:GLY:HA3	2:D:278:ASP:OD1	2.19	0.43
1:E:915:PHE:CZ	1:E:917:LYS:HB2	2.53	0.43
1:E:534:VAL:HG12	1:E:535:TYR:N	2.33	0.43
1:A:534:VAL:HG23	1:A:565:PHE:CE2	2.53	0.43
1:C:656:VAL:HG13	1:C:718:THR:O	2.18	0.43
2:H:611:LYS:HG2	2:H:667:VAL:HB	2.01	0.43
1:A:234:ILE:HD13	1:A:314:ILE:HG23	2.00	0.43
2:F:432:ARG:O	2:F:433:ASP:HB2	2.17	0.43
1:E:1045:VAL:HG22	1:E:1046:SER:N	2.34	0.43
2:D:455:ILE:HG22	2:D:494:GLN:CD	2.37	0.43
1:E:464:TYR:HD2	1:E:472:GLN:HB2	1.83	0.43
1:C:71:MET:SD	1:C:90:GLY:HA3	2.59	0.43
1:C:1024:LEU:HD23	1:C:1024:LEU:C	2.38	0.43
1:G:657:THR:HG23	1:G:720:VAL:CB	2.45	0.43
1:E:771:LEU:O	1:G:789:TRP:CZ2	2.71	0.43
1:C:919:LEU:HG	2:D:643:ARG:NH1	2.33	0.43
2:F:75:GLN:O	2:F:97:PHE:CD1	2.72	0.43
2:H:587:LEU:N	2:H:587:LEU:CD1	2.80	0.43
1:E:1:PHE:CE2	1:E:599:VAL:HG11	2.54	0.43
2:D:616:PRO:HB2	2:D:620:ASN:CA	2.47	0.43
2:D:158:VAL:HB	2:D:207:ASN:HB2	2.00	0.43
2:F:251:GLY:HA3	2:F:278:ASP:OD1	2.18	0.43
1:G:110:LEU:HG	1:G:115:LEU:CD2	2.48	0.43
2:B:6:PHE:CG	2:B:7:LYS:N	2.86	0.43
1:A:631:VAL:HG11	1:A:746:LEU:CD1	2.49	0.43
2:H:334:ILE:HA	2:H:337:ALA:HB2	2.00	0.43
2:D:611:LYS:HG2	2:D:667:VAL:HB	2.01	0.43
1:E:663:ASP:HB3	1:E:666:ARG:HD3	2.01	0.43
2:H:168:PRO:HG2	2:H:179:PRO:HG3	2.00	0.43
2:H:77:SER:HA	2:H:78:PRO:C	2.37	0.43
1:E:361:PHE:CE2	1:E:371:PHE:CE1	3.07	0.43
1:A:282:LEU:HB3	1:A:294:ILE:HD13	1.99	0.43
2:F:77:SER:HA	2:F:78:PRO:C	2.37	0.43
1:A:790:ASN:O	1:A:853:GLY:O	2.36	0.43
1:G:73:LEU:C	1:G:73:LEU:HD12	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:893:THR:O	1:E:893:THR:HG23	2.19	0.43
1:A:956:VAL:O	1:A:963:VAL:HG23	2.19	0.43
1:A:822:LEU:CG	1:A:823:ARG:N	2.81	0.43
1:A:103:LEU:CD1	2:B:156:PRO:HG3	2.49	0.43
2:F:616:PRO:HB3	2:F:621:CYS:SG	2.59	0.43
1:G:917:LYS:HE3	1:G:1077:VAL:HG23	2.00	0.43
1:C:915:PHE:CZ	1:C:917:LYS:HB2	2.53	0.43
2:B:83:LEU:HD11	2:B:419:VAL:HG13	1.99	0.43
1:E:110:LEU:HG	1:E:115:LEU:CD2	2.48	0.43
1:E:565:PHE:C	1:E:565:PHE:CD2	2.92	0.43
2:B:219:MET:CE	2:B:262:GLY:HA2	2.48	0.43
1:E:934:HIS:ND1	1:E:1074:THR:HB	2.34	0.43
2:F:340:LYS:HA	2:F:343:SER:HB2	2.00	0.43
1:E:930:HIS:O	1:E:931:VAL:C	2.57	0.43
1:E:790:ASN:O	1:E:853:GLY:O	2.36	0.43
2:F:108:TYR:CE2	2:F:147:GLY:HA3	2.53	0.43
1:C:36:GLN:HE21	2:D:255:ALA:HB1	1.83	0.43
1:E:1001:LEU:HD23	1:E:1001:LEU:O	2.18	0.43
1:A:484:ARG:NH1	2:B:586:GLN:NE2	2.67	0.43
1:E:365:PRO:C	1:E:367:MET:H	2.22	0.43
1:A:365:PRO:C	1:A:367:MET:H	2.22	0.43
2:F:587:LEU:CD1	2:F:587:LEU:N	2.80	0.43
2:D:345:VAL:HG11	2:D:387:ILE:HD11	2.01	0.43
1:G:1020:VAL:O	1:G:1021:GLN:HB2	2.18	0.43
2:F:132:LEU:HA	2:F:135:LEU:HB3	2.01	0.43
1:A:402:VAL:CG1	1:A:443:LEU:HD22	2.49	0.43
1:G:402:VAL:CG1	1:G:443:LEU:HD22	2.49	0.43
2:F:277:PHE:CE1	2:F:278:ASP:O	2.71	0.43
2:D:186:LEU:HD21	2:D:198:GLU:HB2	2.01	0.43
1:C:534:VAL:HG23	1:C:565:PHE:CZ	2.54	0.43
2:H:6:PHE:CG	2:H:7:LYS:N	2.86	0.43
1:A:766:PHE:HZ	1:A:877:LEU:HD12	1.83	0.43
2:D:188:LEU:HD12	2:D:230:TRP:HA	1.99	0.43
1:G:1081:TYR:O	1:G:1082:LYS:HB2	2.18	0.43
2:D:432:ARG:O	2:D:433:ASP:HB2	2.18	0.43
2:B:565:ARG:HA	2:B:565:ARG:HD3	1.83	0.43
1:C:402:VAL:CG1	1:C:443:LEU:HD22	2.49	0.43
1:A:919:LEU:CB	1:A:1079:GLU:HB3	2.46	0.43
2:B:75:GLN:O	2:B:97:PHE:CD1	2.72	0.43
1:E:609:ILE:HD12	1:E:632:GLN:OE1	2.19	0.43
2:D:161:HIS:CB	2:D:162:PRO:HA	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:543:HIS:HB3	2:D:544:PRO:HD2	2.00	0.43
2:H:132:LEU:HD22	2:H:192:SER:HB3	2.01	0.43
1:G:956:VAL:O	1:G:963:VAL:HG23	2.19	0.43
2:H:251:GLY:HA3	2:H:278:ASP:OD1	2.19	0.43
1:A:656:VAL:HG13	1:A:718:THR:O	2.19	0.43
2:F:6:PHE:CG	2:F:7:LYS:N	2.86	0.43
1:A:317:ILE:HG23	1:A:317:ILE:O	2.18	0.43
1:C:790:ASN:O	1:C:853:GLY:O	2.37	0.43
2:B:508:TYR:HE2	2:B:516:THR:HG23	1.83	0.43
1:G:893:THR:HG23	1:G:893:THR:O	2.19	0.43
1:C:622:GLU:HG3	1:C:623:GLN:CB	2.46	0.43
1:C:484:ARG:HH21	1:C:1021:GLN:HA	1.73	0.43
1:E:119:LEU:HD23	1:E:124:GLN:HE21	1.83	0.43
1:E:93:VAL:HB	1:E:104:THR:CG2	2.49	0.43
1:A:93:VAL:HB	1:A:104:THR:CG2	2.49	0.43
1:A:119:LEU:HD23	1:A:124:GLN:HE21	1.84	0.43
1:A:1063:LEU:HD12	1:A:1064:PRO:HA	2.01	0.43
2:H:75:GLN:O	2:H:97:PHE:CD1	2.72	0.43
2:D:75:GLN:O	2:D:97:PHE:CD1	2.72	0.43
2:F:169:CYS:HA	2:F:170:PRO:HD3	1.83	0.43
1:E:513:ASN:HA	1:E:599:VAL:HG21	1.99	0.43
1:G:513:ASN:CB	1:G:599:VAL:HG21	2.49	0.43
1:E:797:GLY:HA3	1:E:884:GLU:HB2	2.01	0.43
2:H:132:LEU:HA	2:H:135:LEU:HB3	2.01	0.43
2:D:4:THR:HG21	2:D:539:LYS:HZ2	1.83	0.43
1:G:618:PHE:CD2	1:G:619:GLU:N	2.87	0.43
1:G:915:PHE:CZ	1:G:917:LYS:HB2	2.53	0.43
1:A:525:PRO:HA	1:A:532:GLY:HA2	2.00	0.43
1:A:297:VAL:HG12	1:A:298:GLU:N	2.34	0.43
2:F:234:THR:HG22	2:F:235:ARG:N	2.34	0.43
2:F:219:MET:CE	2:F:262:GLY:HA2	2.48	0.43
1:C:663:ASP:HB3	1:C:666:ARG:HD3	2.01	0.43
2:F:168:PRO:HG2	2:F:179:PRO:HG3	1.99	0.43
1:G:419:GLN:HA	1:G:424:TRP:HA	2.00	0.43
1:A:930:HIS:O	1:A:931:VAL:C	2.57	0.43
2:H:473:GLY:C	2:H:475:CYS:H	2.22	0.43
1:G:790:ASN:O	1:G:853:GLY:O	2.36	0.43
1:G:367:MET:HG2	1:G:368:SER:O	2.18	0.42
1:G:597:ARG:CD	1:G:731:ARG:HG2	2.49	0.42
2:F:215:LEU:HD12	2:F:246:HIS:O	2.19	0.42
2:H:643:ARG:NH2	2:H:649:TRP:HZ2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:918:TYR:C	2:F:643:ARG:HH22	2.22	0.42
1:G:755:ASP:O	1:G:756:HIS:HB3	2.18	0.42
2:F:543:HIS:HB3	2:F:544:PRO:HD2	2.00	0.42
2:H:345:VAL:HG11	2:H:387:ILE:HD11	2.02	0.42
2:H:317:LYS:HA	2:H:344:ARG:HD2	2.00	0.42
1:C:956:VAL:O	1:C:963:VAL:HG23	2.19	0.42
1:A:656:VAL:HG21	1:A:687:LEU:HD11	2.01	0.42
1:E:534:VAL:HG23	1:E:565:PHE:CZ	2.54	0.42
1:A:534:VAL:HG23	1:A:565:PHE:CZ	2.54	0.42
1:E:656:VAL:HG13	1:E:718:THR:O	2.19	0.42
1:E:107:CYS:SG	1:E:348:LEU:CD2	3.07	0.42
2:H:219:MET:CE	2:H:262:GLY:HA2	2.49	0.42
1:G:631:VAL:HG11	1:G:746:LEU:CD1	2.49	0.42
2:B:234:THR:HG22	2:B:235:ARG:N	2.34	0.42
2:B:168:PRO:HG2	2:B:179:PRO:HG3	1.99	0.42
1:E:634:ASN:HB2	1:E:695:ASN:HB3	2.01	0.42
1:G:361:PHE:CE2	1:G:371:PHE:CE1	3.06	0.42
1:C:639:ILE:HG13	1:C:689:LEU:HA	2.01	0.42
1:A:22:VAL:HG22	1:A:23:VAL:N	2.32	0.42
1:G:639:ILE:HG13	1:G:689:LEU:HA	2.01	0.42
1:C:361:PHE:CE2	1:C:371:PHE:CE1	3.06	0.42
1:A:490:VAL:CG1	1:A:491:LEU:N	2.69	0.42
1:A:491:LEU:HD21	1:A:545:ILE:O	2.19	0.42
1:C:491:LEU:HD21	1:C:545:ILE:O	2.19	0.42
1:E:490:VAL:HG12	1:E:491:LEU:HA	1.99	0.42
2:H:215:LEU:HD12	2:H:246:HIS:O	2.19	0.42
2:D:6:PHE:CG	2:D:7:LYS:N	2.87	0.42
1:A:402:VAL:HG12	1:A:443:LEU:HD22	2.00	0.42
1:C:833:PRO:HA	1:C:840:TRP:HB3	2.01	0.42
2:H:186:LEU:HD21	2:H:198:GLU:HB2	2.01	0.42
2:B:251:GLY:HA3	2:B:278:ASP:OD1	2.18	0.42
1:G:534:VAL:HG23	1:G:565:PHE:CZ	2.54	0.42
1:G:656:VAL:HG13	1:G:718:THR:O	2.19	0.42
1:A:934:HIS:ND1	1:A:1074:THR:HB	2.34	0.42
1:E:631:VAL:HG11	1:E:746:LEU:CD1	2.49	0.42
2:D:352:LEU:HD22	2:D:358:VAL:HG23	2.01	0.42
1:A:151:MET:SD	1:A:238:ILE:CG2	3.08	0.42
1:C:461:ALA:N	1:C:462:PRO:HD3	2.34	0.42
1:A:893:THR:HG23	1:A:893:THR:O	2.19	0.42
1:C:402:VAL:HG12	1:C:443:LEU:HD22	2.00	0.42
1:E:491:LEU:HD21	1:E:545:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:H	1:C:120:PRO:CA	2.26	0.42
1:C:365:PRO:C	1:C:367:MET:H	2.23	0.42
1:C:908:VAL:HG12	1:C:909:VAL:N	2.35	0.42
2:B:215:LEU:HD12	2:B:246:HIS:O	2.19	0.42
1:E:374:MET:SD	1:E:417:PHE:CZ	3.13	0.42
2:D:144:ILE:HG22	2:D:195:PHE:CZ	2.53	0.42
1:C:565:PHE:CD2	1:C:565:PHE:C	2.92	0.42
1:C:631:VAL:HG11	1:C:746:LEU:CD1	2.49	0.42
2:D:234:THR:HG22	2:D:235:ARG:N	2.34	0.42
2:D:219:MET:CE	2:D:262:GLY:HA2	2.48	0.42
2:B:611:LYS:HG2	2:B:667:VAL:HB	2.01	0.42
1:G:930:HIS:O	1:G:931:VAL:C	2.57	0.42
1:G:634:ASN:HB2	1:G:695:ASN:HB3	2.01	0.42
1:A:218:HIS:NE2	1:A:256:MET:SD	2.90	0.42
1:C:890:THR:HG22	1:C:891:SER:N	2.34	0.42
1:G:464:TYR:HD2	1:G:472:GLN:HB2	1.82	0.42
1:C:813:VAL:HG23	1:C:823:ARG:NH1	2.34	0.42
1:A:833:PRO:HA	1:A:840:TRP:HB3	2.01	0.42
1:C:832:ALA:O	1:C:840:TRP:HB2	2.19	0.42
1:E:956:VAL:O	1:E:963:VAL:HG23	2.19	0.42
1:C:656:VAL:HG21	1:C:687:LEU:HD11	2.01	0.42
2:H:648:CYS:SG	2:H:673:CYS:N	2.92	0.42
1:C:107:CYS:SG	1:C:348:LEU:CD2	3.08	0.42
2:H:234:THR:HG22	2:H:235:ARG:N	2.34	0.42
1:G:799:THR:HG22	1:G:845:ARG:HB3	2.00	0.42
1:G:663:ASP:HB3	1:G:666:ARG:HD3	2.01	0.42
1:G:1045:VAL:HG22	1:G:1046:SER:N	2.35	0.42
2:H:432:ARG:O	2:H:433:ASP:HB2	2.18	0.42
2:F:569:SER:HB2	2:F:590:CYS:O	2.19	0.42
2:B:569:SER:HB2	2:B:590:CYS:O	2.19	0.42
2:B:256:ILE:HG13	2:B:256:ILE:O	2.19	0.42
2:D:256:ILE:HG13	2:D:256:ILE:O	2.20	0.42
2:H:99:ARG:CG	2:H:100:ALA:H	2.27	0.42
1:A:609:ILE:HD11	1:E:690:LYS:HB3	2.00	0.42
1:A:710:PRO:HG3	1:A:884:GLU:OE2	2.19	0.42
1:G:832:ALA:O	1:G:840:TRP:HB2	2.20	0.42
2:D:132:LEU:HD22	2:D:192:SER:HB3	2.01	0.42
1:A:917:LYS:HE3	1:A:1077:VAL:HG23	2.00	0.42
1:G:656:VAL:HG21	1:G:687:LEU:HD11	2.02	0.42
1:E:525:PRO:HA	1:E:532:GLY:HA2	2.00	0.42
2:B:352:LEU:HD22	2:B:358:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:352:LEU:HD22	2:H:358:VAL:HG23	2.01	0.42
2:F:352:LEU:HD22	2:F:358:VAL:HG23	2.01	0.42
1:C:799:THR:HG22	1:C:845:ARG:HB3	2.00	0.42
1:G:890:THR:HG22	1:G:891:SER:N	2.34	0.42
1:E:41:ALA:O	1:E:42:ASN:C	2.58	0.42
2:D:244:GLY:HA2	2:D:304:MET:CE	2.50	0.42
1:C:419:GLN:HA	1:C:424:TRP:HA	2.01	0.42
1:A:639:ILE:HG13	1:A:689:LEU:HA	2.01	0.42
1:A:461:ALA:N	1:A:462:PRO:HD3	2.34	0.42
1:A:175:SER:HB2	1:A:204:GLN:O	2.20	0.42
1:C:893:THR:HG23	1:C:893:THR:O	2.19	0.42
2:D:455:ILE:HG22	2:D:456:GLY:N	2.35	0.42
1:G:365:PRO:C	1:G:367:MET:H	2.23	0.42
1:G:817:GLN:O	1:G:818:LYS:HG2	2.19	0.42
1:A:71:MET:SD	1:A:90:GLY:HA3	2.59	0.42
1:E:908:VAL:HG11	2:F:595:GLY:CA	2.45	0.42
1:G:562:LEU:HD23	1:G:562:LEU:HA	1.85	0.42
1:A:438:TYR:HD2	1:A:441:ALA:HB2	1.85	0.42
2:D:616:PRO:HB3	2:D:621:CYS:SG	2.59	0.42
1:C:797:GLY:HA3	1:C:884:GLU:HB2	2.01	0.42
2:D:36:ASP:N	2:D:510:GLN:NE2	2.65	0.42
1:G:565:PHE:C	1:G:565:PHE:CD2	2.93	0.42
1:G:86:LEU:HD23	1:G:87:LEU:N	2.34	0.42
1:E:656:VAL:HG21	1:E:687:LEU:HD11	2.02	0.42
1:G:107:CYS:SG	1:G:348:LEU:CD2	3.08	0.42
2:H:656:GLN:HB2	2:H:663:TYR:CE1	2.55	0.42
2:B:334:ILE:HA	2:B:337:ALA:HB2	2.00	0.42
2:B:643:ARG:NH2	2:B:649:TRP:HZ2	2.18	0.42
1:A:790:ASN:O	1:A:854:GLY:HA2	2.20	0.42
2:D:223:ALA:HB1	2:D:263:ARG:HA	2.02	0.42
1:G:41:ALA:O	1:G:42:ASN:C	2.58	0.42
1:C:695:ASN:O	1:G:686:VAL:CG1	2.67	0.42
2:B:315:ILE:HA	2:B:316:PRO:HD3	1.88	0.42
1:A:119:LEU:H	1:A:120:PRO:CA	2.31	0.42
1:A:119:LEU:CD2	1:A:124:GLN:HE21	2.33	0.42
1:C:817:GLN:O	1:C:818:LYS:HG2	2.19	0.42
1:C:438:TYR:HD2	1:C:441:ALA:HB2	1.85	0.42
2:H:616:PRO:HB3	2:H:621:CYS:SG	2.59	0.42
1:E:86:LEU:HD23	1:E:87:LEU:N	2.35	0.42
2:F:466:ARG:HE	2:F:466:ARG:HB3	1.81	0.42
2:B:244:GLY:HA2	2:B:304:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1081:TYR:O	1:C:1082:LYS:HB2	2.18	0.42
2:H:256:ILE:HG13	2:H:256:ILE:O	2.19	0.42
1:C:1020:VAL:O	1:C:1021:GLN:CB	2.68	0.42
1:C:479:PRO:HB3	1:C:1021:GLN:CD	2.39	0.42
1:E:816:GLY:C	1:E:818:LYS:N	2.73	0.42
1:G:93:VAL:HB	1:G:104:THR:CG2	2.49	0.42
1:E:624:VAL:HG23	1:E:625:VAL:N	2.35	0.42
1:A:597:ARG:CD	1:A:731:ARG:HG2	2.50	0.42
2:H:543:HIS:HB3	2:H:544:PRO:HD2	2.00	0.42
1:A:208:TYR:CD1	1:A:246:ASP:HA	2.55	0.42
1:G:833:PRO:HA	1:G:840:TRP:HB3	2.01	0.42
1:A:374:MET:SD	1:A:417:PHE:CZ	3.13	0.42
2:B:74:LYS:CD	2:B:103:TYR:OH	2.68	0.42
1:E:402:VAL:CG1	1:E:443:LEU:HD22	2.49	0.42
1:G:374:MET:SD	1:G:417:PHE:CZ	3.12	0.42
2:D:103:TYR:HB3	2:D:104:PRO:CD	2.49	0.42
1:G:352:GLY:HA2	1:G:356:TRP:HA	2.02	0.42
1:C:575:LEU:HD11	1:C:593:LEU:HD13	2.02	0.42
1:A:565:PHE:C	1:A:565:PHE:CD2	2.92	0.42
2:B:656:GLN:HB2	2:B:663:TYR:CE1	2.55	0.42
2:F:611:LYS:HG2	2:F:667:VAL:HB	2.01	0.42
1:A:1045:VAL:HG22	1:A:1046:SER:N	2.35	0.42
1:G:750:LYS:HG2	1:G:796:TYR:CE1	2.54	0.42
1:A:890:THR:HG22	1:A:891:SER:N	2.34	0.42
2:B:573:ARG:NH2	2:B:575:ARG:HD3	2.35	0.42
2:F:573:ARG:NH2	2:F:575:ARG:HD3	2.35	0.42
1:E:419:GLN:HA	1:E:424:TRP:HA	2.01	0.42
1:E:890:THR:HG22	1:E:891:SER:N	2.34	0.42
1:E:372:ILE:O	1:E:372:ILE:HG13	2.20	0.42
1:G:372:ILE:O	1:G:372:ILE:HG13	2.19	0.42
1:C:1020:VAL:O	1:C:1021:GLN:HB2	2.19	0.42
1:G:491:LEU:HD21	1:G:545:ILE:O	2.20	0.42
2:H:546:PHE:CD2	2:H:554:GLU:HG2	2.55	0.42
1:A:918:TYR:O	1:A:919:LEU:C	2.58	0.42
1:G:918:TYR:O	1:G:919:LEU:C	2.58	0.42
2:B:543:HIS:HB3	2:B:544:PRO:HD2	2.00	0.42
2:H:118:LEU:HD23	2:H:204:ILE:HG21	2.02	0.42
1:E:1003:CYS:HB3	1:E:1008:CYS:HB2	1.89	0.42
1:A:832:ALA:O	1:A:840:TRP:HB2	2.20	0.42
1:E:832:ALA:O	1:E:840:TRP:HB2	2.19	0.42
2:H:105:ILE:HG21	2:H:135:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:656:GLN:HB2	2:F:663:TYR:CE1	2.55	0.42
2:D:334:ILE:HA	2:D:337:ALA:HB2	2.00	0.42
2:D:656:GLN:HB2	2:D:663:TYR:CE1	2.54	0.42
1:E:23:VAL:HG22	1:E:24:GLN:N	2.35	0.42
1:C:634:ASN:HB2	1:C:695:ASN:HB3	2.01	0.42
2:H:244:GLY:HA2	2:H:304:MET:CE	2.50	0.42
2:F:648:CYS:SG	2:F:673:CYS:N	2.93	0.42
1:C:450:SER:HB3	1:E:978:ARG:HH22	1.85	0.42
2:F:256:ILE:HG13	2:F:256:ILE:O	2.20	0.42
1:A:1020:VAL:O	1:A:1021:GLN:CB	2.68	0.42
1:E:491:LEU:CD2	1:E:545:ILE:O	2.68	0.42
1:G:119:LEU:CD2	1:G:124:GLN:HE21	2.33	0.42
1:E:119:LEU:CD2	1:E:124:GLN:HE21	2.33	0.42
1:C:630:LEU:CD2	1:G:653:GLN:OE1	2.67	0.42
1:C:93:VAL:HB	1:C:104:THR:CG2	2.49	0.42
1:G:71:MET:SD	1:G:90:GLY:HA3	2.59	0.42
1:E:908:VAL:HG12	1:E:909:VAL:N	2.35	0.42
2:H:468:SER:HB2	2:H:471:LEU:HD12	2.01	0.42
2:F:118:LEU:HD23	2:F:204:ILE:HG21	2.02	0.42
1:A:413:LYS:HG3	1:A:430:VAL:O	2.20	0.42
1:E:917:LYS:HE3	1:E:1077:VAL:HG23	2.00	0.42
1:G:766:PHE:HZ	1:G:877:LEU:HD12	1.83	0.42
2:F:611:LYS:CB	2:F:667:VAL:HB	2.50	0.42
2:F:304:MET:HE3	2:F:307:THR:HG21	2.02	0.42
3:E:3716:NAG:H4	3:E:3717:NAG:H2	1.69	0.42
2:D:517:ILE:HD12	2:D:518:ASN:N	2.35	0.42
1:G:992:LEU:C	1:G:992:LEU:HD23	2.39	0.42
1:A:985:ALA:CB	1:C:621:ARG:HD3	2.38	0.41
2:H:222:ALA:CB	2:H:294:ILE:HD12	2.50	0.41
2:F:222:ALA:CB	2:F:294:ILE:HD12	2.50	0.41
1:A:673:PHE:HE1	1:A:680:SER:HA	1.84	0.41
1:G:673:PHE:HE1	1:G:680:SER:HA	1.84	0.41
1:E:673:PHE:HE1	1:E:680:SER:HA	1.85	0.41
2:D:342:SER:O	2:D:382:GLN:HA	2.20	0.41
1:G:438:TYR:HD2	1:G:441:ALA:HB2	1.85	0.41
1:A:1003:CYS:HB3	1:A:1008:CYS:HB2	1.89	0.41
1:C:374:MET:SD	1:C:417:PHE:CZ	3.13	0.41
2:B:132:LEU:HA	2:B:135:LEU:HB3	2.01	0.41
1:E:402:VAL:HG12	1:E:443:LEU:HD22	2.01	0.41
2:F:186:LEU:HD21	2:F:198:GLU:HB2	2.01	0.41
1:E:352:GLY:HA2	1:E:356:TRP:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:ILE:HD12	2:B:518:ASN:N	2.35	0.41
2:D:611:LYS:CB	2:D:667:VAL:HB	2.50	0.41
1:G:790:ASN:O	1:G:854:GLY:HA2	2.20	0.41
1:C:622:GLU:C	1:C:623:GLN:CG	2.88	0.41
1:C:625:VAL:CG2	1:C:627:GLU:HG3	2.50	0.41
1:A:490:VAL:HG12	1:A:491:LEU:HA	1.99	0.41
1:G:490:VAL:HG12	1:G:491:LEU:HA	1.99	0.41
1:E:763:GLY:C	1:E:789:TRP:HE3	2.24	0.41
1:A:772:LYS:HB3	1:C:789:TRP:NE1	2.35	0.41
2:D:169:CYS:HB2	2:D:173:GLU:HA	2.02	0.41
2:F:132:LEU:HD22	2:F:192:SER:HB3	2.01	0.41
2:B:105:ILE:HG21	2:B:135:LEU:CD1	2.50	0.41
1:G:575:LEU:HD11	1:G:593:LEU:HD13	2.02	0.41
1:A:352:GLY:HA2	1:A:356:TRP:HA	2.02	0.41
1:G:905:VAL:CG1	1:G:946:LEU:HD21	2.50	0.41
1:E:766:PHE:HZ	1:E:877:LEU:HD12	1.83	0.41
1:C:934:HIS:ND1	1:C:1074:THR:HB	2.34	0.41
1:C:533:ALA:HA	1:C:554:ALA:HA	2.02	0.41
1:G:23:VAL:HG22	1:G:24:GLN:N	2.35	0.41
2:F:244:GLY:HA2	2:F:304:MET:CE	2.50	0.41
1:C:391:GLU:HG2	1:C:445:SER:H	1.85	0.41
1:G:461:ALA:N	1:G:462:PRO:HD3	2.34	0.41
1:A:992:LEU:C	1:A:992:LEU:HD23	2.40	0.41
1:G:464:TYR:O	1:G:465:TYR:HB3	2.21	0.41
1:G:491:LEU:CD2	1:G:545:ILE:O	2.69	0.41
2:D:155:LEU:N	2:D:160:THR:CG2	2.84	0.41
1:G:597:ARG:CG	1:G:731:ARG:CG	2.99	0.41
1:E:1032:LEU:CD2	1:E:1078:LEU:HD21	2.46	0.41
2:D:643:ARG:NH2	2:D:649:TRP:HZ2	2.18	0.41
2:F:643:ARG:NH2	2:F:649:TRP:HZ2	2.17	0.41
2:B:118:LEU:HD23	2:B:204:ILE:HG21	2.02	0.41
2:D:118:LEU:HD23	2:D:204:ILE:HG21	2.02	0.41
2:F:508:TYR:CE1	2:F:514:CYS:CB	3.03	0.41
2:D:35:PRO:O	2:D:38:ILE:HG12	2.20	0.41
1:G:446:VAL:CG1	1:G:456:LEU:HD11	2.50	0.41
1:G:82:SER:HB2	1:G:83:PRO:HD2	2.03	0.41
1:C:47:LEU:HB2	1:C:60:ILE:CG2	2.51	0.41
1:A:800:ILE:HG22	1:A:844:CYS:O	2.21	0.41
1:C:800:ILE:HG22	1:C:844:CYS:O	2.20	0.41
1:G:678:ASN:ND2	6:G:3678:NAG:C7	2.79	0.41
1:G:787:MET:HA	1:G:858:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:GLU:HG2	1:E:445:SER:H	1.85	0.41
2:F:223:ALA:HB1	2:F:263:ARG:HA	2.02	0.41
1:C:372:ILE:O	1:C:372:ILE:HG13	2.20	0.41
2:B:222:ALA:CB	2:B:294:ILE:HD12	2.50	0.41
2:D:215:LEU:HD12	2:D:246:HIS:O	2.19	0.41
2:F:442:PHE:CE1	2:F:449:ARG:HD3	2.55	0.41
2:H:468:SER:HB2	2:H:471:LEU:CD1	2.51	0.41
1:E:1020:VAL:O	1:E:1021:GLN:CB	2.68	0.41
2:B:132:LEU:HD22	2:B:192:SER:HB3	2.01	0.41
2:D:132:LEU:HA	2:D:135:LEU:HB3	2.01	0.41
1:C:352:GLY:HA2	1:C:356:TRP:HA	2.02	0.41
1:C:917:LYS:HE3	1:C:1077:VAL:HG21	2.02	0.41
1:A:107:CYS:SG	1:A:348:LEU:CD2	3.08	0.41
1:A:800:ILE:HG23	1:A:800:ILE:O	2.21	0.41
2:H:35:PRO:O	2:H:38:ILE:HG12	2.21	0.41
2:B:223:ALA:HB1	2:B:263:ARG:HA	2.02	0.41
2:H:573:ARG:NH2	2:H:575:ARG:HD3	2.35	0.41
1:C:384:SER:HB2	1:C:405:ALA:HB1	2.02	0.41
1:C:621:ARG:HG2	1:C:622:GLU:H	1.86	0.41
1:A:491:LEU:CD2	1:A:545:ILE:O	2.68	0.41
1:A:469:ARG:HH22	2:B:287:HIS:HB2	1.85	0.41
1:C:119:LEU:CD2	1:C:124:GLN:HE21	2.33	0.41
9:G:3374:NAG:HO3	9:G:3375:MAN:H2	1.83	0.41
1:E:354:PHE:HB2	1:E:355:THR:H	1.67	0.41
1:A:194:LEU:HD23	1:A:197:LEU:HD12	2.00	0.41
1:E:772:LYS:HB3	1:G:789:TRP:NE1	2.35	0.41
2:D:468:SER:HB2	2:D:471:LEU:HD12	2.01	0.41
1:G:438:TYR:CD2	1:G:441:ALA:HB2	2.56	0.41
2:F:169:CYS:CB	2:F:173:GLU:HA	2.50	0.41
1:A:797:GLY:HA3	1:A:884:GLU:HB2	2.01	0.41
2:F:105:ILE:HG21	2:F:135:LEU:CD1	2.50	0.41
1:A:82:SER:HB2	1:A:83:PRO:HD2	2.03	0.41
1:G:917:LYS:HE3	1:G:1077:VAL:HG21	2.03	0.41
1:C:354:PHE:CE2	3:C:3373:NAG:O5	2.73	0.41
1:A:663:ASP:HB3	1:A:666:ARG:HD3	2.01	0.41
1:A:533:ALA:HA	1:A:554:ALA:HA	2.03	0.41
1:E:533:ALA:HA	1:E:554:ALA:HA	2.03	0.41
1:C:790:ASN:O	1:C:854:GLY:HA2	2.19	0.41
2:F:517:ILE:HD12	2:F:518:ASN:N	2.35	0.41
2:H:223:ALA:HB1	2:H:263:ARG:HA	2.02	0.41
1:C:1045:VAL:HG22	1:C:1046:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ALA:O	1:A:42:ASN:C	2.59	0.41
1:G:752:CYS:SG	1:G:758:CYS:N	2.93	0.41
2:H:639:THR:HG23	2:H:639:THR:O	2.21	0.41
1:A:464:TYR:O	1:A:465:TYR:HB3	2.21	0.41
2:B:285:LEU:C	2:B:287:HIS:N	2.74	0.41
1:E:103:LEU:HD13	1:E:334:GLN:NE2	2.36	0.41
2:H:155:LEU:N	2:H:160:THR:CG2	2.84	0.41
1:G:720:VAL:HG22	1:G:721:GLY:N	2.36	0.41
1:C:662:LEU:HD21	1:C:698:LEU:HD23	2.03	0.41
1:G:662:LEU:HD21	1:G:698:LEU:HD23	2.02	0.41
2:D:99:ARG:O	2:D:383:ILE:O	2.39	0.41
2:F:468:SER:HB2	2:F:471:LEU:CD1	2.50	0.41
1:G:797:GLY:HA3	1:G:884:GLU:HB2	2.01	0.41
1:G:1003:CYS:HB3	1:G:1008:CYS:HB2	1.89	0.41
1:E:833:PRO:HA	1:E:840:TRP:HB3	2.01	0.41
1:E:413:LYS:HG3	1:E:430:VAL:O	2.21	0.41
1:G:430:VAL:O	1:G:430:VAL:HG23	2.20	0.41
1:E:446:VAL:CG1	1:E:456:LEU:HD11	2.51	0.41
1:C:82:SER:HB2	1:C:83:PRO:HD2	2.02	0.41
1:E:917:LYS:HE3	1:E:1077:VAL:HG21	2.02	0.41
2:F:334:ILE:HA	2:F:337:ALA:HB2	2.00	0.41
2:B:611:LYS:CB	2:B:667:VAL:HB	2.51	0.41
2:D:569:SER:HB2	2:D:590:CYS:O	2.20	0.41
1:E:358:GLY:HA3	1:E:386:LEU:HB3	2.03	0.41
2:D:302:SER:HB3	2:D:322:GLU:CG	2.51	0.41
2:B:35:PRO:O	2:B:38:ILE:HG12	2.20	0.41
1:A:372:ILE:O	1:A:372:ILE:HG13	2.20	0.41
1:E:822:LEU:CG	1:E:823:ARG:N	2.82	0.41
1:A:103:LEU:HD13	1:A:334:GLN:NE2	2.36	0.41
2:D:468:SER:HB2	2:D:471:LEU:CD1	2.51	0.41
2:B:468:SER:HB2	2:B:471:LEU:CD1	2.51	0.41
1:E:438:TYR:HD2	1:E:441:ALA:HB2	1.85	0.41
2:B:186:LEU:HD21	2:B:198:GLU:HB2	2.01	0.41
1:C:60:ILE:HD11	1:C:110:LEU:CD2	2.51	0.41
1:C:637:LEU:CD1	1:C:658:LEU:HD21	2.51	0.41
1:C:328:PHE:O	1:C:354:PHE:HA	2.21	0.41
1:G:800:ILE:HG22	1:G:844:CYS:O	2.20	0.41
1:G:848:HIS:HB2	2:H:485:SER:HB3	2.01	0.41
2:F:188:LEU:CD1	2:F:230:TRP:HA	2.51	0.41
1:C:752:CYS:SG	1:C:758:CYS:N	2.94	0.41
1:E:461:ALA:N	1:E:462:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:PRO:O	2:F:38:ILE:HG12	2.20	0.41
1:A:391:GLU:HG2	1:A:445:SER:H	1.85	0.41
2:H:169:CYS:CB	2:H:173:GLU:HA	2.51	0.41
2:H:569:SER:HB2	2:H:590:CYS:O	2.20	0.41
1:G:30:VAL:O	1:G:30:VAL:HG13	2.21	0.41
2:D:614:LYS:HE3	2:D:614:LYS:HB2	1.87	0.41
1:C:413:LYS:HG3	1:C:430:VAL:O	2.20	0.41
2:B:289:LEU:HD11	2:B:294:ILE:HG22	2.03	0.41
1:C:630:LEU:HD22	1:G:653:GLN:OE1	2.21	0.41
1:C:657:THR:HG23	1:C:720:VAL:CB	2.45	0.41
1:C:763:GLY:C	1:C:789:TRP:HE3	2.24	0.41
2:H:546:PHE:CE2	2:H:554:GLU:HG2	2.56	0.41
1:C:985:ALA:HA	1:C:986:PRO:HD3	1.94	0.41
1:A:986:PRO:HB3	1:A:987:PRO:CD	2.51	0.41
1:A:905:VAL:CG1	1:A:946:LEU:HD21	2.50	0.41
1:A:86:LEU:HD23	1:A:87:LEU:N	2.35	0.41
1:C:876:LEU:HB3	1:C:898:GLU:HG3	2.03	0.41
1:E:876:LEU:HB3	1:E:898:GLU:HG3	2.03	0.41
1:E:676:THR:O	1:E:677:LYS:CB	2.69	0.41
1:A:221:PHE:CD1	1:A:233:LYS:HD2	2.56	0.41
1:A:135:PHE:HZ	1:A:158:VAL:HB	1.86	0.41
2:B:648:CYS:SG	2:B:673:CYS:N	2.94	0.41
1:C:931:VAL:HG23	1:C:1030:GLY:H	1.86	0.41
1:G:931:VAL:HG23	1:G:1030:GLY:H	1.86	0.41
1:C:686:VAL:HG11	1:G:695:ASN:O	2.20	0.41
1:E:1081:TYR:O	1:E:1082:LYS:HB2	2.20	0.41
2:D:281:SER:OG	2:D:284:GLN:HB2	2.21	0.41
1:C:970:SER:O	1:C:1026:PHE:HB2	2.21	0.41
1:A:811:ARG:HD3	1:A:864:ASP:OD2	2.21	0.41
2:F:302:SER:HB3	2:F:322:GLU:CG	2.51	0.41
1:E:970:SER:O	1:E:1026:PHE:HB2	2.21	0.41
1:C:486:TRP:C	1:C:488:ASP:H	2.24	0.41
2:D:455:ILE:HG23	2:D:494:GLN:HE22	1.82	0.41
1:C:490:VAL:HG12	1:C:491:LEU:HA	1.99	0.41
2:H:289:LEU:HD11	2:H:294:ILE:HG22	2.03	0.41
1:E:119:LEU:H	1:E:120:PRO:CA	2.26	0.41
1:A:813:VAL:HG23	1:A:823:ARG:NH1	2.36	0.41
1:G:103:LEU:HD11	2:H:155:LEU:HD13	2.02	0.41
1:G:103:LEU:CD1	2:H:156:PRO:HG3	2.50	0.41
2:F:155:LEU:N	2:F:160:THR:CG2	2.83	0.41
1:C:720:VAL:HG22	1:C:721:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:763:GLY:C	1:G:789:TRP:HE3	2.24	0.41
1:A:763:GLY:C	1:A:789:TRP:HE3	2.24	0.41
2:B:468:SER:HB2	2:B:471:LEU:HD12	2.02	0.41
1:A:243:LYS:HD3	1:A:250:TYR:CE2	2.56	0.41
1:C:609:ILE:HD12	1:C:632:GLN:OE1	2.21	0.41
1:A:438:TYR:CD2	1:A:441:ALA:HB2	2.56	0.41
2:B:169:CYS:CB	2:B:173:GLU:HA	2.51	0.41
2:F:468:SER:HB2	2:F:471:LEU:HD12	2.01	0.41
1:A:181:HIS:CG	1:A:200:VAL:CG2	3.04	0.41
2:B:442:PHE:CE1	2:B:449:ARG:HD3	2.56	0.41
1:E:986:PRO:HB3	1:E:987:PRO:CD	2.51	0.41
1:G:1020:VAL:O	1:G:1021:GLN:CB	2.68	0.41
2:D:105:ILE:HG21	2:D:135:LEU:CD1	2.50	0.41
1:G:908:VAL:HG12	1:G:909:VAL:N	2.35	0.41
1:E:905:VAL:CG1	1:E:946:LEU:HD21	2.50	0.41
1:C:86:LEU:HD23	1:C:87:LEU:N	2.35	0.41
1:E:25:TYR:HD2	1:E:29:TRP:HB2	1.86	0.41
1:G:611:ALA:HB1	1:G:886:ASN:ND2	2.36	0.41
2:B:281:SER:OG	2:B:284:GLN:HB2	2.21	0.41
1:E:420:VAL:HG12	1:E:421:SER:N	2.36	0.41
2:F:281:SER:OG	2:F:284:GLN:HB2	2.21	0.41
1:G:800:ILE:O	1:G:800:ILE:HG23	2.21	0.41
2:B:648:CYS:HA	2:B:672:GLU:O	2.21	0.41
2:D:648:CYS:SG	2:D:673:CYS:N	2.94	0.41
1:G:533:ALA:HA	1:G:554:ALA:HA	2.03	0.41
1:C:23:VAL:HG22	1:C:24:GLN:N	2.35	0.41
1:A:23:VAL:HG22	1:A:24:GLN:N	2.35	0.41
2:F:648:CYS:HA	2:F:672:GLU:O	2.21	0.41
1:G:665:GLY:HA3	2:H:498:HIS:HB3	2.01	0.41
2:D:573:ARG:NH2	2:D:575:ARG:HD3	2.35	0.41
2:H:517:ILE:HD12	2:H:518:ASN:N	2.35	0.41
1:G:384:SER:HB2	1:G:405:ALA:HB1	2.02	0.41
2:B:472:GLU:HA	2:B:475:CYS:CB	2.50	0.41
1:A:384:SER:HB2	1:A:405:ALA:HB1	2.02	0.41
2:H:285:LEU:C	2:H:287:HIS:N	2.74	0.41
1:E:1023:GLU:O	1:E:1024:LEU:C	2.60	0.41
2:H:546:PHE:HA	2:H:554:GLU:O	2.21	0.41
1:G:919:LEU:CB	1:G:1079:GLU:HB3	2.46	0.41
2:D:222:ALA:CB	2:D:294:ILE:HD12	2.50	0.41
1:G:1023:GLU:O	1:G:1024:LEU:C	2.59	0.41
1:C:446:VAL:CG1	1:C:456:LEU:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:637:LEU:CD1	1:G:658:LEU:HD21	2.51	0.41
1:C:420:VAL:HG12	1:C:421:SER:N	2.36	0.41
1:G:876:LEU:HB3	1:G:898:GLU:HG3	2.03	0.41
1:A:876:LEU:HB3	1:A:898:GLU:HG3	2.03	0.41
1:G:764:ILE:HD12	1:G:800:ILE:CD1	2.51	0.41
1:A:764:ILE:HD12	1:A:800:ILE:CD1	2.51	0.41
2:F:343:SER:HA	2:F:381:VAL:O	2.21	0.41
1:E:790:ASN:O	1:E:854:GLY:HA2	2.20	0.41
1:C:787:MET:HA	1:C:858:THR:HG22	2.02	0.41
1:E:642:ARG:O	1:E:644:LYS:N	2.54	0.41
2:F:298:PHE:HB2	2:F:319:ALA:O	2.21	0.41
1:G:358:GLY:HA3	1:G:386:LEU:HB3	2.03	0.41
1:A:486:TRP:C	1:A:488:ASP:H	2.24	0.41
1:C:464:TYR:O	1:C:465:TYR:HB3	2.21	0.40
1:E:464:TYR:O	1:E:465:TYR:HB3	2.21	0.40
1:E:376:GLN:C	1:E:378:ASN:N	2.75	0.40
1:A:119:LEU:O	1:A:363:TYR:HE1	1.97	0.40
1:G:1032:LEU:CD2	1:G:1078:LEU:HD21	2.46	0.40
1:C:673:PHE:HE1	1:C:680:SER:HA	1.85	0.40
1:E:698:LEU:C	1:E:699:LEU:HD12	2.42	0.40
1:A:271:LEU:C	1:A:273:PHE:N	2.75	0.40
1:C:586:GLY:HA2	1:C:591:VAL:HG23	2.04	0.40
1:E:438:TYR:CD2	1:E:441:ALA:HB2	2.56	0.40
2:D:169:CYS:CB	2:D:173:GLU:HA	2.51	0.40
2:B:103:TYR:HB3	2:B:104:PRO:CD	2.48	0.40
1:E:575:LEU:HD11	1:E:593:LEU:HD13	2.02	0.40
1:A:575:LEU:HD11	1:A:593:LEU:HD13	2.02	0.40
1:A:446:VAL:CG1	1:A:456:LEU:HD11	2.51	0.40
1:E:60:ILE:HD11	1:E:110:LEU:CD2	2.51	0.40
1:E:47:LEU:HB2	1:E:60:ILE:CG2	2.51	0.40
2:H:648:CYS:HA	2:H:672:GLU:O	2.21	0.40
1:G:642:ARG:O	1:G:644:LYS:N	2.54	0.40
1:E:335:GLU:OE2	1:E:361:PHE:HB2	2.21	0.40
2:B:625:CYS:N	2:B:626:PRO:CD	2.84	0.40
1:E:776:VAL:HG12	1:E:867:PRO:O	2.21	0.40
2:F:285:LEU:C	2:F:287:HIS:N	2.74	0.40
1:C:103:LEU:HD13	1:C:334:GLN:NE2	2.36	0.40
1:C:698:LEU:C	1:C:699:LEU:HD12	2.41	0.40
1:E:662:LEU:HD21	1:E:698:LEU:HD23	2.02	0.40
1:A:273:PHE:CB	1:A:296:LYS:HD2	2.47	0.40
2:F:532:ARG:CD	2:F:554:GLU:HG3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:PHE:CD2	1:C:619:GLU:HG3	2.57	0.40
1:E:430:VAL:O	1:E:430:VAL:HG23	2.21	0.40
1:E:478:LEU:O	1:E:478:LEU:HG	2.21	0.40
1:A:908:VAL:HG12	1:A:909:VAL:N	2.35	0.40
1:C:25:TYR:HD2	1:C:29:TRP:HB2	1.86	0.40
1:A:47:LEU:HB2	1:A:60:ILE:CG2	2.51	0.40
1:G:25:TYR:HD2	1:G:29:TRP:HB2	1.85	0.40
1:E:332:MET:SD	2:F:208:LEU:HD13	2.61	0.40
2:F:596:CYS:HA	2:F:597:PRO:HD3	1.85	0.40
1:A:1075:THR:O	1:A:1075:THR:HG23	2.21	0.40
2:F:230:TRP:CZ3	2:F:235:ARG:HB3	2.56	0.40
2:F:625:CYS:N	2:F:626:PRO:CD	2.85	0.40
1:C:776:VAL:HG12	1:C:867:PRO:O	2.21	0.40
2:D:639:THR:O	2:D:639:THR:HG23	2.21	0.40
2:D:565:ARG:HD3	2:D:565:ARG:HA	1.83	0.40
1:C:625:VAL:HG23	1:C:627:GLU:N	2.37	0.40
1:C:478:LEU:HG	1:C:478:LEU:O	2.21	0.40
1:C:1032:LEU:CD2	1:C:1078:LEU:HD21	2.46	0.40
1:E:720:VAL:HG22	1:E:721:GLY:N	2.36	0.40
2:F:99:ARG:O	2:F:383:ILE:O	2.39	0.40
2:H:97:PHE:O	2:H:387:ILE:HG12	2.22	0.40
2:D:97:PHE:O	2:D:387:ILE:HG12	2.22	0.40
1:G:586:GLY:HA2	1:G:591:VAL:HG23	2.04	0.40
2:B:169:CYS:HA	2:B:170:PRO:HD3	1.82	0.40
2:D:169:CYS:HA	2:D:170:PRO:HD3	1.83	0.40
1:C:438:TYR:CD2	1:C:441:ALA:HB2	2.56	0.40
2:F:169:CYS:HB2	2:F:173:GLU:HA	2.02	0.40
1:A:630:LEU:HD21	1:E:653:GLN:CB	2.51	0.40
2:H:442:PHE:CE1	2:H:449:ARG:HD3	2.56	0.40
2:D:442:PHE:CE1	2:D:449:ARG:HD3	2.56	0.40
2:F:665:ILE:HG22	2:F:666:TYR:N	2.36	0.40
1:A:637:LEU:CD1	1:A:658:LEU:HD21	2.51	0.40
1:A:766:PHE:CE1	1:A:877:LEU:HD11	2.57	0.40
2:D:522:TYR:C	2:D:522:TYR:CD2	2.95	0.40
1:C:631:VAL:HG11	1:C:746:LEU:HD11	2.04	0.40
1:E:800:ILE:HG22	1:E:844:CYS:O	2.20	0.40
1:C:800:ILE:HG23	1:C:800:ILE:O	2.21	0.40
1:G:676:THR:O	1:G:677:LYS:CB	2.69	0.40
1:C:678:ASN:ND2	6:C:3678:NAG:C7	2.78	0.40
2:H:611:LYS:CB	2:H:667:VAL:HB	2.50	0.40
1:A:776:VAL:HG12	1:A:867:PRO:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:THR:OG1	1:E:343:PRO:HD2	2.21	0.40
1:G:103:LEU:HD13	1:G:334:GLN:NE2	2.36	0.40
1:E:812:TYR:HE2	1:E:814:ALA:HB2	1.85	0.40
1:C:918:TYR:O	1:C:919:LEU:C	2.58	0.40
1:C:608:PHE:O	1:C:609:ILE:C	2.59	0.40
2:D:289:LEU:HD11	2:D:294:ILE:HG22	2.03	0.40
2:B:169:CYS:HB2	2:B:173:GLU:HA	2.03	0.40
2:D:176:CYS:HB2	2:D:204:ILE:O	2.22	0.40
1:A:698:LEU:C	1:A:699:LEU:HD12	2.41	0.40
2:B:106:ASP:OD2	2:B:188:LEU:HD13	2.22	0.40
2:B:260:ASN:ND2	2:B:280:PRO:HG3	2.37	0.40
1:G:1076:THR:HG22	1:G:1077:VAL:N	2.36	0.40
1:C:1076:THR:CG2	1:C:1077:VAL:N	2.85	0.40
1:E:82:SER:HB2	1:E:83:PRO:HD2	2.02	0.40
2:H:363:PHE:HB2	2:H:388:THR:HB	2.04	0.40
1:G:60:ILE:HD11	1:G:110:LEU:CD2	2.51	0.40
1:E:637:LEU:CD1	1:E:658:LEU:HD21	2.51	0.40
1:A:631:VAL:HG11	1:A:746:LEU:HD11	2.04	0.40
1:C:958:LEU:O	1:C:959:ASN:HB3	2.21	0.40
1:A:335:GLU:OE2	1:A:361:PHE:HB2	2.21	0.40
1:C:335:GLU:OE2	1:C:361:PHE:HB2	2.21	0.40
2:B:302:SER:HB3	2:B:322:GLU:CG	2.51	0.40
1:A:642:ARG:O	1:A:644:LYS:N	2.54	0.40
1:G:970:SER:O	1:G:1026:PHE:HB2	2.21	0.40
1:E:813:VAL:HG23	1:E:823:ARG:NH1	2.36	0.40
1:E:1069:PHE:CE2	2:F:584:GLY:HA3	2.56	0.40
1:G:698:LEU:C	1:G:699:LEU:HD12	2.41	0.40
1:A:608:PHE:O	1:A:609:ILE:C	2.59	0.40
2:F:260:ASN:ND2	2:F:280:PRO:HG3	2.37	0.40
1:A:917:LYS:HE3	1:A:1077:VAL:HG21	2.03	0.40
2:H:281:SER:OG	2:H:284:GLN:HB2	2.21	0.40
1:E:800:ILE:HG23	1:E:800:ILE:O	2.21	0.40
1:G:971:HIS:N	1:G:972:PRO:HD3	2.37	0.40
1:A:676:THR:O	1:A:677:LYS:CB	2.69	0.40
2:H:158:VAL:CG2	2:H:207:ASN:HA	2.52	0.40
2:D:648:CYS:HA	2:D:672:GLU:O	2.21	0.40
1:G:335:GLU:OE2	1:G:361:PHE:HB2	2.21	0.40
2:H:169:CYS:HB2	2:H:173:GLU:HA	2.02	0.40
1:A:342:THR:OG1	1:A:343:PRO:HD2	2.22	0.40
1:E:384:SER:HB2	1:E:405:ALA:HB1	2.02	0.40
1:E:787:MET:HA	1:E:858:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:477:LYS:HG3	2:B:478:ASP:N	2.37	0.40
2:B:298:PHE:HB2	2:B:319:ALA:O	2.22	0.40
2:D:625:CYS:N	2:D:626:PRO:CD	2.84	0.40
1:E:679:ARG:C	1:E:679:ARG:HD3	2.42	0.40
1:G:679:ARG:HD3	1:G:679:ARG:C	2.42	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	1080/1095 (99%)	839 (78%)	215 (20%)	26 (2%)	7	47
1	C	881/1095 (80%)	663 (75%)	194 (22%)	24 (3%)	6	44
1	E	880/1095 (80%)	665 (76%)	190 (22%)	25 (3%)	6	43
1	G	881/1095 (80%)	666 (76%)	191 (22%)	24 (3%)	6	44
2	B	672/687 (98%)	514 (76%)	147 (22%)	11 (2%)	12	55
2	D	672/687 (98%)	515 (77%)	145 (22%)	12 (2%)	11	53
2	F	672/687 (98%)	514 (76%)	145 (22%)	13 (2%)	10	51
2	H	672/687 (98%)	512 (76%)	146 (22%)	14 (2%)	9	50
All	All	6410/7128 (90%)	4888 (76%)	1373 (21%)	149 (2%)	8	48

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	120	PRO
1	A	757	ILE
1	C	82	SER
1	C	757	ILE

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Mol	Chain	Res	Type
1	E	82	SER
1	E	757	ILE
1	E	817	GLN
1	G	82	SER
1	G	757	ILE
1	G	817	GLN
2	H	99	ARG
1	A	27	ASN
1	A	490	VAL
1	A	624	VAL
1	A	817	GLN
1	A	818	LYS
1	A	847	ASN
1	A	931	VAL
1	A	956	VAL
2	B	163	ASP
2	B	465	GLY
1	C	27	ASN
1	C	490	VAL
1	C	818	LYS
1	C	847	ASN
1	C	931	VAL
1	C	956	VAL
2	D	163	ASP
2	D	465	GLY
1	E	27	ASN
1	E	490	VAL
1	E	624	VAL
1	E	818	LYS
1	E	847	ASN
1	E	931	VAL
1	E	956	VAL
2	F	163	ASP
2	F	465	GLY
1	G	27	ASN
1	G	490	VAL
1	G	624	VAL
1	G	847	ASN
1	G	931	VAL
1	G	956	VAL
2	H	101	LYS
2	H	163	ASP

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Mol	Chain	Res	Type
2	H	465	GLY
1	A	649	SER
2	B	158	VAL
2	B	314	ILE
2	B	467	SER
1	C	649	SER
1	C	817	GLN
2	D	158	VAL
2	D	314	ILE
2	D	467	SER
1	E	649	SER
2	F	158	VAL
2	F	314	ILE
2	F	467	SER
1	G	649	SER
1	G	818	LYS
2	H	158	VAL
2	H	314	ILE
2	H	467	SER
1	A	70	ASN
1	A	123	ARG
1	A	124	GLN
1	A	209	THR
1	A	246	ASP
1	A	643	SER
1	A	654	SER
2	B	69	HIS
1	C	123	ARG
1	C	124	GLN
1	C	454	THR
1	C	624	VAL
1	C	643	SER
1	C	654	SER
1	C	816	GLY
2	D	69	HIS
1	E	123	ARG
1	E	124	GLN
1	E	454	THR
1	E	654	SER
1	E	758	CYS
2	F	69	HIS
2	F	463	THR

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Mol	Chain	Res	Type
1	G	123	ARG
1	G	124	GLN
1	G	643	SER
1	G	654	SER
2	H	69	HIS
1	A	454	THR
1	A	579	GLY
1	A	816	GLY
2	B	639	THR
1	C	70	ASN
1	C	579	GLY
2	D	99	ARG
1	E	70	ASN
1	E	579	GLY
1	E	643	SER
1	E	722	LYS
2	F	99	ARG
2	F	639	THR
1	G	70	ASN
1	G	454	THR
1	G	579	GLY
2	H	639	THR
1	A	722	LYS
1	A	773	SER
2	B	660	MET
1	C	722	LYS
1	C	773	SER
2	D	639	THR
2	D	660	MET
1	E	773	SER
1	E	816	GLY
2	F	652	TYR
2	F	660	MET
1	G	722	LYS
1	G	773	SER
1	G	816	GLY
2	H	660	MET
1	A	540	VAL
1	C	540	VAL
1	C	846	ILE
1	E	540	VAL
1	E	846	ILE

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Mol	Chain	Res	Type
1	G	540	VAL
1	A	846	ILE
1	G	846	ILE
2	H	59	PRO
2	B	517	ILE
2	D	517	ILE
2	F	517	ILE
2	H	399	ILE
2	H	517	ILE
2	B	204	ILE
2	B	399	ILE
2	D	204	ILE
2	D	399	ILE
2	F	204	ILE
2	H	204	ILE
1	C	120	PRO
1	E	120	PRO
1	G	120	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	924/934 (99%)	914 (99%)	10 (1%)	80 92
1	C	754/934 (81%)	742 (98%)	12 (2%)	70 89
1	E	753/934 (81%)	743 (99%)	10 (1%)	76 91
1	G	754/934 (81%)	744 (99%)	10 (1%)	76 91
2	B	583/592 (98%)	583 (100%)	0	100 100
2	D	583/592 (98%)	582 (100%)	1 (0%)	95 99
2	F	583/592 (98%)	582 (100%)	1 (0%)	95 99
2	H	583/592 (98%)	581 (100%)	2 (0%)	94 99
All	All	5517/6104 (90%)	5471 (99%)	46 (1%)	86 95

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	565	PHE
1	A	567	GLN
1	A	578	ASP
1	A	679	ARG
1	A	714	ARG
1	A	731	ARG
1	A	840	TRP
1	A	915	PHE
1	A	964	TRP
1	C	119	LEU
1	C	565	PHE
1	C	567	GLN
1	C	578	ASP
1	C	622	GLU
1	C	625	VAL
1	C	679	ARG
1	C	714	ARG
1	C	731	ARG
1	C	840	TRP
1	C	915	PHE
1	C	964	TRP
2	D	426	ARG
1	E	119	LEU
1	E	565	PHE
1	E	567	GLN
1	E	578	ASP
1	E	679	ARG
1	E	714	ARG
1	E	731	ARG
1	E	840	TRP
1	E	915	PHE
1	E	964	TRP
2	F	598	SER
1	G	119	LEU
1	G	565	PHE
1	G	567	GLN
1	G	578	ASP
1	G	679	ARG
1	G	714	ARG
1	G	731	ARG
1	G	840	TRP
1	G	915	PHE

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Mol	Chain	Res	Type
1	G	964	TRP
2	H	489	ASP
2	H	598	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	334	GLN
1	A	434	GLN
1	A	472	GLN
1	A	567	GLN
2	B	73	GLN
2	B	295	GLN
1	C	124	GLN
1	C	334	GLN
1	C	472	GLN
1	C	567	GLN
1	C	697	ASN
2	D	73	GLN
2	D	293	ASN
2	D	295	GLN
2	D	462	GLN
2	D	510	GLN
1	E	124	GLN
1	E	334	GLN
1	E	472	GLN
1	E	567	GLN
2	F	73	GLN
2	F	295	GLN
1	G	124	GLN
1	G	334	GLN
1	G	434	GLN
1	G	472	GLN
1	G	567	GLN
1	G	886	ASN
2	H	73	GLN
2	H	295	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

29 carbohydrates 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	NAG	A	3042	1,3	14,14,15	0.52	0	15,19,21	0.63	0
3	NAG	A	3043	3	14,14,15	0.54	0	15,19,21	1.07	1 (6%)
4	NAG	A	3373	1,4	14,14,15	0.48	0	15,19,21	1.01	1 (6%)
4	NAG	A	3374	4	14,14,15	0.54	0	15,19,21	1.88	3 (20%)
4	MAN	A	3375	4	11,11,12	0.43	0	14,15,17	2.04	6 (42%)
4	MAN	A	3376	4	11,11,12	0.74	0	14,15,17	1.19	1 (7%)
4	MAN	A	3377	4	11,11,12	0.60	0	14,15,17	1.58	2 (14%)
3	NAG	A	3716	1,3	14,14,15	0.58	0	15,19,21	1.80	1 (6%)
3	NAG	A	3717	3	14,14,15	0.52	0	15,19,21	1.70	1 (6%)
3	NAG	C	3042	1,3	14,14,15	0.52	0	15,19,21	0.61	0
3	NAG	C	3043	3	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
3	NAG	C	3373	1,3	14,14,15	0.46	0	15,19,21	1.01	1 (6%)
3	NAG	C	3374	3	14,14,15	0.50	0	15,19,21	1.66	1 (6%)
3	NAG	C	3716	1,3	14,14,15	0.52	0	15,19,21	2.01	1 (6%)
3	NAG	C	3717	3	14,14,15	0.56	0	15,19,21	1.64	1 (6%)
3	NAG	E	3042	1,3	14,14,15	0.53	0	15,19,21	0.60	0
3	NAG	E	3043	3	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
9	NAG	E	3373	1,9	14,14,15	0.47	0	15,19,21	1.03	1 (6%)
9	NAG	E	3374	9	14,14,15	0.54	0	15,19,21	1.84	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	E	3375	9	11,11,12	0.48	0	14,15,17	1.49	3 (21%)
3	NAG	E	3716	1,3	14,14,15	0.52	0	15,19,21	1.93	1 (6%)
3	NAG	E	3717	3	14,14,15	0.54	0	15,19,21	1.53	1 (6%)
3	NAG	G	3042	1,3	14,14,15	0.51	0	15,19,21	0.63	0
3	NAG	G	3043	3	14,14,15	0.56	0	15,19,21	1.08	1 (6%)
9	NAG	G	3373	1,9	14,14,15	0.45	0	15,19,21	0.99	1 (6%)
9	NAG	G	3374	9	14,14,15	0.53	0	15,19,21	1.90	2 (13%)
9	MAN	G	3375	9	11,11,12	0.50	0	14,15,17	1.51	3 (21%)
3	NAG	G	3716	1,3	14,14,15	0.54	0	15,19,21	1.99	1 (6%)
3	NAG	G	3717	3	14,14,15	0.55	0	15,19,21	1.57	1 (6%)

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	NAG	A	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3043	3	-	0/6/23/26	0/1/1/1
4	NAG	A	3373	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	3374	4	-	0/6/23/26	0/1/1/1
4	MAN	A	3375	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	3376	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3377	4	-	0/2/19/22	0/1/1/1
3	NAG	A	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3717	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3043	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3373	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	3374	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3717	3	-	0/6/23/26	0/1/1/1
3	NAG	E	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	3043	3	-	0/6/23/26	0/1/1/1
9	NAG	E	3373	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	E	3374	9	-	0/6/23/26	0/1/1/1
9	MAN	E	3375	9	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	E	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	3717	3	-	0/6/23/26	0/1/1/1
3	NAG	G	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	3043	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	G	3373	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	G	3374	9	-	0/6/23/26	0/1/1/1
9	MAN	G	3375	9	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	G	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	3717	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3375	MAN	C2-C3-C4	-3.46	105.16	111.04
9	G	3375	MAN	C2-C3-C4	-3.15	105.70	111.04
9	E	3375	MAN	C2-C3-C4	-3.02	105.91	111.04
4	A	3376	MAN	C1-O5-C5	-2.92	108.54	112.25
4	A	3377	MAN	C6-C5-C4	-2.75	106.24	113.02
4	A	3375	MAN	C3-C4-C5	-2.40	106.01	110.20
9	G	3375	MAN	O5-C1-C2	-2.37	107.01	110.86
9	E	3375	MAN	O5-C1-C2	-2.28	107.16	110.86
4	A	3375	MAN	C1-C2-C3	-2.25	106.88	109.54
4	A	3375	MAN	O5-C1-C2	-2.16	107.35	110.86
4	A	3374	NAG	O3-C3-C2	-2.06	105.04	109.11
4	A	3375	MAN	C1-O5-C5	2.24	115.09	112.25
9	G	3375	MAN	O5-C5-C6	2.30	112.33	107.35
3	C	3373	NAG	C1-O5-C5	2.34	115.22	112.25
9	E	3375	MAN	O5-C5-C6	2.37	112.49	107.35
9	G	3373	NAG	C1-O5-C5	2.40	115.30	112.25
4	A	3373	NAG	C1-O5-C5	2.53	115.45	112.25
9	E	3373	NAG	C1-O5-C5	2.56	115.50	112.25
4	A	3374	NAG	O4-C4-C3	2.90	116.86	110.34
3	E	3043	NAG	C1-O5-C5	2.91	115.95	112.25
9	E	3374	NAG	O4-C4-C3	2.92	116.91	110.34
3	C	3043	NAG	C1-O5-C5	2.99	116.04	112.25
9	G	3374	NAG	O4-C4-C3	3.01	117.11	110.34
3	A	3043	NAG	C1-O5-C5	3.04	116.11	112.25
3	G	3043	NAG	C1-O5-C5	3.11	116.19	112.25
4	A	3377	MAN	C1-O5-C5	3.74	117.00	112.25
4	A	3375	MAN	O3-C3-C2	3.82	116.91	110.00
9	E	3374	NAG	C1-O5-C5	5.14	118.77	112.25
4	A	3374	NAG	C1-O5-C5	5.25	118.91	112.25
9	G	3374	NAG	C1-O5-C5	5.32	119.00	112.25
3	E	3717	NAG	C1-O5-C5	5.35	119.04	112.25
3	C	3374	NAG	C1-O5-C5	5.58	119.33	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	3717	NAG	C1-O5-C5	5.60	119.35	112.25
3	C	3717	NAG	C1-O5-C5	5.82	119.63	112.25
3	A	3717	NAG	C1-O5-C5	6.02	119.89	112.25
3	A	3716	NAG	C1-O5-C5	6.45	120.43	112.25
3	E	3716	NAG	C1-O5-C5	6.78	120.85	112.25
3	G	3716	NAG	C1-O5-C5	7.00	121.13	112.25
3	C	3716	NAG	C1-O5-C5	7.14	121.31	112.25

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	E	3375	MAN	C1
9	E	3373	NAG	C1
9	G	3375	MAN	C1
3	C	3373	NAG	C1
4	A	3373	NAG	C1
9	G	3373	NAG	C1
4	A	3375	MAN	C1

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3373	NAG	4	0
4	A	3374	NAG	3	0
4	A	3375	MAN	2	0
4	A	3377	MAN	4	0
3	C	3373	NAG	4	0
3	C	3374	NAG	1	0
9	E	3373	NAG	4	0
9	E	3374	NAG	3	0
9	E	3375	MAN	2	0
3	E	3716	NAG	1	0
3	E	3717	NAG	1	0
9	G	3373	NAG	4	0
9	G	3374	NAG	4	0
9	G	3375	MAN	3	0
3	G	3716	NAG	1	0
3	G	3717	NAG	1	0

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 17 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MAN	A	3378	-	11,11,12	1.03	0	14,15,17	6.14	6 (42%)
6	NAG	A	3678	1	14,14,15	0.49	0	15,19,21	0.95	1 (6%)
6	NAG	A	3880	1	14,14,15	0.41	0	15,19,21	1.25	1 (6%)
6	NAG	B	3094	2	14,14,15	0.47	0	15,19,21	0.74	0
6	NAG	C	3678	1	14,14,15	0.48	0	15,19,21	0.91	1 (6%)
6	NAG	C	3880	1	14,14,15	0.41	0	15,19,21	1.16	1 (6%)
6	NAG	D	3094	2	14,14,15	0.50	0	15,19,21	0.71	0
6	NAG	E	3678	1	14,14,15	0.50	0	15,19,21	0.97	1 (6%)
6	NAG	E	3880	1	14,14,15	0.40	0	15,19,21	1.25	1 (6%)
6	NAG	F	3094	2	14,14,15	0.47	0	15,19,21	0.74	0
6	NAG	G	3678	1	14,14,15	0.49	0	15,19,21	0.94	1 (6%)
6	NAG	G	3880	1	14,14,15	0.42	0	15,19,21	1.12	1 (6%)
6	NAG	H	3094	2	14,14,15	0.48	0	15,19,21	0.73	0

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
5	MAN	A	3378	-	-	0/2/19/22	0/1/1/1
6	NAG	A	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	A	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	C	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	C	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	D	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	E	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	E	3880	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	G	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	G	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	H	3094	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3378	MAN	C1-C2-C3	-18.07	88.17	109.54
5	A	3378	MAN	C1-O5-C5	-12.31	96.63	112.25
5	A	3378	MAN	O2-C2-C1	-2.28	104.64	109.21
5	A	3378	MAN	O3-C3-C2	2.31	114.18	110.00
5	A	3378	MAN	O5-C1-C2	2.51	114.93	110.86
6	C	3678	NAG	C1-O5-C5	2.92	115.96	112.25
6	G	3678	NAG	C1-O5-C5	3.01	116.06	112.25
6	A	3678	NAG	C1-O5-C5	3.05	116.12	112.25
6	G	3880	NAG	C1-O5-C5	3.14	116.24	112.25
6	E	3678	NAG	C1-O5-C5	3.17	116.28	112.25
6	C	3880	NAG	C1-O5-C5	3.32	116.46	112.25
6	E	3880	NAG	C1-O5-C5	3.67	116.90	112.25
6	A	3880	NAG	C1-O5-C5	3.74	117.00	112.25
5	A	3378	MAN	C3-C4-C5	4.91	118.76	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3378	MAN	4	0
6	C	3678	NAG	1	0
6	G	3678	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1082/1095 (98%)	-0.07	25 (2%) 64 54	61, 153, 256, 362	0
1	C	885/1095 (80%)	0.21	52 (5%) 26 20	67, 172, 280, 410	0
1	E	884/1095 (80%)	-0.02	31 (3%) 48 38	65, 157, 266, 337	0
1	G	885/1095 (80%)	-0.06	28 (3%) 51 42	74, 150, 266, 342	0
2	B	674/687 (98%)	0.35	48 (7%) 19 15	100, 205, 286, 421	2 (0%)
2	D	674/687 (98%)	1.09	166 (24%) 1 1	107, 229, 313, 416	2 (0%)
2	F	674/687 (98%)	0.48	66 (9%) 10 9	98, 207, 289, 374	2 (0%)
2	H	674/687 (98%)	0.50	71 (10%) 8 8	100, 210, 293, 390	2 (0%)
All	All	6432/7128 (90%)	0.26	487 (7%) 17 14	61, 185, 283, 421	8 (0%)

All (487) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	72	GLY	16.2
2	B	72	GLY	12.5
2	H	73	GLN	11.2
2	B	92	ALA	9.9
2	D	91	ALA	9.6
1	C	817	GLN	9.4
2	D	92	ALA	9.2
1	A	817	GLN	9.2
2	D	63	ALA	9.0
2	D	32	PRO	8.8
2	F	175	GLU	8.2
2	H	416	THR	7.9
2	B	431	SER	7.7
1	G	817	GLN	7.6
2	D	175	GLU	7.5
1	C	818	LYS	7.3

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Mol	Chain	Res	Type	RSRZ
1	C	721	GLY	7.3
2	D	369	THR	6.9
2	F	92	ALA	6.8
2	F	91	ALA	6.5
2	F	161	HIS	6.3
2	H	469	GLN	6.3
1	G	127	PRO	6.2
2	F	176	CYS	6.2
2	H	431	SER	6.1
1	C	730	LEU	6.1
1	G	818	LYS	6.0
2	D	433	ASP	5.9
2	B	73	GLN	5.9
2	F	629	GLN	5.8
2	D	83	LEU	5.8
2	D	144	ILE	5.8
2	D	379	ASP	5.8
1	C	482	TRP	5.7
1	A	1044	LYS	5.7
2	D	68	ASP	5.7
2	D	109	TYR	5.7
2	H	417	VAL	5.6
2	H	433	ASP	5.6
2	D	76	LEU	5.6
2	B	71	GLY	5.5
2	D	367	GLY	5.5
1	E	128	ARG	5.4
2	D	189	THR	5.4
2	D	82	THR	5.3
2	D	399	ILE	5.3
2	B	433	ASP	5.2
2	F	345	VAL	5.2
2	D	1	GLN	5.2
2	D	97	PHE	5.2
2	D	105	ILE	5.2
1	C	820	GLY	5.2
2	H	206	GLY	5.1
2	D	28	ASN	5.1
2	B	469	GLN	5.1
1	E	729	ASN	5.0
1	A	278	SER	4.9
1	E	482	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
2	D	366	ASN	4.9
1	A	277	ASN	4.8
2	H	432	ARG	4.8
2	B	432	ARG	4.8
1	C	1044	LYS	4.8
2	D	650	VAL	4.8
2	D	62	LEU	4.7
2	B	382	GLN	4.7
1	A	623	GLN	4.7
2	H	470	GLU	4.6
2	F	1	GLN	4.6
2	F	177	GLN	4.6
2	H	71	GLY	4.6
1	A	816	GLY	4.6
2	D	65	THR	4.5
1	C	723	PRO	4.5
2	B	430	GLN	4.5
1	C	816	GLY	4.5
2	D	56	ILE	4.5
2	D	104	PRO	4.5
1	E	100	ASN	4.4
2	D	432	ARG	4.4
2	D	331	VAL	4.4
2	H	32	PRO	4.4
2	B	91	ALA	4.4
1	C	102	TYR	4.4
2	F	669	GLU	4.3
1	G	626	SER	4.3
2	D	136	ASN	4.3
2	D	443	LEU	4.3
1	C	104	THR	4.2
1	C	821	GLN	4.2
1	C	1079	GLU	4.2
2	H	67	GLU	4.2
1	C	729	ASN	4.2
1	C	106	LEU	4.2
2	D	400	GLN	4.2
2	D	391	VAL	4.2
1	E	817	GLN	4.2
2	F	72	GLY	4.1
2	H	82	THR	4.1
1	C	726	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	627	GLU	4.1
1	E	623	GLN	4.1
2	D	39	ARG	4.1
2	D	622	SER	4.0
2	H	80	LYS	4.0
2	D	446	GLY	4.0
2	D	123	ASN	4.0
1	G	128	ARG	3.9
1	C	973	GLN	3.9
2	F	416	THR	3.9
1	A	323	THR	3.9
1	A	818	LYS	3.9
2	H	418	GLN	3.9
2	H	454	TYR	3.9
2	D	38	ILE	3.9
2	D	419	VAL	3.9
1	E	821	GLN	3.9
2	H	91	ALA	3.8
2	H	401	GLU	3.8
2	D	413	ASP	3.8
1	C	1078	LEU	3.8
2	D	133	ARG	3.8
2	D	67	GLU	3.8
2	H	92	ALA	3.8
1	E	973	GLN	3.8
2	D	401	GLU	3.7
1	E	40	ALA	3.7
2	D	185	VAL	3.7
2	D	49	ARG	3.7
2	F	193	ASN	3.7
1	A	821	GLN	3.7
1	G	483	ARG	3.7
2	D	93	PHE	3.7
2	B	145	GLY	3.7
2	D	6	PHE	3.6
1	C	396	LYS	3.6
2	F	160	THR	3.6
2	D	29	PHE	3.6
2	D	130	ASP	3.6
2	D	382	GLN	3.6
2	D	161	HIS	3.6
2	D	345	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	819	GLN	3.6
2	D	69	HIS	3.6
1	C	819	GLN	3.6
2	F	470	GLU	3.6
2	B	1	GLN	3.5
2	D	358	VAL	3.5
2	D	416	THR	3.5
2	D	430	GLN	3.5
2	D	409	LEU	3.5
2	D	129	GLY	3.5
2	B	468	SER	3.5
2	D	378	CYS	3.5
1	C	623	GLN	3.5
2	D	628	LEU	3.5
2	D	64	GLU	3.5
1	E	397	GLY	3.4
2	D	445	CYS	3.4
2	D	126	LYS	3.4
2	B	206	GLY	3.4
2	H	629	GLN	3.4
2	D	613	GLU	3.4
1	C	1081	TYR	3.4
2	F	429	ASP	3.4
2	D	375	ARG	3.4
2	D	234	THR	3.4
2	D	649	TRP	3.4
1	C	466	GLU	3.4
2	H	429	ASP	3.4
2	D	24	CYS	3.4
1	G	396	LYS	3.4
1	C	397	GLY	3.4
1	G	482	TRP	3.4
1	E	483	ARG	3.3
2	B	628	LEU	3.3
2	D	81	VAL	3.3
2	D	368	VAL	3.3
2	D	623	ALA	3.3
2	H	70	ASN	3.3
2	F	366	ASN	3.3
2	D	115	TYR	3.3
2	F	178	PRO	3.3
2	D	107	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	407	ARG	3.3
2	D	614	LYS	3.3
2	H	366	ASN	3.3
2	F	430	GLN	3.3
2	D	625	CYS	3.3
2	D	31	GLY	3.3
2	B	136	ASN	3.3
2	H	328	SER	3.3
2	D	143	ARG	3.3
2	H	79	GLN	3.3
2	D	206	GLY	3.2
1	C	420	VAL	3.2
2	D	53	ALA	3.2
2	H	430	GLN	3.2
2	D	195	PHE	3.2
2	H	1	GLN	3.2
1	C	815	GLU	3.2
1	G	481	GLY	3.2
2	D	404	PHE	3.1
2	D	94	ASN	3.1
2	B	629	GLN	3.1
2	F	390	GLN	3.1
2	H	414	ILE	3.1
2	H	93	PHE	3.1
1	G	619	GLU	3.1
2	D	36	ASP	3.1
1	A	272	ALA	3.1
2	B	107	LEU	3.1
2	D	70	ASN	3.1
2	D	145	GLY	3.1
1	G	821	GLN	3.1
2	B	418	GLN	3.1
2	B	171	ASN	3.1
2	D	171	ASN	3.1
2	D	469	GLN	3.0
2	F	71	GLY	3.0
2	H	386	PRO	3.0
2	H	69	HIS	3.0
2	H	335	LYS	3.0
1	C	398	VAL	3.0
2	H	185	VAL	3.0
2	H	389	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	384	ASN	3.0
2	F	73	GLN	3.0
1	C	46	GLY	3.0
2	D	429	ASP	3.0
2	D	98	ARG	3.0
2	D	395	ALA	3.0
2	D	226	GLU	2.9
2	F	389	PHE	2.9
2	F	385	VAL	2.9
1	E	422	ARG	2.9
2	F	39	ARG	2.9
1	E	108	PHE	2.9
2	D	354	ASP	2.9
2	D	387	ILE	2.9
2	H	68	ASP	2.9
2	H	474	SER	2.9
2	D	651	ALA	2.9
2	B	385	VAL	2.9
2	H	415	VAL	2.8
2	D	635	VAL	2.8
2	F	20	GLY	2.8
2	D	80	LYS	2.8
2	F	81	VAL	2.8
1	A	729	ASN	2.8
1	G	823	ARG	2.8
2	D	95	VAL	2.8
2	F	115	TYR	2.8
2	D	347	LEU	2.8
1	E	10	ALA	2.8
2	D	377	ASP	2.8
1	A	273	PHE	2.8
1	E	466	GLU	2.8
2	D	60	THR	2.8
1	A	724	LEU	2.8
2	D	390	GLN	2.8
2	B	133	ARG	2.8
2	H	175	GLU	2.8
2	D	364	CYS	2.8
2	H	207	ASN	2.8
2	H	66	GLN	2.8
2	D	84	TYR	2.8
1	C	1024	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	429	ASP	2.8
2	D	99	ARG	2.8
2	H	136	ASN	2.8
1	C	1039	GLN	2.8
2	F	335	LYS	2.7
2	D	621	CYS	2.7
1	G	624	VAL	2.7
2	F	191	ASN	2.7
2	B	414	ILE	2.7
2	D	159	ASN	2.7
2	D	383	ILE	2.7
2	H	393	VAL	2.7
1	A	1081	TYR	2.7
2	H	452	THR	2.7
2	D	51	CYS	2.7
1	C	125	GLU	2.7
2	D	139	THR	2.7
1	A	10	ALA	2.7
1	C	488	ASP	2.7
2	F	95	VAL	2.7
2	H	78	PRO	2.7
1	E	730	LEU	2.7
2	F	206	GLY	2.7
2	D	406	ILE	2.7
1	G	563	GLN	2.7
1	C	45	GLY	2.6
2	D	442	PHE	2.6
2	D	667	VAL	2.6
2	D	431	SER	2.6
2	F	391	VAL	2.6
2	D	78	PRO	2.6
2	F	369	THR	2.6
2	H	170	PRO	2.6
2	D	346	PHE	2.6
2	B	202	GLN	2.6
2	F	382	GLN	2.6
2	D	27	LEU	2.6
2	D	318	SER	2.6
1	C	725	LEU	2.6
2	F	674	VAL	2.6
2	H	378	CYS	2.6
1	A	625	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	122	ARG	2.6
1	E	95	HIS	2.6
2	F	163	ASP	2.6
2	D	363	PHE	2.6
1	C	627	GLU	2.6
2	H	81	VAL	2.5
2	F	79	GLN	2.5
2	H	189	THR	2.5
2	D	417	VAL	2.5
2	D	61	SER	2.5
1	A	422	ARG	2.5
1	G	625	VAL	2.5
1	G	1081	TYR	2.5
2	H	84	TYR	2.5
2	D	620	ASN	2.5
2	H	329	ASN	2.5
1	G	1039	GLN	2.5
2	D	415	VAL	2.5
1	C	10	ALA	2.5
2	D	142	GLY	2.5
2	F	67	GLU	2.5
2	F	166	ARG	2.5
2	D	616	PRO	2.5
2	D	470	GLU	2.5
1	E	127	PRO	2.5
2	H	382	GLN	2.5
2	B	185	VAL	2.5
2	B	236	LEU	2.5
2	F	347	LEU	2.5
2	H	205	SER	2.5
2	B	413	ASP	2.5
2	D	615	GLY	2.5
2	D	96	THR	2.4
2	D	642	GLU	2.4
2	F	195	PHE	2.4
2	B	622	SER	2.4
2	B	623	ALA	2.4
1	G	124	GLN	2.4
2	F	103	TYR	2.4
2	B	82	THR	2.4
2	D	30	THR	2.4
2	B	93	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	236	LEU	2.4
2	B	384	ASN	2.4
1	A	726	ALA	2.4
2	D	435	SER	2.4
2	B	305	VAL	2.4
2	D	160	THR	2.4
2	D	436	LEU	2.4
2	F	138	ILE	2.4
2	D	618	GLY	2.4
2	H	115	TYR	2.4
1	C	496	GLY	2.4
2	D	408	ALA	2.4
1	E	1044	LYS	2.4
2	F	610	LEU	2.4
1	C	1045	VAL	2.4
1	A	973	GLN	2.4
1	C	123	ARG	2.4
2	B	101	LYS	2.4
2	D	418	GLN	2.4
2	F	371	ARG	2.4
2	H	463	THR	2.4
1	G	95	HIS	2.4
1	G	480	ARG	2.4
2	F	614	LYS	2.4
1	A	12	ARG	2.3
2	D	25	GLN	2.3
2	F	133	ARG	2.3
2	F	171	ASN	2.3
2	H	423	CYS	2.3
2	F	384	ASN	2.3
2	H	392	LYS	2.3
1	E	1039	GLN	2.3
2	F	49	ARG	2.3
1	C	421	SER	2.3
1	A	322	THR	2.3
1	G	973	GLN	2.3
2	D	34	ASP	2.3
2	D	420	LEU	2.3
1	E	624	VAL	2.3
2	D	393	VAL	2.3
2	H	391	VAL	2.3
1	C	918	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	624	VAL	2.3
2	H	464	GLN	2.3
2	D	103	TYR	2.3
2	H	446	GLY	2.3
2	D	634	PRO	2.2
2	H	462	GLN	2.2
2	F	630	LEU	2.2
2	B	371	ARG	2.2
1	C	722	LYS	2.2
2	D	405	VAL	2.2
2	F	571	ARG	2.2
2	F	622	SER	2.2
2	D	57	MET	2.2
2	F	54	ASP	2.2
2	F	668	ASP	2.2
2	D	108	TYR	2.2
2	D	414	ILE	2.2
1	G	489	ALA	2.2
1	E	97	CYS	2.2
2	D	386	PRO	2.2
2	F	608	GLU	2.2
2	B	70	ASN	2.2
2	H	127	LEU	2.2
1	E	728	ARG	2.2
1	E	12	ARG	2.2
1	G	561	ARG	2.2
2	B	69	HIS	2.2
1	C	621	ARG	2.2
1	C	622	GLU	2.2
2	D	90	ALA	2.2
1	E	37	LYS	2.2
2	F	344	ARG	2.2
2	F	651	ALA	2.2
2	D	132	LEU	2.2
1	E	1045	VAL	2.2
2	D	26	LYS	2.2
2	B	49	ARG	2.1
2	D	72	GLY	2.1
1	A	561	ARG	2.1
2	D	119	ASP	2.1
1	G	922	SER	2.1
2	B	109	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	207	ASN	2.1
1	E	1040	ILE	2.1
1	C	990	ASP	2.1
2	F	346	PHE	2.1
2	D	71	GLY	2.1
2	D	624	ALA	2.1
2	D	643	ARG	2.1
2	D	355	THR	2.1
2	H	628	LEU	2.1
1	C	423	GLN	2.1
1	C	731	ARG	2.1
1	E	117	GLN	2.1
1	C	541	LEU	2.1
2	F	628	LEU	2.1
2	B	470	GLU	2.1
2	B	366	ASN	2.1
2	D	45	GLN	2.1
2	D	73	GLN	2.1
2	B	386	PRO	2.1
2	F	30	THR	2.1
1	C	48	TYR	2.1
2	H	453	GLY	2.1
1	E	1078	LEU	2.1
2	D	227	GLU	2.1
2	F	368	VAL	2.1
2	D	611	LYS	2.1
1	G	102	TYR	2.1
1	E	650	ARG	2.1
2	F	69	HIS	2.1
1	C	57	CYS	2.1
1	G	623	GLN	2.1
2	H	434	ARG	2.1
2	F	47	LEU	2.1
2	D	334	ILE	2.1
2	H	171	ASN	2.1
2	B	367	GLY	2.0
1	E	486	TRP	2.0
2	H	161	HIS	2.0
2	D	320	VAL	2.0
2	F	634	PRO	2.0
2	B	47	LEU	2.0
1	A	56	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	335	GLU	2.0
2	D	236	LEU	2.0
2	H	186	LEU	2.0
2	H	413	ASP	2.0
2	D	619	LYS	2.0
1	G	328	PHE	2.0
2	H	320	VAL	2.0
1	C	56	ALA	2.0
2	B	388	THR	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	G	3716	14/15	0.90	0.22	0.47	77,188,300,303	0
3	NAG	C	3716	14/15	0.91	0.18	0.31	60,167,211,249	0
3	NAG	E	3716	14/15	0.92	0.22	0.31	49,184,277,297	0
3	NAG	A	3716	14/15	0.96	0.17	-1.01	28,156,272,274	0
3	NAG	G	3042	14/15	0.75	0.27	-	193,244,274,279	0
4	MAN	A	3377	11/12	0.70	0.20	-	99,256,308,331	0
3	NAG	C	3374	14/15	0.62	0.63	-	136,238,359,434	0
4	NAG	A	3374	14/15	0.71	0.32	-	91,240,362,435	0
3	NAG	E	3043	14/15	0.62	0.46	-	183,310,366,378	0
3	NAG	G	3043	14/15	0.63	0.26	-	176,248,297,317	0
9	NAG	E	3373	14/15	0.81	0.44	-	146,324,390,464	0
9	MAN	G	3375	11/12	0.65	0.29	-	173,208,309,351	0
3	NAG	C	3043	14/15	0.69	0.42	-	179,305,351,363	0
3	NAG	C	3373	14/15	0.68	0.42	-	198,292,381,425	0
4	NAG	A	3373	14/15	0.85	0.32	-	136,261,376,443	0
3	NAG	A	3043	14/15	0.81	0.26	-	80,233,327,333	0
3	NAG	E	3717	14/15	0.87	0.22	-	117,240,280,337	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	3717	14/15	0.88	0.32	-	185,218,319,381	0
3	NAG	C	3717	14/15	0.61	0.76	-	224,297,342,395	0
3	NAG	C	3042	14/15	0.78	0.28	-	150,232,327,335	0
9	NAG	E	3374	14/15	0.78	0.37	-	201,279,352,410	0
9	MAN	E	3375	11/12	0.36	0.30	-	171,251,305,311	0
4	MAN	A	3376	11/12	0.66	0.22	-	114,259,296,316	0
9	NAG	G	3373	14/15	0.83	0.35	-	106,265,384,401	0
9	NAG	G	3374	14/15	0.69	0.47	-	136,261,326,367	0
3	NAG	G	3717	14/15	0.84	0.30	-	192,216,305,376	0
3	NAG	E	3042	14/15	0.82	0.47	-	198,249,285,287	0
4	MAN	A	3375	11/12	0.80	0.16	-	140,207,283,324	0
3	NAG	A	3042	14/15	0.85	0.18	-	133,175,235,244	0

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	G	3880	14/15	0.90	0.29	1.43	84,176,236,252	0
5	MAN	A	3378	11/12	0.62	0.29	0.35	171,186,272,293	0
6	NAG	C	3880	14/15	0.92	0.23	0.12	60,171,245,293	0
7	CA	C	2006	1/1	0.85	0.16	-0.39	125,125,125,125	0
6	NAG	E	3880	14/15	0.90	0.18	-0.82	80,160,189,194	0
6	NAG	A	3880	14/15	0.91	0.18	-1.16	105,143,196,220	0
7	CA	C	2005	1/1	0.76	0.06	-1.29	200,200,200,200	0
8	MG	A	2009	1/1	0.96	0.10	-1.34	367,367,367,367	0
7	CA	D	2002	1/1	0.62	0.17	-1.34	547,547,547,547	0
7	CA	E	2006	1/1	0.90	0.13	-1.41	137,137,137,137	0
7	CA	C	2007	1/1	0.78	0.07	-1.47	206,206,206,206	0
7	CA	A	2005	1/1	0.70	0.10	-1.49	145,145,145,145	0
7	CA	H	2002	1/1	0.60	0.13	-1.53	510,510,510,510	0
7	CA	A	2007	1/1	0.92	0.08	-1.53	181,181,181,181	0
7	CA	F	2002	1/1	0.93	0.10	-1.59	578,578,578,578	0
7	CA	E	2005	1/1	0.86	0.08	-1.60	176,176,176,176	0
7	CA	E	2007	1/1	0.91	0.13	-1.69	188,188,188,188	0
7	CA	B	2002	1/1	0.80	0.09	-1.74	535,535,535,535	0
7	CA	G	2005	1/1	0.93	0.04	-2.18	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	CA	A	2006	1/1	0.81	0.11	-2.33	107,107,107,107	0
7	CA	G	2007	1/1	0.63	0.06	-2.91	150,150,150,150	0
7	CA	G	2006	1/1	0.86	0.06	-3.45	95,95,95,95	0
6	NAG	C	3678	14/15	0.72	0.48	-	125,245,317,319	0
6	NAG	B	3094	14/15	0.78	0.28	-	107,197,277,325	0
6	NAG	A	3678	14/15	0.82	0.41	-	117,269,324,327	0
6	NAG	D	3094	14/15	0.44	0.82	-	189,258,296,299	0
6	NAG	G	3678	14/15	0.84	0.52	-	132,218,244,251	0
6	NAG	H	3094	14/15	0.80	0.40	-	148,232,292,297	0
6	NAG	E	3678	14/15	0.85	0.24	-	104,227,276,317	0
6	NAG	F	3094	14/15	0.84	0.27	-	124,217,266,291	0

6.5 Other polymers (i)

There are no such residues in this entry.