



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2016 – 04:11 PM EDT

PDB ID : 5L5G  
Title : Plexin A2 full extracellular region, domains 1 to 8 modeled, data to 10 angstrom  
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.  
Deposited on : 2016-05-28  
Resolution : 10.00 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

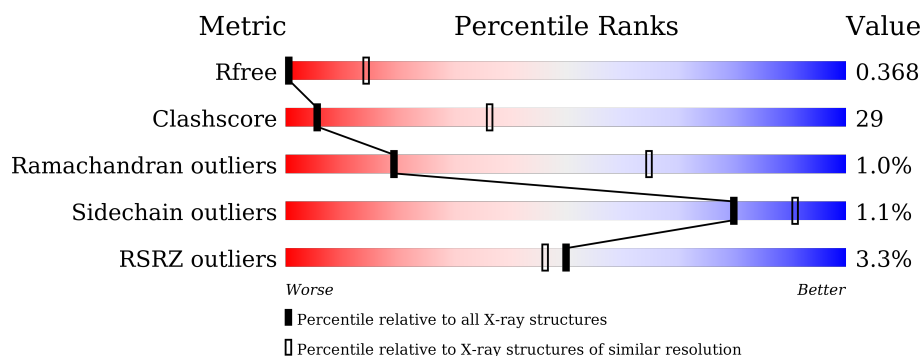
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 10.00 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	1015 (11.50-3.66)
Clashscore	102246	1065 (15.00-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1212	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>23%</div> <div>•</div> <div>25%</div> </div> </div>
1	B	1212	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>19%</div> <div>•</div> <div>33%</div> </div> </div>
1	C	1212	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>27%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	1212	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>27%</div> <div>•</div> <div>18%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28787 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 Plexin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	906	Total	C	N	O	S	0	0	0
			7060	4461	1214	1333	52			
1	B	809	Total	C	N	O	S	0	0	0
			6337	4004	1092	1195	46			
1	C	993	Total	C	N	O	S	0	0	0
			7695	4856	1321	1462	56			
1	D	993	Total	C	N	O	S	0	0	0
			7695	4856	1321	1462	56			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	-	expression tag	UNP P70207
A	1232	GLY	-	expression tag	UNP P70207
A	1233	GLY	-	expression tag	UNP P70207
A	1234	SER	-	expression tag	UNP P70207
A	1235	ARG	-	expression tag	UNP P70207
A	1236	THR	-	expression tag	UNP P70207
A	1237	LYS	-	expression tag	UNP P70207
A	1238	HIS	-	expression tag	UNP P70207
A	1239	HIS	-	expression tag	UNP P70207
A	1240	HIS	-	expression tag	UNP P70207
A	1241	HIS	-	expression tag	UNP P70207
A	1242	HIS	-	expression tag	UNP P70207
A	1243	HIS	-	expression tag	UNP P70207
B	32	GLU	-	expression tag	UNP P70207
B	1232	GLY	-	expression tag	UNP P70207
B	1233	GLY	-	expression tag	UNP P70207
B	1234	SER	-	expression tag	UNP P70207
B	1235	ARG	-	expression tag	UNP P70207
B	1236	THR	-	expression tag	UNP P70207
B	1237	LYS	-	expression tag	UNP P70207
B	1238	HIS	-	expression tag	UNP P70207

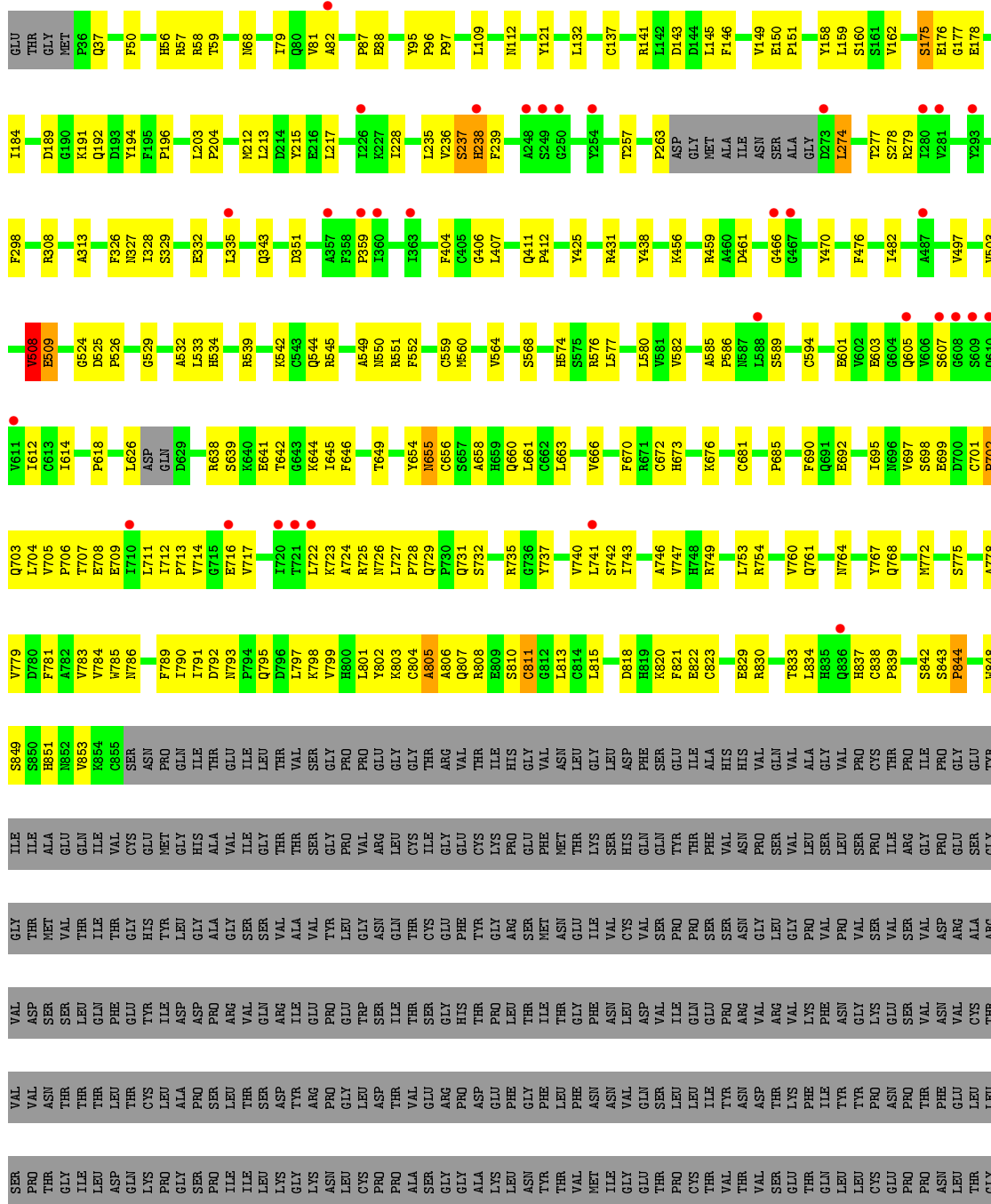
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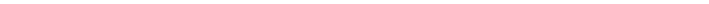
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	HIS	-	expression tag	UNP P70207
B	1240	HIS	-	expression tag	UNP P70207
B	1241	HIS	-	expression tag	UNP P70207
B	1242	HIS	-	expression tag	UNP P70207
B	1243	HIS	-	expression tag	UNP P70207
C	32	GLU	-	expression tag	UNP P70207
C	1232	GLY	-	expression tag	UNP P70207
C	1233	GLY	-	expression tag	UNP P70207
C	1234	SER	-	expression tag	UNP P70207
C	1235	ARG	-	expression tag	UNP P70207
C	1236	THR	-	expression tag	UNP P70207
C	1237	LYS	-	expression tag	UNP P70207
C	1238	HIS	-	expression tag	UNP P70207
C	1239	HIS	-	expression tag	UNP P70207
C	1240	HIS	-	expression tag	UNP P70207
C	1241	HIS	-	expression tag	UNP P70207
C	1242	HIS	-	expression tag	UNP P70207
C	1243	HIS	-	expression tag	UNP P70207
D	32	GLU	-	expression tag	UNP P70207
D	1232	GLY	-	expression tag	UNP P70207
D	1233	GLY	-	expression tag	UNP P70207
D	1234	SER	-	expression tag	UNP P70207
D	1235	ARG	-	expression tag	UNP P70207
D	1236	THR	-	expression tag	UNP P70207
D	1237	LYS	-	expression tag	UNP P70207
D	1238	HIS	-	expression tag	UNP P70207
D	1239	HIS	-	expression tag	UNP P70207
D	1240	HIS	-	expression tag	UNP P70207
D	1241	HIS	-	expression tag	UNP P70207
D	1242	HIS	-	expression tag	UNP P70207
D	1243	HIS	-	expression tag	UNP P70207



Chain B:



Chain C:  53% 27% 18%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	238.40 Å   238.40 Å   642.18 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	63.05 – 10.00 63.05 – 10.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (63.05-10.00) 92.6 (63.05-10.00)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.335 , 0.370 0.327 , 0.368	Depositor DCC
$R_{free}$ test set	520 reflections (4.69%)	DCC
Wilson B-factor (Å <sup>2</sup> )	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 306.7	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.70	EDS
Total number of atoms	28787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	236.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: (*Not available*)

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.68	4/7230 (0.1%)	0.74	8/9821 (0.1%)
1	B	0.64	3/6488 (0.0%)	0.89	7/8804 (0.1%)
1	C	0.65	7/7878 (0.1%)	0.94	13/10705 (0.1%)
1	D	0.68	8/7879 (0.1%)	1.02	23/10708 (0.2%)
All	All	0.66	22/29475 (0.1%)	0.91	51/40038 (0.1%)

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	2
1	B	0	1
1	C	0	4
1	D	0	4
All	All	0	11

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	702	PRO	C-N	26.25	1.94	1.34
1	A	508	VAL	C-N	-24.18	0.78	1.34
1	A	702	PRO	C-N	24.13	1.89	1.34
1	D	655	ASN	C-N	-16.53	0.96	1.34
1	B	655	ASN	C-N	16.05	1.71	1.34
1	D	508	VAL	C-N	-15.27	0.98	1.34
1	B	508	VAL	C-N	-15.08	0.99	1.34
1	D	952	VAL	C-N	14.06	1.66	1.34
1	C	701	CYS	C-N	13.82	1.60	1.34
1	C	508	VAL	C-N	-11.74	1.07	1.34
1	D	988	TYR	CB-CG	-11.45	1.34	1.51
1	C	988	TYR	CB-CG	-11.43	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	701	CYS	C-N	-7.54	1.20	1.34
1	A	803	LYS	C-N	-6.78	1.18	1.34
1	D	559	CYS	C-N	6.25	1.48	1.34
1	C	803	LYS	C-N	-6.09	1.20	1.34
1	C	988	TYR	CD1-CE1	-5.94	1.30	1.39
1	D	988	TYR	CD1-CE1	-5.92	1.30	1.39
1	C	952	VAL	C-N	-5.51	1.21	1.34
1	D	803	LYS	C-N	5.43	1.46	1.34
1	D	988	TYR	CA-CB	5.16	1.65	1.53
1	C	988	TYR	CA-CB	5.09	1.65	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	PRO	O-C-N	-44.19	51.99	122.70
1	C	988	TYR	CB-CG-CD1	-34.32	100.41	121.00
1	D	988	TYR	CB-CG-CD1	-34.12	100.53	121.00
1	B	508	VAL	O-C-N	-33.23	69.54	122.70
1	C	803	LYS	O-C-N	-31.50	72.31	122.70
1	D	559	CYS	O-C-N	-30.43	74.01	122.70
1	C	988	TYR	CG-CD2-CE2	-20.96	104.53	121.30
1	D	988	TYR	CG-CD2-CE2	-20.93	104.56	121.30
1	D	988	TYR	CA-CB-CG	-19.39	76.55	113.40
1	C	988	TYR	CA-CB-CG	-19.37	76.60	113.40
1	C	988	TYR	CD1-CG-CD2	16.26	135.78	117.90
1	D	988	TYR	CD1-CG-CD2	16.17	135.69	117.90
1	D	701	CYS	O-C-N	15.93	151.37	121.10
1	D	952	VAL	O-C-N	-14.95	98.79	122.70
1	D	508	VAL	CA-C-N	-14.47	85.36	117.20
1	D	508	VAL	O-C-N	13.46	144.24	122.70
1	D	559	CYS	CA-C-N	12.75	145.25	117.20
1	B	508	VAL	CA-C-N	12.52	144.74	117.20
1	D	508	VAL	C-N-CA	-11.89	91.97	121.70
1	D	701	CYS	CA-C-N	-11.40	85.18	117.10
1	D	701	CYS	C-N-CD	11.34	152.21	128.40
1	A	702	PRO	O-C-N	-11.10	104.94	122.70
1	A	508	VAL	O-C-N	-10.48	105.93	122.70
1	B	702	PRO	C-N-CA	10.32	147.50	121.70
1	D	559	CYS	C-N-CA	9.34	145.06	121.70
1	C	988	TYR	CG-CD1-CE1	-9.29	113.86	121.30
1	D	988	TYR	CG-CD1-CE1	-9.26	113.89	121.30
1	A	701	CYS	CA-C-N	-9.25	91.19	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	PRO	CA-C-N	9.15	137.34	117.20
1	D	803	LYS	C-N-CA	-8.45	100.58	121.70
1	D	701	CYS	C-N-CA	-8.42	86.63	122.00
1	C	844	PRO	N-CA-C	8.24	133.52	112.10
1	B	844	PRO	N-CA-C	8.23	133.50	112.10
1	A	844	PRO	N-CA-C	8.23	133.50	112.10
1	D	844	PRO	N-CA-C	8.23	133.50	112.10
1	A	508	VAL	C-N-CA	8.20	142.21	121.70
1	A	855	CYS	O-C-N	-8.11	109.73	122.70
1	D	952	VAL	CA-C-N	7.39	133.45	117.20
1	D	952	VAL	C-N-CA	7.36	140.10	121.70
1	A	508	VAL	CA-C-N	7.04	132.68	117.20
1	D	803	LYS	CA-C-N	-6.78	102.29	117.20
1	A	701	CYS	C-N-CA	-6.45	94.92	122.00
1	B	508	VAL	C-N-CA	6.45	137.82	121.70
1	C	803	LYS	C-N-CA	-5.97	106.78	121.70
1	C	655	ASN	C-N-CA	-5.81	107.17	121.70
1	D	988	TYR	CD1-CE1-CZ	-5.79	114.59	119.80
1	C	988	TYR	CD1-CE1-CZ	-5.74	114.64	119.80
1	C	655	ASN	CA-C-N	-5.61	104.87	117.20
1	D	990	GLY	C-N-CA	5.51	135.47	121.70
1	C	990	GLY	C-N-CA	5.50	135.45	121.70
1	C	655	ASN	O-C-N	5.17	130.98	122.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	701	CYS	Mainchain
1	A	855	CYS	Mainchain
1	B	508	VAL	Mainchain
1	C	508	VAL	Mainchain
1	C	803	LYS	Mainchain
1	C	952	VAL	Mainchain
1	C	988	TYR	Sidechain
1	D	508	VAL	Mainchain
1	D	559	CYS	Mainchain
1	D	803	LYS	Mainchain
1	D	988	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7060	0	6854	430	8
1	B	6337	0	6141	353	6
1	C	7695	0	7466	460	5
1	D	7695	0	7468	492	3
All	All	28787	0	27929	1661	11

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 29.

All (1661) 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:463:PRO:HG2	1:B:612:ILE:CG2	1.25	1.55
1:A:407:LEU:CD2	1:C:944:LYS:HD2	1.03	1.48
1:D:533:LEU:CD1	1:D:642:THR:HG23	1.41	1.48
1:A:407:LEU:CD2	1:C:944:LYS:CD	1.93	1.43
1:A:702:PRO:O	1:A:703:GLN:CG	1.65	1.41
1:B:655:ASN:C	1:B:656:CYS:N	1.71	1.40
1:B:533:LEU:CD2	1:B:646:PHE:CG	2.09	1.36
1:C:551:ARG:NH1	1:C:641:GLU:OE2	1.60	1.34
1:B:663:LEU:HD11	1:B:703:GLN:NE2	1.41	1.33
1:B:549:ALA:O	1:B:586:PRO:CB	1.75	1.32
1:D:533:LEU:CB	1:D:642:THR:HG21	1.59	1.30
1:D:533:LEU:O	1:D:644:LYS:HB2	1.32	1.30
1:A:508:VAL:O	1:A:509:GLU:N	1.63	1.28
1:C:663:LEU:HD11	1:C:792:ASP:OD2	1.32	1.27
1:A:407:LEU:HD21	1:C:944:LYS:CD	1.56	1.27
1:B:533:LEU:HD23	1:B:646:PHE:CG	1.67	1.25
1:D:550:ASN:HB2	1:D:586:PRO:CB	1.65	1.25
1:B:775:SER:N	1:B:807:GLN:OE1	1.67	1.25
1:A:702:PRO:C	1:A:703:GLN:N	1.89	1.25
1:B:550:ASN:ND2	1:B:585:ALA:O	1.70	1.24
1:D:550:ASN:CB	1:D:586:PRO:HB3	1.66	1.24
1:A:422:LEU:CD1	1:B:605:GLN:HG2	1.68	1.23
1:A:463:PRO:CG	1:B:612:ILE:CG2	2.18	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:LEU:CD1	1:C:792:ASP:OD2	1.90	1.20
1:D:533:LEU:CD1	1:D:642:THR:CG2	2.21	1.19
1:B:549:ALA:O	1:B:586:PRO:HB3	1.02	1.17
1:D:663:LEU:HD12	1:D:792:ASP:CB	1.73	1.17
1:D:775:SER:CB	1:D:807:GLN:HG3	1.72	1.17
1:B:533:LEU:CD2	1:B:646:PHE:CD1	2.28	1.17
1:C:533:LEU:HB3	1:C:642:THR:HG21	1.24	1.17
1:A:508:VAL:C	1:A:509:GLU:CA	2.13	1.16
1:B:778:ALA:HB1	1:B:798:LYS:HD2	1.15	1.14
1:D:533:LEU:HB3	1:D:642:THR:CG2	1.76	1.14
1:D:778:ALA:HB1	1:D:798:LYS:HD2	1.15	1.13
1:A:655:ASN:HB3	1:A:658:ALA:HB2	1.15	1.13
1:B:663:LEU:CD1	1:B:703:GLN:NE2	2.12	1.13
1:B:533:LEU:HD22	1:B:646:PHE:CD1	1.82	1.13
1:B:545:ARG:NH1	1:B:641:GLU:OE2	1.80	1.13
1:A:810:SER:HB2	1:A:882:ASN:OD1	1.49	1.12
1:C:702:PRO:HB3	1:C:728:PRO:HD3	1.18	1.11
1:A:655:ASN:C	1:A:656:CYS:N	2.03	1.11
1:D:932:LEU:HB3	1:D:943:THR:HG22	1.32	1.11
1:C:932:LEU:HB3	1:C:943:THR:HG22	1.33	1.11
1:D:534:HIS:HA	1:D:644:LYS:HG3	1.32	1.11
1:A:932:LEU:HB3	1:A:943:THR:HG22	1.33	1.10
1:D:533:LEU:HD12	1:D:642:THR:HG23	1.16	1.10
1:A:325:ALA:HB2	1:B:577:LEU:HD13	1.12	1.10
1:C:778:ALA:HB1	1:C:798:LYS:HD2	1.15	1.10
1:A:778:ALA:HB1	1:A:798:LYS:HD2	1.15	1.10
1:A:532:ALA:HB1	1:A:560:MET:HE3	1.23	1.10
1:A:407:LEU:HD22	1:C:944:LYS:HD2	1.24	1.10
1:A:508:VAL:CA	1:A:509:GLU:N	2.14	1.10
1:C:677:TYR:CD1	1:C:731:GLN:HG3	1.86	1.09
1:D:533:LEU:HB3	1:D:642:THR:HG21	1.20	1.09
1:A:325:ALA:HB2	1:B:577:LEU:CD1	1.82	1.09
1:D:533:LEU:HD13	1:D:642:THR:HG23	1.19	1.09
1:A:532:ALA:HB1	1:A:560:MET:CE	1.83	1.09
1:A:463:PRO:HG2	1:B:612:ILE:HG22	1.10	1.08
1:B:532:ALA:HB1	1:B:560:MET:HE3	1.29	1.08
1:D:815:LEU:HD23	1:D:853:VAL:HG11	1.33	1.08
1:A:463:PRO:HG2	1:B:612:ILE:CB	1.83	1.07
1:D:958:SER:HA	1:D:1033:LEU:HD22	1.34	1.07
1:B:815:LEU:HD23	1:B:853:VAL:HG11	1.33	1.07
1:C:815:LEU:HD23	1:C:853:VAL:HG11	1.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:LEU:HD22	1:D:639:SER:CB	1.84	1.06
1:B:692:GLU:CD	1:D:141:ARG:HH22	1.57	1.06
1:C:958:SER:HA	1:C:1033:LEU:HD22	1.34	1.06
1:D:775:SER:HB2	1:D:807:GLN:HG3	1.37	1.06
1:D:533:LEU:CD2	1:D:639:SER:CB	2.34	1.06
1:A:702:PRO:C	1:A:703:GLN:HG3	1.76	1.05
1:A:463:PRO:CG	1:B:612:ILE:HG22	1.83	1.05
1:A:463:PRO:HG2	1:B:612:ILE:HG21	1.33	1.05
1:A:325:ALA:CB	1:B:577:LEU:HD13	1.87	1.04
1:D:550:ASN:HD22	1:D:586:PRO:HA	1.14	1.04
1:A:655:ASN:O	1:A:658:ALA:HB3	1.57	1.04
1:A:815:LEU:HD23	1:A:853:VAL:HG11	1.33	1.04
1:B:533:LEU:HD23	1:B:646:PHE:CD2	1.92	1.03
1:A:464:PRO:HB3	1:B:603:GLU:O	1.56	1.03
1:A:559:CYS:C	1:A:560:MET:N	2.11	1.03
1:B:803:LYS:C	1:B:804:CYS:N	2.12	1.01
1:C:959:LEU:HG	1:C:974:ILE:HG22	1.41	1.01
1:D:533:LEU:HD22	1:D:639:SER:HB3	1.41	1.01
1:D:661:LEU:HD21	1:D:790:ILE:HD11	1.40	1.00
1:D:959:LEU:HG	1:D:974:ILE:HG22	1.41	1.00
1:B:692:GLU:OE2	1:D:141:ARG:NH2	1.94	1.00
1:C:551:ARG:NH1	1:C:641:GLU:CD	2.15	1.00
1:A:676:LYS:HE2	1:A:728:PRO:HB3	1.43	1.00
1:B:676:LYS:HE2	1:B:728:PRO:HB3	1.42	1.00
1:A:407:LEU:HD23	1:C:944:LYS:HD2	1.43	0.99
1:B:663:LEU:HD11	1:B:703:GLN:HE22	0.85	0.99
1:C:775:SER:N	1:C:806:ALA:HB3	1.78	0.99
1:D:534:HIS:CD2	1:D:644:LYS:HZ3	1.81	0.98
1:D:533:LEU:HD21	1:D:639:SER:HB2	1.42	0.98
1:C:533:LEU:HB3	1:C:642:THR:CG2	1.93	0.98
1:D:959:LEU:HD13	1:D:1033:LEU:HD23	1.44	0.98
1:C:959:LEU:HD13	1:C:1033:LEU:HD23	1.44	0.98
1:D:533:LEU:CD2	1:D:639:SER:HB2	1.91	0.98
1:A:655:ASN:CB	1:A:658:ALA:HB2	1.94	0.98
1:D:533:LEU:CB	1:D:642:THR:CG2	2.37	0.98
1:B:532:ALA:HB1	1:B:560:MET:CE	1.93	0.97
1:A:863:ILE:HD12	1:A:878:ILE:HG12	1.46	0.97
1:A:810:SER:HB2	1:A:882:ASN:CG	1.85	0.97
1:C:663:LEU:HD11	1:C:792:ASP:CG	1.85	0.97
1:D:729:GLN:HG3	1:D:754:ARG:HH12	1.26	0.97
1:A:397:PRO:HB2	1:C:947:GLN:HE22	1.25	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:GLN:HG3	1:A:754:ARG:HH12	1.26	0.97
1:C:805:ALA:HB1	1:C:808:ARG:H	1.30	0.97
1:D:663:LEU:CD1	1:D:792:ASP:OD2	2.12	0.97
1:D:863:ILE:HD12	1:D:878:ILE:HG12	1.45	0.97
1:A:407:LEU:HD23	1:C:944:LYS:CE	1.95	0.96
1:A:702:PRO:O	1:A:703:GLN:HG3	0.79	0.96
1:B:729:GLN:HG3	1:B:754:ARG:HH12	1.26	0.96
1:D:805:ALA:HB1	1:D:808:ARG:H	1.30	0.96
1:A:422:LEU:HD11	1:B:605:GLN:HG2	1.46	0.96
1:D:551:ARG:NH1	1:D:641:GLU:OE2	1.99	0.95
1:B:805:ALA:HB1	1:B:808:ARG:H	1.30	0.95
1:A:407:LEU:HD23	1:C:944:LYS:NZ	1.80	0.95
1:D:661:LEU:HD21	1:D:790:ILE:CD1	1.95	0.95
1:B:732:SER:HB2	1:D:83:HIS:CD2	2.01	0.95
1:C:729:GLN:HG3	1:C:754:ARG:HH12	1.26	0.95
1:C:863:ILE:HD12	1:C:878:ILE:HG12	1.45	0.95
1:D:663:LEU:CD1	1:D:792:ASP:CG	2.35	0.94
1:C:533:LEU:CB	1:C:642:THR:HG21	1.97	0.94
1:B:237:SER:HA	1:B:239:PHE:H	1.33	0.94
1:B:735:ARG:HG2	1:B:786:ASN:HA	1.50	0.94
1:C:735:ARG:HG2	1:C:786:ASN:HA	1.50	0.94
1:D:533:LEU:HB2	1:D:642:THR:HG21	1.45	0.94
1:D:735:ARG:HG2	1:D:786:ASN:HA	1.50	0.94
1:B:663:LEU:CD1	1:B:703:GLN:HE22	1.74	0.93
1:C:237:SER:HA	1:C:239:PHE:H	1.33	0.93
1:C:533:LEU:HD13	1:C:642:THR:HG23	1.48	0.93
1:D:533:LEU:O	1:D:644:LYS:CB	2.16	0.93
1:A:805:ALA:HB1	1:A:808:ARG:H	1.30	0.93
1:A:816:LYS:HE3	1:A:910:ILE:CG2	1.98	0.93
1:D:534:HIS:HD2	1:D:644:LYS:NZ	1.66	0.93
1:A:237:SER:HA	1:A:239:PHE:H	1.33	0.92
1:D:663:LEU:HD12	1:D:792:ASP:HB2	1.50	0.92
1:C:702:PRO:CB	1:C:728:PRO:HD3	1.99	0.92
1:B:795:GLN:HB2	1:B:797:LEU:CD1	1.99	0.92
1:B:778:ALA:CB	1:B:798:LYS:HD2	2.00	0.92
1:D:237:SER:HA	1:D:239:PHE:H	1.33	0.92
1:C:778:ALA:CB	1:C:798:LYS:HD2	2.00	0.92
1:A:735:ARG:HG2	1:A:786:ASN:HA	1.50	0.92
1:A:795:GLN:HB2	1:A:797:LEU:CD1	1.99	0.92
1:D:533:LEU:HD13	1:D:642:THR:CG2	1.92	0.92
1:C:795:GLN:HB2	1:C:797:LEU:CD1	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ALA:O	1:B:586:PRO:CA	2.18	0.91
1:D:533:LEU:HB3	1:D:642:THR:CB	2.00	0.91
1:D:795:GLN:HB2	1:D:797:LEU:CD1	1.99	0.91
1:A:655:ASN:OD1	1:A:657:SER:HB2	1.71	0.91
1:A:778:ALA:CB	1:A:798:LYS:HD2	2.00	0.91
1:D:534:HIS:HD2	1:D:644:LYS:HZ3	0.94	0.91
1:C:702:PRO:HB3	1:C:728:PRO:CD	2.01	0.90
1:D:737:TYR:CE1	1:D:754:ARG:HD2	2.06	0.90
1:B:692:GLU:OE2	1:D:141:ARG:NH1	2.05	0.90
1:C:737:TYR:CE1	1:C:754:ARG:HD2	2.06	0.90
1:A:737:TYR:CE1	1:A:754:ARG:HD2	2.06	0.90
1:B:707:THR:HG21	1:B:723:LYS:HD3	1.54	0.90
1:B:737:TYR:CE1	1:B:754:ARG:HD2	2.06	0.90
1:A:422:LEU:CD1	1:B:605:GLN:CG	2.49	0.90
1:A:655:ASN:HB3	1:A:658:ALA:CB	2.02	0.90
1:A:816:LYS:CE	1:A:910:ILE:HG23	2.02	0.89
1:C:533:LEU:CD1	1:C:642:THR:HG23	2.01	0.89
1:D:778:ALA:CB	1:D:798:LYS:HD2	2.00	0.89
1:A:707:THR:HG21	1:A:723:LYS:HD3	1.54	0.89
1:B:533:LEU:HA	1:B:646:PHE:HB2	1.54	0.89
1:B:706:PRO:HA	1:B:797:LEU:HD21	1.55	0.89
1:C:707:THR:HG21	1:C:723:LYS:HD3	1.54	0.89
1:A:810:SER:CB	1:A:882:ASN:OD1	2.22	0.88
1:A:810:SER:HB2	1:A:882:ASN:ND2	1.89	0.88
1:C:533:LEU:HD22	1:C:639:SER:CB	2.04	0.88
1:A:932:LEU:HB3	1:A:943:THR:CG2	2.04	0.88
1:C:663:LEU:HD12	1:C:792:ASP:CB	2.04	0.87
1:C:893:HIS:HB2	1:C:933:CYS:O	1.75	0.87
1:A:655:ASN:O	1:A:658:ALA:CB	2.21	0.87
1:C:959:LEU:CD1	1:C:1033:LEU:HD23	2.04	0.87
1:D:533:LEU:HD12	1:D:642:THR:CG2	1.91	0.87
1:D:959:LEU:CD1	1:D:1033:LEU:HD23	2.04	0.87
1:D:550:ASN:HB2	1:D:586:PRO:HB3	0.89	0.87
1:D:707:THR:HG21	1:D:723:LYS:HD3	1.54	0.87
1:B:533:LEU:HA	1:B:646:PHE:CB	2.04	0.87
1:A:549:ALA:O	1:A:586:PRO:HB3	1.74	0.87
1:D:893:HIS:HB2	1:D:933:CYS:O	1.75	0.87
1:D:551:ARG:NH2	1:D:642:THR:HG22	1.89	0.87
1:D:932:LEU:HB3	1:D:943:THR:CG2	2.04	0.86
1:A:706:PRO:HA	1:A:797:LEU:HD21	1.55	0.86
1:C:706:PRO:HA	1:C:797:LEU:HD21	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:706:PRO:HA	1:D:797:LEU:HD21	1.55	0.86
1:D:711:LEU:HD23	1:D:821:PHE:CD1	2.10	0.86
1:C:934:ILE:HD12	1:C:941:PHE:HD1	1.40	0.86
1:D:550:ASN:CB	1:D:586:PRO:CB	2.39	0.86
1:C:932:LEU:HB3	1:C:943:THR:CG2	2.04	0.86
1:D:663:LEU:HD11	1:D:792:ASP:CG	1.94	0.86
1:B:533:LEU:CD2	1:B:646:PHE:CD2	2.55	0.85
1:B:775:SER:H	1:B:807:GLN:CD	1.79	0.85
1:D:934:ILE:HD12	1:D:941:PHE:HD1	1.40	0.85
1:D:550:ASN:ND2	1:D:586:PRO:HA	1.91	0.85
1:D:775:SER:HB3	1:D:807:GLN:HG3	1.59	0.85
1:A:655:ASN:C	1:A:656:CYS:CA	2.44	0.85
1:A:893:HIS:HB2	1:A:933:CYS:O	1.75	0.85
1:A:934:ILE:HD12	1:A:941:PHE:HD1	1.40	0.85
1:C:533:LEU:HD22	1:C:639:SER:HB2	1.57	0.84
1:D:775:SER:CB	1:D:807:GLN:CG	2.55	0.84
1:C:663:LEU:CD1	1:C:792:ASP:CG	2.44	0.84
1:B:743:ILE:HB	1:B:746:ALA:O	1.78	0.84
1:A:655:ASN:C	1:A:658:ALA:H	1.80	0.84
1:C:743:ILE:HB	1:C:746:ALA:O	1.78	0.84
1:B:702:PRO:HB3	1:B:726:ASN:O	1.76	0.83
1:C:795:GLN:HB2	1:C:797:LEU:HD12	1.60	0.83
1:D:743:ILE:HB	1:D:746:ALA:O	1.78	0.83
1:A:508:VAL:C	1:A:509:GLU:N	0.78	0.83
1:C:818:ASP:HB2	1:C:821:PHE:CD2	2.14	0.83
1:A:407:LEU:CD2	1:C:944:LYS:CE	2.56	0.83
1:B:818:ASP:HB2	1:B:821:PHE:CD2	2.14	0.83
1:A:301:THR:HG21	1:B:589:SER:HB2	1.60	0.83
1:A:743:ILE:HB	1:A:746:ALA:O	1.78	0.83
1:C:893:HIS:CE1	1:C:894:VAL:HG22	2.14	0.83
1:D:663:LEU:HD12	1:D:792:ASP:CG	1.99	0.83
1:A:818:ASP:HB2	1:A:821:PHE:CD2	2.14	0.82
1:B:795:GLN:HB2	1:B:797:LEU:HD12	1.60	0.82
1:A:893:HIS:CE1	1:A:894:VAL:HG22	2.14	0.82
1:D:663:LEU:HD11	1:D:792:ASP:OD2	1.78	0.82
1:D:893:HIS:CE1	1:D:894:VAL:HG22	2.14	0.82
1:D:550:ASN:HD22	1:D:586:PRO:CA	1.93	0.82
1:D:534:HIS:CD2	1:D:644:LYS:NZ	2.43	0.82
1:D:818:ASP:HB2	1:D:821:PHE:CD2	2.14	0.82
1:A:893:HIS:HD1	1:A:932:LEU:HA	1.44	0.81
1:D:795:GLN:HB2	1:D:797:LEU:HD12	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:GLN:HB2	1:A:797:LEU:HD12	1.60	0.81
1:A:816:LYS:HE3	1:A:910:ILE:HG23	1.61	0.81
1:C:907:GLU:OE1	1:C:915:VAL:HG11	1.81	0.81
1:B:741:LEU:O	1:B:747:VAL:HG23	1.81	0.81
1:A:407:LEU:HD23	1:C:944:LYS:CD	1.96	0.81
1:B:711:LEU:HD21	1:B:820:LYS:HB3	1.62	0.81
1:C:893:HIS:HD1	1:C:932:LEU:HA	1.44	0.81
1:A:907:GLU:OE1	1:A:915:VAL:HG11	1.81	0.81
1:C:735:ARG:CG	1:C:786:ASN:HA	2.11	0.81
1:D:893:HIS:HD1	1:D:932:LEU:HA	1.44	0.81
1:D:741:LEU:O	1:D:747:VAL:HG23	1.81	0.81
1:D:907:GLU:OE1	1:D:915:VAL:HG11	1.81	0.81
1:B:802:TYR:CG	1:B:821:PHE:CD1	2.69	0.80
1:C:741:LEU:O	1:C:747:VAL:HG23	1.81	0.80
1:C:883:LEU:HB2	1:C:911:ALA:HA	1.63	0.80
1:D:735:ARG:CG	1:D:786:ASN:HA	2.11	0.80
1:A:784:VAL:HG22	1:A:790:ILE:HG22	1.63	0.80
1:A:422:LEU:HD12	1:B:605:GLN:CD	2.01	0.80
1:B:701:CYS:C	1:B:702:PRO:N	2.35	0.80
1:C:677:TYR:CD1	1:C:731:GLN:CG	2.63	0.80
1:D:883:LEU:HB2	1:D:911:ALA:HA	1.63	0.80
1:B:735:ARG:CG	1:B:786:ASN:HA	2.11	0.80
1:D:904:ILE:CG2	1:D:907:GLU:HB2	2.12	0.80
1:A:904:ILE:CG2	1:A:907:GLU:HB2	2.12	0.80
1:B:692:GLU:OE2	1:D:141:ARG:CZ	2.29	0.80
1:B:784:VAL:HG22	1:B:790:ILE:HG22	1.63	0.80
1:D:551:ARG:NH1	1:D:641:GLU:CD	2.35	0.80
1:D:803:LYS:C	1:D:804:CYS:O	2.17	0.80
1:D:775:SER:HB2	1:D:807:GLN:CG	2.12	0.80
1:A:735:ARG:CG	1:A:786:ASN:HA	2.11	0.80
1:C:904:ILE:CG2	1:C:907:GLU:HB2	2.12	0.80
1:C:893:HIS:CE1	1:C:932:LEU:HG	2.18	0.79
1:D:812:GLY:HA3	1:D:885:LEU:CD2	2.11	0.79
1:A:217:LEU:HD11	1:C:940:GLU:OE1	1.83	0.79
1:A:397:PRO:HB2	1:C:947:GLN:NE2	1.95	0.79
1:D:784:VAL:HG22	1:D:790:ILE:HG22	1.63	0.79
1:A:407:LEU:HD21	1:C:944:LYS:HD2	0.79	0.79
1:A:741:LEU:O	1:A:747:VAL:HG23	1.81	0.79
1:B:690:PHE:HE2	1:B:731:GLN:HB3	1.47	0.79
1:B:775:SER:CB	1:B:807:GLN:OE1	2.30	0.79
1:B:663:LEU:CD1	1:B:703:GLN:HE21	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:VAL:HG22	1:C:790:ILE:HG22	1.63	0.79
1:D:533:LEU:CD1	1:D:639:SER:OG	2.31	0.79
1:D:893:HIS:CE1	1:D:932:LEU:HG	2.18	0.78
1:A:463:PRO:HD2	1:B:577:LEU:HD22	1.65	0.78
1:D:663:LEU:CD1	1:D:792:ASP:CB	2.56	0.78
1:D:823:CYS:HA	1:D:834:LEU:HD23	1.65	0.78
1:A:422:LEU:HD12	1:B:605:GLN:CG	2.14	0.78
1:C:823:CYS:HA	1:C:834:LEU:HD23	1.65	0.78
1:D:958:SER:HA	1:D:1033:LEU:CD2	2.13	0.78
1:A:463:PRO:HG2	1:B:612:ILE:HB	1.66	0.78
1:D:812:GLY:CA	1:D:885:LEU:CD2	2.62	0.78
1:A:893:HIS:CE1	1:A:932:LEU:HG	2.18	0.78
1:A:883:LEU:HB2	1:A:911:ALA:HA	1.63	0.77
1:A:737:TYR:HE1	1:A:754:ARG:HD2	1.50	0.77
1:A:508:VAL:O	1:A:509:GLU:CA	2.29	0.77
1:B:550:ASN:HB2	1:B:586:PRO:CA	2.13	0.77
1:A:890:ILE:HD13	1:A:908:TYR:CE1	2.20	0.77
1:D:786:ASN:HB3	1:D:789:PHE:HD2	1.50	0.77
1:A:655:ASN:C	1:A:656:CYS:C	2.43	0.77
1:D:795:GLN:HB2	1:D:797:LEU:HD11	1.67	0.77
1:B:533:LEU:HD22	1:B:646:PHE:CG	2.00	0.77
1:B:823:CYS:HA	1:B:834:LEU:HD23	1.65	0.77
1:D:890:ILE:HD13	1:D:908:TYR:CE1	2.20	0.77
1:D:729:GLN:HG3	1:D:754:ARG:NH1	2.00	0.76
1:A:795:GLN:HB2	1:A:797:LEU:HD11	1.67	0.76
1:A:823:CYS:HA	1:A:834:LEU:HD23	1.65	0.76
1:C:795:GLN:HB2	1:C:797:LEU:HD11	1.67	0.76
1:D:533:LEU:HB3	1:D:642:THR:OG1	1.86	0.76
1:A:786:ASN:HB3	1:A:789:PHE:HD2	1.50	0.76
1:C:729:GLN:HG3	1:C:754:ARG:NH1	2.00	0.76
1:B:550:ASN:HB2	1:B:586:PRO:N	1.99	0.76
1:D:812:GLY:CA	1:D:885:LEU:HD21	2.16	0.76
1:A:815:LEU:HD23	1:A:853:VAL:CG1	2.15	0.76
1:C:786:ASN:HB3	1:C:789:PHE:HD2	1.50	0.76
1:C:958:SER:HA	1:C:1033:LEU:CD2	2.13	0.76
1:B:729:GLN:HG3	1:B:754:ARG:NH1	2.00	0.76
1:C:890:ILE:HD13	1:C:908:TYR:CE1	2.20	0.76
1:A:463:PRO:CG	1:B:612:ILE:HG21	2.00	0.76
1:D:440:TYR:CE2	1:D:527:HIS:HA	2.21	0.75
1:D:737:TYR:HE1	1:D:754:ARG:HD2	1.50	0.75
1:D:803:LYS:O	1:D:804:CYS:C	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:GLN:HG3	1:A:754:ARG:NH1	2.00	0.75
1:B:559:CYS:C	1:B:560:MET:N	2.40	0.75
1:B:795:GLN:HB2	1:B:797:LEU:HD11	1.67	0.75
1:D:996:PHE:HZ	1:D:999:ARG:HB2	1.51	0.75
1:C:996:PHE:HZ	1:C:999:ARG:HB2	1.51	0.75
1:C:960:SER:OG	1:C:973:THR:HB	1.86	0.75
1:C:707:THR:CG2	1:C:723:LYS:HD3	2.17	0.75
1:B:786:ASN:HB3	1:B:789:PHE:HD2	1.50	0.75
1:B:802:TYR:CD2	1:B:821:PHE:CD1	2.75	0.75
1:C:737:TYR:HE1	1:C:754:ARG:HD2	1.50	0.75
1:A:870:PRO:O	1:A:921:ALA:HB3	1.87	0.75
1:D:870:PRO:O	1:D:921:ALA:HB3	1.87	0.75
1:D:815:LEU:HD23	1:D:853:VAL:CG1	2.15	0.74
1:D:960:SER:OG	1:D:973:THR:HB	1.86	0.74
1:B:459:ARG:NH1	1:B:524:GLY:O	2.20	0.74
1:D:707:THR:CG2	1:D:723:LYS:HD3	2.17	0.74
1:B:775:SER:CA	1:B:807:GLN:OE1	2.36	0.74
1:A:815:LEU:CB	1:A:885:LEU:HD11	2.17	0.74
1:B:550:ASN:HB2	1:B:585:ALA:C	2.08	0.74
1:D:714:VAL:HG13	1:D:767:TYR:O	1.88	0.74
1:A:714:VAL:HG13	1:A:767:TYR:O	1.88	0.73
1:B:714:VAL:HG13	1:B:767:TYR:O	1.88	0.73
1:B:707:THR:CG2	1:B:723:LYS:HD3	2.17	0.73
1:C:873:GLY:HA3	1:C:1026:ARG:HG3	1.70	0.73
1:C:870:PRO:O	1:C:921:ALA:HB3	1.87	0.73
1:A:893:HIS:ND1	1:A:932:LEU:HA	2.02	0.73
1:C:714:VAL:HG13	1:C:767:TYR:O	1.88	0.73
1:C:445:VAL:HG22	1:C:526:PRO:HG2	1.70	0.73
1:A:707:THR:CG2	1:A:723:LYS:HD3	2.17	0.73
1:D:533:LEU:HD21	1:D:639:SER:CB	2.07	0.73
1:B:533:LEU:HD23	1:B:646:PHE:CB	2.19	0.73
1:D:997:TYR:HB3	1:D:1005:VAL:HG23	1.70	0.73
1:D:893:HIS:ND1	1:D:932:LEU:HA	2.02	0.73
1:C:893:HIS:ND1	1:C:932:LEU:HA	2.02	0.73
1:C:997:TYR:HB3	1:C:1005:VAL:HG23	1.70	0.73
1:D:550:ASN:HB2	1:D:586:PRO:CA	2.18	0.73
1:D:786:ASN:HB3	1:D:789:PHE:CD2	2.24	0.72
1:A:702:PRO:O	1:A:703:GLN:CB	2.35	0.72
1:B:775:SER:HB2	1:B:807:GLN:CD	2.08	0.72
1:B:786:ASN:HB3	1:B:789:PHE:CD2	2.24	0.72
1:B:544:GLN:HG2	1:B:545:ARG:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1018:VAL:O	1:C:1034:GLN:HG3	1.88	0.72
1:D:1018:VAL:O	1:D:1034:GLN:HG3	1.88	0.72
1:B:533:LEU:HD21	1:B:646:PHE:CD1	2.24	0.72
1:C:663:LEU:HD12	1:C:792:ASP:HB3	1.72	0.72
1:D:988:TYR:HB3	1:D:1021:SER:HB3	1.70	0.72
1:A:863:ILE:CD1	1:A:878:ILE:HG12	2.20	0.72
1:D:775:SER:HB3	1:D:807:GLN:CG	2.18	0.72
1:A:655:ASN:O	1:A:658:ALA:N	2.22	0.71
1:C:872:GLY:O	1:C:1026:ARG:HB2	1.89	0.71
1:A:422:LEU:HD12	1:B:605:GLN:HG2	1.66	0.71
1:C:988:TYR:HB3	1:C:1021:SER:HB3	1.71	0.71
1:D:893:HIS:NE2	1:D:914:ILE:HD13	2.05	0.71
1:A:786:ASN:HB3	1:A:789:PHE:CD2	2.24	0.71
1:A:883:LEU:HD23	1:A:914:ILE:HD11	1.72	0.71
1:C:863:ILE:CD1	1:C:878:ILE:HG12	2.20	0.71
1:C:893:HIS:NE2	1:C:914:ILE:HD13	2.05	0.71
1:D:883:LEU:HD23	1:D:914:ILE:HD11	1.72	0.71
1:B:711:LEU:CD2	1:B:820:LYS:HB3	2.20	0.71
1:C:815:LEU:HD23	1:C:853:VAL:CG1	2.15	0.71
1:B:732:SER:HB2	1:D:83:HIS:NE2	2.04	0.71
1:A:810:SER:HB2	1:A:882:ASN:HD21	1.53	0.71
1:C:786:ASN:HB3	1:C:789:PHE:CD2	2.24	0.71
1:A:893:HIS:NE2	1:A:914:ILE:HD13	2.05	0.71
1:D:855:CYS:SG	1:D:885:LEU:HD21	2.30	0.71
1:B:532:ALA:CB	1:B:560:MET:HE3	2.16	0.71
1:B:549:ALA:O	1:B:586:PRO:HA	1.91	0.71
1:A:221:PHE:CZ	1:C:830:ARG:HB2	2.25	0.71
1:B:737:TYR:HE1	1:B:754:ARG:HD2	1.50	0.71
1:B:775:SER:CB	1:B:807:GLN:CD	2.59	0.71
1:A:655:ASN:CA	1:A:656:CYS:N	2.54	0.70
1:A:655:ASN:CG	1:A:658:ALA:N	2.45	0.70
1:C:544:GLN:HG2	1:C:545:ARG:HG2	1.71	0.70
1:D:544:GLN:HG2	1:D:545:ARG:HG2	1.71	0.70
1:A:544:GLN:HG2	1:A:545:ARG:HG2	1.71	0.70
1:A:920:HIS:NE2	1:A:922:VAL:HG23	2.06	0.70
1:D:863:ILE:CD1	1:D:878:ILE:HG12	2.20	0.70
1:D:920:HIS:NE2	1:D:922:VAL:HG23	2.06	0.70
1:B:690:PHE:HE2	1:B:731:GLN:CB	2.03	0.70
1:B:697:VAL:HG12	1:B:699:GLU:H	1.57	0.70
1:C:920:HIS:NE2	1:C:922:VAL:HG23	2.06	0.70
1:A:811:CYS:O	1:A:815:LEU:HD13	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:CYS:SG	1:A:839:PRO:HD2	2.32	0.70
1:B:815:LEU:HD23	1:B:853:VAL:CG1	2.15	0.70
1:C:697:VAL:HG12	1:C:699:GLU:H	1.57	0.70
1:C:811:CYS:O	1:C:815:LEU:HD13	1.92	0.70
1:C:883:LEU:HD23	1:C:914:ILE:HD11	1.72	0.70
1:D:838:CYS:SG	1:D:839:PRO:HD2	2.32	0.70
1:B:833:THR:CG2	1:B:837:HIS:HB2	2.22	0.70
1:D:811:CYS:O	1:D:815:LEU:HD13	1.92	0.70
1:A:697:VAL:HG12	1:A:699:GLU:H	1.56	0.70
1:D:938:LYS:HB2	1:D:941:PHE:HD2	1.57	0.70
1:B:838:CYS:SG	1:B:839:PRO:HD2	2.32	0.69
1:C:938:LYS:HB2	1:C:941:PHE:HD2	1.57	0.69
1:A:868:GLY:HA3	1:A:949:TYR:OH	1.92	0.69
1:B:811:CYS:O	1:B:815:LEU:HD13	1.92	0.69
1:C:818:ASP:HB2	1:C:821:PHE:CE2	2.28	0.69
1:D:697:VAL:HG12	1:D:699:GLU:H	1.57	0.69
1:A:810:SER:CB	1:A:882:ASN:HD21	2.06	0.69
1:A:870:PRO:HD3	1:A:952:VAL:O	1.92	0.69
1:D:533:LEU:HD11	1:D:639:SER:OG	1.91	0.69
1:A:818:ASP:HB2	1:A:821:PHE:CE2	2.28	0.69
1:B:470:TYR:CE1	1:B:525:ASP:CG	2.66	0.69
1:A:833:THR:CG2	1:A:837:HIS:HB2	2.22	0.69
1:A:938:LYS:HB2	1:A:941:PHE:HD2	1.57	0.69
1:C:663:LEU:CD1	1:C:792:ASP:CB	2.69	0.69
1:C:838:CYS:SG	1:C:839:PRO:HD2	2.32	0.69
1:C:868:GLY:HA3	1:C:949:TYR:OH	1.92	0.69
1:D:818:ASP:HB2	1:D:821:PHE:CE2	2.28	0.69
1:B:818:ASP:HB2	1:B:821:PHE:CE2	2.28	0.69
1:D:550:ASN:HB3	1:D:586:PRO:HG3	1.73	0.69
1:A:463:PRO:CG	1:B:612:ILE:HB	2.23	0.69
1:C:833:THR:CG2	1:C:837:HIS:HB2	2.22	0.69
1:C:870:PRO:HD3	1:C:952:VAL:O	1.92	0.69
1:D:868:GLY:HA3	1:D:949:TYR:OH	1.92	0.69
1:A:893:HIS:NE2	1:A:894:VAL:HG22	2.08	0.69
1:D:870:PRO:HD3	1:D:952:VAL:O	1.93	0.69
1:A:815:LEU:HB3	1:A:885:LEU:HD11	1.74	0.69
1:D:833:THR:CG2	1:D:837:HIS:HB2	2.22	0.69
1:D:663:LEU:CD1	1:D:792:ASP:HB2	2.23	0.68
1:D:893:HIS:NE2	1:D:894:VAL:HG22	2.08	0.68
1:A:740:VAL:HG22	1:A:749:ARG:HD2	1.76	0.68
1:A:815:LEU:HA	1:A:848:TRP:CD1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:ILE:HB	1:A:893:HIS:HD2	1.58	0.68
1:D:890:ILE:HB	1:D:893:HIS:HD2	1.59	0.68
1:A:79:ILE:HD11	1:A:82:ALA:HB2	1.75	0.68
1:C:550:ASN:CB	1:C:586:PRO:HB3	2.24	0.68
1:D:79:ILE:HD11	1:D:82:ALA:HB2	1.75	0.68
1:B:815:LEU:HA	1:B:848:TRP:CD1	2.29	0.68
1:C:79:ILE:HD11	1:C:82:ALA:HB2	1.75	0.68
1:C:890:ILE:HB	1:C:893:HIS:HD2	1.59	0.68
1:B:737:TYR:CD2	1:B:785:TRP:HB3	2.29	0.68
1:C:737:TYR:CD2	1:C:785:TRP:HB3	2.29	0.68
1:D:564:VAL:HG22	1:D:580:LEU:HD13	1.76	0.68
1:D:815:LEU:HA	1:D:848:TRP:CD1	2.29	0.68
1:D:737:TYR:CD2	1:D:785:TRP:HB3	2.29	0.68
1:A:704:LEU:HD11	1:A:783:VAL:CG2	2.24	0.68
1:A:706:PRO:CA	1:A:797:LEU:HD21	2.24	0.68
1:B:79:ILE:HD11	1:B:82:ALA:HB2	1.75	0.68
1:B:810:SER:OG	1:B:813:LEU:HD13	1.94	0.68
1:C:810:SER:OG	1:C:813:LEU:HD13	1.94	0.68
1:B:740:VAL:HG22	1:B:749:ARG:HD2	1.75	0.67
1:D:704:LEU:HD11	1:D:783:VAL:CG2	2.24	0.67
1:B:550:ASN:CB	1:B:585:ALA:C	2.63	0.67
1:C:704:LEU:HD11	1:C:783:VAL:CG2	2.24	0.67
1:C:713:PRO:HG3	1:C:802:TYR:OH	1.95	0.67
1:B:704:LEU:HD11	1:B:783:VAL:CG2	2.24	0.67
1:B:713:PRO:HG3	1:B:802:TYR:OH	1.95	0.67
1:C:564:VAL:HG22	1:C:580:LEU:HD13	1.76	0.67
1:C:863:ILE:HG13	1:C:877:THR:O	1.94	0.67
1:A:863:ILE:HG13	1:A:877:THR:O	1.95	0.67
1:D:713:PRO:HG3	1:D:802:TYR:OH	1.95	0.67
1:C:815:LEU:HA	1:C:848:TRP:CD1	2.29	0.67
1:D:1015:LEU:HD12	1:D:1015:LEU:H	1.59	0.67
1:D:810:SER:OG	1:D:813:LEU:HD13	1.94	0.67
1:A:737:TYR:CD2	1:A:785:TRP:HB3	2.29	0.67
1:A:810:SER:OG	1:A:813:LEU:HD13	1.94	0.67
1:B:568:SER:HG	1:B:670:PHE:HD1	1.41	0.67
1:A:463:PRO:CD	1:B:612:ILE:HG21	2.24	0.67
1:C:893:HIS:NE2	1:C:894:VAL:HG22	2.08	0.67
1:D:740:VAL:HG22	1:D:749:ARG:HD2	1.76	0.67
1:B:564:VAL:HG22	1:B:580:LEU:HD13	1.76	0.67
1:B:703:GLN:HA	1:B:792:ASP:OD1	1.95	0.67
1:C:1015:LEU:H	1:C:1015:LEU:HD12	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:ASN:OD1	1:C:657:SER:HB2	1.94	0.67
1:B:666:VAL:HG11	1:B:698:SER:N	2.10	0.67
1:B:805:ALA:HB1	1:B:808:ARG:N	2.08	0.67
1:B:237:SER:HA	1:B:239:PHE:N	2.07	0.66
1:B:690:PHE:CD2	1:B:731:GLN:HG3	2.30	0.66
1:C:740:VAL:HG22	1:C:749:ARG:HD2	1.75	0.66
1:A:564:VAL:HG22	1:A:580:LEU:HD13	1.76	0.66
1:B:706:PRO:CA	1:B:797:LEU:HD21	2.24	0.66
1:C:559:CYS:O	1:C:584:ASP:CB	2.43	0.66
1:C:702:PRO:HA	1:C:726:ASN:O	1.95	0.66
1:C:533:LEU:CD2	1:C:639:SER:HB2	2.23	0.66
1:C:956:VAL:HG23	1:C:975:THR:O	1.95	0.66
1:D:666:VAL:HG11	1:D:698:SER:N	2.10	0.66
1:D:956:VAL:HG23	1:D:975:THR:O	1.95	0.66
1:B:714:VAL:HG13	1:B:768:GLN:HA	1.77	0.66
1:D:703:GLN:HA	1:D:792:ASP:OD1	1.95	0.66
1:D:863:ILE:HG13	1:D:877:THR:O	1.94	0.66
1:A:706:PRO:HG3	1:A:795:GLN:HG3	1.78	0.66
1:B:533:LEU:HD21	1:B:646:PHE:CE1	2.31	0.66
1:C:706:PRO:CA	1:C:797:LEU:HD21	2.24	0.66
1:C:677:TYR:HD1	1:C:731:GLN:HG3	1.55	0.66
1:A:324:GLN:HE21	1:B:577:LEU:H	1.42	0.66
1:A:713:PRO:HG3	1:A:802:TYR:OH	1.95	0.66
1:C:237:SER:HA	1:C:239:PHE:N	2.08	0.66
1:D:717:VAL:CG1	1:D:764:ASN:HB3	2.26	0.66
1:A:714:VAL:HG13	1:A:768:GLN:HA	1.78	0.66
1:B:717:VAL:CG1	1:B:764:ASN:HB3	2.26	0.66
1:B:732:SER:CB	1:D:83:HIS:CD2	2.78	0.66
1:C:714:VAL:HG13	1:C:768:GLN:HA	1.77	0.66
1:B:802:TYR:CD1	1:B:821:PHE:CD1	2.84	0.66
1:C:855:CYS:C	1:C:856:SER:N	2.48	0.66
1:D:793:ASN:OD1	1:D:797:LEU:HD13	1.96	0.66
1:A:237:SER:HA	1:A:239:PHE:N	2.08	0.66
1:C:1015:LEU:HD21	1:C:1039:ASP:HB2	1.78	0.65
1:A:666:VAL:HG11	1:A:698:SER:N	2.10	0.65
1:A:703:GLN:HA	1:A:792:ASP:OD1	1.95	0.65
1:B:551:ARG:NH2	1:B:642:THR:HG21	2.11	0.65
1:C:666:VAL:HG11	1:C:698:SER:N	2.10	0.65
1:C:703:GLN:HA	1:C:792:ASP:OD1	1.95	0.65
1:C:717:VAL:CG1	1:C:764:ASN:HB3	2.26	0.65
1:C:793:ASN:OD1	1:C:797:LEU:HD13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:SER:HA	1:D:239:PHE:N	2.08	0.65
1:A:701:CYS:O	1:A:703:GLN:HG3	1.95	0.65
1:D:706:PRO:CA	1:D:797:LEU:HD21	2.24	0.65
1:D:1015:LEU:HD21	1:D:1039:ASP:HB2	1.78	0.65
1:B:711:LEU:HD21	1:B:820:LYS:CB	2.25	0.65
1:C:774:ILE:C	1:C:806:ALA:HB3	2.15	0.65
1:A:717:VAL:CG1	1:A:764:ASN:HB3	2.26	0.65
1:B:793:ASN:OD1	1:B:797:LEU:HD13	1.96	0.65
1:B:803:LYS:C	1:B:804:CYS:CA	2.65	0.65
1:D:864:LEU:HG	1:D:865:THR:N	2.12	0.65
1:D:812:GLY:CA	1:D:885:LEU:HD22	2.26	0.65
1:D:714:VAL:HG13	1:D:768:GLN:HA	1.78	0.65
1:A:742:SER:O	1:A:779:VAL:HG13	1.97	0.65
1:C:864:LEU:HG	1:C:865:THR:N	2.12	0.65
1:A:772:MET:O	1:A:806:ALA:HB1	1.97	0.65
1:A:864:LEU:HG	1:A:865:THR:N	2.12	0.65
1:C:88:GLU:HB2	1:C:132:LEU:HD21	1.79	0.65
1:C:742:SER:O	1:C:779:VAL:HG13	1.97	0.65
1:A:793:ASN:OD1	1:A:797:LEU:HD13	1.96	0.64
1:A:88:GLU:HB2	1:A:132:LEU:HD21	1.79	0.64
1:D:706:PRO:HG3	1:D:795:GLN:HG3	1.78	0.64
1:A:655:ASN:OD1	1:A:658:ALA:N	2.30	0.64
1:D:88:GLU:HB2	1:D:132:LEU:HD21	1.79	0.64
1:D:742:SER:O	1:D:779:VAL:HG13	1.97	0.64
1:A:704:LEU:HD11	1:A:783:VAL:HG21	1.80	0.64
1:A:842:SER:OG	1:A:844:PRO:HD2	1.97	0.64
1:B:695:ILE:CD1	1:B:702:PRO:HD3	2.28	0.64
1:A:805:ALA:HB1	1:A:808:ARG:N	2.08	0.64
1:C:842:SER:OG	1:C:844:PRO:HD2	1.97	0.64
1:D:812:GLY:HA3	1:D:885:LEU:HD22	1.78	0.64
1:B:550:ASN:HB2	1:B:586:PRO:HA	1.80	0.64
1:C:706:PRO:HG3	1:C:795:GLN:HG3	1.78	0.64
1:A:549:ALA:O	1:A:586:PRO:CB	2.45	0.64
1:B:706:PRO:HG3	1:B:795:GLN:HG3	1.78	0.64
1:C:533:LEU:HD13	1:C:639:SER:OG	1.98	0.64
1:A:810:SER:CB	1:A:882:ASN:ND2	2.61	0.63
1:B:742:SER:O	1:B:779:VAL:HG13	1.97	0.63
1:D:931:ARG:HD2	1:D:942:MET:HE3	1.79	0.63
1:B:533:LEU:CD2	1:B:646:PHE:CB	2.76	0.63
1:B:842:SER:OG	1:B:844:PRO:HD2	1.97	0.63
1:C:775:SER:HB2	1:C:807:GLN:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:LEU:HD11	1:C:783:VAL:HG21	1.80	0.63
1:D:959:LEU:HG	1:D:974:ILE:CG2	2.25	0.63
1:B:704:LEU:HD11	1:B:783:VAL:HG21	1.80	0.63
1:C:855:CYS:O	1:C:856:SER:N	2.32	0.63
1:D:1001:MET:HG3	1:D:1002:ASN:N	2.13	0.63
1:D:842:SER:OG	1:D:844:PRO:HD2	1.97	0.63
1:B:706:PRO:HA	1:B:797:LEU:CD2	2.29	0.63
1:A:407:LEU:HD23	1:C:944:LYS:HZ2	1.61	0.63
1:C:1001:MET:HG3	1:C:1002:ASN:N	2.13	0.63
1:C:959:LEU:HG	1:C:974:ILE:CG2	2.25	0.63
1:D:470:TYR:HB2	1:D:523:SER:O	1.98	0.63
1:D:704:LEU:HD11	1:D:783:VAL:HG21	1.80	0.63
1:D:988:TYR:HE1	1:D:992:GLN:C	2.02	0.63
1:B:88:GLU:HB2	1:B:132:LEU:HD21	1.79	0.63
1:C:931:ARG:HD2	1:C:942:MET:HE3	1.79	0.63
1:C:988:TYR:HE1	1:C:992:GLN:C	2.02	0.63
1:D:630:TRP:HB3	1:D:670:PHE:CE2	2.34	0.63
1:C:994:CYS:HA	1:C:1009:PRO:HD3	1.81	0.63
1:C:274:LEU:H	1:C:274:LEU:HD12	1.64	0.63
1:C:904:ILE:HG23	1:C:907:GLU:HB2	1.79	0.63
1:D:904:ILE:HG23	1:D:907:GLU:HB2	1.79	0.63
1:D:994:CYS:HA	1:D:1009:PRO:HD3	1.81	0.63
1:C:989:LEU:HG	1:C:1020:VAL:HG12	1.81	0.62
1:D:661:LEU:HD21	1:D:790:ILE:CG1	2.28	0.62
1:A:274:LEU:H	1:A:274:LEU:HD12	1.64	0.62
1:A:834:LEU:HB2	1:A:837:HIS:HD2	1.64	0.62
1:B:834:LEU:HB2	1:B:837:HIS:HD2	1.64	0.62
1:D:989:LEU:HG	1:D:1020:VAL:HG12	1.81	0.62
1:B:663:LEU:HD12	1:B:703:GLN:HE21	1.63	0.62
1:D:274:LEU:H	1:D:274:LEU:HD12	1.64	0.62
1:A:934:ILE:HD12	1:A:941:PHE:CD1	2.30	0.62
1:A:895:GLN:HG2	1:A:931:ARG:HB3	1.82	0.62
1:C:790:ILE:HG13	1:C:790:ILE:O	2.00	0.62
1:C:885:LEU:HD22	1:C:910:ILE:HD11	1.81	0.62
1:D:885:LEU:CD2	1:D:910:ILE:HD11	2.30	0.62
1:B:274:LEU:H	1:B:274:LEU:HD12	1.64	0.62
1:A:463:PRO:CB	1:B:612:ILE:HG22	2.29	0.62
1:C:805:ALA:HB1	1:C:808:ARG:N	2.08	0.61
1:A:881:VAL:HG13	1:A:882:ASN:N	2.16	0.61
1:A:885:LEU:HD22	1:A:910:ILE:HD11	1.81	0.61
1:A:904:ILE:HG23	1:A:907:GLU:HB2	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:LEU:CD2	1:A:910:ILE:HD11	2.30	0.61
1:B:702:PRO:CB	1:B:726:ASN:O	2.47	0.61
1:D:834:LEU:HB2	1:D:837:HIS:HD2	1.64	0.61
1:C:874:THR:HA	1:C:1025:ASP:OD2	2.00	0.61
1:C:885:LEU:CD2	1:C:910:ILE:HD11	2.30	0.61
1:D:881:VAL:HG13	1:D:882:ASN:N	2.16	0.61
1:B:550:ASN:O	1:B:586:PRO:HG3	2.00	0.61
1:C:834:LEU:HB2	1:C:837:HIS:HD2	1.64	0.61
1:D:706:PRO:HA	1:D:797:LEU:CD2	2.29	0.61
1:C:706:PRO:HA	1:C:797:LEU:CD2	2.29	0.61
1:C:895:GLN:HG2	1:C:931:ARG:HB3	1.82	0.61
1:B:532:ALA:CB	1:B:560:MET:CE	2.75	0.61
1:C:881:VAL:HG13	1:C:882:ASN:N	2.16	0.61
1:A:864:LEU:HG	1:A:865:THR:H	1.66	0.61
1:B:802:TYR:CZ	1:B:821:PHE:HD1	2.19	0.61
1:D:885:LEU:HD22	1:D:910:ILE:HD11	1.81	0.61
1:D:989:LEU:HD12	1:D:989:LEU:N	2.15	0.61
1:B:655:ASN:C	1:B:656:CYS:CA	2.66	0.61
1:B:790:ILE:O	1:B:790:ILE:HG13	2.00	0.61
1:B:786:ASN:HD22	1:B:789:PHE:HE2	1.48	0.60
1:D:551:ARG:NH2	1:D:642:THR:CG2	2.62	0.60
1:A:842:SER:CB	1:A:844:PRO:HD2	2.31	0.60
1:B:508:VAL:CG1	1:B:539:ARG:NH2	2.64	0.60
1:B:802:TYR:CG	1:B:821:PHE:CE1	2.89	0.60
1:D:1015:LEU:HD12	1:D:1015:LEU:N	2.16	0.60
1:D:760:VAL:HG12	1:D:761:GLN:N	2.16	0.60
1:A:815:LEU:HB2	1:A:885:LEU:HD11	1.81	0.60
1:C:661:LEU:HD21	1:C:790:ILE:HD11	1.83	0.60
1:C:842:SER:CB	1:C:844:PRO:HD2	2.31	0.60
1:A:324:GLN:NE2	1:B:577:LEU:H	2.00	0.60
1:A:532:ALA:HB1	1:A:560:MET:HE2	1.78	0.60
1:A:533:LEU:HD23	1:A:646:PHE:CG	2.36	0.60
1:A:760:VAL:HG12	1:A:761:GLN:N	2.16	0.60
1:C:1015:LEU:HD12	1:C:1015:LEU:N	2.16	0.60
1:C:191:LYS:HB3	1:C:194:TYR:HB2	1.83	0.60
1:C:989:LEU:N	1:C:989:LEU:HD12	2.15	0.60
1:D:790:ILE:HG13	1:D:790:ILE:O	2.00	0.60
1:D:842:SER:CB	1:D:844:PRO:HD2	2.31	0.60
1:A:549:ALA:O	1:A:586:PRO:HA	2.02	0.60
1:B:815:LEU:HA	1:B:848:TRP:HD1	1.66	0.60
1:D:786:ASN:HD22	1:D:789:PHE:HE2	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:895:GLN:HG2	1:D:931:ARG:HB3	1.82	0.60
1:C:934:ILE:HD12	1:C:941:PHE:CD1	2.30	0.60
1:B:786:ASN:ND2	1:B:789:PHE:HE2	2.00	0.60
1:B:842:SER:CB	1:B:844:PRO:HD2	2.31	0.60
1:C:663:LEU:HD23	1:C:698:SER:HB2	1.84	0.60
1:A:931:ARG:HH11	1:A:942:MET:HE3	1.66	0.60
1:A:706:PRO:HA	1:A:797:LEU:CD2	2.29	0.60
1:A:790:ILE:O	1:A:790:ILE:HG13	2.00	0.60
1:B:760:VAL:HG12	1:B:761:GLN:N	2.16	0.60
1:B:815:LEU:HB3	1:B:848:TRP:HB3	1.84	0.60
1:C:786:ASN:HD22	1:C:789:PHE:HE2	1.48	0.60
1:D:191:LYS:HB3	1:D:194:TYR:HB2	1.83	0.60
1:A:550:ASN:ND2	1:A:585:ALA:O	2.29	0.59
1:C:864:LEU:HG	1:C:865:THR:H	1.66	0.59
1:D:533:LEU:CG	1:D:642:THR:CG2	2.80	0.59
1:A:786:ASN:HD22	1:A:789:PHE:HE2	1.48	0.59
1:D:550:ASN:HB3	1:D:586:PRO:CG	2.32	0.59
1:D:805:ALA:HB1	1:D:808:ARG:N	2.08	0.59
1:B:191:LYS:HB3	1:B:194:TYR:HB2	1.83	0.59
1:D:663:LEU:HD23	1:D:698:SER:HB2	1.84	0.59
1:D:786:ASN:ND2	1:D:789:PHE:HE2	2.00	0.59
1:A:191:LYS:HB3	1:A:194:TYR:HB2	1.83	0.59
1:C:760:VAL:HG12	1:C:761:GLN:N	2.16	0.59
1:A:786:ASN:ND2	1:A:789:PHE:HE2	2.00	0.59
1:A:855:CYS:SG	1:A:856:SER:N	2.75	0.59
1:C:815:LEU:HA	1:C:848:TRP:HD1	1.66	0.59
1:A:655:ASN:OD1	1:A:657:SER:CB	2.45	0.59
1:A:931:ARG:HD2	1:A:942:MET:HE3	1.84	0.59
1:B:802:TYR:CE2	1:B:821:PHE:HD1	2.19	0.59
1:C:663:LEU:HD12	1:C:792:ASP:OD2	1.95	0.59
1:D:815:LEU:HB3	1:D:848:TRP:HB3	1.84	0.59
1:A:97:PRO:HG2	1:A:158:TYR:CE1	2.38	0.59
1:B:663:LEU:HD23	1:B:698:SER:HB2	1.84	0.59
1:B:802:TYR:CD1	1:B:821:PHE:CE1	2.90	0.59
1:D:97:PRO:HG2	1:D:158:TYR:CE1	2.38	0.59
1:D:864:LEU:HG	1:D:865:THR:H	1.66	0.59
1:C:959:LEU:HD13	1:C:1033:LEU:CD2	2.26	0.59
1:D:887:PHE:O	1:D:890:ILE:HG12	2.02	0.59
1:C:703:GLN:HG2	1:C:792:ASP:OD1	2.03	0.58
1:C:887:PHE:O	1:C:890:ILE:HG12	2.02	0.58
1:C:97:PRO:HG2	1:C:158:TYR:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:VAL:HG22	1:D:526:PRO:HG2	1.85	0.58
1:B:459:ARG:CD	1:B:526:PRO:HG3	2.33	0.58
1:B:803:LYS:CA	1:B:804:CYS:N	2.65	0.58
1:D:443:TYR:HB2	1:D:526:PRO:HB3	1.85	0.58
1:A:703:GLN:HG2	1:A:792:ASP:OD1	2.03	0.58
1:C:815:LEU:HB3	1:C:848:TRP:HB3	1.84	0.58
1:C:853:VAL:HG13	1:C:853:VAL:O	2.04	0.58
1:A:663:LEU:HD23	1:A:698:SER:HB2	1.84	0.58
1:A:815:LEU:HB3	1:A:848:TRP:HB3	1.84	0.58
1:A:887:PHE:O	1:A:890:ILE:HG12	2.02	0.58
1:A:938:LYS:HE3	1:A:941:PHE:CD2	2.38	0.58
1:C:895:GLN:CG	1:C:931:ARG:HB3	2.33	0.58
1:A:815:LEU:HA	1:A:848:TRP:HD1	1.66	0.58
1:B:802:TYR:CE1	1:B:821:PHE:HD1	2.21	0.58
1:C:876:VAL:HG22	1:C:916:CYS:O	2.03	0.58
1:A:853:VAL:HG13	1:A:853:VAL:O	2.04	0.58
1:A:876:VAL:HG22	1:A:916:CYS:O	2.03	0.58
1:A:895:GLN:CG	1:A:931:ARG:HB3	2.33	0.58
1:B:97:PRO:HG2	1:B:158:TYR:CE1	2.38	0.58
1:A:422:LEU:HD13	1:B:605:GLN:HG2	1.78	0.58
1:B:533:LEU:HD13	1:B:639:SER:CB	2.33	0.58
1:D:1015:LEU:HD23	1:D:1039:ASP:N	2.18	0.58
1:D:876:VAL:HG22	1:D:916:CYS:O	2.04	0.58
1:D:550:ASN:HB3	1:D:586:PRO:CB	2.33	0.58
1:D:895:GLN:CG	1:D:931:ARG:HB3	2.34	0.58
1:D:938:LYS:HE3	1:D:941:PHE:CD2	2.39	0.58
1:D:988:TYR:C	1:D:989:LEU:HD12	2.24	0.58
1:C:1017:PRO:HB3	1:C:1034:GLN:NE2	2.19	0.58
1:C:988:TYR:C	1:C:989:LEU:HD12	2.24	0.58
1:D:703:GLN:HG2	1:D:792:ASP:OD1	2.03	0.58
1:D:815:LEU:CD2	1:D:853:VAL:HG11	2.23	0.58
1:D:959:LEU:HD13	1:D:1033:LEU:CD2	2.26	0.58
1:A:815:LEU:N	1:A:815:LEU:HD12	2.19	0.58
1:A:931:ARG:HD3	1:A:943:THR:O	2.04	0.58
1:C:1015:LEU:HD23	1:C:1039:ASP:N	2.18	0.58
1:D:1017:PRO:HB3	1:D:1034:GLN:NE2	2.19	0.58
1:D:815:LEU:HA	1:D:848:TRP:HD1	1.66	0.58
1:D:931:ARG:HD3	1:D:943:THR:O	2.04	0.58
1:A:700:ASP:O	1:A:702:PRO:HD3	2.04	0.57
1:B:703:GLN:HG2	1:B:792:ASP:OD1	2.03	0.57
1:C:786:ASN:ND2	1:C:789:PHE:HE2	2.00	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:988:TYR:CE2	1:C:991:ASN:N	2.71	0.57
1:D:815:LEU:N	1:D:815:LEU:HD12	2.19	0.57
1:C:938:LYS:HE3	1:C:941:PHE:CD2	2.38	0.57
1:D:459:ARG:HD3	1:D:524:GLY:O	2.04	0.57
1:B:690:PHE:HD2	1:B:731:GLN:HG3	1.68	0.57
1:B:843:SER:OG	1:B:844:PRO:HD3	2.05	0.57
1:C:910:ILE:HG23	1:C:910:ILE:O	2.04	0.57
1:A:815:LEU:CD2	1:A:853:VAL:HG11	2.23	0.57
1:B:815:LEU:HD12	1:B:815:LEU:N	2.19	0.57
1:D:853:VAL:HG13	1:D:853:VAL:O	2.04	0.57
1:B:533:LEU:O	1:B:646:PHE:HB3	2.04	0.57
1:B:775:SER:HB3	1:B:807:GLN:OE1	2.04	0.57
1:C:815:LEU:N	1:C:815:LEU:HD12	2.20	0.57
1:D:910:ILE:HG23	1:D:910:ILE:O	2.04	0.57
1:D:934:ILE:HD12	1:D:941:PHE:CD1	2.30	0.57
1:D:988:TYR:CE2	1:D:991:ASN:N	2.71	0.57
1:A:175:SER:OG	1:A:178:GLU:HG2	2.04	0.57
1:C:931:ARG:HD3	1:C:943:THR:O	2.04	0.57
1:C:988:TYR:CZ	1:C:989:LEU:N	2.73	0.57
1:A:910:ILE:HG23	1:A:910:ILE:O	2.04	0.57
1:C:175:SER:OG	1:C:178:GLU:HG2	2.04	0.57
1:C:843:SER:OG	1:C:844:PRO:HD3	2.05	0.57
1:D:988:TYR:CZ	1:D:989:LEU:N	2.73	0.57
1:B:425:TYR:OH	1:B:456:LYS:HE2	2.05	0.57
1:C:550:ASN:HB2	1:C:586:PRO:HB3	1.86	0.57
1:D:175:SER:OG	1:D:178:GLU:HG2	2.04	0.57
1:B:802:TYR:CD2	1:B:821:PHE:HD1	2.23	0.56
1:D:533:LEU:HD13	1:D:642:THR:CB	2.35	0.56
1:B:853:VAL:O	1:B:853:VAL:HG13	2.04	0.56
1:C:775:SER:HB2	1:C:806:ALA:H	1.69	0.56
1:D:407:LEU:O	1:D:411:GLN:HG2	2.05	0.56
1:D:529:GLY:HA3	1:D:552:PHE:CZ	2.40	0.56
1:A:532:ALA:CB	1:A:560:MET:CE	2.73	0.56
1:B:533:LEU:CD2	1:B:646:PHE:CE1	2.85	0.56
1:B:663:LEU:HD12	1:B:703:GLN:NE2	2.12	0.56
1:D:663:LEU:CG	1:D:792:ASP:OD2	2.53	0.56
1:A:529:GLY:HA3	1:A:552:PHE:CZ	2.40	0.56
1:C:425:TYR:OH	1:C:456:LYS:HE2	2.05	0.56
1:C:529:GLY:HA3	1:C:552:PHE:CZ	2.41	0.56
1:D:830:ARG:HG2	1:D:830:ARG:O	2.06	0.56
1:B:175:SER:OG	1:B:178:GLU:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:974:ILE:HD11	1:C:1004:ILE:HB	1.88	0.56
1:D:663:LEU:HD12	1:D:792:ASP:OD2	2.02	0.56
1:D:843:SER:OG	1:D:844:PRO:HD3	2.05	0.56
1:B:407:LEU:O	1:B:411:GLN:HG2	2.05	0.56
1:A:420:GLU:HB3	1:B:607:SER:HB3	1.87	0.56
1:C:407:LEU:O	1:C:411:GLN:HG2	2.05	0.56
1:A:324:GLN:NE2	1:B:576:ARG:HD2	2.20	0.56
1:A:533:LEU:HD23	1:A:646:PHE:CD2	2.41	0.56
1:B:529:GLY:HA3	1:B:552:PHE:CZ	2.40	0.56
1:B:676:LYS:HG3	1:B:702:PRO:HG2	1.86	0.56
1:D:974:ILE:HD11	1:D:1004:ILE:HB	1.88	0.56
1:B:551:ARG:HH22	1:B:642:THR:CG2	2.19	0.56
1:C:985:VAL:HG11	1:C:999:ARG:HD3	1.88	0.56
1:C:815:LEU:CD2	1:C:853:VAL:HG11	2.23	0.56
1:D:508:VAL:HG12	1:D:509:GLU:N	2.20	0.56
1:A:753:LEU:N	1:A:753:LEU:HD12	2.21	0.56
1:C:830:ARG:O	1:C:830:ARG:HG2	2.06	0.56
1:D:985:VAL:HG11	1:D:999:ARG:HD3	1.88	0.56
1:B:551:ARG:HH22	1:B:642:THR:HG21	1.71	0.55
1:A:407:LEU:O	1:A:411:GLN:HG2	2.05	0.55
1:A:425:TYR:OH	1:A:456:LYS:HE2	2.05	0.55
1:A:843:SER:OG	1:A:844:PRO:HD3	2.05	0.55
1:C:235:LEU:HG	1:C:236:VAL:HG23	1.88	0.55
1:D:425:TYR:OH	1:D:456:LYS:HE2	2.05	0.55
1:D:938:LYS:HE3	1:D:941:PHE:CE2	2.41	0.55
1:A:235:LEU:HG	1:A:236:VAL:HG23	1.88	0.55
1:A:830:ARG:HG2	1:A:830:ARG:O	2.06	0.55
1:C:923:ILE:HG12	1:C:924:GLY:H	1.72	0.55
1:D:533:LEU:HD13	1:D:639:SER:OG	2.05	0.55
1:D:663:LEU:HD12	1:D:792:ASP:HB3	1.75	0.55
1:D:904:ILE:HG21	1:D:907:GLU:HB2	1.88	0.55
1:A:508:VAL:O	1:A:509:GLU:HA	2.06	0.55
1:B:753:LEU:HD12	1:B:753:LEU:N	2.21	0.55
1:C:727:LEU:HD11	1:C:760:VAL:CG2	2.37	0.55
1:C:904:ILE:HG21	1:C:907:GLU:HB2	1.88	0.55
1:C:938:LYS:HE3	1:C:941:PHE:CE2	2.41	0.55
1:D:235:LEU:HG	1:D:236:VAL:HG23	1.88	0.55
1:B:830:ARG:HG2	1:B:830:ARG:O	2.06	0.55
1:C:1015:LEU:HD21	1:C:1039:ASP:CA	2.37	0.55
1:A:727:LEU:HD11	1:A:760:VAL:CG2	2.37	0.55
1:A:938:LYS:HE3	1:A:941:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:LEU:HD11	1:B:760:VAL:CG2	2.37	0.55
1:C:747:VAL:HG13	1:C:747:VAL:O	2.07	0.55
1:C:753:LEU:N	1:C:753:LEU:HD12	2.21	0.55
1:D:923:ILE:HG12	1:D:924:GLY:H	1.72	0.55
1:C:894:VAL:HG21	1:C:903:PRO:HG3	1.89	0.55
1:D:1015:LEU:HD21	1:D:1039:ASP:CA	2.37	0.55
1:A:883:LEU:N	1:A:883:LEU:HD12	2.21	0.55
1:B:235:LEU:HG	1:B:236:VAL:HG23	1.88	0.55
1:B:747:VAL:O	1:B:747:VAL:HG13	2.07	0.55
1:C:1024:VAL:O	1:C:1024:VAL:HG13	2.06	0.55
1:C:873:GLY:CA	1:C:1026:ARG:HG3	2.35	0.55
1:C:883:LEU:N	1:C:883:LEU:HD12	2.22	0.55
1:B:775:SER:HB2	1:B:807:GLN:CG	2.37	0.54
1:D:1024:VAL:HG13	1:D:1024:VAL:O	2.06	0.54
1:D:747:VAL:HG13	1:D:747:VAL:O	2.07	0.54
1:A:747:VAL:O	1:A:747:VAL:HG13	2.07	0.54
1:B:87:PRO:HB2	1:B:109:LEU:HD11	1.90	0.54
1:D:663:LEU:HG	1:D:792:ASP:OD2	2.08	0.54
1:D:894:VAL:HG21	1:D:903:PRO:HG3	1.89	0.54
1:A:904:ILE:HG21	1:A:907:GLU:HB2	1.88	0.54
1:B:802:TYR:CD1	1:B:821:PHE:HD1	2.24	0.54
1:C:574:HIS:ND1	1:C:618:PRO:HD3	2.22	0.54
1:D:883:LEU:N	1:D:883:LEU:HD12	2.22	0.54
1:B:550:ASN:CB	1:B:585:ALA:O	2.56	0.54
1:C:887:PHE:CD1	1:C:890:ILE:HD11	2.43	0.54
1:D:1020:VAL:O	1:D:1020:VAL:HG23	2.07	0.54
1:A:890:ILE:HB	1:A:893:HIS:CD2	2.42	0.54
1:B:784:VAL:HG12	1:B:785:TRP:N	2.23	0.54
1:C:1015:LEU:HD21	1:C:1039:ASP:CB	2.38	0.54
1:C:1020:VAL:O	1:C:1020:VAL:HG23	2.07	0.54
1:D:1015:LEU:HD21	1:D:1039:ASP:CB	2.38	0.54
1:D:551:ARG:HH12	1:D:641:GLU:CD	2.06	0.54
1:D:887:PHE:CD1	1:D:890:ILE:HD11	2.43	0.54
1:A:894:VAL:HG21	1:A:903:PRO:HG3	1.89	0.54
1:C:551:ARG:NH2	1:C:642:THR:HG22	2.22	0.54
1:D:574:HIS:ND1	1:D:618:PRO:HD3	2.22	0.54
1:D:775:SER:H	1:D:807:GLN:HG3	1.72	0.54
1:B:574:HIS:ND1	1:B:618:PRO:HD3	2.22	0.54
1:D:775:SER:HB3	1:D:807:GLN:CD	2.28	0.54
1:D:812:GLY:HA2	1:D:885:LEU:CD2	2.36	0.54
1:A:887:PHE:CD1	1:A:890:ILE:HD11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:ASN:O	1:B:658:ALA:CB	2.56	0.54
1:D:1015:LEU:CD1	1:D:1015:LEU:H	2.21	0.54
1:D:753:LEU:N	1:D:753:LEU:HD12	2.21	0.54
1:D:727:LEU:HD11	1:D:760:VAL:CG2	2.37	0.54
1:D:784:VAL:HG12	1:D:785:TRP:N	2.23	0.54
1:A:574:HIS:ND1	1:A:618:PRO:HD3	2.22	0.54
1:C:1015:LEU:H	1:C:1015:LEU:CD1	2.21	0.54
1:A:87:PRO:HB2	1:A:109:LEU:HD11	1.90	0.53
1:A:907:GLU:HB3	1:A:915:VAL:HG21	1.91	0.53
1:C:1038:ILE:HG22	1:C:1039:ASP:N	2.23	0.53
1:C:784:VAL:HG12	1:C:785:TRP:N	2.23	0.53
1:D:812:GLY:HA3	1:D:885:LEU:HD21	1.84	0.53
1:D:885:LEU:HA	1:D:910:ILE:HD11	1.90	0.53
1:A:883:LEU:HD23	1:A:914:ILE:CD1	2.39	0.53
1:D:1038:ILE:HG22	1:D:1039:ASP:N	2.23	0.53
1:D:438:TYR:HH	1:D:527:HIS:CD2	2.23	0.53
1:D:87:PRO:HB2	1:D:109:LEU:HD11	1.90	0.53
1:D:883:LEU:HD23	1:D:914:ILE:CD1	2.39	0.53
1:A:923:ILE:HG12	1:A:924:GLY:H	1.72	0.53
1:B:550:ASN:HB2	1:B:585:ALA:O	2.09	0.53
1:B:723:LYS:HD2	1:B:723:LYS:N	2.24	0.53
1:B:533:LEU:HA	1:B:646:PHE:HB3	1.88	0.53
1:A:705:VAL:HG12	1:A:706:PRO:N	2.24	0.53
1:A:754:ARG:O	1:A:754:ARG:HG3	2.09	0.53
1:C:470:TYR:CE1	1:C:525:ASP:CG	2.82	0.53
1:C:87:PRO:HB2	1:C:109:LEU:HD11	1.90	0.53
1:A:885:LEU:HA	1:A:910:ILE:HD11	1.90	0.53
1:C:876:VAL:CG2	1:C:916:CYS:HB3	2.39	0.53
1:C:883:LEU:HD23	1:C:914:ILE:CD1	2.39	0.53
1:C:988:TYR:OH	1:C:992:GLN:N	2.42	0.53
1:D:907:GLU:HB3	1:D:915:VAL:HG21	1.90	0.53
1:A:723:LYS:N	1:A:723:LYS:HD2	2.24	0.53
1:B:802:TYR:CE2	1:B:821:PHE:CD1	2.97	0.53
1:C:712:ILE:HB	1:C:801:LEU:HD23	1.91	0.53
1:D:876:VAL:CG2	1:D:916:CYS:HB3	2.39	0.53
1:B:712:ILE:HB	1:B:801:LEU:HD23	1.91	0.53
1:C:550:ASN:HB3	1:C:586:PRO:HB3	1.91	0.53
1:D:988:TYR:OH	1:D:992:GLN:N	2.42	0.53
1:A:463:PRO:CD	1:B:612:ILE:CG2	2.84	0.52
1:B:702:PRO:HA	1:B:726:ASN:HB2	1.91	0.52
1:C:907:GLU:HB3	1:C:915:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:958:SER:C	1:C:959:LEU:HD12	2.30	0.52
1:B:550:ASN:C	1:B:586:PRO:HG3	2.29	0.52
1:C:1015:LEU:CD2	1:C:1039:ASP:HB2	2.39	0.52
1:C:885:LEU:HA	1:C:910:ILE:HD11	1.90	0.52
1:D:443:TYR:CB	1:D:526:PRO:HB3	2.39	0.52
1:D:938:LYS:HB2	1:D:941:PHE:CD2	2.42	0.52
1:A:784:VAL:HG12	1:A:785:TRP:N	2.23	0.52
1:D:1015:LEU:CD2	1:D:1039:ASP:HB2	2.39	0.52
1:D:723:LYS:N	1:D:723:LYS:HD2	2.24	0.52
1:D:958:SER:C	1:D:959:LEU:HD12	2.30	0.52
1:A:549:ALA:O	1:A:586:PRO:CA	2.57	0.52
1:A:816:LYS:NZ	1:A:910:ILE:HG23	2.24	0.52
1:B:533:LEU:HD21	1:B:646:PHE:CG	2.34	0.52
1:C:785:TRP:CE3	1:C:786:ASN:HB2	2.45	0.52
1:C:797:LEU:N	1:C:797:LEU:HD12	2.25	0.52
1:A:785:TRP:CE3	1:A:786:ASN:HB2	2.45	0.52
1:A:797:LEU:HD12	1:A:797:LEU:N	2.25	0.52
1:B:754:ARG:HG3	1:B:754:ARG:O	2.09	0.52
1:A:221:PHE:CZ	1:C:830:ARG:CB	2.92	0.52
1:D:712:ILE:HB	1:D:801:LEU:HD23	1.91	0.52
1:A:533:LEU:CD2	1:A:646:PHE:CG	2.93	0.52
1:A:876:VAL:CG2	1:A:916:CYS:HB3	2.39	0.52
1:C:1005:VAL:O	1:C:1005:VAL:HG23	2.09	0.52
1:C:967:SER:O	1:C:1010:PRO:HG3	2.09	0.52
1:C:723:LYS:N	1:C:723:LYS:HD2	2.24	0.52
1:D:785:TRP:CE3	1:D:786:ASN:HB2	2.45	0.52
1:D:996:PHE:CZ	1:D:999:ARG:HB2	2.39	0.52
1:A:702:PRO:C	1:A:703:GLN:CA	2.77	0.52
1:A:890:ILE:O	1:A:893:HIS:HB3	2.09	0.52
1:B:711:LEU:HD12	1:B:711:LEU:N	2.25	0.52
1:B:797:LEU:N	1:B:797:LEU:HD12	2.25	0.52
1:B:815:LEU:CD2	1:B:853:VAL:HG11	2.23	0.52
1:C:533:LEU:HD12	1:C:642:THR:HG23	1.89	0.52
1:D:822:GLU:HG2	1:D:822:GLU:O	2.10	0.52
1:C:533:LEU:CD1	1:C:642:THR:CG2	2.83	0.52
1:C:822:GLU:HG2	1:C:822:GLU:O	2.10	0.52
1:D:967:SER:O	1:D:1010:PRO:HG3	2.09	0.52
1:B:470:TYR:CE1	1:B:525:ASP:OD2	2.63	0.52
1:C:996:PHE:CZ	1:C:999:ARG:HB2	2.39	0.52
1:A:422:LEU:HD12	1:B:605:GLN:NE2	2.25	0.52
1:B:702:PRO:O	1:B:703:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:988:TYR:HB3	1:C:1021:SER:O	2.09	0.52
1:C:711:LEU:HD12	1:C:711:LEU:N	2.25	0.51
1:C:754:ARG:HG3	1:C:754:ARG:O	2.09	0.51
1:D:1005:VAL:O	1:D:1005:VAL:HG23	2.09	0.51
1:D:705:VAL:HG12	1:D:706:PRO:N	2.24	0.51
1:D:711:LEU:HD12	1:D:711:LEU:N	2.25	0.51
1:D:797:LEU:N	1:D:797:LEU:HD12	2.25	0.51
1:D:890:ILE:O	1:D:893:HIS:HB3	2.10	0.51
1:A:712:ILE:HB	1:A:801:LEU:HD23	1.91	0.51
1:A:822:GLU:HG2	1:A:822:GLU:O	2.10	0.51
1:B:274:LEU:N	1:B:274:LEU:HD12	2.25	0.51
1:B:655:ASN:O	1:B:658:ALA:HB3	2.10	0.51
1:B:705:VAL:HG12	1:B:706:PRO:N	2.24	0.51
1:C:655:ASN:C	1:C:657:SER:N	2.62	0.51
1:C:993:THR:HG22	1:C:994:CYS:N	2.25	0.51
1:D:956:VAL:O	1:D:956:VAL:HG13	2.10	0.51
1:B:308:ARG:HB2	1:B:343:GLN:HG2	1.92	0.51
1:D:923:ILE:HG12	1:D:924:GLY:N	2.26	0.51
1:D:988:TYR:HB3	1:D:1021:SER:O	2.09	0.51
1:A:716:GLU:HA	1:A:716:GLU:OE1	2.10	0.51
1:C:533:LEU:CD1	1:C:641:GLU:HB3	2.40	0.51
1:C:890:ILE:HB	1:C:893:HIS:CD2	2.42	0.51
1:C:956:VAL:O	1:C:956:VAL:HG13	2.10	0.51
1:D:754:ARG:HG3	1:D:754:ARG:O	2.09	0.51
1:D:993:THR:HG22	1:D:994:CYS:N	2.25	0.51
1:A:923:ILE:HG12	1:A:924:GLY:N	2.26	0.51
1:C:445:VAL:CG2	1:C:526:PRO:HG2	2.39	0.51
1:C:705:VAL:HG12	1:C:706:PRO:N	2.24	0.51
1:D:896:VAL:O	1:D:897:ALA:HB3	2.10	0.51
1:A:655:ASN:O	1:A:658:ALA:CA	2.58	0.51
1:B:785:TRP:CE3	1:B:786:ASN:HB2	2.45	0.51
1:C:533:LEU:O	1:C:644:LYS:HB2	2.10	0.51
1:D:574:HIS:CE1	1:D:618:PRO:HD3	2.46	0.51
1:D:713:PRO:HG3	1:D:802:TYR:CZ	2.45	0.51
1:D:931:ARG:HH11	1:D:942:MET:HE3	1.75	0.51
1:A:176:GLU:HG3	1:A:177:GLY:N	2.26	0.51
1:A:711:LEU:N	1:A:711:LEU:HD12	2.25	0.51
1:B:235:LEU:HD21	1:B:263:PRO:HG2	1.92	0.51
1:B:676:LYS:HE2	1:B:728:PRO:CB	2.28	0.51
1:B:692:GLU:CD	1:D:141:ARG:NH2	2.42	0.51
1:C:716:GLU:OE1	1:C:716:GLU:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:PRO:HG3	1:C:978:TYR:O	2.10	0.51
1:D:308:ARG:HB2	1:D:343:GLN:HG2	1.92	0.51
1:D:954:PRO:HG3	1:D:978:TYR:O	2.10	0.51
1:A:274:LEU:HD12	1:A:274:LEU:N	2.25	0.51
1:A:574:HIS:CE1	1:A:618:PRO:HD3	2.46	0.51
1:A:896:VAL:O	1:A:897:ALA:HB3	2.10	0.51
1:A:816:LYS:CE	1:A:910:ILE:CG2	2.70	0.51
1:A:938:LYS:HB2	1:A:941:PHE:CD2	2.42	0.51
1:B:822:GLU:HG2	1:B:822:GLU:O	2.10	0.51
1:C:871:GLU:OE1	1:C:1027:ALA:HB2	2.11	0.51
1:C:574:HIS:CE1	1:C:618:PRO:HD3	2.46	0.51
1:D:716:GLU:HA	1:D:716:GLU:OE1	2.10	0.51
1:D:799:VAL:HG23	1:D:799:VAL:O	2.11	0.51
1:C:890:ILE:O	1:C:893:HIS:HB3	2.10	0.51
1:C:923:ILE:HG12	1:C:924:GLY:N	2.26	0.51
1:C:988:TYR:O	1:C:1020:VAL:HA	2.11	0.51
1:C:713:PRO:HG3	1:C:802:TYR:CZ	2.45	0.51
1:C:938:LYS:HB2	1:C:941:PHE:CD2	2.42	0.51
1:D:461:ASP:O	1:D:466:GLY:O	2.29	0.51
1:A:533:LEU:HD22	1:A:646:PHE:CD1	2.46	0.50
1:A:890:ILE:HG13	1:A:891:ALA:N	2.26	0.50
1:B:532:ALA:HB1	1:B:560:MET:HE2	1.89	0.50
1:B:833:THR:HG23	1:B:837:HIS:HB2	1.92	0.50
1:C:461:ASP:O	1:C:466:GLY:O	2.29	0.50
1:A:713:PRO:HG3	1:A:802:TYR:CZ	2.45	0.50
1:A:833:THR:HG23	1:A:837:HIS:HB2	1.91	0.50
1:A:870:PRO:HG2	1:A:871:GLU:OE1	2.11	0.50
1:B:176:GLU:HG3	1:B:177:GLY:N	2.26	0.50
1:B:461:ASP:O	1:B:466:GLY:O	2.29	0.50
1:B:713:PRO:HG3	1:B:802:TYR:CZ	2.46	0.50
1:B:699:GLU:O	1:B:725:ARG:NH2	2.45	0.50
1:C:235:LEU:HD21	1:C:263:PRO:HG2	1.93	0.50
1:C:896:VAL:O	1:C:897:ALA:HB3	2.10	0.50
1:C:988:TYR:HE2	1:C:991:ASN:H	1.55	0.50
1:D:988:TYR:O	1:D:1020:VAL:HA	2.11	0.50
1:D:176:GLU:HG3	1:D:177:GLY:N	2.26	0.50
1:D:274:LEU:N	1:D:274:LEU:HD12	2.25	0.50
1:B:533:LEU:HD21	1:B:646:PHE:CZ	2.45	0.50
1:C:308:ARG:HB2	1:C:343:GLN:HG2	1.92	0.50
1:C:533:LEU:CD1	1:C:639:SER:OG	2.59	0.50
1:C:775:SER:CA	1:C:806:ALA:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:833:THR:HG23	1:C:837:HIS:HB2	1.92	0.50
1:D:833:THR:HG23	1:D:837:HIS:HB2	1.91	0.50
1:D:848:TRP:HA	1:D:853:VAL:HG11	1.94	0.50
1:C:848:TRP:HA	1:C:853:VAL:HG11	1.94	0.50
1:D:863:ILE:HD11	1:D:876:VAL:HB	1.94	0.50
1:D:870:PRO:HG2	1:D:871:GLU:OE1	2.11	0.50
1:A:461:ASP:O	1:A:466:GLY:O	2.29	0.50
1:A:808:ARG:HD2	1:A:813:LEU:C	2.32	0.50
1:B:799:VAL:HG23	1:B:799:VAL:O	2.11	0.50
1:B:808:ARG:HD2	1:B:813:LEU:C	2.32	0.50
1:C:808:ARG:HD2	1:C:813:LEU:C	2.32	0.50
1:C:988:TYR:CE2	1:C:990:GLY:N	2.80	0.50
1:D:988:TYR:CE2	1:D:990:GLY:N	2.80	0.50
1:A:308:ARG:HB2	1:A:343:GLN:HG2	1.92	0.50
1:B:574:HIS:CE1	1:B:618:PRO:HD3	2.46	0.50
1:B:716:GLU:OE1	1:B:716:GLU:HA	2.10	0.50
1:C:931:ARG:CG	1:C:942:MET:HE3	2.41	0.50
1:D:890:ILE:HB	1:D:893:HIS:CD2	2.42	0.50
1:A:863:ILE:HD11	1:A:876:VAL:HB	1.94	0.50
1:D:550:ASN:CB	1:D:586:PRO:CA	2.85	0.50
1:A:815:LEU:CA	1:A:848:TRP:CD1	2.94	0.50
1:C:274:LEU:HD12	1:C:274:LEU:N	2.25	0.50
1:C:815:LEU:CA	1:C:848:TRP:CD1	2.94	0.50
1:D:235:LEU:HD21	1:D:263:PRO:HG2	1.93	0.50
1:A:539:ARG:HD2	1:A:542:LYS:NZ	2.27	0.50
1:C:1017:PRO:HB3	1:C:1034:GLN:CD	2.31	0.50
1:C:539:ARG:HD2	1:C:542:LYS:NZ	2.27	0.50
1:D:508:VAL:CG1	1:D:509:GLU:N	2.67	0.50
1:D:815:LEU:CA	1:D:848:TRP:CD1	2.94	0.50
1:A:235:LEU:HD21	1:A:263:PRO:HG2	1.92	0.49
1:B:815:LEU:CA	1:B:848:TRP:CD1	2.94	0.49
1:C:931:ARG:HH11	1:C:942:MET:HE3	1.77	0.49
1:D:1017:PRO:HB3	1:D:1034:GLN:CD	2.31	0.49
1:A:655:ASN:CG	1:A:658:ALA:HB2	2.32	0.49
1:C:559:CYS:O	1:C:584:ASP:HB3	2.10	0.49
1:C:863:ILE:HD11	1:C:876:VAL:HB	1.93	0.49
1:C:933:CYS:HA	1:C:942:MET:SD	2.53	0.49
1:D:539:ARG:HD2	1:D:542:LYS:NZ	2.27	0.49
1:A:799:VAL:O	1:A:799:VAL:HG23	2.11	0.49
1:A:848:TRP:HA	1:A:853:VAL:HG11	1.94	0.49
1:A:933:CYS:HA	1:A:942:MET:SD	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:893:HIS:CE1	1:C:932:LEU:HA	2.47	0.49
1:D:775:SER:HB2	1:D:807:GLN:CB	2.42	0.49
1:D:808:ARG:HD2	1:D:813:LEU:C	2.32	0.49
1:A:324:GLN:NE2	1:B:576:ARG:HE	2.11	0.49
1:D:974:ILE:CG1	1:D:1004:ILE:HB	2.43	0.49
1:D:533:LEU:O	1:D:644:LYS:CG	2.61	0.49
1:D:988:TYR:HE2	1:D:991:ASN:H	1.55	0.49
1:A:673:HIS:CD2	1:A:685:PRO:HG3	2.48	0.49
1:D:984:SER:O	1:D:1024:VAL:HG23	2.13	0.49
1:B:539:ARG:HD2	1:B:542:LYS:NZ	2.27	0.49
1:C:176:GLU:HG3	1:C:177:GLY:N	2.26	0.49
1:C:673:HIS:CD2	1:C:685:PRO:HG3	2.48	0.49
1:C:774:ILE:C	1:C:806:ALA:CB	2.81	0.49
1:C:799:VAL:O	1:C:799:VAL:HG23	2.11	0.49
1:C:974:ILE:CG1	1:C:1004:ILE:HB	2.43	0.49
1:D:1022:VAL:O	1:D:1022:VAL:HG13	2.12	0.49
1:D:673:HIS:CD2	1:D:685:PRO:HG3	2.48	0.49
1:D:898:GLY:O	1:D:900:PRO:HD3	2.12	0.49
1:D:931:ARG:CG	1:D:942:MET:HE3	2.42	0.49
1:B:560:MET:CE	1:B:586:PRO:HD3	2.43	0.49
1:B:705:VAL:HG13	1:B:706:PRO:HD2	1.95	0.49
1:B:775:SER:N	1:B:807:GLN:CD	2.50	0.49
1:C:1022:VAL:HG13	1:C:1022:VAL:O	2.12	0.49
1:C:677:TYR:HD1	1:C:731:GLN:CG	2.17	0.49
1:C:890:ILE:HG13	1:C:891:ALA:N	2.26	0.49
1:A:217:LEU:CD1	1:C:940:GLU:OE1	2.55	0.49
1:D:893:HIS:CE1	1:D:932:LEU:HA	2.48	0.49
1:D:970:THR:HG22	1:D:1008:SER:OG	2.13	0.49
1:A:864:LEU:HB3	1:A:877:THR:HB	1.95	0.49
1:B:237:SER:OG	1:B:238:HIS:HA	2.13	0.49
1:B:848:TRP:HA	1:B:853:VAL:HG11	1.94	0.49
1:C:137:CYS:SG	1:C:159:LEU:HD11	2.53	0.49
1:C:560:MET:CE	1:C:586:PRO:HD3	2.43	0.49
1:C:870:PRO:HG2	1:C:871:GLU:OE1	2.11	0.49
1:D:959:LEU:CG	1:D:974:ILE:HG22	2.28	0.49
1:A:898:GLY:O	1:A:900:PRO:HD3	2.12	0.49
1:C:970:THR:HG22	1:C:1008:SER:OG	2.13	0.49
1:D:890:ILE:HG13	1:D:891:ALA:N	2.26	0.49
1:A:237:SER:OG	1:A:238:HIS:HA	2.13	0.49
1:A:533:LEU:CD2	1:A:646:PHE:CD1	2.96	0.49
1:A:560:MET:CE	1:A:586:PRO:HD3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:GLN:O	1:B:724:ALA:HB1	2.13	0.49
1:C:984:SER:O	1:C:1024:VAL:HG23	2.13	0.49
1:C:988:TYR:CZ	1:C:991:ASN:N	2.80	0.49
1:D:988:TYR:CZ	1:D:991:ASN:N	2.80	0.49
1:C:859:GLN:HA	1:C:859:GLN:OE1	2.13	0.48
1:C:898:GLY:O	1:C:900:PRO:HD3	2.12	0.48
1:C:938:LYS:CE	1:C:941:PHE:CE2	2.96	0.48
1:A:398:VAL:HG22	1:C:946:HIS:O	2.13	0.48
1:C:959:LEU:CG	1:C:974:ILE:HG22	2.28	0.48
1:D:50:PHE:CE2	1:D:503:VAL:HG23	2.48	0.48
1:D:859:GLN:OE1	1:D:859:GLN:HA	2.13	0.48
1:D:864:LEU:HB3	1:D:877:THR:HB	1.95	0.48
1:D:933:CYS:HA	1:D:942:MET:SD	2.53	0.48
1:A:893:HIS:CE1	1:A:932:LEU:HA	2.48	0.48
1:B:459:ARG:HG3	1:B:526:PRO:HG3	1.94	0.48
1:C:533:LEU:CD2	1:C:639:SER:CB	2.84	0.48
1:A:705:VAL:HG13	1:A:706:PRO:HD2	1.95	0.48
1:C:703:GLN:O	1:C:724:ALA:HB1	2.14	0.48
1:C:804:CYS:SG	1:C:833:THR:HA	2.54	0.48
1:C:864:LEU:HB3	1:C:877:THR:HB	1.95	0.48
1:D:137:CYS:SG	1:D:159:LEU:HD11	2.53	0.48
1:D:711:LEU:HD23	1:D:821:PHE:CE1	2.48	0.48
1:D:661:LEU:HD21	1:D:790:ILE:HG13	1.94	0.48
1:D:829:GLU:O	1:D:830:ARG:HB3	2.14	0.48
1:B:137:CYS:SG	1:B:159:LEU:HD11	2.53	0.48
1:B:804:CYS:SG	1:B:833:THR:HA	2.54	0.48
1:D:703:GLN:O	1:D:724:ALA:HB1	2.14	0.48
1:D:804:CYS:SG	1:D:833:THR:HA	2.53	0.48
1:A:50:PHE:CE2	1:A:503:VAL:HG23	2.48	0.48
1:A:859:GLN:OE1	1:A:859:GLN:HA	2.13	0.48
1:B:50:PHE:CE2	1:B:503:VAL:HG23	2.48	0.48
1:B:732:SER:CB	1:D:83:HIS:NE2	2.75	0.48
1:D:440:TYR:CG	1:D:527:HIS:CD2	3.01	0.48
1:D:705:VAL:HG13	1:D:706:PRO:HD2	1.95	0.48
1:B:829:GLU:O	1:B:830:ARG:HB3	2.14	0.48
1:C:959:LEU:HD12	1:C:1033:LEU:HD23	1.94	0.48
1:C:237:SER:OG	1:C:238:HIS:HA	2.13	0.48
1:C:50:PHE:CE2	1:C:503:VAL:HG23	2.48	0.48
1:D:351:ASP:HA	1:D:431:ARG:HB2	1.96	0.48
1:D:660:GLN:C	1:D:661:LEU:HD12	2.34	0.48
1:D:848:TRP:HA	1:D:853:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:938:LYS:CE	1:D:941:PHE:CE2	2.97	0.48
1:A:938:LYS:CE	1:A:941:PHE:CE2	2.97	0.48
1:B:550:ASN:CG	1:B:585:ALA:O	2.46	0.48
1:B:95:TYR:HA	1:B:96:PRO:C	2.33	0.48
1:C:351:ASP:HA	1:C:431:ARG:HB2	1.96	0.48
1:C:559:CYS:O	1:C:584:ASP:HB2	2.14	0.48
1:C:705:VAL:HG13	1:C:706:PRO:HD2	1.95	0.48
1:A:221:PHE:CE1	1:C:830:ARG:HB2	2.49	0.48
1:C:932:LEU:HD23	1:C:933:CYS:N	2.28	0.48
1:A:594:CYS:O	1:A:601:GLU:HA	2.14	0.48
1:A:660:GLN:C	1:A:661:LEU:HD12	2.34	0.48
1:A:816:LYS:CD	1:A:910:ILE:HG23	2.44	0.48
1:A:95:TYR:HA	1:A:96:PRO:C	2.33	0.48
1:C:848:TRP:HA	1:C:853:VAL:CG1	2.44	0.48
1:D:594:CYS:O	1:D:601:GLU:HA	2.14	0.48
1:D:842:SER:HB2	1:D:844:PRO:HD2	1.96	0.48
1:D:931:ARG:CD	1:D:942:MET:HE3	2.42	0.48
1:D:933:CYS:SG	1:D:937:CYS:N	2.87	0.48
1:A:932:LEU:HD23	1:A:933:CYS:N	2.28	0.48
1:B:594:CYS:O	1:B:601:GLU:HA	2.14	0.48
1:B:660:GLN:C	1:B:661:LEU:HD12	2.34	0.48
1:B:673:HIS:CD2	1:B:685:PRO:HG3	2.48	0.48
1:C:960:SER:CB	1:C:973:THR:HB	2.43	0.48
1:D:237:SER:OG	1:D:238:HIS:HA	2.13	0.48
1:D:875:ARG:HG2	1:D:915:VAL:CG1	2.44	0.48
1:D:95:TYR:HA	1:D:96:PRO:C	2.33	0.48
1:A:137:CYS:SG	1:A:159:LEU:HD11	2.53	0.48
1:A:848:TRP:HA	1:A:853:VAL:CG1	2.44	0.48
1:A:851:HIS:ND1	1:A:886:ASP:OD2	2.47	0.48
1:B:690:PHE:CE2	1:B:731:GLN:HG3	2.49	0.48
1:B:842:SER:HB2	1:B:844:PRO:HD2	1.96	0.48
1:B:848:TRP:HA	1:B:853:VAL:CG1	2.44	0.48
1:C:326:PHE:CG	1:C:359:PRO:HG3	2.49	0.48
1:C:933:CYS:SG	1:C:937:CYS:N	2.87	0.48
1:D:960:SER:CB	1:D:973:THR:HB	2.43	0.48
1:A:695:ILE:CD1	1:A:702:PRO:HD3	2.44	0.47
1:A:797:LEU:HD12	1:A:797:LEU:H	1.79	0.47
1:A:829:GLU:O	1:A:830:ARG:HB3	2.14	0.47
1:A:842:SER:HB2	1:A:844:PRO:HD2	1.96	0.47
1:B:327:ASN:CG	1:B:327:ASN:O	2.52	0.47
1:B:797:LEU:HD12	1:B:797:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:829:GLU:O	1:C:830:ARG:HB3	2.14	0.47
1:D:812:GLY:HA2	1:D:885:LEU:HD22	1.93	0.47
1:D:833:THR:HG21	1:D:837:HIS:CB	2.44	0.47
1:A:141:ARG:HD2	1:A:143:ASP:OD1	2.14	0.47
1:A:804:CYS:SG	1:A:833:THR:HA	2.54	0.47
1:B:326:PHE:CG	1:B:359:PRO:HG3	2.49	0.47
1:C:931:ARG:CD	1:C:942:MET:HE3	2.42	0.47
1:D:932:LEU:HD23	1:D:933:CYS:N	2.28	0.47
1:A:326:PHE:CG	1:A:359:PRO:HG3	2.50	0.47
1:B:470:TYR:HE1	1:B:525:ASP:OD2	1.98	0.47
1:C:327:ASN:CG	1:C:327:ASN:O	2.52	0.47
1:C:594:CYS:O	1:C:601:GLU:HA	2.14	0.47
1:C:660:GLN:C	1:C:661:LEU:HD12	2.34	0.47
1:C:932:LEU:HD23	1:C:932:LEU:C	2.34	0.47
1:D:1022:VAL:HG13	1:D:1029:VAL:HG12	1.94	0.47
1:D:560:MET:CE	1:D:586:PRO:HD3	2.43	0.47
1:A:932:LEU:C	1:A:932:LEU:HD23	2.34	0.47
1:B:141:ARG:HD2	1:B:143:ASP:OD1	2.14	0.47
1:C:833:THR:HG21	1:C:837:HIS:CB	2.44	0.47
1:C:876:VAL:HG23	1:C:876:VAL:O	2.14	0.47
1:D:874:THR:HG22	1:D:875:ARG:N	2.30	0.47
1:D:932:LEU:HD23	1:D:932:LEU:C	2.34	0.47
1:A:351:ASP:HA	1:A:431:ARG:HB2	1.96	0.47
1:A:695:ILE:HD13	1:A:702:PRO:HD3	1.97	0.47
1:A:903:PRO:HA	1:A:916:CYS:HA	1.96	0.47
1:C:1022:VAL:HG13	1:C:1029:VAL:HG12	1.94	0.47
1:C:141:ARG:HD2	1:C:143:ASP:OD1	2.14	0.47
1:D:959:LEU:HD12	1:D:1033:LEU:HD23	1.94	0.47
1:A:703:GLN:O	1:A:724:ALA:HB1	2.13	0.47
1:A:833:THR:HG21	1:A:837:HIS:CB	2.44	0.47
1:A:876:VAL:HG23	1:A:876:VAL:O	2.14	0.47
1:A:933:CYS:SG	1:A:937:CYS:N	2.87	0.47
1:B:712:ILE:HD12	1:B:799:VAL:HB	1.97	0.47
1:D:534:HIS:CD2	1:D:644:LYS:HZ2	2.32	0.47
1:D:551:ARG:HH11	1:D:641:GLU:CD	2.16	0.47
1:A:655:ASN:OD1	1:A:657:SER:CA	2.63	0.47
1:A:874:THR:HG22	1:A:875:ARG:N	2.30	0.47
1:B:655:ASN:CA	1:B:656:CYS:N	2.69	0.47
1:C:95:TYR:HA	1:C:96:PRO:C	2.33	0.47
1:D:326:PHE:CG	1:D:359:PRO:HG3	2.49	0.47
1:A:663:LEU:HD11	1:A:703:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:PRO:O	1:B:577:LEU:HD21	2.14	0.47
1:C:797:LEU:H	1:C:797:LEU:HD12	1.79	0.47
1:C:875:ARG:HG2	1:C:915:VAL:CG1	2.44	0.47
1:C:874:THR:HG22	1:C:875:ARG:N	2.30	0.47
1:D:701:CYS:HA	1:D:702:PRO:HD3	1.75	0.47
1:A:722:LEU:C	1:A:723:LYS:HD2	2.36	0.47
1:A:896:VAL:HG21	1:A:918:MET:CE	2.45	0.47
1:B:833:THR:HG21	1:B:837:HIS:CB	2.44	0.47
1:C:737:TYR:HE1	1:C:754:ARG:CD	2.25	0.47
1:C:896:VAL:HG21	1:C:918:MET:CE	2.45	0.47
1:C:960:SER:HB2	1:C:961:PRO:CD	2.45	0.47
1:D:141:ARG:HD2	1:D:143:ASP:OD1	2.14	0.47
1:D:550:ASN:ND2	1:D:585:ALA:O	2.48	0.47
1:D:638:ARG:HB2	1:D:645:ILE:HD13	1.97	0.47
1:D:960:SER:HB2	1:D:961:PRO:CD	2.45	0.47
1:A:327:ASN:O	1:A:327:ASN:CG	2.52	0.47
1:A:875:ARG:HG2	1:A:915:VAL:CG1	2.44	0.47
1:B:351:ASP:HA	1:B:431:ARG:HB2	1.96	0.47
1:D:327:ASN:CG	1:D:327:ASN:O	2.52	0.47
1:D:869:PRO:HD3	1:D:981:ALA:HB1	1.97	0.47
1:B:722:LEU:C	1:B:723:LYS:HD2	2.35	0.46
1:C:842:SER:HB2	1:C:844:PRO:HD2	1.96	0.46
1:A:655:ASN:CB	1:A:658:ALA:CB	2.77	0.46
1:D:159:LEU:HD13	1:D:184:ILE:HD13	1.98	0.46
1:D:896:VAL:HG21	1:D:918:MET:CE	2.45	0.46
1:A:476:PHE:CE2	1:A:482:ILE:HD13	2.51	0.46
1:A:663:LEU:HD11	1:A:703:GLN:NE2	2.30	0.46
1:A:712:ILE:HD12	1:A:799:VAL:HB	1.97	0.46
1:B:277:THR:HG22	1:B:279:ARG:HG3	1.98	0.46
1:C:328:ILE:HB	1:C:332:GLU:OE1	2.16	0.46
1:C:712:ILE:HD12	1:C:799:VAL:HB	1.97	0.46
1:C:988:TYR:C	1:C:988:TYR:CD2	2.84	0.46
1:D:775:SER:N	1:D:807:GLN:HG3	2.30	0.46
1:D:893:HIS:CG	1:D:894:VAL:N	2.83	0.46
1:A:539:ARG:HB2	1:A:542:LYS:HD3	1.97	0.46
1:B:638:ARG:HB2	1:B:645:ILE:HD13	1.97	0.46
1:C:159:LEU:HD13	1:C:184:ILE:HD13	1.98	0.46
1:C:875:ARG:HD3	1:C:907:GLU:OE1	2.16	0.46
1:D:445:VAL:CG2	1:D:526:PRO:HG2	2.44	0.46
1:D:712:ILE:HD12	1:D:799:VAL:HB	1.97	0.46
1:D:876:VAL:HG23	1:D:876:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD13	1:A:184:ILE:HD13	1.98	0.46
1:A:893:HIS:CG	1:A:894:VAL:N	2.83	0.46
1:B:654:TYR:CD2	1:B:670:PHE:CG	3.04	0.46
1:D:988:TYR:HE1	1:D:992:GLN:O	1.97	0.46
1:A:81:VAL:HG11	1:A:145:LEU:HB2	1.98	0.46
1:A:277:THR:HG22	1:A:279:ARG:HG3	1.98	0.46
1:A:875:ARG:HD3	1:A:907:GLU:OE1	2.16	0.46
1:B:328:ILE:HB	1:B:332:GLU:OE1	2.16	0.46
1:C:903:PRO:HA	1:C:916:CYS:HA	1.96	0.46
1:D:328:ILE:HB	1:D:332:GLU:OE1	2.16	0.46
1:A:328:ILE:HB	1:A:332:GLU:OE1	2.16	0.46
1:C:638:ARG:HB2	1:C:645:ILE:HD13	1.97	0.46
1:C:722:LEU:C	1:C:723:LYS:HD2	2.35	0.46
1:C:893:HIS:CG	1:C:894:VAL:N	2.83	0.46
1:C:896:VAL:HG21	1:C:918:MET:HE3	1.98	0.46
1:B:508:VAL:HG12	1:B:539:ARG:NH2	2.30	0.46
1:C:476:PHE:CE2	1:C:482:ILE:HD13	2.51	0.46
1:C:663:LEU:CG	1:C:792:ASP:OD2	2.59	0.46
1:C:988:TYR:HE1	1:C:992:GLN:O	1.97	0.46
1:D:476:PHE:CE2	1:D:482:ILE:HD13	2.51	0.46
1:D:903:PRO:HA	1:D:916:CYS:HA	1.96	0.46
1:D:988:TYR:CE1	1:D:992:GLN:O	2.68	0.46
1:A:654:TYR:HE1	1:A:656:CYS:SG	2.39	0.46
1:A:655:ASN:C	1:A:657:SER:N	2.68	0.46
1:A:672:CYS:HB3	1:A:681:CYS:SG	2.56	0.46
1:A:737:TYR:CE2	1:A:785:TRP:HB3	2.51	0.46
1:C:988:TYR:CE1	1:C:992:GLN:O	2.68	0.46
1:D:979:LEU:HD12	1:D:1003:GLU:HA	1.97	0.46
1:D:875:ARG:HD3	1:D:907:GLU:OE1	2.16	0.46
1:A:112:ASN:HB2	1:A:132:LEU:HD22	1.98	0.46
1:A:550:ASN:HB2	1:A:585:ALA:O	2.16	0.46
1:B:329:SER:HB3	1:B:332:GLU:HG3	1.98	0.46
1:D:539:ARG:HB2	1:D:542:LYS:HD3	1.97	0.46
1:D:722:LEU:C	1:D:723:LYS:HD2	2.35	0.46
1:D:797:LEU:H	1:D:797:LEU:HD12	1.79	0.46
1:D:904:ILE:HG23	1:D:904:ILE:O	2.15	0.46
1:A:545:ARG:NH1	1:A:641:GLU:OE2	2.49	0.45
1:B:476:PHE:CE2	1:B:482:ILE:HD13	2.51	0.45
1:C:533:LEU:CB	1:C:642:THR:CG2	2.73	0.45
1:C:672:CYS:HB3	1:C:681:CYS:SG	2.56	0.45
1:C:785:TRP:CD1	1:C:791:ILE:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:TYR:CE1	1:D:525:ASP:CG	2.90	0.45
1:A:463:PRO:O	1:B:614:ILE:HG12	2.14	0.45
1:A:904:ILE:HG23	1:A:904:ILE:O	2.15	0.45
1:B:539:ARG:HB2	1:B:542:LYS:HD3	1.97	0.45
1:B:737:TYR:CE2	1:B:785:TRP:HB3	2.51	0.45
1:C:979:LEU:HD12	1:C:1003:GLU:HA	1.98	0.45
1:B:112:ASN:HB2	1:B:132:LEU:HD22	1.98	0.45
1:C:112:ASN:HB2	1:C:132:LEU:HD22	1.98	0.45
1:C:539:ARG:HB2	1:C:542:LYS:HD3	1.97	0.45
1:C:737:TYR:CE2	1:C:785:TRP:HB3	2.51	0.45
1:B:159:LEU:HD13	1:B:184:ILE:HD13	1.98	0.45
1:B:732:SER:HA	1:D:147:ILE:HD11	1.98	0.45
1:D:277:THR:HG22	1:D:279:ARG:HG3	1.98	0.45
1:D:672:CYS:HB3	1:D:681:CYS:SG	2.56	0.45
1:D:988:TYR:CD2	1:D:988:TYR:C	2.84	0.45
1:B:672:CYS:HB3	1:B:681:CYS:SG	2.56	0.45
1:B:81:VAL:HG11	1:B:145:LEU:HB2	1.98	0.45
1:D:735:ARG:HG3	1:D:786:ASN:HA	1.96	0.45
1:B:534:HIS:CD2	1:B:644:LYS:HG3	2.51	0.45
1:B:690:PHE:CE2	1:B:731:GLN:HB3	2.38	0.45
1:D:785:TRP:CD1	1:D:791:ILE:HD11	2.51	0.45
1:B:785:TRP:CD1	1:B:791:ILE:HD11	2.51	0.45
1:A:324:GLN:HE22	1:B:576:ARG:HA	1.82	0.45
1:A:559:CYS:C	1:A:560:MET:CA	2.83	0.45
1:B:802:TYR:CE2	1:B:821:PHE:HB3	2.51	0.45
1:D:112:ASN:HB2	1:D:132:LEU:HD22	1.98	0.45
1:D:551:ARG:HH12	1:D:641:GLU:CG	2.30	0.45
1:A:638:ARG:HB2	1:A:645:ILE:HD13	1.97	0.45
1:C:1022:VAL:CG1	1:C:1029:VAL:CG1	2.94	0.45
1:C:329:SER:HB3	1:C:332:GLU:HG3	1.98	0.45
1:C:808:ARG:HD2	1:C:813:LEU:O	2.17	0.45
1:C:954:PRO:HA	1:C:978:TYR:HB2	1.99	0.45
1:D:1022:VAL:CG1	1:D:1029:VAL:CG1	2.94	0.45
1:A:162:VAL:CG2	1:A:189:ASP:HB2	2.47	0.45
1:A:407:LEU:HD22	1:C:944:LYS:CD	2.04	0.45
1:A:705:VAL:CG1	1:A:706:PRO:N	2.80	0.45
1:B:533:LEU:HA	1:B:533:LEU:HD23	1.84	0.45
1:B:560:MET:HE1	1:B:586:PRO:HD3	1.98	0.45
1:C:162:VAL:CG2	1:C:189:ASP:HB2	2.47	0.45
1:C:533:LEU:HD23	1:C:533:LEU:HA	1.84	0.45
1:D:81:VAL:HG11	1:D:145:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:VAL:CG2	1:D:189:ASP:HB2	2.47	0.45
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.84	0.44
1:D:920:HIS:CD2	1:D:922:VAL:H	2.35	0.44
1:D:954:PRO:HA	1:D:978:TYR:HB2	1.99	0.44
1:A:785:TRP:CD1	1:A:791:ILE:HD11	2.52	0.44
1:B:203:LEU:HA	1:B:203:LEU:HD23	1.84	0.44
1:C:985:VAL:HG23	1:C:985:VAL:O	2.16	0.44
1:D:737:TYR:CE2	1:D:785:TRP:HB3	2.51	0.44
1:D:985:VAL:O	1:D:985:VAL:HG23	2.16	0.44
1:A:329:SER:HB3	1:A:332:GLU:HG3	1.98	0.44
1:C:277:THR:HG22	1:C:279:ARG:HG3	1.98	0.44
1:C:904:ILE:O	1:C:904:ILE:HG23	2.15	0.44
1:C:920:HIS:CD2	1:C:922:VAL:H	2.35	0.44
1:C:992:GLN:OE1	1:C:1012:SER:HB2	2.17	0.44
1:A:655:ASN:CG	1:A:658:ALA:H	2.20	0.44
1:A:920:HIS:CD2	1:A:922:VAL:H	2.35	0.44
1:B:482:ILE:HG23	1:B:497:VAL:HG13	2.00	0.44
1:B:705:VAL:CG1	1:B:706:PRO:N	2.80	0.44
1:C:81:VAL:HG11	1:C:145:LEU:HB2	1.98	0.44
1:D:661:LEU:CD2	1:D:790:ILE:HG13	2.46	0.44
1:D:705:VAL:H	1:D:724:ALA:HA	1.83	0.44
1:D:855:CYS:SG	1:D:885:LEU:CD2	2.96	0.44
1:A:325:ALA:CA	1:B:577:LEU:HD13	2.46	0.44
1:B:808:ARG:HD2	1:B:813:LEU:O	2.17	0.44
1:C:149:VAL:HG22	1:C:150:GLU:N	2.33	0.44
1:C:705:VAL:CG1	1:C:706:PRO:N	2.80	0.44
1:D:992:GLN:OE1	1:D:1012:SER:HB2	2.17	0.44
1:D:808:ARG:HD2	1:D:813:LEU:O	2.17	0.44
1:D:974:ILE:HG13	1:D:974:ILE:O	2.18	0.44
1:B:772:MET:HB3	1:B:806:ALA:HB1	1.98	0.44
1:C:775:SER:CB	1:C:806:ALA:H	2.30	0.44
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.83	0.44
1:D:705:VAL:CG1	1:D:706:PRO:N	2.80	0.44
1:A:559:CYS:CA	1:A:560:MET:N	2.80	0.44
1:A:808:ARG:HD2	1:A:813:LEU:O	2.17	0.44
1:A:890:ILE:HD13	1:A:908:TYR:CZ	2.53	0.44
1:D:1015:LEU:HD21	1:D:1039:ASP:HA	2.00	0.44
1:B:191:LYS:HD2	1:B:191:LYS:N	2.33	0.44
1:C:191:LYS:N	1:C:191:LYS:HD2	2.33	0.44
1:C:482:ILE:HG23	1:C:497:VAL:HG13	2.00	0.44
1:C:525:ASP:HA	1:C:526:PRO:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:HIS:HD2	1:C:644:LYS:NZ	2.15	0.44
1:C:890:ILE:CB	1:C:893:HIS:HD2	2.30	0.44
1:C:974:ILE:O	1:C:974:ILE:HG13	2.18	0.44
1:D:329:SER:HB3	1:D:332:GLU:HG3	1.98	0.44
1:A:760:VAL:CG1	1:A:761:GLN:N	2.81	0.44
1:A:944:LYS:O	1:A:944:LYS:HG3	2.18	0.44
1:B:162:VAL:CG2	1:B:189:ASP:HB2	2.48	0.44
1:B:705:VAL:H	1:B:724:ALA:HA	1.83	0.44
1:C:655:ASN:OD1	1:C:657:SER:CB	2.64	0.44
1:D:149:VAL:HG22	1:D:150:GLU:N	2.33	0.44
1:D:411:GLN:HA	1:D:412:PRO:C	2.38	0.44
1:D:890:ILE:HD13	1:D:908:TYR:CZ	2.53	0.44
1:B:459:ARG:HG3	1:B:526:PRO:CG	2.48	0.43
1:A:463:PRO:HB2	1:B:612:ILE:HG22	2.00	0.43
1:C:959:LEU:H	1:C:1033:LEU:HD21	1.83	0.43
1:D:313:ALA:HB1	1:D:335:LEU:HD11	2.00	0.43
1:D:533:LEU:CD2	1:D:639:SER:OG	2.65	0.43
1:D:959:LEU:H	1:D:1033:LEU:HD21	1.83	0.43
1:A:931:ARG:CG	1:A:942:MET:CE	2.96	0.43
1:C:1015:LEU:HD21	1:C:1039:ASP:HA	2.00	0.43
1:C:1015:LEU:CD2	1:C:1039:ASP:N	2.81	0.43
1:C:775:SER:HB2	1:C:806:ALA:N	2.33	0.43
1:C:995:GLU:O	1:C:1006:CYS:HB2	2.18	0.43
1:D:931:ARG:CG	1:D:942:MET:CE	2.96	0.43
1:A:57:ARG:HG2	1:A:121:TYR:CE1	2.53	0.43
1:C:313:ALA:HB1	1:C:335:LEU:HD11	2.00	0.43
1:C:947:GLN:HG3	1:C:948:GLN:N	2.34	0.43
1:D:1015:LEU:CD2	1:D:1039:ASP:N	2.81	0.43
1:A:313:ALA:HB1	1:A:335:LEU:HD11	2.00	0.43
1:B:533:LEU:HD21	1:B:646:PHE:CD2	2.47	0.43
1:D:482:ILE:HG23	1:D:497:VAL:HG13	2.00	0.43
1:B:735:ARG:HG3	1:B:786:ASN:HA	1.95	0.43
1:C:411:GLN:HA	1:C:412:PRO:C	2.38	0.43
1:C:57:ARG:HG2	1:C:121:TYR:CE1	2.53	0.43
1:C:890:ILE:HD13	1:C:908:TYR:CZ	2.53	0.43
1:C:944:LYS:O	1:C:944:LYS:HG3	2.18	0.43
1:B:741:LEU:HD12	1:B:767:TYR:CD1	2.54	0.43
1:B:802:TYR:CE1	1:B:821:PHE:CD1	3.05	0.43
1:C:56:HIS:HB3	1:C:59:THR:OG1	2.19	0.43
1:D:191:LYS:HD2	1:D:191:LYS:N	2.33	0.43
1:D:890:ILE:CB	1:D:893:HIS:HD2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLN:HA	1:A:412:PRO:C	2.38	0.43
1:B:533:LEU:HD21	1:B:646:PHE:CE2	2.53	0.43
1:B:568:SER:CB	1:B:670:PHE:CE1	3.02	0.43
1:B:833:THR:CG2	1:B:837:HIS:CB	2.95	0.43
1:C:996:PHE:HE1	1:C:1004:ILE:HG23	1.83	0.43
1:C:931:ARG:CG	1:C:942:MET:CE	2.96	0.43
1:D:996:PHE:HE1	1:D:1004:ILE:HG23	1.83	0.43
1:A:149:VAL:HG22	1:A:150:GLU:N	2.33	0.43
1:A:191:LYS:HD2	1:A:191:LYS:N	2.33	0.43
1:B:411:GLN:HA	1:B:412:PRO:C	2.38	0.43
1:D:947:GLN:HG3	1:D:948:GLN:N	2.34	0.43
1:D:995:GLU:O	1:D:1006:CYS:HB2	2.18	0.43
1:A:741:LEU:HD12	1:A:767:TYR:CD1	2.54	0.43
1:A:324:GLN:HE22	1:B:576:ARG:HD2	1.84	0.43
1:B:57:ARG:HG2	1:B:121:TYR:CE1	2.54	0.43
1:B:784:VAL:CG1	1:B:785:TRP:N	2.82	0.43
1:C:1011:SER:HB2	1:C:1037:TYR:CD1	2.54	0.43
1:C:539:ARG:HD2	1:C:542:LYS:HZ2	1.84	0.43
1:C:885:LEU:O	1:C:910:ILE:HD12	2.19	0.43
1:D:57:ARG:HG2	1:D:121:TYR:CE1	2.54	0.43
1:D:775:SER:CA	1:D:807:GLN:HG3	2.42	0.43
1:A:908:TYR:CE1	1:A:914:ILE:HG12	2.54	0.43
1:B:690:PHE:CE2	1:B:731:GLN:CG	3.01	0.43
1:C:705:VAL:H	1:C:724:ALA:HA	1.82	0.43
1:C:741:LEU:HD12	1:C:767:TYR:CD1	2.54	0.43
1:C:908:TYR:CE1	1:C:914:ILE:HG12	2.54	0.43
1:C:987:VAL:HB	1:C:994:CYS:HB3	2.00	0.43
1:D:970:THR:HG22	1:D:1008:SER:CB	2.49	0.43
1:D:533:LEU:HD23	1:D:533:LEU:HA	1.84	0.43
1:D:56:HIS:HB3	1:D:59:THR:OG1	2.19	0.43
1:A:463:PRO:O	1:B:614:ILE:CG1	2.66	0.42
1:A:705:VAL:H	1:A:724:ALA:HA	1.83	0.42
1:A:947:GLN:HG3	1:A:948:GLN:N	2.34	0.42
1:D:1011:SER:HB2	1:D:1037:TYR:CD1	2.54	0.42
1:D:741:LEU:HD12	1:D:767:TYR:CD1	2.54	0.42
1:A:407:LEU:HD21	1:C:944:LYS:HD3	1.77	0.42
1:A:482:ILE:HG23	1:A:497:VAL:HG13	2.00	0.42
1:A:864:LEU:CG	1:A:865:THR:N	2.82	0.42
1:B:196:PRO:HG3	1:B:215:TYR:OH	2.20	0.42
1:C:677:TYR:CE1	1:C:731:GLN:CG	3.02	0.42
1:C:848:TRP:CG	1:C:848:TRP:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:946:HIS:CG	1:C:947:GLN:N	2.87	0.42
1:C:993:THR:CG2	1:C:994:CYS:N	2.82	0.42
1:D:944:LYS:HG3	1:D:944:LYS:O	2.18	0.42
1:D:987:VAL:HB	1:D:994:CYS:HB3	2.00	0.42
1:D:993:THR:CG2	1:D:994:CYS:N	2.82	0.42
1:A:37:GLN:OE1	1:A:37:GLN:HA	2.20	0.42
1:A:655:ASN:HA	1:A:656:CYS:N	2.33	0.42
1:A:784:VAL:CG1	1:A:785:TRP:N	2.82	0.42
1:A:885:LEU:O	1:A:910:ILE:HD12	2.19	0.42
1:B:149:VAL:HG22	1:B:150:GLU:N	2.33	0.42
1:C:970:THR:HG22	1:C:1008:SER:CB	2.49	0.42
1:C:192:GLN:HG3	1:C:228:ILE:O	2.20	0.42
1:D:1001:MET:CG	1:D:1002:ASN:N	2.83	0.42
1:D:881:VAL:CG1	1:D:882:ASN:N	2.82	0.42
1:D:896:VAL:HG21	1:D:918:MET:HE3	2.01	0.42
1:A:192:GLN:HG3	1:A:228:ILE:O	2.20	0.42
1:A:810:SER:OG	1:A:882:ASN:OD1	2.37	0.42
1:B:708:GLU:HG2	1:B:709:GLU:N	2.35	0.42
1:B:760:VAL:CG1	1:B:761:GLN:N	2.81	0.42
1:C:37:GLN:HA	1:C:37:GLN:OE1	2.20	0.42
1:C:735:ARG:HG3	1:C:786:ASN:HA	1.96	0.42
1:D:192:GLN:HG3	1:D:228:ILE:O	2.20	0.42
1:D:482:ILE:HD12	1:D:497:VAL:HG11	2.02	0.42
1:D:440:TYR:CD2	1:D:527:HIS:HA	2.55	0.42
1:D:706:PRO:CG	1:D:795:GLN:HG3	2.49	0.42
1:D:863:ILE:HG13	1:D:877:THR:C	2.40	0.42
1:D:885:LEU:O	1:D:910:ILE:HD12	2.19	0.42
1:A:56:HIS:HB3	1:A:59:THR:OG1	2.19	0.42
1:A:704:LEU:CD1	1:A:783:VAL:HG21	2.49	0.42
1:C:482:ILE:HD12	1:C:497:VAL:HG11	2.02	0.42
1:C:881:VAL:CG1	1:C:882:ASN:N	2.82	0.42
1:D:151:PRO:HG2	1:D:213:LEU:HD12	2.02	0.42
1:D:37:GLN:HA	1:D:37:GLN:OE1	2.20	0.42
1:D:470:TYR:CD1	1:D:525:ASP:HB2	2.55	0.42
1:A:818:ASP:HB2	1:A:821:PHE:HD2	1.79	0.42
1:A:810:SER:CB	1:A:882:ASN:CG	2.71	0.42
1:A:881:VAL:CG1	1:A:882:ASN:N	2.82	0.42
1:C:1001:MET:CG	1:C:1002:ASN:N	2.83	0.42
1:C:151:PRO:HG2	1:C:213:LEU:HD12	2.02	0.42
1:C:863:ILE:HG13	1:C:877:THR:C	2.40	0.42
1:C:988:TYR:OH	1:C:991:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1038:ILE:CG2	1:D:1039:ASP:N	2.82	0.42
1:A:324:GLN:NE2	1:B:576:ARG:NE	2.68	0.42
1:B:37:GLN:OE1	1:B:37:GLN:HA	2.20	0.42
1:B:56:HIS:HB3	1:B:59:THR:OG1	2.19	0.42
1:C:775:SER:H	1:C:807:GLN:HG3	1.85	0.42
1:C:872:GLY:O	1:C:1026:ARG:CB	2.63	0.42
1:D:708:GLU:HG2	1:D:709:GLU:N	2.35	0.42
1:D:908:TYR:CE1	1:D:914:ILE:HG12	2.54	0.42
1:A:708:GLU:HG2	1:A:709:GLU:N	2.35	0.42
1:A:815:LEU:N	1:A:815:LEU:CD1	2.83	0.42
1:C:655:ASN:O	1:C:656:CYS:C	2.54	0.42
1:C:708:GLU:HG2	1:C:709:GLU:N	2.35	0.42
1:C:883:LEU:HG	1:C:932:LEU:HD11	2.02	0.42
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.89	0.42
1:B:151:PRO:HG2	1:B:213:LEU:HD12	2.01	0.42
1:B:508:VAL:HG11	1:B:539:ARG:HH22	1.85	0.42
1:B:549:ALA:C	1:B:586:PRO:HA	2.40	0.42
1:C:1038:ILE:CG2	1:C:1039:ASP:N	2.82	0.42
1:C:933:CYS:SG	1:C:942:MET:SD	3.18	0.42
1:D:815:LEU:CD1	1:D:815:LEU:N	2.83	0.42
1:D:933:CYS:SG	1:D:942:MET:SD	3.18	0.42
1:D:988:TYR:OH	1:D:991:ASN:N	2.53	0.42
1:A:149:VAL:HG22	1:A:151:PRO:HD3	2.02	0.42
1:A:204:PRO:HD2	1:A:212:MET:SD	2.60	0.42
1:A:848:TRP:CG	1:A:848:TRP:O	2.73	0.42
1:C:784:VAL:CG1	1:C:785:TRP:N	2.82	0.42
1:D:791:ILE:HG22	1:D:792:ASP:N	2.35	0.42
1:A:196:PRO:HG3	1:A:215:TYR:OH	2.19	0.41
1:B:313:ALA:HB1	1:B:335:LEU:HD11	2.00	0.41
1:B:57:ARG:HG3	1:B:58:ARG:HG3	2.02	0.41
1:C:938:LYS:CE	1:C:941:PHE:HE2	2.33	0.41
1:D:784:VAL:CG1	1:D:785:TRP:N	2.82	0.41
1:D:864:LEU:CG	1:D:865:THR:N	2.82	0.41
1:D:883:LEU:HG	1:D:932:LEU:HD11	2.02	0.41
1:A:655:ASN:OD1	1:A:657:SER:C	2.58	0.41
1:B:192:GLN:HG3	1:B:228:ILE:O	2.20	0.41
1:B:476:PHE:HE2	1:B:482:ILE:HD13	1.85	0.41
1:B:482:ILE:HD12	1:B:497:VAL:HG11	2.02	0.41
1:C:716:GLU:OE2	1:C:836:GLN:HG2	2.20	0.41
1:C:833:THR:HG21	1:C:837:HIS:HB2	1.99	0.41
1:D:149:VAL:HG22	1:D:151:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:863:ILE:O	1:D:863:ILE:HG23	2.20	0.41
1:D:946:HIS:CG	1:D:947:GLN:N	2.87	0.41
1:A:324:GLN:NE2	1:B:576:ARG:CD	2.84	0.41
1:A:482:ILE:HD12	1:A:497:VAL:HG11	2.02	0.41
1:A:737:TYR:HE1	1:A:754:ARG:CD	2.25	0.41
1:A:791:ILE:HG22	1:A:792:ASP:N	2.36	0.41
1:C:760:VAL:CG1	1:C:761:GLN:N	2.81	0.41
1:D:760:VAL:CG1	1:D:761:GLN:N	2.81	0.41
1:D:848:TRP:CG	1:D:848:TRP:O	2.73	0.41
1:D:931:ARG:HG2	1:D:942:MET:CE	2.50	0.41
1:A:629:ASP:OD1	1:A:659:HIS:CE1	2.72	0.41
1:A:931:ARG:HG2	1:A:942:MET:CE	2.50	0.41
1:C:1015:LEU:CD1	1:C:1015:LEU:N	2.83	0.41
1:C:204:PRO:HD2	1:C:212:MET:SD	2.60	0.41
1:C:843:SER:N	1:C:844:PRO:CD	2.84	0.41
1:C:863:ILE:O	1:C:863:ILE:HG23	2.20	0.41
1:D:815:LEU:O	1:D:848:TRP:CD1	2.74	0.41
1:A:815:LEU:HB3	1:A:885:LEU:CD1	2.46	0.41
1:A:883:LEU:HG	1:A:932:LEU:HD11	2.02	0.41
1:C:203:LEU:HA	1:C:203:LEU:HD23	1.83	0.41
1:C:417:THR:HA	1:C:418:PRO:HD3	1.74	0.41
1:C:560:MET:HE2	1:C:586:PRO:HD3	2.03	0.41
1:C:781:PHE:C	1:C:781:PHE:CD1	2.94	0.41
1:C:815:LEU:CD1	1:C:815:LEU:N	2.83	0.41
1:D:1015:LEU:CD1	1:D:1015:LEU:N	2.83	0.41
1:A:564:VAL:HG23	1:A:649:THR:HG21	2.03	0.41
1:A:781:PHE:CD1	1:A:781:PHE:C	2.94	0.41
1:A:863:ILE:HG13	1:A:877:THR:C	2.40	0.41
1:B:508:VAL:CG1	1:B:539:ARG:HH22	2.33	0.41
1:B:564:VAL:HG23	1:B:649:THR:HG21	2.03	0.41
1:B:815:LEU:O	1:B:848:TRP:CD1	2.74	0.41
1:C:1018:VAL:HG12	1:C:1019:PRO:N	2.35	0.41
1:C:476:PHE:HE2	1:C:482:ILE:HD13	1.85	0.41
1:D:204:PRO:HD2	1:D:212:MET:SD	2.60	0.41
1:D:570:SER:CB	1:D:683:HIS:CG	3.03	0.41
1:D:938:LYS:CE	1:D:941:PHE:HE2	2.34	0.41
1:A:815:LEU:O	1:A:848:TRP:CD1	2.74	0.41
1:A:946:HIS:CG	1:A:947:GLN:N	2.87	0.41
1:B:204:PRO:HD2	1:B:212:MET:SD	2.60	0.41
1:B:582:VAL:CG1	1:B:585:ALA:HB2	2.51	0.41
1:B:848:TRP:CG	1:B:848:TRP:O	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:VAL:HG23	1:C:649:THR:HG21	2.03	0.41
1:C:68:ASN:ND2	1:C:87:PRO:HG3	2.36	0.41
1:D:533:LEU:CD1	1:D:641:GLU:HB3	2.51	0.41
1:D:864:LEU:CG	1:D:865:THR:H	2.32	0.41
1:A:843:SER:N	1:A:844:PRO:CD	2.84	0.41
1:A:87:PRO:HB2	1:A:109:LEU:CD1	2.51	0.41
1:B:843:SER:N	1:B:844:PRO:CD	2.84	0.41
1:C:864:LEU:CG	1:C:865:THR:H	2.32	0.41
1:D:196:PRO:HG3	1:D:215:TYR:OH	2.19	0.41
1:D:843:SER:N	1:D:844:PRO:CD	2.84	0.41
1:D:68:ASN:ND2	1:D:87:PRO:HG3	2.36	0.41
1:A:781:PHE:CE2	1:A:797:LEU:O	2.74	0.41
1:A:933:CYS:SG	1:A:942:MET:SD	3.18	0.41
1:C:149:VAL:HG22	1:C:151:PRO:HD3	2.03	0.41
1:D:1018:VAL:HG12	1:D:1019:PRO:N	2.35	0.41
1:D:404:PHE:CE2	1:D:406:GLY:HA2	2.56	0.41
1:D:533:LEU:HD11	1:D:641:GLU:HB3	2.03	0.41
1:D:709:GLU:O	1:D:711:LEU:HD12	2.21	0.41
1:A:532:ALA:O	1:A:646:PHE:HB2	2.20	0.41
1:A:68:ASN:ND2	1:A:87:PRO:HG3	2.36	0.41
1:A:714:VAL:CG1	1:A:768:GLN:HA	2.49	0.41
1:B:404:PHE:CE2	1:B:406:GLY:HA2	2.56	0.41
1:A:463:PRO:CG	1:B:612:ILE:CB	2.68	0.41
1:C:196:PRO:HG3	1:C:215:TYR:OH	2.20	0.41
1:C:315:LEU:HD11	1:C:333:ASP:HB3	2.03	0.41
1:C:709:GLU:OE1	1:C:709:GLU:HA	2.21	0.41
1:C:791:ILE:HG22	1:C:792:ASP:N	2.36	0.41
1:D:476:PHE:HE2	1:D:482:ILE:HD13	1.85	0.41
1:D:781:PHE:CE2	1:D:797:LEU:O	2.74	0.41
1:A:582:VAL:CG1	1:A:585:ALA:HB2	2.51	0.41
1:A:57:ARG:HG3	1:A:58:ARG:HG3	2.02	0.41
1:A:709:GLU:O	1:A:711:LEU:HD12	2.21	0.41
1:A:883:LEU:HD13	1:A:911:ALA:O	2.21	0.41
1:B:781:PHE:CE2	1:B:797:LEU:O	2.74	0.41
1:B:68:ASN:ND2	1:B:87:PRO:HG3	2.36	0.41
1:C:815:LEU:O	1:C:848:TRP:CD1	2.74	0.41
1:C:931:ARG:HG2	1:C:942:MET:CE	2.50	0.41
1:D:309:LEU:HA	1:D:309:LEU:HD23	1.89	0.41
1:D:807:GLN:HE21	1:D:807:GLN:HB3	1.65	0.41
1:A:151:PRO:HG2	1:A:213:LEU:HD12	2.02	0.40
1:A:709:GLU:HA	1:A:709:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:GLU:O	1:B:711:LEU:HD12	2.21	0.40
1:B:815:LEU:CD1	1:B:815:LEU:N	2.83	0.40
1:B:815:LEU:HD23	1:B:848:TRP:HB3	2.04	0.40
1:C:709:GLU:O	1:C:711:LEU:HD12	2.21	0.40
1:C:864:LEU:CG	1:C:865:THR:N	2.82	0.40
1:C:979:LEU:HD12	1:C:1002:ASN:C	2.41	0.40
1:D:539:ARG:HD2	1:D:542:LYS:HZ2	1.86	0.40
1:D:582:VAL:CG1	1:D:585:ALA:HB2	2.51	0.40
1:D:619:LYS:HA	1:D:619:LYS:HD3	1.91	0.40
1:D:564:VAL:HG23	1:D:649:THR:HG21	2.03	0.40
1:D:979:LEU:HD12	1:D:1002:ASN:C	2.41	0.40
1:A:404:PHE:CE2	1:A:406:GLY:HA2	2.56	0.40
1:A:407:LEU:HD22	1:C:944:LYS:CG	2.48	0.40
1:A:863:ILE:HG23	1:A:863:ILE:O	2.20	0.40
1:A:931:ARG:HG2	1:A:942:MET:HE1	2.03	0.40
1:B:257:THR:O	1:B:278:SER:HA	2.22	0.40
1:A:463:PRO:HD2	1:B:612:ILE:HG21	2.03	0.40
1:B:781:PHE:CD1	1:B:781:PHE:C	2.94	0.40
1:C:404:PHE:CE2	1:C:406:GLY:HA2	2.56	0.40
1:C:883:LEU:HD13	1:C:911:ALA:O	2.21	0.40
1:A:550:ASN:O	1:A:586:PRO:HG3	2.21	0.40
1:A:815:LEU:HD23	1:A:848:TRP:HB3	2.04	0.40
1:A:864:LEU:CG	1:A:865:THR:H	2.32	0.40
1:A:923:ILE:CG1	1:A:924:GLY:H	2.35	0.40
1:C:702:PRO:HB3	1:C:728:PRO:CG	2.52	0.40
1:C:781:PHE:CE2	1:C:797:LEU:O	2.74	0.40
1:C:952:VAL:HG23	1:C:954:PRO:HD3	2.03	0.40
1:D:315:LEU:HD11	1:D:333:ASP:HB3	2.03	0.40
1:A:931:ARG:CG	1:A:942:MET:HE1	2.52	0.40
1:B:149:VAL:HG22	1:B:151:PRO:HD3	2.02	0.40
1:D:57:ARG:HG3	1:D:58:ARG:HG3	2.02	0.40
1:D:781:PHE:CD1	1:D:781:PHE:C	2.94	0.40
1:D:87:PRO:HB2	1:D:109:LEU:CD1	2.51	0.40
1:D:993:THR:HG22	1:D:994:CYS:O	2.22	0.40
1:A:810:SER:HB3	1:A:882:ASN:HD21	1.83	0.40
1:C:1013:ASN:HB3	1:C:1014:GLY:H	1.68	0.40
1:C:349:PRO:HA	1:C:350:PRO:HD3	1.96	0.40
1:C:979:LEU:HB2	1:C:1000:SER:O	2.21	0.40
1:D:883:LEU:HD13	1:D:911:ALA:O	2.21	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLN:OE1	1:C:146:PHE:CD1[3_455]	1.56	0.64
1:B:407:LEU:CD2	1:D:944:LYS:CD[2_564]	1.79	0.41
1:A:731:GLN:NE2	1:C:146:PHE:CE1[3_455]	1.87	0.33
1:A:766:SER:OG	1:B:839:PRO:CA[5_665]	1.98	0.22
1:A:839:PRO:CG	1:B:768:GLN:OE1[5_665]	2.02	0.18
1:B:146:PHE:CE1	1:C:677:TYR:OH[4_565]	2.03	0.17
1:A:731:GLN:CD	1:C:146:PHE:CD1[3_455]	2.08	0.12
1:A:766:SER:OG	1:B:839:PRO:CB[5_665]	2.12	0.08
1:A:731:GLN:CD	1:C:146:PHE:CE1[3_455]	2.15	0.05
1:A:84:LYS:CB	1:D:732:SER:OG[5_555]	2.15	0.05
1:B:217:LEU:CD1	1:D:940:GLU:OE1[2_564]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	896/1212 (74%)	861 (96%)	26 (3%)	9 (1%)	19	65
1	B	797/1212 (66%)	771 (97%)	19 (2%)	7 (1%)	21	67
1	C	981/1212 (81%)	937 (96%)	35 (4%)	9 (1%)	21	67
1	D	983/1212 (81%)	942 (96%)	31 (3%)	10 (1%)	19	65
All	All	3657/4848 (75%)	3511 (96%)	111 (3%)	35 (1%)	19	65

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	702	PRO
1	A	851	HIS
1	B	508	VAL
1	B	509	GLU
1	B	851	HIS
1	C	804	CYS
1	C	851	HIS

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Mol	Chain	Res	Type
1	D	804	CYS
1	D	851	HIS
1	A	703	GLN
1	A	160	SER
1	A	175	SER
1	A	805	ALA
1	B	160	SER
1	B	175	SER
1	B	805	ALA
1	C	160	SER
1	C	175	SER
1	C	805	ALA
1	D	160	SER
1	D	175	SER
1	D	805	ALA
1	A	849	SER
1	B	849	SER
1	C	849	SER
1	D	559	CYS
1	D	849	SER
1	A	935	GLY
1	C	935	GLY
1	C	952	VAL
1	D	935	GLY
1	D	952	VAL
1	A	922	VAL
1	C	922	VAL
1	D	922	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	796/1064 (75%)	787 (99%)	9 (1%)	80	91
1	B	714/1064 (67%)	706 (99%)	8 (1%)	80	91
1	C	870/1064 (82%)	860 (99%)	10 (1%)	80	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	870/1064 (82%)	860 (99%)	10 (1%)	80	91
All	All	3250/4256 (76%)	3213 (99%)	37 (1%)	80	91

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	A	238	HIS
1	A	274	LEU
1	A	298	PHE
1	A	438	TYR
1	A	509	GLU
1	A	626	LEU
1	A	811	CYS
1	A	893	HIS
1	B	237	SER
1	B	238	HIS
1	B	274	LEU
1	B	298	PHE
1	B	438	TYR
1	B	509	GLU
1	B	626	LEU
1	B	811	CYS
1	C	237	SER
1	C	238	HIS
1	C	274	LEU
1	C	298	PHE
1	C	438	TYR
1	C	509	GLU
1	C	626	LEU
1	C	811	CYS
1	C	893	HIS
1	C	953	ASN
1	D	237	SER
1	D	238	HIS
1	D	274	LEU
1	D	298	PHE
1	D	438	TYR
1	D	509	GLU
1	D	626	LEU
1	D	811	CYS
1	D	893	HIS

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Mol	Chain	Res	Type
1	D	953	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	726	ASN
1	A	731	GLN
1	A	761	GLN
1	A	837	HIS
1	B	513	GLN
1	B	534	HIS
1	B	703	GLN
1	B	761	GLN
1	B	837	HIS
1	C	534	HIS
1	C	726	ASN
1	C	761	GLN
1	C	807	GLN
1	C	837	HIS
1	C	953	ASN
1	C	1034	GLN
1	D	513	GLN
1	D	534	HIS
1	D	550	ASN
1	D	726	ASN
1	D	761	GLN
1	D	807	GLN
1	D	837	HIS
1	D	953	ASN
1	D	1034	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	6
1	A	6
1	C	6
1	D	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	855:CYS	C	856:SER	N	5.61
1	C	702:PRO	C	703:GLN	N	3.75
1	D	702:PRO	C	703:GLN	N	3.35
1	C	559:CYS	C	560:MET	N	2.82
1	C	855:CYS	C	856:SER	N	2.48
1	B	559:CYS	C	560:MET	N	2.40
1	B	701:CYS	C	702:PRO	N	2.35
1	B	803:LYS	C	804:CYS	N	2.12
1	A	559:CYS	C	560:MET	N	2.11
1	A	655:ASN	C	656:CYS	N	2.03
1	B	702:PRO	C	703:GLN	N	1.94
1	A	702:PRO	C	703:GLN	N	1.89
1	B	655:ASN	C	656:CYS	N	1.71
1	D	952:VAL	C	953:ASN	N	1.66
1	C	701:CYS	C	702:PRO	N	1.60
1	C	803:LYS	C	804:CYS	N	1.20
1	A	701:CYS	C	702:PRO	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	803:LYS	C	804:CYS	N	1.18
1	C	508:VAL	C	509:GLU	N	1.07
1	B	508:VAL	C	509:GLU	N	0.99
1	D	508:VAL	C	509:GLU	N	0.98
1	D	655:ASN	C	656:CYS	N	0.96
1	A	508:VAL	C	509:GLU	N	0.78

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	906/1212 (74%)	0.08	63 (6%)	19	22	153, 176, 433, 433	0
1	B	809/1212 (66%)	-0.09	33 (4%)	41	39	147, 209, 350, 350	0
1	C	993/1212 (81%)	-0.28	15 (1%)	76	70	200, 270, 340, 340	0
1	D	993/1212 (81%)	-0.28	10 (1%)	84	79	184, 270, 345, 345	0
All	All	3701/4848 (76%)	-0.15	121 (3%)	50	46	147, 228, 345, 433	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	THR	9.9
1	A	708	GLU	8.1
1	B	721	THR	6.4
1	A	709	GLU	6.1
1	A	710	ILE	6.0
1	A	867	SER	5.8
1	A	466	GLY	5.2
1	A	866	VAL	5.2
1	A	865	THR	4.6
1	A	462	GLY	4.3
1	A	948	GLN	4.2
1	A	950	THR	4.1
1	A	947	GLN	3.9
1	B	609	SER	3.9
1	A	799	VAL	3.9
1	A	424	LEU	3.8
1	A	357	ALA	3.7
1	B	716	GLU	3.5
1	A	36	PRO	3.5
1	B	610	GLN	3.4
1	B	363	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	588	LEU	3.3
1	B	836	GLN	3.3
1	A	585	ALA	3.3
1	C	861	THR	3.2
1	A	721	THR	3.1
1	B	720	ILE	3.1
1	A	868	GLY	3.1
1	A	927	SER	3.1
1	C	238	HIS	3.0
1	A	862	GLU	3.0
1	A	906	GLY	3.0
1	C	623	VAL	3.0
1	D	166	GLY	3.0
1	B	249	SER	3.0
1	A	422	LEU	3.0
1	C	793	ASN	2.9
1	A	722	LEU	2.9
1	B	710	ILE	2.9
1	C	947	GLN	2.9
1	B	722	LEU	2.9
1	B	281	VAL	2.8
1	A	895	GLN	2.8
1	A	952	VAL	2.8
1	A	907	GLU	2.8
1	A	358	PHE	2.8
1	A	928	GLY	2.8
1	A	461	ASP	2.8
1	D	851	HIS	2.7
1	A	931	ARG	2.7
1	A	864	LEU	2.7
1	A	465	HIS	2.7
1	A	720	ILE	2.6
1	D	969	GLY	2.6
1	B	248	ALA	2.6
1	A	609	SER	2.6
1	B	273	ASP	2.6
1	A	335	LEU	2.6
1	C	854	LYS	2.5
1	D	854	LYS	2.5
1	A	706	PRO	2.5
1	A	723	LYS	2.5
1	D	36	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	929	PRO	2.5
1	C	783	VAL	2.5
1	B	238	HIS	2.5
1	A	463	PRO	2.5
1	B	226	ILE	2.5
1	A	582	VAL	2.5
1	B	466	GLY	2.5
1	D	273	ASP	2.5
1	A	949	TYR	2.5
1	B	250	GLY	2.5
1	C	862	GLU	2.5
1	B	607	SER	2.5
1	B	467	GLY	2.4
1	A	930	VAL	2.4
1	A	608	GLY	2.4
1	B	280	ILE	2.4
1	B	359	PRO	2.4
1	B	360	ILE	2.4
1	A	467	GLY	2.4
1	A	460	ALA	2.4
1	A	905	PRO	2.3
1	A	322	LEU	2.3
1	B	611	VAL	2.3
1	B	357	ALA	2.3
1	C	399	PRO	2.3
1	A	926	THR	2.3
1	A	893	HIS	2.3
1	B	605	GLN	2.3
1	A	863	ILE	2.3
1	B	254	TYR	2.3
1	D	852	ASN	2.2
1	C	237	SER	2.2
1	B	82	ALA	2.2
1	A	359	PRO	2.2
1	B	741	LEU	2.2
1	A	945	SER	2.2
1	C	273	ASP	2.2
1	A	622	PRO	2.2
1	A	487	ALA	2.2
1	A	879	HIS	2.2
1	C	408	ASP	2.1
1	A	599	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	770	ASP	2.1
1	A	877	THR	2.1
1	D	710	ILE	2.1
1	A	53	LEU	2.1
1	B	293	TYR	2.1
1	D	850	SER	2.1
1	C	138	LYS	2.1
1	C	924	GLY	2.1
1	A	82	ALA	2.1
1	D	605	GLN	2.1
1	A	745	GLY	2.1
1	B	487	ALA	2.1
1	B	335	LEU	2.0
1	A	798	LYS	2.0
1	B	608	GLY	2.0
1	C	836	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.