



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:12 PM UTC

PDB ID : 1XNW / pdb_00001xnw
Title : Acyl-CoA Carboxylase Beta Subunit from *S. coelicolor* (PccB), apo form #2, mutant D422I
Authors : Diacovich, L.; Mitchell, D.L.; Pham, H.; Gago, G.; Melgar, M.M.; Khosla, C.; Gramajo, H.; Tsai, S.-C.
Deposited on : 2004-10-05
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

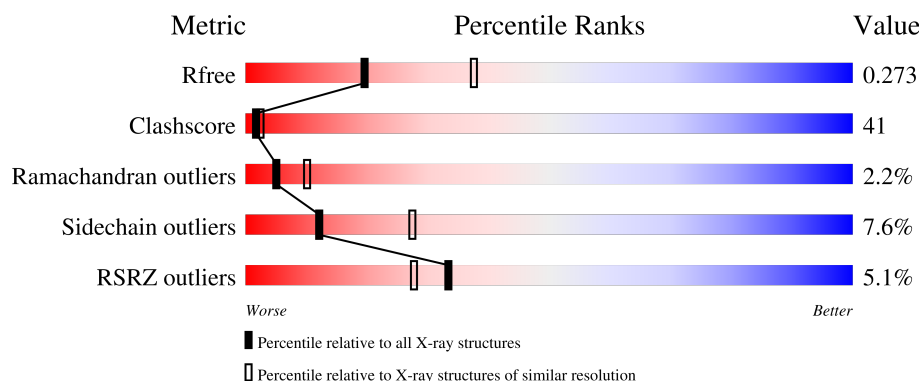
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	530	5% 42% 50% 6%
1	B	530	3% 46% 47% 5%
1	C	530	6% 38% 51% 10%
1	D	530	5% 47% 46% 6%
1	E	530	6% 43% 49% 6%

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Mol	Chain	Length	Quality of chain
1	F	530	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: 5% (red), 39% (green), 52% (yellow), and 7% (orange). A small grey dot is at the end of the bar.

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 24754 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 propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			3953	2483	698	759	13			
1	B	521	Total	C	N	O	S	0	0	0
			3953	2483	698	759	13			
1	C	521	Total	C	N	O	S	0	0	0
			3953	2483	698	759	13			
1	D	521	Total	C	N	O	S	0	0	0
			3953	2483	698	759	13			
1	E	521	Total	C	N	O	S	0	0	0
			3953	2483	698	759	13			
1	F	521	Total	C	N	O	S	0	0	0
			3953	2483	698	759	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	ILE	ASP	engineered mutation	UNP Q9X4K7
B	422	ILE	ASP	engineered mutation	UNP Q9X4K7
C	422	ILE	ASP	engineered mutation	UNP Q9X4K7
D	422	ILE	ASP	engineered mutation	UNP Q9X4K7
E	422	ILE	ASP	engineered mutation	UNP Q9X4K7
F	422	ILE	ASP	engineered mutation	UNP Q9X4K7

- Molecule 2 is water.

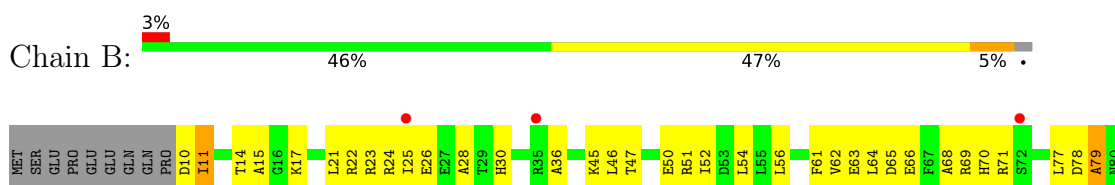
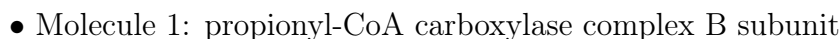
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	173	Total	O	0	0
			173	173		
2	B	167	Total	O	0	0
			167	167		
2	C	184	Total	O	0	0
			184	184		

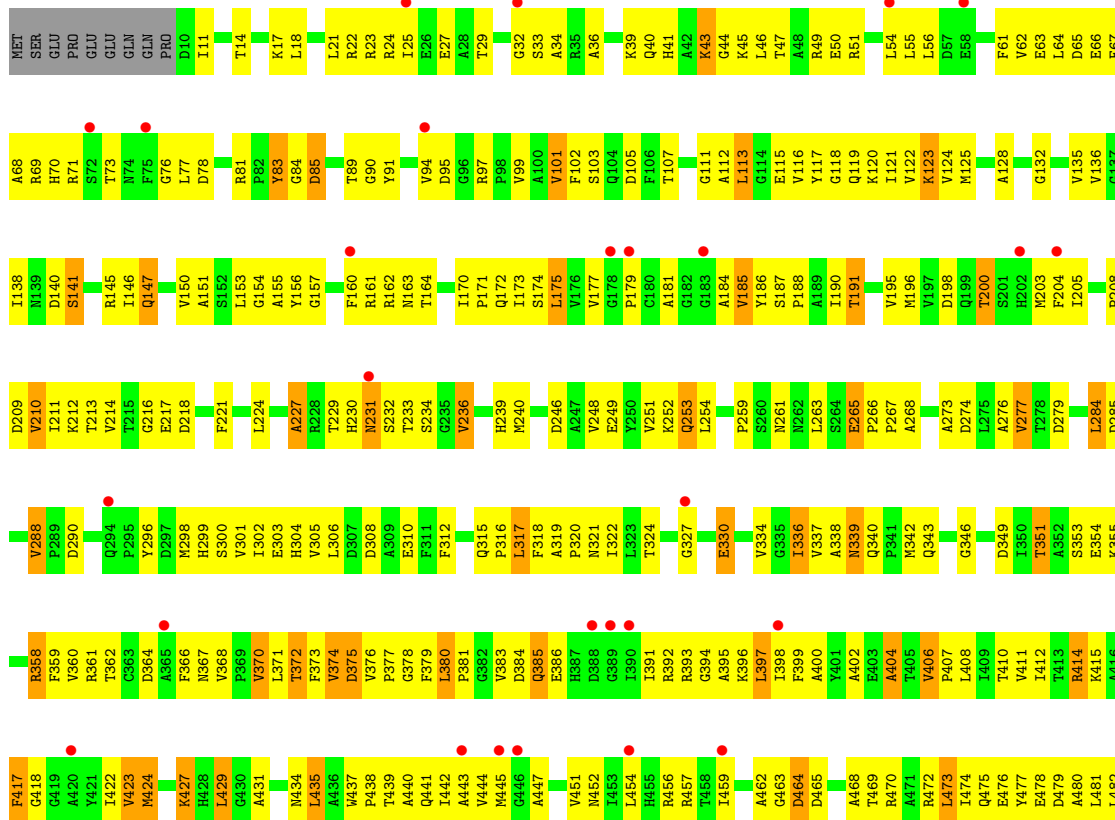
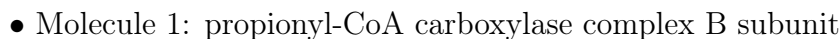
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	154	Total 154	O 154	0	0
2	E	176	Total 176	O 176	0	0
2	F	182	Total 182	O 182	0	0

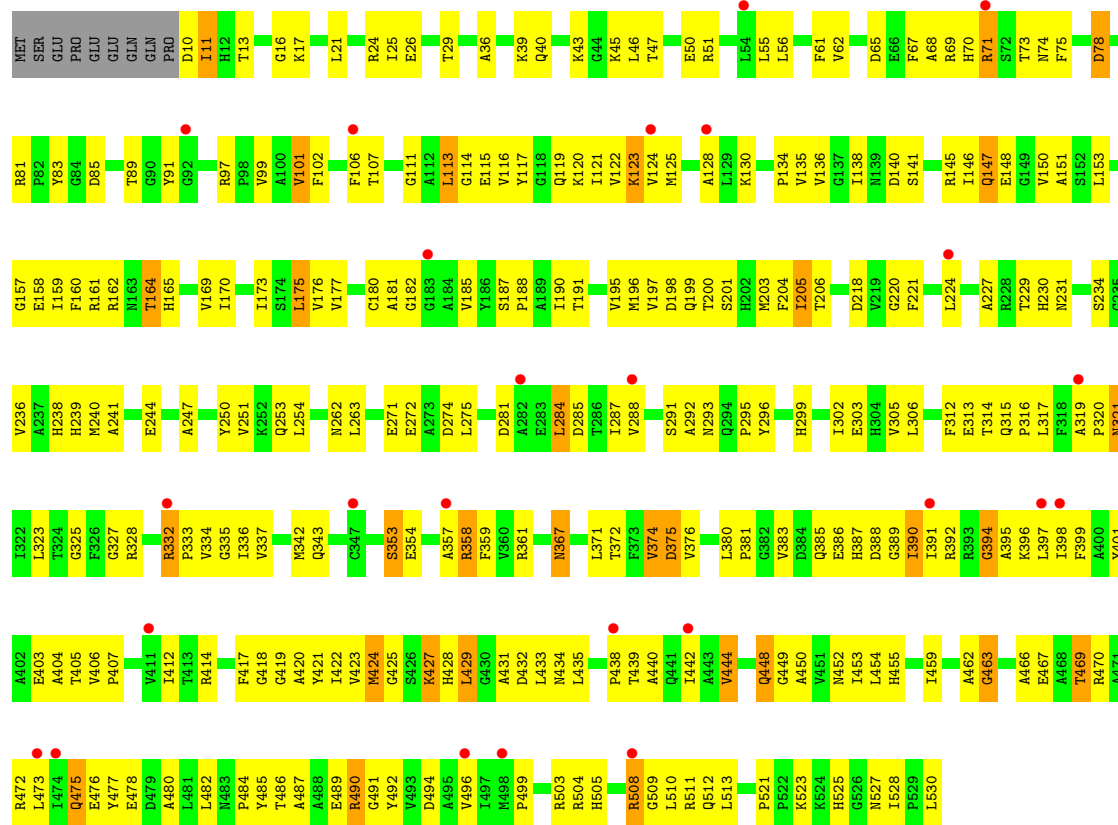
- Molecule 1: propionyl-CoA carboxylase complex B subunit



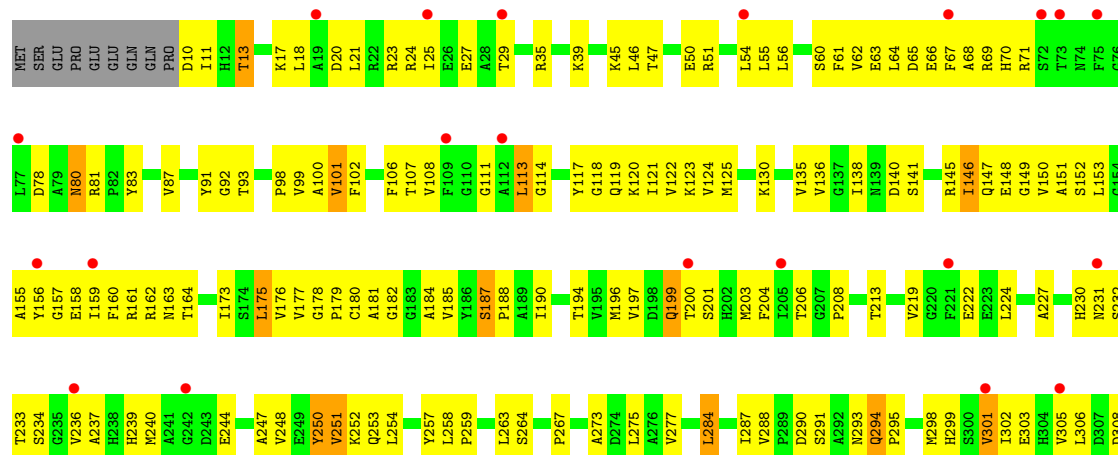
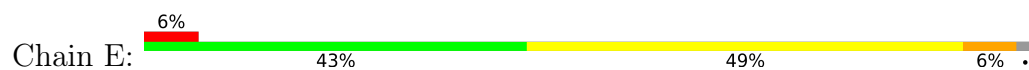




- Molecule 1: propionyl-CoA carboxylase complex B subunit



- Molecule 1: propionyl-CoA carboxylase complex B subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.85Å 219.49Å 135.69Å 90.00° 102.99° 90.00°	Depositor
Resolution (Å)	49.05 – 2.60 49.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.7 (49.05-2.60) 87.7 (49.05-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.276 0.267 , 0.273	Depositor DCC
R_{free} test set	2808 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.956	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24754	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.60	0/4033	0.98	12/5478 (0.2%)
1	B	0.60	0/4033	0.98	9/5478 (0.2%)
1	C	0.60	0/4033	0.95	7/5478 (0.1%)
1	D	0.60	0/4033	0.98	10/5478 (0.2%)
1	E	0.63	0/4033	0.99	15/5478 (0.3%)
1	F	0.58	0/4033	0.98	18/5478 (0.3%)
All	All	0.60	0/24198	0.98	71/32868 (0.2%)

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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	VAL	N-CA-C	9.09	119.69	108.06
1	A	288	VAL	N-CA-C	8.47	115.27	107.56
1	C	463	GLY	N-CA-C	-7.80	104.00	113.99
1	F	463	GLY	N-CA-C	-7.50	104.39	113.99
1	D	374	VAL	N-CA-C	7.38	119.71	108.71
1	B	374	VAL	N-CA-C	7.11	119.99	108.97
1	C	469	THR	N-CA-C	-7.01	105.34	114.04
1	E	374	VAL	N-CA-C	6.96	119.47	108.89
1	E	101	VAL	N-CA-C	6.89	117.39	107.88
1	E	367	ASN	N-CA-C	6.87	120.88	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	126	ASP	N-CA-C	-6.82	104.78	113.23
1	D	463	GLY	N-CA-C	-6.79	105.95	114.16
1	E	294	GLN	CA-C-N	6.79	127.33	120.14
1	E	294	GLN	C-N-CA	6.79	127.33	120.14
1	B	469	THR	N-CA-C	-6.73	105.63	114.31
1	B	336	ILE	N-CA-C	6.72	117.58	108.17
1	F	374	VAL	N-CA-C	6.71	118.27	108.53
1	C	101	VAL	N-CA-C	6.56	119.43	108.81
1	A	370	VAL	N-CA-C	6.54	116.13	106.85
1	F	469	THR	N-CA-C	-6.49	105.29	113.72
1	F	207	GLY	CA-C-N	6.48	125.98	119.24
1	F	207	GLY	C-N-CA	6.48	125.98	119.24
1	E	423	VAL	N-CA-C	6.45	117.98	110.62
1	E	469	THR	N-CA-C	-6.40	104.42	112.93
1	C	367	ASN	N-CA-C	6.31	120.26	111.74
1	A	520	LEU	CA-C-N	-6.30	115.06	119.66
1	A	520	LEU	C-N-CA	-6.30	115.06	119.66
1	F	120	LYS	N-CA-C	-6.26	104.09	111.03
1	B	101	VAL	N-CA-C	6.22	116.57	108.35
1	B	207	GLY	CA-C-N	6.12	125.61	119.24
1	B	207	GLY	C-N-CA	6.12	125.61	119.24
1	D	332	ARG	CA-C-N	6.11	125.87	119.76
1	D	332	ARG	C-N-CA	6.11	125.87	119.76
1	F	367	ASN	N-CA-C	6.04	119.73	111.39
1	E	336	ILE	N-CA-C	6.03	116.55	108.11
1	F	101	VAL	N-CA-C	6.03	117.04	108.42
1	A	469	THR	N-CA-C	-5.99	104.68	112.23
1	C	417	PHE	N-CA-C	5.95	118.61	108.90
1	A	265	GLU	CA-C-N	-5.89	115.36	119.66
1	A	265	GLU	C-N-CA	-5.89	115.36	119.66
1	D	469	THR	N-CA-C	-5.86	105.98	114.12
1	B	192	ASP	N-CA-C	5.85	117.33	111.07
1	D	101	VAL	N-CA-C	5.83	115.52	108.06
1	F	332	ARG	CA-C-N	5.74	125.75	119.90
1	F	332	ARG	C-N-CA	5.74	125.75	119.90
1	F	497	ILE	N-CA-C	5.72	117.66	108.85
1	D	367	ASN	N-CA-C	5.67	119.25	111.54
1	E	332	ARG	CA-C-N	5.63	125.64	119.90
1	E	332	ARG	C-N-CA	5.63	125.64	119.90
1	F	181	ALA	N-CA-C	5.59	118.81	110.14
1	A	524	LYS	N-CA-C	-5.55	105.23	111.28
1	B	79	ALA	N-CA-C	-5.55	106.35	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	463	GLY	N-CA-C	-5.50	106.95	113.99
1	F	495	ALA	N-CA-C	5.43	117.34	108.76
1	F	81	ARG	CA-C-N	5.35	125.11	119.76
1	F	81	ARG	C-N-CA	5.35	125.11	119.76
1	A	192	ASP	N-CA-C	5.35	116.91	111.14
1	E	485	TYR	N-CA-C	5.29	118.52	111.75
1	C	374	VAL	N-CA-C	5.28	117.16	108.97
1	A	97	ARG	CA-C-N	5.28	125.04	119.76
1	A	97	ARG	C-N-CA	5.28	125.04	119.76
1	D	394	GLY	N-CA-C	-5.27	108.42	115.32
1	C	370	VAL	N-CA-C	5.26	115.16	107.37
1	D	485	TYR	N-CA-C	5.26	118.86	112.23
1	E	524	LYS	N-CA-C	-5.22	105.48	111.07
1	E	101	VAL	CB-CA-C	-5.21	104.56	111.80
1	F	370	VAL	N-CA-C	5.17	114.94	106.72
1	B	370	VAL	N-CA-C	5.14	114.98	107.37
1	F	87	VAL	N-CA-C	5.11	115.10	108.35
1	D	417	PHE	N-CA-C	5.06	117.81	109.72
1	E	417	PHE	N-CA-C	5.04	117.27	108.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	83	TYR	Sidechain
1	C	83	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3953	0	3887	352	0
1	B	3953	0	3887	318	0
1	C	3953	0	3887	370	0
1	D	3953	0	3887	303	0
1	E	3953	0	3887	348	0
1	F	3953	0	3887	410	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	173	0	0	69	0
2	B	167	0	0	63	0
2	C	184	0	0	69	0
2	D	154	0	0	50	0
2	E	176	0	0	73	0
2	F	182	0	0	76	0
All	All	24754	0	23322	1909	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (1909) 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:F:47:THR:HG23	1:F:50:GLU:HB2	1.39	1.00
1:B:147:GLN:H	1:B:147:GLN:NE2	1.60	1.00
1:D:147:GLN:HE21	1:D:147:GLN:H	1.06	0.99
1:F:187:SER:HB3	1:F:188:PRO:HD3	1.46	0.96
1:C:173:ILE:HG21	1:C:251:VAL:HG23	1.48	0.95
1:F:99:VAL:HA	2:F:607:HOH:O	1.64	0.94
1:A:35:ARG:HH12	1:A:39:LYS:HD2	1.32	0.94
1:C:40:GLN:HE21	1:C:45:LYS:HD2	1.32	0.94
1:B:147:GLN:HE21	1:B:147:GLN:N	1.66	0.93
1:D:328:ARG:HA	2:D:602:HOH:O	1.70	0.92
1:A:113:LEU:HD22	1:A:117:TYR:CE1	2.05	0.91
1:C:65:ASP:HB2	1:C:120:LYS:HE3	1.50	0.91
1:A:169:VAL:HG23	2:D:594:HOH:O	1.72	0.90
1:A:146:ILE:H	1:A:146:ILE:HD12	1.37	0.89
1:C:440:ALA:O	1:C:484:PRO:HD3	1.73	0.89
1:C:151:ALA:HB2	1:F:490:ARG:NH1	1.88	0.88
1:F:305:VAL:HG21	1:F:506:ILE:HD12	1.56	0.87
1:B:122:VAL:HG22	2:B:586:HOH:O	1.74	0.86
1:F:173:ILE:HG21	1:F:251:VAL:HG23	1.57	0.86
1:F:398:ILE:HG13	1:F:429:LEU:HD21	1.57	0.86
1:F:65:ASP:HB2	1:F:120:LYS:HE3	1.58	0.86
1:F:372:THR:HB	2:F:546:HOH:O	1.76	0.85
1:E:62:VAL:HG11	1:F:508:ARG:HH21	1.41	0.85
1:B:508:ARG:HD3	1:B:509:GLY:N	1.92	0.85
1:B:147:GLN:H	1:B:147:GLN:HE21	0.85	0.84
1:C:113:LEU:HD22	1:C:117:TYR:CE1	2.13	0.83
1:C:408:LEU:HD23	2:C:681:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ALA:HB1	1:D:240:MET:HG3	1.61	0.83
1:B:325:GLY:O	1:B:359:PHE:HZ	1.60	0.83
1:A:170:ILE:HG21	2:A:570:HOH:O	1.78	0.82
1:D:62:VAL:HG11	1:E:508:ARG:HH21	1.42	0.82
1:E:148:GLU:HG3	2:E:699:HOH:O	1.80	0.82
1:D:422:ILE:HG23	2:D:547:HOH:O	1.80	0.81
1:A:509:GLY:O	1:A:513:LEU:HD23	1.80	0.81
1:A:510:LEU:HA	2:A:537:HOH:O	1.79	0.81
1:B:173:ILE:HG21	1:B:251:VAL:HG23	1.63	0.81
1:B:138:ILE:HG12	1:B:175:LEU:HD23	1.63	0.81
1:B:497:ILE:HG21	1:B:505:HIS:HE2	1.46	0.81
1:B:64:LEU:HG	2:B:562:HOH:O	1.80	0.80
1:C:408:LEU:HA	2:C:681:HOH:O	1.80	0.80
1:D:508:ARG:HH21	1:F:62:VAL:HG11	1.45	0.80
1:E:254:LEU:HB2	2:E:700:HOH:O	1.80	0.80
1:B:433:LEU:HA	1:B:494:ASP:OD1	1.81	0.80
1:A:489:GLU:HA	1:B:68:ALA:HA	1.63	0.80
1:B:113:LEU:HD22	1:B:117:TYR:CE1	2.16	0.80
1:C:334:VAL:HB	2:C:584:HOH:O	1.82	0.80
1:C:231:ASN:HB3	1:C:317:LEU:HD13	1.62	0.79
1:B:306:LEU:HD13	1:B:327:GLY:HA3	1.64	0.79
1:A:393:ARG:HA	1:A:396:LYS:HE3	1.64	0.79
1:C:211:ILE:HG23	2:C:713:HOH:O	1.82	0.79
1:F:104:GLN:HE21	1:F:140:ASP:H	1.30	0.79
1:D:89:THR:HB	1:D:124:VAL:HG21	1.63	0.79
1:F:451:VAL:HG11	1:F:474:ILE:HA	1.62	0.79
1:F:465:ASP:HB3	1:F:468:ALA:HB3	1.65	0.79
1:D:99:VAL:HA	2:D:603:HOH:O	1.82	0.79
1:B:315:GLN:HB3	2:B:625:HOH:O	1.83	0.78
1:A:267:PRO:HG3	2:A:572:HOH:O	1.83	0.78
1:F:348:LEU:HD21	1:F:424:MET:HE3	1.63	0.78
1:D:148:GLU:HG3	2:D:655:HOH:O	1.81	0.78
1:C:151:ALA:HB2	1:F:490:ARG:HH12	1.47	0.78
1:C:170:ILE:HG21	2:C:641:HOH:O	1.83	0.78
1:D:321:ASN:HA	1:D:343:GLN:HB2	1.66	0.78
1:D:62:VAL:HG11	1:E:508:ARG:NH2	1.99	0.78
1:A:295:PRO:HB2	1:A:342:MET:CE	2.13	0.77
1:C:164:THR:HG23	1:F:399:PHE:CD1	2.20	0.77
1:F:299:HIS:O	1:F:303:GLU:HG3	1.85	0.77
1:C:187:SER:HB3	1:C:188:PRO:HD3	1.66	0.77
1:C:371:LEU:HG	2:C:584:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:PRO:HG2	2:C:651:HOH:O	1.83	0.77
1:D:230:HIS:HA	1:D:234:SER:OG	1.84	0.77
1:C:208:PRO:HG3	1:C:224:LEU:HD22	1.65	0.76
1:D:499:PRO:HB3	2:D:581:HOH:O	1.85	0.76
1:D:508:ARG:HD3	1:D:509:GLY:N	2.01	0.76
1:C:45:LYS:HE2	1:C:200:THR:HG22	1.67	0.76
1:F:472:ARG:NH2	1:F:473:LEU:HD22	2.01	0.76
1:E:146:ILE:H	1:E:146:ILE:HD12	1.51	0.76
1:B:89:THR:HB	1:B:124:VAL:HG21	1.66	0.76
1:C:97:ARG:NH1	1:C:267:PRO:HG3	2.01	0.75
1:C:418:GLY:HA2	1:F:153:LEU:HD21	1.68	0.75
1:C:40:GLN:NE2	1:C:45:LYS:HD2	2.01	0.75
1:C:64:LEU:HG	2:C:571:HOH:O	1.87	0.75
1:D:147:GLN:HE21	1:D:147:GLN:N	1.82	0.75
1:E:161:ARG:HG3	1:E:161:ARG:HH11	1.50	0.75
1:D:432:ASP:O	1:D:433:LEU:HD12	1.86	0.75
1:E:111:GLY:HA2	2:E:598:HOH:O	1.87	0.75
1:F:437:TRP:HB2	2:F:648:HOH:O	1.86	0.75
1:A:62:VAL:HG11	1:C:508:ARG:NH2	2.01	0.75
1:A:422:ILE:HG23	2:A:543:HOH:O	1.87	0.75
1:B:414:ARG:HB2	2:B:597:HOH:O	1.87	0.75
1:D:313:GLU:HG2	1:D:316:PRO:HG3	1.69	0.75
1:A:391:ILE:H	1:A:391:ILE:HD12	1.51	0.74
1:A:424:MET:HB3	2:A:594:HOH:O	1.87	0.74
1:C:153:LEU:HD21	1:F:418:GLY:HA2	1.69	0.74
1:C:483:ASN:HD22	1:C:485:TYR:H	1.35	0.74
1:F:101:VAL:HG23	1:F:136:VAL:O	1.87	0.74
1:A:483:ASN:HD22	1:A:485:TYR:HD2	1.36	0.74
1:C:529:PRO:HG3	1:F:190:ILE:HA	1.69	0.74
1:B:497:ILE:HG21	1:B:505:HIS:NE2	2.02	0.74
1:C:399:PHE:CE1	1:F:164:THR:HG23	2.22	0.74
1:F:125:MET:HE1	1:F:163:ASN:ND2	2.02	0.74
1:F:125:MET:HE1	1:F:163:ASN:HD21	1.50	0.74
1:B:325:GLY:O	1:B:359:PHE:CZ	2.40	0.74
1:B:398:ILE:HD12	1:E:160:PHE:HB3	1.67	0.74
1:B:159:ILE:HA	2:B:586:HOH:O	1.88	0.74
1:A:230:HIS:HA	1:A:234:SER:OG	1.88	0.74
1:B:69:ARG:HD2	1:B:81:ARG:HB3	1.67	0.74
1:C:273:ALA:HB2	1:C:330:GLU:HG3	1.69	0.74
1:C:319:ALA:HB2	1:C:351:THR:HB	1.69	0.73
1:E:527:ASN:ND2	2:E:584:HOH:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:508:ARG:HD3	1:F:509:GLY:N	2.03	0.73
1:A:398:ILE:HD12	1:D:160:PHE:HB3	1.69	0.73
1:E:412:ILE:HG23	2:E:627:HOH:O	1.88	0.73
1:F:478:GLU:HA	1:F:482:LEU:HB2	1.69	0.73
1:A:162:ARG:HG2	1:A:162:ARG:HH11	1.53	0.73
1:D:69:ARG:HD2	1:D:81:ARG:O	1.89	0.73
1:D:187:SER:HB3	1:D:188:PRO:HD3	1.69	0.73
1:B:153:LEU:HD21	1:E:418:GLY:HA2	1.69	0.73
1:C:89:THR:HB	1:C:124:VAL:HG21	1.71	0.73
1:A:295:PRO:HB2	1:A:342:MET:HE2	1.71	0.73
1:B:421:TYR:HA	2:B:629:HOH:O	1.88	0.73
1:E:306:LEU:HD21	1:E:336:ILE:HD11	1.70	0.73
1:C:56:LEU:HD12	1:C:61:PHE:HB2	1.71	0.73
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.72	0.72
1:C:40:GLN:HG3	1:C:45:LYS:HB2	1.71	0.72
1:E:319:ALA:HB3	1:E:355:LYS:HD2	1.71	0.72
1:F:451:VAL:HG21	1:F:474:ILE:HG12	1.71	0.72
1:A:62:VAL:HG11	1:C:508:ARG:HH21	1.52	0.72
1:A:508:ARG:NE	1:B:91:TYR:OH	2.22	0.72
1:C:317:LEU:H	1:C:317:LEU:HD12	1.54	0.72
1:A:97:ARG:NH1	2:A:572:HOH:O	2.22	0.72
1:B:305:VAL:HB	2:B:580:HOH:O	1.89	0.72
1:F:49:ARG:HE	1:F:88:VAL:HG21	1.54	0.72
1:D:427:LYS:NZ	1:D:434:ASN:OD1	2.23	0.72
1:F:118:GLY:HA2	2:F:654:HOH:O	1.89	0.72
1:A:28:ALA:HB2	1:A:83:TYR:HD1	1.53	0.72
1:C:372:THR:HG23	1:C:410:THR:HA	1.70	0.72
1:F:337:VAL:HB	2:F:546:HOH:O	1.90	0.72
1:A:427:LYS:HB2	1:A:434:ASN:OD1	1.90	0.72
1:E:395:ALA:O	1:E:398:ILE:HG23	1.90	0.72
1:C:444:VAL:HA	1:F:153:LEU:HD11	1.72	0.72
1:D:197:VAL:O	1:D:227:ALA:HB2	1.89	0.72
1:B:160:PHE:HB3	1:E:398:ILE:HD11	1.71	0.71
1:C:162:ARG:HG2	1:C:162:ARG:HH11	1.55	0.71
1:A:508:ARG:HD3	1:A:509:GLY:N	2.04	0.71
1:D:68:ALA:HA	1:E:489:GLU:HA	1.71	0.71
1:F:505:HIS:HA	1:F:508:ARG:HD2	1.72	0.71
1:A:254:LEU:HB2	2:A:660:HOH:O	1.89	0.71
1:A:386:GLU:HG3	1:D:224:LEU:HD11	1.72	0.71
1:A:398:ILE:HG22	1:A:423:VAL:HG22	1.71	0.71
1:D:147:GLN:H	1:D:147:GLN:NE2	1.87	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:374:VAL:HB	1:E:412:ILE:HD13	1.72	0.71
1:F:483:ASN:HD22	1:F:485:TYR:HD2	1.38	0.71
1:D:467:GLU:HA	1:D:470:ARG:HB3	1.71	0.71
1:C:434:ASN:HB2	2:C:690:HOH:O	1.90	0.71
1:F:140:ASP:OD1	1:F:178:GLY:HA3	1.90	0.70
1:F:13:THR:O	1:F:17:LYS:HG2	1.91	0.70
1:A:63:GLU:OE2	1:A:88:VAL:HG13	1.91	0.70
1:C:248:VAL:O	1:C:251:VAL:HG12	1.90	0.70
1:B:69:ARG:HD3	1:B:81:ARG:O	1.91	0.70
1:A:84:GLY:HA2	1:A:120:LYS:HZ2	1.56	0.70
1:E:182:GLY:O	1:E:185:VAL:HG22	1.91	0.70
1:E:465:ASP:HB3	1:E:468:ALA:HB3	1.73	0.70
1:B:495:ALA:HB2	2:B:534:HOH:O	1.91	0.70
1:D:505:HIS:HA	1:D:508:ARG:HD2	1.73	0.70
1:E:185:VAL:O	1:E:188:PRO:HD2	1.91	0.70
1:E:406:VAL:HG22	2:E:677:HOH:O	1.91	0.70
1:F:372:THR:HG23	1:F:410:THR:HA	1.74	0.69
1:C:391:ILE:HG23	2:F:651:HOH:O	1.92	0.69
1:A:508:ARG:NH2	1:B:62:VAL:HG11	2.07	0.69
1:B:160:PHE:HB3	1:E:398:ILE:CD1	2.22	0.69
1:B:422:ILE:HD11	1:E:153:LEU:HB3	1.73	0.69
1:E:158:GLU:HB3	2:E:688:HOH:O	1.92	0.69
1:E:313:GLU:HG2	1:E:316:PRO:HG3	1.73	0.69
1:D:158:GLU:O	1:D:162:ARG:HG2	1.92	0.69
1:A:71:ARG:CZ	1:C:490:ARG:HE	2.05	0.69
1:D:247:ALA:HA	2:D:614:HOH:O	1.92	0.69
1:A:187:SER:HB3	1:A:188:PRO:HD3	1.73	0.69
1:E:302:ILE:HD13	1:E:336:ILE:HG21	1.75	0.69
1:E:356:ALA:O	1:E:360:VAL:HG23	1.92	0.69
1:B:335:GLY:C	1:B:336:ILE:HD12	2.18	0.69
1:B:478:GLU:HA	1:B:482:LEU:HB2	1.73	0.68
1:F:487:ALA:HB1	1:F:492:TYR:HB2	1.74	0.68
1:B:483:ASN:HD22	1:B:485:TYR:H	1.41	0.68
1:B:302:ILE:HD13	1:B:336:ILE:HG21	1.76	0.68
1:B:432:ASP:O	1:B:433:LEU:HD12	1.93	0.68
1:E:523:LYS:NZ	2:E:599:HOH:O	2.26	0.68
1:F:348:LEU:HD21	1:F:424:MET:CE	2.23	0.68
1:F:434:ASN:HB2	2:F:622:HOH:O	1.93	0.68
1:E:179:PRO:HG3	2:E:625:HOH:O	1.94	0.68
1:F:527:ASN:ND2	2:F:593:HOH:O	2.27	0.68
1:C:427:LYS:HB2	1:C:427:LYS:NZ	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LEU:HD22	1:A:513:LEU:N	2.08	0.68
1:F:175:LEU:HA	1:F:195:VAL:HG13	1.76	0.68
1:C:524:LYS:HD2	2:F:650:HOH:O	1.93	0.68
1:D:336:ILE:N	1:D:336:ILE:HD12	2.09	0.68
1:E:240:MET:HG2	2:E:624:HOH:O	1.93	0.68
1:E:414:ARG:HA	1:E:440:ALA:HA	1.76	0.68
1:A:70:HIS:HB3	1:A:85:ASP:OD1	1.94	0.68
1:D:528:ILE:O	1:D:530:LEU:HD22	1.94	0.68
1:E:254:LEU:HD13	1:E:312:PHE:HE2	1.58	0.68
1:F:305:VAL:HG21	1:F:506:ILE:CD1	2.23	0.68
1:B:318:PHE:HB3	2:B:625:HOH:O	1.95	0.67
1:C:318:PHE:CZ	1:C:351:THR:HG22	2.29	0.67
1:C:408:LEU:HB2	1:C:431:ALA:HA	1.76	0.67
1:D:74:ASN:HB2	2:D:623:HOH:O	1.94	0.67
1:B:231:ASN:HD21	1:B:239:HIS:C	2.01	0.67
1:F:302:ILE:O	1:F:305:VAL:HG12	1.94	0.67
1:F:472:ARG:HH21	1:F:473:LEU:HD22	1.57	0.67
1:B:65:ASP:HB2	1:B:120:LYS:HE3	1.76	0.67
1:D:114:GLY:H	1:D:117:TYR:HB3	1.58	0.67
1:A:113:LEU:HD22	1:A:117:TYR:HE1	1.60	0.67
1:B:324:THR:HG23	1:B:355:LYS:HE2	1.75	0.67
1:E:231:ASN:O	1:E:317:LEU:HB2	1.93	0.67
1:F:162:ARG:HG2	1:F:162:ARG:HH11	1.59	0.67
1:D:508:ARG:NH2	1:F:62:VAL:HG11	2.09	0.67
1:C:470:ARG:HH11	1:C:470:ARG:HG3	1.60	0.67
1:A:35:ARG:HB3	1:A:35:ARG:NH1	2.09	0.67
1:E:113:LEU:HD22	1:E:117:TYR:CE1	2.30	0.67
1:F:70:HIS:HB2	2:F:605:HOH:O	1.95	0.67
1:F:104:GLN:HG2	2:F:708:HOH:O	1.94	0.67
1:F:231:ASN:O	1:F:317:LEU:HB2	1.95	0.67
1:E:120:LYS:HD3	2:E:689:HOH:O	1.93	0.67
1:C:321:ASN:HA	1:C:343:GLN:HB2	1.77	0.66
1:C:156:TYR:HB3	1:C:160:PHE:CE2	2.31	0.66
1:D:197:VAL:HA	2:D:633:HOH:O	1.95	0.66
1:F:150:VAL:O	1:F:153:LEU:HB2	1.96	0.66
1:C:229:THR:HA	2:C:595:HOH:O	1.94	0.66
1:E:230:HIS:HB3	1:E:236:VAL:HG22	1.78	0.66
1:A:433:LEU:HA	1:A:494:ASP:OD1	1.96	0.66
1:A:529:PRO:O	1:A:530:LEU:HD13	1.96	0.66
1:C:299:HIS:O	1:C:303:GLU:HG3	1.96	0.66
2:C:698:HOH:O	1:F:358:ARG:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TYR:OH	1:C:508:ARG:NE	2.28	0.66
1:C:417:PHE:HA	1:C:443:ALA:O	1.96	0.66
1:B:438:PRO:HG3	1:C:21:LEU:HD22	1.78	0.66
1:C:434:ASN:N	1:C:494:ASP:OD1	2.23	0.66
1:F:514:ARG:HD2	2:F:700:HOH:O	1.94	0.66
1:C:190:ILE:HD12	1:F:399:PHE:HD1	1.60	0.66
1:C:211:ILE:HD11	2:C:579:HOH:O	1.96	0.66
1:E:62:VAL:HG21	1:F:508:ARG:HE	1.61	0.66
1:F:101:VAL:HG23	1:F:136:VAL:HB	1.77	0.66
1:F:523:LYS:HE3	2:F:688:HOH:O	1.96	0.66
1:C:196:MET:HB3	2:C:620:HOH:O	1.94	0.66
1:E:175:LEU:HB3	2:E:593:HOH:O	1.96	0.66
1:F:328:ARG:HB3	2:F:550:HOH:O	1.95	0.66
1:A:14:THR:HB	2:A:574:HOH:O	1.94	0.65
1:B:101:VAL:HG23	1:B:136:VAL:O	1.96	0.65
1:F:377:PRO:HA	1:F:417:PHE:HD2	1.61	0.65
1:A:391:ILE:HD13	2:A:650:HOH:O	1.96	0.65
1:B:459:ILE:HD11	1:B:470:ARG:HB2	1.78	0.65
1:C:45:LYS:CE	1:C:200:THR:HG22	2.25	0.65
1:F:32:GLY:HA3	1:F:107:THR:OG1	1.96	0.65
1:F:198:ASP:HA	1:F:227:ALA:HB3	1.78	0.65
1:A:494:ASP:HB3	1:B:64:LEU:HD22	1.79	0.65
1:D:429:LEU:HD13	2:D:547:HOH:O	1.97	0.65
1:E:334:VAL:HG23	2:E:612:HOH:O	1.96	0.65
1:F:177:VAL:HG12	1:F:197:VAL:CG2	2.26	0.65
1:F:354:GLU:HG3	2:F:628:HOH:O	1.95	0.65
1:F:104:GLN:HE21	1:F:140:ASP:N	1.93	0.65
1:A:84:GLY:HA2	1:A:120:LYS:NZ	2.11	0.65
1:C:437:TRP:HB2	2:C:618:HOH:O	1.95	0.65
1:B:11:ILE:HG13	1:B:11:ILE:O	1.97	0.65
1:B:102:PHE:CD1	1:B:121:ILE:HG23	2.32	0.65
1:C:101:VAL:HG23	1:C:136:VAL:O	1.97	0.65
1:D:296:TYR:C	1:D:342:MET:HE3	2.22	0.65
1:F:162:ARG:HB2	2:F:630:HOH:O	1.95	0.64
1:A:319:ALA:HB3	1:A:355:LYS:HD2	1.78	0.64
1:A:354:GLU:OE1	1:A:393:ARG:HB3	1.97	0.64
2:C:692:HOH:O	1:F:402:ALA:HB1	1.97	0.64
1:E:117:TYR:HA	2:E:689:HOH:O	1.96	0.64
1:C:61:PHE:HE1	1:C:90:GLY:HA3	1.60	0.64
1:C:508:ARG:HD3	1:C:509:GLY:N	2.12	0.64
1:E:258:LEU:HB2	2:E:571:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:HG23	1:D:399:PHE:CD1	2.32	0.64
1:B:315:GLN:N	1:B:316:PRO:HD3	2.12	0.64
1:B:361:ARG:HD2	1:B:403:GLU:OE2	1.98	0.64
1:C:164:THR:HG23	1:F:399:PHE:CE1	2.33	0.64
1:D:337:VAL:HG11	2:D:601:HOH:O	1.96	0.64
1:E:396:LYS:HG2	2:E:592:HOH:O	1.96	0.64
1:F:340:GLN:CD	1:F:342:MET:HB2	2.22	0.64
1:B:162:ARG:HG3	2:B:586:HOH:O	1.96	0.64
1:E:298:MET:SD	1:E:301:VAL:HG21	2.38	0.64
1:F:208:PRO:HA	1:F:211:ILE:HD12	1.79	0.64
1:A:71:ARG:NH2	1:C:490:ARG:HE	1.95	0.64
1:B:508:ARG:NH2	1:C:62:VAL:HG11	2.12	0.64
1:C:336:ILE:HD12	1:C:336:ILE:N	2.13	0.64
1:B:448:GLN:O	1:B:451:VAL:HG22	1.98	0.64
1:D:433:LEU:HA	1:D:494:ASP:OD1	1.97	0.64
1:F:196:MET:HE3	1:F:203:MET:HG3	1.79	0.64
1:A:180:CYS:O	1:A:203:MET:HA	1.98	0.64
1:A:315:GLN:N	1:A:316:PRO:HD3	2.13	0.64
1:B:190:ILE:HD12	1:E:399:PHE:HD1	1.63	0.64
1:E:21:LEU:O	1:E:25:ILE:HG23	1.98	0.64
1:F:175:LEU:HA	1:F:195:VAL:CG1	2.28	0.64
1:B:162:ARG:HG2	1:B:162:ARG:HH11	1.63	0.64
1:C:399:PHE:CD1	1:F:164:THR:HG23	2.33	0.64
1:E:141:SER:O	1:E:179:PRO:HB2	1.98	0.64
1:A:71:ARG:HH21	1:C:490:ARG:HA	1.63	0.63
1:B:527:ASN:ND2	1:E:358:ARG:HE	1.94	0.63
1:C:319:ALA:N	1:C:320:PRO:HD3	2.13	0.63
1:E:529:PRO:O	1:E:530:LEU:HD12	1.97	0.63
1:B:52:ILE:HG13	2:B:590:HOH:O	1.97	0.63
1:E:145:ARG:HB2	2:E:608:HOH:O	1.97	0.63
1:D:173:ILE:HG21	1:D:251:VAL:HG23	1.79	0.63
1:B:279:ASP:O	1:B:282:ALA:HB3	1.98	0.63
1:B:527:ASN:ND2	2:B:585:HOH:O	2.32	0.63
1:C:427:LYS:HB2	1:C:427:LYS:HZ2	1.63	0.63
1:B:499:PRO:HB3	2:B:646:HOH:O	1.97	0.63
1:D:374:VAL:HG13	1:D:424:MET:HG3	1.80	0.63
1:E:398:ILE:HB	2:E:706:HOH:O	1.97	0.63
1:D:65:ASP:HB2	1:D:120:LYS:HE3	1.81	0.63
1:E:505:HIS:HA	1:E:508:ARG:HD2	1.81	0.63
1:C:393:ARG:HA	1:C:396:LYS:HE3	1.81	0.62
1:F:316:PRO:HA	2:F:567:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG11	1:D:381:PRO:HG2	1.80	0.62
1:C:284:LEU:HD13	1:C:304:HIS:CD2	2.33	0.62
1:C:147:GLN:N	1:C:147:GLN:OE1	2.31	0.62
1:C:483:ASN:ND2	1:C:485:TYR:HB2	2.14	0.62
1:E:113:LEU:HD12	2:E:665:HOH:O	1.99	0.62
1:A:392:ARG:HH11	1:A:392:ARG:HG3	1.64	0.62
1:E:18:LEU:HD11	1:F:285:ASP:O	1.98	0.62
1:F:295:PRO:HB2	2:F:536:HOH:O	1.99	0.62
1:F:483:ASN:ND2	1:F:485:TYR:HB2	2.13	0.62
1:F:97:ARG:NH1	1:F:267:PRO:HG3	2.14	0.62
1:C:411:VAL:HG22	1:C:435:LEU:HB2	1.80	0.62
1:D:361:ARG:HD2	1:D:403:GLU:OE2	1.99	0.62
1:E:113:LEU:HD13	1:E:117:TYR:CD1	2.34	0.62
1:E:422:ILE:HG23	2:E:539:HOH:O	1.99	0.62
1:A:424:MET:HE3	2:A:594:HOH:O	2.00	0.62
1:B:121:ILE:HG22	2:B:575:HOH:O	2.00	0.62
1:E:336:ILE:HG13	2:E:612:HOH:O	1.98	0.62
1:D:397:LEU:HD22	1:D:423:VAL:HG13	1.82	0.62
1:F:169:VAL:HG12	1:F:170:ILE:HG23	1.82	0.62
1:F:234:SER:HB2	1:F:236:VAL:HG13	1.81	0.62
1:B:456:ARG:O	1:B:459:ILE:HG22	1.99	0.62
1:D:469:THR:O	1:D:473:LEU:HB2	1.99	0.62
1:A:483:ASN:ND2	1:A:485:TYR:HB2	2.15	0.61
1:B:306:LEU:HB2	2:B:642:HOH:O	2.00	0.61
1:C:71:ARG:NH2	1:C:119:GLN:HE22	1.98	0.61
1:D:503:ARG:O	1:D:504:ARG:C	2.43	0.61
1:A:231:ASN:O	1:A:318:PHE:HB2	1.99	0.61
1:A:472:ARG:O	1:A:476:GLU:HG3	1.99	0.61
1:A:61:PHE:CZ	1:A:63:GLU:HB2	2.35	0.61
1:E:91:TYR:OH	1:F:508:ARG:NE	2.34	0.61
1:E:505:HIS:O	1:E:508:ARG:HD3	2.00	0.61
1:F:177:VAL:HG12	1:F:197:VAL:HG23	1.80	0.61
1:A:224:LEU:HD12	1:D:383:VAL:HG13	1.80	0.61
1:C:322:ILE:HA	1:C:339:ASN:HA	1.81	0.61
1:F:342:MET:HG2	2:F:657:HOH:O	2.00	0.61
1:A:371:LEU:HD23	2:A:558:HOH:O	1.99	0.61
1:B:505:HIS:C	1:B:508:ARG:HH11	2.08	0.61
1:E:208:PRO:HG3	1:E:224:LEU:HD22	1.80	0.61
1:F:185:VAL:HG23	2:F:651:HOH:O	2.00	0.61
1:C:70:HIS:NE2	1:C:81:ARG:HG2	2.14	0.61
1:D:113:LEU:HD22	1:D:117:TYR:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:ASP:CG	1:F:414:ARG:HB3	2.26	0.61
1:B:47:THR:HG23	1:B:50:GLU:CD	2.25	0.61
1:C:70:HIS:HB2	2:C:533:HOH:O	2.00	0.61
1:A:418:GLY:HA2	1:D:153:LEU:HD21	1.83	0.61
1:D:496:VAL:HB	1:F:67:PHE:HE2	1.66	0.61
1:A:453:ILE:HG21	1:D:146:ILE:HD12	1.82	0.61
1:A:47:THR:OG1	1:A:50:GLU:HG3	2.01	0.61
1:A:454:LEU:HD13	1:D:75:PHE:CZ	2.36	0.61
1:A:524:LYS:HD3	1:D:405:THR:OG1	2.01	0.61
1:C:24:ARG:HD3	1:C:83:TYR:OH	2.00	0.61
1:C:173:ILE:HD12	1:C:254:LEU:HD23	1.82	0.61
1:D:508:ARG:HE	1:F:62:VAL:HG21	1.65	0.61
1:E:101:VAL:HG23	1:E:136:VAL:O	2.00	0.61
1:A:396:LYS:HG2	2:A:677:HOH:O	2.00	0.60
1:A:425:GLY:HA3	2:A:670:HOH:O	2.01	0.60
1:C:456:ARG:O	1:C:459:ILE:HG22	2.01	0.60
1:E:56:LEU:HD13	1:E:92:GLY:HA3	1.83	0.60
1:F:55:LEU:CD2	1:F:136:VAL:HG11	2.31	0.60
1:F:291:SER:HB3	1:F:294:GLN:HB2	1.84	0.60
1:C:435:LEU:HD12	2:C:683:HOH:O	2.01	0.60
1:A:169:VAL:HG21	1:D:521:PRO:HB2	1.84	0.60
1:A:291:SER:HB3	1:A:294:GLN:HB2	1.84	0.60
1:A:302:ILE:HD13	1:A:336:ILE:HG21	1.84	0.60
1:A:459:ILE:HD11	1:A:470:ARG:HB2	1.82	0.60
1:C:231:ASN:O	1:C:317:LEU:HB2	2.01	0.60
1:E:161:ARG:HG3	1:E:161:ARG:NH1	2.16	0.60
1:E:339:ASN:HB2	2:E:569:HOH:O	2.01	0.60
1:F:440:ALA:O	1:F:484:PRO:HD3	2.01	0.60
1:B:508:ARG:HD3	1:B:508:ARG:C	2.26	0.60
1:C:208:PRO:HB3	2:C:591:HOH:O	2.00	0.60
1:C:395:ALA:HB2	1:F:186:TYR:HD1	1.66	0.60
1:D:62:VAL:CG1	1:E:508:ARG:HH21	2.13	0.60
1:D:505:HIS:C	1:D:508:ARG:HH11	2.08	0.60
1:F:65:ASP:CB	1:F:120:LYS:HE3	2.31	0.60
1:A:73:THR:HG22	1:A:78:ASP:OD2	2.02	0.60
1:E:138:ILE:HG23	2:E:593:HOH:O	2.01	0.60
1:B:70:HIS:HB2	2:B:621:HOH:O	2.02	0.60
1:B:87:VAL:HG23	1:B:104:GLN:HA	1.83	0.60
1:C:392:ARG:HH11	1:C:392:ARG:HG3	1.67	0.60
1:E:483:ASN:HD22	1:E:485:TYR:H	1.48	0.60
1:A:273:ALA:HB2	1:A:330:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:MET:HE1	2:D:648:HOH:O	2.01	0.60
1:D:391:ILE:HA	2:D:640:HOH:O	2.02	0.60
1:E:472:ARG:O	1:E:476:GLU:HG3	2.02	0.60
1:F:505:HIS:C	1:F:508:ARG:HH11	2.10	0.60
1:B:22:ARG:O	1:B:25:ILE:HG12	2.02	0.60
1:B:397:LEU:HD13	1:B:423:VAL:CG1	2.32	0.59
1:C:386:GLU:OE1	1:F:204:PHE:HA	2.01	0.59
1:A:159:ILE:HG22	2:A:562:HOH:O	2.02	0.59
1:A:487:ALA:HB1	1:A:492:TYR:HB2	1.84	0.59
1:D:39:LYS:O	1:D:43:LYS:HG3	2.03	0.59
1:E:322:ILE:HG13	1:E:338:ALA:O	2.02	0.59
1:F:238:HIS:HA	1:F:315:GLN:HG2	1.84	0.59
1:A:24:ARG:HB3	1:A:83:TYR:HE1	1.67	0.59
1:A:175:LEU:HD22	1:A:177:VAL:HG13	1.84	0.59
1:E:259:PRO:HB2	2:E:600:HOH:O	2.02	0.59
1:E:464:ASP:O	1:E:465:ASP:HB2	2.02	0.59
1:F:198:ASP:HB2	1:F:240:MET:HE3	1.84	0.59
1:C:186:TYR:HD1	1:F:395:ALA:HB2	1.68	0.59
1:D:284:LEU:O	1:D:287:ILE:HG22	2.02	0.59
1:E:416:ALA:HB3	1:E:442:ILE:HA	1.85	0.59
1:F:198:ASP:HB2	1:F:240:MET:SD	2.43	0.59
1:F:288:VAL:HG23	2:F:677:HOH:O	2.02	0.59
1:A:377:PRO:O	1:A:417:PHE:HB2	2.02	0.59
1:A:508:ARG:HD3	1:A:508:ARG:C	2.27	0.59
1:B:151:ALA:HB2	1:E:490:ARG:NH2	2.18	0.59
1:B:527:ASN:HD21	1:E:358:ARG:HE	1.50	0.59
1:C:398:ILE:HD12	1:F:160:PHE:HD2	1.66	0.59
1:F:414:ARG:HA	1:F:439:THR:O	2.02	0.59
1:A:71:ARG:NH2	1:C:490:ARG:HA	2.16	0.59
1:A:151:ALA:HB2	1:D:490:ARG:NH1	2.18	0.59
2:A:694:HOH:O	1:D:358:ARG:HA	2.03	0.59
1:B:169:VAL:HG23	2:E:599:HOH:O	2.01	0.59
1:B:498:MET:HE1	1:C:18:LEU:HD13	1.85	0.59
1:B:529:PRO:HA	2:B:649:HOH:O	2.02	0.59
1:C:172:GLN:O	1:C:191:THR:HB	2.02	0.59
1:F:97:ARG:CZ	1:F:267:PRO:HG3	2.32	0.59
1:F:121:ILE:O	1:F:125:MET:HG3	2.03	0.59
1:F:472:ARG:HG2	1:F:472:ARG:HH11	1.67	0.59
1:F:377:PRO:O	1:F:417:PHE:HB2	2.02	0.59
1:D:525:HIS:HB2	2:D:573:HOH:O	2.02	0.59
1:F:187:SER:CB	1:F:188:PRO:HD3	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:ARG:NE	1:C:91:TYR:OH	2.36	0.58
1:C:89:THR:HG22	1:C:102:PHE:HB2	1.84	0.58
1:C:370:VAL:HB	2:C:681:HOH:O	2.01	0.58
1:D:496:VAL:HB	1:F:67:PHE:CE2	2.38	0.58
1:A:69:ARG:HD2	1:A:81:ARG:O	2.03	0.58
1:E:199:GLN:HB3	2:E:687:HOH:O	2.02	0.58
1:F:231:ASN:HD21	1:F:239:HIS:CA	2.16	0.58
1:D:175:LEU:HD22	1:D:177:VAL:HG13	1.85	0.58
1:D:427:LYS:NZ	1:D:427:LYS:HB2	2.17	0.58
1:D:472:ARG:HG2	2:D:624:HOH:O	2.03	0.58
1:E:185:VAL:C	1:E:188:PRO:HD2	2.28	0.58
1:D:478:GLU:HA	1:D:482:LEU:HB2	1.84	0.58
1:F:336:ILE:N	1:F:336:ILE:HD12	2.17	0.58
1:B:427:LYS:NZ	1:B:434:ASN:OD1	2.36	0.58
1:C:230:HIS:HB3	1:C:236:VAL:HG22	1.85	0.58
1:F:55:LEU:HD21	1:F:136:VAL:HG11	1.86	0.58
1:F:63:GLU:CD	1:F:66:GLU:HB2	2.29	0.58
1:A:302:ILE:HD12	2:A:678:HOH:O	2.04	0.58
1:A:451:VAL:HG13	2:A:681:HOH:O	2.03	0.58
1:E:17:LYS:HE2	2:F:625:HOH:O	2.03	0.58
1:F:104:GLN:HG3	1:F:139:ASN:HA	1.85	0.58
1:F:266:PRO:HG2	2:F:604:HOH:O	2.04	0.58
1:C:525:HIS:HE1	1:F:361:ARG:HE	1.52	0.58
1:E:176:VAL:HG12	1:E:201:SER:HB2	1.84	0.58
1:D:70:HIS:HA	1:D:116:VAL:HG21	1.84	0.58
1:D:490:ARG:HH21	1:F:71:ARG:CZ	2.17	0.58
1:E:24:ARG:NH1	1:E:83:TYR:OH	2.37	0.58
1:F:175:LEU:HD23	1:F:195:VAL:HG13	1.85	0.58
1:A:21:LEU:HD22	1:C:438:PRO:HG3	1.84	0.58
1:C:496:VAL:HG21	2:C:651:HOH:O	2.04	0.58
1:D:414:ARG:HD2	2:D:564:HOH:O	2.03	0.58
1:D:10:ASP:CG	1:D:11:ILE:H	2.12	0.58
1:D:25:ILE:O	1:D:29:THR:HG23	2.04	0.58
1:D:181:ALA:HB2	1:D:204:PHE:CE1	2.39	0.58
1:D:197:VAL:HG12	1:D:198:ASP:H	1.69	0.58
1:E:208:PRO:HG3	1:E:224:LEU:CD2	2.33	0.58
1:F:64:LEU:HG	2:F:551:HOH:O	2.03	0.58
1:B:164:THR:HG23	1:E:399:PHE:CD1	2.39	0.57
1:D:181:ALA:HA	1:D:204:PHE:O	2.03	0.57
1:F:193:PHE:HA	1:F:238:HIS:CE1	2.39	0.57
1:F:196:MET:O	1:F:240:MET:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:392:ARG:HH11	1:F:392:ARG:HG3	1.69	0.57
1:F:427:LYS:HB2	1:F:427:LYS:NZ	2.19	0.57
1:B:508:ARG:CZ	1:C:62:VAL:HG11	2.35	0.57
1:D:176:VAL:HB	1:D:196:MET:HB3	1.86	0.57
1:D:428:HIS:HB2	2:D:547:HOH:O	2.04	0.57
1:E:91:TYR:CD1	1:E:91:TYR:C	2.82	0.57
1:C:94:VAL:HG23	1:C:99:VAL:HG11	1.85	0.57
1:C:147:GLN:CD	1:C:147:GLN:H	2.11	0.57
1:D:302:ILE:HD13	1:D:336:ILE:HG21	1.87	0.57
1:E:512:GLN:N	2:E:611:HOH:O	2.30	0.57
1:F:195:VAL:HG23	2:F:600:HOH:O	2.03	0.57
1:F:314:THR:HG23	1:F:325:GLY:HA2	1.85	0.57
1:B:324:THR:HA	1:B:336:ILE:O	2.04	0.57
1:A:321:ASN:OD1	1:A:321:ASN:N	2.32	0.57
1:B:70:HIS:NE2	1:B:77:LEU:HD22	2.20	0.57
1:C:63:GLU:HG2	1:C:66:GLU:HB2	1.87	0.57
1:D:505:HIS:O	1:D:508:ARG:HD3	2.05	0.57
1:F:111:GLY:O	1:F:141:SER:HB2	2.03	0.57
1:A:442:ILE:HG22	1:D:150:VAL:HG11	1.84	0.57
1:B:302:ILE:O	1:B:305:VAL:HG22	2.04	0.57
1:C:338:ALA:CB	1:C:373:PHE:HB2	2.33	0.57
1:C:368:VAL:HG23	2:C:550:HOH:O	2.03	0.57
1:D:197:VAL:HG12	1:D:198:ASP:N	2.19	0.57
1:F:319:ALA:N	1:F:320:PRO:HD3	2.19	0.57
1:F:329:VAL:N	2:F:550:HOH:O	2.37	0.57
1:A:177:VAL:HG12	1:A:197:VAL:HG23	1.86	0.57
1:B:36:ALA:HB1	1:B:107:THR:HB	1.87	0.57
1:C:520:LEU:H	1:C:520:LEU:HD12	1.69	0.57
1:D:147:GLN:HB2	2:D:655:HOH:O	2.02	0.57
1:D:432:ASP:C	1:D:433:LEU:HD12	2.30	0.57
1:A:124:VAL:HG11	2:A:546:HOH:O	2.03	0.57
1:E:386:GLU:HA	1:E:390:ILE:HG22	1.85	0.57
1:B:393:ARG:HA	1:B:396:LYS:HE3	1.87	0.57
1:B:470:ARG:HG2	2:B:682:HOH:O	2.05	0.57
2:B:649:HOH:O	1:E:358:ARG:CZ	2.53	0.57
1:D:180:CYS:HB3	1:D:203:MET:HG2	1.87	0.57
1:F:77:LEU:HD12	2:F:655:HOH:O	2.05	0.57
1:F:278:THR:OG1	1:F:281:ASP:HB2	2.04	0.57
1:A:197:VAL:HG12	1:A:198:ASP:N	2.20	0.57
1:B:262:ASN:OD1	1:B:263:LEU:N	2.37	0.57
1:B:120:LYS:NZ	2:B:531:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:LEU:HD22	2:B:596:HOH:O	2.05	0.56
1:B:464:ASP:O	1:B:465:ASP:HB2	2.04	0.56
1:C:124:VAL:HG12	2:C:574:HOH:O	2.05	0.56
1:C:342:MET:HG2	2:C:646:HOH:O	2.04	0.56
1:F:49:ARG:HG3	1:F:49:ARG:HH11	1.69	0.56
1:F:205:ILE:HG23	1:F:206:THR:HG23	1.85	0.56
1:A:173:ILE:HG21	1:A:251:VAL:HG23	1.87	0.56
1:E:431:ALA:HB1	1:E:434:ASN:HD21	1.70	0.56
1:A:505:HIS:O	1:A:508:ARG:NH1	2.38	0.56
1:C:338:ALA:HB2	1:C:373:PHE:HB2	1.87	0.56
1:C:402:ALA:HA	1:C:429:LEU:O	2.05	0.56
1:D:315:GLN:N	1:D:316:PRO:HD3	2.20	0.56
1:D:412:ILE:HG23	2:D:620:HOH:O	2.04	0.56
1:D:422:ILE:O	1:D:429:LEU:HD22	2.05	0.56
1:E:145:ARG:NE	2:E:608:HOH:O	2.38	0.56
1:B:250:TYR:OH	1:B:314:THR:HG22	2.05	0.56
1:B:307:ASP:OD2	1:B:330:GLU:N	2.38	0.56
1:C:51:ARG:HH12	1:C:140:ASP:HB2	1.71	0.56
1:C:208:PRO:C	1:C:210:VAL:H	2.13	0.56
1:E:483:ASN:HB2	1:E:484:PRO:HD2	1.88	0.56
1:A:87:VAL:HG13	1:A:87:VAL:O	2.05	0.56
1:D:177:VAL:HG12	1:D:197:VAL:CG2	2.35	0.56
1:E:177:VAL:HG22	2:E:593:HOH:O	2.05	0.56
1:F:521:PRO:HB2	2:F:688:HOH:O	2.05	0.56
1:C:177:VAL:HG11	2:C:605:HOH:O	2.05	0.56
1:C:315:GLN:N	1:C:316:PRO:HD3	2.20	0.56
1:D:467:GLU:HA	1:D:470:ARG:CB	2.36	0.56
1:A:206:THR:CG2	1:A:210:VAL:HB	2.36	0.56
1:B:278:THR:HG23	2:B:693:HOH:O	2.06	0.56
1:C:447:ALA:O	1:C:451:VAL:HG22	2.06	0.56
1:D:238:HIS:HA	1:D:315:GLN:HG2	1.88	0.56
1:D:241:ALA:N	2:D:633:HOH:O	2.38	0.56
1:E:431:ALA:CB	1:E:434:ASN:HD21	2.19	0.56
1:C:472:ARG:HD2	1:C:476:GLU:OE2	2.05	0.56
1:F:517:ARG:O	1:F:518:GLU:HG2	2.05	0.56
1:B:494:ASP:HB3	1:C:64:LEU:HD22	1.88	0.56
1:D:177:VAL:HG12	1:D:197:VAL:HG23	1.88	0.56
1:F:497:ILE:HG13	2:F:687:HOH:O	2.06	0.56
1:C:156:TYR:HB3	1:C:160:PHE:CZ	2.40	0.55
1:D:122:VAL:O	1:D:125:MET:N	2.39	0.55
1:D:398:ILE:CG2	1:D:423:VAL:HG22	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:LEU:HD22	1:E:117:TYR:HE1	1.70	0.55
1:A:399:PHE:CD1	1:D:164:THR:HG23	2.42	0.55
1:A:480:ALA:O	1:A:481:LEU:HD12	2.06	0.55
1:D:24:ARG:HD3	1:D:83:TYR:OH	2.06	0.55
1:E:504:ARG:O	1:E:508:ARG:HD2	2.05	0.55
1:A:153:LEU:HD11	1:D:418:GLY:HA2	1.88	0.55
1:E:10:ASP:HB3	1:E:13:THR:OG1	2.07	0.55
1:E:87:VAL:HG13	1:E:120:LYS:HE2	1.88	0.55
1:F:71:ARG:NH1	1:F:71:ARG:HB2	2.21	0.55
1:A:375:ASP:CG	1:A:414:ARG:HB3	2.32	0.55
1:B:10:ASP:OD1	1:B:11:ILE:N	2.39	0.55
1:B:135:VAL:O	1:B:135:VAL:HG12	2.07	0.55
1:C:121:ILE:O	1:C:125:MET:HG3	2.07	0.55
1:C:398:ILE:HD12	1:F:160:PHE:CD2	2.42	0.55
1:C:306:LEU:HD13	1:C:327:GLY:HA3	1.87	0.55
1:E:180:CYS:SG	1:E:185:VAL:HA	2.47	0.55
1:B:508:ARG:HE	1:C:62:VAL:HG21	1.70	0.55
1:D:69:ARG:HA	2:D:539:HOH:O	2.07	0.55
1:E:24:ARG:HG2	1:E:24:ARG:HH11	1.70	0.55
1:E:364:ASP:CG	2:E:677:HOH:O	2.50	0.55
1:E:419:GLY:O	1:E:423:VAL:HG23	2.07	0.55
1:A:101:VAL:HG23	1:A:136:VAL:O	2.05	0.55
1:C:24:ARG:HG3	2:C:562:HOH:O	2.06	0.55
1:C:91:TYR:CD1	1:C:91:TYR:C	2.84	0.55
1:D:231:ASN:HB3	1:D:317:LEU:HD12	1.89	0.55
1:B:490:ARG:NH1	1:E:151:ALA:HB2	2.21	0.55
1:F:441:GLN:HB3	1:F:482:LEU:HG	1.87	0.55
1:A:299:HIS:O	1:A:303:GLU:HG3	2.07	0.55
2:C:698:HOH:O	1:F:358:ARG:HA	2.06	0.55
1:A:146:ILE:HG12	1:D:453:ILE:HG21	1.87	0.55
1:A:206:THR:HG23	1:A:210:VAL:HB	1.88	0.55
1:A:434:ASN:HB3	2:A:568:HOH:O	2.06	0.55
1:C:337:VAL:O	1:C:372:THR:HA	2.07	0.55
1:D:101:VAL:HG23	1:D:136:VAL:O	2.06	0.55
1:E:121:ILE:HG13	2:E:670:HOH:O	2.07	0.55
1:E:197:VAL:HA	2:E:624:HOH:O	2.07	0.55
1:F:315:GLN:N	1:F:316:PRO:HD3	2.21	0.55
1:F:472:ARG:HG2	1:F:472:ARG:NH1	2.22	0.55
1:D:397:LEU:HD22	1:D:423:VAL:CG1	2.36	0.54
1:C:150:VAL:O	1:C:153:LEU:N	2.38	0.54
1:C:153:LEU:HD21	1:F:418:GLY:CA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:GLN:HB2	1:C:355:LYS:HE3	1.89	0.54
1:B:427:LYS:HZ2	1:B:427:LYS:HB2	1.73	0.54
1:D:262:ASN:OD1	1:D:263:LEU:HD13	2.06	0.54
1:F:447:ALA:HA	1:F:477:TYR:CD1	2.42	0.54
1:F:486:THR:O	1:F:489:GLU:HB2	2.08	0.54
2:B:624:HOH:O	1:E:490:ARG:HG3	2.08	0.54
1:E:358:ARG:O	1:E:358:ARG:HD3	2.08	0.54
1:A:374:VAL:HG22	1:A:424:MET:HB3	1.90	0.54
1:C:231:ASN:HD21	1:C:239:HIS:CA	2.20	0.54
1:D:51:ARG:HB3	1:D:138:ILE:HD13	1.90	0.54
1:D:65:ASP:OD1	1:D:123:LYS:HD2	2.07	0.54
1:D:450:ALA:HB1	1:D:477:TYR:CE2	2.42	0.54
1:F:456:ARG:O	1:F:459:ILE:HG22	2.07	0.54
1:C:268:ALA:HB2	2:C:610:HOH:O	2.08	0.54
1:E:478:GLU:HA	1:E:482:LEU:HB2	1.89	0.54
1:F:49:ARG:H	1:F:49:ARG:HD2	1.73	0.54
1:F:359:PHE:O	1:F:362:THR:N	2.41	0.54
1:A:339:ASN:O	1:A:341:PRO:HD3	2.07	0.54
1:D:288:VAL:HG11	1:D:439:THR:HB	1.89	0.54
1:D:513:LEU:HD22	1:D:513:LEU:N	2.22	0.54
1:A:414:ARG:HA	1:A:439:THR:O	2.08	0.54
1:B:87:VAL:HG11	2:B:657:HOH:O	2.08	0.54
1:E:80:ASN:HD22	1:E:80:ASN:N	2.06	0.54
1:E:432:ASP:O	1:E:433:LEU:HD12	2.08	0.54
1:F:344:PHE:O	1:F:345:ALA:HB3	2.07	0.54
1:A:528:ILE:HG12	2:A:677:HOH:O	2.08	0.54
1:B:173:ILE:HG21	1:B:251:VAL:CG2	2.35	0.54
1:B:346:GLY:HA2	2:B:623:HOH:O	2.07	0.54
1:C:265:GLU:HG2	1:C:266:PRO:HD2	1.90	0.54
1:E:157:GLY:O	1:E:160:PHE:N	2.41	0.54
1:A:146:ILE:H	1:A:146:ILE:CD1	2.11	0.54
1:A:527:ASN:HD21	1:D:358:ARG:CD	2.21	0.54
1:C:353:SER:CB	1:C:394:GLY:HA2	2.38	0.54
1:D:241:ALA:HB2	2:D:614:HOH:O	2.07	0.54
1:D:414:ARG:HA	1:D:440:ALA:HA	1.90	0.54
1:E:451:VAL:C	1:E:453:ILE:H	2.15	0.54
1:F:139:ASN:OD1	1:F:176:VAL:HG22	2.08	0.54
1:F:176:VAL:HG12	1:F:201:SER:HB2	1.90	0.54
1:F:203:MET:HB2	1:F:230:HIS:CD2	2.42	0.54
1:A:10:ASP:CG	1:A:11:ILE:H	2.16	0.53
1:A:159:ILE:HA	2:A:583:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:VAL:HG12	1:A:197:VAL:CG2	2.38	0.53
1:B:230:HIS:HA	1:B:234:SER:OG	2.07	0.53
1:C:196:MET:HE2	2:C:620:HOH:O	2.07	0.53
1:C:234:SER:HB2	1:C:236:VAL:HG13	1.89	0.53
1:D:111:GLY:O	1:D:141:SER:HA	2.08	0.53
1:E:46:LEU:HD12	1:E:244:GLU:OE2	2.07	0.53
1:E:175:LEU:HD22	1:E:177:VAL:HG13	1.89	0.53
1:E:428:HIS:HB2	2:E:539:HOH:O	2.08	0.53
1:F:177:VAL:HG22	2:F:644:HOH:O	2.07	0.53
1:A:11:ILE:HG23	1:A:12:HIS:ND1	2.23	0.53
1:B:313:GLU:HG2	1:B:316:PRO:HG3	1.90	0.53
1:B:398:ILE:HD11	1:E:190:ILE:HD11	1.89	0.53
1:C:346:GLY:O	1:C:376:VAL:HG23	2.08	0.53
1:C:442:ILE:HB	2:C:547:HOH:O	2.07	0.53
1:B:132:GLY:O	1:B:261:ASN:ND2	2.41	0.53
1:C:185:VAL:O	1:F:391:ILE:HG23	2.08	0.53
1:E:47:THR:OG1	1:E:50:GLU:HG3	2.08	0.53
1:E:147:GLN:HB2	2:E:699:HOH:O	2.06	0.53
1:F:341:PRO:HB2	2:F:657:HOH:O	2.08	0.53
1:F:346:GLY:O	1:F:376:VAL:HG23	2.08	0.53
1:C:364:ASP:O	1:F:524:LYS:HD2	2.08	0.53
1:D:376:VAL:HG21	1:D:420:ALA:HB1	1.90	0.53
1:E:123:LYS:HD2	2:E:609:HOH:O	2.07	0.53
1:E:398:ILE:HG12	1:E:399:PHE:N	2.23	0.53
1:F:497:ILE:HG21	1:F:505:HIS:NE2	2.24	0.53
1:A:55:LEU:HD11	2:A:671:HOH:O	2.08	0.53
1:A:163:ASN:ND2	2:A:562:HOH:O	2.41	0.53
1:A:486:THR:HG23	2:A:598:HOH:O	2.08	0.53
1:B:469:THR:O	1:B:473:LEU:HB2	2.08	0.53
1:C:70:HIS:CE1	1:C:81:ARG:HG2	2.43	0.53
1:C:505:HIS:CA	1:C:508:ARG:HH11	2.22	0.53
1:D:176:VAL:O	1:D:196:MET:HA	2.09	0.53
1:E:67:PHE:CE2	1:F:496:VAL:HB	2.43	0.53
1:D:376:VAL:CG2	1:D:420:ALA:HB1	2.39	0.53
1:E:125:MET:HE1	1:E:163:ASN:HD21	1.74	0.53
1:F:375:ASP:OD1	1:F:414:ARG:HB3	2.08	0.53
1:C:45:LYS:HE2	1:C:200:THR:O	2.08	0.53
1:C:288:VAL:HG23	2:C:558:HOH:O	2.08	0.53
1:E:483:ASN:ND2	1:E:485:TYR:HB2	2.23	0.53
1:F:212:LYS:C	1:F:214:VAL:H	2.17	0.53
1:A:28:ALA:HB2	1:A:83:TYR:CD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:O	1:A:179:PRO:HB2	2.08	0.53
1:A:450:ALA:HB3	2:A:681:HOH:O	2.09	0.53
1:B:10:ASP:CG	1:B:11:ILE:H	2.17	0.53
1:C:324:THR:HA	1:C:336:ILE:O	2.09	0.53
1:C:530:LEU:HD21	1:F:528:ILE:HD13	1.90	0.53
2:C:650:HOH:O	1:F:149:GLY:HA2	2.08	0.53
1:E:374:VAL:HG13	1:E:424:MET:HG3	1.91	0.53
1:A:227:ALA:HB1	2:A:597:HOH:O	2.09	0.53
2:A:698:HOH:O	1:B:91:TYR:HB2	2.09	0.53
1:C:373:PHE:HA	1:C:411:VAL:O	2.08	0.53
1:C:456:ARG:NH1	1:C:456:ARG:HB3	2.23	0.53
1:D:45:LYS:HA	1:D:244:GLU:OE1	2.09	0.53
1:F:101:VAL:CG2	1:F:136:VAL:HB	2.39	0.53
1:C:475:GLN:HE22	1:C:476:GLU:HG3	1.74	0.53
1:D:459:ILE:HD11	1:D:466:ALA:O	2.08	0.53
1:E:321:ASN:OD1	1:E:321:ASN:N	2.38	0.53
1:A:510:LEU:HD23	2:A:537:HOH:O	2.09	0.52
1:B:36:ALA:CB	1:B:107:THR:HB	2.39	0.52
1:B:125:MET:SD	2:B:560:HOH:O	2.58	0.52
1:D:85:ASP:OD2	1:D:116:VAL:HB	2.09	0.52
1:E:315:GLN:N	1:E:316:PRO:HD3	2.24	0.52
1:E:319:ALA:N	1:E:320:PRO:HD3	2.25	0.52
1:A:76:GLY:HA3	2:A:673:HOH:O	2.10	0.52
1:A:164:THR:O	1:A:166:ALA:N	2.42	0.52
1:A:354:GLU:HG2	1:A:396:LYS:HD2	1.91	0.52
1:A:392:ARG:HD3	1:D:236:VAL:HG12	1.91	0.52
1:B:113:LEU:HD22	1:B:117:TYR:HE1	1.72	0.52
1:B:114:GLY:H	1:B:117:TYR:HB3	1.74	0.52
1:C:212:LYS:HG3	1:C:216:GLY:HA2	1.91	0.52
1:C:362:THR:O	1:C:366:PHE:HD2	1.92	0.52
1:E:67:PHE:HE2	1:F:496:VAL:HB	1.73	0.52
1:E:466:ALA:HB2	2:E:602:HOH:O	2.09	0.52
1:F:25:ILE:O	1:F:29:THR:HG23	2.08	0.52
1:F:45:LYS:HB3	2:F:665:HOH:O	2.09	0.52
1:A:62:VAL:HG21	1:C:508:ARG:HE	1.73	0.52
1:A:70:HIS:C	1:A:70:HIS:ND1	2.67	0.52
1:C:122:VAL:O	1:C:125:MET:N	2.42	0.52
1:C:132:GLY:C	1:C:261:ASN:HD22	2.17	0.52
1:D:205:ILE:HG22	1:D:206:THR:HG23	1.91	0.52
1:E:528:ILE:O	1:E:530:LEU:HD13	2.10	0.52
1:F:227:ALA:HB2	2:F:554:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:508:ARG:HD3	1:F:508:ARG:C	2.34	0.52
1:B:375:ASP:CG	1:B:414:ARG:HB3	2.33	0.52
1:C:236:VAL:HG12	1:F:392:ARG:HD3	1.92	0.52
1:C:525:HIS:CE1	1:F:361:ARG:HE	2.28	0.52
1:A:319:ALA:N	1:A:320:PRO:HD3	2.24	0.52
1:B:77:LEU:C	1:B:79:ALA:H	2.17	0.52
1:B:309:ALA:HA	2:B:642:HOH:O	2.10	0.52
1:C:41:HIS:O	1:C:44:GLY:N	2.35	0.52
1:D:169:VAL:HA	2:D:570:HOH:O	2.10	0.52
1:A:508:ARG:HH21	1:B:62:VAL:HG11	1.75	0.52
1:B:505:HIS:O	1:B:508:ARG:NH1	2.38	0.52
1:D:271:GLU:O	1:D:271:GLU:HG3	2.10	0.52
1:D:513:LEU:HD22	1:D:513:LEU:H	1.74	0.52
1:E:125:MET:HE1	1:E:163:ASN:ND2	2.24	0.52
1:F:46:LEU:HB3	1:F:50:GLU:OE1	2.09	0.52
1:A:328:ARG:HD3	1:A:331:GLY:O	2.10	0.52
1:A:504:ARG:HG3	2:A:531:HOH:O	2.09	0.52
1:D:295:PRO:HB2	1:D:342:MET:CE	2.40	0.52
1:F:321:ASN:OD1	1:F:321:ASN:N	2.38	0.52
1:F:323:LEU:HA	2:F:537:HOH:O	2.10	0.52
1:F:335:GLY:O	1:F:371:LEU:N	2.41	0.52
1:F:397:LEU:HD22	2:F:592:HOH:O	2.10	0.52
1:C:480:ALA:C	1:C:481:LEU:HD22	2.34	0.52
1:E:45:LYS:HG2	1:E:200:THR:HG23	1.92	0.52
1:F:91:TYR:C	1:F:91:TYR:CD1	2.86	0.52
1:F:483:ASN:HD21	1:F:485:TYR:HB2	1.74	0.52
1:A:231:ASN:HD21	1:A:239:HIS:C	2.18	0.52
1:A:495:ALA:HB1	2:A:541:HOH:O	2.10	0.52
1:B:496:VAL:HB	1:C:67:PHE:HE2	1.74	0.52
1:F:483:ASN:HB2	1:F:484:PRO:HD2	1.91	0.52
1:A:432:ASP:O	1:A:433:LEU:HD23	2.09	0.52
1:B:21:LEU:O	1:B:25:ILE:HG23	2.09	0.52
1:B:405:THR:O	1:B:516:LYS:HE2	2.10	0.52
1:C:29:THR:HA	1:C:49:ARG:NE	2.25	0.52
1:F:45:LYS:HE3	1:F:200:THR:HG22	1.92	0.52
1:F:90:GLY:HA2	2:F:551:HOH:O	2.10	0.52
1:F:427:LYS:NZ	1:F:434:ASN:OD1	2.42	0.52
1:A:156:TYR:CE1	1:A:184:ALA:HB2	2.45	0.51
1:A:380:LEU:HD23	1:A:385:GLN:CD	2.35	0.51
2:A:622:HOH:O	1:B:65:ASP:HA	2.10	0.51
1:C:116:VAL:HG23	2:C:656:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:GLN:HG2	2:C:599:HOH:O	2.11	0.51
1:D:187:SER:CB	1:D:188:PRO:HD3	2.40	0.51
1:D:291:SER:C	1:D:293:ASN:H	2.18	0.51
1:F:274:ASP:C	1:F:274:ASP:OD1	2.53	0.51
1:F:447:ALA:O	1:F:451:VAL:HG13	2.09	0.51
1:A:507:VAL:HG12	1:A:508:ARG:N	2.24	0.51
1:B:17:LYS:HB2	2:B:593:HOH:O	2.11	0.51
1:B:356:ALA:O	1:B:360:VAL:HG23	2.09	0.51
1:B:442:ILE:HG13	2:B:665:HOH:O	2.09	0.51
1:E:298:MET:HA	1:E:301:VAL:HG23	1.93	0.51
1:E:403:GLU:HG2	2:E:540:HOH:O	2.08	0.51
1:F:238:HIS:HD2	1:F:315:GLN:NE2	2.08	0.51
1:B:231:ASN:ND2	1:B:239:HIS:C	2.68	0.51
1:D:121:ILE:O	1:D:125:MET:HG3	2.10	0.51
1:D:395:ALA:O	1:D:398:ILE:HG12	2.10	0.51
1:E:473:LEU:O	1:E:474:ILE:C	2.54	0.51
1:F:472:ARG:HH12	1:F:476:GLU:CD	2.17	0.51
1:A:188:PRO:O	1:A:191:THR:OG1	2.28	0.51
1:A:398:ILE:CG2	1:A:423:VAL:HG22	2.40	0.51
1:A:509:GLY:O	1:A:513:LEU:CD2	2.56	0.51
1:B:65:ASP:CB	1:B:120:LYS:HE3	2.40	0.51
1:B:427:LYS:NZ	1:B:427:LYS:HB2	2.25	0.51
1:D:284:LEU:HD23	1:D:499:PRO:O	2.10	0.51
1:D:334:VAL:HG13	2:D:602:HOH:O	2.10	0.51
1:E:122:VAL:HG22	2:E:688:HOH:O	2.10	0.51
1:F:523:LYS:CE	2:F:688:HOH:O	2.58	0.51
1:A:483:ASN:ND2	1:A:485:TYR:HD2	2.05	0.51
1:C:71:ARG:HH22	1:C:119:GLN:HE22	1.57	0.51
1:C:150:VAL:O	1:C:151:ALA:C	2.53	0.51
1:C:470:ARG:HG3	1:C:470:ARG:NH1	2.26	0.51
1:C:497:ILE:HG23	2:C:683:HOH:O	2.10	0.51
1:E:302:ILE:CG2	1:E:336:ILE:HD13	2.41	0.51
1:E:459:ILE:HG12	1:E:470:ARG:HH21	1.76	0.51
1:F:297:ASP:HA	1:F:342:MET:HG3	1.92	0.51
1:F:427:LYS:NZ	2:F:622:HOH:O	2.43	0.51
1:A:69:ARG:CD	1:A:81:ARG:O	2.58	0.51
1:A:391:ILE:HD12	1:A:391:ILE:N	2.23	0.51
2:A:694:HOH:O	1:D:358:ARG:HD3	2.09	0.51
1:D:444:VAL:HG23	2:D:540:HOH:O	2.10	0.51
1:E:231:ASN:HD21	1:E:239:HIS:C	2.18	0.51
1:A:228:ARG:NH2	1:A:240:MET:HE1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASN:HD21	1:A:485:TYR:HB2	1.74	0.51
1:B:322:ILE:CG2	1:B:355:LYS:HD3	2.41	0.51
1:D:102:PHE:CD1	1:D:121:ILE:HG23	2.46	0.51
1:D:275:LEU:HD11	1:D:511:ARG:HH12	1.75	0.51
1:F:324:THR:HA	1:F:336:ILE:O	2.10	0.51
1:F:427:LYS:HB2	1:F:427:LYS:HZ3	1.74	0.51
1:D:65:ASP:CB	1:D:120:LYS:HE3	2.41	0.51
1:E:11:ILE:C	1:E:13:THR:H	2.18	0.51
1:E:291:SER:C	1:E:293:ASN:H	2.19	0.51
1:A:13:THR:HG22	1:C:290:ASP:CG	2.36	0.51
1:B:396:LYS:HE2	1:B:529:PRO:O	2.10	0.51
1:C:170:ILE:HD13	2:C:641:HOH:O	2.11	0.51
1:C:392:ARG:HG3	1:C:392:ARG:NH1	2.23	0.51
1:C:530:LEU:HD21	1:F:528:ILE:CD1	2.40	0.51
1:F:113:LEU:HD22	1:F:117:TYR:CD1	2.45	0.51
1:A:164:THR:O	1:A:165:HIS:C	2.54	0.51
1:A:427:LYS:NZ	1:A:434:ASN:OD1	2.42	0.51
1:A:505:HIS:C	1:A:508:ARG:HH11	2.19	0.51
1:C:364:ASP:OD2	1:C:404:ALA:HA	2.11	0.51
1:D:523:LYS:NZ	2:D:594:HOH:O	2.39	0.51
1:E:101:VAL:HG22	1:E:102:PHE:N	2.25	0.51
1:A:469:THR:O	1:A:473:LEU:HD13	2.10	0.50
1:C:103:SER:HB2	1:C:138:ILE:HD12	1.92	0.50
1:C:285:ASP:N	2:C:670:HOH:O	2.41	0.50
1:E:156:TYR:CZ	1:E:184:ALA:HB2	2.47	0.50
1:E:264:SER:HB3	2:E:600:HOH:O	2.12	0.50
1:E:395:ALA:O	1:E:396:LYS:C	2.54	0.50
1:F:55:LEU:HD12	1:F:252:LYS:HG3	1.91	0.50
1:F:56:LEU:HD12	1:F:61:PHE:HB2	1.93	0.50
1:F:224:LEU:O	1:F:229:THR:HG21	2.11	0.50
1:A:64:LEU:HD22	1:C:494:ASP:HB3	1.93	0.50
1:B:102:PHE:C	1:B:102:PHE:CD2	2.89	0.50
1:B:147:GLN:NE2	1:B:147:GLN:N	2.42	0.50
1:B:399:PHE:CE2	1:B:528:ILE:HB	2.46	0.50
1:C:407:PRO:HB3	1:C:513:LEU:HB3	1.92	0.50
1:D:319:ALA:N	1:D:320:PRO:HD3	2.27	0.50
1:E:10:ASP:CG	1:E:11:ILE:H	2.19	0.50
1:E:324:THR:HA	1:E:336:ILE:O	2.10	0.50
1:E:404:ALA:HB1	2:E:677:HOH:O	2.10	0.50
1:E:440:ALA:O	1:E:484:PRO:HD3	2.11	0.50
1:F:305:VAL:CG2	1:F:506:ILE:HD12	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:HB3	2:A:546:HOH:O	2.11	0.50
1:C:162:ARG:HG2	1:C:162:ARG:NH1	2.24	0.50
1:E:230:HIS:HA	1:E:234:SER:OG	2.11	0.50
1:F:75:PHE:CD2	1:F:75:PHE:N	2.80	0.50
1:F:301:VAL:HG21	2:F:663:HOH:O	2.12	0.50
1:F:509:GLY:O	1:F:513:LEU:HD23	2.11	0.50
1:A:349:ASP:O	1:A:350:ILE:C	2.55	0.50
1:A:392:ARG:HG3	1:A:392:ARG:NH1	2.26	0.50
1:B:435:LEU:CD2	2:B:596:HOH:O	2.58	0.50
1:C:175:LEU:HD22	1:C:177:VAL:HG13	1.93	0.50
1:C:505:HIS:C	1:C:508:ARG:HH11	2.20	0.50
1:F:238:HIS:HA	1:F:315:GLN:CG	2.41	0.50
1:A:68:ALA:HA	1:C:489:GLU:HA	1.93	0.50
1:A:258:LEU:HD12	2:A:612:HOH:O	2.12	0.50
1:A:298:MET:O	1:A:301:VAL:N	2.44	0.50
1:B:102:PHE:CD2	1:B:102:PHE:O	2.64	0.50
1:B:179:PRO:HD2	2:B:679:HOH:O	2.11	0.50
1:C:161:ARG:HD3	2:F:578:HOH:O	2.12	0.50
1:C:229:THR:HG23	2:C:595:HOH:O	2.11	0.50
2:C:658:HOH:O	1:F:527:ASN:HB3	2.12	0.50
1:D:392:ARG:HH11	1:D:392:ARG:HG3	1.76	0.50
1:D:390:ILE:HG13	2:D:640:HOH:O	2.11	0.50
1:E:490:ARG:HG2	1:E:490:ARG:HH11	1.76	0.50
1:A:374:VAL:HG12	1:A:375:ASP:N	2.26	0.50
1:E:152:SER:HA	2:E:665:HOH:O	2.10	0.50
1:E:250:TYR:O	1:E:253:GLN:N	2.44	0.50
1:B:52:ILE:N	2:B:590:HOH:O	2.43	0.50
1:B:215:THR:C	1:B:217:GLU:H	2.17	0.50
1:C:375:ASP:CG	1:C:414:ARG:HB3	2.36	0.50
1:C:475:GLN:NE2	1:C:476:GLU:HG3	2.27	0.50
1:D:389:GLY:O	1:D:390:ILE:C	2.55	0.50
1:D:438:PRO:HG3	1:F:21:LEU:HD22	1.94	0.50
1:A:121:ILE:O	1:A:124:VAL:HG22	2.12	0.50
1:A:202:HIS:HD2	1:A:222:GLU:HA	1.76	0.50
1:B:111:GLY:HA3	2:B:675:HOH:O	2.10	0.50
1:B:212:LYS:C	1:B:214:VAL:H	2.20	0.50
1:B:247:ALA:O	1:B:250:TYR:N	2.45	0.50
1:C:161:ARG:O	1:C:162:ARG:C	2.55	0.50
1:C:211:ILE:CG2	1:C:217:GLU:HB2	2.41	0.50
1:C:454:LEU:HD13	1:F:75:PHE:CE1	2.47	0.50
1:D:197:VAL:HB	1:D:200:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ALA:HB3	2:D:672:HOH:O	2.10	0.50
1:F:408:LEU:HB2	1:F:431:ALA:HA	1.94	0.50
1:A:29:THR:HG23	2:A:641:HOH:O	2.12	0.49
1:A:122:VAL:HG22	2:A:583:HOH:O	2.11	0.49
1:A:391:ILE:H	1:A:391:ILE:CD1	2.24	0.49
1:A:453:ILE:HD12	1:A:453:ILE:N	2.26	0.49
1:C:89:THR:HA	2:C:707:HOH:O	2.12	0.49
1:D:231:ASN:HD21	1:D:239:HIS:CA	2.24	0.49
1:E:173:ILE:HD11	2:E:632:HOH:O	2.12	0.49
1:E:520:LEU:HD12	1:E:520:LEU:N	2.27	0.49
1:A:296:TYR:N	1:A:342:MET:HE3	2.27	0.49
1:B:150:VAL:HG23	2:B:624:HOH:O	2.12	0.49
1:B:173:ILE:HD13	1:B:251:VAL:HG23	1.94	0.49
1:B:350:ILE:HG21	1:B:393:ARG:NH2	2.27	0.49
1:B:355:LYS:HD2	2:B:625:HOH:O	2.12	0.49
1:B:494:ASP:HA	2:C:696:HOH:O	2.11	0.49
2:B:611:HOH:O	1:E:530:LEU:HG	2.10	0.49
1:C:184:ALA:C	1:C:186:TYR:H	2.19	0.49
1:C:493:VAL:HA	2:C:690:HOH:O	2.13	0.49
1:E:61:PHE:CE2	1:E:63:GLU:HB2	2.47	0.49
1:F:35:ARG:HH21	1:F:39:LYS:NZ	2.10	0.49
1:A:14:THR:HG23	1:C:439:THR:HG21	1.93	0.49
1:B:483:ASN:HD22	1:B:485:TYR:N	2.09	0.49
1:C:63:GLU:HG3	1:C:64:LEU:N	2.26	0.49
1:C:374:VAL:HG22	1:C:424:MET:HB3	1.94	0.49
1:D:508:ARG:NE	1:F:91:TYR:OH	2.45	0.49
1:E:175:LEU:HD21	1:E:247:ALA:HB1	1.94	0.49
1:E:337:VAL:O	1:E:372:THR:HA	2.12	0.49
1:A:91:TYR:HD1	1:A:92:GLY:N	2.10	0.49
1:A:513:LEU:N	1:A:513:LEU:CD2	2.74	0.49
1:B:89:THR:HB	1:B:124:VAL:CG2	2.38	0.49
1:B:166:ALA:C	2:E:599:HOH:O	2.54	0.49
1:B:360:VAL:HB	1:B:400:ALA:HB1	1.94	0.49
1:C:373:PHE:HD2	1:C:411:VAL:HB	1.77	0.49
1:D:55:LEU:HD21	1:D:136:VAL:HG11	1.93	0.49
1:D:262:ASN:ND2	2:D:570:HOH:O	2.45	0.49
1:D:296:TYR:O	1:D:342:MET:HE3	2.12	0.49
1:D:302:ILE:HA	2:D:639:HOH:O	2.11	0.49
1:D:491:GLY:O	1:D:492:TYR:C	2.56	0.49
1:D:503:ARG:HG2	1:D:503:ARG:HH11	1.77	0.49
1:B:161:ARG:HD2	2:B:598:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASP:HB3	2:B:587:HOH:O	2.13	0.49
1:B:268:ALA:CB	1:B:332:ARG:HG2	2.42	0.49
1:B:336:ILE:HD12	1:B:336:ILE:N	2.28	0.49
1:C:113:LEU:HD22	1:C:117:TYR:CD1	2.47	0.49
1:C:495:ALA:HB3	2:C:683:HOH:O	2.12	0.49
1:D:221:PHE:O	1:D:224:LEU:HB3	2.12	0.49
1:D:335:GLY:O	1:D:371:LEU:N	2.45	0.49
1:E:62:VAL:HG11	1:F:508:ARG:NH2	2.18	0.49
1:E:65:ASP:HB2	1:E:120:LYS:HE3	1.94	0.49
1:E:177:VAL:CA	1:E:201:SER:HB3	2.42	0.49
1:F:497:ILE:HG21	1:F:505:HIS:CE1	2.48	0.49
1:A:48:ALA:O	1:A:51:ARG:HB2	2.12	0.49
1:A:411:VAL:C	2:A:636:HOH:O	2.55	0.49
1:A:438:PRO:HG3	1:B:21:LEU:HD22	1.93	0.49
1:A:196:MET:HE1	1:A:203:MET:HG3	1.94	0.49
1:A:280:GLU:OE2	1:A:280:GLU:N	2.43	0.49
1:A:377:PRO:HG2	1:A:378:GLY:H	1.78	0.49
1:B:47:THR:OG1	1:B:50:GLU:HG3	2.13	0.49
1:B:90:GLY:N	2:B:606:HOH:O	2.46	0.49
1:B:300:SER:O	1:B:304:HIS:ND1	2.46	0.49
1:B:339:ASN:HB2	2:B:696:HOH:O	2.12	0.49
1:C:73:THR:HG22	1:C:78:ASP:HB3	1.95	0.49
1:C:399:PHE:CZ	1:F:164:THR:HG23	2.47	0.49
1:C:418:GLY:HA2	1:F:153:LEU:HD11	1.94	0.49
1:D:185:VAL:HG21	1:D:205:ILE:HG12	1.95	0.49
1:E:273:ALA:O	1:E:275:LEU:HD22	2.13	0.49
1:E:460:ALA:HA	2:E:680:HOH:O	2.11	0.49
1:F:11:ILE:O	1:F:11:ILE:HG13	2.13	0.49
1:A:347:CYS:SG	1:A:377:PRO:HG2	2.53	0.49
1:C:70:HIS:HB3	1:C:85:ASP:OD1	2.13	0.49
1:C:505:HIS:ND1	1:C:508:ARG:NH1	2.60	0.49
1:D:13:THR:HB	1:E:290:ASP:OD1	2.13	0.49
1:D:407:PRO:HB3	1:D:513:LEU:HB3	1.95	0.49
1:D:489:GLU:HA	1:F:68:ALA:HA	1.93	0.49
1:E:121:ILE:O	1:E:124:VAL:HG22	2.12	0.49
1:E:376:VAL:N	1:E:415:LYS:HB2	2.28	0.49
1:E:407:PRO:HB3	1:E:513:LEU:HB3	1.94	0.49
1:F:124:VAL:HB	2:F:565:HOH:O	2.12	0.49
1:F:287:ILE:HG23	1:F:288:VAL:N	2.27	0.49
1:B:399:PHE:CE1	1:E:164:THR:HG23	2.48	0.49
1:C:525:HIS:ND1	1:F:361:ARG:NH2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:HD12	1:D:61:PHE:HB2	1.94	0.49
1:E:55:LEU:HD21	1:E:136:VAL:HG21	1.94	0.49
1:E:145:ARG:HD2	1:E:148:GLU:OE2	2.13	0.49
1:E:181:ALA:HA	1:E:204:PHE:O	2.13	0.49
1:E:485:TYR:HA	1:E:488:ALA:HB3	1.93	0.49
1:A:124:VAL:HG21	2:A:546:HOH:O	2.11	0.49
1:A:389:GLY:HA2	2:A:650:HOH:O	2.13	0.49
1:B:484:PRO:HB2	2:B:662:HOH:O	2.12	0.49
1:C:524:LYS:HD3	1:F:405:THR:OG1	2.13	0.49
1:D:475:GLN:HA	1:D:478:GLU:OE1	2.12	0.49
1:E:150:VAL:HG23	2:E:596:HOH:O	2.13	0.49
1:F:208:PRO:HG2	1:F:221:PHE:CE1	2.47	0.49
1:A:262:ASN:C	1:A:262:ASN:OD1	2.56	0.48
2:A:589:HOH:O	1:C:495:ALA:HA	2.13	0.48
1:B:403:GLU:HG2	2:B:537:HOH:O	2.12	0.48
1:C:415:LYS:HD3	1:C:417:PHE:HE2	1.77	0.48
1:D:291:SER:C	1:D:293:ASN:N	2.70	0.48
1:D:397:LEU:HD23	1:D:401:TYR:HD2	1.78	0.48
1:D:449:GLY:O	1:D:453:ILE:HD13	2.12	0.48
1:E:302:ILE:HG23	1:E:336:ILE:HD13	1.95	0.48
1:E:312:PHE:HZ	2:E:700:HOH:O	1.95	0.48
1:E:372:THR:CG2	2:E:544:HOH:O	2.60	0.48
1:E:411:VAL:HG22	1:E:435:LEU:HD23	1.94	0.48
1:A:129:LEU:HD13	1:A:166:ALA:HB2	1.95	0.48
1:B:383:VAL:HG21	1:E:219:VAL:HG11	1.95	0.48
1:C:339:ASN:HB3	2:C:543:HOH:O	2.13	0.48
1:D:46:LEU:HB2	1:D:51:ARG:HD2	1.95	0.48
1:D:115:GLU:HB2	1:D:148:GLU:OE1	2.12	0.48
1:D:299:HIS:O	1:D:303:GLU:HG3	2.13	0.48
1:E:63:GLU:HG2	1:E:66:GLU:HB2	1.94	0.48
1:E:507:VAL:HG12	1:E:508:ARG:N	2.26	0.48
1:F:187:SER:HB3	1:F:188:PRO:CD	2.31	0.48
1:F:391:ILE:HA	2:F:709:HOH:O	2.12	0.48
1:A:398:ILE:HD12	1:D:160:PHE:CB	2.42	0.48
1:A:498:MET:C	1:A:500:SER:N	2.69	0.48
1:B:473:LEU:HA	1:B:476:GLU:OE1	2.13	0.48
1:B:505:HIS:HA	1:B:508:ARG:HD2	1.95	0.48
1:C:101:VAL:HG22	1:C:102:PHE:N	2.28	0.48
1:C:349:ASP:OD2	1:C:351:THR:OG1	2.30	0.48
1:D:254:LEU:HD13	1:D:312:PHE:HE2	1.78	0.48
1:D:427:LYS:HB2	1:D:427:LYS:HZ2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ARG:NH2	1:E:244:GLU:OE1	2.41	0.48
1:E:326:PHE:HA	2:E:612:HOH:O	2.14	0.48
1:F:510:LEU:O	1:F:511:ARG:C	2.55	0.48
1:A:35:ARG:HB3	1:A:35:ARG:HH11	1.77	0.48
1:B:56:LEU:HD12	1:B:61:PHE:HB2	1.96	0.48
1:C:174:SER:OG	1:C:191:THR:HG21	2.13	0.48
1:A:195:VAL:HG23	2:A:683:HOH:O	2.14	0.48
1:B:208:PRO:HG3	1:B:224:LEU:HD22	1.95	0.48
1:D:395:ALA:O	1:D:396:LYS:C	2.54	0.48
1:E:146:ILE:H	1:E:146:ILE:CD1	2.16	0.48
1:F:113:LEU:C	1:F:113:LEU:HD13	2.39	0.48
1:B:122:VAL:C	1:B:124:VAL:N	2.69	0.48
1:B:318:PHE:O	1:B:319:ALA:C	2.56	0.48
1:B:374:VAL:HG11	2:B:629:HOH:O	2.13	0.48
1:D:224:LEU:O	1:D:229:THR:HG21	2.13	0.48
1:E:24:ARG:HD3	1:F:485:TYR:CE1	2.49	0.48
1:F:392:ARG:HG3	1:F:392:ARG:NH1	2.26	0.48
1:A:155:ALA:O	1:A:156:TYR:C	2.56	0.48
1:B:308:ASP:O	1:B:309:ALA:HB3	2.14	0.48
1:B:509:GLY:O	1:B:513:LEU:CD2	2.61	0.48
1:B:509:GLY:O	1:B:513:LEU:HD22	2.13	0.48
1:C:489:GLU:HB3	2:C:532:HOH:O	2.12	0.48
1:C:508:ARG:HD3	1:C:508:ARG:C	2.38	0.48
1:D:509:GLY:O	1:D:513:LEU:CD2	2.60	0.48
1:E:64:LEU:HD22	1:F:494:ASP:HB3	1.95	0.48
1:E:69:ARG:HB2	1:F:489:GLU:HG2	1.95	0.48
1:E:324:THR:HB	1:E:359:PHE:CD2	2.49	0.48
1:E:367:ASN:N	1:E:367:ASN:ND2	2.61	0.48
1:E:427:LYS:HB2	1:E:434:ASN:OD1	2.14	0.48
1:F:173:ILE:HG21	1:F:251:VAL:CG2	2.37	0.48
1:B:234:SER:HB2	1:B:236:VAL:HG13	1.95	0.48
1:B:346:GLY:HA3	2:B:628:HOH:O	2.12	0.48
1:D:47:THR:HG23	1:D:50:GLU:CD	2.39	0.48
1:D:73:THR:HA	1:D:78:ASP:OD1	2.12	0.48
1:D:386:GLU:C	1:D:388:ASP:H	2.20	0.48
1:E:62:VAL:O	1:E:62:VAL:HG12	2.12	0.48
1:E:177:VAL:C	1:E:201:SER:HB3	2.39	0.48
1:F:33:SER:HB2	1:F:36:ALA:HB2	1.96	0.48
1:F:414:ARG:HG2	1:F:414:ARG:NH1	2.29	0.48
1:F:460:ALA:HA	2:F:697:HOH:O	2.12	0.48
1:F:468:ALA:O	1:F:472:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:528:ILE:O	1:F:530:LEU:HD13	2.14	0.48
1:C:231:ASN:HD21	1:C:239:HIS:C	2.22	0.48
1:C:320:PRO:O	1:C:343:GLN:HG3	2.14	0.48
1:D:425:GLY:O	1:D:431:ALA:HB2	2.13	0.48
1:E:376:VAL:HG13	1:E:376:VAL:O	2.12	0.48
1:A:160:PHE:HA	2:A:562:HOH:O	2.13	0.48
1:A:288:VAL:O	1:B:14:THR:OG1	2.32	0.48
1:B:299:HIS:HD2	2:B:677:HOH:O	1.96	0.48
1:E:155:ALA:HB3	2:E:665:HOH:O	2.14	0.48
1:E:250:TYR:O	1:E:251:VAL:C	2.56	0.48
1:E:508:ARG:HD3	1:E:508:ARG:C	2.37	0.48
1:A:406:VAL:HG12	2:A:643:HOH:O	2.12	0.47
1:B:387:HIS:O	1:E:233:THR:HG22	2.14	0.47
2:B:561:HOH:O	1:C:65:ASP:HA	2.14	0.47
1:C:318:PHE:CE1	1:C:351:THR:HG22	2.49	0.47
1:D:158:GLU:OE2	1:D:161:ARG:NH2	2.47	0.47
1:F:75:PHE:N	1:F:75:PHE:HD2	2.12	0.47
1:F:182:GLY:O	1:F:185:VAL:HG22	2.14	0.47
1:A:135:VAL:HG13	2:A:701:HOH:O	2.14	0.47
1:D:145:ARG:HG2	2:D:655:HOH:O	2.13	0.47
1:E:21:LEU:HD22	1:F:438:PRO:HG3	1.96	0.47
1:E:35:ARG:O	1:E:39:LYS:HG3	2.14	0.47
1:E:118:GLY:O	1:E:121:ILE:N	2.47	0.47
1:F:23:ARG:O	1:F:27:GLU:HG3	2.14	0.47
1:F:70:HIS:C	1:F:70:HIS:ND1	2.72	0.47
1:F:291:SER:C	1:F:293:ASN:H	2.22	0.47
1:A:131:THR:O	1:C:515:THR:OG1	2.26	0.47
1:A:160:PHE:CE2	1:D:422:ILE:HG21	2.50	0.47
1:B:118:GLY:HA3	1:B:155:ALA:HB1	1.96	0.47
1:B:389:GLY:O	1:B:390:ILE:C	2.57	0.47
1:C:154:GLY:O	1:C:155:ALA:C	2.58	0.47
1:C:259:PRO:HD3	2:C:550:HOH:O	2.13	0.47
1:C:374:VAL:HB	1:C:412:ILE:HG12	1.96	0.47
1:D:71:ARG:HD3	2:E:668:HOH:O	2.14	0.47
1:D:122:VAL:O	1:D:123:LYS:C	2.56	0.47
1:D:302:ILE:O	1:D:305:VAL:HG22	2.14	0.47
1:E:322:ILE:HD12	2:E:658:HOH:O	2.13	0.47
1:E:436:ALA:O	1:E:496:VAL:HA	2.14	0.47
1:A:75:PHE:CE2	1:D:454:LEU:HD13	2.49	0.47
1:A:512:GLN:NE2	2:A:698:HOH:O	2.46	0.47
1:A:527:ASN:O	1:A:527:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:VAL:HG22	2:D:602:HOH:O	2.14	0.47
1:E:364:ASP:OD2	1:E:404:ALA:HA	2.14	0.47
1:E:528:ILE:HG21	2:E:579:HOH:O	2.13	0.47
1:F:451:VAL:HG21	1:F:474:ILE:CG1	2.42	0.47
1:A:377:PRO:HD3	2:A:534:HOH:O	2.15	0.47
1:A:508:ARG:CZ	1:B:91:TYR:OH	2.63	0.47
1:B:427:LYS:HB2	1:B:434:ASN:OD1	2.13	0.47
1:E:299:HIS:O	1:E:303:GLU:HG3	2.14	0.47
1:E:505:HIS:HA	1:E:508:ARG:CD	2.43	0.47
1:A:89:THR:HB	1:A:124:VAL:HG11	1.97	0.47
1:A:176:VAL:HB	1:A:196:MET:HB3	1.97	0.47
1:A:527:ASN:HD21	1:D:358:ARG:HD3	1.78	0.47
1:B:70:HIS:HE1	1:B:81:ARG:HG2	1.80	0.47
1:B:444:VAL:HA	1:E:153:LEU:HD11	1.95	0.47
1:C:55:LEU:HA	2:C:666:HOH:O	2.14	0.47
1:E:24:ARG:NH1	1:E:24:ARG:HG2	2.30	0.47
1:F:345:ALA:HB1	2:F:626:HOH:O	2.15	0.47
1:A:170:ILE:HG13	1:A:170:ILE:O	2.15	0.47
1:A:379:PHE:O	1:A:380:LEU:C	2.57	0.47
1:A:397:LEU:HD22	1:A:401:TYR:CE2	2.50	0.47
1:C:51:ARG:HH12	1:C:140:ASP:CB	2.27	0.47
1:C:111:GLY:O	1:C:141:SER:HB2	2.15	0.47
1:C:175:LEU:CD2	1:C:177:VAL:HG13	2.45	0.47
1:C:203:MET:CE	1:F:391:ILE:HG21	2.44	0.47
1:C:239:HIS:HA	2:C:601:HOH:O	2.15	0.47
1:C:284:LEU:CD1	1:C:304:HIS:CD2	2.97	0.47
1:D:45:LYS:HD2	2:D:567:HOH:O	2.13	0.47
1:D:115:GLU:O	1:D:119:GLN:HG3	2.15	0.47
1:D:272:GLU:HG2	2:D:600:HOH:O	2.14	0.47
1:D:291:SER:O	1:D:293:ASN:N	2.47	0.47
1:E:162:ARG:HH11	1:E:162:ARG:HG2	1.79	0.47
1:F:177:VAL:HG12	1:F:197:VAL:HG21	1.95	0.47
1:F:198:ASP:HB2	1:F:240:MET:CE	2.44	0.47
1:F:291:SER:C	1:F:293:ASN:N	2.72	0.47
1:A:185:VAL:O	1:A:188:PRO:HD2	2.15	0.47
1:B:322:ILE:HG23	1:B:355:LYS:HD3	1.97	0.47
1:C:47:THR:O	1:C:51:ARG:HG3	2.15	0.47
1:C:173:ILE:HG21	1:C:251:VAL:CG2	2.34	0.47
1:C:302:ILE:O	1:C:305:VAL:HG22	2.15	0.47
1:C:490:ARG:HH12	1:F:151:ALA:HB2	1.80	0.47
1:D:91:TYR:OH	1:E:508:ARG:CZ	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:PHE:HB2	2:D:607:HOH:O	2.15	0.47
1:E:68:ALA:HA	1:F:489:GLU:HA	1.97	0.47
1:E:298:MET:O	1:E:299:HIS:C	2.58	0.47
1:B:448:GLN:HA	1:B:474:ILE:HD13	1.95	0.47
1:C:422:ILE:HD11	1:F:153:LEU:O	2.15	0.47
1:C:452:ASN:HD22	1:C:452:ASN:N	2.12	0.47
1:E:432:ASP:HB2	1:E:513:LEU:HD21	1.97	0.47
1:F:163:ASN:N	2:F:630:HOH:O	2.47	0.47
1:F:521:PRO:HD2	2:F:688:HOH:O	2.15	0.47
1:B:45:LYS:CE	1:B:200:THR:HG22	2.45	0.47
1:B:350:ILE:HG21	1:B:393:ARG:CZ	2.45	0.47
1:B:483:ASN:HB2	1:B:484:PRO:HD2	1.96	0.47
1:C:195:VAL:HG23	1:C:239:HIS:HB3	1.96	0.47
1:C:230:HIS:HA	1:C:234:SER:OG	2.14	0.47
1:D:89:THR:HB	1:D:124:VAL:CG2	2.40	0.47
1:E:284:LEU:O	1:E:287:ILE:HG22	2.15	0.47
1:E:322:ILE:HG23	1:E:355:LYS:HD3	1.96	0.47
1:F:396:LYS:HD3	2:F:594:HOH:O	2.14	0.47
1:F:459:ILE:HD11	1:F:470:ARG:HB2	1.96	0.47
1:A:10:ASP:HB3	1:A:13:THR:OG1	2.15	0.46
1:C:36:ALA:O	1:C:39:LYS:HB2	2.15	0.46
1:C:65:ASP:HB3	1:C:68:ALA:HB2	1.97	0.46
1:C:392:ARG:HD3	1:F:236:VAL:HG12	1.96	0.46
1:D:419:GLY:O	1:D:420:ALA:C	2.58	0.46
1:E:339:ASN:O	1:E:341:PRO:HD3	2.15	0.46
1:E:462:ALA:C	1:E:464:ASP:N	2.72	0.46
1:F:190:ILE:O	1:F:191:THR:C	2.59	0.46
1:A:499:PRO:N	2:A:690:HOH:O	2.47	0.46
1:A:502:THR:O	1:A:506:ILE:HG13	2.15	0.46
1:A:508:ARG:CZ	1:B:62:VAL:HG11	2.44	0.46
1:B:46:LEU:HB3	1:B:50:GLU:HB2	1.97	0.46
1:C:77:LEU:HD11	1:C:147:GLN:HB2	1.96	0.46
1:C:187:SER:CB	1:C:188:PRO:HD3	2.41	0.46
1:C:529:PRO:CG	1:F:190:ILE:HA	2.44	0.46
1:D:91:TYR:C	1:D:91:TYR:CD1	2.93	0.46
1:E:135:VAL:HG13	2:E:557:HOH:O	2.13	0.46
1:E:160:PHE:O	1:E:163:ASN:HB2	2.15	0.46
1:F:231:ASN:HD21	1:F:239:HIS:C	2.23	0.46
1:F:398:ILE:HG13	1:F:429:LEU:CD2	2.36	0.46
1:A:498:MET:O	1:A:500:SER:N	2.49	0.46
1:B:497:ILE:HD12	2:B:600:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:PHE:CD2	1:C:411:VAL:HB	2.50	0.46
1:C:380:LEU:HD23	1:C:385:GLN:CD	2.40	0.46
1:C:381:PRO:HA	1:F:206:THR:HG21	1.97	0.46
1:D:122:VAL:O	1:D:124:VAL:N	2.49	0.46
1:D:176:VAL:HG12	1:D:201:SER:HB2	1.97	0.46
1:D:180:CYS:O	1:D:203:MET:HA	2.15	0.46
1:E:415:LYS:HD3	1:E:417:PHE:HE2	1.80	0.46
1:A:62:VAL:HG11	1:C:508:ARG:CZ	2.46	0.46
1:A:162:ARG:HH11	1:A:162:ARG:CG	2.24	0.46
1:A:374:VAL:HG23	2:A:636:HOH:O	2.16	0.46
1:B:444:VAL:HB	1:E:149:GLY:C	2.41	0.46
1:E:277:VAL:HG23	1:E:277:VAL:O	2.15	0.46
1:F:325:GLY:O	1:F:359:PHE:HZ	1.98	0.46
1:F:380:LEU:HD23	1:F:380:LEU:C	2.41	0.46
1:A:234:SER:HB2	1:A:236:VAL:HG13	1.98	0.46
1:A:494:ASP:HB3	1:B:64:LEU:CD2	2.43	0.46
1:A:504:ARG:NH2	2:A:556:HOH:O	2.48	0.46
1:A:508:ARG:C	1:A:508:ARG:CD	2.87	0.46
1:B:157:GLY:C	1:B:159:ILE:N	2.73	0.46
1:C:55:LEU:HD13	1:C:248:VAL:HG13	1.97	0.46
1:D:220:GLY:O	1:D:221:PHE:C	2.58	0.46
1:D:398:ILE:HG22	1:D:423:VAL:HG22	1.97	0.46
1:F:205:ILE:O	1:F:205:ILE:HD13	2.14	0.46
1:F:397:LEU:HB3	2:F:592:HOH:O	2.15	0.46
1:A:150:VAL:O	1:A:151:ALA:C	2.59	0.46
1:A:271:GLU:O	1:A:272:GLU:C	2.59	0.46
1:B:28:ALA:C	1:B:30:HIS:H	2.23	0.46
1:B:273:ALA:N	1:B:330:GLU:OE1	2.48	0.46
1:B:350:ILE:HG13	1:B:390:ILE:HD13	1.97	0.46
1:C:89:THR:HB	1:C:124:VAL:CG2	2.42	0.46
1:D:334:VAL:N	2:D:602:HOH:O	2.48	0.46
1:D:336:ILE:HA	1:D:371:LEU:O	2.15	0.46
1:D:508:ARG:NE	1:F:62:VAL:HG21	2.31	0.46
1:E:455:HIS:C	1:E:457:ARG:N	2.72	0.46
1:F:339:ASN:OD1	1:F:376:VAL:HB	2.16	0.46
1:A:24:ARG:C	1:A:26:GLU:N	2.73	0.46
1:A:167:SER:HA	2:A:532:HOH:O	2.16	0.46
1:A:376:VAL:HA	2:A:534:HOH:O	2.15	0.46
1:B:121:ILE:O	1:B:125:MET:HG3	2.16	0.46
1:B:361:ARG:HB2	2:E:584:HOH:O	2.16	0.46
1:C:457:ARG:HH11	1:C:457:ARG:HG3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:N	1:D:244:GLU:OE1	2.49	0.46
1:E:55:LEU:CD2	1:E:136:VAL:HG11	2.46	0.46
1:E:180:CYS:HB3	1:E:203:MET:HG2	1.98	0.46
1:F:132:GLY:O	1:F:261:ASN:ND2	2.47	0.46
1:F:202:HIS:HA	1:F:225:GLY:O	2.15	0.46
1:F:302:ILE:HD11	2:F:613:HOH:O	2.15	0.46
1:A:70:HIS:NE2	1:A:77:LEU:HD23	2.31	0.46
1:A:462:ALA:O	1:A:466:ALA:HB2	2.16	0.46
1:A:508:ARG:HG3	1:B:62:VAL:HG21	1.98	0.46
1:B:490:ARG:NH2	1:C:71:ARG:HD3	2.30	0.46
1:F:111:GLY:O	1:F:141:SER:CB	2.63	0.46
1:F:483:ASN:ND2	1:F:485:TYR:H	2.14	0.46
1:A:114:GLY:H	1:A:117:TYR:HB3	1.81	0.46
1:A:437:TRP:CD1	2:A:690:HOH:O	2.69	0.46
1:B:322:ILE:HG23	1:B:322:ILE:O	2.15	0.46
1:B:490:ARG:HH21	1:C:71:ARG:HD3	1.81	0.46
1:C:298:MET:O	1:C:301:VAL:N	2.49	0.46
1:C:445:MET:HA	2:C:561:HOH:O	2.16	0.46
1:C:483:ASN:HB2	1:C:484:PRO:HD2	1.98	0.46
1:D:440:ALA:O	1:D:484:PRO:HD3	2.15	0.46
1:D:530:LEU:HD22	1:D:530:LEU:N	2.31	0.46
1:F:85:ASP:CG	1:F:85:ASP:O	2.59	0.46
1:F:257:TYR:CE1	1:F:328:ARG:NH1	2.84	0.46
1:F:291:SER:O	1:F:293:ASN:N	2.49	0.46
1:F:419:GLY:O	1:F:423:VAL:HG23	2.16	0.46
1:F:437:TRP:HD1	2:F:687:HOH:O	1.99	0.46
1:F:512:GLN:HE21	1:F:512:GLN:HB3	1.56	0.46
1:B:397:LEU:HB3	1:B:423:VAL:HG13	1.98	0.46
1:C:186:TYR:CD1	1:F:395:ALA:HB2	2.50	0.46
1:C:364:ASP:CG	1:C:404:ALA:HA	2.40	0.46
1:C:379:PHE:HZ	1:C:423:VAL:HG21	1.81	0.46
1:E:47:THR:HG23	1:E:50:GLU:OE1	2.16	0.46
1:E:257:TYR:CE1	1:E:328:ARG:NH1	2.84	0.46
1:F:122:VAL:HG11	1:F:162:ARG:HH21	1.80	0.46
1:F:505:HIS:O	1:F:508:ARG:HD3	2.16	0.46
1:F:511:ARG:HG2	2:F:596:HOH:O	2.16	0.46
1:A:55:LEU:HD21	1:A:136:VAL:HG11	1.98	0.45
1:A:161:ARG:HH11	1:A:161:ARG:HG3	1.81	0.45
1:A:513:LEU:HB2	2:A:537:HOH:O	2.16	0.45
1:B:448:GLN:HA	1:B:474:ILE:CD1	2.46	0.45
1:B:474:ILE:O	1:B:478:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ARG:HB3	1:C:456:ARG:CZ	2.46	0.45
1:D:13:THR:O	1:D:17:LYS:HG3	2.16	0.45
1:D:295:PRO:HB2	1:D:342:MET:HE1	1.98	0.45
1:D:317:LEU:O	1:D:320:PRO:HG3	2.17	0.45
1:E:55:LEU:HD13	1:E:248:VAL:HG13	1.97	0.45
1:E:199:GLN:HG3	1:E:222:GLU:OE1	2.16	0.45
1:F:352:ALA:HB3	2:F:561:HOH:O	2.15	0.45
1:A:199:GLN:HA	1:A:222:GLU:OE1	2.16	0.45
1:B:14:THR:O	1:B:15:ALA:C	2.58	0.45
1:C:22:ARG:O	1:C:25:ILE:HG12	2.16	0.45
1:C:40:GLN:O	1:C:41:HIS:C	2.59	0.45
1:C:208:PRO:HG3	1:C:224:LEU:CD2	2.42	0.45
1:C:229:THR:O	1:C:233:THR:HB	2.16	0.45
1:C:377:PRO:HG2	1:C:378:GLY:H	1.81	0.45
1:D:321:ASN:OD1	1:D:321:ASN:N	2.41	0.45
1:D:375:ASP:OD1	1:D:414:ARG:HB3	2.15	0.45
1:D:478:GLU:C	1:D:480:ALA:H	2.23	0.45
1:F:160:PHE:CZ	1:F:186:TYR:HB2	2.51	0.45
1:F:398:ILE:HD11	1:F:429:LEU:HD11	1.99	0.45
1:F:423:VAL:HG13	2:F:592:HOH:O	2.15	0.45
1:F:493:VAL:HA	2:F:622:HOH:O	2.15	0.45
1:A:146:ILE:HD12	1:A:146:ILE:N	2.18	0.45
1:A:180:CYS:HB3	1:A:203:MET:HG2	1.99	0.45
1:A:185:VAL:HG22	2:A:548:HOH:O	2.16	0.45
1:A:397:LEU:HD13	1:A:423:VAL:CG1	2.45	0.45
1:C:41:HIS:HE1	1:C:50:GLU:OE1	1.99	0.45
1:C:146:ILE:HG22	1:F:454:LEU:HD21	1.96	0.45
1:D:99:VAL:HG22	2:D:603:HOH:O	2.16	0.45
1:E:20:ASP:O	1:E:23:ARG:HB3	2.17	0.45
1:E:45:LYS:HG2	1:E:200:THR:CG2	2.46	0.45
1:E:306:LEU:HD11	1:E:336:ILE:CD1	2.47	0.45
1:E:374:VAL:HB	2:E:627:HOH:O	2.15	0.45
1:F:21:LEU:O	1:F:25:ILE:HG23	2.17	0.45
1:A:25:ILE:O	1:A:29:THR:HG23	2.17	0.45
1:A:386:GLU:OE1	1:A:391:ILE:HD11	2.17	0.45
1:B:91:TYR:CD1	1:B:91:TYR:C	2.94	0.45
1:B:508:ARG:C	1:B:508:ARG:CD	2.89	0.45
1:C:198:ASP:HB2	1:C:240:MET:HG2	1.97	0.45
1:C:354:GLU:HG2	1:C:396:LYS:HD2	1.99	0.45
1:C:376:VAL:O	1:C:415:LYS:HB3	2.17	0.45
1:C:422:ILE:O	1:C:423:VAL:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:LEU:HD12	1:C:520:LEU:N	2.30	0.45
1:E:178:GLY:N	1:E:201:SER:HB3	2.31	0.45
1:E:344:PHE:CD1	1:E:344:PHE:N	2.84	0.45
1:F:113:LEU:HD13	1:F:114:GLY:N	2.32	0.45
1:F:176:VAL:O	1:F:196:MET:HA	2.16	0.45
1:B:24:ARG:HD3	1:B:83:TYR:OH	2.16	0.45
1:B:236:VAL:HG23	1:B:237:ALA:N	2.30	0.45
1:C:277:VAL:HA	2:C:712:HOH:O	2.17	0.45
1:C:504:ARG:NH2	2:C:669:HOH:O	2.50	0.45
1:C:521:PRO:HB2	1:F:169:VAL:HG21	1.98	0.45
1:D:250:TYR:OH	1:D:314:THR:HG22	2.17	0.45
1:D:306:LEU:HD13	1:D:327:GLY:HA3	1.98	0.45
1:D:397:LEU:HD21	1:D:401:TYR:HE2	1.82	0.45
1:E:275:LEU:HD22	1:E:275:LEU:N	2.31	0.45
1:F:234:SER:CB	1:F:236:VAL:HG13	2.45	0.45
1:F:349:ASP:OD1	1:F:349:ASP:N	2.49	0.45
1:F:359:PHE:O	1:F:360:VAL:C	2.58	0.45
1:A:91:TYR:HH	1:C:508:ARG:NE	2.15	0.45
1:A:104:GLN:OE1	1:A:140:ASP:N	2.47	0.45
1:A:372:THR:HG21	1:A:401:TYR:OH	2.17	0.45
1:A:494:ASP:O	1:A:495:ALA:HB2	2.17	0.45
1:B:307:ASP:CG	1:B:330:GLU:H	2.24	0.45
1:C:251:VAL:HG13	1:C:252:LYS:N	2.32	0.45
1:C:379:PHE:O	1:C:381:PRO:HD3	2.16	0.45
1:E:70:HIS:CE1	1:E:78:ASP:HA	2.52	0.45
1:E:113:LEU:HD13	1:E:117:TYR:HD1	1.78	0.45
1:F:48:ALA:C	1:F:50:GLU:N	2.74	0.45
1:F:48:ALA:O	1:F:50:GLU:N	2.49	0.45
1:F:122:VAL:O	1:F:123:LYS:C	2.57	0.45
1:F:284:LEU:O	1:F:287:ILE:HG22	2.16	0.45
1:A:193:PHE:HA	1:A:238:HIS:CE1	2.52	0.45
1:B:129:LEU:HA	1:B:170:ILE:HD13	1.99	0.45
1:B:508:ARG:NE	1:C:62:VAL:HG11	2.32	0.45
1:C:118:GLY:HA3	1:C:155:ALA:HB1	1.98	0.45
1:D:170:ILE:HG22	2:D:611:HOH:O	2.15	0.45
1:E:177:VAL:HA	1:E:201:SER:HB3	1.99	0.45
1:A:113:LEU:HD11	2:A:633:HOH:O	2.17	0.45
1:A:224:LEU:HD11	1:D:386:GLU:HG3	1.99	0.45
1:B:23:ARG:O	1:B:26:GLU:HB3	2.17	0.45
1:B:160:PHE:HB3	1:E:398:ILE:HD12	1.98	0.45
1:B:340:GLN:O	1:B:340:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:GLN:HB3	1:D:312:PHE:CE1	2.51	0.45
1:E:114:GLY:H	1:E:117:TYR:HB3	1.81	0.45
1:E:157:GLY:O	1:E:158:GLU:C	2.60	0.45
1:A:62:VAL:HG21	1:C:508:ARG:NE	2.32	0.45
1:B:169:VAL:HG21	1:E:521:PRO:HB2	1.98	0.45
1:B:437:TRP:HD1	2:B:600:HOH:O	1.99	0.45
1:B:512:GLN:HG3	1:C:91:TYR:CE1	2.52	0.45
2:B:585:HOH:O	1:E:361:ARG:HB2	2.16	0.45
1:E:99:VAL:CG1	1:E:100:ALA:N	2.80	0.45
1:E:206:THR:HB	2:E:617:HOH:O	2.17	0.45
1:E:395:ALA:HA	1:E:398:ILE:HG23	1.98	0.45
1:E:483:ASN:HD22	1:E:485:TYR:N	2.14	0.45
1:F:89:THR:HG22	1:F:102:PHE:HB2	1.99	0.45
1:F:251:VAL:HG13	1:F:252:LYS:N	2.31	0.45
1:F:472:ARG:HH21	1:F:473:LEU:CD2	2.28	0.45
1:F:518:GLU:HB3	2:F:543:HOH:O	2.16	0.45
1:A:361:ARG:HD2	1:A:403:GLU:OE2	2.16	0.45
1:A:490:ARG:HH12	1:D:151:ALA:HB2	1.81	0.45
1:B:212:LYS:O	1:B:214:VAL:N	2.50	0.45
1:B:284:LEU:HD13	1:B:304:HIS:CD2	2.52	0.45
1:B:457:ARG:HA	1:B:457:ARG:HE	1.82	0.45
1:B:475:GLN:HA	1:B:478:GLU:OE1	2.17	0.45
1:D:299:HIS:CD2	1:D:323:LEU:HD13	2.52	0.45
1:D:354:GLU:HA	2:D:672:HOH:O	2.17	0.45
1:E:487:ALA:HB1	1:E:492:TYR:HB2	1.98	0.45
1:F:141:SER:O	1:F:179:PRO:HB2	2.16	0.45
1:F:449:GLY:O	1:F:453:ILE:HG13	2.17	0.45
1:A:124:VAL:HG23	1:A:125:MET:N	2.32	0.44
1:A:417:PHE:O	1:A:420:ALA:HB3	2.17	0.44
1:B:246:ASP:O	1:B:249:GLU:HB3	2.17	0.44
1:B:430:GLY:O	1:B:431:ALA:C	2.60	0.44
1:C:39:LYS:O	1:C:43:LYS:HG2	2.16	0.44
1:C:418:GLY:HA2	1:F:153:LEU:CD2	2.43	0.44
1:D:528:ILE:O	1:D:528:ILE:HG23	2.17	0.44
1:E:70:HIS:NE2	1:E:81:ARG:HG2	2.32	0.44
1:E:377:PRO:HA	1:E:417:PHE:HD2	1.81	0.44
1:F:74:ASN:HB2	2:F:655:HOH:O	2.17	0.44
1:A:153:LEU:O	1:D:422:ILE:HD11	2.17	0.44
1:A:278:THR:HB	1:A:280:GLU:OE2	2.17	0.44
1:A:412:ILE:C	2:A:544:HOH:O	2.60	0.44
1:B:146:ILE:H	1:B:146:ILE:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:GLY:HA2	2:C:636:HOH:O	2.15	0.44
1:C:203:MET:HE2	1:F:391:ILE:HD13	1.98	0.44
1:C:359:PHE:C	1:C:361:ARG:N	2.74	0.44
1:E:177:VAL:HG12	1:E:197:VAL:HG21	1.99	0.44
1:F:69:ARG:HD3	1:F:81:ARG:O	2.18	0.44
1:F:377:PRO:HA	1:F:417:PHE:CD2	2.47	0.44
1:F:396:LYS:NZ	2:F:594:HOH:O	2.51	0.44
1:A:161:ARG:O	1:A:162:ARG:C	2.58	0.44
1:B:106:PHE:C	1:B:106:PHE:CD2	2.95	0.44
1:C:61:PHE:CE1	1:C:90:GLY:HA3	2.48	0.44
1:D:177:VAL:HA	1:D:201:SER:HB3	1.99	0.44
1:F:104:GLN:CG	1:F:139:ASN:HA	2.47	0.44
1:F:389:GLY:O	1:F:393:ARG:HG3	2.16	0.44
1:A:63:GLU:OE1	1:A:66:GLU:HG3	2.18	0.44
1:A:486:THR:HB	2:A:588:HOH:O	2.17	0.44
1:B:253:GLN:HB3	1:B:312:PHE:CE1	2.52	0.44
1:C:69:ARG:O	1:C:116:VAL:HG21	2.17	0.44
1:C:153:LEU:HD21	1:F:418:GLY:C	2.41	0.44
1:C:298:MET:C	1:C:300:SER:N	2.74	0.44
1:C:478:GLU:HA	1:C:482:LEU:HB2	2.00	0.44
1:E:375:ASP:OD1	1:E:415:LYS:HG3	2.16	0.44
1:F:417:PHE:HE1	1:F:482:LEU:HD11	1.83	0.44
1:A:372:THR:CG2	2:A:594:HOH:O	2.65	0.44
1:A:527:ASN:HD21	1:D:358:ARG:NE	2.15	0.44
1:B:121:ILE:HG13	2:B:657:HOH:O	2.18	0.44
1:B:156:TYR:CE1	1:B:184:ALA:HB2	2.53	0.44
1:C:284:LEU:HD11	1:C:304:HIS:CG	2.52	0.44
1:C:359:PHE:O	1:C:360:VAL:C	2.61	0.44
1:C:399:PHE:O	1:C:400:ALA:C	2.60	0.44
1:C:509:GLY:O	1:C:513:LEU:CD2	2.64	0.44
1:D:128:ALA:CB	1:D:135:VAL:HG22	2.48	0.44
1:E:251:VAL:HG23	1:E:252:LYS:N	2.31	0.44
1:F:227:ALA:HB1	1:F:240:MET:HG3	2.00	0.44
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.98	0.44
1:B:200:THR:HG22	1:B:200:THR:O	2.17	0.44
1:B:204:PHE:HA	1:E:386:GLU:OE2	2.17	0.44
1:C:393:ARG:NH2	1:F:393:ARG:CZ	2.81	0.44
1:C:495:ALA:HB2	2:C:566:HOH:O	2.18	0.44
1:D:122:VAL:C	1:D:124:VAL:N	2.74	0.44
1:E:106:PHE:C	1:E:108:VAL:H	2.25	0.44
1:F:91:TYR:HB2	2:F:535:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:GLN:HB2	1:F:140:ASP:H	1.83	0.44
1:A:166:ALA:C	2:D:594:HOH:O	2.61	0.44
1:A:324:THR:HA	1:A:336:ILE:O	2.16	0.44
1:A:372:THR:CG2	1:A:401:TYR:OH	2.66	0.44
1:C:274:ASP:OD1	1:C:276:ALA:HB3	2.18	0.44
1:C:437:TRP:CD1	2:C:537:HOH:O	2.69	0.44
1:D:120:LYS:O	1:D:121:ILE:C	2.61	0.44
1:E:311:PHE:CD1	1:E:311:PHE:C	2.94	0.44
1:E:374:VAL:HG12	1:E:375:ASP:N	2.33	0.44
1:F:472:ARG:HH12	1:F:476:GLU:CG	2.30	0.44
1:A:91:TYR:OH	1:C:508:ARG:CZ	2.65	0.44
1:B:45:LYS:HE2	1:B:200:THR:HG22	2.00	0.44
1:B:180:CYS:O	1:B:203:MET:HA	2.18	0.44
1:C:451:VAL:HG21	1:C:474:ILE:HG12	1.99	0.44
1:D:134:PRO:HB2	2:D:603:HOH:O	2.18	0.44
1:E:65:ASP:OD2	1:E:120:LYS:HG2	2.17	0.44
1:E:227:ALA:HB3	2:E:675:HOH:O	2.18	0.44
1:E:287:ILE:HG23	1:E:288:VAL:N	2.32	0.44
1:E:361:ARG:HD2	1:E:403:GLU:OE2	2.17	0.44
1:A:69:ARG:O	1:A:116:VAL:HG21	2.18	0.44
1:B:63:GLU:HG2	1:B:66:GLU:HB2	1.98	0.44
1:B:384:ASP:O	1:B:385:GLN:C	2.61	0.44
1:D:353:SER:OG	1:D:394:GLY:HA2	2.18	0.44
1:E:155:ALA:O	1:E:159:ILE:HG13	2.18	0.44
1:E:230:HIS:HB3	1:E:236:VAL:CG2	2.47	0.44
1:F:187:SER:CB	1:F:188:PRO:CD	2.94	0.44
1:A:203:MET:HB2	1:A:230:HIS:CD2	2.53	0.43
1:A:377:PRO:HA	1:A:417:PHE:HD2	1.83	0.43
1:A:389:GLY:O	1:A:393:ARG:HG3	2.18	0.43
1:B:215:THR:C	1:B:217:GLU:N	2.74	0.43
1:D:157:GLY:C	1:D:159:ILE:N	2.75	0.43
1:D:354:GLU:HG2	1:D:396:LYS:HD2	2.00	0.43
1:E:21:LEU:O	1:E:21:LEU:HD12	2.18	0.43
1:E:71:ARG:NH1	1:F:490:ARG:NH2	2.66	0.43
1:E:177:VAL:HB	1:E:244:GLU:OE1	2.18	0.43
1:E:239:HIS:HA	2:E:673:HOH:O	2.18	0.43
1:F:35:ARG:HH21	1:F:39:LYS:HZ1	1.66	0.43
1:F:440:ALA:HB2	2:F:648:HOH:O	2.18	0.43
1:A:10:ASP:CG	1:A:11:ILE:N	2.76	0.43
1:A:101:VAL:C	2:A:546:HOH:O	2.61	0.43
1:A:464:ASP:O	1:A:465:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:MET:O	1:A:499:PRO:C	2.60	0.43
1:A:512:GLN:HG3	1:B:91:TYR:CE1	2.52	0.43
1:A:523:LYS:HE2	1:D:169:VAL:CG2	2.48	0.43
1:B:167:SER:N	2:E:599:HOH:O	2.50	0.43
1:B:182:GLY:O	1:B:185:VAL:HG22	2.18	0.43
1:C:94:VAL:O	1:C:95:ASP:HB2	2.16	0.43
1:D:85:ASP:CG	1:D:85:ASP:O	2.62	0.43
1:D:315:GLN:HA	2:D:542:HOH:O	2.18	0.43
1:E:447:ALA:O	1:E:451:VAL:HG22	2.17	0.43
1:F:323:LEU:HD11	2:F:686:HOH:O	2.17	0.43
1:F:448:GLN:O	1:F:451:VAL:HG22	2.17	0.43
1:A:91:TYR:CD1	1:A:92:GLY:N	2.85	0.43
1:A:508:ARG:CG	1:B:62:VAL:HG21	2.48	0.43
1:B:432:ASP:C	1:B:433:LEU:HD12	2.43	0.43
1:B:528:ILE:O	1:B:530:LEU:HD13	2.18	0.43
1:C:33:SER:O	1:C:36:ALA:N	2.50	0.43
1:C:298:MET:O	1:C:300:SER:N	2.50	0.43
1:D:36:ALA:HB1	1:D:107:THR:HB	2.00	0.43
1:E:25:ILE:O	1:E:29:THR:HG23	2.18	0.43
1:E:294:GLN:HA	1:E:295:PRO:HD3	1.75	0.43
1:E:490:ARG:HH11	1:E:490:ARG:CG	2.30	0.43
1:F:215:THR:C	1:F:217:GLU:H	2.26	0.43
1:F:376:VAL:O	1:F:376:VAL:HG13	2.17	0.43
1:A:300:SER:O	1:A:304:HIS:ND1	2.49	0.43
1:B:172:GLN:HG2	2:B:666:HOH:O	2.17	0.43
1:B:254:LEU:HD22	2:B:607:HOH:O	2.18	0.43
1:C:473:LEU:HD12	1:C:473:LEU:HA	1.82	0.43
1:C:491:GLY:C	1:C:493:VAL:N	2.75	0.43
1:D:40:GLN:HE22	1:D:106:PHE:HD2	1.64	0.43
1:E:62:VAL:CG1	1:F:508:ARG:HH21	2.20	0.43
1:E:414:ARG:HG3	1:E:439:THR:O	2.18	0.43
1:F:161:ARG:O	1:F:164:THR:N	2.47	0.43
1:F:402:ALA:HA	1:F:429:LEU:O	2.18	0.43
1:A:40:GLN:HE21	1:A:40:GLN:HA	1.83	0.43
1:B:180:CYS:HB3	1:B:203:MET:HG2	2.01	0.43
1:B:386:GLU:HG3	1:E:224:LEU:HD11	2.00	0.43
1:C:84:GLY:HA2	1:C:120:LYS:NZ	2.34	0.43
1:E:51:ARG:CZ	1:E:177:VAL:CG2	2.97	0.43
1:E:146:ILE:HD12	1:E:146:ILE:N	2.26	0.43
1:E:451:VAL:C	1:E:453:ILE:N	2.76	0.43
1:A:24:ARG:HD2	1:C:485:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:HD12	1:A:484:PRO:HA	2.00	0.43
1:B:158:GLU:OE2	1:B:161:ARG:NH2	2.52	0.43
2:B:649:HOH:O	1:E:358:ARG:HG2	2.19	0.43
1:C:285:ASP:HA	1:C:499:PRO:HB2	2.00	0.43
1:C:462:ALA:C	1:C:464:ASP:N	2.73	0.43
1:D:274:ASP:OD2	1:D:274:ASP:C	2.61	0.43
1:E:199:GLN:HE21	1:E:199:GLN:HB2	1.53	0.43
1:E:234:SER:HB2	1:E:236:VAL:HG13	2.00	0.43
1:F:313:GLU:HG2	1:F:316:PRO:HG3	2.00	0.43
1:F:528:ILE:O	1:F:530:LEU:CD1	2.67	0.43
1:B:125:MET:HE1	1:B:163:ASN:ND2	2.34	0.43
1:B:491:GLY:C	1:B:493:VAL:N	2.76	0.43
1:C:308:ASP:HB2	1:C:310:GLU:HG3	2.00	0.43
1:D:177:VAL:C	1:D:201:SER:HB3	2.43	0.43
1:F:472:ARG:HH22	1:F:476:GLU:CD	2.25	0.43
1:F:518:GLU:CB	2:F:543:HOH:O	2.67	0.43
1:A:145:ARG:HD2	1:A:148:GLU:OE2	2.19	0.43
1:A:164:THR:HG23	1:D:399:PHE:CE1	2.53	0.43
1:A:527:ASN:ND2	1:A:527:ASN:C	2.76	0.43
1:B:374:VAL:HG12	1:B:375:ASP:N	2.33	0.43
1:B:380:LEU:HD23	1:B:380:LEU:C	2.44	0.43
1:C:512:GLN:HE21	1:C:512:GLN:HB3	1.52	0.43
1:C:527:ASN:HD22	1:C:527:ASN:C	2.26	0.43
1:D:70:HIS:ND1	1:D:70:HIS:C	2.77	0.43
1:D:423:VAL:O	1:D:425:GLY:N	2.51	0.43
1:E:397:LEU:HD13	1:E:423:VAL:CG1	2.49	0.43
1:E:412:ILE:HG22	1:E:440:ALA:HB1	2.01	0.43
1:F:154:GLY:O	1:F:155:ALA:C	2.60	0.43
1:F:174:SER:O	1:F:195:VAL:HG12	2.19	0.43
1:F:393:ARG:HB3	2:F:628:HOH:O	2.18	0.43
1:F:491:GLY:C	1:F:493:VAL:N	2.77	0.43
1:A:24:ARG:C	1:A:26:GLU:H	2.25	0.43
1:A:102:PHE:CD2	1:A:102:PHE:C	2.96	0.43
1:A:193:PHE:HA	1:A:238:HIS:ND1	2.33	0.43
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.84	0.43
1:A:375:ASP:OD1	1:A:414:ARG:HB3	2.19	0.43
1:B:231:ASN:HD21	1:B:239:HIS:CA	2.32	0.43
1:C:214:VAL:O	1:C:214:VAL:HG12	2.18	0.43
1:D:21:LEU:O	1:D:25:ILE:HG23	2.19	0.43
1:D:367:ASN:HA	1:D:406:VAL:CG1	2.49	0.43
1:D:510:LEU:O	1:D:511:ARG:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:ILE:C	1:E:13:THR:N	2.75	0.43
1:E:405:THR:N	2:E:677:HOH:O	2.41	0.43
1:F:132:GLY:C	1:F:261:ASN:HD22	2.27	0.43
1:F:318:PHE:HA	2:F:614:HOH:O	2.19	0.43
1:A:21:LEU:O	1:A:25:ILE:HG23	2.18	0.43
1:A:118:GLY:O	1:A:119:GLN:C	2.62	0.43
1:A:141:SER:OG	1:A:142:GLY:N	2.50	0.43
1:A:306:LEU:HD13	1:A:327:GLY:HA3	2.01	0.43
1:C:414:ARG:HA	1:C:440:ALA:HA	2.00	0.43
1:D:190:ILE:O	1:D:191:THR:C	2.59	0.43
1:D:231:ASN:HD21	1:D:239:HIS:C	2.26	0.43
1:D:442:ILE:HG13	2:D:644:HOH:O	2.18	0.43
1:E:47:THR:N	1:E:50:GLU:OE1	2.50	0.43
1:E:157:GLY:O	1:E:160:PHE:HB2	2.19	0.43
1:F:121:ILE:HD12	2:F:654:HOH:O	2.19	0.43
1:F:208:PRO:HG2	1:F:221:PHE:CZ	2.54	0.43
1:F:238:HIS:HD2	1:F:315:GLN:HE21	1.67	0.43
1:B:85:ASP:O	1:B:85:ASP:OD2	2.37	0.42
1:B:157:GLY:O	1:B:159:ILE:N	2.51	0.42
1:B:236:VAL:CG2	1:B:237:ALA:N	2.82	0.42
1:B:377:PRO:HG3	2:B:650:HOH:O	2.19	0.42
1:B:449:GLY:HA2	1:B:452:ASN:ND2	2.34	0.42
1:B:512:GLN:NE2	2:B:545:HOH:O	2.52	0.42
1:C:135:VAL:HG22	2:C:574:HOH:O	2.19	0.42
1:E:87:VAL:HG13	1:E:87:VAL:O	2.18	0.42
1:E:161:ARG:NH1	1:E:161:ARG:CG	2.80	0.42
1:E:197:VAL:HB	1:E:200:THR:HB	2.01	0.42
1:E:455:HIS:O	1:E:457:ARG:N	2.52	0.42
1:F:55:LEU:CD1	1:F:252:LYS:HG3	2.49	0.42
1:F:106:PHE:O	1:F:106:PHE:CD2	2.71	0.42
1:F:134:PRO:N	2:F:607:HOH:O	2.52	0.42
1:A:157:GLY:C	1:A:159:ILE:N	2.75	0.42
1:B:24:ARG:C	1:B:26:GLU:N	2.76	0.42
1:B:335:GLY:O	1:B:371:LEU:N	2.49	0.42
1:C:122:VAL:C	1:C:124:VAL:N	2.77	0.42
1:C:246:ASP:O	1:C:249:GLU:HB3	2.20	0.42
1:C:316:PRO:HD2	2:C:601:HOH:O	2.19	0.42
1:D:486:THR:HB	2:D:599:HOH:O	2.18	0.42
1:E:302:ILE:O	1:E:305:VAL:HG22	2.19	0.42
1:E:313:GLU:HG3	2:E:561:HOH:O	2.19	0.42
1:B:268:ALA:HB2	1:B:332:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ALA:HB2	2:C:620:HOH:O	2.19	0.42
1:C:232:SER:HB3	1:C:317:LEU:CB	2.49	0.42
1:C:253:GLN:HB3	1:C:312:PHE:CE1	2.55	0.42
1:E:199:GLN:HB2	2:E:691:HOH:O	2.19	0.42
1:E:397:LEU:HD13	1:E:423:VAL:HG11	2.02	0.42
1:E:505:HIS:CD2	2:E:640:HOH:O	2.72	0.42
1:F:322:ILE:HG13	2:F:608:HOH:O	2.18	0.42
1:F:445:MET:HG3	1:F:450:ALA:HB2	2.01	0.42
1:A:353:SER:CB	1:A:394:GLY:HA2	2.49	0.42
1:A:485:TYR:HA	1:A:488:ALA:HB3	2.02	0.42
1:A:530:LEU:HB3	2:D:672:HOH:O	2.20	0.42
1:B:11:ILE:O	1:B:11:ILE:CG1	2.67	0.42
1:B:198:ASP:CG	1:B:199:GLN:HG2	2.43	0.42
1:B:334:VAL:HG23	1:B:336:ILE:HD11	2.01	0.42
1:B:503:ARG:NH2	2:B:693:HOH:O	2.51	0.42
1:C:32:GLY:HA3	1:C:107:THR:OG1	2.19	0.42
1:C:128:ALA:HB2	2:C:574:HOH:O	2.19	0.42
1:C:170:ILE:CD1	2:C:641:HOH:O	2.67	0.42
1:C:443:ALA:HB1	2:C:629:HOH:O	2.18	0.42
1:D:180:CYS:HB3	1:D:203:MET:CG	2.50	0.42
1:E:306:LEU:CD2	1:E:336:ILE:HD11	2.45	0.42
1:E:332:ARG:NH1	1:E:332:ARG:HB2	2.34	0.42
1:E:473:LEU:O	1:E:476:GLU:N	2.52	0.42
1:F:55:LEU:HD21	1:F:136:VAL:HG21	2.00	0.42
1:F:414:ARG:HA	1:F:440:ALA:HA	2.00	0.42
1:A:147:GLN:OE1	1:A:147:GLN:N	2.49	0.42
1:A:410:THR:HG22	2:A:636:HOH:O	2.19	0.42
1:C:285:ASP:OD1	1:C:499:PRO:HD2	2.19	0.42
1:C:305:VAL:HG23	1:C:306:LEU:N	2.34	0.42
1:C:358:ARG:HB3	2:C:653:HOH:O	2.20	0.42
1:D:503:ARG:C	1:D:505:HIS:N	2.78	0.42
1:D:509:GLY:O	1:D:513:LEU:HD22	2.20	0.42
1:E:118:GLY:O	1:E:119:GLN:C	2.62	0.42
1:E:298:MET:SD	1:E:301:VAL:CG2	3.07	0.42
1:F:325:GLY:O	1:F:359:PHE:CZ	2.72	0.42
1:F:380:LEU:HD23	1:F:380:LEU:O	2.19	0.42
1:A:136:VAL:HG21	2:A:671:HOH:O	2.19	0.42
1:A:287:ILE:O	1:A:287:ILE:HG13	2.19	0.42
1:A:318:PHE:O	1:A:319:ALA:C	2.62	0.42
1:A:332:ARG:NH1	1:A:514:ARG:HH21	2.17	0.42
1:A:344:PHE:CD1	1:A:344:PHE:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HB3	1:A:423:VAL:HG13	2.02	0.42
1:A:513:LEU:C	1:A:515:THR:H	2.28	0.42
1:B:505:HIS:CA	1:B:508:ARG:HH11	2.32	0.42
1:C:50:GLU:O	1:C:54:LEU:HB2	2.20	0.42
1:C:181:ALA:HB2	1:C:204:PHE:CE1	2.54	0.42
1:D:510:LEU:C	1:D:512:GLN:N	2.76	0.42
1:E:62:VAL:HG21	1:F:508:ARG:CG	2.50	0.42
1:E:98:PRO:HB2	2:E:662:HOH:O	2.19	0.42
1:E:177:VAL:HG12	1:E:197:VAL:CG2	2.49	0.42
1:E:291:SER:C	1:E:293:ASN:N	2.77	0.42
1:E:398:ILE:CG1	1:E:399:PHE:N	2.81	0.42
1:E:427:LYS:NZ	2:E:694:HOH:O	2.50	0.42
1:E:459:ILE:HD11	1:E:470:ARG:HB2	2.02	0.42
1:A:374:VAL:CG1	1:A:375:ASP:N	2.83	0.42
1:A:527:ASN:ND2	1:D:358:ARG:HE	2.18	0.42
1:B:146:ILE:HD12	1:B:146:ILE:N	2.35	0.42
1:B:175:LEU:HD12	1:B:195:VAL:HG13	2.01	0.42
1:C:154:GLY:O	1:C:157:GLY:N	2.53	0.42
1:E:469:THR:O	1:E:473:LEU:HD13	2.19	0.42
1:F:173:ILE:HD13	1:F:254:LEU:HD23	2.02	0.42
1:F:291:SER:HB3	1:F:294:GLN:CB	2.49	0.42
1:F:332:ARG:N	2:F:550:HOH:O	2.53	0.42
1:F:337:VAL:HG21	1:F:360:VAL:HG22	2.01	0.42
1:F:382:GLY:O	1:F:385:GLN:HB2	2.20	0.42
1:A:39:LYS:O	1:A:43:LYS:HB2	2.19	0.42
1:A:313:GLU:OE1	1:A:323:LEU:HD22	2.20	0.42
1:A:427:LYS:HE2	1:A:494:ASP:OD2	2.20	0.42
1:B:61:PHE:HE1	1:B:90:GLY:HA3	1.84	0.42
1:B:87:VAL:O	1:B:87:VAL:HG13	2.20	0.42
1:B:336:ILE:N	1:B:336:ILE:CD1	2.82	0.42
1:B:396:LYS:HD3	1:E:530:LEU:HG	2.02	0.42
1:D:453:ILE:HD12	1:D:453:ILE:N	2.34	0.42
1:E:498:MET:O	1:E:499:PRO:C	2.61	0.42
1:F:150:VAL:O	1:F:153:LEU:N	2.44	0.42
1:F:198:ASP:HA	1:F:227:ALA:CB	2.46	0.42
1:A:91:TYR:CD1	1:A:91:TYR:C	2.98	0.42
1:A:397:LEU:HD13	1:A:423:VAL:HG12	2.01	0.42
1:A:398:ILE:HD11	1:D:190:ILE:HD11	2.01	0.42
1:B:51:ARG:HB2	2:B:590:HOH:O	2.19	0.42
1:B:69:ARG:O	1:B:116:VAL:HG21	2.20	0.42
1:B:90:GLY:HA2	2:B:562:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLY:O	1:E:444:VAL:HB	2.20	0.42
1:C:171:PRO:HG3	1:C:366:PHE:CE1	2.55	0.42
1:C:459:ILE:HD11	1:C:470:ARG:HB2	2.00	0.42
1:C:468:ALA:O	1:C:472:ARG:HB2	2.20	0.42
1:D:99:VAL:HG13	2:D:603:HOH:O	2.19	0.42
1:D:181:ALA:CB	1:D:204:PHE:CE1	3.01	0.42
1:D:182:GLY:O	1:D:205:ILE:HD13	2.20	0.42
1:D:380:LEU:HD23	1:D:385:GLN:CD	2.44	0.42
1:E:196:MET:HE3	1:E:203:MET:HG3	2.01	0.42
1:E:343:GLN:O	1:E:344:PHE:C	2.63	0.42
1:E:361:ARG:CZ	2:E:579:HOH:O	2.68	0.42
1:F:193:PHE:HA	1:F:238:HIS:ND1	2.34	0.42
1:F:372:THR:HG21	2:F:568:HOH:O	2.19	0.42
1:F:374:VAL:HG13	1:F:424:MET:HG3	2.01	0.42
1:F:461:ASP:HB3	2:F:627:HOH:O	2.19	0.42
1:A:203:MET:HB2	1:A:230:HIS:NE2	2.35	0.42
1:A:315:GLN:N	1:A:316:PRO:CD	2.82	0.42
1:B:85:ASP:OD1	1:B:116:VAL:HB	2.20	0.42
1:B:177:VAL:HG12	1:B:197:VAL:CG2	2.50	0.42
1:B:375:ASP:OD2	1:B:414:ARG:HB3	2.20	0.42
1:C:23:ARG:NH2	1:C:27:GLU:OE2	2.52	0.42
1:C:248:VAL:HG12	2:C:666:HOH:O	2.20	0.42
1:C:383:VAL:HG22	1:F:219:VAL:HG21	2.02	0.42
1:C:505:HIS:HA	1:C:508:ARG:HH11	1.85	0.42
1:E:51:ARG:CZ	1:E:177:VAL:HG21	2.50	0.42
1:E:258:LEU:HG	2:E:560:HOH:O	2.19	0.42
1:E:505:HIS:O	1:E:508:ARG:NH1	2.52	0.42
1:F:116:VAL:O	1:F:120:LYS:HG3	2.20	0.42
1:F:248:VAL:O	1:F:251:VAL:HG12	2.20	0.42
1:F:315:GLN:HB2	1:F:355:LYS:HE3	2.01	0.42
1:A:11:ILE:O	1:A:11:ILE:HG13	2.20	0.41
1:A:160:PHE:HE2	1:D:422:ILE:HG21	1.84	0.41
1:A:197:VAL:O	1:A:227:ALA:HB2	2.20	0.41
1:A:406:VAL:HB	1:A:407:PRO:CD	2.50	0.41
1:A:461:ASP:O	1:A:462:ALA:HB3	2.20	0.41
1:C:115:GLU:O	1:C:116:VAL:C	2.63	0.41
1:C:523:LYS:O	1:C:523:LYS:HG2	2.19	0.41
2:C:713:HOH:O	1:F:382:GLY:HA2	2.20	0.41
1:D:197:VAL:C	2:D:633:HOH:O	2.63	0.41
1:D:234:SER:HB2	1:D:236:VAL:HG13	2.02	0.41
1:D:448:GLN:C	1:D:450:ALA:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:GLY:O	1:E:371:LEU:N	2.53	0.41
1:E:456:ARG:HD2	1:E:456:ARG:C	2.45	0.41
1:F:122:VAL:HG13	1:F:162:ARG:NE	2.35	0.41
1:F:281:ASP:O	1:F:500:SER:HA	2.20	0.41
1:F:294:GLN:HA	1:F:295:PRO:HD3	1.84	0.41
1:F:344:PHE:CD1	1:F:344:PHE:N	2.88	0.41
1:A:94:VAL:HG13	1:A:252:LYS:HD2	2.02	0.41
1:A:153:LEU:HD11	1:D:418:GLY:CA	2.50	0.41
1:A:206:THR:HG22	1:A:211:ILE:HG13	2.02	0.41
1:A:398:ILE:CD1	1:D:160:PHE:HB3	2.43	0.41
1:A:528:ILE:O	1:A:530:LEU:HD22	2.21	0.41
1:B:122:VAL:O	1:B:125:MET:N	2.53	0.41
1:B:196:MET:HB2	2:B:609:HOH:O	2.20	0.41
1:B:319:ALA:N	1:B:320:PRO:HD3	2.35	0.41
1:B:420:ALA:O	1:B:421:TYR:C	2.63	0.41
1:B:487:ALA:HB1	1:B:492:TYR:HB2	2.01	0.41
1:C:185:VAL:CG2	1:F:391:ILE:HG12	2.50	0.41
1:C:353:SER:HB3	1:C:394:GLY:HA2	2.01	0.41
1:C:400:ALA:HA	2:C:693:HOH:O	2.20	0.41
2:C:660:HOH:O	1:F:525:HIS:HB2	2.20	0.41
1:D:134:PRO:C	2:D:603:HOH:O	2.63	0.41
1:D:285:ASP:OD1	1:D:499:PRO:HD2	2.20	0.41
1:D:397:LEU:HD23	1:D:401:TYR:CD2	2.55	0.41
1:D:418:GLY:O	1:D:421:TYR:HB3	2.20	0.41
1:D:439:THR:HG21	1:F:14:THR:HG23	2.02	0.41
1:A:101:VAL:HG22	1:A:102:PHE:N	2.35	0.41
1:A:413:THR:HA	2:A:544:HOH:O	2.19	0.41
1:A:527:ASN:C	1:A:527:ASN:HD22	2.27	0.41
1:B:389:GLY:C	1:B:391:ILE:N	2.77	0.41
1:B:498:MET:HE1	1:C:18:LEU:HB3	2.03	0.41
1:C:161:ARG:HG3	1:C:161:ARG:HH11	1.85	0.41
1:C:397:LEU:C	1:C:399:PHE:N	2.77	0.41
1:D:113:LEU:HD22	1:D:117:TYR:HE1	1.84	0.41
1:D:281:ASP:O	1:D:284:LEU:HB2	2.19	0.41
1:D:527:ASN:O	1:D:528:ILE:C	2.63	0.41
1:E:130:LYS:HG3	1:F:516:LYS:HG3	2.02	0.41
1:F:212:LYS:C	1:F:214:VAL:N	2.79	0.41
1:F:517:ARG:C	1:F:518:GLU:HG2	2.45	0.41
1:A:26:GLU:O	1:A:30:HIS:HD2	2.04	0.41
1:A:162:ARG:HG2	1:A:162:ARG:H	1.71	0.41
1:A:490:ARG:NH1	2:A:579:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:N	2:B:657:HOH:O	2.52	0.41
1:B:154:GLY:O	1:B:155:ALA:C	2.62	0.41
1:B:262:ASN:OD1	1:B:262:ASN:C	2.63	0.41
1:B:380:LEU:HD23	1:B:380:LEU:O	2.20	0.41
1:B:473:LEU:HD12	1:B:476:GLU:OE1	2.19	0.41
1:B:517:ARG:NH2	2:B:533:HOH:O	2.34	0.41
1:C:14:THR:O	1:C:17:LYS:HB2	2.21	0.41
1:C:208:PRO:C	1:C:210:VAL:N	2.79	0.41
1:C:364:ASP:OD1	1:C:406:VAL:HG22	2.21	0.41
1:D:21:LEU:HD22	1:E:438:PRO:HG3	2.01	0.41
1:D:47:THR:O	1:D:51:ARG:HD3	2.20	0.41
1:D:449:GLY:HA2	1:D:452:ASN:HD22	1.85	0.41
1:E:55:LEU:HD21	1:E:136:VAL:HG11	2.02	0.41
1:E:308:ASP:C	1:E:310:GLU:N	2.77	0.41
1:F:181:ALA:HB2	1:F:204:PHE:CE1	2.55	0.41
1:F:422:ILE:HA	1:F:426:SER:HB3	2.01	0.41
1:C:122:VAL:O	1:C:124:VAL:N	2.53	0.41
1:C:360:VAL:HB	1:C:400:ALA:HB1	2.03	0.41
1:D:231:ASN:O	1:D:317:LEU:HB2	2.20	0.41
1:D:380:LEU:HD23	1:D:385:GLN:NE2	2.35	0.41
1:E:427:LYS:HB2	1:E:427:LYS:NZ	2.36	0.41
1:F:16:GLY:HA3	2:F:573:HOH:O	2.20	0.41
1:F:71:ARG:HB2	1:F:71:ARG:HH11	1.86	0.41
1:F:230:HIS:HB3	1:F:236:VAL:HG22	2.03	0.41
1:F:342:MET:O	1:F:343:GLN:HG2	2.21	0.41
1:F:423:VAL:CG1	2:F:592:HOH:O	2.68	0.41
1:A:324:THR:HB	1:A:359:PHE:CD2	2.55	0.41
1:A:508:ARG:NE	1:B:62:VAL:HG21	2.35	0.41
1:B:125:MET:HE3	1:B:135:VAL:HG11	2.03	0.41
1:B:269:PHE:O	1:B:331:GLY:HA3	2.21	0.41
1:B:456:ARG:HH12	1:B:457:ARG:CZ	2.32	0.41
2:B:649:HOH:O	1:E:358:ARG:CG	2.69	0.41
1:D:46:LEU:N	1:D:46:LEU:HD12	2.36	0.41
1:D:284:LEU:HA	1:D:284:LEU:HD12	1.81	0.41
1:D:336:ILE:N	1:D:336:ILE:CD1	2.79	0.41
1:E:62:VAL:HG21	1:F:508:ARG:NE	2.32	0.41
1:E:156:TYR:OH	1:E:184:ALA:HB2	2.19	0.41
1:E:486:THR:O	1:E:489:GLU:HB2	2.20	0.41
1:F:147:GLN:HB3	2:F:655:HOH:O	2.18	0.41
1:F:203:MET:HB2	1:F:230:HIS:NE2	2.36	0.41
1:A:100:ALA:HB3	2:A:578:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:O	1:A:159:ILE:HB	2.20	0.41
1:A:521:PRO:HD2	1:D:165:HIS:O	2.21	0.41
1:B:122:VAL:O	1:B:123:LYS:C	2.64	0.41
1:B:162:ARG:HH11	1:B:162:ARG:CG	2.30	0.41
1:B:344:PHE:CD1	1:B:344:PHE:N	2.88	0.41
1:D:463:GLY:HA2	2:D:657:HOH:O	2.21	0.41
1:E:10:ASP:N	2:E:629:HOH:O	2.53	0.41
1:E:316:PRO:HD2	2:E:567:HOH:O	2.20	0.41
1:F:122:VAL:HG11	1:F:162:ARG:NH2	2.36	0.41
1:F:157:GLY:O	1:F:160:PHE:N	2.53	0.41
1:A:24:ARG:HB3	1:A:83:TYR:CE1	2.51	0.41
1:A:28:ALA:HB3	2:A:641:HOH:O	2.20	0.41
1:A:162:ARG:HG2	1:A:162:ARG:NH1	2.29	0.41
1:A:164:THR:O	1:A:167:SER:N	2.45	0.41
1:A:399:PHE:CG	1:D:164:THR:HG23	2.56	0.41
1:B:437:TRP:HA	2:B:600:HOH:O	2.20	0.41
1:B:489:GLU:O	1:C:68:ALA:HA	2.20	0.41
1:C:112:ALA:HB3	1:C:145:ARG:HE	1.86	0.41
1:C:153:LEU:O	1:F:422:ILE:HD11	2.20	0.41
1:C:319:ALA:N	1:C:320:PRO:CD	2.84	0.41
1:C:346:GLY:O	1:C:377:PRO:HD2	2.20	0.41
1:C:440:ALA:O	1:C:483:ASN:HA	2.20	0.41
1:D:67:PHE:CE2	1:E:496:VAL:HB	2.56	0.41
1:D:295:PRO:HB2	1:D:342:MET:HE2	2.03	0.41
1:D:325:GLY:O	1:D:359:PHE:CZ	2.74	0.41
1:E:254:LEU:CD1	1:E:312:PHE:HE2	2.30	0.41
1:E:322:ILE:CG2	1:E:355:LYS:HD3	2.51	0.41
1:F:41:HIS:HA	1:F:45:LYS:O	2.21	0.41
1:F:52:ILE:O	1:F:53:ASP:C	2.64	0.41
1:F:336:ILE:HA	1:F:371:LEU:O	2.21	0.41
1:A:40:GLN:HA	1:A:40:GLN:NE2	2.36	0.41
1:A:103:SER:HA	1:A:138:ILE:HB	2.03	0.41
1:A:132:GLY:N	2:A:609:HOH:O	2.54	0.41
1:A:150:VAL:HG23	1:A:151:ALA:N	2.36	0.41
1:A:164:THR:C	1:A:166:ALA:N	2.77	0.41
1:A:298:MET:HE2	1:A:339:ASN:O	2.21	0.41
1:A:299:HIS:HA	2:A:678:HOH:O	2.21	0.41
1:A:490:ARG:HA	1:B:71:ARG:HH21	1.86	0.41
1:A:513:LEU:C	1:A:515:THR:N	2.77	0.41
1:B:61:PHE:CE1	1:B:90:GLY:HA3	2.55	0.41
1:B:155:ALA:O	1:B:159:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:HA	1:B:201:SER:HB3	2.03	0.41
1:B:197:VAL:O	1:B:227:ALA:HB2	2.21	0.41
1:C:105:ASP:HA	2:C:614:HOH:O	2.21	0.41
1:C:122:VAL:O	1:C:123:LYS:C	2.63	0.41
1:C:156:TYR:CE1	1:C:184:ALA:HB2	2.56	0.41
1:C:184:ALA:C	1:C:186:TYR:N	2.79	0.41
1:C:393:ARG:NH2	1:F:393:ARG:NH1	2.69	0.41
1:C:407:PRO:HB3	1:C:513:LEU:CB	2.51	0.41
2:C:705:HOH:O	1:F:211:ILE:HD13	2.20	0.41
1:D:16:GLY:HA3	2:D:579:HOH:O	2.20	0.41
1:D:55:LEU:CD2	1:D:136:VAL:HG11	2.50	0.41
1:E:101:VAL:CG2	1:E:102:PHE:N	2.84	0.41
1:E:339:ASN:ND2	2:E:658:HOH:O	2.48	0.41
1:E:350:ILE:O	1:E:354:GLU:HG3	2.21	0.41
1:F:70:HIS:O	1:F:81:ARG:HD2	2.21	0.41
1:F:150:VAL:O	1:F:151:ALA:C	2.64	0.41
1:F:196:MET:CE	1:F:203:MET:HG3	2.47	0.41
1:F:322:ILE:HG21	2:F:710:HOH:O	2.20	0.41
1:F:377:PRO:HG3	2:F:632:HOH:O	2.20	0.41
1:F:475:GLN:HE21	1:F:475:GLN:HB3	1.72	0.41
1:A:46:LEU:HD12	1:A:244:GLU:OE2	2.21	0.41
1:B:157:GLY:O	1:B:160:PHE:N	2.54	0.41
1:D:439:THR:CG2	1:F:14:THR:HG23	2.51	0.41
1:E:113:LEU:C	2:E:608:HOH:O	2.64	0.41
1:E:148:GLU:HB3	2:E:587:HOH:O	2.21	0.41
1:E:156:TYR:CE1	1:E:184:ALA:HB2	2.55	0.41
1:E:194:THR:OG1	1:E:237:ALA:HA	2.21	0.41
1:F:120:LYS:O	1:F:121:ILE:C	2.63	0.41
1:A:33:SER:C	1:A:35:ARG:N	2.78	0.40
1:B:329:VAL:O	1:B:330:GLU:HB2	2.21	0.40
1:C:141:SER:O	1:C:179:PRO:O	2.39	0.40
1:C:434:ASN:O	1:C:494:ASP:OD1	2.37	0.40
1:D:24:ARG:C	1:D:26:GLU:N	2.79	0.40
1:E:62:VAL:HG21	1:F:508:ARG:HG3	2.03	0.40
1:F:157:GLY:O	1:F:158:GLU:C	2.65	0.40
1:F:162:ARG:NH1	1:F:162:ARG:CG	2.83	0.40
1:F:212:LYS:O	1:F:214:VAL:N	2.54	0.40
1:F:440:ALA:O	1:F:483:ASN:HA	2.21	0.40
1:A:181:ALA:C	2:A:548:HOH:O	2.65	0.40
1:A:344:PHE:O	1:A:345:ALA:HB3	2.22	0.40
1:C:212:LYS:HD3	1:C:218:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ASN:HB3	2:C:573:HOH:O	2.20	0.40
1:E:459:ILE:HG23	1:E:460:ALA:N	2.36	0.40
1:B:181:ALA:HB2	1:B:204:PHE:CE1	2.57	0.40
1:B:185:VAL:HB	1:E:391:ILE:HD13	2.04	0.40
1:B:232:SER:HB3	1:B:317:LEU:HB3	2.03	0.40
1:B:337:VAL:O	1:B:372:THR:HA	2.21	0.40
1:C:163:ASN:N	2:C:539:HOH:O	2.54	0.40
1:C:511:ARG:HD2	2:C:556:HOH:O	2.22	0.40
1:D:429:LEU:HA	1:D:429:LEU:HD12	1.80	0.40
1:D:487:ALA:HB1	1:D:492:TYR:HB2	2.03	0.40
1:E:60:SER:HB2	1:E:93:THR:H	1.87	0.40
1:E:101:VAL:HG13	2:E:607:HOH:O	2.21	0.40
1:E:244:GLU:O	1:E:248:VAL:HG23	2.22	0.40
1:E:344:PHE:O	1:E:345:ALA:HB3	2.20	0.40
1:F:482:LEU:HD13	2:F:691:HOH:O	2.21	0.40
1:A:508:ARG:HE	1:B:62:VAL:HG21	1.87	0.40
1:C:33:SER:O	1:C:34:ALA:C	2.63	0.40
1:D:157:GLY:O	1:D:158:GLU:C	2.63	0.40
1:E:65:ASP:HA	2:F:590:HOH:O	2.21	0.40
1:E:187:SER:N	1:E:188:PRO:CD	2.84	0.40
1:E:445:MET:HG3	1:E:450:ALA:HB2	2.04	0.40
1:F:101:VAL:HG22	1:F:102:PHE:N	2.36	0.40
1:A:454:LEU:HD13	1:D:75:PHE:CE1	2.57	0.40
1:B:174:SER:OG	1:B:191:THR:HG21	2.22	0.40
1:B:374:VAL:HG13	1:B:424:MET:HG3	2.04	0.40
1:B:451:VAL:HG21	1:B:474:ILE:CG1	2.52	0.40
1:C:208:PRO:O	1:C:210:VAL:N	2.55	0.40
1:C:298:MET:O	1:C:299:HIS:C	2.63	0.40
1:C:472:ARG:CD	1:C:476:GLU:OE2	2.70	0.40
1:D:332:ARG:HA	1:D:333:PRO:HD3	1.88	0.40
1:D:397:LEU:HD21	1:D:401:TYR:CE2	2.56	0.40
1:D:455:HIS:O	1:D:459:ILE:HG22	2.22	0.40
1:D:508:ARG:HD3	1:D:508:ARG:C	2.45	0.40
1:E:114:GLY:O	1:E:117:TYR:HB3	2.22	0.40
1:F:301:VAL:HG13	1:F:437:TRP:HH2	1.85	0.40
1:F:418:GLY:O	1:F:421:TYR:HB3	2.21	0.40
1:F:436:ALA:O	1:F:496:VAL:HA	2.20	0.40

There are no symmetry-related clashes.

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	519/530 (98%)	444 (86%)	65 (12%)	10 (2%)	6	13
1	B	519/530 (98%)	440 (85%)	68 (13%)	11 (2%)	5	11
1	C	519/530 (98%)	430 (83%)	70 (14%)	19 (4%)	2	3
1	D	519/530 (98%)	437 (84%)	71 (14%)	11 (2%)	5	11
1	E	519/530 (98%)	441 (85%)	71 (14%)	7 (1%)	9	21
1	F	519/530 (98%)	435 (84%)	73 (14%)	11 (2%)	5	11
All	All	3114/3180 (98%)	2627 (84%)	418 (13%)	69 (2%)	5	10

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ASP
1	B	11	ILE
1	D	448	GLN
1	F	448	GLN
1	A	11	ILE
1	A	115	GLU
1	A	165	HIS
1	A	350	ILE
1	B	213	THR
1	B	375	ASP
1	C	11	ILE
1	C	85	ASP
1	C	209	ASP
1	C	227	ALA
1	C	375	ASP
1	C	404	ALA
1	C	464	ASP
1	D	140	ASP
1	D	424	MET
1	E	140	ASP

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Mol	Chain	Res	Type
1	E	232	SER
1	F	213	THR
1	B	78	ASP
1	B	140	ASP
1	C	191	THR
1	C	414	ARG
1	D	375	ASP
1	D	387	HIS
1	E	375	ASP
1	F	48	ALA
1	F	167	SER
1	F	414	ARG
1	F	452	ASN
1	F	462	ALA
1	A	221	PHE
1	B	167	SER
1	B	424	MET
1	D	11	ILE
1	E	250	TYR
1	F	47	THR
1	A	31	ALA
1	A	85	ASP
1	A	507	VAL
1	B	158	GLU
1	B	404	ALA
1	C	123	LYS
1	C	296	TYR
1	C	385	GLN
1	C	423	VAL
1	C	424	MET
1	C	477	TYR
1	C	529	PRO
1	D	123	LYS
1	D	292	ALA
1	D	462	ALA
1	E	107	THR
1	E	267	PRO
1	F	146	ILE
1	F	292	ALA
1	B	414	ARG
1	C	185	VAL
1	C	221	PHE

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Mol	Chain	Res	Type
1	D	404	ALA
1	E	251	VAL
1	F	296	TYR
1	C	210	VAL
1	B	146	ILE
1	A	377	PRO
1	D	390	ILE

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	412/421 (98%)	380 (92%)	32 (8%)	11	26
1	B	412/421 (98%)	389 (94%)	23 (6%)	19	40
1	C	412/421 (98%)	370 (90%)	42 (10%)	7	15
1	D	412/421 (98%)	387 (94%)	25 (6%)	17	37
1	E	412/421 (98%)	381 (92%)	31 (8%)	12	28
1	F	412/421 (98%)	377 (92%)	35 (8%)	10	22
All	All	2472/2526 (98%)	2284 (92%)	188 (8%)	12	27

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	53	ASP
1	A	70	HIS
1	A	78	ASP
1	A	113	LEU
1	A	123	LYS
1	A	146	ILE
1	A	161	ARG
1	A	162	ARG
1	A	164	THR
1	A	175	LEU

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Mol	Chain	Res	Type
1	A	195	VAL
1	A	200	THR
1	A	263	LEU
1	A	321	ASN
1	A	330	GLU
1	A	358	ARG
1	A	372	THR
1	A	384	ASP
1	A	397	LEU
1	A	398	ILE
1	A	429	LEU
1	A	435	LEU
1	A	448	GLN
1	A	473	LEU
1	A	508	ARG
1	A	513	LEU
1	A	517	ARG
1	A	518	GLU
1	A	519	SER
1	A	520	LEU
1	A	530	LEU
1	B	54	LEU
1	B	97	ARG
1	B	113	LEU
1	B	147	GLN
1	B	162	ARG
1	B	164	THR
1	B	195	VAL
1	B	209	ASP
1	B	218	ASP
1	B	277	VAL
1	B	284	LEU
1	B	294	GLN
1	B	324	THR
1	B	347	CYS
1	B	358	ARG
1	B	372	THR
1	B	397	LEU
1	B	427	LYS
1	B	429	LEU
1	B	435	LEU
1	B	448	GLN

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Mol	Chain	Res	Type
1	B	508	ARG
1	B	530	LEU
1	C	43	LYS
1	C	46	LEU
1	C	113	LEU
1	C	141	SER
1	C	147	GLN
1	C	175	LEU
1	C	200	THR
1	C	205	ILE
1	C	213	THR
1	C	231	ASN
1	C	236	VAL
1	C	253	GLN
1	C	263	LEU
1	C	265	GLU
1	C	277	VAL
1	C	279	ASP
1	C	284	LEU
1	C	288	VAL
1	C	317	LEU
1	C	330	GLU
1	C	336	ILE
1	C	339	ASN
1	C	351	THR
1	C	358	ARG
1	C	372	THR
1	C	380	LEU
1	C	384	ASP
1	C	397	LEU
1	C	406	VAL
1	C	427	LYS
1	C	429	LEU
1	C	435	LEU
1	C	441	GLN
1	C	465	ASP
1	C	473	LEU
1	C	479	ASP
1	C	494	ASP
1	C	508	ARG
1	C	512	GLN
1	C	517	ARG

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Mol	Chain	Res	Type
1	C	520	LEU
1	C	530	LEU
1	D	71	ARG
1	D	78	ASP
1	D	97	ARG
1	D	113	LEU
1	D	130	LYS
1	D	147	GLN
1	D	164	THR
1	D	175	LEU
1	D	195	VAL
1	D	199	GLN
1	D	205	ILE
1	D	218	ASP
1	D	284	LEU
1	D	321	ASN
1	D	353	SER
1	D	358	ARG
1	D	372	THR
1	D	427	LYS
1	D	429	LEU
1	D	435	LEU
1	D	444	VAL
1	D	475	GLN
1	D	476	GLU
1	D	490	ARG
1	D	508	ARG
1	E	13	THR
1	E	27	GLU
1	E	54	LEU
1	E	80	ASN
1	E	113	LEU
1	E	146	ILE
1	E	175	LEU
1	E	187	SER
1	E	199	GLN
1	E	213	THR
1	E	263	LEU
1	E	284	LEU
1	E	301	VAL
1	E	330	GLU
1	E	358	ARG

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Mol	Chain	Res	Type
1	E	367	ASN
1	E	372	THR
1	E	398	ILE
1	E	427	LYS
1	E	429	LEU
1	E	433	LEU
1	E	435	LEU
1	E	441	GLN
1	E	475	GLN
1	E	481	LEU
1	E	494	ASP
1	E	505	HIS
1	E	508	ARG
1	E	512	GLN
1	E	513	LEU
1	E	530	LEU
1	F	46	LEU
1	F	47	THR
1	F	49	ARG
1	F	107	THR
1	F	113	LEU
1	F	124	VAL
1	F	162	ARG
1	F	175	LEU
1	F	200	THR
1	F	205	ILE
1	F	231	ASN
1	F	263	LEU
1	F	272	GLU
1	F	277	VAL
1	F	281	ASP
1	F	288	VAL
1	F	290	ASP
1	F	301	VAL
1	F	321	ASN
1	F	358	ARG
1	F	372	THR
1	F	384	ASP
1	F	397	LEU
1	F	406	VAL
1	F	414	ARG
1	F	427	LYS

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Mol	Chain	Res	Type
1	F	429	LEU
1	F	435	LEU
1	F	465	ASP
1	F	473	LEU
1	F	475	GLN
1	F	482	LEU
1	F	494	ASP
1	F	508	ARG
1	F	512	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	40	GLN
1	A	172	GLN
1	A	202	HIS
1	A	231	ASN
1	A	239	HIS
1	A	294	GLN
1	A	315	GLN
1	A	367	ASN
1	A	452	ASN
1	A	455	HIS
1	A	483	ASN
1	A	512	GLN
1	A	527	ASN
1	B	30	HIS
1	B	70	HIS
1	B	119	GLN
1	B	147	GLN
1	B	163	ASN
1	B	231	ASN
1	B	253	GLN
1	B	293	ASN
1	B	343	GLN
1	B	452	ASN
1	B	475	GLN
1	B	483	ASN
1	B	512	GLN
1	B	527	ASN
1	C	30	HIS

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Mol	Chain	Res	Type
1	C	40	GLN
1	C	41	HIS
1	C	119	GLN
1	C	163	ASN
1	C	172	GLN
1	C	231	ASN
1	C	261	ASN
1	C	367	ASN
1	C	441	GLN
1	C	452	ASN
1	C	455	HIS
1	C	475	GLN
1	C	483	ASN
1	C	512	GLN
1	C	527	ASN
1	D	30	HIS
1	D	40	GLN
1	D	119	GLN
1	D	147	GLN
1	D	163	ASN
1	D	199	GLN
1	D	231	ASN
1	D	294	GLN
1	D	452	ASN
1	D	512	GLN
1	D	527	ASN
1	E	40	GLN
1	E	80	ASN
1	E	163	ASN
1	E	172	GLN
1	E	199	GLN
1	E	231	ASN
1	E	299	HIS
1	E	315	GLN
1	E	343	GLN
1	E	367	ASN
1	E	434	ASN
1	E	441	GLN
1	E	448	GLN
1	E	455	HIS
1	E	483	ASN
1	E	512	GLN

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Mol	Chain	Res	Type
1	E	527	ASN
1	F	30	HIS
1	F	40	GLN
1	F	74	ASN
1	F	104	GLN
1	F	147	GLN
1	F	163	ASN
1	F	231	ASN
1	F	253	GLN
1	F	294	GLN
1	F	315	GLN
1	F	367	ASN
1	F	385	GLN
1	F	475	GLN
1	F	483	ASN
1	F	512	GLN
1	F	527	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	521/530 (98%)	0.71	25 (4%)	35	30	36, 57, 77, 113	0
1	B	521/530 (98%)	0.69	17 (3%)	49	43	37, 57, 78, 116	0
1	C	521/530 (98%)	0.74	32 (6%)	27	22	37, 59, 76, 111	0
1	D	521/530 (98%)	0.66	25 (4%)	35	30	38, 57, 77, 117	0
1	E	521/530 (98%)	0.73	31 (5%)	27	22	35, 57, 77, 115	0
1	F	521/530 (98%)	0.76	28 (5%)	31	26	40, 60, 76, 113	0
All	All	3126/3180 (98%)	0.72	158 (5%)	33	28	35, 58, 77, 117	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	508	ARG	5.7
1	F	225	GLY	4.5
1	A	109	PHE	4.4
1	B	72	SER	4.3
1	E	508	ARG	4.3
1	F	454	LEU	4.1
1	B	508	ARG	4.1
1	E	242	GLY	3.9
1	E	221	PHE	3.9
1	F	508	ARG	3.8
1	A	508	ARG	3.8
1	A	83	TYR	3.8
1	C	508	ARG	3.6
1	B	417	PHE	3.6
1	B	152	SER	3.6
1	A	365	ALA	3.5
1	D	411	VAL	3.4
1	E	231	ASN	3.3
1	C	25	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	398	ILE	3.3
1	A	245	LYS	3.3
1	F	236	VAL	3.3
1	D	347	CYS	3.2
1	C	294	GLN	3.2
1	F	224	LEU	3.2
1	B	35	ARG	3.2
1	F	181	ALA	3.1
1	E	73	THR	3.1
1	A	87	VAL	3.1
1	F	221	PHE	3.1
1	F	477	TYR	3.1
1	F	347	CYS	3.0
1	E	109	PHE	3.0
1	B	504	ARG	3.0
1	D	498	MET	2.9
1	E	453	ILE	2.9
1	E	72	SER	2.8
1	E	54	LEU	2.8
1	F	237	ALA	2.8
1	C	94	VAL	2.8
1	C	160	PHE	2.8
1	E	347	CYS	2.8
1	F	205	ILE	2.8
1	C	72	SER	2.8
1	E	25	ILE	2.7
1	C	443	ALA	2.7
1	E	67	PHE	2.7
1	E	383	VAL	2.7
1	C	179	PRO	2.7
1	D	183	GLY	2.7
1	A	332	ARG	2.7
1	F	231	ASN	2.7
1	A	459	ILE	2.6
1	D	224	LEU	2.6
1	A	160	PHE	2.6
1	F	296	TYR	2.6
1	C	32	GLY	2.6
1	E	320	PRO	2.6
1	E	200	THR	2.5
1	D	397	LEU	2.5
1	C	445	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	388	ASP	2.5
1	C	454	LEU	2.5
1	D	282	ALA	2.5
1	C	202	HIS	2.5
1	C	75	PHE	2.5
1	E	159	ILE	2.4
1	F	242	GLY	2.4
1	F	342	MET	2.4
1	C	507	VAL	2.4
1	D	496	VAL	2.4
1	C	204	PHE	2.4
1	D	54	LEU	2.4
1	F	463	GLY	2.4
1	F	480	ALA	2.4
1	B	412	ILE	2.4
1	B	155	ALA	2.4
1	A	366	PHE	2.4
1	B	397	LEU	2.3
1	C	499	PRO	2.3
1	D	438	PRO	2.3
1	D	332	ARG	2.3
1	D	124	VAL	2.3
1	E	236	VAL	2.3
1	E	301	VAL	2.3
1	A	237	ALA	2.3
1	C	420	ALA	2.3
1	D	473	LEU	2.3
1	F	319	ALA	2.3
1	B	477	TYR	2.3
1	A	80	ASN	2.3
1	A	140	ASP	2.3
1	C	365	ALA	2.3
1	A	398	ILE	2.3
1	B	391	ILE	2.3
1	D	391	ILE	2.3
1	D	474	ILE	2.3
1	E	336	ILE	2.3
1	B	461	ASP	2.3
1	C	504	ARG	2.3
1	E	382	GLY	2.3
1	C	390	ILE	2.2
1	E	112	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	58	GLU	2.2
1	A	231	ASN	2.2
1	C	389	GLY	2.2
1	E	77	LEU	2.2
1	E	156	TYR	2.2
1	E	470	ARG	2.2
1	C	388	ASP	2.2
1	E	75	PHE	2.2
1	D	92	GLY	2.2
1	F	183	GLY	2.2
1	F	453	ILE	2.2
1	F	31	ALA	2.2
1	C	183	GLY	2.2
1	C	327	GLY	2.2
1	A	387	HIS	2.2
1	B	202	HIS	2.2
1	E	305	VAL	2.2
1	A	443	ALA	2.1
1	E	19	ALA	2.1
1	E	462	ALA	2.1
1	F	338	ALA	2.1
1	A	77	LEU	2.1
1	A	72	SER	2.1
1	C	398	ILE	2.1
1	D	106	PHE	2.1
1	F	67	PHE	2.1
1	F	344	PHE	2.1
1	A	462	ALA	2.1
1	E	29	THR	2.1
1	F	499	PRO	2.1
1	A	159	ILE	2.1
1	A	391	ILE	2.1
1	D	288	VAL	2.1
1	D	442	ILE	2.1
1	F	28	ALA	2.1
1	B	25	ILE	2.1
1	C	500	SER	2.1
1	D	128	ALA	2.1
1	D	319	ALA	2.1
1	C	178	GLY	2.1
1	A	485	TYR	2.1
1	A	236	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	373	PHE	2.1
1	C	231	ASN	2.0
1	F	70	HIS	2.0
1	C	446	GLY	2.0
1	E	205	ILE	2.0
1	D	71	ARG	2.0
1	B	365	ALA	2.0
1	D	357	ALA	2.0
1	C	54	LEU	2.0
1	C	459	ILE	2.0
1	B	370	VAL	2.0
1	E	332	ARG	2.0
1	F	374	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.