Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:03 PM EDT

PDB ID	:	6IWQ
Title	:	Crystal structure of GalNAc-T7 with Mn2+
Authors	:	Yu, C.; Yin, Y.X.
Deposited on	:	2018-12-06
Resolution	:	2.95 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

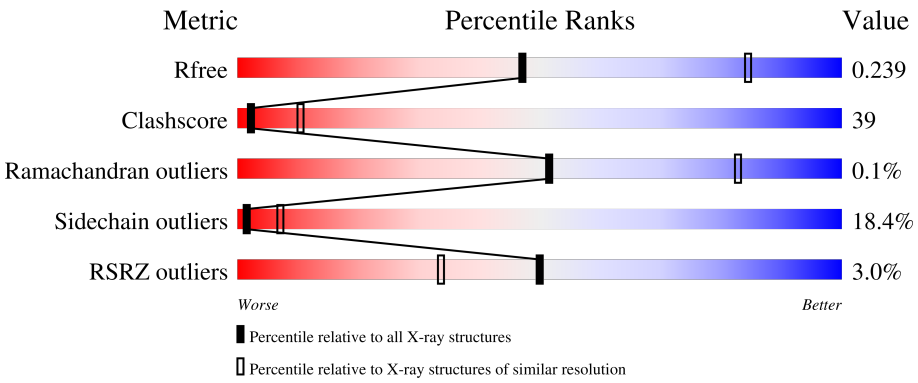
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	597	.% 46% 34% 11% • 9%
1	B	597	4% 41% 38% 12% • 9%
1	C	597	2% 49% 34% 9% • 9%
1	D	597	2% 41% 39% 12% 9%
1	E	597	4% 40% 42% 10% 9%

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Mol	Chain	Length	Quality of chain
1	F	597	4% 42% 39% 10% • 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26834 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 N-acetylgalactosaminyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	546	4440	2855	757	805	23	0	0	0
1	B	546	4440	2855	757	805	23	0	0	0
1	C	546	4440	2855	757	805	23	0	0	0
1	D	546	4440	2855	757	805	23	0	0	0
1	E	546	4440	2855	757	805	23	0	0	0
1	F	546	4440	2855	757	805	23	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

- Molecule 3 is water.

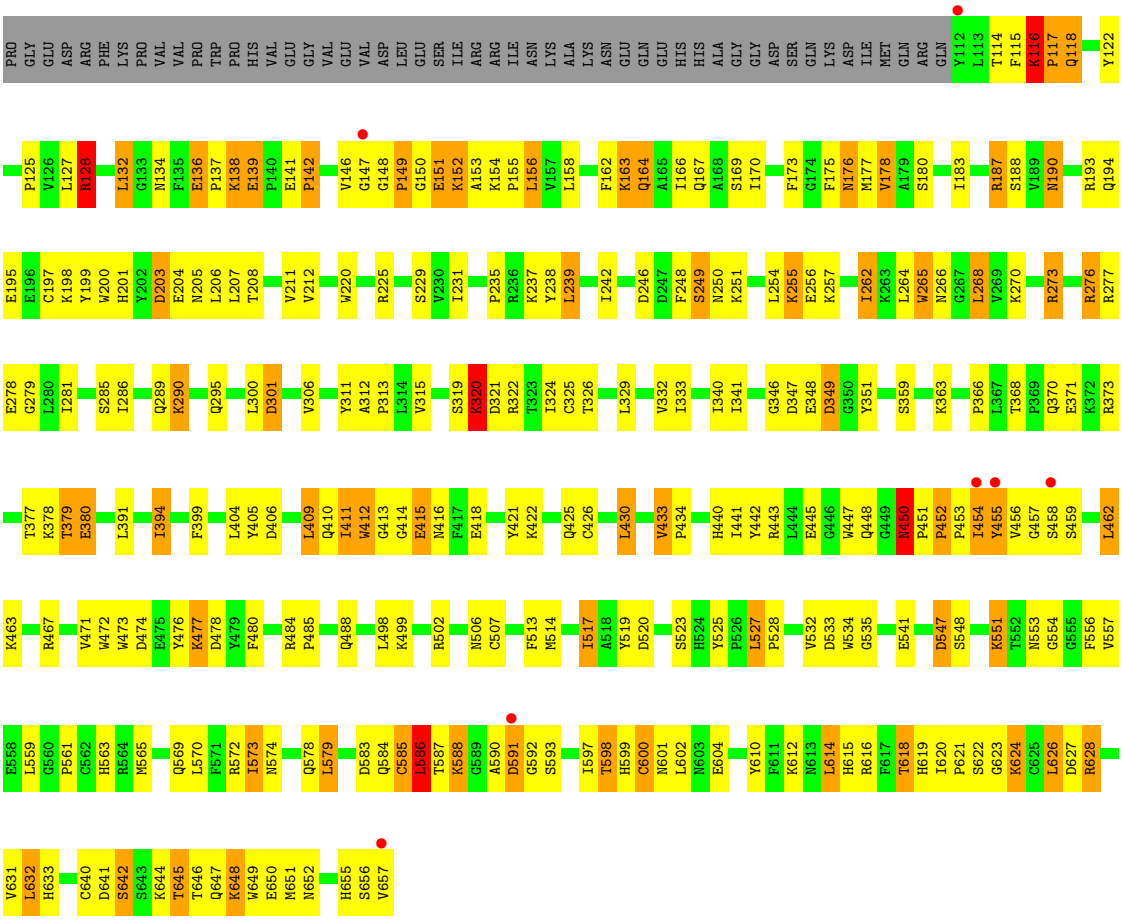
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	42	42	42	0	0
			Total	O		
3	B	31	31	31	0	0
			Total	O		
3	C	42	42	42	0	0
			Total	O		
3	D	25	25	25	0	0
			Total	O		
3	E	30	30	30	0	0
			Total	O		
3	F	18	18	18	0	0

3 Residue-property plots (i)

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

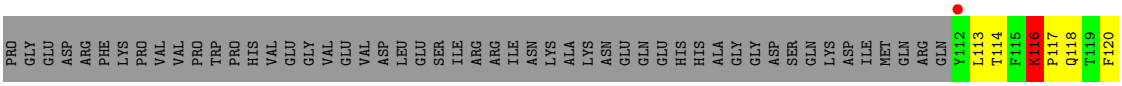
• Molecule 1: N-acetylgalactosaminyltransferase 7

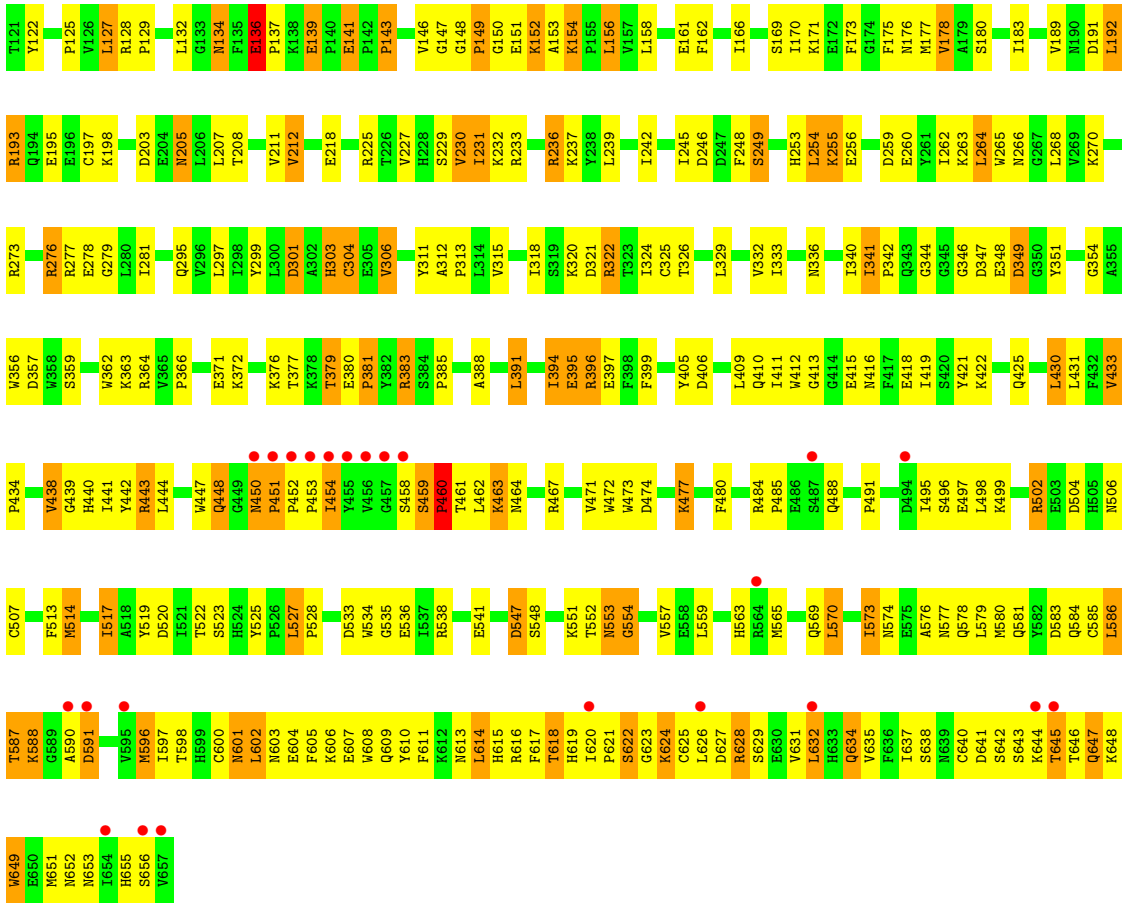
Chain A:



• Molecule 1: N-acetylgalactosaminyltransferase 7

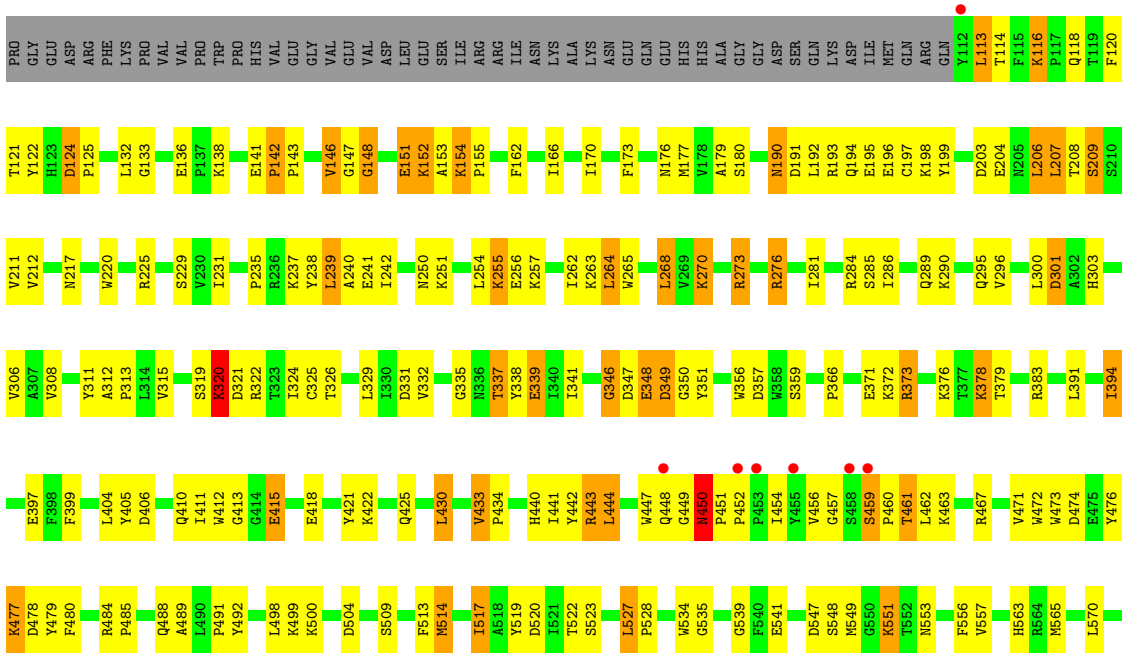
Chain B:

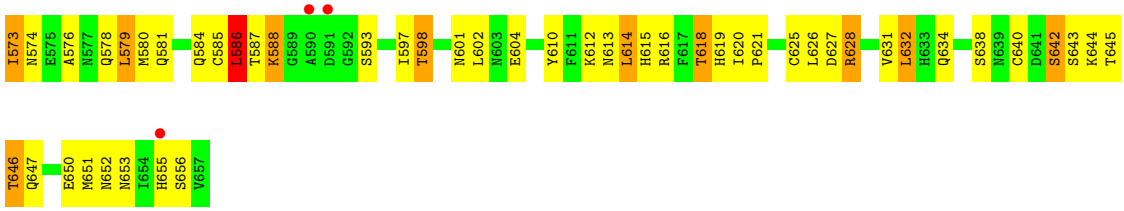




• Molecule 1: N-acetylgalactosaminyltransferase 7

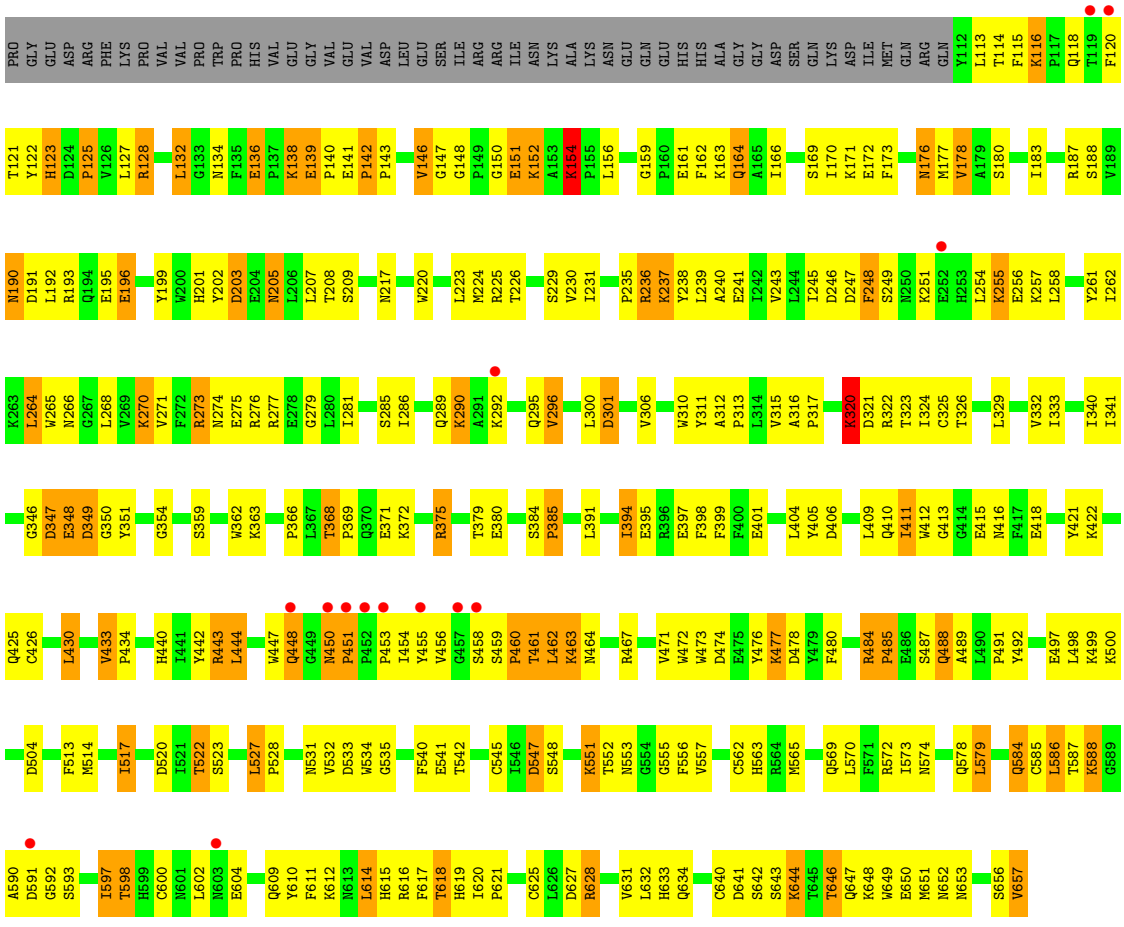
Chain C:





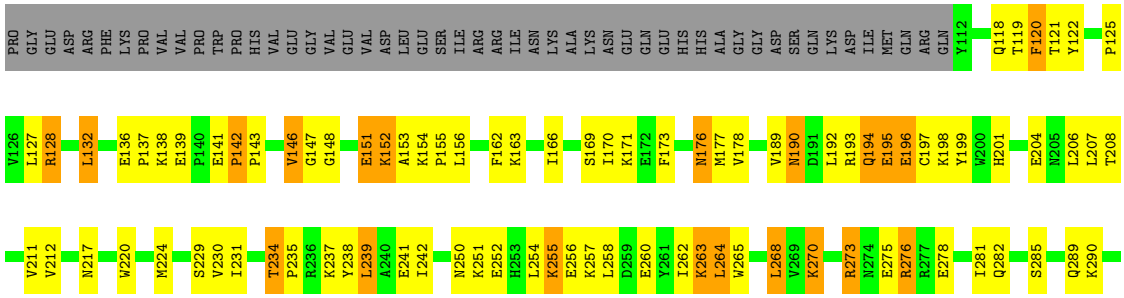
• Molecule 1: N-acetylgalactosaminyltransferase 7

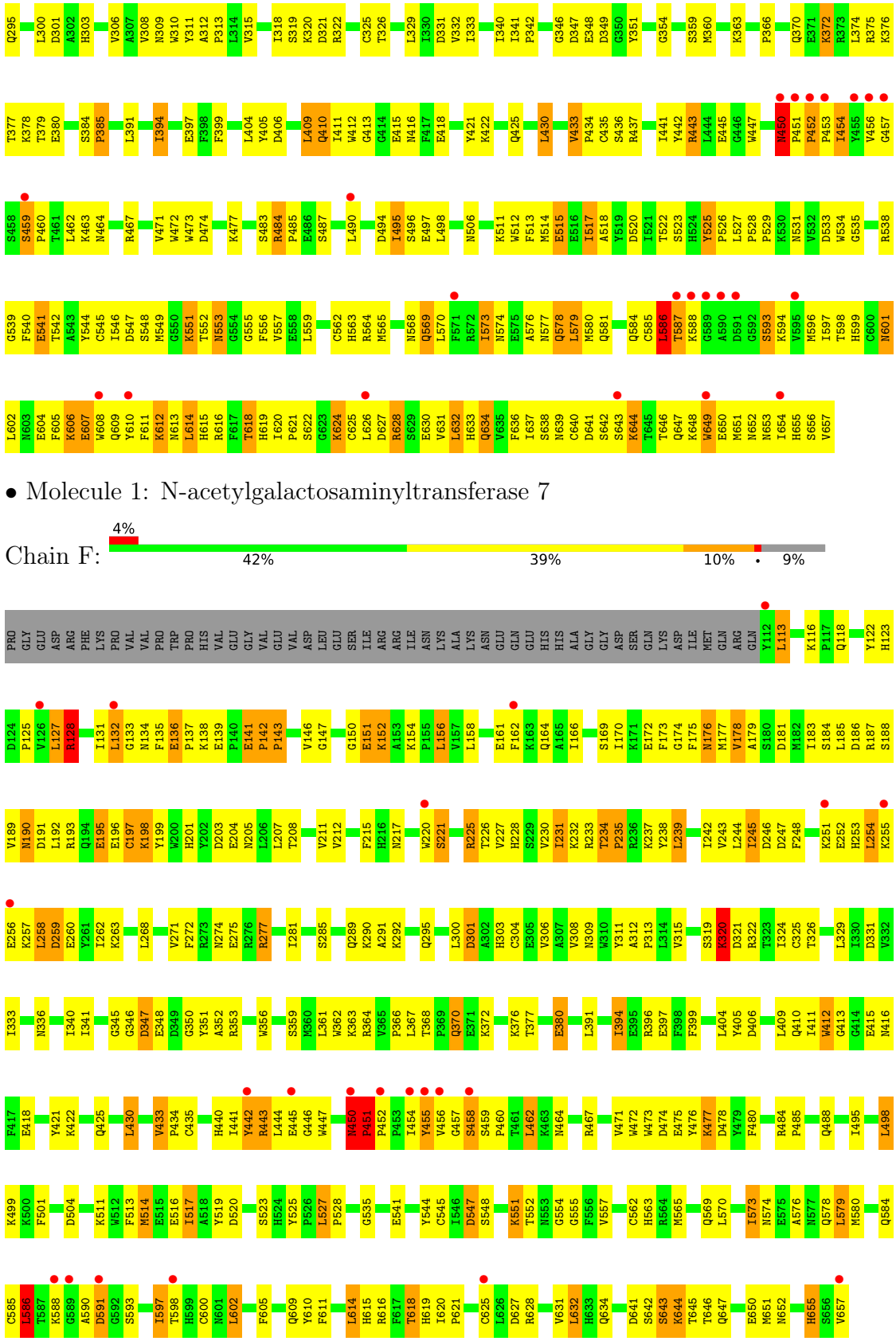
Chain D:



• Molecule 1: N-acetylgalactosaminyltransferase 7

Chain E:





• Molecule 1: N-acetylgalactosaminyltransferase 7

Chain F: 4% 42% 39% 10% • 9%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.69Å 158.23Å 251.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 2.95 49.27 – 2.95	Depositor EDS
% Data completeness (in resolution range)	88.9 (49.25-2.95) 89.0 (49.27-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.96Å)	Xtriage
Refinement program	PHENIX (dev_2400: ???)	Depositor
R, R_{free}	0.225 , 0.239 0.225 , 0.239	Depositor DCC
R_{free} test set	5179 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	26834	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.92	9/4569 (0.2%)	0.86	19/6192 (0.3%)
1	B	0.80	9/4569 (0.2%)	0.85	17/6192 (0.3%)
1	C	0.82	5/4569 (0.1%)	0.84	15/6192 (0.2%)
1	D	0.76	5/4569 (0.1%)	0.82	15/6192 (0.2%)
1	E	0.74	7/4569 (0.2%)	0.80	17/6192 (0.3%)
1	F	0.70	6/4569 (0.1%)	0.81	11/6192 (0.2%)
All	All	0.79	41/27414 (0.1%)	0.83	94/37152 (0.3%)

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	2
1	C	0	2
All	All	0	4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	PRO	N-CD	9.43	1.61	1.47
1	E	137	PRO	N-CD	8.29	1.59	1.47
1	E	212	VAL	CB-CG2	-7.39	1.37	1.52
1	A	212	VAL	CB-CG2	-7.38	1.37	1.52
1	F	212	VAL	CB-CG2	-7.37	1.37	1.52
1	C	212	VAL	CB-CG2	-7.36	1.37	1.52
1	B	212	VAL	CB-CG2	-7.35	1.37	1.52
1	B	460	PRO	N-CD	5.76	1.55	1.47
1	A	265	TRP	CE3-CZ3	-5.59	1.28	1.38
1	E	451	PRO	N-CD	5.47	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	GLU	CD-OE1	-5.46	1.19	1.25
1	C	451	PRO	N-CD	5.43	1.55	1.47
1	E	452	PRO	N-CD	5.40	1.55	1.47
1	B	149	PRO	N-CD	5.37	1.55	1.47
1	F	452	PRO	N-CD	5.27	1.55	1.47
1	C	452	PRO	N-CD	5.25	1.55	1.47
1	B	117	PRO	N-CD	5.24	1.55	1.47
1	A	125	PRO	N-CD	5.19	1.55	1.47
1	E	385	PRO	N-CD	5.18	1.55	1.47
1	D	460	PRO	N-CD	5.18	1.55	1.47
1	E	125	PRO	N-CD	5.18	1.55	1.47
1	B	125	PRO	N-CD	5.17	1.55	1.47
1	F	125	PRO	N-CD	5.17	1.55	1.47
1	A	117	PRO	N-CD	5.16	1.55	1.47
1	C	125	PRO	N-CD	5.14	1.55	1.47
1	F	320	LYS	CD-CE	5.14	1.64	1.51
1	C	320	LYS	CD-CE	5.14	1.64	1.51
1	A	320	LYS	CD-CE	5.12	1.64	1.51
1	D	125	PRO	N-CD	5.12	1.55	1.47
1	B	129	PRO	N-CD	5.12	1.55	1.47
1	D	320	LYS	CD-CE	5.12	1.64	1.51
1	B	143	PRO	N-CD	5.10	1.54	1.47
1	A	155	PRO	N-CD	5.04	1.54	1.47
1	D	485	PRO	N-CD	5.04	1.54	1.47
1	F	143	PRO	N-CD	5.03	1.54	1.47
1	B	381	PRO	N-CD	5.03	1.54	1.47
1	B	137	PRO	N-CD	5.03	1.54	1.47
1	F	235	PRO	N-CD	5.02	1.54	1.47
1	A	453	PRO	N-CD	5.01	1.54	1.47
1	D	385	PRO	N-CD	5.01	1.54	1.47
1	E	155	PRO	N-CD	5.01	1.54	1.47

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	133	GLY	N-CA-C	-8.75	91.23	113.10
1	C	586	LEU	CA-CB-CG	7.68	132.98	115.30
1	E	586	LEU	CA-CB-CG	7.68	132.96	115.30
1	F	586	LEU	CA-CB-CG	7.67	132.94	115.30
1	C	459	SER	C-N-CD	6.37	141.79	128.40
1	B	451	PRO	C-N-CD	6.29	141.60	128.40
1	D	451	PRO	C-N-CD	6.28	141.59	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	484	ARG	C-N-CD	6.27	141.56	128.40
1	C	484	ARG	C-N-CD	6.26	141.55	128.40
1	E	525	TYR	C-N-CD	6.26	141.55	128.40
1	A	484	ARG	C-N-CD	6.26	141.55	128.40
1	B	484	ARG	C-N-CD	6.26	141.55	128.40
1	A	527	LEU	C-N-CD	6.22	141.47	128.40
1	A	452	PRO	C-N-CD	6.20	141.43	128.40
1	B	514	MET	CG-SD-CE	-6.17	90.32	100.20
1	B	554	GLY	N-CA-C	-6.17	97.67	113.10
1	F	450	ASN	C-N-CD	6.17	141.36	128.40
1	F	514	MET	CG-SD-CE	-6.16	90.34	100.20
1	A	514	MET	CG-SD-CE	-6.16	90.35	100.20
1	C	514	MET	CG-SD-CE	-6.15	90.36	100.20
1	D	514	MET	CG-SD-CE	-6.14	90.37	100.20
1	A	137	PRO	CA-N-CD	-6.10	102.96	111.50
1	E	528	PRO	C-N-CD	6.09	141.19	128.40
1	B	452	PRO	C-N-CD	6.08	141.16	128.40
1	D	527	LEU	C-N-CD	6.03	141.07	128.40
1	C	527	LEU	C-N-CD	6.03	141.06	128.40
1	B	527	LEU	C-N-CD	6.03	141.06	128.40
1	A	528	PRO	C-N-CD	6.01	141.01	128.40
1	E	459	SER	C-N-CD	6.00	140.99	128.40
1	F	527	LEU	C-N-CD	6.00	140.99	128.40
1	A	128	ARG	C-N-CD	5.99	140.98	128.40
1	D	136	GLU	C-N-CD	5.98	140.95	128.40
1	E	139	GLU	C-N-CD	5.95	140.90	128.40
1	D	139	GLU	C-N-CD	5.94	140.87	128.40
1	D	154	LYS	C-N-CD	5.93	140.85	128.40
1	E	137	PRO	CA-N-CD	-5.93	103.20	111.50
1	B	341	ILE	C-N-CD	5.91	140.81	128.40
1	B	433	VAL	C-N-CD	5.91	140.81	128.40
1	C	142	PRO	C-N-CD	5.91	140.81	128.40
1	A	142	PRO	C-N-CD	5.90	140.79	128.40
1	A	433	VAL	C-N-CD	5.89	140.78	128.40
1	C	433	VAL	C-N-CD	5.89	140.78	128.40
1	E	142	PRO	C-N-CD	5.89	140.77	128.40
1	D	142	PRO	C-N-CD	5.89	140.77	128.40
1	E	234	THR	C-N-CD	5.89	140.76	128.40
1	F	528	PRO	C-N-CD	5.89	140.76	128.40
1	D	433	VAL	C-N-CD	5.88	140.75	128.40
1	E	433	VAL	C-N-CD	5.88	140.74	128.40
1	F	433	VAL	C-N-CD	5.87	140.74	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	459	SER	C-N-CD	5.87	140.73	128.40
1	B	528	PRO	C-N-CD	5.87	140.73	128.40
1	B	141	GLU	C-N-CD	5.87	140.72	128.40
1	C	528	PRO	C-N-CD	5.86	140.71	128.40
1	D	528	PRO	C-N-CD	5.86	140.71	128.40
1	B	128	ARG	C-N-CD	5.84	140.67	128.40
1	F	128	ARG	C-N-CD	5.84	140.66	128.40
1	A	139	GLU	C-N-CD	5.83	140.65	128.40
1	A	450	ASN	C-N-CD	5.83	140.64	128.40
1	D	384	SER	C-N-CD	5.80	140.59	128.40
1	B	139	GLU	C-N-CD	5.79	140.55	128.40
1	A	380	GLU	C-N-CD	5.77	140.52	128.40
1	D	484	ARG	C-N-CD	5.70	140.38	128.40
1	D	368	THR	C-N-CD	5.68	140.33	128.40
1	C	124	ASP	C-N-CD	5.68	140.33	128.40
1	F	451	PRO	C-N-CD	5.67	140.31	128.40
1	C	451	PRO	C-N-CD	5.67	140.30	128.40
1	B	116	LYS	C-N-CD	5.66	140.28	128.40
1	B	154	LYS	C-N-CD	5.64	140.25	128.40
1	C	154	LYS	C-N-CD	5.61	140.18	128.40
1	A	116	LYS	C-N-CD	5.60	140.16	128.40
1	A	149	PRO	CA-N-CD	-5.59	103.68	111.50
1	E	384	SER	C-N-CD	5.58	140.12	128.40
1	B	136	GLU	C-N-CD	5.55	140.06	128.40
1	E	451	PRO	C-N-CD	5.50	139.96	128.40
1	E	154	LYS	C-N-CD	5.49	139.94	128.40
1	B	148	GLY	N-CA-C	-5.42	99.56	113.10
1	E	450	ASN	C-N-CD	5.41	139.76	128.40
1	F	430	LEU	CA-CB-CG	5.33	127.56	115.30
1	C	430	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	430	LEU	CA-CB-CG	5.33	127.55	115.30
1	D	430	LEU	CA-CB-CG	5.32	127.54	115.30
1	E	430	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	430	LEU	CA-CB-CG	5.31	127.51	115.30
1	C	450	ASN	C-N-CD	5.28	139.48	128.40
1	A	148	GLY	C-N-CD	5.23	139.38	128.40
1	A	586	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	159	GLY	C-N-CD	5.18	139.28	128.40
1	A	136	GLU	C-N-CD	5.14	139.19	128.40
1	E	136	GLU	C-N-CD	5.11	139.13	128.40
1	F	247	ASP	N-CA-C	-5.08	97.28	111.00
1	D	148	GLY	N-CA-C	-5.06	100.45	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	148	GLY	N-CA-C	-5.04	100.50	113.10
1	E	119	THR	C-N-CA	-5.03	109.11	121.70
1	C	148	GLY	N-CA-C	-5.02	100.54	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	553	ASN	Peptide
1	B	645	THR	Peptide
1	C	346	GLY	Peptide
1	C	348	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4440	0	4329	269	0
1	B	4440	0	4329	441	0
1	C	4440	0	4327	268	0
1	D	4440	0	4331	374	0
1	E	4440	0	4329	387	0
1	F	4440	0	4331	356	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	42	0	0	9	0
3	B	31	0	0	10	0
3	C	42	0	0	7	0
3	D	25	0	0	4	0
3	E	30	0	0	6	0
3	F	18	0	0	8	0
All	All	26834	0	25976	2060	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (2060) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:545:CYS:HB3	1:E:562:CYS:SG	1.57	1.43
1:B:614:LEU:CD1	1:B:616:ARG:HD3	1.55	1.36
1:F:128:ARG:HG3	1:F:201:HIS:CD2	1.62	1.32
1:A:332:VAL:HG13	1:A:442:TYR:CD2	1.65	1.30
1:E:513:PHE:CE1	1:E:517:ILE:HD11	1.67	1.30
1:E:545:CYS:CB	1:E:562:CYS:HG	1.44	1.29
1:B:616:ARG:CG	1:B:648:LYS:HE3	1.61	1.29
1:D:585:CYS:SG	1:D:600:CYS:HB3	1.71	1.28
1:E:363:LYS:HD2	1:E:525:TYR:CE2	1.68	1.28
1:B:554:GLY:HA3	1:B:597:ILE:O	1.28	1.28
1:B:608:TRP:CZ3	1:B:626:LEU:HD21	1.68	1.27
1:B:614:LEU:HD13	1:B:616:ARG:CD	1.63	1.27
1:E:545:CYS:CB	1:E:562:CYS:SG	2.23	1.26
1:F:141:GLU:OE2	1:F:142:PRO:HD3	1.35	1.25
1:D:456:VAL:HG13	1:D:657:VAL:C	1.56	1.25
1:F:226:THR:HG22	1:F:304:CYS:O	1.31	1.24
1:C:625:CYS:SG	1:C:640:CYS:HB2	1.76	1.24
1:D:625:CYS:CB	1:D:640:CYS:SG	2.27	1.23
1:F:585:CYS:CB	1:F:600:CYS:SG	2.26	1.23
1:B:625:CYS:SG	1:B:640:CYS:HA	1.77	1.22
1:C:627:ASP:OD1	1:C:646:THR:HB	1.41	1.20
1:D:443:ARG:HD2	1:D:447:TRP:CE3	1.76	1.20
1:F:258:LEU:CD2	1:F:262:ILE:HD11	1.71	1.19
1:F:141:GLU:OE2	1:F:142:PRO:CD	1.92	1.18
1:D:643:SER:HB3	1:D:648:LYS:NZ	1.60	1.17
1:F:166:ILE:HG23	1:F:176:ASN:ND2	1.60	1.17
1:B:495:ILE:HD12	1:B:498:LEU:CD1	1.75	1.16
1:F:226:THR:HG21	1:F:304:CYS:H	1.07	1.16
1:D:522:THR:CG2	1:D:527:LEU:HD11	1.76	1.16
1:E:625:CYS:SG	1:E:640:CYS:HB2	1.85	1.16
1:F:545:CYS:SG	1:F:562:CYS:SG	1.44	1.16
1:D:590:ALA:HA	1:D:592:GLY:H	1.11	1.15
1:B:495:ILE:CD1	1:B:498:LEU:HD12	1.76	1.15
1:B:601:ASN:CB	1:B:604:GLU:HG3	1.77	1.14
1:F:226:THR:CG2	1:F:304:CYS:H	1.59	1.14
1:A:132:LEU:HD23	1:A:199:TYR:CE1	1.82	1.14
1:A:153:ALA:HB3	1:A:190:ASN:HD22	1.12	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:CYS:HB3	1:B:640:CYS:SG	1.88	1.13
1:F:258:LEU:HD22	1:F:262:ILE:HD11	1.30	1.13
1:F:585:CYS:SG	1:F:600:CYS:SG	1.14	1.13
1:D:545:CYS:SG	1:D:562:CYS:CB	2.38	1.12
1:A:414:GLY:HA2	1:A:415:GLU:HB3	1.26	1.11
1:B:333:ILE:CG2	1:B:441:ILE:HD13	1.81	1.11
1:D:522:THR:HG22	1:D:527:LEU:CD1	1.82	1.10
1:D:258:LEU:O	1:D:262:ILE:HG12	1.50	1.10
1:B:585:CYS:HB2	1:B:600:CYS:HB2	1.28	1.10
1:A:132:LEU:CD2	1:A:199:TYR:HE1	1.63	1.10
1:D:348:GLU:HA	1:D:350:GLY:H	1.14	1.10
1:F:133:GLY:H	1:F:136:GLU:HG2	0.99	1.10
1:B:304:CYS:HB3	1:B:439:GLY:O	1.52	1.09
1:E:193:ARG:HH22	1:E:310:TRP:HA	1.05	1.09
1:E:627:ASP:HB2	1:E:647:GLN:HG3	1.22	1.09
1:A:455:TYR:HB2	1:A:456:VAL:HG23	1.35	1.09
1:C:457:GLY:HA2	1:C:459:SER:H	1.10	1.09
1:D:132:LEU:HD23	1:D:199:TYR:HE1	1.10	1.09
1:F:136:GLU:OE2	1:F:138:LYS:HG3	1.53	1.09
1:F:197:CYS:SG	1:F:435:CYS:SG	1.21	1.09
1:A:132:LEU:CD2	1:A:199:TYR:CE1	2.36	1.08
1:B:616:ARG:CD	1:B:648:LYS:HE3	1.84	1.08
1:E:627:ASP:HB2	1:E:647:GLN:CG	1.83	1.08
1:B:608:TRP:HZ3	1:B:626:LEU:HD21	0.92	1.08
1:D:347:ASP:HB2	1:D:351:TYR:H	1.19	1.08
1:B:626:LEU:HB2	1:B:649:TRP:CH2	1.88	1.08
1:F:116:LYS:HD3	1:F:397:GLU:OE1	1.52	1.08
1:F:348:GLU:HA	1:F:350:GLY:H	1.13	1.08
1:B:538:ARG:O	1:B:649:TRP:HB3	1.52	1.07
1:D:443:ARG:CD	1:D:447:TRP:CE3	2.36	1.07
1:D:545:CYS:SG	1:D:562:CYS:SG	1.09	1.07
1:B:495:ILE:CD1	1:B:498:LEU:CD1	2.31	1.06
1:E:625:CYS:SG	1:E:640:CYS:CB	2.43	1.06
1:C:162:PHE:O	1:C:166:ILE:HG13	1.55	1.05
1:D:208:THR:CG2	1:D:240:ALA:HB2	1.85	1.05
1:A:153:ALA:HB3	1:A:190:ASN:ND2	1.70	1.05
1:B:616:ARG:HG2	1:B:648:LYS:HE3	1.38	1.05
1:F:133:GLY:HA2	1:F:136:GLU:HG3	1.30	1.05
1:F:348:GLU:N	1:F:348:GLU:OE1	1.89	1.05
1:B:552:THR:HB	1:B:584:GLN:HE22	1.20	1.05
1:B:333:ILE:CG2	1:B:441:ILE:CD1	2.34	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:CYS:CB	1:B:640:CYS:SG	2.45	1.05
1:A:153:ALA:CB	1:A:190:ASN:ND2	2.21	1.04
1:B:574:ASN:HD22	1:B:578:GLN:HG3	1.18	1.04
1:C:203:ASP:O	1:C:204:GLU:HB2	1.55	1.04
1:C:574:ASN:HD22	1:C:578:GLN:HG3	1.18	1.04
1:D:584:GLN:HG2	1:D:597:ILE:HG23	1.40	1.04
1:E:627:ASP:HB3	3:E:808:HOH:O	1.58	1.03
1:F:574:ASN:HD22	1:F:578:GLN:HG3	1.18	1.03
1:E:332:VAL:HG13	1:E:442:TYR:CD2	1.94	1.03
1:C:116:LYS:HE2	1:C:397:GLU:OE1	1.59	1.03
1:A:132:LEU:HD23	1:A:199:TYR:HE1	0.91	1.02
1:D:585:CYS:SG	1:D:600:CYS:CB	2.46	1.02
1:D:139:GLU:HG3	1:D:140:PRO:HD2	1.35	1.02
1:D:236:ARG:HG3	1:D:236:ARG:HH11	1.22	1.02
1:A:276:ARG:HD2	1:A:278:GLU:OE2	1.59	1.02
1:C:632:LEU:H	1:C:632:LEU:HD12	1.21	1.02
1:B:301:ASP:OD2	1:B:440:HIS:HE1	1.40	1.01
1:E:193:ARG:HH22	1:E:310:TRP:CA	1.72	1.01
1:C:155:PRO:HD3	1:C:339:GLU:HG3	1.39	1.01
1:D:485:PRO:O	1:D:488:GLN:HG3	1.60	1.01
1:E:627:ASP:CB	1:E:647:GLN:HG3	1.89	1.01
1:B:333:ILE:HG21	1:B:441:ILE:CD1	1.90	1.01
1:F:133:GLY:N	1:F:136:GLU:HG2	1.74	1.01
1:F:243:VAL:HG12	1:F:245:ILE:CD1	1.90	1.01
1:B:506:ASN:HB3	3:B:804:HOH:O	1.59	1.01
1:D:625:CYS:SG	1:D:640:CYS:SG	1.11	1.00
1:A:574:ASN:HD22	1:A:578:GLN:HG3	1.26	1.00
1:E:457:GLY:HA2	1:E:459:SER:H	1.23	1.00
1:B:583:ASP:OD1	1:B:584:GLN:HG3	1.61	1.00
1:C:372:LYS:HE3	1:C:378:LYS:HZ1	1.25	0.99
1:E:413:GLY:CA	1:E:464:ASN:HD22	1.74	0.99
1:A:332:VAL:HG13	1:A:442:TYR:HD2	1.00	0.99
1:D:348:GLU:OE1	1:D:348:GLU:N	1.96	0.98
1:A:456:VAL:HG13	1:A:458:SER:HB3	1.44	0.98
1:E:370:GLN:OE1	1:E:370:GLN:N	1.96	0.98
1:C:625:CYS:SG	1:C:640:CYS:CB	2.51	0.98
1:D:132:LEU:HD23	1:D:199:TYR:CE1	1.98	0.98
1:E:632:LEU:HD12	1:E:632:LEU:H	1.26	0.97
1:E:625:CYS:HG	1:E:640:CYS:CB	1.77	0.97
1:F:172:GLU:HG2	1:F:173:PHE:CE2	1.98	0.97
1:B:150:GLY:HA3	1:B:183:ILE:HG23	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ILE:HG21	1:B:441:ILE:HD11	1.46	0.97
1:E:363:LYS:CD	1:E:525:TYR:CE2	2.48	0.97
1:A:454:ILE:HD12	1:A:455:TYR:N	1.79	0.96
1:E:193:ARG:NH2	1:E:310:TRP:HA	1.78	0.96
1:D:443:ARG:HD2	1:D:447:TRP:CZ3	1.99	0.96
1:A:456:VAL:HG13	1:A:458:SER:CB	1.95	0.96
1:B:534:TRP:HA	1:B:651:MET:CE	1.96	0.96
1:B:603:ASN:HB3	1:B:606:LYS:HE2	1.48	0.96
1:C:207:LEU:HD21	1:C:319:SER:HA	1.46	0.96
1:F:363:LYS:HD2	1:F:525:TYR:CZ	2.01	0.95
1:E:627:ASP:OD1	1:E:646:THR:HB	1.67	0.95
1:F:136:GLU:CD	1:F:138:LYS:HG3	1.87	0.95
1:F:545:CYS:CB	1:F:562:CYS:SG	2.53	0.95
1:F:197:CYS:SG	1:F:435:CYS:CB	2.54	0.95
1:E:166:ILE:HG12	1:E:178:VAL:HG21	1.48	0.95
1:B:458:SER:O	1:B:462:LEU:HB3	1.65	0.95
1:B:626:LEU:HD23	1:B:637:ILE:HG22	1.46	0.95
1:B:601:ASN:O	1:B:604:GLU:HB2	1.66	0.94
1:E:556:PHE:CD2	1:E:594:LYS:HD3	2.02	0.94
1:E:363:LYS:HD2	1:E:525:TYR:CZ	2.02	0.94
1:B:534:TRP:N	1:B:651:MET:HE2	1.82	0.94
1:A:332:VAL:CG1	1:A:442:TYR:HD2	1.80	0.94
1:F:128:ARG:HG3	1:F:201:HIS:HD2	1.26	0.94
1:D:522:THR:HG22	1:D:527:LEU:HD11	1.38	0.94
1:B:625:CYS:SG	1:B:640:CYS:CA	2.55	0.94
1:B:246:ASP:OD1	1:B:249:SER:HB2	1.68	0.94
1:D:171:LYS:HD3	1:D:448:GLN:HE22	1.32	0.94
1:D:456:VAL:HG13	1:D:657:VAL:O	1.67	0.94
1:A:347:ASP:HB2	1:A:351:TYR:O	1.68	0.94
1:B:587:THR:HG21	1:B:605:PHE:CG	2.04	0.93
1:B:301:ASP:OD2	1:B:440:HIS:CE1	2.21	0.93
1:D:590:ALA:HA	1:D:592:GLY:N	1.83	0.93
1:D:132:LEU:CD2	1:D:199:TYR:HE1	1.81	0.93
1:D:348:GLU:HB2	1:D:349:ASP:HA	1.47	0.93
1:B:391:LEU:HD13	1:B:438:VAL:HG21	1.50	0.93
1:F:641:ASP:H	1:F:647:GLN:HE22	1.12	0.92
1:A:147:GLY:O	1:D:489:ALA:HB1	1.70	0.92
1:D:132:LEU:CD2	1:D:199:TYR:CE1	2.52	0.92
1:D:161:GLU:OE1	1:D:161:GLU:N	2.03	0.92
1:F:243:VAL:HG12	1:F:245:ILE:HD11	1.49	0.92
1:B:588:LYS:NZ	1:B:588:LYS:HB3	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:ARG:HD2	1:B:648:LYS:HE3	1.52	0.91
1:E:624:LYS:HG3	1:E:638:SER:C	1.90	0.91
1:B:626:LEU:CB	1:B:649:TRP:CH2	2.52	0.91
1:D:522:THR:HG21	1:D:527:LEU:HD11	1.51	0.91
1:F:226:THR:CG2	1:F:304:CYS:N	2.32	0.91
1:D:237:LYS:HG3	1:D:238:TYR:CD2	2.06	0.91
1:D:443:ARG:NE	1:D:447:TRP:CZ3	2.38	0.91
1:A:414:GLY:HA2	1:A:415:GLU:CB	1.96	0.91
1:D:456:VAL:CG1	1:D:657:VAL:C	2.38	0.91
1:C:474:ASP:O	1:C:477:LYS:HG2	1.71	0.91
1:F:396:ARG:HG2	1:F:396:ARG:HH11	1.36	0.91
1:B:495:ILE:HD12	1:B:498:LEU:HD12	0.93	0.91
1:F:226:THR:HG21	1:F:304:CYS:N	1.86	0.91
1:B:333:ILE:CB	1:B:441:ILE:HD13	2.01	0.91
1:A:153:ALA:CB	1:A:190:ASN:HD22	1.78	0.90
1:B:552:THR:HB	1:B:584:GLN:NE2	1.85	0.90
1:E:281:ILE:HD11	1:E:413:GLY:H	1.37	0.90
1:B:619:HIS:NE2	1:B:621:PRO:HG2	1.86	0.90
1:D:248:PHE:CE1	1:D:275:GLU:O	2.24	0.89
1:D:273:ARG:HG2	1:D:273:ARG:HH11	1.34	0.89
1:E:462:LEU:HD11	1:E:487:SER:OG	1.72	0.89
1:B:616:ARG:CG	1:B:648:LYS:CE	2.50	0.89
1:B:626:LEU:C	1:B:649:TRP:HH2	1.76	0.89
1:C:457:GLY:HA2	1:C:459:SER:N	1.88	0.89
1:F:348:GLU:HA	1:F:350:GLY:N	1.87	0.89
1:D:347:ASP:HB3	1:D:348:GLU:CA	2.01	0.89
1:F:258:LEU:O	1:F:262:ILE:HG12	1.71	0.89
1:A:147:GLY:O	1:D:489:ALA:CB	2.21	0.89
1:C:208:THR:CG2	1:C:240:ALA:HB2	2.01	0.89
1:F:641:ASP:H	1:F:647:GLN:NE2	1.70	0.89
1:D:643:SER:HB3	1:D:648:LYS:HZ1	1.21	0.89
1:B:534:TRP:CA	1:B:651:MET:CE	2.52	0.88
1:B:458:SER:HB3	1:B:459:SER:OG	1.71	0.88
1:B:626:LEU:O	1:B:649:TRP:CH2	2.26	0.88
1:F:133:GLY:H	1:F:136:GLU:CG	1.85	0.88
1:F:475:GLU:OE1	1:F:511:LYS:HE2	1.74	0.88
1:A:474:ASP:O	1:A:477:LYS:HG2	1.74	0.88
1:E:474:ASP:O	1:E:477:LYS:HG2	1.74	0.88
1:E:514:MET:HE2	1:E:518:ALA:HB3	1.52	0.88
1:D:122:TYR:CE1	1:D:203:ASP:HB3	2.08	0.87
1:D:584:GLN:HG3	1:D:598:THR:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:LYS:CD	1:F:397:GLU:OE1	2.22	0.87
1:C:485:PRO:O	1:C:488:GLN:HG3	1.74	0.87
1:F:474:ASP:O	1:F:477:LYS:HG2	1.74	0.87
1:B:485:PRO:O	1:B:488:GLN:HG3	1.74	0.87
1:F:215:PHE:CE1	1:F:254:LEU:HD13	2.10	0.87
1:B:608:TRP:HZ3	1:B:626:LEU:CD2	1.82	0.87
1:B:626:LEU:CB	1:B:649:TRP:HH2	1.84	0.87
1:E:624:LYS:HG3	1:E:638:SER:O	1.75	0.87
1:B:474:ASP:O	1:B:477:LYS:HG2	1.75	0.86
1:D:237:LYS:HD2	1:D:238:TYR:CE2	2.10	0.86
1:E:548:SER:O	1:E:551:LYS:HG3	1.74	0.86
1:F:346:GLY:HA2	1:F:366:PRO:HB3	1.56	0.86
1:A:590:ALA:HB1	1:A:591:ASP:HA	1.55	0.86
1:F:485:PRO:O	1:F:488:GLN:HG3	1.74	0.86
1:A:485:PRO:O	1:A:488:GLN:HG3	1.74	0.86
1:F:186:ASP:OD1	1:F:228:HIS:HD2	1.57	0.86
1:A:533:ASP:OD2	1:A:612:LYS:HE2	1.76	0.86
1:C:346:GLY:HA2	1:C:366:PRO:HB3	1.55	0.86
1:D:208:THR:HB	1:D:295:GLN:HG3	1.58	0.86
1:E:556:PHE:CE2	1:E:594:LYS:HD3	2.10	0.86
1:B:495:ILE:HD11	1:B:498:LEU:HD13	1.57	0.86
1:B:616:ARG:HD2	1:B:648:LYS:CE	2.05	0.86
1:D:348:GLU:HA	1:D:350:GLY:N	1.89	0.86
1:D:450:ASN:HB2	1:D:451:PRO:HD2	1.57	0.86
1:F:454:ILE:HD12	1:F:460:PRO:CD	2.04	0.86
1:C:207:LEU:HD23	1:C:319:SER:OG	1.76	0.86
1:F:128:ARG:CG	1:F:201:HIS:CD2	2.56	0.86
1:F:655:HIS:CA	3:F:809:HOH:O	2.23	0.85
1:B:304:CYS:CB	1:B:439:GLY:O	2.24	0.85
1:B:333:ILE:HB	1:B:441:ILE:HD13	1.58	0.85
1:B:587:THR:HG21	1:B:605:PHE:CD2	2.11	0.85
1:D:258:LEU:CD1	1:D:262:ILE:HD11	2.06	0.85
1:D:443:ARG:CD	1:D:447:TRP:CZ3	2.56	0.85
1:F:454:ILE:HD12	1:F:460:PRO:HD3	1.55	0.85
1:D:166:ILE:HG12	1:D:178:VAL:HG21	1.58	0.85
1:E:143:PRO:HG2	1:E:146:VAL:HG12	1.59	0.85
1:E:276:ARG:HD2	1:E:278:GLU:OE2	1.76	0.85
1:A:147:GLY:C	1:D:489:ALA:HB1	1.97	0.85
1:A:641:ASP:H	1:A:647:GLN:HE22	1.21	0.85
1:C:207:LEU:CD2	1:C:319:SER:OG	2.24	0.85
1:D:208:THR:HG21	1:D:240:ALA:HB2	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:628:ARG:HG2	1:E:628:ARG:HH11	1.38	0.85
1:F:456:VAL:C	1:F:458:SER:HA	1.96	0.85
1:B:346:GLY:HA3	1:B:366:PRO:HB3	1.58	0.85
1:D:122:TYR:HE1	1:D:203:ASP:HB3	1.41	0.85
1:E:513:PHE:CE1	1:E:517:ILE:CD1	2.58	0.84
1:B:601:ASN:HB2	1:B:604:GLU:HG3	1.59	0.84
1:B:534:TRP:HA	1:B:651:MET:HE3	1.56	0.84
1:D:600:CYS:SG	1:D:604:GLU:O	2.36	0.84
1:F:632:LEU:H	1:F:632:LEU:HD12	1.42	0.84
1:D:347:ASP:OD2	1:D:351:TYR:HB2	1.76	0.84
1:B:450:ASN:HB2	1:B:451:PRO:HD2	1.57	0.84
1:F:457:GLY:N	1:F:458:SER:HA	1.90	0.84
1:B:122:TYR:CE1	1:B:203:ASP:HB2	2.13	0.84
1:F:253:HIS:CE1	1:F:254:LEU:HD21	2.13	0.84
1:D:332:VAL:HG13	1:D:442:TYR:CD1	2.13	0.84
1:E:413:GLY:HA3	1:E:464:ASN:HD22	1.40	0.84
1:B:644:LYS:HA	1:B:645:THR:C	1.98	0.84
1:D:625:CYS:SG	1:D:640:CYS:CB	2.66	0.84
1:C:281:ILE:HG12	1:C:415:GLU:HG2	1.60	0.83
1:B:281:ILE:HD11	1:B:413:GLY:H	1.41	0.83
1:F:413:GLY:HA3	1:F:464:ASN:HD22	1.41	0.83
1:B:495:ILE:CD1	1:B:498:LEU:HD13	2.08	0.83
1:F:133:GLY:CA	1:F:136:GLU:HG3	2.08	0.83
1:A:346:GLY:HA3	1:A:366:PRO:HB3	1.60	0.83
1:D:574:ASN:HD22	1:D:578:GLN:HG3	1.43	0.83
1:F:150:GLY:HA3	1:F:183:ILE:HG23	1.60	0.83
1:D:143:PRO:HG2	1:D:146:VAL:HG12	1.59	0.83
1:C:628:ARG:O	1:C:646:THR:HG21	1.78	0.82
1:B:147:GLY:O	1:C:489:ALA:HB1	1.78	0.82
1:B:342:PRO:O	1:D:632:LEU:HD12	1.79	0.82
1:E:457:GLY:HA2	1:E:459:SER:N	1.95	0.82
1:D:173:PHE:CD2	1:D:177:MET:HG3	2.15	0.82
1:E:346:GLY:HA2	1:E:366:PRO:HA	1.59	0.82
1:C:628:ARG:CD	1:C:646:THR:HG22	2.09	0.82
1:D:236:ARG:HG3	1:D:236:ARG:NH1	1.93	0.82
1:B:588:LYS:HD3	1:B:637:ILE:HD11	1.61	0.82
1:B:601:ASN:HB3	1:B:604:GLU:HG3	1.60	0.82
1:F:226:THR:CG2	1:F:304:CYS:O	2.24	0.81
1:E:162:PHE:O	1:E:166:ILE:HG13	1.80	0.81
1:E:545:CYS:SG	1:E:562:CYS:HA	2.19	0.81
1:E:627:ASP:OD1	1:E:646:THR:CB	2.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:655:HIS:HA	3:F:809:HOH:O	1.79	0.81
1:B:645:THR:OG1	1:B:646:THR:HA	1.79	0.81
1:B:628:ARG:HG2	1:B:629:SER:N	1.96	0.81
1:E:132:LEU:HD23	1:E:199:TYR:HE1	1.43	0.81
1:B:563:HIS:ND1	1:B:565:MET:HB2	1.96	0.81
1:C:153:ALA:O	1:C:339:GLU:HG2	1.80	0.81
1:F:368:THR:O	1:F:372:LYS:HG3	1.80	0.81
1:F:547:ASP:HB2	1:F:569:GLN:HG2	1.63	0.81
1:C:563:HIS:ND1	1:C:565:MET:HB2	1.96	0.81
1:D:347:ASP:HB3	1:D:348:GLU:C	2.01	0.81
1:F:574:ASN:HD22	1:F:578:GLN:CG	1.94	0.81
1:B:266:ASN:HD21	1:C:500:LYS:HZ1	1.28	0.81
1:B:626:LEU:C	1:B:649:TRP:CH2	2.54	0.81
1:D:563:HIS:ND1	1:D:565:MET:HB2	1.96	0.81
1:B:391:LEU:CD1	1:B:438:VAL:CG2	2.59	0.80
1:A:347:ASP:HB3	1:A:351:TYR:H	1.47	0.80
1:F:166:ILE:HG23	1:F:176:ASN:HD21	1.42	0.80
1:F:442:TYR:HD1	1:F:443:ARG:H	1.28	0.80
1:B:547:ASP:HB2	1:B:569:GLN:HG2	1.63	0.80
1:E:332:VAL:HG13	1:E:442:TYR:HD2	1.39	0.80
1:E:545:CYS:N	1:E:562:CYS:SG	2.54	0.80
1:A:136:GLU:HG2	3:A:829:HOH:O	1.79	0.80
1:D:443:ARG:HH11	1:D:443:ARG:HG3	1.46	0.80
1:D:611:PHE:CD1	1:E:204:GLU:HB2	2.16	0.80
1:F:133:GLY:HA2	1:F:136:GLU:CG	2.12	0.80
1:F:243:VAL:CG1	1:F:245:ILE:HD11	2.11	0.80
1:C:454:ILE:HD13	1:C:460:PRO:HD3	1.62	0.80
1:F:614:LEU:O	1:F:615:HIS:HB2	1.82	0.80
1:D:584:GLN:HG2	1:D:597:ILE:CG2	2.11	0.80
1:D:547:ASP:HB2	1:D:569:GLN:HG2	1.63	0.80
1:B:614:LEU:O	1:B:615:HIS:HB2	1.79	0.79
1:D:122:TYR:CE1	1:D:203:ASP:CB	2.65	0.79
1:A:547:ASP:HB2	1:A:569:GLN:HG2	1.63	0.79
1:A:563:HIS:ND1	1:A:565:MET:HB2	1.96	0.79
1:A:585:CYS:HB2	1:A:600:CYS:SG	2.22	0.79
1:A:628:ARG:HG2	1:A:649:TRP:CH2	2.17	0.79
1:E:551:LYS:HZ2	1:E:551:LYS:HB3	1.47	0.79
1:F:136:GLU:OE1	1:F:138:LYS:HG3	1.82	0.79
1:F:363:LYS:HD2	1:F:525:TYR:CE1	2.17	0.79
1:B:162:PHE:O	1:B:166:ILE:HG13	1.82	0.79
1:B:413:GLY:HA3	1:B:464:ASN:HD22	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:545:CYS:SG	3:E:806:HOH:O	2.41	0.79
1:A:368:THR:HB	1:A:370:GLN:OE1	1.83	0.78
1:D:522:THR:HG22	1:D:527:LEU:HD12	1.64	0.78
1:F:166:ILE:CG2	1:F:176:ASN:ND2	2.43	0.78
1:F:580:MET:HG2	1:F:585:CYS:SG	2.23	0.78
1:B:538:ARG:O	1:B:649:TRP:CB	2.30	0.78
1:F:655:HIS:CG	3:F:809:HOH:O	2.34	0.78
3:A:813:HOH:O	1:C:631:VAL:CG1	2.30	0.78
1:C:456:VAL:HG22	3:C:810:HOH:O	1.83	0.78
1:E:574:ASN:ND2	1:E:578:GLN:HG3	1.98	0.78
1:E:196:GLU:HG3	3:E:813:HOH:O	1.84	0.78
1:C:207:LEU:HD21	1:C:319:SER:CA	2.14	0.78
1:E:193:ARG:CZ	1:E:435:CYS:O	2.32	0.78
1:B:554:GLY:N	1:B:598:THR:HG22	1.99	0.78
1:B:453:PRO:HB3	1:D:164:GLN:OE1	1.83	0.78
1:B:626:LEU:HD23	1:B:637:ILE:CG2	2.14	0.78
1:B:459:SER:H	1:B:462:LEU:H	1.30	0.78
1:C:574:ASN:HD22	1:C:578:GLN:CG	1.94	0.78
1:C:155:PRO:HB3	1:C:337:THR:CG2	2.14	0.78
1:A:332:VAL:CG1	1:A:442:TYR:CD2	2.58	0.77
1:B:625:CYS:SG	1:B:640:CYS:CB	2.72	0.77
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.49	0.77
1:C:443:ARG:HG3	1:C:443:ARG:HH11	1.50	0.77
1:F:444:LEU:N	1:F:444:LEU:HD12	1.99	0.77
1:B:574:ASN:HD22	1:B:578:GLN:CG	1.94	0.77
1:E:513:PHE:CZ	1:E:517:ILE:HD11	2.20	0.77
1:A:628:ARG:HH11	1:A:628:ARG:HG3	1.49	0.77
1:B:474:ASP:O	1:B:477:LYS:CG	2.31	0.77
1:B:348:GLU:N	1:B:349:ASP:O	2.17	0.77
1:B:625:CYS:SG	1:B:647:GLN:NE2	2.58	0.77
1:D:347:ASP:HB3	1:D:348:GLU:HA	1.64	0.77
1:D:258:LEU:HD12	1:D:262:ILE:HD11	1.65	0.77
1:B:191:ASP:OD1	1:B:193:ARG:HG3	1.83	0.77
1:B:347:ASP:HB3	1:B:351:TYR:H	1.49	0.77
1:D:139:GLU:HG3	1:D:140:PRO:CD	2.14	0.77
1:D:116:LYS:HD2	1:D:401:GLU:OE2	1.85	0.76
1:E:415:GLU:HG2	1:E:416:ASN:N	1.99	0.76
1:D:143:PRO:CG	1:D:146:VAL:HG12	2.15	0.76
1:E:189:VAL:CG1	1:E:340:ILE:HD12	2.15	0.76
1:D:474:ASP:O	1:D:477:LYS:HG2	1.86	0.76
1:E:625:CYS:HG	1:E:640:CYS:HG	0.81	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASP:HB3	1:B:324:ILE:HG13	1.67	0.76
1:A:128:ARG:HG3	1:A:201:HIS:CD2	2.21	0.76
1:B:586:LEU:N	1:B:586:LEU:HD23	2.01	0.76
1:F:545:CYS:SG	1:F:562:CYS:CB	2.74	0.76
1:C:155:PRO:CB	1:C:337:THR:HG23	2.16	0.76
1:C:113:LEU:N	1:C:113:LEU:HD23	2.01	0.75
1:E:143:PRO:CG	1:E:146:VAL:HG12	2.15	0.75
1:A:332:VAL:HG13	1:A:442:TYR:CE2	2.21	0.75
1:E:189:VAL:HG11	1:E:340:ILE:HD12	1.69	0.75
1:B:585:CYS:HB2	1:B:600:CYS:CB	2.12	0.75
1:B:615:HIS:O	1:B:648:LYS:HB3	1.87	0.75
1:D:632:LEU:HD23	1:D:633:HIS:N	2.02	0.75
1:E:132:LEU:HD23	1:E:199:TYR:CE1	2.22	0.75
1:C:132:LEU:HB3	1:C:199:TYR:CE1	2.22	0.75
1:E:514:MET:HE2	1:E:518:ALA:CB	2.16	0.75
1:F:143:PRO:HG2	1:F:146:VAL:HG12	1.69	0.75
1:A:166:ILE:HG23	1:A:176:ASN:ND2	2.02	0.75
1:B:447:TRP:C	1:B:448:GLN:HE21	1.89	0.75
1:E:614:LEU:O	1:E:615:HIS:HB2	1.85	0.75
1:B:534:TRP:CA	1:B:651:MET:HE2	2.15	0.75
1:F:226:THR:HG22	1:F:304:CYS:H	1.52	0.75
1:D:180:SER:OG	1:D:225:ARG:NH1	2.20	0.74
1:D:208:THR:H	1:D:295:GLN:HE21	1.33	0.74
1:E:176:ASN:HD21	1:E:178:VAL:HG22	1.52	0.74
1:F:348:GLU:CA	1:F:350:GLY:H	1.95	0.74
1:F:175:PHE:CE1	1:F:441:ILE:HG22	2.22	0.74
1:F:563:HIS:ND1	1:F:565:MET:HB2	2.02	0.74
1:E:454:ILE:HB	1:E:457:GLY:H	1.52	0.74
1:B:533:ASP:C	1:B:651:MET:HE2	2.07	0.74
1:F:172:GLU:HG2	1:F:173:PHE:CD2	2.22	0.74
1:B:601:ASN:CA	1:B:604:GLU:HG3	2.17	0.74
1:D:443:ARG:HD2	1:D:447:TRP:HE3	1.48	0.74
1:F:197:CYS:CB	1:F:435:CYS:SG	2.71	0.74
1:A:281:ILE:HD12	1:A:410:GLN:O	1.88	0.74
1:D:348:GLU:CA	1:D:350:GLY:H	1.99	0.74
1:F:133:GLY:N	1:F:136:GLU:CG	2.44	0.74
1:A:559:LEU:HB3	1:A:633:HIS:HB3	1.70	0.74
1:E:176:ASN:HD21	1:E:178:VAL:CG2	2.00	0.74
1:F:258:LEU:O	1:F:262:ILE:CG1	2.35	0.74
1:F:442:TYR:HD1	1:F:443:ARG:N	1.84	0.74
1:F:228:HIS:O	1:F:231:ILE:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:LEU:HD23	1:F:254:LEU:N	2.03	0.74
1:D:497:GLU:HG3	3:D:821:HOH:O	1.87	0.73
1:F:195:GLU:OE1	1:F:195:GLU:HA	1.87	0.73
1:A:632:LEU:HD23	3:A:817:HOH:O	1.89	0.73
1:E:628:ARG:HG2	1:E:628:ARG:NH1	1.98	0.73
1:F:226:THR:HG22	1:F:304:CYS:C	2.08	0.73
1:A:147:GLY:HA3	1:D:489:ALA:HB2	1.70	0.73
1:B:266:ASN:HD21	1:C:500:LYS:NZ	1.87	0.73
1:C:456:VAL:O	1:C:459:SER:HB3	1.87	0.73
1:F:268:LEU:O	1:F:268:LEU:HD13	1.88	0.73
1:F:351:TYR:O	1:F:367:LEU:HB2	1.87	0.73
1:B:632:LEU:HD12	1:B:632:LEU:N	2.04	0.73
1:D:456:VAL:CG1	1:D:657:VAL:O	2.36	0.73
1:E:207:LEU:CD1	1:E:319:SER:OG	2.36	0.73
1:E:413:GLY:HA3	1:E:464:ASN:ND2	2.02	0.73
1:E:471:VAL:HB	1:E:495:ILE:HD11	1.70	0.73
1:F:192:LEU:HD12	1:F:331:ASP:OD2	1.88	0.73
1:F:226:THR:HG22	1:F:304:CYS:N	2.03	0.73
1:B:554:GLY:CA	1:B:597:ILE:O	2.23	0.73
1:B:585:CYS:CB	1:B:600:CYS:HB2	2.14	0.73
1:E:363:LYS:CD	1:E:525:TYR:CZ	2.68	0.73
1:A:190:ASN:ND2	1:A:190:ASN:H	1.86	0.73
1:D:347:ASP:HB2	1:D:351:TYR:N	1.99	0.73
1:E:580:MET:HG2	1:E:585:CYS:SG	2.28	0.73
1:A:301:ASP:OD2	1:A:440:HIS:NE2	2.22	0.73
1:A:377:THR:HG22	1:A:379:THR:H	1.54	0.73
1:D:346:GLY:HA2	1:D:366:PRO:HB3	1.69	0.73
1:E:569:GLN:HB2	3:E:806:HOH:O	1.87	0.73
1:E:545:CYS:CA	1:E:562:CYS:HG	2.00	0.72
1:E:556:PHE:HD2	1:E:594:LYS:HD3	1.53	0.72
1:B:391:LEU:CD1	1:B:438:VAL:HG21	2.18	0.72
1:D:176:ASN:HD21	1:D:178:VAL:HG22	1.54	0.72
1:D:611:PHE:CD1	1:E:204:GLU:CB	2.71	0.72
1:E:413:GLY:HA2	1:E:464:ASN:HD22	1.54	0.72
1:D:281:ILE:HD11	1:D:413:GLY:H	1.53	0.72
1:B:628:ARG:HG2	1:B:629:SER:H	1.52	0.72
1:D:231:ILE:HD12	1:D:265:TRP:CD1	2.25	0.72
1:E:176:ASN:ND2	1:E:178:VAL:HG22	2.04	0.72
1:E:614:LEU:CD1	1:E:616:ARG:CZ	2.67	0.72
1:D:641:ASP:HB3	1:D:644:LYS:HG2	1.70	0.72
1:E:552:THR:HB	1:E:584:GLN:OE1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:454:ILE:N	1:F:455:TYR:HA	2.04	0.72
1:C:371:GLU:HG2	1:C:519:TYR:OH	1.89	0.72
1:E:196:GLU:OE2	1:E:196:GLU:HA	1.87	0.72
1:B:551:LYS:O	1:B:552:THR:CG2	2.37	0.72
1:F:346:GLY:HA2	1:F:366:PRO:CB	2.20	0.72
1:A:628:ARG:NH1	1:A:646:THR:HA	2.05	0.72
1:F:141:GLU:OE2	1:F:142:PRO:HD2	1.88	0.72
1:A:574:ASN:HD22	1:A:578:GLN:CG	2.02	0.72
1:B:333:ILE:HG22	1:B:441:ILE:CD1	2.19	0.72
1:C:264:LEU:O	1:C:265:TRP:HB2	1.90	0.72
1:B:413:GLY:CA	1:B:464:ASN:HD22	2.02	0.72
1:E:462:LEU:HG	1:E:490:LEU:CD2	2.20	0.71
1:F:215:PHE:HE1	1:F:254:LEU:HD13	1.55	0.71
1:F:627:ASP:OD1	1:F:646:THR:HB	1.89	0.71
1:F:632:LEU:HD12	1:F:632:LEU:N	2.04	0.71
1:B:459:SER:N	1:B:462:LEU:H	1.87	0.71
1:E:193:ARG:HH21	1:E:437:ARG:H	1.36	0.71
1:D:456:VAL:HB	1:D:459:SER:OG	1.89	0.71
1:D:643:SER:HB3	1:D:648:LYS:HZ2	1.50	0.71
1:F:234:THR:HG21	1:F:239:LEU:HG	1.71	0.71
1:A:162:PHE:O	1:A:166:ILE:HG13	1.91	0.71
1:B:122:TYR:CE1	1:B:203:ASP:CB	2.73	0.71
1:B:333:ILE:HG22	1:B:441:ILE:HD13	1.73	0.71
1:E:624:LYS:CG	1:E:638:SER:C	2.59	0.71
1:B:127:LEU:HD12	1:B:377:THR:HG21	1.73	0.71
1:B:587:THR:CG2	1:B:605:PHE:CD2	2.72	0.71
1:E:456:VAL:HG23	1:E:459:SER:CB	2.21	0.71
1:E:545:CYS:CA	1:E:562:CYS:SG	2.79	0.71
1:F:184:SER:O	1:F:225:ARG:NH2	2.24	0.71
1:A:279:GLY:HA2	1:A:411:ILE:HD12	1.73	0.71
1:A:450:ASN:HD22	1:A:450:ASN:N	1.88	0.71
1:B:645:THR:N	1:B:646:THR:OG1	2.24	0.71
1:E:551:LYS:HB3	1:E:551:LYS:NZ	2.05	0.71
1:F:166:ILE:O	1:F:170:ILE:HG13	1.91	0.70
1:F:345:GLY:O	1:F:350:GLY:CA	2.39	0.70
1:B:554:GLY:CA	1:B:598:THR:HG22	2.21	0.70
1:E:456:VAL:HG23	1:E:459:SER:HB3	1.73	0.70
1:A:162:PHE:CD1	1:D:455:TYR:HD2	2.09	0.70
1:D:485:PRO:O	1:D:488:GLN:CG	2.39	0.70
1:F:454:ILE:HG21	1:F:458:SER:O	1.92	0.70
1:D:166:ILE:HG23	1:D:176:ASN:ND2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:LYS:HB2	1:F:256:GLU:OE2	1.92	0.70
1:A:346:GLY:HA2	3:A:822:HOH:O	1.92	0.70
1:D:614:LEU:O	1:D:615:HIS:HB2	1.89	0.70
1:A:136:GLU:OE2	1:A:193:ARG:NH2	2.24	0.70
1:F:655:HIS:CB	3:F:809:HOH:O	2.39	0.70
1:C:628:ARG:HH11	1:C:646:THR:HG22	1.56	0.70
1:F:413:GLY:CA	1:F:464:ASN:HD22	2.05	0.70
1:E:120:PHE:CZ	1:E:207:LEU:HD11	2.27	0.69
1:F:215:PHE:HE1	1:F:254:LEU:CD1	2.04	0.69
1:C:372:LYS:HE3	1:C:378:LYS:NZ	2.04	0.69
1:E:632:LEU:HD12	1:E:632:LEU:N	2.04	0.69
1:C:628:ARG:NH1	1:C:646:THR:HA	2.07	0.69
1:E:540:PHE:O	1:E:542:THR:HG23	1.92	0.69
1:F:258:LEU:HD22	1:F:262:ILE:CD1	2.18	0.69
1:A:455:TYR:CB	1:A:456:VAL:HG23	2.20	0.69
1:F:228:HIS:O	1:F:231:ILE:CG2	2.40	0.69
1:C:422:LYS:HG2	1:C:472:TRP:CZ2	2.28	0.69
1:E:120:PHE:HZ	1:E:207:LEU:CD1	2.06	0.69
1:A:162:PHE:CE1	1:D:455:TYR:HD2	2.11	0.69
1:A:190:ASN:HD22	1:A:190:ASN:H	1.41	0.69
1:A:422:LYS:HG2	1:A:472:TRP:CZ2	2.28	0.69
1:A:456:VAL:HG13	1:A:458:SER:HB2	1.73	0.69
1:B:527:LEU:N	1:B:527:LEU:HD12	2.08	0.69
1:C:207:LEU:CD2	1:C:207:LEU:H	2.05	0.69
1:E:193:ARG:NH2	1:E:436:SER:HA	2.07	0.69
1:F:377:THR:OG1	1:F:380:GLU:HG2	1.91	0.69
1:B:422:LYS:HG2	1:B:472:TRP:CZ2	2.28	0.69
1:E:411:ILE:HD13	1:E:411:ILE:N	2.08	0.69
1:A:347:ASP:HB3	1:A:351:TYR:N	2.08	0.69
1:C:627:ASP:CG	1:C:647:GLN:HG2	2.14	0.69
1:E:224:MET:HE3	1:E:258:LEU:CD1	2.23	0.68
1:C:196:GLU:CB	3:C:801:HOH:O	2.40	0.68
1:D:237:LYS:HG3	1:D:238:TYR:CE2	2.27	0.68
1:B:548:SER:HB2	1:B:581:GLN:HE22	1.58	0.68
1:B:625:CYS:N	1:B:640:CYS:SG	2.66	0.68
1:A:584:GLN:HG2	1:A:598:THR:O	1.92	0.68
1:C:632:LEU:H	1:C:632:LEU:CD1	1.93	0.68
1:F:422:LYS:HG2	1:F:472:TRP:CZ2	2.28	0.68
1:E:166:ILE:O	1:E:170:ILE:HG13	1.93	0.68
1:E:454:ILE:HD13	1:E:457:GLY:HA3	1.75	0.68
1:D:171:LYS:HG2	1:D:448:GLN:NE2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:VAL:CG2	1:D:273:ARG:HH12	2.06	0.68
1:D:422:LYS:HG2	1:D:472:TRP:CZ2	2.28	0.68
1:D:584:GLN:HG3	1:D:598:THR:C	2.13	0.68
1:E:646:THR:O	1:E:647:GLN:HB2	1.94	0.68
1:B:623:GLY:C	3:B:802:HOH:O	2.32	0.68
1:C:527:LEU:HD12	1:C:527:LEU:N	2.08	0.68
1:E:224:MET:CE	1:E:258:LEU:CD1	2.71	0.68
1:F:136:GLU:OE1	1:F:138:LYS:N	2.27	0.68
1:F:164:GLN:OE1	1:F:164:GLN:HA	1.93	0.68
1:B:574:ASN:ND2	1:B:578:GLN:HG3	2.03	0.68
1:B:601:ASN:CB	1:B:604:GLU:CG	2.65	0.68
1:D:128:ARG:HG3	1:D:201:HIS:CD2	2.29	0.68
1:F:253:HIS:ND1	1:F:254:LEU:CD2	2.57	0.68
1:A:414:GLY:CA	1:A:415:GLU:HB3	2.12	0.68
1:F:627:ASP:OD1	1:F:628:ARG:N	2.26	0.68
1:C:628:ARG:HD3	1:C:646:THR:HG22	1.76	0.68
1:D:273:ARG:HG2	1:D:273:ARG:NH1	2.05	0.68
1:F:255:LYS:O	1:F:256:GLU:HB2	1.94	0.68
1:A:646:THR:O	1:A:647:GLN:HB2	1.92	0.67
1:C:122:TYR:CE1	1:C:203:ASP:HB3	2.29	0.67
1:C:474:ASP:O	1:C:477:LYS:CG	2.40	0.67
1:F:133:GLY:CA	1:F:136:GLU:CG	2.68	0.67
1:A:474:ASP:O	1:A:477:LYS:CG	2.42	0.67
1:D:586:LEU:HD22	1:D:597:ILE:HG12	1.76	0.67
1:F:122:TYR:CZ	1:F:203:ASP:HB3	2.30	0.67
1:B:535:GLY:HA3	1:B:652:ASN:O	1.94	0.67
1:C:116:LYS:CE	1:C:397:GLU:OE1	2.37	0.67
1:D:208:THR:HB	1:D:295:GLN:CG	2.25	0.67
1:D:258:LEU:HD11	1:D:262:ILE:HD11	1.75	0.67
1:B:620:ILE:HG22	1:B:621:PRO:HD3	1.75	0.67
1:D:527:LEU:HD12	1:D:527:LEU:N	2.08	0.67
1:E:422:LYS:HG2	1:E:472:TRP:CZ2	2.29	0.67
1:D:138:LYS:H	1:D:138:LYS:CD	2.07	0.67
1:E:527:LEU:CD1	1:E:527:LEU:H	2.07	0.67
1:E:627:ASP:CG	1:E:647:GLN:HG3	2.14	0.67
1:F:231:ILE:HD13	1:F:231:ILE:C	2.15	0.67
1:F:268:LEU:HD13	1:F:268:LEU:C	2.14	0.67
1:F:301:ASP:OD2	1:F:440:HIS:NE2	2.27	0.67
1:A:414:GLY:HA2	1:A:415:GLU:OE2	1.94	0.67
1:D:347:ASP:CB	1:D:351:TYR:H	2.04	0.67
1:A:348:GLU:HA	1:A:348:GLU:OE1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:VAL:O	1:B:231:ILE:HG23	1.95	0.67
1:E:545:CYS:N	1:E:562:CYS:HG	1.91	0.67
1:C:509:SER:HB2	3:C:839:HOH:O	1.95	0.67
1:E:527:LEU:N	1:E:527:LEU:HD12	2.08	0.67
1:B:454:ILE:HG13	1:B:454:ILE:O	1.92	0.67
1:B:626:LEU:CA	1:B:649:TRP:HH2	2.07	0.67
1:C:628:ARG:HD2	1:C:646:THR:HG22	1.75	0.67
1:C:132:LEU:C	1:C:132:LEU:HD12	2.14	0.67
1:D:235:PRO:HB2	1:D:238:TYR:CD2	2.30	0.67
1:F:585:CYS:HB2	1:F:600:CYS:SG	2.28	0.67
1:A:447:TRP:O	1:A:448:GLN:HG2	1.95	0.66
1:B:391:LEU:HD13	1:B:438:VAL:CG2	2.20	0.66
1:E:120:PHE:HZ	1:E:207:LEU:HD11	1.58	0.66
1:D:279:GLY:HA2	1:D:411:ILE:HD12	1.77	0.66
1:E:166:ILE:HG12	1:E:178:VAL:CG2	2.25	0.66
1:E:484:ARG:CG	1:E:484:ARG:HH11	2.08	0.66
1:F:573:ILE:HD11	1:F:610:TYR:CD2	2.30	0.66
1:B:619:HIS:HE2	1:B:621:PRO:HG2	1.58	0.66
1:B:627:ASP:OD1	1:B:628:ARG:N	2.28	0.66
1:B:347:ASP:HB3	1:B:349:ASP:O	1.95	0.66
1:B:580:MET:HG2	1:B:585:CYS:SG	2.35	0.66
1:B:616:ARG:HG3	1:B:648:LYS:HE3	1.72	0.66
1:C:196:GLU:HB3	3:C:801:HOH:O	1.94	0.66
1:D:643:SER:CB	1:D:648:LYS:NZ	2.50	0.66
1:C:573:ILE:HD11	1:C:610:TYR:CD2	2.30	0.66
1:D:443:ARG:CZ	1:D:447:TRP:CZ3	2.78	0.66
1:D:241:GLU:HG3	1:D:243:VAL:HG23	1.77	0.66
1:D:413:GLY:HA3	1:D:464:ASN:HD22	1.61	0.66
1:E:576:ALA:O	1:E:606:LYS:HB2	1.96	0.66
1:F:396:ARG:HG2	1:F:396:ARG:NH1	2.04	0.66
1:F:474:ASP:O	1:F:477:LYS:CG	2.42	0.66
1:C:195:GLU:OE2	1:C:198:LYS:HE2	1.96	0.66
1:C:642:SER:O	1:C:643:SER:OG	2.08	0.66
1:D:563:HIS:CE1	1:D:565:MET:HB2	2.31	0.66
1:D:190:ASN:HD22	1:D:190:ASN:N	1.94	0.66
1:A:457:GLY:HA2	1:A:463:LYS:NZ	2.11	0.65
1:A:563:HIS:CE1	1:A:565:MET:HB2	2.31	0.65
1:A:583:ASP:OD2	1:A:599:HIS:HD2	1.78	0.65
1:C:563:HIS:CE1	1:C:565:MET:HB2	2.31	0.65
1:D:241:GLU:HB2	1:D:270:LYS:NZ	2.12	0.65
1:E:529:PRO:HG2	1:E:574:ASN:ND2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:TRP:O	1:B:653:ASN:ND2	2.29	0.65
1:B:603:ASN:CB	1:B:606:LYS:HE2	2.26	0.65
1:B:617:PHE:CB	1:B:626:LEU:HD12	2.26	0.65
1:D:161:GLU:H	1:D:161:GLU:CD	1.97	0.65
1:F:258:LEU:HD22	1:F:258:LEU:O	1.97	0.65
1:A:147:GLY:C	1:D:489:ALA:CB	2.61	0.65
1:B:563:HIS:CE1	1:B:565:MET:HB2	2.31	0.65
1:F:139:GLU:OE1	1:F:139:GLU:HA	1.96	0.65
1:A:363:LYS:HD2	1:A:525:TYR:CZ	2.32	0.65
1:C:632:LEU:HD12	1:C:632:LEU:N	2.04	0.65
1:E:241:GLU:OE1	1:E:270:LYS:HE3	1.96	0.65
1:E:132:LEU:CD2	1:E:199:TYR:CE1	2.79	0.65
1:D:237:LYS:CD	1:D:238:TYR:CE2	2.80	0.65
1:D:220:TRP:HZ2	1:D:261:TYR:CD2	2.15	0.64
1:B:347:ASP:HB2	1:B:351:TYR:O	1.97	0.64
1:B:472:TRP:CZ3	1:B:502:ARG:HG3	2.31	0.64
1:B:620:ILE:HB	1:B:621:PRO:CD	2.27	0.64
1:F:231:ILE:HD13	1:F:231:ILE:O	1.96	0.64
1:B:279:GLY:HA2	1:B:411:ILE:HD12	1.79	0.64
1:D:349:ASP:OD1	1:D:349:ASP:N	2.23	0.64
1:E:377:THR:OG1	1:E:380:GLU:HG2	1.97	0.64
1:C:281:ILE:HD11	1:C:413:GLY:H	1.60	0.64
1:C:467:ARG:O	1:C:471:VAL:HG12	1.98	0.64
1:D:454:ILE:CG2	1:D:459:SER:OG	2.46	0.64
1:E:346:GLY:HA2	1:E:366:PRO:CA	2.26	0.64
1:F:641:ASP:N	1:F:647:GLN:HE22	1.89	0.64
1:B:588:LYS:HB3	1:B:588:LYS:HZ1	1.60	0.64
1:A:561:PRO:HG3	1:C:337:THR:HG21	1.77	0.64
1:B:259:ASP:OD2	1:B:273:ARG:NH2	2.30	0.64
1:B:585:CYS:C	1:B:586:LEU:HD23	2.18	0.64
1:D:574:ASN:HD22	1:D:578:GLN:CG	2.10	0.64
1:E:641:ASP:O	1:E:642:SER:HB3	1.96	0.64
1:B:620:ILE:CB	1:B:621:PRO:CD	2.76	0.64
1:D:467:ARG:O	1:D:471:VAL:HG12	1.98	0.64
1:F:454:ILE:CG2	1:F:460:PRO:HD3	2.28	0.64
1:B:189:VAL:HG13	1:B:340:ILE:HD12	1.79	0.64
1:B:601:ASN:HB3	1:B:604:GLU:CG	2.26	0.64
1:B:641:ASP:O	1:B:642:SER:HB3	1.96	0.64
1:F:187:ARG:NE	1:F:225:ARG:HH12	1.96	0.64
1:F:444:LEU:N	1:F:444:LEU:CD1	2.61	0.64
1:B:616:ARG:HG2	1:B:648:LYS:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:ARG:O	1:E:471:VAL:HG12	1.98	0.64
1:F:207:LEU:HD11	1:F:319:SER:HA	1.80	0.64
1:C:371:GLU:OE2	1:C:383:ARG:NH2	2.31	0.64
1:E:276:ARG:CD	1:E:278:GLU:OE2	2.46	0.64
1:C:454:ILE:HD13	1:C:460:PRO:CD	2.28	0.63
1:D:371:GLU:O	1:D:375:ARG:HG2	1.97	0.63
1:F:345:GLY:O	1:F:350:GLY:HA2	1.98	0.63
1:A:132:LEU:HD22	1:A:199:TYR:CE1	2.31	0.63
1:C:155:PRO:CD	1:C:339:GLU:HG3	2.21	0.63
1:B:132:LEU:HG	1:B:136:GLU:OE1	1.98	0.63
1:E:563:HIS:ND1	1:E:565:MET:HB2	2.14	0.63
1:F:574:ASN:HB2	1:F:578:GLN:H	1.64	0.63
1:A:414:GLY:HA3	1:A:416:ASN:H	1.63	0.63
1:A:467:ARG:O	1:A:471:VAL:HG12	1.98	0.63
1:B:587:THR:CG2	1:B:605:PHE:CG	2.80	0.63
1:F:467:ARG:O	1:F:471:VAL:HG12	1.98	0.63
1:B:467:ARG:O	1:B:471:VAL:HG12	1.98	0.63
1:D:241:GLU:HB2	1:D:270:LYS:HZ3	1.64	0.63
1:A:632:LEU:HA	1:C:341:ILE:HG23	1.78	0.63
1:B:609:GLN:NE2	1:B:611:PHE:HZ	1.96	0.63
1:B:624:LYS:N	3:B:802:HOH:O	2.31	0.63
1:C:173:PHE:CD2	1:C:177:MET:HG3	2.34	0.63
1:C:255:LYS:O	1:C:256:GLU:HB2	1.99	0.63
1:D:237:LYS:HD2	1:D:238:TYR:CZ	2.33	0.63
1:D:456:VAL:HG12	1:D:458:SER:H	1.62	0.63
1:B:626:LEU:HB2	1:B:649:TRP:HH2	1.39	0.63
1:C:231:ILE:HD12	1:C:265:TRP:NE1	2.14	0.63
1:A:207:LEU:HD11	1:A:319:SER:HA	1.80	0.62
1:A:587:THR:OG1	1:A:588:LYS:N	2.32	0.62
1:C:208:THR:HB	1:C:295:GLN:HG3	1.80	0.62
1:E:255:LYS:O	1:E:256:GLU:HB2	1.99	0.62
1:F:272:PHE:CD2	1:F:290:LYS:HB3	2.33	0.62
1:A:641:ASP:O	1:A:647:GLN:NE2	2.32	0.62
1:D:522:THR:CG2	1:D:527:LEU:CD1	2.51	0.62
1:D:166:ILE:HG12	1:D:178:VAL:CG2	2.28	0.62
1:A:116:LYS:O	1:A:322:ARG:NH2	2.33	0.62
1:B:395:GLU:OE1	1:B:397:GLU:HG3	2.00	0.62
1:C:412:TRP:O	1:C:461:THR:HG23	2.00	0.62
1:D:235:PRO:HB2	1:D:238:TYR:HD2	1.63	0.62
1:D:333:ILE:HG12	1:D:340:ILE:HG12	1.81	0.62
1:E:276:ARG:HH11	1:E:276:ARG:CG	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:VAL:O	1:F:230:VAL:HG22	1.98	0.62
1:F:346:GLY:HA2	1:F:366:PRO:CA	2.29	0.62
1:F:353:ARG:NH2	1:F:520:ASP:OD2	2.30	0.62
1:B:602:LEU:HD22	1:B:603:ASN:HA	1.82	0.62
1:D:171:LYS:HD3	1:D:448:GLN:NE2	2.09	0.62
1:D:271:VAL:HG22	1:D:273:ARG:HH12	1.64	0.62
1:E:128:ARG:HG3	1:E:201:HIS:CD2	2.34	0.62
1:E:372:LYS:C	1:E:372:LYS:HD3	2.19	0.62
1:F:183:ILE:HG21	1:F:225:ARG:NH1	2.14	0.62
1:F:258:LEU:O	1:F:262:ILE:CD1	2.47	0.62
1:F:574:ASN:ND2	1:F:578:GLN:HG3	2.03	0.62
1:B:230:VAL:C	1:B:231:ILE:HG23	2.20	0.62
1:E:193:ARG:HG2	1:E:437:ARG:HD2	1.80	0.62
1:A:455:TYR:O	1:A:455:TYR:HD1	1.82	0.62
1:B:333:ILE:HG12	1:B:340:ILE:HG12	1.81	0.62
1:E:406:ASP:CG	1:E:498:LEU:HD21	2.20	0.62
1:E:540:PHE:CD2	1:E:541:GLU:HG3	2.35	0.62
1:A:203:ASP:C	1:A:204:GLU:HG3	2.19	0.62
1:A:454:ILE:HD12	1:A:454:ILE:C	2.19	0.62
1:B:533:ASP:C	1:B:651:MET:CE	2.68	0.62
1:C:206:LEU:HD13	1:C:206:LEU:N	2.14	0.62
1:C:627:ASP:CB	1:C:647:GLN:HG2	2.30	0.62
1:A:122:TYR:OH	1:A:206:LEU:CD2	2.48	0.62
1:E:454:ILE:HB	1:E:457:GLY:N	2.13	0.62
1:C:527:LEU:CD1	1:C:527:LEU:H	2.13	0.61
1:C:574:ASN:HB2	1:C:578:GLN:H	1.64	0.61
1:E:333:ILE:HG12	1:E:340:ILE:HG12	1.81	0.61
1:F:347:ASP:HB3	3:F:804:HOH:O	2.00	0.61
1:A:255:LYS:O	1:A:256:GLU:HB2	1.99	0.61
1:B:574:ASN:HB2	1:B:578:GLN:H	1.64	0.61
1:F:220:TRP:CZ3	1:F:257:LYS:HG2	2.34	0.61
1:B:547:ASP:CB	1:B:569:GLN:HG2	2.31	0.61
1:E:363:LYS:HD3	1:E:525:TYR:OH	2.00	0.61
1:C:347:ASP:HB3	1:C:351:TYR:H	1.65	0.61
1:D:354:GLY:HA3	1:D:362:TRP:CH2	2.35	0.61
1:E:252:GLU:OE1	1:E:255:LYS:HE3	2.00	0.61
1:A:333:ILE:HG12	1:A:340:ILE:HG12	1.81	0.61
1:A:627:ASP:OD1	1:A:646:THR:HB	2.01	0.61
1:F:333:ILE:HG12	1:F:340:ILE:HG12	1.81	0.61
1:A:628:ARG:HD2	1:A:646:THR:HG22	1.83	0.61
1:F:211:VAL:HG22	1:F:242:ILE:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LYS:O	1:B:256:GLU:HB2	2.00	0.61
1:C:118:GLN:OE1	1:C:120:PHE:HB3	1.99	0.61
1:C:241:GLU:HB2	1:C:270:LYS:NZ	2.14	0.61
1:C:456:VAL:O	1:C:459:SER:CB	2.47	0.61
1:D:527:LEU:CD1	1:D:527:LEU:H	2.13	0.61
1:D:547:ASP:CB	1:D:569:GLN:HG2	2.30	0.61
1:E:552:THR:HB	1:E:553:ASN:OD1	1.99	0.61
1:F:258:LEU:HD23	1:F:262:ILE:HD11	1.77	0.61
1:A:162:PHE:CD1	1:D:455:TYR:CD2	2.88	0.61
1:C:203:ASP:O	1:C:204:GLU:CB	2.34	0.61
1:D:136:GLU:OE1	1:D:193:ARG:NH2	2.29	0.61
1:E:413:GLY:CA	1:E:464:ASN:ND2	2.55	0.61
1:E:619:HIS:CE1	1:E:621:PRO:HG2	2.36	0.61
1:A:619:HIS:CE1	1:A:621:PRO:HG2	2.36	0.61
1:B:629:SER:N	1:B:634:GLN:O	2.33	0.61
1:C:132:LEU:HB3	1:C:199:TYR:HE1	1.63	0.61
1:C:207:LEU:HD21	1:C:319:SER:CB	2.31	0.61
1:E:281:ILE:HD11	1:E:413:GLY:N	2.11	0.61
1:A:211:VAL:HG22	1:A:242:ILE:HG12	1.83	0.61
1:D:610:TYR:OH	1:D:612:LYS:HD2	2.01	0.61
1:F:253:HIS:H	1:F:253:HIS:CD2	2.19	0.61
1:A:122:TYR:CZ	1:A:206:LEU:HD23	2.36	0.60
1:A:451:PRO:HB2	1:A:452:PRO:HD2	1.81	0.60
1:B:551:LYS:O	1:B:552:THR:HG22	2.01	0.60
1:E:264:LEU:O	1:E:265:TRP:HB2	2.00	0.60
1:E:609:GLN:CD	1:E:611:PHE:CZ	2.74	0.60
1:F:253:HIS:ND1	1:F:254:LEU:HD23	2.15	0.60
1:F:619:HIS:CE1	1:F:621:PRO:HG2	2.36	0.60
1:F:657:VAL:O	1:F:657:VAL:HG12	2.00	0.60
1:A:207:LEU:HD12	1:A:207:LEU:N	2.16	0.60
1:A:592:GLY:HA3	3:A:820:HOH:O	2.00	0.60
1:A:614:LEU:O	1:A:615:HIS:HB2	2.01	0.60
1:E:207:LEU:N	1:E:207:LEU:HD12	2.16	0.60
1:E:495:ILE:O	1:E:495:ILE:HG13	2.01	0.60
1:E:627:ASP:HB2	1:E:647:GLN:HG2	1.78	0.60
1:F:175:PHE:CE1	1:F:441:ILE:CG2	2.84	0.60
1:A:118:GLN:NE2	1:A:322:ARG:H	1.99	0.60
1:B:211:VAL:HG22	1:B:242:ILE:HG12	1.83	0.60
1:D:172:GLU:HG2	1:D:251:LYS:NZ	2.17	0.60
1:E:207:LEU:HD11	1:E:319:SER:HA	1.82	0.60
1:E:551:LYS:HE3	1:E:555:GLY:CA	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:THR:OG1	1:A:295:GLN:HG3	2.02	0.60
1:C:619:HIS:CE1	1:C:621:PRO:HG2	2.36	0.60
1:F:161:GLU:HG2	1:F:162:PHE:N	2.16	0.60
1:B:175:PHE:CE1	1:B:441:ILE:HG22	2.37	0.60
1:C:628:ARG:HD3	1:C:646:THR:CG2	2.31	0.60
1:E:605:PHE:HA	1:E:607:GLU:OE2	2.02	0.60
1:F:547:ASP:CB	1:F:569:GLN:HG2	2.30	0.60
1:A:255:LYS:NZ	3:A:801:HOH:O	2.34	0.60
1:C:573:ILE:CD1	1:C:610:TYR:CD2	2.84	0.60
1:E:211:VAL:HG22	1:E:242:ILE:HG12	1.83	0.60
1:C:211:VAL:HG22	1:C:242:ILE:HG12	1.83	0.60
1:D:208:THR:HG22	1:D:240:ALA:HB2	1.81	0.60
1:E:456:VAL:O	1:E:459:SER:HB3	2.01	0.60
1:E:641:ASP:HB3	1:E:644:LYS:HD2	1.82	0.60
1:B:527:LEU:H	1:B:527:LEU:CD1	2.13	0.60
1:C:122:TYR:HE1	1:C:203:ASP:HB3	1.66	0.60
1:C:631:VAL:O	1:C:631:VAL:HG23	2.02	0.60
1:E:173:PHE:CD2	1:E:177:MET:HG3	2.36	0.60
1:F:253:HIS:CE1	1:F:254:LEU:CD2	2.84	0.60
1:A:547:ASP:CB	1:A:569:GLN:HG2	2.31	0.60
1:A:554:GLY:N	1:A:597:ILE:O	2.24	0.60
1:B:150:GLY:CA	1:B:183:ILE:HG23	2.28	0.60
1:B:459:SER:H	1:B:462:LEU:N	1.99	0.60
1:B:649:TRP:HE3	1:B:649:TRP:H	1.50	0.60
1:C:347:ASP:HB2	1:C:351:TYR:O	2.02	0.60
1:D:619:HIS:CE1	1:D:621:PRO:HG2	2.36	0.60
1:F:611:PHE:HE1	1:F:618:THR:CG2	2.14	0.60
1:A:574:ASN:HB2	1:A:578:GLN:H	1.65	0.60
1:B:264:LEU:HD22	1:B:265:TRP:N	2.17	0.60
1:E:208:THR:OG1	1:E:295:GLN:HG3	2.02	0.60
1:F:573:ILE:CD1	1:F:610:TYR:CD2	2.84	0.60
1:D:346:GLY:HA2	1:D:366:PRO:CB	2.30	0.59
1:E:207:LEU:HD13	1:E:319:SER:OG	2.02	0.59
1:A:246:ASP:OD1	1:A:249:SER:OG	2.20	0.59
1:B:459:SER:H	1:B:461:THR:N	1.99	0.59
1:B:577:ASN:HB2	1:B:606:LYS:HB3	1.83	0.59
1:C:614:LEU:O	1:C:615:HIS:HB2	2.01	0.59
1:D:138:LYS:N	1:D:138:LYS:HD2	2.16	0.59
1:E:190:ASN:HD22	1:E:190:ASN:C	2.05	0.59
1:F:193:ARG:NH2	1:F:308:VAL:CG2	2.66	0.59
1:B:450:ASN:CB	1:B:451:PRO:HD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:GLU:CD	1:D:193:ARG:HH22	2.04	0.59
1:D:203:ASP:OD2	1:D:205:ASN:HB2	2.02	0.59
1:D:224:MET:HE3	1:D:258:LEU:HD13	1.83	0.59
1:E:540:PHE:CD2	1:E:541:GLU:CG	2.85	0.59
1:D:412:TRP:O	1:D:461:THR:HG23	2.02	0.59
1:F:590:ALA:HB1	1:F:591:ASP:HA	1.83	0.59
1:F:641:ASP:O	1:F:642:SER:HB3	2.01	0.59
1:A:118:GLN:HE22	1:A:322:ARG:N	1.99	0.59
1:A:349:ASP:OD2	1:A:378:LYS:HE3	2.02	0.59
1:C:347:ASP:CB	1:C:351:TYR:H	2.15	0.59
1:D:395:GLU:OE1	1:D:397:GLU:HB3	2.03	0.59
1:F:351:TYR:O	1:F:367:LEU:CB	2.49	0.59
1:B:588:LYS:HB3	1:B:588:LYS:HZ2	1.66	0.59
1:B:641:ASP:HB3	1:B:643:SER:HB3	1.84	0.59
1:C:443:ARG:HH11	1:C:443:ARG:CG	2.14	0.59
1:D:191:ASP:OD1	1:D:193:ARG:HD3	2.03	0.59
1:F:136:GLU:OE2	1:F:138:LYS:CG	2.41	0.59
1:F:187:ARG:NE	1:F:225:ARG:NH1	2.51	0.59
1:B:588:LYS:CD	1:B:637:ILE:HD11	2.33	0.59
1:D:346:GLY:HA2	1:D:366:PRO:CA	2.32	0.59
1:E:276:ARG:HH11	1:E:276:ARG:HG3	1.67	0.59
1:E:564:ARG:H	1:E:569:GLN:HE22	1.49	0.59
1:A:262:ILE:HD13	1:A:265:TRP:HZ3	1.66	0.59
1:C:143:PRO:HG3	1:C:146:VAL:HB	1.85	0.59
1:C:625:CYS:HG	1:C:640:CYS:CB	2.06	0.59
1:D:255:LYS:O	1:D:256:GLU:HB2	2.01	0.59
1:A:118:GLN:NE2	1:A:321:ASP:HA	2.17	0.59
1:A:574:ASN:ND2	1:A:578:GLN:HG3	2.09	0.59
1:B:527:LEU:N	1:B:527:LEU:CD1	2.66	0.59
1:C:281:ILE:HD11	1:C:413:GLY:N	2.18	0.59
1:C:527:LEU:N	1:C:527:LEU:CD1	2.66	0.59
1:C:574:ASN:ND2	1:C:578:GLN:HG3	2.03	0.59
1:D:150:GLY:HA3	1:D:183:ILE:HG23	1.85	0.59
1:A:584:GLN:HB3	1:A:597:ILE:CG2	2.32	0.58
1:C:155:PRO:HB3	1:C:337:THR:HG23	1.79	0.58
1:C:231:ILE:HD12	1:C:265:TRP:CD1	2.38	0.58
1:C:335:GLY:HA3	1:C:444:LEU:HD21	1.85	0.58
1:A:169:SER:HB2	1:A:177:MET:HB2	1.84	0.58
1:A:231:ILE:HD12	1:A:265:TRP:NE1	2.18	0.58
1:B:116:LYS:O	1:B:322:ARG:NH2	2.36	0.58
1:C:410:GLN:O	1:C:411:ILE:CG2	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HD12	1:D:504:ASP:HB3	1.85	0.58
1:F:208:THR:OG1	1:F:295:GLN:HG3	2.02	0.58
1:F:243:VAL:CG1	1:F:245:ILE:CD1	2.73	0.58
1:F:410:GLN:O	1:F:464:ASN:ND2	2.34	0.58
1:B:156:LEU:HD22	1:B:158:LEU:HD21	1.85	0.58
1:B:412:TRP:HE3	1:B:461:THR:HG21	1.68	0.58
1:B:632:LEU:HD12	1:B:632:LEU:H	1.68	0.58
1:D:208:THR:CB	1:D:295:GLN:HG3	2.33	0.58
1:D:450:ASN:HB2	1:D:451:PRO:CD	2.32	0.58
1:A:590:ALA:HB1	1:A:591:ASP:CA	2.30	0.58
1:D:548:SER:O	1:D:551:LYS:HB2	2.04	0.58
1:F:641:ASP:O	1:F:643:SER:N	2.34	0.58
1:D:246:ASP:O	1:D:274:ASN:HB2	2.03	0.58
1:E:192:LEU:HD12	1:E:331:ASP:OD2	2.03	0.58
1:E:260:GLU:O	1:E:263:LYS:HB2	2.03	0.58
1:E:527:LEU:H	1:E:527:LEU:HD12	1.66	0.58
1:B:322:ARG:HD2	1:B:395:GLU:OE2	2.03	0.58
1:C:207:LEU:CD2	1:C:319:SER:CB	2.80	0.58
1:E:533:ASP:OD2	1:E:612:LYS:NZ	2.35	0.58
1:D:162:PHE:O	1:D:166:ILE:HG13	2.03	0.58
1:D:271:VAL:HG22	1:D:273:ARG:NH1	2.19	0.58
1:B:616:ARG:HG3	1:B:648:LYS:CE	2.32	0.58
1:C:136:GLU:CD	1:C:193:ARG:HH12	2.06	0.58
1:C:539:GLY:HA3	1:C:628:ARG:HH21	1.69	0.58
1:D:125:PRO:HB3	1:D:202:TYR:HD1	1.69	0.58
1:B:166:ILE:HG23	1:B:176:ASN:OD1	2.03	0.58
1:C:192:LEU:HD12	1:C:331:ASP:OD2	2.04	0.58
1:D:231:ILE:HD12	1:D:265:TRP:NE1	2.19	0.58
1:E:231:ILE:HD12	1:E:265:TRP:NE1	2.19	0.58
1:A:456:VAL:CG1	1:A:458:SER:HB3	2.27	0.58
1:B:551:LYS:C	1:B:552:THR:HG23	2.24	0.58
1:D:450:ASN:CB	1:D:451:PRO:HD2	2.32	0.58
1:E:235:PRO:HB2	1:E:238:TYR:HD2	1.68	0.58
1:F:137:PRO:O	1:F:138:LYS:HB2	2.04	0.58
1:A:457:GLY:HA2	1:A:463:LYS:HZ3	1.69	0.57
3:A:813:HOH:O	1:C:631:VAL:HG11	2.01	0.57
1:B:534:TRP:N	1:B:651:MET:CE	2.59	0.57
1:D:224:MET:HE3	1:D:258:LEU:CD1	2.34	0.57
1:F:187:ARG:CD	1:F:225:ARG:HH12	2.17	0.57
1:F:190:ASN:C	1:F:190:ASN:HD22	2.05	0.57
1:A:153:ALA:CB	1:A:190:ASN:HD21	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:SER:HB2	1:D:177:MET:HB2	1.86	0.57
1:E:471:VAL:HG13	1:E:472:TRP:CD1	2.38	0.57
1:E:498:LEU:HD12	1:E:498:LEU:H	1.69	0.57
1:A:548:SER:O	1:A:551:LYS:HB2	2.04	0.57
1:B:377:THR:OG1	1:B:380:GLU:HG2	2.03	0.57
1:D:315:VAL:O	1:D:315:VAL:HG12	2.04	0.57
1:D:527:LEU:CD1	1:D:527:LEU:N	2.66	0.57
1:D:574:ASN:HB2	1:D:578:GLN:H	1.70	0.57
1:E:193:ARG:HH12	1:E:309:ASN:C	2.06	0.57
1:E:527:LEU:CD1	1:E:527:LEU:N	2.66	0.57
1:E:538:ARG:NH1	1:E:564:ARG:HE	2.01	0.57
1:F:600:CYS:HB3	1:F:605:PHE:HD2	1.69	0.57
1:B:534:TRP:CA	1:B:651:MET:HE3	2.23	0.57
1:C:194:GLN:O	1:C:197:CYS:HB2	2.04	0.57
1:C:220:TRP:CZ3	1:C:257:LYS:HG2	2.39	0.57
1:D:474:ASP:O	1:D:477:LYS:CG	2.52	0.57
1:E:483:SER:C	1:E:485:PRO:HD3	2.24	0.57
1:E:564:ARG:CA	1:E:569:GLN:OE1	2.52	0.57
1:A:553:ASN:HA	1:A:598:THR:HA	1.85	0.57
1:B:450:ASN:HB2	1:B:451:PRO:CD	2.32	0.57
1:B:649:TRP:N	1:B:649:TRP:CE3	2.73	0.57
1:D:264:LEU:HD22	1:D:265:TRP:N	2.20	0.57
1:D:320:LYS:NZ	3:D:803:HOH:O	2.35	0.57
1:F:127:LEU:HD23	1:F:199:TYR:O	2.04	0.57
1:B:614:LEU:O	1:B:648:LYS:HD3	2.04	0.57
1:F:172:GLU:HG2	1:F:173:PHE:CZ	2.39	0.57
1:F:225:ARG:HH21	1:F:225:ARG:CG	2.17	0.57
1:B:596:MET:HE2	1:B:598:THR:HG23	1.85	0.57
1:D:122:TYR:CE1	1:D:203:ASP:HB2	2.38	0.57
1:E:220:TRP:CZ3	1:E:257:LYS:HG2	2.39	0.57
1:E:614:LEU:HD11	1:E:616:ARG:CZ	2.33	0.57
1:E:649:TRP:CD1	1:E:649:TRP:N	2.73	0.57
1:A:150:GLY:O	1:A:187:ARG:NH2	2.38	0.57
1:B:620:ILE:HB	1:B:621:PRO:HD2	1.86	0.57
1:C:627:ASP:HB2	1:C:647:GLN:HG2	1.87	0.57
1:D:631:VAL:HG23	1:D:631:VAL:O	2.03	0.57
1:E:471:VAL:CB	1:E:495:ILE:HD11	2.35	0.57
1:F:455:TYR:N	1:F:455:TYR:CD1	2.73	0.57
1:B:116:LYS:NZ	1:B:397:GLU:OE1	2.35	0.57
1:B:551:LYS:O	1:B:552:THR:HG23	2.05	0.57
1:B:553:ASN:HA	1:B:598:THR:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:GLY:HA3	1:B:598:THR:HG22	1.86	0.57
1:D:346:GLY:HA2	1:D:366:PRO:HA	1.87	0.57
1:E:513:PHE:HE1	1:E:517:ILE:HD11	1.52	0.57
1:F:136:GLU:OE1	1:F:138:LYS:CG	2.53	0.57
1:A:220:TRP:CZ3	1:A:257:LYS:HG2	2.39	0.56
1:B:301:ASP:H	1:B:391:LEU:HD22	1.70	0.56
1:C:264:LEU:CD2	1:C:265:TRP:N	2.67	0.56
1:C:301:ASP:OD2	1:C:440:HIS:NE2	2.36	0.56
1:E:609:GLN:NE2	1:E:611:PHE:HZ	2.03	0.56
1:A:207:LEU:CD1	1:A:319:SER:OG	2.53	0.56
1:B:647:GLN:HG3	1:B:647:GLN:O	2.04	0.56
1:C:548:SER:O	1:C:549:MET:HB2	2.05	0.56
1:D:447:TRP:CD1	1:D:448:GLN:N	2.73	0.56
1:E:189:VAL:HG11	1:E:340:ILE:CD1	2.36	0.56
1:F:346:GLY:CA	1:F:366:PRO:HB3	2.33	0.56
1:A:194:GLN:HG3	1:A:351:TYR:OH	2.05	0.56
1:A:585:CYS:CB	1:A:600:CYS:SG	2.92	0.56
1:B:626:LEU:HB2	1:B:649:TRP:CZ3	2.39	0.56
1:B:653:ASN:HD22	1:B:653:ASN:N	2.02	0.56
1:D:236:ARG:HH11	1:D:236:ARG:CG	2.07	0.56
1:E:152:LYS:H	1:E:152:LYS:HD3	1.70	0.56
1:E:484:ARG:N	1:E:485:PRO:HD3	2.21	0.56
1:C:180:SER:HB2	1:C:338:TYR:CZ	2.39	0.56
1:C:190:ASN:HD22	1:C:190:ASN:C	2.05	0.56
1:E:332:VAL:HG13	1:E:442:TYR:CE2	2.41	0.56
1:A:412:TRP:CD1	1:A:413:GLY:N	2.73	0.56
1:C:264:LEU:O	1:C:265:TRP:CB	2.50	0.56
1:E:151:GLU:HA	1:E:153:ALA:H	1.70	0.56
1:E:194:GLN:HG3	1:E:351:TYR:OH	2.05	0.56
1:A:122:TYR:OH	1:A:206:LEU:HD21	2.05	0.56
1:B:626:LEU:O	1:B:649:TRP:HH2	1.76	0.56
1:E:574:ASN:HB2	1:E:578:GLN:H	1.70	0.56
1:A:628:ARG:HH11	1:A:628:ARG:CG	2.13	0.56
1:E:576:ALA:O	1:E:577:ASN:HB2	2.04	0.56
1:F:207:LEU:CD1	1:F:319:SER:OG	2.53	0.56
1:B:506:ASN:CB	3:B:804:HOH:O	2.32	0.56
1:B:536:GLU:HA	1:B:569:GLN:O	2.06	0.56
1:E:193:ARG:HG2	1:E:437:ARG:CD	2.34	0.56
1:F:609:GLN:HG3	1:F:611:PHE:CE1	2.41	0.56
1:A:414:GLY:HA3	1:A:416:ASN:OD1	2.04	0.56
1:B:266:ASN:ND2	1:C:500:LYS:NZ	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:LEU:HD22	1:C:265:TRP:N	2.21	0.56
1:D:412:TRP:O	1:D:461:THR:CG2	2.53	0.56
1:E:494:ASP:OD1	1:E:496:SER:OG	2.24	0.56
1:F:162:PHE:O	1:F:166:ILE:HG13	2.06	0.56
1:B:233:ARG:NH2	1:B:306:VAL:O	2.35	0.56
1:C:179:ALA:O	1:C:180:SER:C	2.43	0.56
1:C:348:GLU:O	1:C:348:GLU:HG2	2.05	0.56
1:D:164:GLN:HA	1:D:164:GLN:HE21	1.71	0.56
1:E:234:THR:HG22	1:E:310:TRP:HE1	1.71	0.56
1:E:443:ARG:HD3	1:E:447:TRP:CZ3	2.41	0.56
1:B:585:CYS:SG	1:B:600:CYS:CB	2.94	0.55
1:B:645:THR:OG1	1:B:646:THR:CA	2.52	0.55
1:E:605:PHE:C	1:E:607:GLU:HG3	2.26	0.55
1:F:352:ALA:HB3	1:F:364:ARG:NH2	2.22	0.55
1:B:458:SER:O	1:B:462:LEU:CB	2.48	0.55
1:B:458:SER:C	1:B:462:LEU:HB3	2.26	0.55
1:B:591:ASP:N	1:B:591:ASP:OD1	2.39	0.55
1:C:155:PRO:CB	1:C:337:THR:CG2	2.80	0.55
1:C:457:GLY:CA	1:C:459:SER:H	2.02	0.55
1:D:411:ILE:HG23	1:D:411:ILE:O	2.06	0.55
1:E:644:LYS:O	1:E:646:THR:O	2.24	0.55
1:B:197:CYS:SG	1:B:379:THR:CG2	2.94	0.55
1:B:297:LEU:HG	1:B:396:ARG:HG2	1.86	0.55
1:E:120:PHE:CZ	1:E:207:LEU:CD1	2.86	0.55
1:A:346:GLY:CA	1:A:366:PRO:HB3	2.33	0.55
1:C:239:LEU:HD13	1:C:268:LEU:HD11	1.89	0.55
1:C:573:ILE:HD13	1:C:610:TYR:CB	2.37	0.55
1:C:122:TYR:CE1	1:C:203:ASP:CB	2.89	0.55
1:E:189:VAL:HG12	1:E:190:ASN:N	2.21	0.55
1:F:573:ILE:HD13	1:F:610:TYR:CB	2.36	0.55
1:F:351:TYR:O	1:F:367:LEU:N	2.40	0.55
1:B:620:ILE:CG2	1:B:621:PRO:HD3	2.37	0.55
1:C:132:LEU:HB3	1:C:199:TYR:CD1	2.41	0.55
1:E:627:ASP:OD1	1:E:646:THR:OG1	2.24	0.55
1:F:454:ILE:HG23	1:F:460:PRO:HD3	1.89	0.55
1:B:354:GLY:O	1:B:385:PRO:HD2	2.07	0.55
1:B:444:LEU:HD12	1:B:444:LEU:N	2.22	0.55
1:B:538:ARG:C	1:B:649:TRP:HB3	2.25	0.55
1:D:643:SER:CB	1:D:648:LYS:HZ2	2.17	0.55
1:A:262:ILE:CD1	1:A:265:TRP:HZ3	2.19	0.55
1:E:239:LEU:HD13	1:E:268:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:TYR:CD1	1:F:123:HIS:N	2.75	0.55
1:E:169:SER:HB2	1:E:177:MET:HB2	1.89	0.55
1:E:494:ASP:CG	1:E:496:SER:HG	2.09	0.55
1:B:415:GLU:HG2	1:B:416:ASN:N	2.21	0.54
1:B:533:ASP:O	1:B:651:MET:HE1	2.07	0.54
1:B:616:ARG:HG2	1:B:648:LYS:CE	2.22	0.54
1:E:552:THR:HB	1:E:584:GLN:HE22	1.72	0.54
1:F:415:GLU:HG2	1:F:416:ASN:N	2.21	0.54
1:B:611:PHE:HE2	1:B:618:THR:CG2	2.20	0.54
1:B:617:PHE:HB3	1:B:626:LEU:HD12	1.89	0.54
1:C:166:ILE:O	1:C:170:ILE:HG13	2.08	0.54
1:D:533:ASP:OD2	1:D:612:LYS:CE	2.55	0.54
1:E:194:GLN:O	1:E:197:CYS:HB2	2.07	0.54
1:A:166:ILE:O	1:A:170:ILE:HG13	2.07	0.54
1:B:231:ILE:HG13	1:B:232:LYS:N	2.22	0.54
1:B:548:SER:HB2	1:B:581:GLN:NE2	2.22	0.54
1:B:552:THR:HB	1:B:584:GLN:CD	2.28	0.54
1:C:449:GLY:C	3:C:806:HOH:O	2.45	0.54
1:D:286:ILE:CG2	1:D:290:LYS:HD2	2.38	0.54
1:E:207:LEU:HD12	1:E:207:LEU:H	1.72	0.54
1:E:224:MET:CE	1:E:258:LEU:HD13	2.36	0.54
1:E:471:VAL:CG1	1:E:495:ILE:HD11	2.37	0.54
1:A:231:ILE:HD12	1:A:265:TRP:CD1	2.42	0.54
1:A:279:GLY:CA	1:A:411:ILE:HD12	2.38	0.54
1:A:373:ARG:HD2	1:A:373:ARG:O	2.07	0.54
1:B:411:ILE:HG23	1:B:411:ILE:O	2.07	0.54
1:B:611:PHE:HE2	1:B:618:THR:HG23	1.72	0.54
1:E:118:GLN:NE2	1:E:120:PHE:O	2.41	0.54
1:A:626:LEU:O	1:A:647:GLN:HA	2.07	0.54
1:B:371:GLU:HG2	1:B:519:TYR:OH	2.08	0.54
1:C:372:LYS:HG3	3:C:823:HOH:O	2.08	0.54
1:D:625:CYS:HB2	1:D:640:CYS:SG	2.40	0.54
1:E:193:ARG:NH2	1:E:310:TRP:CA	2.54	0.54
1:E:443:ARG:HD3	1:E:447:TRP:CE3	2.43	0.54
1:A:346:GLY:HA3	1:A:366:PRO:CB	2.35	0.54
1:A:641:ASP:OD1	1:A:642:SER:N	2.41	0.54
1:D:551:LYS:HG2	1:D:555:GLY:HA3	1.88	0.54
1:E:512:TRP:HE1	1:F:516:GLU:HB2	1.73	0.54
1:E:598:THR:HG22	1:E:599:HIS:N	2.23	0.54
1:A:286:ILE:CG2	1:A:290:LYS:HD2	2.37	0.54
1:B:474:ASP:O	1:B:477:LYS:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:585:CYS:HG	1:D:600:CYS:CB	2.07	0.54
1:E:192:LEU:HD22	1:E:342:PRO:HD3	1.89	0.54
1:E:552:THR:CB	1:E:584:GLN:OE1	2.54	0.54
1:E:593:SER:O	1:E:636:PHE:HB2	2.07	0.54
1:F:128:ARG:CG	1:F:201:HIS:HD2	2.11	0.54
1:F:548:SER:O	1:F:551:LYS:HB2	2.08	0.54
1:B:166:ILE:O	1:B:170:ILE:HG13	2.08	0.54
1:C:194:GLN:HG3	1:C:351:TYR:OH	2.08	0.54
1:C:450:ASN:H	1:C:450:ASN:ND2	2.05	0.54
1:B:614:LEU:HD13	1:B:616:ARG:HD3	0.68	0.54
1:C:463:LYS:HE3	1:C:491:PRO:O	2.08	0.54
1:D:286:ILE:HG22	1:D:290:LYS:HD2	1.90	0.54
1:E:587:THR:HB	1:E:605:PHE:CD1	2.42	0.54
1:A:207:LEU:HD12	1:A:207:LEU:H	1.72	0.53
1:A:485:PRO:O	1:A:488:GLN:CG	2.54	0.53
1:B:299:TYR:O	1:B:391:LEU:HA	2.07	0.53
1:B:388:ALA:CB	3:B:803:HOH:O	2.55	0.53
1:D:191:ASP:OD2	1:D:193:ARG:NH1	2.41	0.53
1:D:443:ARG:NE	1:D:447:TRP:CE3	2.71	0.53
1:F:197:CYS:SG	1:F:435:CYS:CA	2.95	0.53
1:A:583:ASP:OD2	1:A:599:HIS:CD2	2.61	0.53
1:A:632:LEU:HB2	1:C:341:ILE:CG2	2.38	0.53
1:B:626:LEU:CD2	1:B:637:ILE:HG22	2.29	0.53
1:E:544:TYR:C	1:E:562:CYS:SG	2.87	0.53
1:E:557:VAL:HG21	1:E:586:LEU:HD13	1.90	0.53
1:E:622:SER:OG	1:E:624:LYS:HB2	2.08	0.53
1:A:122:TYR:O	1:A:320:LYS:HG2	2.08	0.53
1:B:596:MET:CE	1:B:598:THR:CG2	2.86	0.53
1:E:552:THR:HB	1:E:584:GLN:NE2	2.24	0.53
1:A:276:ARG:CD	1:A:278:GLU:OE2	2.46	0.53
1:B:212:VAL:HG21	1:B:299:TYR:CE1	2.43	0.53
1:C:349:ASP:N	1:C:349:ASP:OD1	2.40	0.53
1:C:646:THR:O	1:C:647:GLN:HG3	2.09	0.53
1:D:125:PRO:HB3	1:D:202:TYR:CD1	2.43	0.53
1:E:332:VAL:CG1	1:E:442:TYR:HD2	2.18	0.53
1:E:485:PRO:HG3	1:E:531:ASN:ND2	2.23	0.53
1:E:627:ASP:OD1	1:E:628:ARG:N	2.36	0.53
1:A:286:ILE:HG22	1:A:290:LYS:HD2	1.90	0.53
1:D:166:ILE:O	1:D:170:ILE:HG13	2.08	0.53
1:D:611:PHE:CD1	1:E:204:GLU:HB3	2.42	0.53
1:F:346:GLY:HA2	1:F:366:PRO:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:454:ILE:CD1	1:F:460:PRO:HD3	2.33	0.53
1:B:197:CYS:SG	1:B:379:THR:HG21	2.49	0.53
1:B:552:THR:CB	1:B:584:GLN:HE22	2.07	0.53
1:B:596:MET:HE3	1:B:598:THR:HG21	1.89	0.53
1:D:258:LEU:HD12	1:D:262:ILE:CD1	2.36	0.53
1:F:215:PHE:CE1	1:F:254:LEU:CD1	2.81	0.53
1:B:231:ILE:HD13	1:B:265:TRP:NE1	2.24	0.53
1:D:220:TRP:CZ3	1:D:257:LYS:HG2	2.43	0.53
1:F:197:CYS:SG	1:F:435:CYS:HA	2.49	0.53
1:F:413:GLY:O	1:F:415:GLU:OE2	2.26	0.53
1:F:551:LYS:HG2	1:F:555:GLY:HA3	1.91	0.53
1:A:447:TRP:CD1	1:A:448:GLN:N	2.75	0.53
1:F:272:PHE:CE2	1:F:290:LYS:HB3	2.44	0.53
1:A:239:LEU:HD13	1:A:268:LEU:HD11	1.89	0.53
1:A:532:VAL:HB	1:A:573:ILE:HG23	1.90	0.53
1:B:132:LEU:CD2	1:B:136:GLU:OE1	2.57	0.53
1:E:452:PRO:HB2	1:E:453:PRO:HD2	1.91	0.53
1:E:553:ASN:OD1	1:E:553:ASN:N	2.42	0.53
1:F:166:ILE:CG2	1:F:176:ASN:CG	2.77	0.53
1:A:136:GLU:OE2	1:A:193:ARG:NH1	2.42	0.52
1:B:459:SER:N	1:B:460:PRO:CA	2.72	0.52
1:C:346:GLY:HA2	1:C:366:PRO:CB	2.32	0.52
1:C:626:LEU:O	1:C:647:GLN:HA	2.08	0.52
1:F:141:GLU:OE2	1:F:141:GLU:HA	2.08	0.52
1:B:127:LEU:HD12	1:B:377:THR:CG2	2.38	0.52
1:D:443:ARG:C	1:D:444:LEU:HD12	2.29	0.52
1:E:217:ASN:HD21	1:E:250:ASN:HB2	1.75	0.52
1:A:586:LEU:N	1:A:586:LEU:CD2	2.73	0.52
1:B:264:LEU:O	1:B:265:TRP:HB2	2.09	0.52
1:D:410:GLN:HB2	1:D:460:PRO:HB2	1.91	0.52
1:F:136:GLU:OE1	1:F:138:LYS:CA	2.57	0.52
1:A:414:GLY:CA	1:A:415:GLU:CB	2.79	0.52
1:B:189:VAL:CG1	1:B:340:ILE:HD12	2.38	0.52
1:B:264:LEU:CD2	1:B:265:TRP:N	2.73	0.52
1:C:155:PRO:HB3	1:C:337:THR:HG21	1.89	0.52
1:C:410:GLN:C	1:C:411:ILE:HG23	2.30	0.52
1:D:329:LEU:HG	1:D:434:PRO:HA	1.92	0.52
1:E:551:LYS:HE3	1:E:555:GLY:HA3	1.92	0.52
1:C:193:ARG:NH2	1:C:308:VAL:CG2	2.73	0.52
1:D:271:VAL:CG2	1:D:273:ARG:NH1	2.73	0.52
1:A:183:ILE:CG2	1:A:187:ARG:HD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLY:HA3	1:B:183:ILE:CG2	2.29	0.52
1:B:573:ILE:HD11	1:B:610:TYR:CD2	2.45	0.52
1:E:454:ILE:HD13	1:E:457:GLY:CA	2.40	0.52
1:F:195:GLU:OE1	1:F:198:LYS:HE3	2.08	0.52
1:F:230:VAL:O	1:F:234:THR:HG22	2.09	0.52
1:A:533:ASP:OD2	1:A:612:LYS:CE	2.52	0.52
1:D:171:LYS:HG2	1:D:448:GLN:CD	2.30	0.52
1:E:626:LEU:O	1:E:647:GLN:HA	2.10	0.52
1:A:329:LEU:HG	1:A:434:PRO:HA	1.92	0.52
1:B:147:GLY:O	1:C:489:ALA:CB	2.53	0.52
1:B:388:ALA:HB3	3:B:803:HOH:O	2.08	0.52
1:B:444:LEU:N	1:B:444:LEU:CD1	2.73	0.52
1:B:450:ASN:ND2	1:B:450:ASN:H	2.08	0.52
1:C:628:ARG:HB2	1:C:634:GLN:O	2.10	0.52
1:D:223:LEU:HD12	1:D:223:LEU:O	2.10	0.52
1:D:262:ILE:O	1:D:264:LEU:O	2.27	0.52
1:F:281:ILE:HD11	1:F:413:GLY:H	1.75	0.52
1:C:207:LEU:CD2	1:C:207:LEU:N	2.73	0.52
1:C:217:ASN:HD21	1:C:250:ASN:HB2	1.74	0.52
1:C:329:LEU:HG	1:C:434:PRO:HA	1.92	0.52
1:D:264:LEU:CD2	1:D:265:TRP:N	2.73	0.52
1:E:176:ASN:C	1:E:176:ASN:HD22	2.11	0.52
1:E:574:ASN:HD22	1:E:578:GLN:CG	2.23	0.52
1:F:258:LEU:O	1:F:262:ILE:HD11	2.09	0.52
1:B:576:ALA:O	1:B:606:LYS:HB3	2.10	0.52
1:E:207:LEU:CD1	1:E:319:SER:CB	2.88	0.52
1:E:556:PHE:HE2	1:E:594:LYS:HD3	1.70	0.52
1:F:225:ARG:NH2	1:F:225:ARG:CG	2.73	0.52
1:A:266:ASN:HD21	1:D:500:LYS:NZ	2.08	0.51
1:C:286:ILE:HG22	1:C:290:LYS:HD2	1.91	0.51
1:D:444:LEU:N	1:D:444:LEU:CD1	2.73	0.51
1:E:329:LEU:HG	1:E:434:PRO:HA	1.92	0.51
1:E:354:GLY:O	1:E:385:PRO:HD2	2.09	0.51
1:E:452:PRO:HB2	1:E:453:PRO:CD	2.41	0.51
1:F:520:ASP:OD1	1:F:520:ASP:N	2.41	0.51
1:A:588:LYS:HD2	1:A:588:LYS:O	2.10	0.51
1:E:411:ILE:HD13	1:E:411:ILE:H	1.74	0.51
1:E:514:MET:CE	1:E:518:ALA:CB	2.86	0.51
1:E:653:ASN:HD22	1:E:653:ASN:N	2.07	0.51
1:F:363:LYS:HD2	1:F:525:TYR:OH	2.10	0.51
1:B:443:ARG:HD2	1:B:447:TRP:CE3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ASN:ND2	1:B:578:GLN:CG	2.69	0.51
1:D:138:LYS:CD	1:D:138:LYS:N	2.73	0.51
1:E:193:ARG:NE	1:E:435:CYS:O	2.43	0.51
1:E:234:THR:HG22	1:E:310:TRP:NE1	2.25	0.51
1:E:535:GLY:HA3	1:E:652:ASN:O	2.10	0.51
1:F:329:LEU:HG	1:F:434:PRO:HA	1.92	0.51
1:B:586:LEU:HA	1:B:596:MET:O	2.09	0.51
1:C:574:ASN:ND2	1:C:578:GLN:CG	2.69	0.51
1:D:485:PRO:HG3	1:D:531:ASN:ND2	2.25	0.51
1:E:534:TRP:CH2	1:E:653:ASN:HB3	2.45	0.51
1:B:149:PRO:HG2	1:C:491:PRO:HG3	1.92	0.51
1:B:443:ARG:HH11	1:B:443:ARG:CG	2.16	0.51
1:B:459:SER:N	1:B:460:PRO:HA	2.25	0.51
1:D:176:ASN:HD22	1:D:176:ASN:C	2.14	0.51
1:B:329:LEU:HG	1:B:434:PRO:HA	1.92	0.51
1:B:576:ALA:O	1:B:606:LYS:HD2	2.10	0.51
1:C:207:LEU:N	1:C:207:LEU:HD22	2.25	0.51
1:D:136:GLU:OE2	1:D:193:ARG:NH2	2.43	0.51
1:D:413:GLY:CA	1:D:464:ASN:HD22	2.22	0.51
1:E:511:LYS:O	1:E:515:GLU:HG3	2.10	0.51
1:E:514:MET:HE2	1:E:514:MET:HA	1.92	0.51
1:E:605:PHE:HD1	1:E:607:GLU:OE2	1.92	0.51
1:E:624:LYS:HD2	1:E:639:ASN:OD1	2.11	0.51
1:B:134:ASN:OD1	1:B:134:ASN:N	2.32	0.51
1:B:362:TRP:O	1:B:363:LYS:HG2	2.10	0.51
1:B:522:THR:CG2	1:B:527:LEU:HD11	2.41	0.51
1:C:372:LYS:CE	1:C:378:LYS:HZ1	2.11	0.51
1:E:608:TRP:CZ3	1:E:626:LEU:HD13	2.46	0.51
1:F:345:GLY:O	1:F:350:GLY:HA3	2.09	0.51
1:F:641:ASP:C	1:F:643:SER:H	2.14	0.51
1:A:628:ARG:NH1	1:A:628:ARG:CG	2.73	0.51
1:B:342:PRO:O	1:D:632:LEU:CD1	2.56	0.51
1:B:462:LEU:O	1:B:462:LEU:HG	2.10	0.51
1:B:552:THR:CG2	1:B:584:GLN:OE1	2.58	0.51
1:C:207:LEU:H	1:C:207:LEU:HD22	1.73	0.51
1:D:208:THR:H	1:D:295:GLN:NE2	2.06	0.51
1:D:237:LYS:CG	1:D:238:TYR:CE2	2.93	0.51
1:F:232:LYS:NZ	1:F:233:ARG:HH11	2.08	0.51
1:F:454:ILE:CG2	1:F:458:SER:O	2.58	0.51
1:A:371:GLU:HG2	1:A:519:TYR:OH	2.10	0.51
1:B:203:ASP:OD2	1:B:205:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:CYS:HG	1:B:600:CYS:CB	2.23	0.51
1:B:629:SER:HB3	1:B:634:GLN:CB	2.41	0.51
1:C:522:THR:CG2	1:C:527:LEU:HD11	2.41	0.51
1:D:209:SER:HG	1:D:311:TYR:HE1	1.57	0.51
1:D:632:LEU:HD23	1:D:633:HIS:H	1.76	0.51
1:E:563:HIS:CD2	1:E:563:HIS:N	2.78	0.51
1:B:362:TRP:C	1:B:363:LYS:HG2	2.32	0.51
1:B:459:SER:N	1:B:461:THR:N	2.59	0.51
1:B:616:ARG:CD	1:B:648:LYS:CE	2.65	0.51
1:F:177:MET:CE	1:F:221:SER:OG	2.59	0.51
1:A:641:ASP:HB3	1:A:644:LYS:HG3	1.93	0.50
1:D:138:LYS:H	1:D:138:LYS:HD2	1.71	0.50
1:D:264:LEU:CD2	1:D:265:TRP:H	2.25	0.50
1:D:533:ASP:OD2	1:D:612:LYS:HE2	2.11	0.50
1:E:564:ARG:HA	1:E:569:GLN:OE1	2.12	0.50
1:F:362:TRP:O	1:F:363:LYS:HG2	2.11	0.50
1:A:502:ARG:HG3	1:A:507:CYS:HB2	1.93	0.50
1:C:443:ARG:CG	1:C:443:ARG:NH1	2.73	0.50
1:C:534:TRP:CH2	1:C:653:ASN:HB3	2.47	0.50
1:D:220:TRP:CZ2	1:D:261:TYR:CD2	2.97	0.50
1:D:264:LEU:O	1:D:265:TRP:HB2	2.11	0.50
1:D:454:ILE:HG21	1:D:459:SER:OG	2.11	0.50
1:E:574:ASN:ND2	1:E:578:GLN:CG	2.73	0.50
1:F:152:LYS:O	1:F:189:VAL:HA	2.12	0.50
1:B:443:ARG:CG	1:B:443:ARG:NH1	2.73	0.50
1:C:456:VAL:O	1:C:456:VAL:HG23	2.12	0.50
1:D:143:PRO:HG3	1:D:146:VAL:HG12	1.94	0.50
1:D:348:GLU:CB	1:D:349:ASP:HA	2.22	0.50
1:D:415:GLU:HG2	1:D:416:ASN:N	2.25	0.50
1:E:152:LYS:N	1:E:152:LYS:CD	2.73	0.50
1:A:628:ARG:HG2	1:A:649:TRP:CZ2	2.46	0.50
1:E:143:PRO:HG3	1:E:146:VAL:HG12	1.94	0.50
1:E:285:SER:O	1:E:289:GLN:HG3	2.12	0.50
1:E:526:PRO:HG2	1:E:602:LEU:HD13	1.91	0.50
1:E:573:ILE:HD13	1:E:610:TYR:HB2	1.94	0.50
1:F:186:ASP:OD1	1:F:228:HIS:CD2	2.49	0.50
1:A:457:GLY:N	1:A:458:SER:CA	2.74	0.50
1:B:192:LEU:HG	1:B:342:PRO:HG3	1.93	0.50
1:D:354:GLY:HA3	1:D:362:TRP:HH2	1.75	0.50
1:D:553:ASN:N	1:D:584:GLN:OE1	2.43	0.50
1:E:462:LEU:HG	1:E:490:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:TYR:N	1:E:525:TYR:CD1	2.79	0.50
1:E:573:ILE:CD1	1:E:610:TYR:CD2	2.94	0.50
1:A:118:GLN:NE2	1:A:322:ARG:N	2.58	0.50
1:B:614:LEU:HD22	1:B:648:LYS:HE2	1.94	0.50
1:C:347:ASP:HB3	1:C:350:GLY:H	1.76	0.50
1:D:443:ARG:CZ	1:D:447:TRP:CH2	2.95	0.50
1:D:611:PHE:HD1	1:E:204:GLU:CB	2.23	0.50
1:E:363:LYS:CD	1:E:525:TYR:HE2	2.20	0.50
1:B:601:ASN:C	1:B:604:GLU:HG3	2.32	0.50
1:C:628:ARG:NH1	1:C:646:THR:HG22	2.25	0.50
1:D:196:GLU:OE2	1:D:379:THR:OG1	2.28	0.50
1:D:248:PHE:CZ	1:D:275:GLU:O	2.63	0.50
1:F:230:VAL:HG21	1:F:242:ILE:HD13	1.94	0.50
1:A:600:CYS:O	1:A:601:ASN:OD1	2.29	0.50
1:E:630:GLU:O	1:E:633:HIS:ND1	2.45	0.50
1:E:653:ASN:N	1:E:653:ASN:ND2	2.60	0.50
1:F:156:LEU:HD22	1:F:158:LEU:CD2	2.42	0.50
1:F:254:LEU:N	1:F:254:LEU:CD2	2.73	0.50
1:F:443:ARG:NH1	1:F:447:TRP:CH2	2.79	0.50
1:A:122:TYR:OH	1:A:206:LEU:HD23	2.11	0.50
1:E:462:LEU:HG	1:E:490:LEU:HD22	1.94	0.50
1:A:450:ASN:N	1:A:450:ASN:ND2	2.60	0.49
1:A:579:LEU:O	1:A:586:LEU:HD23	2.11	0.49
1:A:632:LEU:CB	1:C:341:ILE:CG2	2.90	0.49
1:B:260:GLU:OE1	1:B:263:LYS:NZ	2.44	0.49
1:D:273:ARG:NH1	1:D:273:ARG:CG	2.73	0.49
1:D:456:VAL:HG11	1:D:463:LYS:HZ2	1.76	0.49
1:E:231:ILE:HD12	1:E:265:TRP:CD1	2.47	0.49
1:F:203:ASP:OD1	1:F:205:ASN:HB2	2.12	0.49
1:A:281:ILE:HD13	1:A:409:LEU:HB3	1.93	0.49
1:A:414:GLY:CA	1:A:416:ASN:H	2.25	0.49
1:C:155:PRO:HD3	1:C:339:GLU:CG	2.28	0.49
1:C:348:GLU:N	1:C:350:GLY:N	2.60	0.49
1:C:447:TRP:CD1	1:C:448:GLN:N	2.80	0.49
1:C:459:SER:O	1:C:463:LYS:CB	2.60	0.49
1:D:552:THR:CA	1:D:584:GLN:OE1	2.60	0.49
1:F:244:LEU:C	1:F:245:ILE:HD12	2.32	0.49
1:F:655:HIS:CD2	3:F:809:HOH:O	2.62	0.49
1:A:162:PHE:CE1	1:D:455:TYR:CD2	2.98	0.49
1:A:532:VAL:HB	1:A:573:ILE:CG2	2.42	0.49
1:C:373:ARG:O	1:C:373:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:LYS:CD	1:D:448:GLN:HE22	2.15	0.49
1:D:450:ASN:N	1:D:450:ASN:ND2	2.60	0.49
1:E:282:GLN:NE2	1:E:409:LEU:O	2.41	0.49
1:E:410:GLN:HB3	1:E:411:ILE:HG12	1.93	0.49
1:F:406:ASP:HB2	1:F:498:LEU:HD21	1.95	0.49
1:C:180:SER:OG	1:C:225:ARG:NH1	2.46	0.49
1:C:235:PRO:HB2	1:C:238:TYR:HD2	1.78	0.49
1:D:447:TRP:HD1	1:D:448:GLN:H	1.59	0.49
1:F:271:VAL:O	1:F:272:PHE:HD1	1.95	0.49
1:F:272:PHE:HD2	1:F:290:LYS:HB3	1.76	0.49
1:F:585:CYS:HB2	1:F:600:CYS:HB3	1.94	0.49
1:A:173:PHE:CD2	1:A:177:MET:HG3	2.47	0.49
1:A:601:ASN:HB2	1:A:604:GLU:OE1	2.13	0.49
1:C:485:PRO:O	1:C:488:GLN:CG	2.54	0.49
1:C:584:GLN:HG2	1:C:598:THR:C	2.32	0.49
1:D:312:ALA:N	1:D:313:PRO:CD	2.75	0.49
1:E:484:ARG:HH11	1:E:484:ARG:HG3	1.77	0.49
1:A:128:ARG:HG3	1:A:201:HIS:HD2	1.72	0.49
1:B:122:TYR:CE1	1:B:203:ASP:HB3	2.46	0.49
1:B:570:LEU:O	1:B:581:GLN:HG3	2.12	0.49
1:B:653:ASN:ND2	1:B:653:ASN:N	2.60	0.49
1:D:458:SER:OG	1:D:656:SER:OG	2.31	0.49
1:A:156:LEU:HD22	1:A:158:LEU:CD2	2.42	0.49
1:B:461:THR:O	1:B:464:ASN:N	2.45	0.49
1:B:551:LYS:C	1:B:552:THR:CG2	2.80	0.49
1:B:615:HIS:O	1:B:648:LYS:CB	2.56	0.49
1:D:281:ILE:HD12	1:D:410:GLN:O	2.13	0.49
1:B:624:LYS:HG3	1:B:638:SER:C	2.32	0.49
1:D:115:PHE:HE2	1:D:426:CYS:O	1.96	0.49
1:D:203:ASP:C	1:D:205:ASN:H	2.15	0.49
1:E:552:THR:CA	1:E:584:GLN:OE1	2.61	0.49
1:E:627:ASP:CB	3:E:808:HOH:O	2.37	0.49
1:F:176:ASN:C	1:F:176:ASN:HD22	2.15	0.49
1:F:353:ARG:NH2	1:F:520:ASP:CG	2.66	0.49
1:F:450:ASN:N	1:F:450:ASN:ND2	2.60	0.49
1:A:152:LYS:CD	1:A:152:LYS:N	2.76	0.49
1:B:149:PRO:CG	1:C:491:PRO:HG3	2.43	0.49
1:B:614:LEU:O	1:B:615:HIS:CB	2.51	0.49
1:C:584:GLN:HG2	1:C:598:THR:O	2.13	0.49
1:E:473:TRP:O	1:E:474:ASP:HB2	2.13	0.49
1:F:230:VAL:HG23	1:F:231:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:NZ	3:A:806:HOH:O	2.46	0.49
1:B:450:ASN:ND2	1:B:450:ASN:N	2.60	0.49
1:B:485:PRO:O	1:B:488:GLN:CG	2.54	0.49
1:C:601:ASN:HB2	1:C:604:GLU:OE1	2.13	0.49
1:D:266:ASN:N	1:D:266:ASN:ND2	2.60	0.49
1:E:598:THR:HG22	1:E:599:HIS:H	1.77	0.49
1:F:442:TYR:CD1	1:F:443:ARG:N	2.73	0.49
1:F:544:TYR:CE2	3:F:812:HOH:O	2.55	0.49
1:A:641:ASP:H	1:A:647:GLN:NE2	1.99	0.48
1:B:169:SER:HB2	1:B:177:MET:HB2	1.95	0.48
1:B:180:SER:OG	1:B:225:ARG:NH1	2.46	0.48
1:D:180:SER:CB	1:D:225:ARG:HH12	2.26	0.48
1:E:230:VAL:O	1:E:234:THR:HG23	2.12	0.48
1:E:264:LEU:O	1:E:265:TRP:CB	2.61	0.48
1:E:454:ILE:HB	1:E:457:GLY:CA	2.43	0.48
1:F:183:ILE:CG2	1:F:225:ARG:NH1	2.75	0.48
1:B:281:ILE:HD12	1:B:410:GLN:O	2.13	0.48
1:B:318:ILE:O	1:B:321:ASP:O	2.30	0.48
1:D:136:GLU:CD	1:D:193:ARG:NH2	2.67	0.48
1:E:262:ILE:O	1:E:262:ILE:CG2	2.60	0.48
1:E:637:ILE:O	1:E:637:ILE:HG13	2.13	0.48
1:F:232:LYS:NZ	3:F:802:HOH:O	2.43	0.48
1:D:485:PRO:HB2	1:D:534:TRP:CD2	2.48	0.48
1:D:600:CYS:SG	1:D:604:GLU:HB3	2.53	0.48
1:E:193:ARG:NH1	1:E:308:VAL:O	2.45	0.48
1:E:552:THR:HB	1:E:584:GLN:CD	2.33	0.48
1:E:614:LEU:HD12	1:E:616:ARG:CZ	2.43	0.48
1:E:632:LEU:H	1:E:632:LEU:CD1	1.96	0.48
1:A:363:LYS:HD2	1:A:525:TYR:OH	2.14	0.48
1:A:412:TRP:CD1	1:A:412:TRP:C	2.86	0.48
1:B:246:ASP:HB3	1:B:273:ARG:HA	1.95	0.48
1:B:347:ASP:CB	1:B:349:ASP:O	2.61	0.48
1:B:520:ASP:OD1	1:B:520:ASP:N	2.41	0.48
1:C:141:GLU:HG2	1:C:142:PRO:HD2	1.96	0.48
1:D:586:LEU:N	1:D:586:LEU:HD23	2.29	0.48
1:E:548:SER:O	1:E:549:MET:HB3	2.13	0.48
1:E:573:ILE:HD13	1:E:610:TYR:CB	2.44	0.48
1:F:177:MET:HE3	1:F:221:SER:OG	2.14	0.48
1:C:166:ILE:HG23	1:C:176:ASN:ND2	2.28	0.48
1:C:208:THR:HG21	1:C:240:ALA:HB2	1.89	0.48
1:C:410:GLN:O	1:C:411:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ILE:O	1:E:262:ILE:HG22	2.13	0.48
1:E:276:ARG:CG	1:E:276:ARG:NH1	2.73	0.48
1:E:454:ILE:CB	1:E:457:GLY:HA3	2.43	0.48
1:A:176:ASN:C	1:A:176:ASN:HD22	2.15	0.48
1:D:116:LYS:O	1:D:322:ARG:NH2	2.45	0.48
1:F:574:ASN:ND2	1:F:578:GLN:CG	2.69	0.48
1:B:620:ILE:HG22	1:B:621:PRO:CD	2.42	0.48
1:B:624:LYS:HG3	1:B:638:SER:O	2.13	0.48
1:C:264:LEU:HD23	1:C:265:TRP:H	1.79	0.48
1:C:348:GLU:H	1:C:350:GLY:N	2.12	0.48
1:D:586:LEU:N	1:D:586:LEU:CD2	2.76	0.48
1:D:614:LEU:HD13	1:D:616:ARG:HB3	1.96	0.48
1:F:143:PRO:CB	1:F:151:GLU:OE2	2.62	0.48
1:F:475:GLU:OE1	1:F:511:LYS:CE	2.56	0.48
1:B:195:GLU:OE1	1:B:198:LYS:NZ	2.47	0.48
1:C:154:LYS:NZ	3:C:805:HOH:O	2.46	0.48
1:C:209:SER:OG	1:C:296:VAL:HG22	2.14	0.48
1:C:551:LYS:HE3	1:C:556:PHE:O	2.14	0.48
1:D:375:ARG:NH1	1:D:380:GLU:O	2.38	0.48
1:F:207:LEU:H	1:F:207:LEU:HD12	1.78	0.48
1:A:312:ALA:N	1:A:313:PRO:CD	2.77	0.48
1:B:601:ASN:HB2	1:B:604:GLU:CG	2.36	0.48
1:B:632:LEU:HD22	1:B:634:GLN:HE22	1.78	0.48
1:C:113:LEU:HG	1:C:504:ASP:HB3	1.96	0.48
1:C:476:TYR:O	1:C:477:LYS:C	2.51	0.48
1:E:152:LYS:H	1:E:152:LYS:CD	2.24	0.48
1:A:180:SER:OG	1:A:225:ARG:NH1	2.46	0.48
1:A:195:GLU:OE2	1:A:198:LYS:HE3	2.14	0.48
1:C:208:THR:HG22	1:C:240:ALA:HB2	1.90	0.48
1:D:301:ASP:OD2	1:D:440:HIS:NE2	2.47	0.48
1:D:642:SER:HA	1:D:643:SER:HA	1.69	0.48
1:E:152:LYS:HD3	1:E:152:LYS:N	2.28	0.48
1:E:539:GLY:O	1:E:542:THR:OG1	2.29	0.48
1:F:113:LEU:HD12	1:F:504:ASP:HB3	1.96	0.48
1:F:312:ALA:N	1:F:313:PRO:CD	2.77	0.48
1:A:220:TRP:CE3	1:A:257:LYS:HE3	2.49	0.47
1:A:551:LYS:HE3	1:A:556:PHE:O	2.14	0.47
1:A:590:ALA:HA	1:A:591:ASP:C	2.34	0.47
1:B:312:ALA:N	1:B:313:PRO:CD	2.77	0.47
1:D:190:ASN:HD22	1:D:190:ASN:H	1.61	0.47
1:D:321:ASP:HB3	1:D:324:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:GLU:HG2	1:E:142:PRO:HD2	1.96	0.47
1:E:552:THR:CB	1:E:553:ASN:OD1	2.62	0.47
1:E:563:HIS:CD2	1:E:563:HIS:H	2.31	0.47
1:F:146:VAL:HA	1:F:147:GLY:HA2	1.64	0.47
1:F:177:MET:HE3	1:F:181:ASP:OD1	2.14	0.47
1:A:122:TYR:CD2	1:A:205:ASN:HB3	2.49	0.47
1:C:220:TRP:CE3	1:C:257:LYS:HE3	2.49	0.47
1:C:312:ALA:N	1:C:313:PRO:CD	2.77	0.47
1:C:587:THR:OG1	1:C:588:LYS:N	2.47	0.47
1:D:323:THR:HG22	1:D:398:PHE:CE1	2.49	0.47
1:F:134:ASN:ND2	1:F:204:GLU:OE2	2.47	0.47
1:F:454:ILE:CB	1:F:458:SER:O	2.62	0.47
1:B:208:THR:OG1	1:B:295:GLN:HG3	2.14	0.47
1:B:254:LEU:O	1:B:273:ARG:NH1	2.39	0.47
1:B:458:SER:C	1:B:460:PRO:HA	2.34	0.47
1:B:463:LYS:HE3	1:B:491:PRO:O	2.15	0.47
1:D:120:PHE:CE2	1:D:207:LEU:HD21	2.49	0.47
1:D:141:GLU:HG2	1:D:142:PRO:HD2	1.96	0.47
1:D:346:GLY:CA	1:D:366:PRO:HA	2.44	0.47
1:E:189:VAL:HG13	1:E:340:ILE:HD12	1.95	0.47
1:E:220:TRP:CE3	1:E:257:LYS:HE3	2.49	0.47
1:E:370:GLN:H	1:E:370:GLN:CD	2.05	0.47
1:E:564:ARG:H	1:E:569:GLN:NE2	2.12	0.47
1:F:444:LEU:CD1	1:F:444:LEU:H	2.26	0.47
1:F:485:PRO:O	1:F:488:GLN:CG	2.54	0.47
1:B:626:LEU:CD2	1:B:637:ILE:CG2	2.88	0.47
1:C:415:GLU:H	1:C:415:GLU:HG3	1.50	0.47
1:D:552:THR:HA	1:D:584:GLN:OE1	2.13	0.47
1:E:347:ASP:N	1:E:347:ASP:OD1	2.45	0.47
1:F:187:ARG:HG2	1:F:225:ARG:HH22	1.79	0.47
1:B:356:TRP:HZ2	1:B:514:MET:HE3	1.78	0.47
1:B:363:LYS:HD2	1:B:525:TYR:CE1	2.49	0.47
1:B:412:TRP:O	1:B:461:THR:HG22	2.14	0.47
1:D:173:PHE:HD2	1:D:177:MET:HG3	1.75	0.47
1:D:264:LEU:HD23	1:D:265:TRP:H	1.80	0.47
1:D:627:ASP:OD1	1:D:646:THR:HB	2.14	0.47
1:E:193:ARG:HH22	1:E:310:TRP:N	2.11	0.47
1:A:147:GLY:CA	1:D:489:ALA:HB2	2.42	0.47
1:A:152:LYS:CD	1:A:152:LYS:H	2.27	0.47
1:B:552:THR:HG22	1:B:584:GLN:OE1	2.15	0.47
1:D:262:ILE:O	1:D:262:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:ASN:N	1:D:653:ASN:ND2	2.63	0.47
1:F:573:ILE:HD13	1:F:610:TYR:HB3	1.96	0.47
1:A:138:LYS:HB2	1:A:138:LYS:HE3	1.55	0.47
1:A:235:PRO:HB2	1:A:238:TYR:HD2	1.78	0.47
1:A:377:THR:HB	1:A:380:GLU:HG2	1.95	0.47
1:A:622:SER:OG	1:A:624:LYS:CG	2.63	0.47
1:A:622:SER:OG	1:A:624:LYS:HG3	2.14	0.47
1:B:227:VAL:O	1:B:231:ILE:HG23	2.14	0.47
1:B:502:ARG:HG2	1:B:507:CYS:HB2	1.96	0.47
1:B:506:ASN:ND2	3:B:804:HOH:O	2.46	0.47
1:B:601:ASN:O	1:B:604:GLU:CB	2.52	0.47
1:C:254:LEU:O	1:C:273:ARG:NH2	2.48	0.47
1:C:450:ASN:ND2	1:C:450:ASN:N	2.60	0.47
1:D:316:ALA:N	1:D:317:PRO:HD2	2.29	0.47
1:D:551:LYS:HE3	1:D:556:PHE:O	2.14	0.47
1:D:642:SER:HA	1:D:644:LYS:HB2	1.97	0.47
1:E:312:ALA:N	1:E:313:PRO:CD	2.77	0.47
1:E:556:PHE:CD2	1:E:594:LYS:CD	2.89	0.47
1:F:203:ASP:O	1:F:204:GLU:HB2	2.15	0.47
1:F:611:PHE:HB2	1:F:614:LEU:HB2	1.96	0.47
1:A:632:LEU:HA	1:C:341:ILE:CG2	2.45	0.47
1:E:325:CYS:HB2	1:E:394:ILE:HG23	1.97	0.47
1:E:494:ASP:CG	1:E:496:SER:OG	2.52	0.47
1:E:606:LYS:HG3	1:E:606:LYS:O	2.15	0.47
1:F:132:LEU:CD2	1:F:199:TYR:HE1	2.28	0.47
1:F:246:ASP:O	1:F:274:ASN:HB2	2.15	0.47
1:A:457:GLY:N	1:A:458:SER:HA	2.29	0.47
1:B:588:LYS:CG	1:B:637:ILE:HD11	2.45	0.47
1:D:164:GLN:HA	1:D:164:GLN:NE2	2.30	0.47
1:D:520:ASP:O	1:D:523:SER:HB3	2.15	0.47
1:E:189:VAL:CG1	1:E:190:ASN:N	2.78	0.47
1:E:318:ILE:O	1:E:321:ASP:O	2.32	0.47
1:A:200:TRP:HZ2	1:A:377:THR:HG21	1.79	0.47
1:B:113:LEU:N	1:B:113:LEU:HD23	2.30	0.47
1:B:325:CYS:HB2	1:B:394:ILE:HG23	1.97	0.47
1:B:346:GLY:N	3:B:806:HOH:O	2.48	0.47
1:C:476:TYR:C	1:C:478:ASP:N	2.68	0.47
1:C:627:ASP:CG	1:C:647:GLN:CG	2.82	0.47
1:E:556:PHE:HD2	1:E:594:LYS:CD	2.23	0.47
1:F:132:LEU:HD23	1:F:199:TYR:HE1	1.80	0.47
1:F:217:ASN:OD1	1:F:251:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:579:LEU:O	1:F:586:LEU:HD23	2.15	0.47
1:C:206:LEU:N	1:C:206:LEU:CD1	2.78	0.46
1:C:579:LEU:O	1:C:586:LEU:HD23	2.15	0.46
1:D:217:ASN:HA	1:D:254:LEU:CD1	2.45	0.46
1:E:224:MET:CE	1:E:258:LEU:HD11	2.45	0.46
1:E:454:ILE:HB	1:E:457:GLY:HA3	1.97	0.46
1:A:262:ILE:HD13	1:A:262:ILE:HA	1.73	0.46
1:A:321:ASP:HB3	1:A:324:ILE:HD12	1.96	0.46
1:C:321:ASP:HB3	1:C:324:ILE:HD12	1.96	0.46
1:D:492:TYR:HE2	3:D:825:HOH:O	1.98	0.46
1:E:624:LYS:CG	1:E:638:SER:O	2.54	0.46
1:F:325:CYS:HB2	1:F:394:ILE:HG23	1.97	0.46
1:A:141:GLU:HG2	1:A:142:PRO:HD2	1.96	0.46
1:B:218:GLU:OE1	1:B:303:HIS:HD2	1.97	0.46
1:C:580:MET:HG2	1:C:585:CYS:SG	2.56	0.46
1:D:190:ASN:H	1:D:190:ASN:ND2	2.13	0.46
1:D:316:ALA:HB3	1:D:317:PRO:HD3	1.96	0.46
1:D:587:THR:OG1	1:D:588:LYS:N	2.47	0.46
1:E:609:GLN:NE2	1:E:611:PHE:CZ	2.83	0.46
1:F:253:HIS:CG	1:F:254:LEU:HD23	2.50	0.46
1:F:258:LEU:HD22	1:F:258:LEU:C	2.36	0.46
1:F:321:ASP:HB3	1:F:324:ILE:HD12	1.96	0.46
1:F:554:GLY:N	1:F:597:ILE:O	2.22	0.46
1:A:156:LEU:HD22	1:A:158:LEU:HD21	1.96	0.46
1:B:590:ALA:HA	1:B:591:ASP:HA	1.66	0.46
1:D:266:ASN:N	1:D:266:ASN:HD22	2.12	0.46
1:D:271:VAL:HG21	1:D:273:ARG:HH12	1.76	0.46
1:E:207:LEU:HD12	1:E:319:SER:OG	2.14	0.46
1:B:276:ARG:HB3	1:B:276:ARG:NH1	2.30	0.46
1:D:443:ARG:HG3	1:D:443:ARG:NH1	2.20	0.46
1:A:325:CYS:HB2	1:A:394:ILE:HG23	1.97	0.46
1:D:226:THR:O	1:D:230:VAL:HG23	2.16	0.46
1:D:443:ARG:HD3	1:D:447:TRP:CE3	2.44	0.46
1:D:456:VAL:HG11	1:D:463:LYS:NZ	2.31	0.46
1:D:640:CYS:HA	1:D:647:GLN:HE22	1.81	0.46
1:E:303:HIS:O	1:E:441:ILE:HG13	2.15	0.46
1:E:490:LEU:CD1	1:E:656:SER:O	2.63	0.46
1:B:616:ARG:HD2	1:B:648:LYS:HE2	1.96	0.46
1:B:655:HIS:N	1:B:655:HIS:CD2	2.83	0.46
1:C:534:TRP:CZ2	1:C:653:ASN:HB3	2.51	0.46
1:D:453:PRO:C	1:D:454:ILE:HD13	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:GLN:CG	1:D:597:ILE:HG23	2.29	0.46
1:F:151:GLU:H	1:F:151:GLU:HG2	1.45	0.46
1:F:156:LEU:HD22	1:F:158:LEU:HD21	1.96	0.46
1:A:195:GLU:O	1:A:198:LYS:HG3	2.16	0.46
1:A:476:TYR:O	1:A:477:LYS:C	2.53	0.46
1:B:212:VAL:CG2	1:B:299:TYR:CE1	2.99	0.46
1:C:463:LYS:HG3	1:C:492:TYR:HA	1.98	0.46
1:E:548:SER:O	1:E:549:MET:CB	2.63	0.46
1:E:593:SER:O	1:E:636:PHE:CB	2.64	0.46
1:A:254:LEU:O	1:A:273:ARG:NH2	2.48	0.46
1:A:473:TRP:CZ3	1:A:480:PHE:HB2	2.51	0.46
1:C:573:ILE:HD13	1:C:610:TYR:HB3	1.97	0.46
1:D:443:ARG:NH1	1:D:443:ARG:CG	2.73	0.46
1:D:520:ASP:OD1	1:D:520:ASP:N	2.41	0.46
1:F:136:GLU:OE1	1:F:138:LYS:CB	2.64	0.46
1:F:413:GLY:HA3	1:F:464:ASN:ND2	2.22	0.46
1:B:473:TRP:CZ3	1:B:480:PHE:HB2	2.51	0.46
1:C:241:GLU:CB	1:C:270:LYS:NZ	2.78	0.46
1:D:151:GLU:HA	1:D:152:LYS:HA	1.71	0.46
1:D:473:TRP:O	1:D:474:ASP:HB2	2.17	0.46
1:E:122:TYR:HB3	1:E:320:LYS:HA	1.98	0.46
1:E:556:PHE:CE2	1:E:594:LYS:HB3	2.51	0.46
1:F:177:MET:O	1:F:181:ASP:OD1	2.34	0.46
1:F:225:ARG:NH2	1:F:225:ARG:HG2	2.30	0.46
1:A:262:ILE:HD13	1:A:265:TRP:CZ3	2.50	0.45
1:B:559:LEU:HD22	1:B:628:ARG:HG3	1.98	0.45
1:C:473:TRP:CZ3	1:C:480:PHE:HB2	2.51	0.45
1:E:608:TRP:HZ3	1:E:626:LEU:HD13	1.80	0.45
1:F:336:ASN:HB2	1:F:444:LEU:HD21	1.98	0.45
1:A:377:THR:HG22	1:A:378:LYS:N	2.32	0.45
1:A:590:ALA:HA	1:A:592:GLY:N	2.30	0.45
1:A:632:LEU:CB	1:C:341:ILE:HG22	2.46	0.45
1:B:212:VAL:CG2	1:B:299:TYR:CD1	2.99	0.45
1:B:552:THR:HB	1:B:584:GLN:OE1	2.16	0.45
1:B:585:CYS:CB	1:B:600:CYS:CB	2.85	0.45
1:C:573:ILE:CD1	1:C:610:TYR:HD2	2.29	0.45
1:F:191:ASP:OD1	1:F:193:ARG:HB2	2.16	0.45
1:A:574:ASN:ND2	1:A:578:GLN:CG	2.76	0.45
1:B:122:TYR:O	1:B:320:LYS:HE2	2.16	0.45
1:B:156:LEU:CD2	1:B:158:LEU:HD21	2.47	0.45
1:B:326:THR:HG23	1:B:433:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:TYR:O	1:B:406:ASP:C	2.55	0.45
1:E:193:ARG:NH1	1:E:435:CYS:O	2.50	0.45
1:E:454:ILE:CD1	1:E:457:GLY:HA3	2.45	0.45
1:E:522:THR:HG22	1:E:527:LEU:HD11	1.97	0.45
1:A:463:LYS:HB2	1:A:463:LYS:HE3	1.59	0.45
1:C:276:ARG:HG3	1:C:276:ARG:NH1	2.31	0.45
1:C:326:THR:HG23	1:C:433:VAL:HG23	1.99	0.45
1:D:476:TYR:C	1:D:478:ASP:N	2.70	0.45
1:E:375:ARG:NH2	1:E:380:GLU:O	2.30	0.45
1:E:412:TRP:O	1:E:412:TRP:CE3	2.70	0.45
1:E:540:PHE:CE2	1:E:541:GLU:CG	3.00	0.45
1:E:609:GLN:CD	1:E:611:PHE:HZ	2.18	0.45
1:F:230:VAL:HG23	1:F:242:ILE:HD11	1.99	0.45
1:A:447:TRP:C	1:A:448:GLN:CG	2.85	0.45
1:B:262:ILE:O	1:B:262:ILE:HG22	2.16	0.45
1:C:325:CYS:HB2	1:C:394:ILE:HG23	1.97	0.45
1:E:405:TYR:O	1:E:406:ASP:C	2.55	0.45
1:E:494:ASP:OD2	1:E:496:SER:OG	2.33	0.45
1:E:540:PHE:CE2	1:E:541:GLU:CD	2.90	0.45
1:F:230:VAL:CG2	1:F:242:ILE:CD1	2.95	0.45
1:F:473:TRP:CZ3	1:F:480:PHE:HB2	2.51	0.45
1:B:391:LEU:HD12	1:B:438:VAL:CG2	2.43	0.45
1:C:206:LEU:HD13	1:C:206:LEU:H	1.82	0.45
1:C:412:TRP:O	1:C:412:TRP:CG	2.70	0.45
1:D:609:GLN:HG2	1:D:618:THR:HG23	1.98	0.45
1:F:179:ALA:O	1:F:183:ILE:HG13	2.16	0.45
1:F:405:TYR:O	1:F:406:ASP:C	2.55	0.45
1:B:152:LYS:O	1:B:153:ALA:HB3	2.16	0.45
1:B:161:GLU:HG2	1:B:162:PHE:N	2.32	0.45
1:B:412:TRP:O	1:B:412:TRP:CE3	2.70	0.45
1:C:405:TYR:O	1:C:406:ASP:C	2.55	0.45
1:C:627:ASP:OD1	1:C:647:GLN:N	2.49	0.45
1:D:118:GLN:NE2	1:D:120:PHE:HB3	2.32	0.45
1:D:325:CYS:HB2	1:D:394:ILE:HG23	1.97	0.45
1:D:326:THR:HG23	1:D:433:VAL:HG23	1.99	0.45
1:F:346:GLY:CA	1:F:366:PRO:HA	2.47	0.45
1:F:495:ILE:HD12	1:F:495:ILE:HA	1.85	0.45
1:A:586:LEU:N	1:A:586:LEU:HD23	2.32	0.45
1:B:336:ASN:HB2	1:B:444:LEU:HD21	1.99	0.45
1:B:383:ARG:HA	1:B:431:LEU:HD23	1.99	0.45
1:D:644:LYS:HA	1:D:644:LYS:HD3	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:PHE:O	1:E:120:PHE:CD1	2.70	0.45
1:E:569:GLN:CB	3:E:806:HOH:O	2.56	0.45
1:A:363:LYS:HD2	1:A:525:TYR:CE1	2.51	0.45
1:D:405:TYR:O	1:D:406:ASP:C	2.55	0.45
1:D:443:ARG:HH11	1:D:443:ARG:CG	2.15	0.45
1:D:450:ASN:CB	1:D:451:PRO:CD	2.93	0.45
1:D:585:CYS:HB2	1:D:600:CYS:HB2	1.98	0.45
1:E:459:SER:O	1:E:463:LYS:N	2.45	0.45
1:E:463:LYS:O	1:E:463:LYS:HG2	2.17	0.45
1:E:498:LEU:HD12	1:E:498:LEU:N	2.32	0.45
1:E:553:ASN:N	1:E:584:GLN:OE1	2.49	0.45
1:B:173:PHE:CD2	1:B:177:MET:HG3	2.52	0.45
1:B:443:ARG:CD	1:B:447:TRP:CE3	2.99	0.45
1:D:368:THR:O	1:D:372:LYS:HG3	2.17	0.45
1:E:176:ASN:HD21	1:E:178:VAL:HG23	1.80	0.45
1:E:565:MET:N	1:E:569:GLN:OE1	2.50	0.45
1:F:245:ILE:CD1	1:F:245:ILE:N	2.79	0.45
1:A:326:THR:HG23	1:A:433:VAL:HG23	1.99	0.44
1:B:596:MET:CE	1:B:598:THR:HG23	2.46	0.44
1:E:326:THR:HG23	1:E:433:VAL:HG23	1.99	0.44
1:E:460:PRO:O	1:E:464:ASN:CG	2.56	0.44
1:E:615:HIS:O	1:E:648:LYS:HA	2.16	0.44
1:E:628:ARG:HH11	1:E:628:ARG:CG	2.15	0.44
1:B:301:ASP:H	1:B:391:LEU:CD2	2.29	0.44
1:B:559:LEU:HD22	1:B:628:ARG:CG	2.46	0.44
1:C:463:LYS:HE3	1:C:492:TYR:HA	1.99	0.44
1:D:532:VAL:HB	1:D:573:ILE:HG23	1.98	0.44
1:D:653:ASN:N	1:D:653:ASN:HD22	2.13	0.44
1:F:471:VAL:HG13	1:F:472:TRP:CD1	2.53	0.44
1:B:231:ILE:CD1	1:B:265:TRP:NE1	2.80	0.44
1:D:412:TRP:O	1:D:412:TRP:CE3	2.70	0.44
1:E:281:ILE:CD1	1:E:413:GLY:H	2.20	0.44
1:E:522:THR:CG2	1:E:527:LEU:HD11	2.47	0.44
1:F:631:VAL:HA	1:F:632:LEU:C	2.37	0.44
1:A:118:GLN:HE21	1:A:321:ASP:HA	1.80	0.44
1:A:200:TRP:CZ2	1:A:377:THR:HG21	2.52	0.44
1:A:368:THR:CB	1:A:370:GLN:OE1	2.61	0.44
1:A:414:GLY:HA2	1:A:415:GLU:CD	2.37	0.44
1:A:645:THR:O	1:A:648:LYS:HB2	2.17	0.44
1:B:332:VAL:HG13	1:B:442:TYR:CD1	2.53	0.44
1:B:611:PHE:CE2	1:B:618:THR:HG23	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:TRP:CZ3	1:D:480:PHE:HB2	2.51	0.44
1:E:303:HIS:HB2	1:E:441:ILE:HD12	1.98	0.44
1:E:579:LEU:O	1:E:586:LEU:HD23	2.17	0.44
1:E:605:PHE:CD1	1:E:607:GLU:OE2	2.70	0.44
1:F:221:SER:O	1:F:225:ARG:HB2	2.18	0.44
1:F:268:LEU:C	1:F:268:LEU:CD1	2.86	0.44
1:F:454:ILE:HD12	1:F:460:PRO:CG	2.46	0.44
1:F:545:CYS:N	1:F:562:CYS:SG	2.90	0.44
1:F:627:ASP:OD1	1:F:646:THR:CB	2.61	0.44
1:A:152:LYS:H	1:A:152:LYS:HD3	1.83	0.44
1:B:132:LEU:CG	1:B:136:GLU:OE1	2.63	0.44
1:B:495:ILE:HD12	1:B:495:ILE:HA	1.79	0.44
1:B:609:GLN:NE2	1:B:611:PHE:CZ	2.81	0.44
1:C:471:VAL:HG13	1:C:472:TRP:CD1	2.53	0.44
1:C:616:ARG:HG2	1:C:618:THR:HG22	2.00	0.44
1:D:208:THR:O	1:D:296:VAL:HG13	2.17	0.44
1:F:226:THR:HG22	1:F:304:CYS:CA	2.47	0.44
1:F:254:LEU:O	1:F:258:LEU:HB3	2.17	0.44
1:F:326:THR:HG23	1:F:433:VAL:HG23	1.99	0.44
1:F:412:TRP:CE3	1:F:412:TRP:O	2.70	0.44
1:F:609:GLN:NE2	1:F:611:PHE:HZ	2.15	0.44
1:A:405:TYR:O	1:A:406:ASP:C	2.55	0.44
1:B:230:VAL:C	1:B:231:ILE:CG2	2.85	0.44
1:B:450:ASN:CB	1:B:451:PRO:CD	2.93	0.44
1:B:587:THR:HB	1:B:607:GLU:OE2	2.17	0.44
1:B:617:PHE:HB3	1:B:626:LEU:CD1	2.47	0.44
1:C:191:ASP:OD1	1:C:193:ARG:HB2	2.18	0.44
1:C:303:HIS:HB2	1:C:441:ILE:HD12	2.00	0.44
1:C:346:GLY:HA3	1:C:366:PRO:HA	2.00	0.44
1:D:573:ILE:HD12	1:D:579:LEU:HG	1.98	0.44
1:F:143:PRO:CG	1:F:146:VAL:HG12	2.44	0.44
1:F:220:TRP:CD1	1:F:220:TRP:C	2.91	0.44
1:F:454:ILE:HG21	1:F:460:PRO:HD3	1.99	0.44
1:B:471:VAL:HG13	1:B:472:TRP:CD1	2.52	0.44
1:C:655:HIS:CD2	1:C:655:HIS:O	2.70	0.44
1:D:614:LEU:O	1:D:615:HIS:CB	2.60	0.44
1:E:193:ARG:CG	1:E:437:ARG:CD	2.95	0.44
1:F:235:PRO:HB2	1:F:238:TYR:HD2	1.83	0.44
1:A:456:VAL:O	1:A:657:VAL:O	2.35	0.44
1:A:471:VAL:HG13	1:A:472:TRP:CD1	2.53	0.44
1:B:236:ARG:HA	1:B:236:ARG:HD2	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ILE:HD11	1:B:498:LEU:CD1	2.16	0.44
1:B:596:MET:HE2	1:B:598:THR:CG2	2.48	0.44
1:B:624:LYS:CG	1:B:638:SER:C	2.86	0.44
1:D:513:PHE:CE1	1:D:517:ILE:HD11	2.53	0.44
1:E:450:ASN:ND2	1:E:450:ASN:N	2.65	0.44
1:F:513:PHE:CE1	1:F:517:ILE:HD11	2.53	0.44
1:B:175:PHE:CE1	1:B:441:ILE:CG2	3.01	0.44
1:B:625:CYS:CA	1:B:640:CYS:SG	3.05	0.44
1:C:241:GLU:HB2	1:C:270:LYS:HZ3	1.82	0.44
1:C:476:TYR:O	1:C:479:TYR:N	2.51	0.44
1:C:527:LEU:HD12	1:C:527:LEU:H	1.74	0.44
1:D:190:ASN:N	1:D:190:ASN:ND2	2.60	0.44
1:D:362:TRP:C	1:D:363:LYS:HG2	2.37	0.44
1:D:443:ARG:NE	1:D:447:TRP:CH2	2.82	0.44
1:E:195:GLU:O	1:E:198:LYS:CG	2.66	0.44
1:E:654:ILE:HD13	1:E:654:ILE:HA	1.71	0.44
1:E:551:LYS:NZ	1:E:551:LYS:CB	2.73	0.43
1:F:152:LYS:O	1:F:188:SER:O	2.36	0.43
1:F:230:VAL:HG21	1:F:242:ILE:CD1	2.48	0.43
1:B:143:PRO:HG2	1:B:146:VAL:HG22	1.98	0.43
1:B:628:ARG:HE	1:B:628:ARG:HB3	1.67	0.43
1:C:264:LEU:HD23	1:C:265:TRP:N	2.32	0.43
1:C:513:PHE:CE1	1:C:517:ILE:HD11	2.53	0.43
1:D:123:HIS:CD2	3:D:803:HOH:O	2.71	0.43
1:D:166:ILE:HG23	1:D:176:ASN:CG	2.38	0.43
1:D:243:VAL:HG12	1:D:245:ILE:HD11	2.00	0.43
1:D:471:VAL:HG13	1:D:472:TRP:CD1	2.52	0.43
1:F:231:ILE:C	1:F:231:ILE:CD1	2.86	0.43
1:A:122:TYR:CE2	1:A:206:LEU:HD23	2.53	0.43
1:B:122:TYR:HE1	1:B:203:ASP:CB	2.28	0.43
1:E:122:TYR:CE1	1:E:206:LEU:HD23	2.53	0.43
1:E:254:LEU:O	1:E:273:ARG:NH2	2.51	0.43
1:E:462:LEU:HD12	1:E:462:LEU:HA	1.81	0.43
1:E:484:ARG:O	1:E:487:SER:HB2	2.18	0.43
1:E:614:LEU:HD12	1:E:616:ARG:NE	2.33	0.43
1:F:217:ASN:CG	1:F:251:LYS:HG2	2.39	0.43
1:F:476:TYR:O	1:F:477:LYS:C	2.53	0.43
1:A:455:TYR:HB2	1:A:456:VAL:CG2	2.27	0.43
1:A:584:GLN:HG2	1:A:598:THR:C	2.39	0.43
1:B:596:MET:HG2	1:B:597:ILE:N	2.33	0.43
1:B:613:ASN:ND2	3:B:807:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:LEU:HB3	1:B:649:TRP:CH2	2.47	0.43
1:C:476:TYR:O	1:C:478:ASP:N	2.51	0.43
1:C:520:ASP:OD1	1:C:520:ASP:N	2.51	0.43
1:D:476:TYR:O	1:D:477:LYS:C	2.54	0.43
1:E:311:TYR:CE1	1:E:315:VAL:HG21	2.54	0.43
1:E:520:ASP:OD1	1:E:520:ASP:N	2.41	0.43
1:F:573:ILE:CD1	1:F:610:TYR:HD2	2.30	0.43
1:A:513:PHE:CE1	1:A:517:ILE:HD11	2.53	0.43
1:B:218:GLU:O	1:B:253:HIS:HE1	2.01	0.43
1:B:347:ASP:O	1:B:348:GLU:C	2.54	0.43
1:B:447:TRP:CD1	1:B:448:GLN:N	2.87	0.43
1:B:450:ASN:H	1:B:450:ASN:HD22	1.66	0.43
1:D:310:TRP:O	1:D:313:PRO:HD2	2.18	0.43
1:D:540:PHE:O	1:D:542:THR:HG23	2.18	0.43
1:D:616:ARG:HG2	1:D:618:THR:HG22	2.00	0.43
1:F:228:HIS:C	1:F:231:ILE:HG22	2.38	0.43
1:F:641:ASP:HB3	1:F:644:LYS:HD3	2.01	0.43
1:A:220:TRP:CZ3	1:A:257:LYS:HE3	2.53	0.43
1:A:311:TYR:CE1	1:A:315:VAL:HG21	2.54	0.43
1:A:616:ARG:HG2	1:A:618:THR:HG22	2.00	0.43
1:C:284:ARG:NH1	1:C:415:GLU:OE1	2.48	0.43
1:E:360:MET:O	1:E:360:MET:HG2	2.18	0.43
1:B:156:LEU:HD22	1:B:158:LEU:CD2	2.47	0.43
1:B:412:TRP:O	1:B:461:THR:CG2	2.67	0.43
1:C:166:ILE:CG2	1:C:176:ASN:ND2	2.81	0.43
1:D:224:MET:CE	1:D:258:LEU:CD1	2.96	0.43
1:E:363:LYS:CD	1:E:525:TYR:OH	2.65	0.43
1:E:553:ASN:HA	1:E:598:THR:HA	2.01	0.43
1:B:348:GLU:N	1:B:349:ASP:C	2.72	0.43
1:B:597:ILE:C	1:B:598:THR:HG23	2.39	0.43
1:B:603:ASN:HB3	1:B:606:LYS:CE	2.33	0.43
1:D:609:GLN:CD	1:D:611:PHE:CZ	2.92	0.43
1:E:556:PHE:CE1	1:E:596:MET:HB2	2.54	0.43
1:F:215:PHE:HE1	1:F:254:LEU:HD12	1.81	0.43
1:B:166:ILE:HG12	1:B:178:VAL:HG21	2.01	0.43
1:B:644:LYS:HA	1:B:646:THR:N	2.31	0.43
1:C:146:VAL:HA	1:C:147:GLY:HA2	1.80	0.43
1:C:194:GLN:H	1:C:194:GLN:HG2	1.68	0.43
1:D:171:LYS:CG	1:D:448:GLN:NE2	2.80	0.43
1:D:332:VAL:HG13	1:D:442:TYR:HD1	1.79	0.43
1:D:369:PRO:HA	1:D:372:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:H	1:A:138:LYS:HG3	1.59	0.43
1:A:166:ILE:HG12	1:A:178:VAL:HG21	2.01	0.43
1:A:370:GLN:CD	1:A:370:GLN:H	2.22	0.43
1:A:412:TRP:CG	1:A:413:GLY:N	2.87	0.43
1:A:610:TYR:OH	1:A:612:LYS:HG3	2.19	0.43
1:A:623:GLY:O	1:A:640:CYS:SG	2.77	0.43
1:C:118:GLN:NE2	1:C:322:ARG:H	2.17	0.43
1:D:484:ARG:O	1:D:487:SER:HB3	2.19	0.43
1:D:534:TRP:CH2	1:D:653:ASN:HB3	2.54	0.43
1:F:281:ILE:HD13	1:F:409:LEU:HB3	2.00	0.43
1:F:370:GLN:HG3	1:F:519:TYR:CE1	2.54	0.43
1:A:535:GLY:HA3	1:A:652:ASN:O	2.19	0.42
1:B:118:GLN:NE2	1:B:120:PHE:O	2.52	0.42
1:C:220:TRP:CZ3	1:C:257:LYS:HE3	2.53	0.42
1:C:311:TYR:CE1	1:C:315:VAL:HG21	2.54	0.42
1:D:166:ILE:HA	1:D:178:VAL:CG1	2.49	0.42
1:E:220:TRP:CZ3	1:E:257:LYS:HE3	2.53	0.42
1:E:545:CYS:SG	1:E:562:CYS:CA	2.98	0.42
1:E:614:LEU:CD1	1:E:616:ARG:NE	2.82	0.42
1:F:207:LEU:HD12	1:F:207:LEU:N	2.34	0.42
1:A:421:TYR:HB3	1:A:425:GLN:NE2	2.35	0.42
1:C:410:GLN:C	1:C:411:ILE:CG2	2.87	0.42
1:C:553:ASN:HA	1:C:598:THR:HA	2.01	0.42
1:D:132:LEU:HD22	1:D:199:TYR:CE1	2.47	0.42
1:D:217:ASN:HA	1:D:254:LEU:HD11	2.01	0.42
1:E:122:TYR:O	1:E:320:LYS:HG3	2.19	0.42
1:E:276:ARG:NE	1:E:278:GLU:OE2	2.51	0.42
1:E:484:ARG:CG	1:E:484:ARG:NH1	2.73	0.42
1:F:311:TYR:CE1	1:F:315:VAL:HG21	2.54	0.42
1:B:122:TYR:HE1	1:B:203:ASP:HB3	1.84	0.42
1:C:264:LEU:CD2	1:C:264:LEU:C	2.87	0.42
1:C:410:GLN:O	1:C:411:ILE:HG22	2.17	0.42
1:C:421:TYR:HB3	1:C:425:GLN:NE2	2.34	0.42
1:D:281:ILE:HD13	1:D:409:LEU:HB3	2.01	0.42
1:F:362:TRP:C	1:F:363:LYS:HG2	2.40	0.42
1:A:455:TYR:HA	1:A:456:VAL:HA	1.64	0.42
1:B:260:GLU:CD	1:B:263:LYS:NZ	2.73	0.42
1:B:301:ASP:O	1:B:304:CYS:SG	2.75	0.42
1:B:311:TYR:CE1	1:B:315:VAL:HG21	2.54	0.42
1:D:146:VAL:HA	1:D:147:GLY:HA2	1.70	0.42
1:E:176:ASN:ND2	1:E:176:ASN:C	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:ILE:O	1:F:411:ILE:HG23	2.19	0.42
1:F:421:TYR:HB3	1:F:425:GLN:NE2	2.35	0.42
1:A:149:PRO:O	1:A:149:PRO:HD2	2.19	0.42
1:A:285:SER:O	1:A:289:GLN:HG3	2.19	0.42
1:B:276:ARG:HG3	1:B:278:GLU:OE2	2.19	0.42
1:B:347:ASP:HB3	1:B:351:TYR:N	2.27	0.42
1:B:587:THR:HG22	1:B:605:PHE:HB3	2.02	0.42
1:B:596:MET:CE	1:B:598:THR:HG21	2.49	0.42
1:B:619:HIS:CD2	1:B:621:PRO:HG2	2.54	0.42
1:B:646:THR:O	1:B:647:GLN:HG2	2.18	0.42
1:D:208:THR:H	1:D:295:GLN:HG3	1.85	0.42
1:D:375:ARG:HH21	1:D:375:ARG:HG3	1.84	0.42
1:D:610:TYR:HB2	1:D:617:PHE:CE1	2.55	0.42
1:E:190:ASN:C	1:E:190:ASN:ND2	2.73	0.42
1:E:192:LEU:HD11	1:E:340:ILE:HG22	2.02	0.42
1:E:235:PRO:HB2	1:E:238:TYR:CD2	2.51	0.42
1:E:578:GLN:HE21	1:E:578:GLN:HB3	1.68	0.42
1:E:632:LEU:HD22	1:E:634:GLN:NE2	2.34	0.42
1:B:237:LYS:H	1:B:237:LYS:HG2	1.62	0.42
1:B:459:SER:N	1:B:460:PRO:C	2.72	0.42
1:B:513:PHE:CE1	1:B:517:ILE:HD11	2.53	0.42
1:C:151:GLU:HA	1:C:152:LYS:HA	1.81	0.42
1:C:646:THR:C	1:C:647:GLN:HG3	2.40	0.42
1:D:285:SER:O	1:D:289:GLN:HG3	2.19	0.42
1:D:354:GLY:CA	1:D:362:TRP:CH2	3.02	0.42
1:D:450:ASN:ND2	1:D:450:ASN:H	2.17	0.42
1:D:462:LEU:HD11	1:D:487:SER:HB2	2.01	0.42
1:D:641:ASP:O	1:D:644:LYS:HB2	2.18	0.42
1:E:411:ILE:N	1:E:411:ILE:CD1	2.76	0.42
1:E:616:ARG:HG2	1:E:618:THR:HG22	2.00	0.42
1:F:135:PHE:HB3	1:F:309:ASN:OD1	2.19	0.42
1:F:285:SER:O	1:F:289:GLN:HG3	2.19	0.42
1:F:445:GLU:HG2	1:F:446:GLY:N	2.33	0.42
1:F:473:TRP:O	1:F:474:ASP:HB2	2.19	0.42
1:B:443:ARG:HD2	1:B:447:TRP:CZ3	2.54	0.42
1:B:627:ASP:HA	1:B:647:GLN:HB2	2.02	0.42
1:C:241:GLU:HB2	1:C:270:LYS:HZ2	1.83	0.42
1:D:154:LYS:HB3	1:D:154:LYS:HE3	1.74	0.42
1:E:544:TYR:HD2	1:E:630:GLU:OE1	2.03	0.42
1:F:176:ASN:HD21	1:F:178:VAL:HG22	1.84	0.42
1:F:399:PHE:CE1	1:F:404:LEU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:NE2	1:A:321:ASP:CA	2.83	0.42
1:A:134:ASN:OD1	1:A:134:ASN:N	2.47	0.42
1:B:321:ASP:CB	1:B:324:ILE:HG13	2.43	0.42
1:B:344:GLY:O	1:B:364:ARG:NH1	2.53	0.42
1:B:620:ILE:CB	1:B:621:PRO:HD3	2.48	0.42
1:C:152:LYS:O	1:C:153:ALA:HB3	2.20	0.42
1:C:399:PHE:CE1	1:C:404:LEU:HA	2.55	0.42
1:D:553:ASN:HA	1:D:598:THR:HA	2.01	0.42
1:E:421:TYR:HB3	1:E:425:GLN:NE2	2.35	0.42
1:E:580:MET:CG	1:E:585:CYS:SG	3.04	0.42
1:F:185:LEU:HA	1:F:225:ARG:HG3	2.01	0.42
1:F:585:CYS:HB2	1:F:600:CYS:CB	2.50	0.42
1:B:276:ARG:HB3	1:B:276:ARG:CZ	2.50	0.42
1:B:533:ASP:O	1:B:651:MET:CE	2.67	0.42
1:C:262:ILE:HD13	1:C:262:ILE:HA	1.76	0.42
1:D:176:ASN:ND2	1:D:176:ASN:C	2.73	0.42
1:D:399:PHE:CE1	1:D:404:LEU:HA	2.55	0.42
1:D:421:TYR:HB3	1:D:425:GLN:NE2	2.35	0.42
1:F:459:SER:OG	1:F:462:LEU:HB2	2.19	0.42
1:A:175:PHE:CE1	1:A:441:ILE:HG22	2.54	0.42
1:A:414:GLY:CA	1:A:415:GLU:OE2	2.65	0.42
1:B:281:ILE:HD13	1:B:409:LEU:HB3	2.01	0.42
1:B:614:LEU:HD11	1:B:616:ARG:HH11	1.85	0.42
1:C:285:SER:O	1:C:289:GLN:HG3	2.19	0.42
1:E:399:PHE:CE1	1:E:404:LEU:HA	2.55	0.42
1:E:512:TRP:NE1	1:F:516:GLU:HB2	2.33	0.42
1:E:568:ASN:O	1:E:581:GLN:NE2	2.53	0.42
1:E:573:ILE:CD1	1:E:610:TYR:CB	2.97	0.42
1:E:601:ASN:O	1:E:604:GLU:HB2	2.20	0.42
1:F:172:GLU:CG	1:F:173:PHE:CE2	2.86	0.42
1:F:189:VAL:HG13	1:F:340:ILE:HD12	2.02	0.42
1:F:230:VAL:CG2	1:F:242:ILE:HD13	2.49	0.42
1:A:153:ALA:HB1	1:A:190:ASN:HD21	1.85	0.41
1:A:346:GLY:C	1:A:366:PRO:HB3	2.41	0.41
1:B:399:PHE:HE1	1:B:419:ILE:HD13	1.85	0.41
1:B:552:THR:C	1:B:554:GLY:HA2	2.40	0.41
1:B:574:ASN:HB3	1:B:576:ALA:N	2.35	0.41
1:B:628:ARG:HA	1:B:635:VAL:HA	2.01	0.41
1:B:646:THR:HG22	1:B:647:GLN:N	2.35	0.41
1:C:625:CYS:HG	1:C:640:CYS:HG	1.63	0.41
1:F:356:TRP:HZ2	1:F:514:MET:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:457:GLY:N	1:F:458:SER:CA	2.72	0.41
1:F:476:TYR:O	1:F:478:ASP:N	2.53	0.41
1:F:602:LEU:HD23	1:F:602:LEU:HA	1.95	0.41
1:F:641:ASP:C	1:F:643:SER:N	2.73	0.41
1:A:207:LEU:HD13	1:A:319:SER:OG	2.19	0.41
1:A:473:TRP:O	1:A:474:ASP:HB2	2.19	0.41
1:A:476:TYR:O	1:A:478:ASP:N	2.53	0.41
1:B:576:ALA:O	1:B:606:LYS:CD	2.68	0.41
1:C:241:GLU:CB	1:C:270:LYS:HZ3	2.33	0.41
1:C:356:TRP:HZ2	1:C:514:MET:HE3	1.85	0.41
1:C:371:GLU:HG2	1:C:519:TYR:HH	1.83	0.41
1:C:539:GLY:CA	1:C:628:ARG:HH21	2.31	0.41
1:D:458:SER:HG	1:D:656:SER:CB	2.32	0.41
1:E:262:ILE:O	1:E:264:LEU:O	2.38	0.41
1:E:546:ILE:CG2	1:E:557:VAL:HG11	2.50	0.41
1:E:596:MET:HE2	1:E:596:MET:HB3	1.93	0.41
1:F:228:HIS:O	1:F:231:ILE:HG23	2.16	0.41
1:A:520:ASP:OD1	1:A:520:ASP:N	2.41	0.41
1:B:380:GLU:O	1:B:381:PRO:C	2.56	0.41
1:B:596:MET:HE3	1:B:598:THR:CG2	2.48	0.41
1:B:622:SER:O	1:B:624:LYS:HB2	2.20	0.41
1:D:163:LYS:HG3	1:D:164:GLN:N	2.33	0.41
1:E:374:LEU:HD23	1:E:374:LEU:HA	1.89	0.41
1:F:303:HIS:HB2	1:F:441:ILE:HD12	2.02	0.41
1:A:115:PHE:HE2	1:A:426:CYS:O	2.03	0.41
1:A:311:TYR:CZ	1:A:315:VAL:HG21	2.56	0.41
1:B:245:ILE:HD13	1:B:245:ILE:HA	1.90	0.41
1:B:573:ILE:CD1	1:B:610:TYR:CD2	3.03	0.41
1:C:547:ASP:OD2	1:C:549:MET:SD	2.79	0.41
1:D:354:GLY:O	1:D:385:PRO:HD2	2.20	0.41
1:D:535:GLY:HA3	1:D:652:ASN:O	2.19	0.41
1:D:628:ARG:HD2	1:D:649:TRP:CH2	2.55	0.41
1:E:146:VAL:HA	1:E:147:GLY:HA2	1.70	0.41
1:F:258:LEU:CD2	1:F:262:ILE:CD1	2.66	0.41
1:F:535:GLY:HA3	1:F:652:ASN:O	2.19	0.41
1:F:574:ASN:HB3	1:F:576:ALA:N	2.35	0.41
1:F:641:ASP:CB	1:F:644:LYS:HD3	2.51	0.41
1:A:176:ASN:HD21	1:A:178:VAL:HG22	1.84	0.41
1:A:462:LEU:HD23	1:A:462:LEU:HA	1.92	0.41
1:B:348:GLU:CA	1:B:349:ASP:C	2.88	0.41
1:B:388:ALA:N	3:B:803:HOH:O	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:TYR:HB3	1:B:425:GLN:NE2	2.35	0.41
1:B:573:ILE:HD13	1:B:610:TYR:HB3	2.03	0.41
1:B:620:ILE:HB	1:B:621:PRO:HD3	2.01	0.41
1:C:644:LYS:N	1:C:645:THR:HA	2.35	0.41
1:F:128:ARG:O	1:F:199:TYR:HB3	2.21	0.41
1:F:170:ILE:O	1:F:174:GLY:N	2.45	0.41
1:F:501:PHE:CD1	1:F:501:PHE:C	2.93	0.41
1:F:611:PHE:HE1	1:F:618:THR:HG21	1.85	0.41
1:A:122:TYR:CE2	1:A:205:ASN:HB3	2.55	0.41
1:A:399:PHE:CE1	1:A:404:LEU:HA	2.55	0.41
1:B:632:LEU:H	1:B:632:LEU:CD1	2.27	0.41
1:C:454:ILE:CD1	1:C:460:PRO:HD3	2.42	0.41
1:C:574:ASN:HB3	1:C:576:ALA:N	2.35	0.41
1:C:653:ASN:N	1:C:653:ASN:HD22	2.19	0.41
1:D:190:ASN:HD21	1:D:340:ILE:HB	1.86	0.41
1:D:203:ASP:C	1:D:205:ASN:N	2.73	0.41
1:E:406:ASP:CB	1:E:498:LEU:HD21	2.50	0.41
1:E:454:ILE:CG1	1:E:457:GLY:HA3	2.51	0.41
1:F:156:LEU:HD12	1:F:183:ILE:HD11	2.01	0.41
1:F:192:LEU:HD11	1:F:340:ILE:HG22	2.01	0.41
1:F:207:LEU:HD13	1:F:319:SER:OG	2.19	0.41
1:F:256:GLU:CA	1:F:259:ASP:OD1	2.68	0.41
1:F:311:TYR:CZ	1:F:315:VAL:HG21	2.56	0.41
1:F:590:ALA:HA	1:F:591:ASP:C	2.41	0.41
1:B:619:HIS:O	1:B:623:GLY:HA2	2.21	0.41
1:D:191:ASP:CG	1:D:193:ARG:HH11	2.24	0.41
1:D:208:THR:N	1:D:295:GLN:HG3	2.35	0.41
1:E:584:GLN:HG2	1:E:598:THR:C	2.41	0.41
1:A:153:ALA:HB1	1:A:190:ASN:ND2	2.23	0.41
1:B:642:SER:O	1:B:642:SER:OG	2.30	0.41
1:C:548:SER:HB2	1:C:581:GLN:HE22	1.85	0.41
1:E:194:GLN:HE21	1:E:194:GLN:HB3	1.65	0.41
1:F:116:LYS:O	1:F:322:ARG:NH2	2.51	0.41
1:A:451:PRO:HB2	1:A:452:PRO:CD	2.50	0.41
1:A:590:ALA:CB	1:A:591:ASP:CA	2.95	0.41
1:B:311:TYR:CZ	1:B:315:VAL:HG21	2.56	0.41
1:B:347:ASP:CB	1:B:351:TYR:O	2.65	0.41
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.23	0.41
1:B:627:ASP:CB	1:B:647:GLN:HB2	2.51	0.41
1:C:124:ASP:OD2	1:C:320:LYS:HD2	2.21	0.41
1:C:143:PRO:CG	1:C:146:VAL:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLY:C	1:C:148:GLY:O	2.60	0.41
1:C:262:ILE:HD13	1:C:265:TRP:HZ3	1.86	0.41
1:C:262:ILE:O	1:C:262:ILE:HG22	2.21	0.41
1:C:443:ARG:HD2	1:C:447:TRP:CE3	2.56	0.41
1:C:535:GLY:HA3	1:C:652:ASN:O	2.19	0.41
1:D:243:VAL:HG22	1:D:270:LYS:HD2	2.01	0.41
1:E:311:TYR:CZ	1:E:315:VAL:HG21	2.56	0.41
1:E:322:ARG:HH11	1:E:397:GLU:HB3	1.86	0.41
1:E:573:ILE:HD12	1:E:610:TYR:CD2	2.55	0.41
1:F:174:GLY:CA	1:F:447:TRP:HB2	2.51	0.41
1:F:193:ARG:NH2	1:F:308:VAL:HG22	2.36	0.41
1:F:248:PHE:HB3	1:F:277:ARG:HB2	2.03	0.41
1:F:394:ILE:HG21	1:F:394:ILE:HD13	1.73	0.41
1:F:614:LEU:HD13	1:F:616:ARG:HH21	1.85	0.41
1:C:311:TYR:CZ	1:C:315:VAL:HG21	2.56	0.41
1:D:217:ASN:OD1	1:D:249:SER:HB3	2.19	0.41
1:D:632:LEU:HD22	1:D:634:GLN:HG3	2.02	0.41
1:E:551:LYS:HD3	1:E:556:PHE:O	2.21	0.41
1:A:163:LYS:HG3	1:A:164:GLN:N	2.36	0.40
1:B:207:LEU:HB3	1:B:295:GLN:HB2	2.02	0.40
1:B:629:SER:O	1:B:632:LEU:O	2.40	0.40
1:C:286:ILE:CG2	1:C:290:LYS:HD2	2.52	0.40
1:D:134:ASN:OD1	1:D:134:ASN:N	2.37	0.40
1:D:187:ARG:O	1:D:187:ARG:HG3	2.20	0.40
1:D:476:TYR:O	1:D:478:ASP:N	2.54	0.40
1:D:534:TRP:CZ2	1:D:653:ASN:HB3	2.56	0.40
1:E:141:GLU:HA	1:E:142:PRO:HD3	1.84	0.40
1:E:454:ILE:H	1:E:454:ILE:HG13	1.70	0.40
1:F:118:GLN:NE2	1:F:320:LYS:O	2.54	0.40
1:F:243:VAL:HG21	1:F:291:ALA:HB2	2.02	0.40
1:F:450:ASN:HD22	1:F:450:ASN:H	1.69	0.40
1:F:552:THR:HB	1:F:584:GLN:OE1	2.21	0.40
1:F:616:ARG:HD3	1:F:625:CYS:SG	2.61	0.40
1:A:183:ILE:HG21	1:A:187:ARG:HD2	2.02	0.40
1:B:113:LEU:HG	1:B:504:ASP:HB3	2.03	0.40
1:B:147:GLY:H	1:C:489:ALA:HB2	1.87	0.40
1:B:453:PRO:CB	1:D:164:GLN:OE1	2.62	0.40
1:C:263:LYS:HE3	1:C:263:LYS:HB3	1.58	0.40
1:C:332:VAL:HG13	1:C:442:TYR:CD1	2.56	0.40
1:D:183:ILE:CG2	1:D:187:ARG:HD3	2.51	0.40
1:F:356:TRP:HA	1:F:361:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLN:NE2	3:A:810:HOH:O	2.54	0.40
1:A:485:PRO:HB2	1:A:534:TRP:CD2	2.57	0.40
1:B:230:VAL:CG2	1:B:231:ILE:N	2.85	0.40
1:D:394:ILE:HG21	1:D:394:ILE:HD13	1.73	0.40
1:D:453:PRO:O	1:D:454:ILE:HD13	2.21	0.40
1:E:415:GLU:CG	1:E:416:ASN:N	2.79	0.40
1:E:626:LEU:HD12	1:E:637:ILE:HG22	2.04	0.40
1:B:171:LYS:HG2	1:B:448:GLN:CD	2.42	0.40
1:C:357:ASP:OD1	1:C:357:ASP:C	2.60	0.40
1:D:173:PHE:CD2	1:D:177:MET:CG	2.94	0.40
1:D:371:GLU:O	1:D:375:ARG:CG	2.68	0.40
1:E:326:THR:HG23	1:E:433:VAL:CG2	2.52	0.40
1:B:357:ASP:C	1:B:357:ASP:OD1	2.60	0.40
1:D:264:LEU:O	1:D:265:TRP:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	544/597 (91%)	515 (95%)	29 (5%)	0	100	100
1	B	544/597 (91%)	518 (95%)	25 (5%)	1 (0%)	47	79
1	C	544/597 (91%)	517 (95%)	27 (5%)	0	100	100
1	D	544/597 (91%)	521 (96%)	22 (4%)	1 (0%)	47	79
1	E	544/597 (91%)	520 (96%)	24 (4%)	0	100	100
1	F	544/597 (91%)	518 (95%)	25 (5%)	1 (0%)	47	79
All	All	3264/3582 (91%)	3109 (95%)	152 (5%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	459	SER
1	F	451	PRO
1	D	491	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	480/525 (91%)	381 (79%)	99 (21%)	1 4
1	B	480/525 (91%)	395 (82%)	85 (18%)	2 8
1	C	480/525 (91%)	406 (85%)	74 (15%)	2 11
1	D	480/525 (91%)	389 (81%)	91 (19%)	1 6
1	E	480/525 (91%)	387 (81%)	93 (19%)	1 6
1	F	480/525 (91%)	391 (82%)	89 (18%)	1 7
All	All	2880/3150 (91%)	2349 (82%)	531 (18%)	1 7

All (531) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	116	LYS
1	A	117	PRO
1	A	118	GLN
1	A	127	LEU
1	A	128	ARG
1	A	132	LEU
1	A	138	LYS
1	A	139	GLU
1	A	146	VAL
1	A	151	GLU
1	A	152	LYS
1	A	154	LYS
1	A	156	LEU
1	A	163	LYS
1	A	164	GLN

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Mol	Chain	Res	Type
1	A	176	ASN
1	A	178	VAL
1	A	187	ARG
1	A	188	SER
1	A	190	ASN
1	A	197	CYS
1	A	203	ASP
1	A	229	SER
1	A	237	LYS
1	A	239	LEU
1	A	248	PHE
1	A	249	SER
1	A	250	ASN
1	A	251	LYS
1	A	255	LYS
1	A	262	ILE
1	A	264	LEU
1	A	268	LEU
1	A	270	LYS
1	A	273	ARG
1	A	276	ARG
1	A	277	ARG
1	A	290	LYS
1	A	300	LEU
1	A	301	ASP
1	A	306	VAL
1	A	320	LYS
1	A	341	ILE
1	A	349	ASP
1	A	359	SER
1	A	379	THR
1	A	391	LEU
1	A	394	ILE
1	A	409	LEU
1	A	411	ILE
1	A	412	TRP
1	A	415	GLU
1	A	418	GLU
1	A	430	LEU
1	A	443	ARG
1	A	445	GLU
1	A	450	ASN

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Mol	Chain	Res	Type
1	A	454	ILE
1	A	455	TYR
1	A	462	LEU
1	A	477	LYS
1	A	498	LEU
1	A	499	LYS
1	A	506	ASN
1	A	517	ILE
1	A	523	SER
1	A	527	LEU
1	A	541	GLU
1	A	547	ASP
1	A	551	LYS
1	A	557	VAL
1	A	570	LEU
1	A	572	ARG
1	A	573	ILE
1	A	579	LEU
1	A	585	CYS
1	A	586	LEU
1	A	588	LYS
1	A	591	ASP
1	A	593	SER
1	A	598	THR
1	A	600	CYS
1	A	602	LEU
1	A	614	LEU
1	A	618	THR
1	A	620	ILE
1	A	624	LYS
1	A	626	LEU
1	A	628	ARG
1	A	631	VAL
1	A	632	LEU
1	A	642	SER
1	A	645	THR
1	A	648	LYS
1	A	650	GLU
1	A	651	MET
1	A	655	HIS
1	A	656	SER
1	B	114	THR

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Mol	Chain	Res	Type
1	B	116	LYS
1	B	127	LEU
1	B	134	ASN
1	B	136	GLU
1	B	139	GLU
1	B	141	GLU
1	B	151	GLU
1	B	152	LYS
1	B	154	LYS
1	B	156	LEU
1	B	178	VAL
1	B	192	LEU
1	B	193	ARG
1	B	205	ASN
1	B	229	SER
1	B	230	VAL
1	B	231	ILE
1	B	236	ARG
1	B	239	LEU
1	B	248	PHE
1	B	249	SER
1	B	254	LEU
1	B	255	LYS
1	B	264	LEU
1	B	268	LEU
1	B	270	LYS
1	B	276	ARG
1	B	277	ARG
1	B	301	ASP
1	B	303	HIS
1	B	304	CYS
1	B	306	VAL
1	B	322	ARG
1	B	341	ILE
1	B	349	ASP
1	B	359	SER
1	B	372	LYS
1	B	376	LYS
1	B	379	THR
1	B	383	ARG
1	B	391	LEU
1	B	394	ILE

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Mol	Chain	Res	Type
1	B	395	GLU
1	B	396	ARG
1	B	418	GLU
1	B	430	LEU
1	B	438	VAL
1	B	443	ARG
1	B	448	GLN
1	B	450	ASN
1	B	454	ILE
1	B	460	PRO
1	B	463	LYS
1	B	477	LYS
1	B	496	SER
1	B	497	GLU
1	B	499	LYS
1	B	502	ARG
1	B	517	ILE
1	B	523	SER
1	B	541	GLU
1	B	547	ASP
1	B	557	VAL
1	B	570	LEU
1	B	573	ILE
1	B	579	LEU
1	B	586	LEU
1	B	587	THR
1	B	588	LYS
1	B	591	ASP
1	B	596	MET
1	B	601	ASN
1	B	602	LEU
1	B	614	LEU
1	B	618	THR
1	B	622	SER
1	B	624	LYS
1	B	628	ARG
1	B	631	VAL
1	B	632	LEU
1	B	634	GLN
1	B	647	GLN
1	B	649	TRP
1	B	656	SER

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Mol	Chain	Res	Type
1	C	113	LEU
1	C	114	THR
1	C	116	LYS
1	C	121	THR
1	C	138	LYS
1	C	146	VAL
1	C	151	GLU
1	C	152	LYS
1	C	190	ASN
1	C	206	LEU
1	C	207	LEU
1	C	209	SER
1	C	229	SER
1	C	237	LYS
1	C	239	LEU
1	C	251	LYS
1	C	255	LYS
1	C	264	LEU
1	C	268	LEU
1	C	270	LYS
1	C	273	ARG
1	C	276	ARG
1	C	300	LEU
1	C	301	ASP
1	C	306	VAL
1	C	320	LYS
1	C	337	THR
1	C	339	GLU
1	C	349	ASP
1	C	359	SER
1	C	373	ARG
1	C	376	LYS
1	C	378	LYS
1	C	379	THR
1	C	391	LEU
1	C	394	ILE
1	C	415	GLU
1	C	418	GLU
1	C	430	LEU
1	C	443	ARG
1	C	444	LEU
1	C	450	ASN

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Mol	Chain	Res	Type
1	C	461	THR
1	C	462	LEU
1	C	477	LYS
1	C	498	LEU
1	C	499	LYS
1	C	517	ILE
1	C	523	SER
1	C	541	GLU
1	C	551	LYS
1	C	557	VAL
1	C	570	LEU
1	C	573	ILE
1	C	579	LEU
1	C	586	LEU
1	C	588	LYS
1	C	593	SER
1	C	597	ILE
1	C	598	THR
1	C	602	LEU
1	C	612	LYS
1	C	613	ASN
1	C	614	LEU
1	C	618	THR
1	C	620	ILE
1	C	628	ARG
1	C	632	LEU
1	C	638	SER
1	C	642	SER
1	C	646	THR
1	C	650	GLU
1	C	651	MET
1	C	656	SER
1	D	114	THR
1	D	116	LYS
1	D	121	THR
1	D	123	HIS
1	D	127	LEU
1	D	128	ARG
1	D	132	LEU
1	D	138	LYS
1	D	146	VAL
1	D	151	GLU

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Mol	Chain	Res	Type
1	D	152	LYS
1	D	154	LYS
1	D	156	LEU
1	D	164	GLN
1	D	176	ASN
1	D	178	VAL
1	D	188	SER
1	D	190	ASN
1	D	192	LEU
1	D	195	GLU
1	D	196	GLU
1	D	203	ASP
1	D	205	ASN
1	D	229	SER
1	D	236	ARG
1	D	237	LYS
1	D	239	LEU
1	D	247	ASP
1	D	248	PHE
1	D	255	LYS
1	D	264	LEU
1	D	268	LEU
1	D	270	LYS
1	D	273	ARG
1	D	276	ARG
1	D	277	ARG
1	D	290	LYS
1	D	292	LYS
1	D	296	VAL
1	D	300	LEU
1	D	301	ASP
1	D	306	VAL
1	D	320	LYS
1	D	341	ILE
1	D	347	ASP
1	D	348	GLU
1	D	349	ASP
1	D	359	SER
1	D	375	ARG
1	D	391	LEU
1	D	394	ILE
1	D	411	ILE

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Mol	Chain	Res	Type
1	D	418	GLU
1	D	430	LEU
1	D	443	ARG
1	D	444	LEU
1	D	448	GLN
1	D	450	ASN
1	D	461	THR
1	D	462	LEU
1	D	463	LYS
1	D	477	LYS
1	D	488	GLN
1	D	498	LEU
1	D	499	LYS
1	D	517	ILE
1	D	522	THR
1	D	541	GLU
1	D	547	ASP
1	D	551	LYS
1	D	557	VAL
1	D	570	LEU
1	D	572	ARG
1	D	579	LEU
1	D	584	GLN
1	D	586	LEU
1	D	588	LYS
1	D	591	ASP
1	D	593	SER
1	D	597	ILE
1	D	598	THR
1	D	602	LEU
1	D	614	LEU
1	D	618	THR
1	D	620	ILE
1	D	628	ARG
1	D	644	LYS
1	D	646	THR
1	D	650	GLU
1	D	651	MET
1	D	657	VAL
1	E	120	PHE
1	E	121	THR
1	E	127	LEU

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Mol	Chain	Res	Type
1	E	128	ARG
1	E	132	LEU
1	E	138	LYS
1	E	146	VAL
1	E	151	GLU
1	E	152	LYS
1	E	156	LEU
1	E	163	LYS
1	E	171	LYS
1	E	176	ASN
1	E	190	ASN
1	E	194	GLN
1	E	195	GLU
1	E	196	GLU
1	E	229	SER
1	E	237	LYS
1	E	239	LEU
1	E	251	LYS
1	E	255	LYS
1	E	263	LYS
1	E	264	LEU
1	E	268	LEU
1	E	270	LYS
1	E	273	ARG
1	E	275	GLU
1	E	276	ARG
1	E	290	LYS
1	E	300	LEU
1	E	301	ASP
1	E	306	VAL
1	E	341	ILE
1	E	348	GLU
1	E	349	ASP
1	E	359	SER
1	E	372	LYS
1	E	376	LYS
1	E	378	LYS
1	E	379	THR
1	E	391	LEU
1	E	394	ILE
1	E	409	LEU
1	E	410	GLN

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Mol	Chain	Res	Type
1	E	418	GLU
1	E	430	LEU
1	E	443	ARG
1	E	445	GLU
1	E	450	ASN
1	E	454	ILE
1	E	484	ARG
1	E	495	ILE
1	E	497	GLU
1	E	506	ASN
1	E	515	GLU
1	E	517	ILE
1	E	523	SER
1	E	541	GLU
1	E	547	ASP
1	E	551	LYS
1	E	553	ASN
1	E	559	LEU
1	E	569	GLN
1	E	570	LEU
1	E	573	ILE
1	E	578	GLN
1	E	579	LEU
1	E	586	LEU
1	E	587	THR
1	E	588	LYS
1	E	593	SER
1	E	597	ILE
1	E	601	ASN
1	E	606	LYS
1	E	607	GLU
1	E	612	LYS
1	E	613	ASN
1	E	614	LEU
1	E	618	THR
1	E	620	ILE
1	E	624	LYS
1	E	628	ARG
1	E	631	VAL
1	E	632	LEU
1	E	634	GLN
1	E	643	SER

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Mol	Chain	Res	Type
1	E	644	LYS
1	E	649	TRP
1	E	650	GLU
1	E	651	MET
1	E	655	HIS
1	E	657	VAL
1	F	113	LEU
1	F	127	LEU
1	F	128	ARG
1	F	131	ILE
1	F	132	LEU
1	F	136	GLU
1	F	141	GLU
1	F	142	PRO
1	F	151	GLU
1	F	152	LYS
1	F	154	LYS
1	F	156	LEU
1	F	169	SER
1	F	176	ASN
1	F	178	VAL
1	F	190	ASN
1	F	195	GLU
1	F	196	GLU
1	F	197	CYS
1	F	198	LYS
1	F	221	SER
1	F	225	ARG
1	F	231	ILE
1	F	234	THR
1	F	237	LYS
1	F	239	LEU
1	F	245	ILE
1	F	252	GLU
1	F	254	LEU
1	F	258	LEU
1	F	259	ASP
1	F	260	GLU
1	F	263	LYS
1	F	275	GLU
1	F	277	ARG
1	F	292	LYS

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Mol	Chain	Res	Type
1	F	300	LEU
1	F	301	ASP
1	F	306	VAL
1	F	320	LYS
1	F	341	ILE
1	F	347	ASP
1	F	359	SER
1	F	370	GLN
1	F	376	LYS
1	F	380	GLU
1	F	391	LEU
1	F	394	ILE
1	F	412	TRP
1	F	418	GLU
1	F	430	LEU
1	F	442	TYR
1	F	443	ARG
1	F	450	ASN
1	F	451	PRO
1	F	455	TYR
1	F	458	SER
1	F	462	LEU
1	F	477	LYS
1	F	498	LEU
1	F	499	LYS
1	F	517	ILE
1	F	523	SER
1	F	527	LEU
1	F	541	GLU
1	F	547	ASP
1	F	551	LYS
1	F	557	VAL
1	F	570	LEU
1	F	573	ILE
1	F	579	LEU
1	F	586	LEU
1	F	588	LYS
1	F	591	ASP
1	F	593	SER
1	F	597	ILE
1	F	598	THR
1	F	602	LEU

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Mol	Chain	Res	Type
1	F	614	LEU
1	F	618	THR
1	F	620	ILE
1	F	632	LEU
1	F	634	GLN
1	F	643	SER
1	F	644	LYS
1	F	645	THR
1	F	650	GLU
1	F	651	MET
1	F	655	HIS

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

Mol	Chain	Res	Type
1	A	118	GLN
1	A	167	GLN
1	A	176	ASN
1	A	190	ASN
1	A	201	HIS
1	A	266	ASN
1	A	425	GLN
1	A	450	ASN
1	A	568	ASN
1	A	574	ASN
1	A	578	GLN
1	A	599	HIS
1	A	603	ASN
1	A	647	GLN
1	A	653	ASN
1	B	123	HIS
1	B	253	HIS
1	B	266	ASN
1	B	303	HIS
1	B	370	GLN
1	B	425	GLN
1	B	440	HIS
1	B	448	GLN
1	B	450	ASN
1	B	464	ASN
1	B	568	ASN
1	B	574	ASN

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Mol	Chain	Res	Type
1	B	578	GLN
1	B	581	GLN
1	B	601	ASN
1	B	634	GLN
1	B	647	GLN
1	B	653	ASN
1	B	655	HIS
1	C	118	GLN
1	C	190	ASN
1	C	266	ASN
1	C	370	GLN
1	C	425	GLN
1	C	450	ASN
1	C	568	ASN
1	C	574	ASN
1	C	578	GLN
1	C	599	HIS
1	C	603	ASN
1	C	653	ASN
1	C	655	HIS
1	D	176	ASN
1	D	190	ASN
1	D	201	HIS
1	D	266	ASN
1	D	295	GLN
1	D	410	GLN
1	D	425	GLN
1	D	448	GLN
1	D	450	ASN
1	D	464	ASN
1	D	524	HIS
1	D	531	ASN
1	D	568	ASN
1	D	574	ASN
1	D	578	GLN
1	D	603	ASN
1	D	613	ASN
1	D	647	GLN
1	D	653	ASN
1	E	176	ASN
1	E	190	ASN
1	E	194	GLN

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Mol	Chain	Res	Type
1	E	201	HIS
1	E	266	ASN
1	E	425	GLN
1	E	450	ASN
1	E	464	ASN
1	E	506	ASN
1	E	568	ASN
1	E	574	ASN
1	E	577	ASN
1	E	578	GLN
1	E	634	GLN
1	E	647	GLN
1	E	653	ASN
1	F	134	ASN
1	F	176	ASN
1	F	190	ASN
1	F	194	GLN
1	F	201	HIS
1	F	228	HIS
1	F	250	ASN
1	F	274	ASN
1	F	425	GLN
1	F	450	ASN
1	F	464	ASN
1	F	505	HIS
1	F	568	ASN
1	F	574	ASN
1	F	578	GLN
1	F	603	ASN
1	F	647	GLN
1	F	653	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	546/597 (91%)	-0.23	7 (1%)	77	61	19, 33, 61, 95	0
1	B	546/597 (91%)	0.19	24 (4%)	34	21	21, 42, 89, 153	0
1	C	546/597 (91%)	-0.03	10 (1%)	68	51	26, 38, 70, 109	0
1	D	546/597 (91%)	0.08	14 (2%)	56	39	27, 52, 81, 121	0
1	E	546/597 (91%)	0.14	22 (4%)	38	25	27, 48, 86, 142	0
1	F	546/597 (91%)	0.32	22 (4%)	38	25	37, 65, 91, 129	0
All	All	3276/3582 (91%)	0.08	99 (3%)	50	34	19, 46, 85, 153	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	657	VAL	11.1
1	B	456	VAL	8.4
1	B	656	SER	8.2
1	B	455	TYR	6.1
1	A	458	SER	5.7
1	E	591	ASP	5.4
1	E	590	ALA	5.3
1	C	112	TYR	5.1
1	B	458	SER	5.1
1	B	452	PRO	5.0
1	F	458	SER	4.9
1	D	451	PRO	4.9
1	B	591	ASP	4.9
1	B	645	THR	4.9
1	B	590	ALA	4.8
1	B	626	LEU	4.7
1	C	458	SER	4.6
1	B	453	PRO	4.5
1	D	458	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	455	TYR	4.5
1	F	455	TYR	4.4
1	E	456	VAL	4.3
1	F	456	VAL	4.2
1	D	457	GLY	4.2
1	E	451	PRO	4.1
1	B	450	ASN	4.0
1	F	591	ASP	3.9
1	C	455	TYR	3.9
1	F	132	LEU	3.9
1	D	591	ASP	3.8
1	F	454	ILE	3.8
1	B	644	LYS	3.7
1	C	452	PRO	3.6
1	E	459	SER	3.5
1	D	450	ASN	3.4
1	B	451	PRO	3.4
1	D	452	PRO	3.4
1	E	654	ILE	3.4
1	C	655	HIS	3.3
1	E	452	PRO	3.2
1	D	453	PRO	3.2
1	F	112	TYR	3.1
1	E	610	TYR	3.1
1	E	608	TRP	3.1
1	F	442	TYR	3.1
1	E	588	LYS	3.0
1	A	657	VAL	3.0
1	C	591	ASP	2.9
1	C	453	PRO	2.9
1	B	494	ASP	2.9
1	D	455	TYR	2.8
1	B	112	TYR	2.8
1	D	119	THR	2.8
1	E	490	LEU	2.8
1	E	450	ASN	2.7
1	D	448	GLN	2.7
1	E	453	PRO	2.7
1	A	454	ILE	2.6
1	E	587	THR	2.6
1	C	459	SER	2.6
1	B	454	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	590	ALA	2.5
1	E	457	GLY	2.5
1	E	589	GLY	2.4
1	E	649	TRP	2.4
1	B	654	ILE	2.4
1	F	255	LYS	2.4
1	F	588	LYS	2.4
1	B	457	GLY	2.4
1	E	626	LEU	2.4
1	B	487	SER	2.3
1	F	256	GLU	2.3
1	E	643	SER	2.3
1	F	589	GLY	2.3
1	A	591	ASP	2.3
1	B	620	ILE	2.3
1	D	603	ASN	2.3
1	E	595	VAL	2.3
1	D	120	PHE	2.3
1	F	251	LYS	2.3
1	F	598	THR	2.2
1	E	571	PHE	2.2
1	F	445	GLU	2.2
1	D	252	GLU	2.2
1	A	147	GLY	2.2
1	A	112	TYR	2.2
1	B	632	LEU	2.1
1	F	657	VAL	2.1
1	A	455	TYR	2.1
1	B	595	VAL	2.1
1	F	162	PHE	2.1
1	D	292	LYS	2.1
1	F	625	CYS	2.1
1	F	452	PRO	2.0
1	F	220	TRP	2.0
1	F	126	VAL	2.0
1	C	448	GLN	2.0
1	F	450	ASN	2.0
1	B	564	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	A	701	1/1	0.55	0.25	87,87,87,87	0
2	MN	B	701	1/1	0.88	0.19	80,80,80,80	0
2	MN	E	701	1/1	0.88	0.18	90,90,90,90	0
2	MN	D	701	1/1	0.92	0.28	74,74,74,74	0
2	MN	F	701	1/1	0.92	0.19	82,82,82,82	0
2	MN	C	701	1/1	0.95	0.29	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.