



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:22 PM BST

PDB ID : 5FTN
EMDB ID: : EMD-3299
Title : Cryo-EM structure of human p97 bound to ATPgS (Conformation III)
Authors : Banerjee, S.; Bartesaghi, A.; Merk, A.; Rao, P.; Bulfer, S.L.; Yan, Y.; Green, N.; Mroczkowski, B.; Neitz, R.J.; Wipf, P.; Falconieri, V.; Deshaies, R.J.; Milne, J.L.S.; Hury, D.; Arkin, M.; Subramaniam, S.
Deposited on : 2016-01-14
Resolution : 3.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

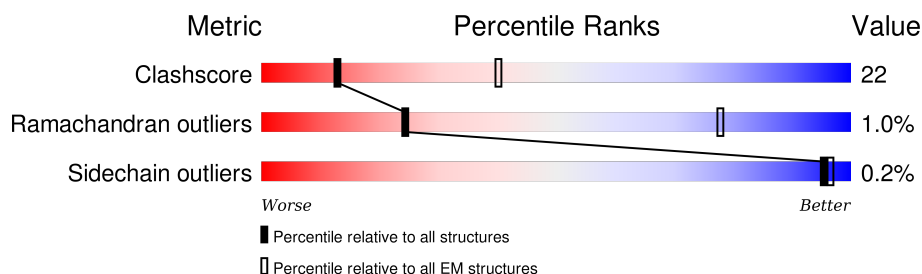
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	806	59% 31% • 9%
1	B	806	59% 31% • 9%
1	C	806	59% 31% • 9%
1	D	806	59% 31% • 9%
1	E	806	59% 31% • 9%
1	F	806	59% 31% • 9%

2 Entry composition [i](#)

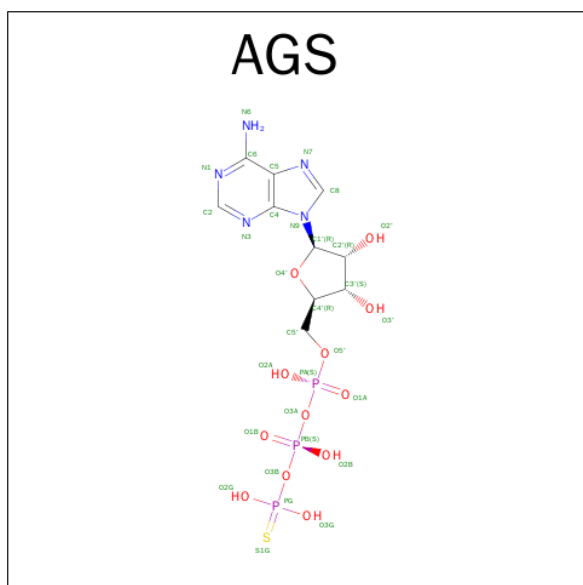
There are 3 unique types of molecules in this entry. The entry contains 34956 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	B	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	C	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	D	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	E	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	F	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	A	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	B	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	B	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	C	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	C	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	D	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	D	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	E	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	E	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	F	1	Total 62	C 20	N 10	O 24	P 6	S 2	0
2	F	1	Total 62	C 20	N 10	O 24	P 6	S 2	0

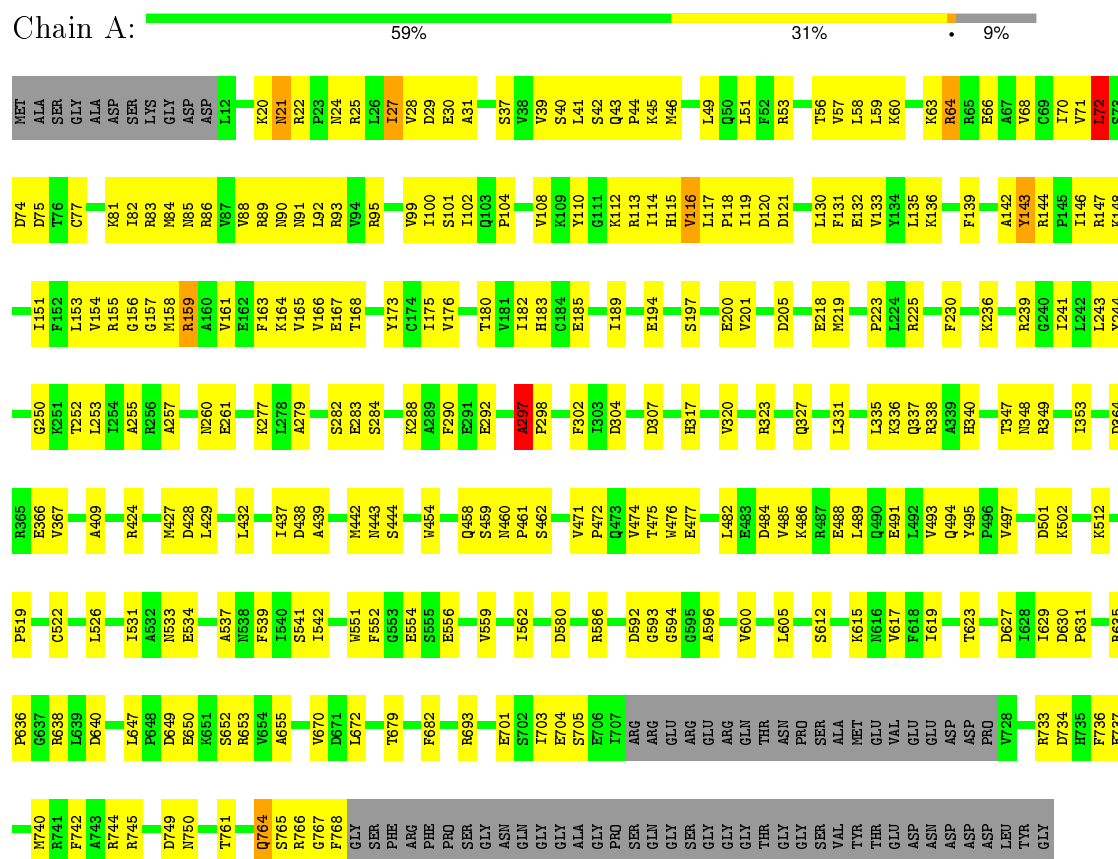
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	D	2	Total 2	Mg 2	0
3	E	2	Total 2	Mg 2	0
3	B	2	Total 2	Mg 2	0
3	C	2	Total 2	Mg 2	0
3	A	2	Total 2	Mg 2	0
3	F	2	Total 2	Mg 2	0

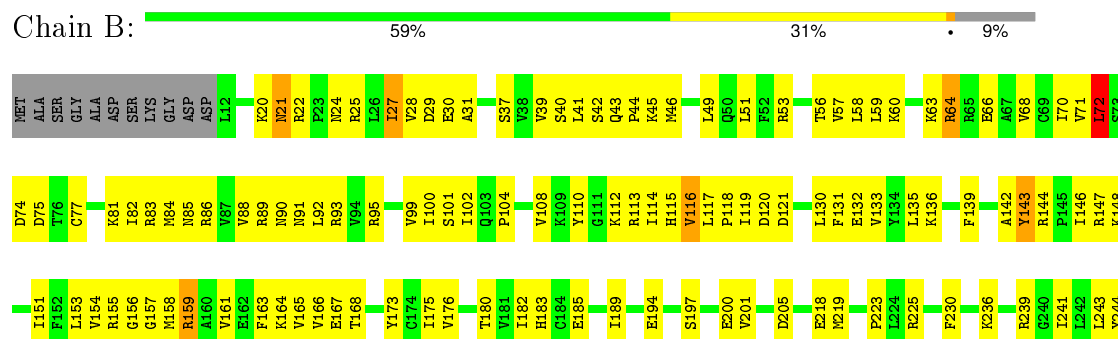
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



M740	P636	P519	R366	G250	I151	D74
R741	G637	C522	E366	K251	L152	D75
F742	R638	L526	V367	T252	L153	C77
A743	L639	L531	A409	L253	V154	K81
R744	D640	A532	R424	L254	R155	
R745	L647	N533	M427	A255	G156	
D749	P648	E534	D428	K256	R83	
N750	D649	S537	L429	A257	M158	R84
T761	S652	A537	L432	N260	R159	N85
	R653	N538	F539	E261	A160	R86
	V654	F539	I437	K277	V161	V87
	A655	S541	D438	L278	F163	V88
R766	V670	I542	A439	A279	K164	N90
F767	D671	W551	M442	S282	V165	N91
F768	L672	F552	N443	E283	V166	L92
GLY	SER	G553	S444	S284	E167	R93
PHE	T679	E554	W454	K288	T168	V94
ARG	F682	S555	Q458	A289	Y173	R95
PHE	PRO	E556	S459	F290	C174	V99
SER	R693	V559	M460	E291	V176	I100
GLY	E701	I562	P461	E292	T180	S101
ASN	S702	D580	S462	K297	V181	I102
GLN	I703	R586	V471	P298	I182	Q103
GLY	E704	D592	P472	F302	H183	P104
ALA	S705	G593	Q473	I303	G184	V108
GLY	E706	G594	E477	D304	E185	
PRO	I707	G595	V474	D307	I189	
SER	ARG	A596	T475	E194	K112	
GLN	ARG	V600	W476	S197	I113	R113
GLY	GLU	L605	E487	V320	I114	H115
SER	ARG	S612	E488	R323	V116	V116
GLY	GLN	R615	L489	Q327	L117	L117
GLY	GLN	N616	Q490	L331	P118	P118
THR	THR	V617	E491	L335	I119	I119
GLY	ASN	F618	L492	K336	D120	D120
GLY	ASP	I619	V493	Q337	D205	D121
GLY	ASP	T623	Q494	R338	E218	L130
ASP	ASP	R627	P496	A339	M219	F131
ASP	PRO	D627	V497	H340	P223	E132
LEU	V728	I628	D501	R349	L224	V133
THR	GLY	R733	K502	R349	R225	V134
GLY	R734	I629	K512	R349	R235	L135
	H735	D630	R512	R349	R235	K136
	F736	P631	R512	R349	F230	F139
	E737	R635	R512	R349	K236	A142
					R239	Y143
					G240	R144
					I241	P145
					L242	I146
					L243	R147
					Y244	K148

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	950	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

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: MG, AGS

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.50	0/5855	0.65	3/7905 (0.0%)
1	B	0.50	0/5855	0.65	3/7905 (0.0%)
1	C	0.50	0/5855	0.65	3/7905 (0.0%)
1	D	0.50	0/5855	0.65	3/7905 (0.0%)
1	E	0.50	0/5855	0.65	3/7905 (0.0%)
1	F	0.50	0/5855	0.65	3/7905 (0.0%)
All	All	0.50	0/35130	0.65	18/47430 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	6
1	D	0	6
1	E	0	6
1	F	0	6
All	All	0	36

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	143	TYR	C-N-CA	5.73	136.03	121.70
1	C	143	TYR	C-N-CA	5.73	136.02	121.70
1	A	143	TYR	C-N-CA	5.71	135.98	121.70
1	D	143	TYR	C-N-CA	5.71	135.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	143	TYR	C-N-CA	5.71	135.98	121.70
1	B	143	TYR	C-N-CA	5.70	135.96	121.70
1	C	72	LEU	CA-CB-CG	5.60	128.19	115.30
1	D	72	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	72	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	72	LEU	CA-CB-CG	5.60	128.17	115.30
1	F	72	LEU	CA-CB-CG	5.59	128.16	115.30
1	E	72	LEU	CA-CB-CG	5.58	128.14	115.30
1	C	297	ALA	C-N-CD	5.40	139.74	128.40
1	F	297	ALA	C-N-CD	5.40	139.74	128.40
1	E	297	ALA	C-N-CD	5.40	139.73	128.40
1	D	297	ALA	C-N-CD	5.39	139.73	128.40
1	B	297	ALA	C-N-CD	5.38	139.71	128.40
1	A	297	ALA	C-N-CD	5.38	139.70	128.40

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ALA	Peptide
1	A	144	ARG	Peptide
1	A	156	GLY	Peptide
1	A	159	ARG	Peptide
1	A	64	ARG	Peptide
1	A	72	LEU	Peptide
1	B	142	ALA	Peptide
1	B	144	ARG	Peptide
1	B	156	GLY	Peptide
1	B	159	ARG	Peptide
1	B	64	ARG	Peptide
1	B	72	LEU	Peptide
1	C	142	ALA	Peptide
1	C	144	ARG	Peptide
1	C	156	GLY	Peptide
1	C	159	ARG	Peptide
1	C	64	ARG	Peptide
1	C	72	LEU	Peptide
1	D	142	ALA	Peptide
1	D	144	ARG	Peptide
1	D	156	GLY	Peptide
1	D	159	ARG	Peptide
1	D	64	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	D	72	LEU	Peptide
1	E	142	ALA	Peptide
1	E	144	ARG	Peptide
1	E	156	GLY	Peptide
1	E	159	ARG	Peptide
1	E	64	ARG	Peptide
1	E	72	LEU	Peptide
1	F	142	ALA	Peptide
1	F	144	ARG	Peptide
1	F	156	GLY	Peptide
1	F	159	ARG	Peptide
1	F	64	ARG	Peptide
1	F	72	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5762	0	5841	259	0
1	B	5762	0	5841	258	0
1	C	5762	0	5841	261	0
1	D	5762	0	5841	261	0
1	E	5762	0	5841	258	0
1	F	5762	0	5841	261	0
2	A	62	0	24	10	0
2	B	62	0	24	10	0
2	C	62	0	24	10	0
2	D	62	0	24	9	0
2	E	62	0	24	10	0
2	F	62	0	24	10	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	34956	0	35190	1518	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 22.

All (1518) 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:B:113:ARG:NH2	1:B:131:PHE:CE2	2.26	1.03
1:C:113:ARG:NH2	1:C:131:PHE:CE2	2.26	1.03
1:D:113:ARG:NH2	1:D:131:PHE:CE2	2.26	1.03
1:A:113:ARG:NH2	1:A:131:PHE:CE2	2.26	1.03
1:F:113:ARG:NH2	1:F:131:PHE:CE2	2.26	1.02
1:E:113:ARG:NH2	1:E:131:PHE:CE2	2.26	1.02
1:E:596:ALA:HB3	1:E:630:ASP:HB3	1.47	0.97
1:B:596:ALA:HB3	1:B:630:ASP:HB3	1.47	0.97
1:C:113:ARG:HH22	1:C:131:PHE:HE2	1.10	0.97
1:A:596:ALA:HB3	1:A:630:ASP:HB3	1.47	0.96
1:D:596:ALA:HB3	1:D:630:ASP:HB3	1.47	0.96
1:F:596:ALA:HB3	1:F:630:ASP:HB3	1.47	0.96
1:B:113:ARG:HH22	1:B:131:PHE:HE2	1.10	0.95
1:C:113:ARG:HD3	1:C:182:ILE:CG2	1.96	0.95
1:C:596:ALA:HB3	1:C:630:ASP:HB3	1.47	0.95
1:E:113:ARG:HD3	1:E:182:ILE:CG2	1.96	0.95
1:D:113:ARG:HD3	1:D:182:ILE:CG2	1.96	0.95
1:B:113:ARG:HD3	1:B:182:ILE:CG2	1.96	0.95
1:F:113:ARG:HD3	1:F:182:ILE:CG2	1.96	0.95
1:A:113:ARG:HD3	1:A:182:ILE:CG2	1.96	0.95
1:D:113:ARG:HH22	1:D:131:PHE:HE2	1.10	0.93
1:A:113:ARG:HH22	1:A:131:PHE:HE2	1.10	0.91
1:F:113:ARG:HH22	1:F:131:PHE:HE2	1.10	0.91
1:B:113:ARG:HD3	1:B:182:ILE:HG23	1.53	0.90
1:E:113:ARG:HH22	1:E:131:PHE:HE2	1.10	0.89
1:B:297:ALA:HB1	1:B:298:PRO:HD3	1.55	0.89
1:F:113:ARG:HD3	1:F:182:ILE:HG23	1.53	0.89
1:E:113:ARG:HD3	1:E:182:ILE:HG23	1.53	0.89
1:C:297:ALA:HB1	1:C:298:PRO:HD3	1.55	0.89
1:A:113:ARG:HD3	1:A:182:ILE:HG23	1.53	0.88
1:C:113:ARG:HD3	1:C:182:ILE:HG23	1.53	0.88
1:D:297:ALA:HB1	1:D:298:PRO:HD3	1.55	0.88
1:B:250:GLY:HA2	2:B:901:AGS:O2A	1.74	0.88
1:A:297:ALA:HB1	1:A:298:PRO:HD3	1.55	0.88
1:C:250:GLY:HA2	2:C:901:AGS:O2A	1.74	0.87
1:D:113:ARG:HD3	1:D:182:ILE:HG23	1.53	0.87
1:A:250:GLY:HA2	2:A:901:AGS:O2A	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HD12	1:A:176:VAL:HG11	1.57	0.87
1:F:297:ALA:HB1	1:F:298:PRO:HD3	1.55	0.86
1:B:114:ILE:HD12	1:B:176:VAL:HG11	1.57	0.86
1:D:114:ILE:HD12	1:D:176:VAL:HG11	1.57	0.86
1:E:297:ALA:HB1	1:E:298:PRO:HD3	1.55	0.86
1:F:250:GLY:HA2	2:F:901:AGS:O2A	1.74	0.86
1:D:250:GLY:HA2	2:D:901:AGS:O2A	1.74	0.86
1:E:250:GLY:HA2	2:E:901:AGS:O2A	1.74	0.86
1:E:225:ARG:HH21	1:F:432:LEU:HD22	1.40	0.85
1:C:114:ILE:HD12	1:C:176:VAL:HG11	1.57	0.85
1:F:114:ILE:HD12	1:F:176:VAL:HG11	1.57	0.85
1:D:132:GLU:HG3	1:D:136:LYS:HD3	1.59	0.85
1:B:113:ARG:O	1:B:114:ILE:HG13	1.77	0.84
1:A:113:ARG:O	1:A:114:ILE:HG13	1.77	0.84
1:E:132:GLU:HG3	1:E:136:LYS:HD3	1.59	0.84
1:C:25:ARG:HG3	1:C:99:VAL:HG11	1.60	0.84
1:E:114:ILE:HD12	1:E:176:VAL:HG11	1.57	0.84
1:D:25:ARG:HG3	1:D:99:VAL:HG11	1.60	0.84
1:D:114:ILE:HD12	1:D:176:VAL:CG1	2.08	0.84
1:B:25:ARG:HG3	1:B:99:VAL:HG11	1.60	0.84
1:A:114:ILE:HD12	1:A:176:VAL:CG1	2.08	0.84
1:E:25:ARG:HG3	1:E:99:VAL:HG11	1.60	0.84
1:B:225:ARG:HH21	1:C:432:LEU:HD22	1.41	0.84
1:B:114:ILE:HD12	1:B:176:VAL:CG1	2.08	0.84
1:F:114:ILE:HD12	1:F:176:VAL:CG1	2.08	0.83
1:C:53:ARG:HA	1:C:72:LEU:HD11	1.60	0.83
1:F:25:ARG:HG3	1:F:99:VAL:HG11	1.60	0.83
1:C:132:GLU:HG3	1:C:136:LYS:HD3	1.59	0.83
1:A:225:ARG:HH21	1:B:432:LEU:HD22	1.43	0.83
1:F:113:ARG:O	1:F:114:ILE:HG13	1.77	0.83
1:D:53:ARG:HA	1:D:72:LEU:HD11	1.60	0.83
1:D:225:ARG:HH21	1:E:432:LEU:HD22	1.42	0.83
1:C:113:ARG:O	1:C:114:ILE:HG13	1.77	0.83
1:E:113:ARG:O	1:E:114:ILE:HG13	1.77	0.83
1:A:432:LEU:HD22	1:F:225:ARG:HH21	1.42	0.83
1:B:53:ARG:HA	1:B:72:LEU:HD11	1.60	0.83
1:C:114:ILE:HD12	1:C:176:VAL:CG1	2.08	0.83
1:D:113:ARG:O	1:D:114:ILE:HG13	1.77	0.83
1:A:25:ARG:HG3	1:A:99:VAL:HG11	1.60	0.83
1:A:132:GLU:HG3	1:A:136:LYS:HD3	1.59	0.83
1:A:53:ARG:HA	1:A:72:LEU:HD11	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:ILE:HD12	1:E:176:VAL:CG1	2.08	0.82
1:C:225:ARG:HH21	1:D:432:LEU:HD22	1.42	0.82
1:E:53:ARG:HA	1:E:72:LEU:HD11	1.60	0.82
1:E:64:ARG:HH12	1:E:260:ASN:HA	1.45	0.82
1:F:53:ARG:HA	1:F:72:LEU:HD11	1.60	0.82
1:B:132:GLU:HG3	1:B:136:LYS:HD3	1.59	0.81
1:F:64:ARG:HH12	1:F:260:ASN:HA	1.44	0.81
1:B:64:ARG:HH12	1:B:260:ASN:HA	1.44	0.81
1:F:132:GLU:HG3	1:F:136:LYS:HD3	1.59	0.81
1:C:64:ARG:HH12	1:C:260:ASN:HA	1.44	0.81
1:A:64:ARG:HH12	1:A:260:ASN:HA	1.45	0.80
1:D:64:ARG:HH12	1:D:260:ASN:HA	1.45	0.80
1:D:57:VAL:HA	1:D:104:PRO:HA	1.64	0.80
1:A:22:ARG:NH1	1:A:24:ASN:HB3	1.98	0.79
1:C:57:VAL:HA	1:C:104:PRO:HA	1.64	0.79
1:B:57:VAL:HA	1:B:104:PRO:HA	1.64	0.79
1:B:22:ARG:NH1	1:B:24:ASN:HB3	1.98	0.79
1:F:22:ARG:NH1	1:F:24:ASN:HB3	1.98	0.79
1:C:22:ARG:NH1	1:C:24:ASN:HB3	1.98	0.79
1:D:22:ARG:NH1	1:D:24:ASN:HB3	1.98	0.78
1:E:586:ARG:HD3	1:E:594:GLY:HA3	1.65	0.78
2:A:901:AGS:H8	2:A:901:AGS:H5'1	1.65	0.78
1:E:57:VAL:HA	1:E:104:PRO:HA	1.64	0.78
1:F:586:ARG:HD3	1:F:594:GLY:HA3	1.65	0.78
1:E:22:ARG:NH1	1:E:24:ASN:HB3	1.98	0.78
2:E:901:AGS:H5'1	2:E:901:AGS:H8	1.65	0.78
1:A:586:ARG:HD3	1:A:594:GLY:HA3	1.65	0.78
1:D:586:ARG:HD3	1:D:594:GLY:HA3	1.65	0.78
1:F:57:VAL:HA	1:F:104:PRO:HA	1.64	0.78
1:A:57:VAL:HA	1:A:104:PRO:HA	1.64	0.78
1:B:586:ARG:HD3	1:B:594:GLY:HA3	1.65	0.78
2:D:901:AGS:H8	2:D:901:AGS:H5'1	1.65	0.78
1:C:28:VAL:HA	1:C:82:ILE:HG22	1.66	0.78
1:D:28:VAL:HA	1:D:82:ILE:HG22	1.66	0.78
2:C:901:AGS:H8	2:C:901:AGS:H5'1	1.65	0.77
2:F:901:AGS:H5'1	2:F:901:AGS:H8	1.65	0.77
1:B:28:VAL:HA	1:B:82:ILE:HG22	1.66	0.77
1:C:586:ARG:HD3	1:C:594:GLY:HA3	1.65	0.77
2:B:901:AGS:H8	2:B:901:AGS:H5'1	1.65	0.77
1:A:28:VAL:HA	1:A:82:ILE:HG22	1.66	0.76
1:D:148:LYS:HG2	1:D:165:VAL:HG11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:VAL:HA	1:E:82:ILE:HG22	1.66	0.76
1:F:28:VAL:HA	1:F:82:ILE:HG22	1.66	0.76
1:E:60:LYS:HB2	1:E:101:SER:HB3	1.68	0.76
1:F:60:LYS:HB2	1:F:101:SER:HB3	1.68	0.76
1:C:148:LYS:HG2	1:C:165:VAL:HG11	1.68	0.75
1:B:148:LYS:HG2	1:B:165:VAL:HG11	1.68	0.75
1:E:148:LYS:HG2	1:E:165:VAL:HG11	1.68	0.75
1:C:670:VAL:HA	1:C:733:ARG:HD3	1.69	0.75
1:E:670:VAL:HA	1:E:733:ARG:HD3	1.69	0.75
1:D:60:LYS:HB2	1:D:101:SER:HB3	1.68	0.74
1:D:670:VAL:HA	1:D:733:ARG:HD3	1.69	0.74
1:F:670:VAL:HA	1:F:733:ARG:HD3	1.69	0.74
1:B:670:VAL:HA	1:B:733:ARG:HD3	1.69	0.74
1:B:60:LYS:HB2	1:B:101:SER:HB3	1.68	0.74
1:C:60:LYS:HB2	1:C:101:SER:HB3	1.68	0.74
1:A:612:SER:HB3	1:A:615:LYS:HG2	1.70	0.74
1:A:148:LYS:HG2	1:A:165:VAL:HG11	1.68	0.74
1:E:113:ARG:HD3	1:E:182:ILE:HG21	1.70	0.74
1:C:113:ARG:HD3	1:C:182:ILE:HG21	1.70	0.74
1:A:670:VAL:HA	1:A:733:ARG:HD3	1.69	0.74
1:E:112:LYS:O	1:E:113:ARG:HB3	1.87	0.73
1:E:612:SER:HB3	1:E:615:LYS:HG2	1.70	0.73
1:F:612:SER:HB3	1:F:615:LYS:HG2	1.70	0.73
1:D:112:LYS:O	1:D:113:ARG:HB3	1.87	0.73
1:A:112:LYS:O	1:A:113:ARG:HB3	1.87	0.73
1:B:113:ARG:HD3	1:B:182:ILE:HG21	1.70	0.73
1:B:612:SER:HB3	1:B:615:LYS:HG2	1.70	0.73
1:F:112:LYS:O	1:F:113:ARG:HB3	1.87	0.73
1:F:148:LYS:HG2	1:F:165:VAL:HG11	1.68	0.73
1:B:112:LYS:O	1:B:113:ARG:HB3	1.87	0.73
1:C:112:LYS:O	1:C:113:ARG:HB3	1.87	0.73
1:D:612:SER:HB3	1:D:615:LYS:HG2	1.70	0.73
1:B:20:LYS:O	1:B:21:ASN:CG	2.28	0.73
1:C:164:LYS:HG2	1:C:165:VAL:H	1.54	0.73
1:A:164:LYS:HG2	1:A:165:VAL:H	1.54	0.73
1:A:113:ARG:HD3	1:A:182:ILE:HG21	1.70	0.72
1:D:164:LYS:HG2	1:D:165:VAL:H	1.54	0.72
1:A:60:LYS:HB2	1:A:101:SER:HB3	1.68	0.72
1:F:164:LYS:HG2	1:F:165:VAL:H	1.54	0.72
1:E:20:LYS:O	1:E:21:ASN:CG	2.28	0.72
1:D:20:LYS:O	1:D:21:ASN:CG	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:ARG:HD3	1:F:182:ILE:HG21	1.70	0.72
1:C:612:SER:HB3	1:C:615:LYS:HG2	1.70	0.72
1:A:20:LYS:O	1:A:21:ASN:CG	2.28	0.72
1:E:164:LYS:HG2	1:E:165:VAL:H	1.54	0.72
1:D:113:ARG:HD3	1:D:182:ILE:HG21	1.70	0.72
1:C:20:LYS:O	1:C:21:ASN:CG	2.28	0.72
1:F:20:LYS:O	1:F:21:ASN:CG	2.28	0.72
1:B:164:LYS:HG2	1:B:165:VAL:H	1.54	0.71
1:F:476:TRP:NE1	1:F:534:GLU:OE1	2.23	0.71
1:A:476:TRP:NE1	1:A:534:GLU:OE1	2.23	0.71
1:F:236:LYS:HG3	1:F:337:GLN:HE21	1.57	0.70
1:B:130:LEU:O	1:B:133:VAL:N	2.25	0.70
1:A:236:LYS:HG3	1:A:337:GLN:HE21	1.57	0.70
1:F:130:LEU:O	1:F:133:VAL:N	2.25	0.70
1:E:476:TRP:NE1	1:E:534:GLU:OE1	2.23	0.69
1:B:476:TRP:NE1	1:B:534:GLU:OE1	2.23	0.69
1:E:236:LYS:HG3	1:E:337:GLN:HE21	1.57	0.69
1:C:130:LEU:O	1:C:133:VAL:N	2.25	0.69
1:B:236:LYS:HG3	1:B:337:GLN:HE21	1.57	0.69
1:B:766:ARG:NH2	2:C:902:AGS:O3G	2.26	0.69
1:A:130:LEU:O	1:A:133:VAL:N	2.25	0.69
1:E:113:ARG:CD	1:E:182:ILE:HG21	2.23	0.69
1:B:113:ARG:CD	1:B:182:ILE:HG21	2.23	0.69
1:D:113:ARG:CD	1:D:182:ILE:HG21	2.23	0.69
1:A:113:ARG:CD	1:A:182:ILE:HG21	2.23	0.69
1:D:236:LYS:HG3	1:D:337:GLN:HE21	1.57	0.69
1:E:250:GLY:CA	2:E:901:AGS:O2A	2.41	0.69
1:C:236:LYS:HG3	1:C:337:GLN:HE21	1.57	0.69
1:C:113:ARG:CD	1:C:182:ILE:HG21	2.23	0.69
1:A:336:LYS:HB2	1:A:338:ARG:HG2	1.75	0.69
1:F:277:LYS:HB2	1:F:282:SER:HB3	1.75	0.69
1:D:250:GLY:CA	2:D:901:AGS:O2A	2.41	0.68
1:C:277:LYS:HB2	1:C:282:SER:HB3	1.75	0.68
1:C:336:LYS:HB2	1:C:338:ARG:HG2	1.75	0.68
1:B:526:LEU:HD11	2:B:902:AGS:H2'	1.76	0.68
1:B:277:LYS:HB2	1:B:282:SER:HB3	1.75	0.68
1:E:766:ARG:NH2	2:F:902:AGS:O3G	2.27	0.68
1:F:526:LEU:HD11	2:F:902:AGS:H2'	1.76	0.68
1:F:113:ARG:CD	1:F:182:ILE:HG21	2.23	0.68
1:D:766:ARG:NH2	2:E:902:AGS:O3G	2.27	0.68
1:E:526:LEU:HD11	2:E:902:AGS:H2'	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:HB2	1:B:338:ARG:HG2	1.75	0.68
1:E:130:LEU:O	1:E:133:VAL:N	2.25	0.68
1:D:277:LYS:HB2	1:D:282:SER:HB3	1.75	0.68
1:F:250:GLY:CA	2:F:901:AGS:O2A	2.41	0.68
1:C:476:TRP:NE1	1:C:534:GLU:OE1	2.23	0.68
1:C:121:ASP:HB3	1:C:161:VAL:HG22	1.76	0.68
1:A:526:LEU:HD11	2:A:902:AGS:H2'	1.76	0.68
2:A:902:AGS:O3G	1:F:766:ARG:NH2	2.26	0.68
1:F:336:LYS:HB2	1:F:338:ARG:HG2	1.75	0.68
1:F:121:ASP:HB3	1:F:161:VAL:HG22	1.76	0.68
1:C:526:LEU:HD11	2:C:902:AGS:H2'	1.76	0.68
1:A:277:LYS:HB2	1:A:282:SER:HB3	1.75	0.68
1:C:766:ARG:NH2	2:D:902:AGS:O3G	2.27	0.68
1:D:121:ASP:HB3	1:D:161:VAL:HG22	1.76	0.68
1:C:250:GLY:CA	2:C:901:AGS:O2A	2.41	0.67
1:E:121:ASP:HB3	1:E:161:VAL:HG22	1.76	0.67
1:B:250:GLY:CA	2:B:901:AGS:O2A	2.41	0.67
1:B:60:LYS:N	1:B:101:SER:O	2.27	0.67
1:D:476:TRP:NE1	1:D:534:GLU:OE1	2.23	0.67
1:E:277:LYS:HB2	1:E:282:SER:HB3	1.75	0.67
1:A:60:LYS:N	1:A:101:SER:O	2.27	0.67
1:D:526:LEU:HD11	2:D:902:AGS:H2'	1.76	0.67
1:A:250:GLY:CA	2:A:901:AGS:O2A	2.41	0.67
1:D:336:LYS:HB2	1:D:338:ARG:HG2	1.75	0.67
1:B:90:ASN:OD1	1:B:91:ASN:N	2.28	0.67
1:A:121:ASP:HB3	1:A:161:VAL:HG22	1.76	0.67
1:E:336:LYS:HB2	1:E:338:ARG:HG2	1.75	0.67
1:D:90:ASN:OD1	1:D:91:ASN:N	2.28	0.67
1:B:121:ASP:HB3	1:B:161:VAL:HG22	1.76	0.67
1:B:131:PHE:CE1	1:B:135:LEU:HD22	2.30	0.66
1:C:131:PHE:CE1	1:C:135:LEU:HD22	2.30	0.66
1:F:60:LYS:N	1:F:101:SER:O	2.27	0.66
1:F:90:ASN:OD1	1:F:91:ASN:N	2.28	0.66
1:A:766:ARG:NH2	2:B:902:AGS:O3G	2.28	0.66
1:F:347:THR:HG21	1:F:353:ILE:HD11	1.78	0.66
1:E:90:ASN:OD1	1:E:91:ASN:N	2.28	0.66
1:E:60:LYS:N	1:E:101:SER:O	2.27	0.66
1:C:117:LEU:HD13	1:C:166:VAL:HG11	1.77	0.66
1:D:117:LEU:HD13	1:D:166:VAL:HG11	1.77	0.66
1:C:90:ASN:OD1	1:C:91:ASN:N	2.28	0.66
1:E:347:THR:HG21	1:E:353:ILE:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:THR:HG21	1:D:353:ILE:HD11	1.77	0.66
1:C:472:PRO:O	1:C:533:ASN:ND2	2.29	0.66
1:A:117:LEU:HD13	1:A:166:VAL:HG11	1.77	0.66
1:C:60:LYS:N	1:C:101:SER:O	2.27	0.66
1:B:113:ARG:NH2	1:B:131:PHE:CZ	2.64	0.66
1:F:472:PRO:O	1:F:533:ASN:ND2	2.29	0.66
1:D:472:PRO:O	1:D:533:ASN:ND2	2.29	0.66
1:F:297:ALA:HB1	1:F:298:PRO:CD	2.26	0.65
1:D:512:LYS:HG2	1:D:512:LYS:O	1.97	0.65
1:E:113:ARG:NH2	1:E:131:PHE:CZ	2.64	0.65
1:E:131:PHE:CE1	1:E:135:LEU:HD22	2.30	0.65
1:D:409:ALA:HB2	2:D:901:AGS:H5'2	1.79	0.65
1:E:472:PRO:O	1:E:533:ASN:ND2	2.29	0.65
1:A:472:PRO:O	1:A:533:ASN:ND2	2.29	0.65
1:B:472:PRO:O	1:B:533:ASN:ND2	2.29	0.65
1:E:512:LYS:HG2	1:E:512:LYS:O	1.96	0.65
1:F:131:PHE:CE1	1:F:135:LEU:HD22	2.30	0.65
1:D:60:LYS:N	1:D:101:SER:O	2.27	0.65
1:B:30:GLU:HA	1:B:86:ARG:NH2	2.12	0.65
1:E:117:LEU:HD13	1:E:166:VAL:HG11	1.77	0.65
1:A:30:GLU:HA	1:A:86:ARG:NH2	2.12	0.65
1:A:90:ASN:OD1	1:A:91:ASN:N	2.28	0.65
1:C:113:ARG:NH2	1:C:131:PHE:CZ	2.64	0.65
1:A:347:THR:HG21	1:A:353:ILE:HD11	1.77	0.65
1:C:512:LYS:O	1:C:512:LYS:HG2	1.97	0.65
1:F:113:ARG:NH2	1:F:131:PHE:CZ	2.64	0.65
1:D:130:LEU:O	1:D:133:VAL:N	2.25	0.65
1:D:113:ARG:NH2	1:D:131:PHE:CZ	2.64	0.65
1:A:131:PHE:CE1	1:A:135:LEU:HD22	2.30	0.65
1:C:409:ALA:HB2	2:C:901:AGS:H5'2	1.79	0.65
1:D:491:GLU:HG2	1:D:495:TYR:CE2	2.32	0.65
1:B:512:LYS:HG2	1:B:512:LYS:O	1.96	0.65
1:C:491:GLU:HG2	1:C:495:TYR:CE2	2.32	0.65
1:B:117:LEU:HD13	1:B:166:VAL:HG11	1.77	0.65
1:C:347:THR:HG21	1:C:353:ILE:HD11	1.77	0.65
1:F:512:LYS:HG2	1:F:512:LYS:O	1.97	0.65
1:D:131:PHE:CE1	1:D:135:LEU:HD22	2.30	0.65
1:F:117:LEU:HD13	1:F:166:VAL:HG11	1.77	0.65
1:A:512:LYS:O	1:A:512:LYS:HG2	1.97	0.65
1:B:491:GLU:HG2	1:B:495:TYR:CE2	2.32	0.65
1:A:297:ALA:HB1	1:A:298:PRO:CD	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:NH2	1:A:131:PHE:CZ	2.64	0.65
1:B:297:ALA:HB1	1:B:298:PRO:CD	2.26	0.65
1:E:409:ALA:HB2	2:E:901:AGS:H5'2	1.79	0.65
1:E:491:GLU:HG2	1:E:495:TYR:CE2	2.32	0.64
1:F:491:GLU:HG2	1:F:495:TYR:CE2	2.32	0.64
1:B:409:ALA:HB2	2:B:901:AGS:H5'2	1.79	0.64
1:C:42:SER:HB2	1:C:45:LYS:HB3	1.79	0.64
1:D:42:SER:HB2	1:D:45:LYS:HB3	1.79	0.64
1:E:42:SER:HB2	1:E:45:LYS:HB3	1.79	0.64
1:A:42:SER:HB2	1:A:45:LYS:HB3	1.79	0.64
1:B:347:THR:HG21	1:B:353:ILE:HD11	1.78	0.64
1:C:30:GLU:HA	1:C:86:ARG:NH2	2.12	0.64
1:D:22:ARG:HH11	1:D:24:ASN:HB3	1.63	0.64
1:B:42:SER:HB2	1:B:45:LYS:HB3	1.79	0.64
1:F:42:SER:HB2	1:F:45:LYS:HB3	1.79	0.64
1:A:491:GLU:HG2	1:A:495:TYR:CE2	2.32	0.64
1:F:409:ALA:HB2	2:F:901:AGS:H5'2	1.79	0.64
1:E:30:GLU:HA	1:E:86:ARG:NH2	2.12	0.64
1:D:30:GLU:HA	1:D:86:ARG:NH2	2.12	0.64
1:E:218:GLU:OE1	1:F:424:ARG:NH2	2.31	0.64
1:F:30:GLU:HA	1:F:86:ARG:NH2	2.12	0.64
1:C:297:ALA:HB1	1:C:298:PRO:CD	2.26	0.63
1:D:297:ALA:HB1	1:D:298:PRO:CD	2.26	0.63
1:A:409:ALA:HB2	2:A:901:AGS:H5'2	1.79	0.63
1:C:239:ARG:NH1	1:C:335:LEU:O	2.32	0.63
1:F:22:ARG:HH11	1:F:24:ASN:HB3	1.63	0.63
1:B:764:GLN:OE1	1:B:764:GLN:N	2.32	0.63
1:C:764:GLN:N	1:C:764:GLN:OE1	2.32	0.63
1:B:114:ILE:O	1:B:115:HIS:CG	2.52	0.63
1:A:114:ILE:CD1	1:A:176:VAL:CG1	2.77	0.63
1:E:297:ALA:HB1	1:E:298:PRO:CD	2.26	0.63
1:B:239:ARG:NH1	1:B:335:LEU:O	2.32	0.63
1:D:239:ARG:NH1	1:D:335:LEU:O	2.32	0.63
1:F:239:ARG:NH1	1:F:335:LEU:O	2.31	0.63
1:C:114:ILE:O	1:C:115:HIS:CG	2.52	0.62
1:C:114:ILE:CD1	1:C:176:VAL:CG1	2.77	0.62
1:D:114:ILE:CD1	1:D:176:VAL:CG1	2.77	0.62
1:E:114:ILE:CD1	1:E:176:VAL:CG1	2.77	0.62
1:E:22:ARG:HH11	1:E:24:ASN:HB3	1.63	0.62
1:A:764:GLN:N	1:A:764:GLN:OE1	2.32	0.62
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:OE1	1:C:424:ARG:NH2	2.32	0.62
1:E:239:ARG:NH1	1:E:335:LEU:O	2.32	0.62
1:D:113:ARG:CD	1:D:182:ILE:CG2	2.76	0.62
1:A:22:ARG:HH11	1:A:24:ASN:HB3	1.63	0.62
1:C:218:GLU:OE1	1:D:424:ARG:NH2	2.33	0.62
1:A:114:ILE:O	1:A:115:HIS:CG	2.52	0.62
1:E:114:ILE:O	1:E:115:HIS:CG	2.52	0.62
1:A:424:ARG:NH2	1:F:218:GLU:OE1	2.33	0.62
1:D:764:GLN:N	1:D:764:GLN:OE1	2.32	0.62
1:D:40:SER:HB2	1:D:83:ARG:HB3	1.82	0.62
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.40	0.62
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.40	0.62
1:C:22:ARG:HH11	1:C:24:ASN:HB3	1.63	0.62
1:A:40:SER:HB2	1:A:83:ARG:HB3	1.82	0.62
1:F:114:ILE:O	1:F:115:HIS:CG	2.52	0.62
1:F:63:LYS:HG2	1:F:261:GLU:OE2	2.00	0.62
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.40	0.62
1:A:239:ARG:NH1	1:A:335:LEU:O	2.32	0.62
1:F:764:GLN:N	1:F:764:GLN:OE1	2.32	0.62
1:D:218:GLU:OE1	1:E:424:ARG:NH2	2.33	0.62
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.40	0.62
1:D:114:ILE:O	1:D:115:HIS:CG	2.52	0.62
1:E:113:ARG:CD	1:E:182:ILE:CG2	2.76	0.61
1:F:46:MET:HA	1:F:49:LEU:HB2	1.82	0.61
1:B:40:SER:HB2	1:B:83:ARG:HB3	1.82	0.61
1:D:475:THR:HG22	1:D:476:TRP:H	1.65	0.61
1:F:114:ILE:CD1	1:F:176:VAL:CG1	2.77	0.61
1:C:40:SER:HB2	1:C:83:ARG:HB3	1.82	0.61
1:F:475:THR:HG22	1:F:476:TRP:H	1.65	0.61
1:E:764:GLN:OE1	1:E:764:GLN:N	2.32	0.61
1:E:63:LYS:HG2	1:E:261:GLU:OE2	2.00	0.61
1:A:475:THR:HG22	1:A:476:TRP:H	1.65	0.61
1:A:74:ASP:OD2	1:A:83:ARG:HB2	2.01	0.61
1:C:556:GLU:HB3	1:D:552:PHE:CD2	2.35	0.61
1:B:22:ARG:HH11	1:B:24:ASN:HB3	1.63	0.61
1:E:46:MET:HA	1:E:49:LEU:HB2	1.83	0.61
1:D:84:MET:HG2	1:D:88:VAL:HG21	1.82	0.61
1:C:74:ASP:OD2	1:C:83:ARG:HB2	2.01	0.61
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.40	0.61
1:C:459:SER:O	1:C:462:SER:N	2.31	0.61
1:D:556:GLU:HB3	1:E:552:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:HE1	1:A:135:LEU:HD22	1.66	0.61
1:C:586:ARG:CD	1:C:594:GLY:HA3	2.31	0.61
1:E:84:MET:HG2	1:E:88:VAL:HG21	1.82	0.61
1:B:475:THR:HG22	1:B:476:TRP:H	1.65	0.61
1:A:218:GLU:OE1	1:B:424:ARG:NH2	2.33	0.61
1:B:63:LYS:HG2	1:B:261:GLU:OE2	2.00	0.61
1:C:63:LYS:HG2	1:C:261:GLU:OE2	2.00	0.61
1:D:63:LYS:HG2	1:D:261:GLU:OE2	2.00	0.61
1:D:22:ARG:NE	1:D:25:ARG:HB2	2.16	0.61
1:A:552:PHE:CD2	1:F:556:GLU:HB3	2.36	0.61
1:B:586:ARG:CD	1:B:594:GLY:HA3	2.31	0.61
1:A:63:LYS:HG2	1:A:261:GLU:OE2	2.00	0.61
1:B:114:ILE:CD1	1:B:176:VAL:CG1	2.77	0.60
1:F:22:ARG:NE	1:F:25:ARG:HB2	2.16	0.60
1:A:22:ARG:NE	1:A:25:ARG:HB2	2.16	0.60
1:B:40:SER:HB3	1:B:82:ILE:HG13	1.83	0.60
1:F:74:ASP:OD2	1:F:83:ARG:HB2	2.01	0.60
1:E:22:ARG:NE	1:E:25:ARG:HB2	2.16	0.60
1:C:84:MET:HG2	1:C:88:VAL:HG21	1.82	0.60
1:D:119:ILE:HG23	1:D:164:LYS:HB2	1.83	0.60
1:E:40:SER:HB2	1:E:83:ARG:HB3	1.82	0.60
1:F:84:MET:HG2	1:F:88:VAL:HG21	1.82	0.60
1:E:119:ILE:HG23	1:E:164:LYS:HB2	1.83	0.60
1:C:74:ASP:CG	1:C:75:ASP:H	2.05	0.60
1:E:74:ASP:OD2	1:E:83:ARG:HB2	2.01	0.60
1:C:119:ILE:HG23	1:C:164:LYS:HB2	1.83	0.60
1:B:119:ILE:HG23	1:B:164:LYS:HB2	1.83	0.60
1:A:556:GLU:HB3	1:B:552:PHE:CD2	2.36	0.60
1:D:459:SER:O	1:D:462:SER:N	2.31	0.60
1:F:586:ARG:CD	1:F:594:GLY:HA3	2.31	0.60
1:F:40:SER:HB2	1:F:83:ARG:HB3	1.82	0.60
1:A:519:PRO:HG3	1:A:647:LEU:HD12	1.84	0.60
1:E:131:PHE:HE1	1:E:135:LEU:HD22	1.66	0.60
1:B:22:ARG:NE	1:B:25:ARG:HB2	2.16	0.60
1:D:74:ASP:OD2	1:D:83:ARG:HB2	2.01	0.60
1:C:475:THR:HG22	1:C:476:TRP:H	1.65	0.60
1:C:519:PRO:HG3	1:C:647:LEU:HD12	1.84	0.60
1:C:131:PHE:HE1	1:C:135:LEU:HD22	1.66	0.60
1:C:46:MET:HA	1:C:49:LEU:HB2	1.83	0.60
1:E:586:ARG:CD	1:E:594:GLY:HA3	2.31	0.60
1:B:74:ASP:OD2	1:B:83:ARG:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ASP:CG	1:E:75:ASP:H	2.05	0.60
1:B:519:PRO:HG3	1:B:647:LEU:HD12	1.84	0.60
1:A:40:SER:HB3	1:A:82:ILE:HG13	1.83	0.60
1:A:46:MET:HA	1:A:49:LEU:HB2	1.83	0.60
1:D:586:ARG:CD	1:D:594:GLY:HA3	2.31	0.60
1:E:475:THR:HG22	1:E:476:TRP:H	1.65	0.60
1:C:22:ARG:NE	1:C:25:ARG:HB2	2.16	0.60
1:F:74:ASP:CG	1:F:75:ASP:H	2.05	0.60
1:E:556:GLU:HB3	1:F:552:PHE:CD2	2.37	0.60
1:B:46:MET:HA	1:B:49:LEU:HB2	1.83	0.60
1:D:519:PRO:HG3	1:D:647:LEU:HD12	1.84	0.60
1:F:113:ARG:CD	1:F:182:ILE:CG2	2.76	0.59
1:A:586:ARG:CD	1:A:594:GLY:HA3	2.31	0.59
1:F:519:PRO:HG3	1:F:647:LEU:HD12	1.84	0.59
1:B:556:GLU:HB3	1:C:552:PHE:CD2	2.36	0.59
1:C:40:SER:HB3	1:C:82:ILE:HG13	1.83	0.59
1:D:46:MET:HA	1:D:49:LEU:HB2	1.83	0.59
1:B:84:MET:HG2	1:B:88:VAL:HG21	1.82	0.59
1:A:84:MET:HG2	1:A:88:VAL:HG21	1.82	0.59
1:F:40:SER:HB3	1:F:82:ILE:HG13	1.83	0.59
1:A:119:ILE:HG23	1:A:164:LYS:HB2	1.83	0.59
1:F:119:ILE:HG23	1:F:164:LYS:HB2	1.84	0.59
1:E:519:PRO:HG3	1:E:647:LEU:HD12	1.84	0.59
1:B:74:ASP:CG	1:B:75:ASP:H	2.05	0.59
1:E:40:SER:HB3	1:E:82:ILE:HG13	1.83	0.59
1:D:40:SER:HB3	1:D:82:ILE:HG13	1.83	0.59
1:B:66:GLU:O	1:B:147:ARG:NH2	2.36	0.59
1:F:66:GLU:O	1:F:147:ARG:NH2	2.36	0.59
1:C:45:LYS:HE3	1:C:49:LEU:HD21	1.85	0.59
1:E:201:VAL:HG13	1:E:205:ASP:HB2	1.85	0.59
1:C:66:GLU:O	1:C:147:ARG:NH2	2.36	0.59
1:F:201:VAL:HG13	1:F:205:ASP:HB2	1.85	0.59
1:A:201:VAL:HG13	1:A:205:ASP:HB2	1.85	0.59
1:D:512:LYS:HZ2	1:D:619:ILE:HG13	1.68	0.59
1:D:131:PHE:HE1	1:D:135:LEU:HD22	1.66	0.58
1:E:112:LYS:O	1:E:113:ARG:CB	2.51	0.58
1:D:45:LYS:HE3	1:D:49:LEU:HD21	1.85	0.58
1:B:115:HIS:O	1:B:116:VAL:HB	2.04	0.58
1:B:131:PHE:HE1	1:B:135:LEU:HD22	1.66	0.58
1:D:115:HIS:O	1:D:116:VAL:HB	2.04	0.58
1:A:45:LYS:HE3	1:A:49:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:VAL:HG13	1:D:205:ASP:HB2	1.85	0.58
1:D:74:ASP:CG	1:D:75:ASP:H	2.05	0.58
1:E:66:GLU:O	1:E:147:ARG:NH2	2.36	0.58
1:A:66:GLU:O	1:A:147:ARG:NH2	2.36	0.58
1:F:428:ASP:OD1	1:F:429:LEU:N	2.36	0.58
1:B:45:LYS:HE3	1:B:49:LEU:HD21	1.85	0.58
1:C:59:LEU:HD13	1:C:100:ILE:HD11	1.84	0.58
1:C:132:GLU:HA	1:C:136:LYS:HB3	1.86	0.58
1:C:201:VAL:HG13	1:C:205:ASP:HB2	1.85	0.58
1:A:59:LEU:HD13	1:A:100:ILE:HD11	1.84	0.58
1:A:424:ARG:HA	1:A:427:MET:HG2	1.86	0.58
1:A:428:ASP:OD1	1:A:429:LEU:N	2.37	0.58
1:F:131:PHE:HE1	1:F:135:LEU:HD22	1.66	0.58
1:E:45:LYS:HE3	1:E:49:LEU:HD21	1.85	0.58
1:F:424:ARG:HA	1:F:427:MET:HG2	1.86	0.58
1:E:424:ARG:HA	1:E:427:MET:HG2	1.86	0.58
1:F:108:VAL:HG23	1:F:175:ILE:HG13	1.86	0.58
1:E:108:VAL:HG23	1:E:175:ILE:HG13	1.86	0.58
1:E:428:ASP:OD1	1:E:429:LEU:N	2.37	0.58
1:B:112:LYS:O	1:B:113:ARG:CB	2.51	0.58
1:C:115:HIS:O	1:C:116:VAL:HB	2.04	0.58
1:F:115:HIS:O	1:F:116:VAL:HB	2.04	0.58
1:D:66:GLU:O	1:D:147:ARG:NH2	2.36	0.58
1:C:493:VAL:HG21	1:C:531:ILE:HG12	1.86	0.58
1:F:45:LYS:HE3	1:F:49:LEU:HD21	1.85	0.58
1:F:59:LEU:HD13	1:F:100:ILE:HD11	1.84	0.58
1:B:201:VAL:HG13	1:B:205:ASP:HB2	1.85	0.58
1:F:132:GLU:HA	1:F:136:LYS:HB3	1.86	0.58
1:B:424:ARG:HA	1:B:427:MET:HG2	1.86	0.58
1:D:59:LEU:HD13	1:D:100:ILE:HD11	1.84	0.57
1:E:493:VAL:HG21	1:E:531:ILE:HG12	1.86	0.57
1:B:512:LYS:HZ2	1:B:619:ILE:HG13	1.69	0.57
1:E:59:LEU:HD13	1:E:100:ILE:HD11	1.84	0.57
1:B:493:VAL:HG21	1:B:531:ILE:HG12	1.86	0.57
1:D:424:ARG:HA	1:D:427:MET:HG2	1.86	0.57
1:A:108:VAL:HG23	1:A:175:ILE:HG13	1.86	0.57
1:A:112:LYS:O	1:A:113:ARG:CB	2.51	0.57
1:E:132:GLU:HA	1:E:136:LYS:HB3	1.86	0.57
1:B:59:LEU:HD13	1:B:100:ILE:HD11	1.84	0.57
1:A:74:ASP:CG	1:A:75:ASP:H	2.05	0.57
1:C:424:ARG:HA	1:C:427:MET:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PRO:HG3	1:B:230:PHE:CE2	2.40	0.57
1:B:428:ASP:OD1	1:B:429:LEU:N	2.37	0.57
1:D:132:GLU:HA	1:D:136:LYS:HB3	1.86	0.57
1:D:693:ARG:HH12	1:D:742:PHE:HD2	1.53	0.57
1:C:693:ARG:HH12	1:C:742:PHE:HD2	1.53	0.57
1:C:428:ASP:OD1	1:C:429:LEU:N	2.36	0.57
1:A:693:ARG:HH12	1:A:742:PHE:HD2	1.53	0.57
1:F:693:ARG:HH12	1:F:742:PHE:HD2	1.53	0.57
1:E:223:PRO:HG3	1:E:230:PHE:CE2	2.40	0.57
1:B:132:GLU:HA	1:B:136:LYS:HB3	1.86	0.57
1:C:91:ASN:HD21	1:C:151:ILE:H	1.53	0.57
1:D:428:ASP:OD1	1:D:429:LEU:N	2.37	0.57
1:D:108:VAL:HG23	1:D:175:ILE:HG13	1.86	0.57
1:F:223:PRO:HG3	1:F:230:PHE:CE2	2.40	0.57
1:D:493:VAL:HG21	1:D:531:ILE:HG12	1.86	0.57
1:D:112:LYS:O	1:D:113:ARG:CB	2.51	0.57
1:E:115:HIS:O	1:E:116:VAL:HB	2.04	0.57
1:E:20:LYS:HE3	1:E:25:ARG:HH22	1.70	0.57
1:A:20:LYS:HE3	1:A:25:ARG:HH22	1.70	0.57
1:E:693:ARG:HH12	1:E:742:PHE:HD2	1.53	0.57
1:B:20:LYS:HE3	1:B:25:ARG:HH22	1.70	0.57
1:F:20:LYS:HE3	1:F:25:ARG:HH22	1.70	0.57
1:C:112:LYS:O	1:C:113:ARG:CB	2.51	0.56
1:A:115:HIS:O	1:A:116:VAL:HB	2.04	0.56
1:D:297:ALA:CB	1:D:298:PRO:HD3	2.33	0.56
1:F:297:ALA:CB	1:F:298:PRO:HD3	2.33	0.56
1:B:91:ASN:HD21	1:B:151:ILE:H	1.53	0.56
1:B:693:ARG:HH12	1:B:742:PHE:HD2	1.53	0.56
1:A:223:PRO:HG3	1:A:230:PHE:CE2	2.40	0.56
1:E:297:ALA:CB	1:E:298:PRO:HD3	2.33	0.56
1:C:20:LYS:HE3	1:C:25:ARG:HH22	1.70	0.56
1:B:22:ARG:HB3	1:B:25:ARG:CB	2.36	0.56
1:F:112:LYS:O	1:F:113:ARG:CB	2.51	0.56
1:A:297:ALA:CB	1:A:298:PRO:CD	2.84	0.56
1:D:27:ILE:HG13	1:D:81:LYS:HA	1.86	0.56
1:E:27:ILE:HG13	1:E:81:LYS:HA	1.86	0.56
1:F:679:THR:HB	1:F:682:PHE:CD2	2.41	0.56
1:A:679:THR:HB	1:A:682:PHE:CD2	2.41	0.56
1:D:20:LYS:HE3	1:D:25:ARG:HH22	1.70	0.56
1:E:22:ARG:HB3	1:E:25:ARG:CB	2.36	0.56
1:A:132:GLU:HA	1:A:136:LYS:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ASN:HD21	1:D:151:ILE:H	1.53	0.56
1:E:512:LYS:HZ2	1:E:619:ILE:HG13	1.70	0.56
1:E:155:ARG:HD3	1:E:161:VAL:HG23	1.88	0.56
1:B:297:ALA:CB	1:B:298:PRO:CD	2.83	0.56
1:C:297:ALA:CB	1:C:298:PRO:CD	2.84	0.56
1:D:297:ALA:CB	1:D:298:PRO:CD	2.84	0.56
1:A:22:ARG:HB3	1:A:25:ARG:CB	2.36	0.56
1:F:493:VAL:HG21	1:F:531:ILE:HG12	1.86	0.56
1:A:493:VAL:HG21	1:A:531:ILE:HG12	1.86	0.56
1:C:223:PRO:HG3	1:C:230:PHE:CE2	2.40	0.56
1:B:679:THR:HB	1:B:682:PHE:CD2	2.41	0.56
1:C:22:ARG:HB3	1:C:25:ARG:CB	2.36	0.56
1:C:108:VAL:HG23	1:C:175:ILE:HG13	1.86	0.56
1:B:27:ILE:HG13	1:B:81:LYS:HA	1.86	0.56
1:C:679:THR:HB	1:C:682:PHE:CD2	2.40	0.56
1:F:27:ILE:HG13	1:F:81:LYS:HA	1.86	0.56
1:E:679:THR:HB	1:E:682:PHE:CD2	2.40	0.56
1:B:108:VAL:HG23	1:B:175:ILE:HG13	1.86	0.56
1:F:64:ARG:NH1	1:F:260:ASN:O	2.39	0.56
1:C:155:ARG:HD3	1:C:161:VAL:HG23	1.88	0.56
1:C:27:ILE:HG13	1:C:81:LYS:HA	1.86	0.56
1:A:27:ILE:HG13	1:A:81:LYS:HA	1.86	0.56
1:D:22:ARG:HB3	1:D:25:ARG:CB	2.36	0.56
1:A:512:LYS:HZ2	1:A:619:ILE:HG13	1.71	0.56
1:A:64:ARG:NH1	1:A:260:ASN:O	2.39	0.55
1:A:91:ASN:HD21	1:A:151:ILE:H	1.53	0.55
1:F:297:ALA:CB	1:F:298:PRO:CD	2.84	0.55
1:D:223:PRO:HG3	1:D:230:PHE:CE2	2.40	0.55
1:F:155:ARG:HD3	1:F:161:VAL:HG23	1.88	0.55
1:F:91:ASN:HD21	1:F:151:ILE:H	1.53	0.55
1:E:91:ASN:HD21	1:E:151:ILE:H	1.53	0.55
1:F:22:ARG:HB3	1:F:25:ARG:CB	2.36	0.55
1:C:39:VAL:HB	1:C:71:VAL:HG12	1.89	0.55
1:D:39:VAL:HB	1:D:71:VAL:HG12	1.89	0.55
1:B:39:VAL:HB	1:B:71:VAL:HG12	1.89	0.55
1:B:155:ARG:HD3	1:B:161:VAL:HG23	1.88	0.55
1:B:459:SER:O	1:B:462:SER:N	2.31	0.55
1:B:114:ILE:HG22	1:B:115:HIS:N	2.22	0.55
1:F:114:ILE:HG22	1:F:115:HIS:N	2.21	0.55
1:F:135:LEU:HD12	1:F:154:VAL:HG11	1.89	0.55
1:C:201:VAL:O	1:C:260:ASN:ND2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:679:THR:HB	1:D:682:PHE:CD2	2.40	0.55
1:E:297:ALA:CB	1:E:298:PRO:CD	2.84	0.55
1:E:64:ARG:NH1	1:E:260:ASN:O	2.39	0.55
1:A:114:ILE:HG22	1:A:115:HIS:N	2.22	0.55
1:A:135:LEU:HD12	1:A:154:VAL:HG11	1.89	0.55
1:A:297:ALA:CB	1:A:298:PRO:HD3	2.33	0.55
1:A:155:ARG:HD3	1:A:161:VAL:HG23	1.88	0.55
1:F:146:ILE:O	1:F:173:TYR:HB2	2.07	0.55
1:B:64:ARG:NH1	1:B:260:ASN:O	2.39	0.55
1:D:155:ARG:HD3	1:D:161:VAL:HG23	1.88	0.55
1:F:459:SER:O	1:F:462:SER:N	2.31	0.55
1:C:114:ILE:HG22	1:C:115:HIS:N	2.22	0.54
1:B:147:ARG:NH1	1:B:148:LYS:O	2.41	0.54
1:E:39:VAL:HB	1:E:71:VAL:HG12	1.89	0.54
1:D:135:LEU:HD12	1:D:154:VAL:HG11	1.89	0.54
1:E:114:ILE:HG22	1:E:115:HIS:N	2.21	0.54
1:B:201:VAL:O	1:B:260:ASN:ND2	2.32	0.54
1:D:146:ILE:O	1:D:173:TYR:HB2	2.07	0.54
1:A:39:VAL:HB	1:A:71:VAL:HG12	1.89	0.54
1:B:113:ARG:CD	1:B:182:ILE:CG2	2.76	0.54
1:D:114:ILE:HG22	1:D:115:HIS:N	2.22	0.54
1:E:135:LEU:HD12	1:E:154:VAL:HG11	1.88	0.54
1:D:22:ARG:CZ	1:D:25:ARG:HB2	2.38	0.54
1:C:64:ARG:NH1	1:C:260:ASN:O	2.39	0.54
1:A:201:VAL:O	1:A:260:ASN:ND2	2.32	0.54
1:D:64:ARG:NH1	1:D:260:ASN:O	2.39	0.54
1:E:147:ARG:NH1	1:E:148:LYS:O	2.41	0.54
1:D:489:LEU:O	1:D:493:VAL:HG22	2.08	0.54
1:D:223:PRO:HG3	1:D:230:PHE:HE2	1.72	0.54
1:C:115:HIS:ND1	1:C:116:VAL:N	2.56	0.54
1:F:115:HIS:ND1	1:F:116:VAL:N	2.56	0.54
1:E:68:VAL:HG11	1:E:173:TYR:CE2	2.43	0.54
1:A:459:SER:O	1:A:462:SER:N	2.31	0.54
1:F:39:VAL:HB	1:F:71:VAL:HG12	1.89	0.54
1:C:147:ARG:NH1	1:C:148:LYS:O	2.41	0.54
1:C:489:LEU:O	1:C:493:VAL:HG22	2.08	0.54
1:E:115:HIS:ND1	1:E:116:VAL:N	2.56	0.54
1:E:22:ARG:CZ	1:E:25:ARG:HB2	2.38	0.54
1:D:147:ARG:NH1	1:D:148:LYS:O	2.41	0.54
1:C:512:LYS:HZ2	1:C:619:ILE:HG13	1.72	0.54
1:F:68:VAL:HG11	1:F:173:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ILE:O	1:E:173:TYR:HB2	2.07	0.54
1:A:146:ILE:O	1:A:173:TYR:HB2	2.07	0.54
1:E:223:PRO:HG3	1:E:230:PHE:HE2	1.72	0.54
1:E:484:ASP:OD1	1:E:485:VAL:N	2.41	0.54
1:B:135:LEU:HD12	1:B:154:VAL:HG11	1.88	0.54
1:C:113:ARG:CD	1:C:182:ILE:CG2	2.76	0.54
1:B:223:PRO:HG3	1:B:230:PHE:HE2	1.72	0.54
1:A:22:ARG:CZ	1:A:25:ARG:HB2	2.38	0.54
1:F:83:ARG:O	1:F:84:MET:HB2	2.08	0.54
1:A:147:ARG:NH1	1:A:148:LYS:O	2.41	0.54
1:E:489:LEU:O	1:E:493:VAL:HG22	2.08	0.54
1:F:512:LYS:HZ2	1:F:619:ILE:HG13	1.73	0.54
1:E:108:VAL:HG11	1:E:173:TYR:CE2	2.43	0.54
1:B:146:ILE:O	1:B:173:TYR:HB2	2.07	0.54
1:E:559:VAL:HG21	1:E:600:VAL:HG13	1.90	0.54
1:F:484:ASP:OD1	1:F:485:VAL:N	2.41	0.54
1:D:559:VAL:HG21	1:D:600:VAL:HG13	1.90	0.54
1:D:83:ARG:O	1:D:84:MET:HB2	2.08	0.54
1:E:83:ARG:O	1:E:84:MET:HB2	2.08	0.54
1:F:147:ARG:NH1	1:F:148:LYS:O	2.41	0.54
1:C:223:PRO:HG3	1:C:230:PHE:HE2	1.72	0.54
1:C:146:ILE:O	1:C:173:TYR:HB2	2.07	0.54
1:B:108:VAL:HG11	1:B:173:TYR:CE2	2.43	0.54
1:E:635:ARG:HE	1:E:638:ARG:NH1	2.06	0.54
1:C:83:ARG:O	1:C:84:MET:HB2	2.08	0.53
1:A:223:PRO:HG3	1:A:230:PHE:HE2	1.72	0.53
1:B:115:HIS:ND1	1:B:116:VAL:N	2.56	0.53
1:B:489:LEU:O	1:B:493:VAL:HG22	2.08	0.53
1:D:236:LYS:HG3	1:D:337:GLN:NE2	2.24	0.53
1:F:223:PRO:HG3	1:F:230:PHE:HE2	1.72	0.53
1:A:539:PHE:CE2	1:A:541:SER:HB2	2.44	0.53
1:D:635:ARG:HE	1:D:638:ARG:NH1	2.06	0.53
1:F:635:ARG:HE	1:F:638:ARG:NH1	2.06	0.53
1:C:135:LEU:HD12	1:C:154:VAL:HG11	1.89	0.53
1:C:22:ARG:CZ	1:C:25:ARG:HB2	2.38	0.53
1:A:108:VAL:HG11	1:A:173:TYR:CE2	2.43	0.53
1:D:108:VAL:HG11	1:D:173:TYR:CE2	2.43	0.53
1:D:484:ASP:OD1	1:D:485:VAL:N	2.41	0.53
1:C:635:ARG:HE	1:C:638:ARG:NH1	2.06	0.53
1:B:539:PHE:CE2	1:B:541:SER:HB2	2.44	0.53
1:D:115:HIS:ND1	1:D:116:VAL:N	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:489:LEU:O	1:F:493:VAL:HG22	2.08	0.53
1:F:22:ARG:CZ	1:F:25:ARG:HB2	2.38	0.53
1:C:108:VAL:HG11	1:C:173:TYR:CE2	2.43	0.53
1:E:636:PRO:HA	1:E:640:ASP:HB3	1.90	0.53
1:C:559:VAL:HG21	1:C:600:VAL:HG13	1.90	0.53
1:B:635:ARG:HE	1:B:638:ARG:NH1	2.06	0.53
1:F:108:VAL:HG11	1:F:173:TYR:CE2	2.43	0.53
1:A:68:VAL:HG11	1:A:173:TYR:CE2	2.43	0.53
1:C:68:VAL:HG11	1:C:173:TYR:CE2	2.43	0.53
1:C:551:TRP:CZ2	1:C:600:VAL:HG22	2.44	0.53
1:F:636:PRO:HA	1:F:640:ASP:HB3	1.90	0.53
1:F:559:VAL:HG21	1:F:600:VAL:HG13	1.90	0.53
1:C:539:PHE:CE2	1:C:541:SER:HB2	2.44	0.53
1:A:489:LEU:O	1:A:493:VAL:HG22	2.08	0.53
1:E:482:LEU:O	1:E:486:LYS:HG3	2.09	0.53
1:D:68:VAL:HG11	1:D:173:TYR:CE2	2.43	0.53
1:B:68:VAL:HG11	1:B:173:TYR:CE2	2.43	0.53
1:E:551:TRP:CZ2	1:E:600:VAL:HG22	2.44	0.53
1:F:539:PHE:CE2	1:F:541:SER:HB2	2.44	0.53
1:B:484:ASP:OD1	1:B:485:VAL:N	2.41	0.53
1:A:484:ASP:OD1	1:A:485:VAL:N	2.41	0.53
1:C:113:ARG:CZ	1:C:182:ILE:HG12	2.39	0.53
1:E:113:ARG:CZ	1:E:182:ILE:HG12	2.39	0.53
1:B:22:ARG:CZ	1:B:25:ARG:HB2	2.38	0.53
1:A:482:LEU:O	1:A:486:LYS:HG3	2.09	0.53
1:A:115:HIS:ND1	1:A:116:VAL:N	2.56	0.53
1:A:113:ARG:CZ	1:A:182:ILE:HG12	2.39	0.53
1:B:83:ARG:O	1:B:84:MET:HB2	2.08	0.53
1:B:493:VAL:HG23	1:B:494:GLN:H	1.74	0.53
1:A:636:PRO:HA	1:A:640:ASP:HB3	1.90	0.53
1:B:551:TRP:CZ2	1:B:600:VAL:HG22	2.44	0.53
1:E:113:ARG:C	1:E:114:ILE:HG13	2.30	0.53
1:A:635:ARG:HE	1:A:638:ARG:NH1	2.06	0.53
1:A:113:ARG:C	1:A:114:ILE:HG13	2.30	0.52
1:A:493:VAL:HG23	1:A:494:GLN:H	1.74	0.52
1:B:482:LEU:O	1:B:486:LYS:HG3	2.09	0.52
1:D:482:LEU:O	1:D:486:LYS:HG3	2.09	0.52
1:D:551:TRP:CZ2	1:D:600:VAL:HG22	2.44	0.52
1:A:605:LEU:HD22	1:A:638:ARG:HD3	1.91	0.52
1:C:484:ASP:OD1	1:C:485:VAL:N	2.41	0.52
1:A:493:VAL:HG21	1:A:531:ILE:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:VAL:HG21	1:B:531:ILE:CG1	2.40	0.52
1:E:236:LYS:HG3	1:E:337:GLN:NE2	2.24	0.52
1:F:113:ARG:CZ	1:F:182:ILE:HG12	2.39	0.52
1:F:493:VAL:HG21	1:F:531:ILE:CG1	2.40	0.52
1:C:236:LYS:HG3	1:C:337:GLN:NE2	2.24	0.52
1:B:559:VAL:HG21	1:B:600:VAL:HG13	1.90	0.52
1:A:559:VAL:HG21	1:A:600:VAL:HG13	1.90	0.52
1:B:113:ARG:C	1:B:114:ILE:HG13	2.30	0.52
1:D:113:ARG:CZ	1:D:182:ILE:HG12	2.39	0.52
1:F:482:LEU:O	1:F:486:LYS:HG3	2.09	0.52
1:D:693:ARG:NH1	1:D:742:PHE:HB3	2.25	0.52
1:D:323:ARG:O	1:D:327:GLN:N	2.41	0.52
1:B:636:PRO:HA	1:B:640:ASP:HB3	1.90	0.52
1:E:539:PHE:CE2	1:E:541:SER:HB2	2.44	0.52
1:E:493:VAL:HG21	1:E:531:ILE:CG1	2.40	0.52
1:C:493:VAL:HG23	1:C:494:GLN:H	1.74	0.52
1:F:605:LEU:HD22	1:F:638:ARG:HD3	1.91	0.52
1:B:605:LEU:HD22	1:B:638:ARG:HD3	1.91	0.52
1:F:551:TRP:CZ2	1:F:600:VAL:HG22	2.44	0.52
1:A:551:TRP:CZ2	1:A:600:VAL:HG22	2.44	0.52
1:A:183:HIS:HB3	1:A:185:GLU:HG2	1.92	0.52
1:D:539:PHE:CE2	1:D:541:SER:HB2	2.44	0.52
1:B:113:ARG:CZ	1:B:182:ILE:HG12	2.39	0.52
1:F:693:ARG:NH1	1:F:742:PHE:HB3	2.25	0.52
1:D:605:LEU:HD22	1:D:638:ARG:HD3	1.91	0.52
1:B:183:HIS:HB3	1:B:185:GLU:HG2	1.92	0.52
1:D:636:PRO:HA	1:D:640:ASP:HB3	1.90	0.52
1:F:41:LEU:HD22	1:F:46:MET:SD	2.50	0.52
1:C:493:VAL:HG21	1:C:531:ILE:CG1	2.40	0.52
1:E:93:ARG:NH1	1:E:99:VAL:O	2.43	0.52
1:F:93:ARG:NH1	1:F:99:VAL:O	2.43	0.52
1:D:74:ASP:OD2	1:D:83:ARG:CB	2.58	0.52
1:B:92:LEU:HD21	1:B:100:ILE:HD13	1.92	0.52
1:A:83:ARG:O	1:A:84:MET:HB2	2.08	0.52
1:B:323:ARG:O	1:B:327:GLN:N	2.41	0.52
1:D:113:ARG:C	1:D:114:ILE:HG13	2.30	0.51
1:F:113:ARG:C	1:F:114:ILE:HG13	2.30	0.51
1:D:201:VAL:O	1:D:260:ASN:ND2	2.32	0.51
1:E:30:GLU:HA	1:E:86:ARG:HH22	1.75	0.51
1:F:74:ASP:OD2	1:F:83:ARG:CB	2.58	0.51
1:E:471:VAL:HG12	1:E:537:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:471:VAL:HG12	1:F:537:ALA:O	2.11	0.51
1:C:113:ARG:C	1:C:114:ILE:HG13	2.30	0.51
1:A:92:LEU:HD21	1:A:100:ILE:HD13	1.92	0.51
1:F:92:LEU:HD21	1:F:100:ILE:HD13	1.92	0.51
1:F:493:VAL:HG23	1:F:494:GLN:H	1.74	0.51
1:C:482:LEU:O	1:C:486:LYS:HG3	2.09	0.51
1:B:471:VAL:HG12	1:B:537:ALA:O	2.11	0.51
1:C:93:ARG:NH1	1:C:99:VAL:O	2.43	0.51
1:A:93:ARG:NH1	1:A:99:VAL:O	2.43	0.51
1:B:74:ASP:OD2	1:B:83:ARG:CB	2.58	0.51
1:E:493:VAL:HG23	1:E:494:GLN:H	1.74	0.51
1:D:493:VAL:HG23	1:D:494:GLN:H	1.74	0.51
1:C:693:ARG:NH1	1:C:742:PHE:HB3	2.25	0.51
1:E:693:ARG:NH1	1:E:742:PHE:HB3	2.25	0.51
1:C:605:LEU:HD22	1:C:638:ARG:HD3	1.91	0.51
1:C:636:PRO:HA	1:C:640:ASP:HB3	1.90	0.51
1:C:471:VAL:HG12	1:C:537:ALA:O	2.11	0.51
1:B:297:ALA:CB	1:B:298:PRO:HD3	2.33	0.51
1:D:93:ARG:NH1	1:D:99:VAL:O	2.43	0.51
1:F:22:ARG:HB3	1:F:25:ARG:HB2	1.93	0.51
1:E:92:LEU:HD21	1:E:100:ILE:HD13	1.92	0.51
1:E:605:LEU:HD22	1:E:638:ARG:HD3	1.91	0.51
1:F:183:HIS:HB3	1:F:185:GLU:HG2	1.92	0.51
1:A:250:GLY:N	2:A:901:AGS:O2A	2.44	0.51
1:F:250:GLY:N	2:F:901:AGS:O2A	2.44	0.51
1:F:201:VAL:O	1:F:260:ASN:ND2	2.32	0.51
1:A:74:ASP:OD2	1:A:83:ARG:CB	2.58	0.51
1:A:693:ARG:NH1	1:A:742:PHE:HB3	2.25	0.51
1:A:471:VAL:HG12	1:A:537:ALA:O	2.11	0.51
1:C:250:GLY:N	2:C:901:AGS:O2A	2.44	0.51
1:C:41:LEU:HD22	1:C:46:MET:SD	2.50	0.51
1:A:22:ARG:HB3	1:A:25:ARG:HB2	1.93	0.51
1:A:41:LEU:HD22	1:A:46:MET:SD	2.50	0.51
1:C:92:LEU:HD21	1:C:100:ILE:HD13	1.92	0.51
1:D:493:VAL:HG21	1:D:531:ILE:CG1	2.40	0.51
1:E:290:PHE:CD1	1:E:331:LEU:HD13	2.46	0.51
1:B:93:ARG:NH1	1:B:99:VAL:O	2.43	0.51
1:E:74:ASP:OD2	1:E:83:ARG:CB	2.58	0.51
1:F:236:LYS:HG3	1:F:337:GLN:NE2	2.24	0.51
1:D:471:VAL:HG12	1:D:537:ALA:O	2.11	0.51
1:B:290:PHE:CD1	1:B:331:LEU:HD13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:HIS:HB3	1:C:185:GLU:HG2	1.92	0.51
1:F:290:PHE:CD1	1:F:331:LEU:HD13	2.46	0.51
1:D:43:GLN:HB2	1:D:44:PRO:HD3	1.92	0.51
1:B:30:GLU:HA	1:B:86:ARG:HH22	1.75	0.51
1:B:236:LYS:HG3	1:B:337:GLN:NE2	2.24	0.51
1:E:459:SER:O	1:E:462:SER:N	2.31	0.51
1:A:290:PHE:CD1	1:A:331:LEU:HD13	2.46	0.51
1:F:43:GLN:HB2	1:F:44:PRO:HD3	1.92	0.51
1:A:364:ASP:OD1	1:A:364:ASP:N	2.44	0.51
1:E:41:LEU:HD22	1:E:46:MET:SD	2.50	0.51
1:E:631:PRO:HB3	1:E:766:ARG:CB	2.41	0.51
1:E:323:ARG:O	1:E:327:GLN:N	2.41	0.51
1:B:364:ASP:N	1:B:364:ASP:OD1	2.44	0.51
1:B:250:GLY:N	2:B:901:AGS:O2A	2.44	0.50
1:B:41:LEU:HD22	1:B:46:MET:SD	2.50	0.50
1:C:74:ASP:OD2	1:C:83:ARG:CB	2.58	0.50
1:B:693:ARG:NH1	1:B:742:PHE:HB3	2.25	0.50
1:E:183:HIS:HB3	1:E:185:GLU:HG2	1.92	0.50
1:A:627:ASP:N	1:A:627:ASP:OD1	2.44	0.50
1:D:627:ASP:OD1	1:D:627:ASP:N	2.44	0.50
1:D:92:LEU:HD21	1:D:100:ILE:HD13	1.92	0.50
1:B:85:ASN:O	1:B:88:VAL:HG22	2.12	0.50
1:F:631:PRO:HB3	1:F:766:ARG:CB	2.41	0.50
1:C:631:PRO:HB3	1:C:766:ARG:CB	2.42	0.50
1:E:43:GLN:HB2	1:E:44:PRO:HD3	1.92	0.50
1:A:43:GLN:HB2	1:A:44:PRO:HD3	1.92	0.50
1:F:364:ASP:N	1:F:364:ASP:OD1	2.44	0.50
1:D:250:GLY:N	2:D:901:AGS:O2A	2.44	0.50
1:F:84:MET:CG	1:F:88:VAL:HG21	2.42	0.50
1:F:85:ASN:O	1:F:88:VAL:HG22	2.11	0.50
1:A:236:LYS:HG3	1:A:337:GLN:NE2	2.24	0.50
1:C:30:GLU:HA	1:C:86:ARG:HH22	1.75	0.50
1:C:290:PHE:CD1	1:C:331:LEU:HD13	2.46	0.50
1:D:114:ILE:O	1:D:115:HIS:CD2	2.65	0.50
1:E:22:ARG:HB3	1:E:25:ARG:HB2	1.93	0.50
1:C:200:GLU:HG3	1:C:260:ASN:ND2	2.27	0.50
1:C:84:MET:CG	1:C:88:VAL:HG21	2.42	0.50
1:B:22:ARG:HB3	1:B:25:ARG:HB2	1.93	0.50
1:B:200:GLU:HG3	1:B:260:ASN:ND2	2.27	0.50
1:E:85:ASN:O	1:E:88:VAL:HG22	2.12	0.50
1:A:30:GLU:HA	1:A:86:ARG:HH22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PHE:CD1	1:D:331:LEU:HD13	2.46	0.50
1:B:623:THR:HG21	1:B:629:ILE:HG21	1.94	0.50
1:E:114:ILE:O	1:E:115:HIS:CD2	2.65	0.50
1:E:250:GLY:N	2:E:901:AGS:O2A	2.44	0.50
1:C:85:ASN:O	1:C:88:VAL:HG22	2.12	0.50
1:B:631:PRO:HB3	1:B:766:ARG:CB	2.42	0.50
1:C:623:THR:HG21	1:C:629:ILE:HG21	1.94	0.50
1:D:183:HIS:HB3	1:D:185:GLU:HG2	1.92	0.50
1:B:114:ILE:O	1:B:115:HIS:CD2	2.65	0.50
1:C:114:ILE:O	1:C:115:HIS:CD2	2.65	0.50
1:C:22:ARG:HB3	1:C:25:ARG:HB2	1.93	0.50
1:D:41:LEU:HD22	1:D:46:MET:SD	2.50	0.50
1:A:631:PRO:HB3	1:A:766:ARG:CB	2.42	0.50
1:D:631:PRO:HB3	1:D:766:ARG:CB	2.42	0.50
1:B:22:ARG:NH1	1:B:24:ASN:CB	2.74	0.50
1:B:551:TRP:CD1	1:B:551:TRP:N	2.79	0.50
1:C:627:ASP:N	1:C:627:ASP:OD1	2.44	0.50
1:A:85:ASN:O	1:A:88:VAL:HG22	2.12	0.50
1:B:43:GLN:HB2	1:B:44:PRO:HD3	1.92	0.50
1:D:22:ARG:HB3	1:D:25:ARG:HB2	1.93	0.49
1:D:200:GLU:HG3	1:D:260:ASN:ND2	2.27	0.49
1:E:84:MET:CG	1:E:88:VAL:HG21	2.42	0.49
1:F:114:ILE:O	1:F:115:HIS:CD2	2.65	0.49
1:D:84:MET:CG	1:D:88:VAL:HG21	2.42	0.49
1:D:85:ASN:O	1:D:88:VAL:HG22	2.12	0.49
1:A:84:MET:CG	1:A:88:VAL:HG21	2.42	0.49
1:C:43:GLN:HB2	1:C:44:PRO:HD3	1.92	0.49
1:A:114:ILE:O	1:A:115:HIS:CD2	2.65	0.49
1:E:201:VAL:O	1:E:260:ASN:ND2	2.32	0.49
1:B:84:MET:CG	1:B:88:VAL:HG21	2.42	0.49
1:D:623:THR:HG21	1:D:629:ILE:HG21	1.94	0.49
1:A:200:GLU:HG3	1:A:260:ASN:ND2	2.27	0.49
1:A:623:THR:HG21	1:A:629:ILE:HG21	1.94	0.49
1:A:650:GLU:OE1	1:A:650:GLU:N	2.31	0.49
1:F:200:GLU:HG3	1:F:260:ASN:ND2	2.27	0.49
1:C:551:TRP:CD1	1:C:551:TRP:N	2.79	0.49
1:F:627:ASP:OD1	1:F:627:ASP:N	2.44	0.49
1:A:477:GLU:OE1	1:A:477:GLU:N	2.44	0.49
1:C:298:PRO:HA	1:C:340:HIS:O	2.13	0.49
1:F:551:TRP:N	1:F:551:TRP:CD1	2.79	0.49
1:A:551:TRP:CD1	1:A:551:TRP:N	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:PRO:HA	1:B:340:HIS:O	2.13	0.49
1:A:493:VAL:HG23	1:A:494:GLN:N	2.28	0.49
1:F:491:GLU:HG2	1:F:495:TYR:HE2	1.78	0.49
1:F:623:THR:HG21	1:F:629:ILE:HG21	1.94	0.49
1:B:477:GLU:N	1:B:477:GLU:OE1	2.44	0.49
1:F:298:PRO:HA	1:F:340:HIS:O	2.13	0.49
1:E:22:ARG:NH1	1:E:24:ASN:CB	2.74	0.49
1:B:627:ASP:OD1	1:B:627:ASP:N	2.44	0.49
1:E:200:GLU:HG3	1:E:260:ASN:ND2	2.27	0.49
1:D:30:GLU:HA	1:D:86:ARG:HH22	1.75	0.49
1:D:493:VAL:HG23	1:D:494:GLN:N	2.28	0.48
1:C:491:GLU:HG2	1:C:495:TYR:HE2	1.78	0.48
1:E:554:GLU:HG3	1:F:552:PHE:CZ	2.48	0.48
1:E:551:TRP:CD1	1:E:551:TRP:N	2.79	0.48
1:E:623:THR:HG21	1:E:629:ILE:HG21	1.94	0.48
1:D:74:ASP:OD2	1:D:83:ARG:HD3	2.14	0.48
1:F:30:GLU:HA	1:F:86:ARG:HH22	1.75	0.48
1:E:493:VAL:HG23	1:E:494:GLN:N	2.28	0.48
1:A:491:GLU:HG2	1:A:495:TYR:HE2	1.78	0.48
1:D:551:TRP:N	1:D:551:TRP:CD1	2.79	0.48
1:A:323:ARG:O	1:A:327:GLN:N	2.41	0.48
1:A:701:GLU:O	1:A:705:SER:N	2.35	0.48
1:D:298:PRO:HA	1:D:340:HIS:O	2.13	0.48
1:E:298:PRO:HA	1:E:340:HIS:O	2.13	0.48
1:B:493:VAL:HG23	1:B:494:GLN:N	2.28	0.48
1:E:74:ASP:OD2	1:E:83:ARG:HD3	2.14	0.48
1:F:493:VAL:HG23	1:F:494:GLN:N	2.28	0.48
1:C:364:ASP:N	1:C:364:ASP:OD1	2.44	0.48
1:A:298:PRO:HA	1:A:340:HIS:O	2.13	0.48
1:A:22:ARG:NH1	1:A:24:ASN:CB	2.74	0.48
1:B:74:ASP:OD2	1:B:83:ARG:HD3	2.14	0.48
1:A:74:ASP:OD2	1:A:83:ARG:HD3	2.14	0.48
1:F:323:ARG:O	1:F:327:GLN:N	2.41	0.48
1:C:88:VAL:O	1:C:92:LEU:HB3	2.14	0.48
1:C:493:VAL:HG23	1:C:494:GLN:N	2.28	0.48
1:C:323:ARG:O	1:C:327:GLN:N	2.41	0.48
1:D:114:ILE:CD1	1:D:176:VAL:HG12	2.44	0.48
1:F:74:ASP:OD2	1:F:83:ARG:HD3	2.14	0.48
1:D:631:PRO:HB3	1:D:766:ARG:HB3	1.96	0.48
1:C:631:PRO:HB3	1:C:766:ARG:HB3	1.96	0.48
1:A:554:GLU:HG3	1:B:552:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ASP:OD2	1:C:83:ARG:HD3	2.14	0.48
1:D:512:LYS:NZ	1:D:619:ILE:HG13	2.29	0.48
1:C:512:LYS:NZ	1:C:619:ILE:HG13	2.29	0.48
1:B:554:GLU:HG3	1:C:552:PHE:CZ	2.49	0.48
1:D:88:VAL:O	1:D:92:LEU:HB3	2.14	0.47
1:F:631:PRO:HB3	1:F:766:ARG:HB3	1.96	0.47
1:E:703:ILE:HG13	1:E:704:GLU:N	2.29	0.47
1:F:477:GLU:N	1:F:477:GLU:OE1	2.44	0.47
1:C:58:LEU:O	1:C:102:ILE:HA	2.15	0.47
1:D:554:GLU:HG3	1:E:552:PHE:CZ	2.49	0.47
1:C:114:ILE:CD1	1:C:176:VAL:HG12	2.44	0.47
1:A:58:LEU:O	1:A:102:ILE:HA	2.15	0.47
1:B:703:ILE:HG13	1:B:704:GLU:N	2.29	0.47
1:E:114:ILE:CD1	1:E:176:VAL:HG12	2.44	0.47
1:B:88:VAL:O	1:B:92:LEU:HB3	2.14	0.47
1:A:631:PRO:HB3	1:A:766:ARG:HB3	1.96	0.47
1:D:443:ASN:OD1	1:D:444:SER:N	2.48	0.47
1:C:37:SER:O	1:C:70:ILE:HG13	2.15	0.47
1:C:554:GLU:HG3	1:D:552:PHE:CZ	2.49	0.47
1:E:701:GLU:O	1:E:705:SER:N	2.35	0.47
1:F:703:ILE:HG13	1:F:704:GLU:N	2.29	0.47
1:A:454:TRP:O	1:A:458:GLN:HG2	2.15	0.47
1:C:454:TRP:O	1:C:458:GLN:HG2	2.15	0.47
1:C:477:GLU:OE1	1:C:477:GLU:N	2.44	0.47
1:B:114:ILE:CD1	1:B:176:VAL:HG12	2.44	0.47
1:A:88:VAL:O	1:A:92:LEU:HB3	2.14	0.47
1:E:58:LEU:O	1:E:102:ILE:HA	2.15	0.47
1:E:512:LYS:NZ	1:E:619:ILE:HG13	2.29	0.47
1:B:512:LYS:NZ	1:B:619:ILE:HG13	2.29	0.47
1:A:512:LYS:NZ	1:A:619:ILE:HG13	2.29	0.47
1:B:491:GLU:HG2	1:B:495:TYR:HE2	1.78	0.47
1:A:552:PHE:CZ	1:F:554:GLU:HG3	2.49	0.47
1:A:443:ASN:OD1	1:A:444:SER:N	2.48	0.47
1:D:37:SER:O	1:D:70:ILE:HG13	2.15	0.47
1:A:37:SER:O	1:A:70:ILE:HG13	2.15	0.47
1:D:703:ILE:HG13	1:D:704:GLU:N	2.29	0.47
1:B:37:SER:O	1:B:70:ILE:HG13	2.15	0.47
1:E:112:LYS:O	1:E:180:THR:HB	2.15	0.47
1:D:58:LEU:O	1:D:102:ILE:HA	2.15	0.47
1:B:77:CYS:SG	1:B:83:ARG:HB2	2.55	0.47
1:B:494:GLN:HE21	1:B:534:GLU:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:GLN:HE21	1:E:534:GLU:HG2	1.79	0.47
1:E:37:SER:O	1:E:70:ILE:HG13	2.14	0.47
1:F:37:SER:O	1:F:70:ILE:HG13	2.15	0.47
1:B:454:TRP:O	1:B:458:GLN:HG2	2.15	0.47
1:E:443:ASN:OD1	1:E:444:SER:N	2.48	0.47
1:F:58:LEU:O	1:F:102:ILE:HA	2.15	0.47
1:F:88:VAL:O	1:F:92:LEU:HB3	2.14	0.47
1:E:631:PRO:HB3	1:E:766:ARG:HB3	1.96	0.47
1:B:443:ASN:OD1	1:B:444:SER:N	2.48	0.47
1:F:114:ILE:CD1	1:F:176:VAL:HG12	2.44	0.47
1:C:77:CYS:SG	1:C:83:ARG:HB2	2.55	0.47
1:E:120:ASP:OD1	1:E:120:ASP:N	2.46	0.47
1:F:120:ASP:OD1	1:F:120:ASP:N	2.46	0.47
1:F:512:LYS:NZ	1:F:619:ILE:HG13	2.29	0.47
1:F:443:ASN:OD1	1:F:444:SER:N	2.48	0.47
1:E:454:TRP:O	1:E:458:GLN:HG2	2.15	0.47
1:C:703:ILE:HG13	1:C:704:GLU:N	2.29	0.47
1:A:114:ILE:CD1	1:A:176:VAL:HG12	2.44	0.46
1:A:77:CYS:SG	1:A:83:ARG:HB2	2.55	0.46
1:E:88:VAL:O	1:E:92:LEU:HB3	2.14	0.46
1:F:454:TRP:O	1:F:458:GLN:HG2	2.15	0.46
1:E:364:ASP:N	1:E:364:ASP:OD1	2.44	0.46
1:F:494:GLN:HE21	1:F:534:GLU:HG2	1.79	0.46
1:E:652:SER:O	1:E:655:ALA:N	2.49	0.46
1:F:649:ASP:O	1:F:653:ARG:HG3	2.16	0.46
1:C:443:ASN:OD1	1:C:444:SER:N	2.48	0.46
1:D:364:ASP:OD1	1:D:364:ASP:N	2.44	0.46
1:B:112:LYS:O	1:B:180:THR:HB	2.15	0.46
1:A:112:LYS:O	1:A:180:THR:HB	2.15	0.46
1:A:494:GLN:HE21	1:A:534:GLU:HG2	1.79	0.46
1:E:494:GLN:HE21	1:E:534:GLU:HG2	1.79	0.46
1:A:649:ASP:O	1:A:653:ARG:HG3	2.16	0.46
1:C:649:ASP:O	1:C:653:ARG:HG3	2.16	0.46
1:D:244:TYR:HE1	1:D:366:GLU:HB3	1.81	0.46
1:C:112:LYS:O	1:C:180:THR:HB	2.15	0.46
1:F:112:LYS:O	1:F:180:THR:HB	2.15	0.46
1:D:77:CYS:SG	1:D:83:ARG:HB2	2.55	0.46
1:F:494:GLN:O	1:F:497:VAL:HG12	2.16	0.46
1:B:475:THR:HG22	1:B:476:TRP:N	2.31	0.46
1:B:494:GLN:O	1:B:497:VAL:HG12	2.16	0.46
1:B:512:LYS:HE2	1:B:617:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ASP:O	1:B:653:ARG:HG3	2.16	0.46
1:A:244:TYR:HE1	1:A:366:GLU:HB3	1.81	0.46
1:A:288:LYS:O	1:A:292:GLU:HG2	2.16	0.46
1:B:58:LEU:O	1:B:102:ILE:HA	2.15	0.46
1:E:77:CYS:SG	1:E:83:ARG:HB2	2.55	0.46
1:F:252:THR:O	1:F:255:ALA:HB3	2.16	0.46
1:D:284:SER:O	1:D:288:LYS:HG2	2.16	0.46
1:F:244:TYR:HE1	1:F:366:GLU:HB3	1.81	0.46
1:B:244:TYR:HE1	1:B:366:GLU:HB3	1.81	0.46
1:B:252:THR:O	1:B:255:ALA:HB3	2.16	0.46
1:D:494:GLN:HE21	1:D:534:GLU:HG2	1.79	0.46
1:E:243:LEU:HD23	1:E:367:VAL:HB	1.98	0.46
1:D:652:SER:O	1:D:655:ALA:N	2.49	0.46
1:C:243:LEU:HD23	1:C:367:VAL:HB	1.98	0.46
1:E:252:THR:O	1:E:255:ALA:HB3	2.16	0.46
1:A:652:SER:O	1:A:655:ALA:N	2.49	0.46
1:B:288:LYS:O	1:B:292:GLU:HG2	2.16	0.46
1:D:454:TRP:O	1:D:458:GLN:HG2	2.15	0.46
1:D:243:LEU:HD23	1:D:367:VAL:HB	1.98	0.46
1:C:84:MET:SD	1:C:88:VAL:HG21	2.56	0.46
1:B:631:PRO:HB3	1:B:766:ARG:HB3	1.96	0.46
1:E:288:LYS:O	1:E:292:GLU:HG2	2.16	0.46
1:E:302:PHE:CE2	1:E:304:ASP:HB2	2.51	0.46
1:B:652:SER:O	1:B:655:ALA:N	2.49	0.46
1:C:749:ASP:OD1	1:C:750:ASN:N	2.49	0.46
1:D:22:ARG:NH1	1:D:24:ASN:CB	2.74	0.46
1:F:22:ARG:NH2	1:F:25:ARG:HA	2.31	0.46
1:E:649:ASP:O	1:E:653:ARG:HG3	2.16	0.46
1:D:288:LYS:O	1:D:292:GLU:HG2	2.16	0.46
1:E:284:SER:O	1:E:288:LYS:HG2	2.16	0.46
1:E:244:TYR:HE1	1:E:366:GLU:HB3	1.81	0.46
1:D:749:ASP:OD1	1:D:750:ASN:N	2.49	0.46
1:C:302:PHE:CE2	1:C:304:ASP:HB2	2.51	0.46
1:D:302:PHE:CE2	1:D:304:ASP:HB2	2.51	0.46
1:F:652:SER:O	1:F:655:ALA:N	2.49	0.46
1:F:302:PHE:CE2	1:F:304:ASP:HB2	2.51	0.46
1:C:244:TYR:HE1	1:C:366:GLU:HB3	1.81	0.46
1:B:749:ASP:OD1	1:B:750:ASN:N	2.49	0.46
1:C:744:ARG:HD2	1:C:744:ARG:HA	1.76	0.46
1:B:84:MET:SD	1:B:88:VAL:HG21	2.56	0.46
1:C:494:GLN:O	1:C:497:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:SER:O	1:C:288:LYS:HG2	2.16	0.46
1:A:703:ILE:HG13	1:A:704:GLU:N	2.29	0.46
1:A:302:PHE:CE2	1:A:304:ASP:HB2	2.51	0.46
1:D:252:THR:O	1:D:255:ALA:HB3	2.16	0.46
1:F:135:LEU:HD23	1:F:135:LEU:O	2.17	0.45
1:B:22:ARG:NH2	1:B:25:ARG:HA	2.31	0.45
1:C:74:ASP:OD1	1:C:75:ASP:N	2.49	0.45
1:C:82:ILE:HA	1:C:82:ILE:HD12	1.88	0.45
1:D:84:MET:SD	1:D:88:VAL:HG21	2.56	0.45
1:E:494:GLN:O	1:E:497:VAL:HG12	2.16	0.45
1:E:157:GLY:O	1:E:159:ARG:N	2.50	0.45
1:D:512:LYS:HE2	1:D:617:VAL:O	2.16	0.45
1:C:288:LYS:O	1:C:292:GLU:HG2	2.16	0.45
1:A:252:THR:O	1:A:255:ALA:HB3	2.16	0.45
1:F:749:ASP:OD1	1:F:750:ASN:N	2.49	0.45
1:D:112:LYS:O	1:D:180:THR:HB	2.15	0.45
1:C:22:ARG:NH2	1:C:25:ARG:HA	2.31	0.45
1:C:475:THR:HG22	1:C:476:TRP:N	2.31	0.45
1:D:157:GLY:O	1:D:159:ARG:N	2.49	0.45
1:D:494:GLN:O	1:D:497:VAL:HG12	2.16	0.45
1:C:512:LYS:HE2	1:C:617:VAL:O	2.16	0.45
1:A:512:LYS:HE2	1:A:617:VAL:O	2.16	0.45
1:D:616:ASN:OD1	1:D:616:ASN:N	2.37	0.45
1:B:116:VAL:HA	1:B:163:PHE:HZ	1.81	0.45
1:D:74:ASP:OD1	1:D:75:ASP:N	2.49	0.45
1:F:77:CYS:SG	1:F:83:ARG:HB2	2.55	0.45
1:A:494:GLN:O	1:A:497:VAL:HG12	2.16	0.45
1:E:749:ASP:OD1	1:E:750:ASN:N	2.49	0.45
1:F:288:LYS:O	1:F:292:GLU:HG2	2.16	0.45
1:C:652:SER:O	1:C:655:ALA:N	2.49	0.45
1:E:477:GLU:N	1:E:477:GLU:OE1	2.44	0.45
1:D:116:VAL:HA	1:D:163:PHE:HZ	1.81	0.45
1:E:22:ARG:NH2	1:E:25:ARG:HA	2.31	0.45
1:E:119:ILE:HG13	1:E:120:ASP:H	1.82	0.45
1:F:157:GLY:O	1:F:159:ARG:N	2.49	0.45
1:D:485:VAL:HA	1:D:488:GLU:HB3	1.99	0.45
1:A:284:SER:O	1:A:288:LYS:HG2	2.16	0.45
1:B:302:PHE:CE2	1:B:304:ASP:HB2	2.51	0.45
1:D:119:ILE:HG13	1:D:120:ASP:H	1.82	0.45
1:E:84:MET:SD	1:E:88:VAL:HG21	2.56	0.45
1:D:649:ASP:O	1:D:653:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:458:GLN:C	1:E:461:PRO:HD2	2.37	0.45
1:B:135:LEU:O	1:B:135:LEU:HD23	2.17	0.45
1:C:135:LEU:O	1:C:135:LEU:HD23	2.17	0.45
1:F:74:ASP:OD1	1:F:75:ASP:N	2.49	0.45
1:E:475:THR:HG22	1:E:476:TRP:N	2.31	0.45
1:F:512:LYS:HE2	1:F:617:VAL:O	2.16	0.45
1:F:117:LEU:HA	1:F:118:PRO:HD3	1.82	0.45
1:D:139:PHE:HD2	1:D:143:TYR:HE1	1.64	0.45
1:D:114:ILE:CG2	1:D:115:HIS:N	2.80	0.45
1:E:116:VAL:HA	1:E:163:PHE:HZ	1.81	0.45
1:A:22:ARG:NH2	1:A:25:ARG:HA	2.31	0.45
1:A:74:ASP:OD1	1:A:75:ASP:N	2.49	0.45
1:F:84:MET:SD	1:F:88:VAL:HG21	2.56	0.45
1:B:764:GLN:NE2	1:C:745:ARG:O	2.50	0.45
1:C:458:GLN:C	1:C:461:PRO:HD2	2.37	0.45
1:B:458:GLN:C	1:B:461:PRO:HD2	2.37	0.45
1:B:284:SER:O	1:B:288:LYS:HG2	2.16	0.45
1:D:458:GLN:C	1:D:461:PRO:HD2	2.37	0.45
1:B:243:LEU:HD23	1:B:367:VAL:HB	1.98	0.45
1:A:744:ARG:HD2	1:A:744:ARG:HA	1.76	0.45
1:A:749:ASP:OD1	1:A:750:ASN:N	2.49	0.45
1:F:243:LEU:HD23	1:F:367:VAL:HB	1.98	0.45
1:C:114:ILE:CG2	1:C:115:HIS:N	2.80	0.45
1:C:166:VAL:HG23	1:C:167:GLU:H	1.82	0.45
1:E:512:LYS:HE2	1:E:617:VAL:O	2.16	0.45
1:A:139:PHE:HD2	1:A:143:TYR:HE1	1.64	0.45
1:D:135:LEU:O	1:D:135:LEU:HD23	2.17	0.45
1:E:114:ILE:HD12	1:E:176:VAL:HG12	1.96	0.45
1:D:22:ARG:NH2	1:D:25:ARG:HA	2.31	0.45
1:F:22:ARG:NH1	1:F:24:ASN:CB	2.74	0.45
1:D:74:ASP:HB2	1:D:83:ARG:CZ	2.47	0.45
1:A:84:MET:SD	1:A:88:VAL:HG21	2.56	0.45
1:C:157:GLY:O	1:C:159:ARG:N	2.49	0.45
1:A:243:LEU:HD23	1:A:367:VAL:HB	1.98	0.45
1:C:252:THR:O	1:C:255:ALA:HB3	2.16	0.45
1:D:119:ILE:HG13	1:D:120:ASP:OD1	2.17	0.45
1:F:31:ALA:HB2	1:F:83:ARG:HG2	1.99	0.45
1:A:157:GLY:O	1:A:159:ARG:N	2.49	0.45
1:F:284:SER:O	1:F:288:LYS:HG2	2.16	0.45
1:F:439:ALA:HA	1:F:442:MET:HB2	1.99	0.45
1:E:139:PHE:HD2	1:E:143:TYR:HE1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ARG:HB3	1:C:25:ARG:HB3	1.99	0.44
1:A:31:ALA:HB2	1:A:83:ARG:HG2	1.99	0.44
1:F:605:LEU:HD22	1:F:638:ARG:CD	2.48	0.44
1:A:605:LEU:HD22	1:A:638:ARG:CD	2.48	0.44
1:A:458:GLN:C	1:A:461:PRO:HD2	2.37	0.44
1:F:458:GLN:C	1:F:461:PRO:HD2	2.37	0.44
1:B:501:ASP:OD1	1:B:502:LYS:N	2.51	0.44
1:C:593:GLY:HA3	1:D:592:ASP:HA	1.99	0.44
1:C:139:PHE:HD2	1:C:143:TYR:HE1	1.64	0.44
1:D:501:ASP:OD1	1:D:502:LYS:N	2.51	0.44
1:C:437:ILE:HG13	1:C:438:ASP:OD1	2.18	0.44
1:F:139:PHE:HD2	1:F:143:TYR:HE1	1.64	0.44
1:C:116:VAL:HA	1:C:163:PHE:HZ	1.81	0.44
1:F:116:VAL:HA	1:F:163:PHE:HZ	1.81	0.44
1:B:31:ALA:HB2	1:B:83:ARG:HG2	1.99	0.44
1:B:74:ASP:HB2	1:B:83:ARG:CZ	2.47	0.44
1:B:119:ILE:HG13	1:B:120:ASP:OD1	2.17	0.44
1:A:119:ILE:HG13	1:A:120:ASP:OD1	2.17	0.44
1:D:166:VAL:HG23	1:D:167:GLU:H	1.82	0.44
1:A:56:THR:HB	1:A:68:VAL:HG13	2.00	0.44
1:E:279:ALA:HB1	1:E:320:VAL:HG21	1.99	0.44
1:C:501:ASP:OD1	1:C:502:LYS:N	2.51	0.44
1:B:701:GLU:O	1:B:705:SER:N	2.35	0.44
1:C:439:ALA:HA	1:C:442:MET:HB2	1.99	0.44
1:D:701:GLU:O	1:D:705:SER:N	2.35	0.44
1:C:736:PHE:O	1:C:740:MET:HG2	2.18	0.44
1:A:135:LEU:HD23	1:A:135:LEU:O	2.17	0.44
1:B:22:ARG:HB3	1:B:25:ARG:HB3	1.99	0.44
1:F:82:ILE:HD12	1:F:82:ILE:HA	1.88	0.44
1:E:119:ILE:HG13	1:E:120:ASP:OD1	2.17	0.44
1:F:119:ILE:HG13	1:F:120:ASP:H	1.82	0.44
1:A:166:VAL:HG23	1:A:167:GLU:H	1.82	0.44
1:B:485:VAL:HA	1:B:488:GLU:HB3	1.99	0.44
1:C:485:VAL:HA	1:C:488:GLU:HB3	1.99	0.44
1:F:501:ASP:OD1	1:F:502:LYS:N	2.51	0.44
1:A:116:VAL:HA	1:A:163:PHE:HZ	1.81	0.44
1:E:135:LEU:O	1:E:135:LEU:HD23	2.17	0.44
1:F:74:ASP:HB2	1:F:83:ARG:CZ	2.47	0.44
1:C:119:ILE:HG13	1:C:120:ASP:H	1.82	0.44
1:B:119:ILE:HG13	1:B:120:ASP:H	1.82	0.44
1:B:157:GLY:O	1:B:159:ARG:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ARG:O	1:F:764:GLN:NE2	2.50	0.44
1:F:437:ILE:HG13	1:F:438:ASP:OD1	2.18	0.44
1:D:736:PHE:O	1:D:740:MET:HG2	2.18	0.44
1:B:593:GLY:HA3	1:C:592:ASP:HA	1.99	0.44
1:A:437:ILE:HG13	1:A:438:ASP:OD1	2.18	0.44
1:F:279:ALA:HB1	1:F:320:VAL:HG21	2.00	0.44
1:A:672:LEU:HD23	1:A:672:LEU:HA	1.78	0.44
1:A:580:ASP:N	1:A:580:ASP:OD1	2.51	0.44
1:F:701:GLU:O	1:F:705:SER:N	2.35	0.44
1:C:114:ILE:HD12	1:C:176:VAL:HG12	1.96	0.44
1:C:29:ASP:N	1:C:82:ILE:O	2.34	0.44
1:B:74:ASP:OD1	1:B:75:ASP:N	2.49	0.44
1:F:119:ILE:HG13	1:F:120:ASP:OD1	2.17	0.44
1:F:166:VAL:HG23	1:F:167:GLU:H	1.82	0.44
1:D:605:LEU:HD22	1:D:638:ARG:CD	2.48	0.44
1:D:439:ALA:HA	1:D:442:MET:HB2	1.99	0.44
1:D:477:GLU:OE1	1:D:477:GLU:N	2.44	0.44
1:A:501:ASP:OD1	1:A:502:LYS:N	2.51	0.44
1:D:22:ARG:HB3	1:D:25:ARG:HB3	1.99	0.44
1:A:29:ASP:N	1:A:82:ILE:O	2.34	0.44
1:E:74:ASP:OD1	1:E:75:ASP:N	2.49	0.44
1:E:74:ASP:HB2	1:E:83:ARG:CZ	2.47	0.44
1:F:475:THR:HG22	1:F:476:TRP:N	2.31	0.44
1:A:117:LEU:HA	1:A:118:PRO:HD3	1.82	0.44
1:B:166:VAL:HG23	1:B:167:GLU:H	1.82	0.44
1:D:764:GLN:NE2	1:E:745:ARG:O	2.51	0.44
1:E:764:GLN:NE2	1:F:745:ARG:O	2.51	0.44
1:A:593:GLY:HA3	1:B:592:ASP:HA	1.99	0.44
1:B:650:GLU:OE1	1:B:650:GLU:N	2.31	0.44
1:B:114:ILE:HD12	1:B:176:VAL:HG12	1.96	0.44
1:C:74:ASP:HB2	1:C:83:ARG:CZ	2.47	0.44
1:A:74:ASP:HB2	1:A:83:ARG:CZ	2.47	0.44
1:E:31:ALA:HB2	1:E:83:ARG:HG2	1.99	0.44
1:E:119:ILE:HG22	1:E:189:ILE:HG12	2.00	0.44
1:A:119:ILE:HG13	1:A:120:ASP:H	1.82	0.44
1:F:653:ARG:NE	1:F:679:THR:O	2.51	0.44
1:B:139:PHE:HD2	1:B:143:TYR:HE1	1.64	0.44
1:B:437:ILE:HG13	1:B:438:ASP:OD1	2.17	0.44
1:B:46:MET:HG2	1:B:51:LEU:HB3	2.00	0.44
1:C:764:GLN:NE2	1:D:745:ARG:O	2.51	0.44
1:F:110:TYR:HA	1:F:175:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:TYR:HA	1:D:175:ILE:O	2.18	0.44
1:A:653:ARG:NE	1:A:679:THR:O	2.51	0.44
1:B:56:THR:HB	1:B:68:VAL:HG13	2.00	0.44
1:B:605:LEU:HD22	1:B:638:ARG:CD	2.48	0.44
1:F:736:PHE:O	1:F:740:MET:HG2	2.18	0.44
1:E:650:GLU:OE1	1:E:650:GLU:N	2.31	0.44
1:F:580:ASP:N	1:F:580:ASP:OD1	2.51	0.44
1:B:460:ASN:OD1	1:B:460:ASN:N	2.51	0.44
1:E:114:ILE:CG2	1:E:115:HIS:N	2.80	0.44
1:A:253:LEU:HD22	2:A:901:AGS:H2'	2.00	0.44
1:F:253:LEU:HD22	2:F:901:AGS:H2'	2.00	0.44
1:D:119:ILE:HG22	1:D:189:ILE:HG12	2.00	0.44
1:C:119:ILE:HG13	1:C:120:ASP:OD1	2.17	0.44
1:E:117:LEU:HA	1:E:118:PRO:HD3	1.82	0.44
1:F:56:THR:HB	1:F:68:VAL:HG13	2.00	0.44
1:C:653:ARG:NE	1:C:679:THR:O	2.51	0.44
1:E:653:ARG:NE	1:E:679:THR:O	2.51	0.44
1:E:605:LEU:HD22	1:E:638:ARG:CD	2.48	0.44
1:A:485:VAL:HA	1:A:488:GLU:HB3	1.99	0.44
1:B:114:ILE:CG2	1:B:115:HIS:N	2.80	0.43
1:D:114:ILE:HD12	1:D:176:VAL:HG12	1.96	0.43
1:B:253:LEU:HD22	2:B:901:AGS:H2'	2.00	0.43
1:E:253:LEU:HD22	2:E:901:AGS:H2'	2.00	0.43
1:D:46:MET:HG2	1:D:51:LEU:HB3	2.00	0.43
1:E:40:SER:CB	1:E:83:ARG:HB3	2.48	0.43
1:E:485:VAL:HA	1:E:488:GLU:HB3	1.99	0.43
1:B:736:PHE:O	1:B:740:MET:HG2	2.18	0.43
1:A:592:ASP:HA	1:F:593:GLY:HA3	1.99	0.43
1:B:672:LEU:HD23	1:B:672:LEU:HA	1.78	0.43
1:C:580:ASP:N	1:C:580:ASP:OD1	2.51	0.43
1:C:307:ASP:OD1	1:C:307:ASP:N	2.51	0.43
1:E:580:ASP:OD1	1:E:580:ASP:N	2.51	0.43
1:F:307:ASP:OD1	1:F:307:ASP:N	2.51	0.43
1:B:115:HIS:O	1:B:116:VAL:CB	2.66	0.43
1:F:114:ILE:CG2	1:F:115:HIS:N	2.80	0.43
1:C:253:LEU:HD22	2:C:901:AGS:H2'	2.00	0.43
1:D:253:LEU:HD22	2:D:901:AGS:H2'	2.00	0.43
1:B:41:LEU:HB3	1:B:72:LEU:HA	2.00	0.43
1:A:59:LEU:HB3	1:A:102:ILE:HG22	2.01	0.43
1:F:59:LEU:HB3	1:F:102:ILE:HG22	2.00	0.43
1:C:476:TRP:CZ3	1:C:486:LYS:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:VAL:HG23	1:E:167:GLU:H	1.82	0.43
1:A:279:ALA:HB1	1:A:320:VAL:HG21	1.99	0.43
1:E:437:ILE:HG13	1:E:438:ASP:OD1	2.17	0.43
1:E:616:ASN:N	1:E:616:ASN:OD1	2.37	0.43
1:D:650:GLU:OE1	1:D:650:GLU:N	2.31	0.43
1:A:114:ILE:CG2	1:A:115:HIS:N	2.80	0.43
1:C:64:ARG:HH12	1:C:260:ASN:CA	2.25	0.43
1:F:58:LEU:N	1:F:103:GLN:O	2.38	0.43
1:B:119:ILE:HG22	1:B:189:ILE:HG12	2.00	0.43
1:E:167:GLU:HG2	1:E:168:THR:N	2.33	0.43
1:A:764:GLN:NE2	1:B:745:ARG:O	2.52	0.43
1:E:110:TYR:HA	1:E:175:ILE:O	2.18	0.43
1:B:110:TYR:HA	1:B:175:ILE:O	2.18	0.43
1:D:653:ARG:NE	1:D:679:THR:O	2.51	0.43
1:F:485:VAL:HA	1:F:488:GLU:HB3	1.99	0.43
1:A:439:ALA:HA	1:A:442:MET:HB2	1.99	0.43
1:D:279:ALA:HB1	1:D:320:VAL:HG21	2.00	0.43
1:C:672:LEU:HD23	1:C:672:LEU:HA	1.78	0.43
1:C:31:ALA:HB2	1:C:83:ARG:HG2	1.99	0.43
1:B:476:TRP:CZ3	1:B:486:LYS:HG2	2.54	0.43
1:D:476:TRP:CZ3	1:D:486:LYS:HG2	2.54	0.43
1:D:167:GLU:HG2	1:D:168:THR:N	2.33	0.43
1:D:491:GLU:HG2	1:D:495:TYR:HE2	1.78	0.43
1:B:653:ARG:NE	1:B:679:THR:O	2.51	0.43
1:B:279:ALA:HB1	1:B:320:VAL:HG21	1.99	0.43
1:D:437:ILE:HG13	1:D:438:ASP:OD1	2.18	0.43
1:C:542:ILE:HG12	1:C:562:ILE:HD13	2.01	0.43
1:A:307:ASP:N	1:A:307:ASP:OD1	2.51	0.43
1:D:31:ALA:HB2	1:D:83:ARG:HG2	1.99	0.43
1:B:59:LEU:HB3	1:B:102:ILE:HG22	2.01	0.43
1:E:58:LEU:N	1:E:103:GLN:O	2.38	0.43
1:C:119:ILE:HG22	1:C:189:ILE:HG12	2.00	0.43
1:D:56:THR:HB	1:D:68:VAL:HG13	2.00	0.43
1:D:593:GLY:HA3	1:E:592:ASP:HA	1.99	0.43
1:B:542:ILE:HG12	1:B:562:ILE:HD13	2.00	0.43
1:B:307:ASP:OD1	1:B:307:ASP:N	2.51	0.43
1:D:62:LYS:HE3	1:D:62:LYS:HB3	1.82	0.43
1:D:307:ASP:N	1:D:307:ASP:OD1	2.51	0.43
1:E:439:ALA:HA	1:E:442:MET:HB2	1.99	0.43
1:E:250:GLY:N	2:E:901:AGS:O2B	2.51	0.43
1:A:41:LEU:HB3	1:A:72:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:HA	1:D:82:ILE:HD12	1.88	0.43
1:A:593:GLY:O	1:B:592:ASP:N	2.52	0.43
1:E:736:PHE:O	1:E:740:MET:HG2	2.18	0.43
1:C:279:ALA:HB1	1:C:320:VAL:HG21	1.99	0.43
1:F:194:GLU:O	1:F:197:SER:HB3	2.19	0.43
1:A:194:GLU:O	1:A:197:SER:HB3	2.19	0.43
1:E:501:ASP:OD1	1:E:502:LYS:N	2.51	0.43
2:A:901:AGS:C8	2:A:901:AGS:H5'1	2.44	0.43
1:F:250:GLY:N	2:F:901:AGS:O2B	2.51	0.43
1:E:22:ARG:HB3	1:E:25:ARG:HB3	1.99	0.43
1:A:46:MET:HG2	1:A:51:LEU:HB3	2.00	0.43
1:E:491:GLU:HG2	1:E:495:TYR:HE2	1.78	0.43
1:A:110:TYR:HA	1:A:175:ILE:O	2.18	0.43
1:C:110:TYR:HA	1:C:175:ILE:O	2.18	0.43
1:C:56:THR:HB	1:C:68:VAL:HG13	2.00	0.43
1:C:593:GLY:O	1:D:592:ASP:N	2.52	0.43
1:E:460:ASN:N	1:E:460:ASN:OD1	2.51	0.43
1:A:113:ARG:CD	1:A:182:ILE:CG2	2.76	0.43
1:E:115:HIS:O	1:E:116:VAL:CB	2.66	0.43
1:B:250:GLY:N	2:B:901:AGS:O2B	2.51	0.43
1:C:41:LEU:HB3	1:C:72:LEU:HA	2.00	0.43
1:C:167:GLU:HG2	1:C:168:THR:N	2.33	0.43
1:A:167:GLU:HG2	1:A:168:THR:N	2.33	0.43
1:B:439:ALA:HA	1:B:442:MET:HB2	1.99	0.43
1:A:460:ASN:N	1:A:460:ASN:OD1	2.51	0.43
1:C:22:ARG:NH1	1:C:24:ASN:CB	2.74	0.43
1:E:46:MET:HG2	1:E:51:LEU:HB3	2.00	0.43
1:B:40:SER:CB	1:B:83:ARG:HB3	2.48	0.43
1:E:744:ARG:HD2	1:E:744:ARG:HA	1.76	0.43
1:A:736:PHE:O	1:A:740:MET:HG2	2.18	0.43
1:C:701:GLU:O	1:C:705:SER:N	2.35	0.43
1:C:460:ASN:N	1:C:460:ASN:OD1	2.51	0.43
1:B:580:ASP:OD1	1:B:580:ASP:N	2.51	0.43
1:D:460:ASN:OD1	1:D:460:ASN:N	2.51	0.43
2:B:901:AGS:C8	2:B:901:AGS:H5'1	2.44	0.43
1:E:59:LEU:HB3	1:E:102:ILE:HG22	2.00	0.43
1:A:476:TRP:CZ3	1:A:486:LYS:HG2	2.54	0.43
1:B:631:PRO:HB3	1:B:766:ARG:HA	2.01	0.43
1:B:167:GLU:HG2	1:B:168:THR:N	2.33	0.43
1:E:56:THR:HB	1:E:68:VAL:HG13	2.00	0.43
1:F:22:ARG:HB3	1:F:25:ARG:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:LEU:HB3	1:F:72:LEU:HA	2.00	0.42
1:C:59:LEU:HB3	1:C:102:ILE:HG22	2.00	0.42
1:E:476:TRP:CZ3	1:E:486:LYS:HG2	2.54	0.42
1:F:167:GLU:HG2	1:F:168:THR:N	2.33	0.42
1:C:605:LEU:HD22	1:C:638:ARG:CD	2.48	0.42
1:D:542:ILE:HG12	1:D:562:ILE:HD13	2.01	0.42
1:E:194:GLU:O	1:E:197:SER:HB3	2.19	0.42
1:B:194:GLU:O	1:B:197:SER:HB3	2.19	0.42
1:D:580:ASP:OD1	1:D:580:ASP:N	2.51	0.42
1:D:153:LEU:O	1:D:153:LEU:HD12	2.19	0.42
1:A:115:HIS:O	1:A:116:VAL:CB	2.66	0.42
1:F:115:HIS:O	1:F:116:VAL:CB	2.66	0.42
1:C:46:MET:HG2	1:C:51:LEU:HB3	2.00	0.42
1:E:41:LEU:HB3	1:E:72:LEU:HA	2.00	0.42
1:F:119:ILE:HG22	1:F:189:ILE:CG1	2.50	0.42
1:F:119:ILE:HG22	1:F:189:ILE:HG12	2.00	0.42
1:D:475:THR:HG22	1:D:476:TRP:N	2.31	0.42
1:B:761:THR:HG22	1:C:744:ARG:HE	1.84	0.42
1:E:593:GLY:HA3	1:F:592:ASP:HA	2.00	0.42
1:F:616:ASN:OD1	1:F:616:ASN:N	2.37	0.42
1:F:460:ASN:N	1:F:460:ASN:OD1	2.51	0.42
1:F:672:LEU:HD23	1:F:672:LEU:HA	1.78	0.42
1:F:64:ARG:HH12	1:F:260:ASN:CA	2.25	0.42
1:D:631:PRO:HB3	1:D:766:ARG:HA	2.01	0.42
1:C:40:SER:CB	1:C:83:ARG:HB3	2.48	0.42
1:A:542:ILE:HG12	1:A:562:ILE:HD13	2.01	0.42
1:A:153:LEU:HD12	1:A:153:LEU:O	2.19	0.42
1:C:119:ILE:HG22	1:C:189:ILE:CG1	2.50	0.42
1:F:476:TRP:CZ3	1:F:486:LYS:HG2	2.54	0.42
1:E:476:TRP:HE3	1:E:486:LYS:HE2	1.84	0.42
1:A:155:ARG:HH21	1:A:157:GLY:HA3	1.84	0.42
1:B:593:GLY:O	1:C:592:ASP:N	2.52	0.42
1:C:115:HIS:O	1:C:116:VAL:CB	2.66	0.42
1:F:46:MET:HG2	1:F:51:LEU:HB3	2.00	0.42
1:D:59:LEU:HB3	1:D:102:ILE:HG22	2.01	0.42
1:D:40:SER:CB	1:D:83:ARG:HB3	2.48	0.42
1:E:119:ILE:HG22	1:E:189:ILE:CG1	2.50	0.42
1:A:119:ILE:HG22	1:A:189:ILE:HG12	2.00	0.42
1:A:475:THR:HG22	1:A:476:TRP:N	2.31	0.42
1:D:194:GLU:O	1:D:197:SER:HB3	2.19	0.42
1:D:115:HIS:O	1:D:116:VAL:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:SER:CB	1:A:83:ARG:HB3	2.48	0.42
1:E:28:VAL:HG13	1:E:89:ARG:HH22	1.84	0.42
1:F:28:VAL:HG13	1:F:89:ARG:HH22	1.84	0.42
1:C:631:PRO:HB3	1:C:766:ARG:HA	2.01	0.42
2:C:901:AGS:C8	2:C:901:AGS:H5'1	2.44	0.42
1:B:119:ILE:HG22	1:B:189:ILE:CG1	2.50	0.42
1:C:155:ARG:HH21	1:C:157:GLY:HA3	1.84	0.42
1:D:155:ARG:HH21	1:D:157:GLY:HA3	1.84	0.42
1:D:476:TRP:HE3	1:D:486:LYS:HE2	1.84	0.42
1:E:761:THR:HG22	1:F:744:ARG:HE	1.84	0.42
1:C:650:GLU:OE1	1:C:650:GLU:N	2.31	0.42
1:E:153:LEU:O	1:E:153:LEU:HD12	2.19	0.42
1:D:250:GLY:N	2:D:901:AGS:O2B	2.51	0.42
1:F:29:ASP:N	1:F:82:ILE:O	2.34	0.42
1:A:476:TRP:HE3	1:A:486:LYS:HE2	1.84	0.42
1:A:631:PRO:HB3	1:A:766:ARG:HA	2.01	0.42
1:F:336:LYS:CB	1:F:338:ARG:HG2	2.49	0.42
1:A:592:ASP:N	1:F:593:GLY:O	2.52	0.42
1:D:593:GLY:O	1:E:592:ASP:N	2.52	0.42
1:F:542:ILE:HG12	1:F:562:ILE:HD13	2.00	0.42
1:C:194:GLU:O	1:C:197:SER:HB3	2.19	0.42
1:B:153:LEU:O	1:B:153:LEU:HD12	2.20	0.42
1:C:153:LEU:O	1:C:153:LEU:HD12	2.19	0.42
1:E:307:ASP:N	1:E:307:ASP:OD1	2.51	0.42
1:D:119:ILE:HG22	1:D:189:ILE:CG1	2.50	0.42
1:A:119:ILE:HG22	1:A:189:ILE:CG1	2.50	0.42
1:E:631:PRO:HB3	1:E:766:ARG:HA	2.00	0.42
1:E:542:ILE:HG12	1:E:562:ILE:HD13	2.01	0.42
1:D:41:LEU:HB3	1:D:72:LEU:HA	2.00	0.41
1:B:24:ASN:HA	1:B:45:LYS:NZ	2.35	0.41
1:D:28:VAL:HG13	1:D:89:ARG:HH22	1.84	0.41
1:B:164:LYS:HG2	1:B:165:VAL:N	2.30	0.41
1:B:476:TRP:HE3	1:B:486:LYS:HE2	1.84	0.41
1:A:117:LEU:HD23	1:A:118:PRO:O	2.20	0.41
1:B:117:LEU:HD23	1:B:118:PRO:O	2.21	0.41
1:C:113:ARG:HG2	1:C:114:ILE:N	2.36	0.41
1:C:132:GLU:O	1:C:136:LYS:NZ	2.43	0.41
1:A:22:ARG:HB3	1:A:25:ARG:HB3	1.99	0.41
1:A:24:ASN:HA	1:A:45:LYS:NZ	2.35	0.41
1:B:29:ASP:N	1:B:82:ILE:O	2.34	0.41
1:A:164:LYS:HG2	1:A:165:VAL:N	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:734:ASP:O	1:F:737:GLU:HB2	2.21	0.41
1:D:64:ARG:HH12	1:D:260:ASN:CA	2.25	0.41
1:D:117:LEU:HD23	1:D:118:PRO:O	2.20	0.41
1:A:734:ASP:O	1:A:737:GLU:HB2	2.21	0.41
1:F:153:LEU:HD12	1:F:153:LEU:O	2.19	0.41
1:D:113:ARG:HG2	1:D:114:ILE:N	2.35	0.41
1:B:120:ASP:OD1	1:B:120:ASP:N	2.46	0.41
1:F:476:TRP:HE3	1:F:486:LYS:HE2	1.84	0.41
1:F:494:GLN:NE2	1:F:534:GLU:HG2	2.36	0.41
1:E:494:GLN:NE2	1:E:534:GLU:HG2	2.36	0.41
1:F:155:ARG:HH21	1:F:157:GLY:HA3	1.84	0.41
1:B:155:ARG:HH21	1:B:157:GLY:HA3	1.84	0.41
1:C:117:LEU:HD23	1:C:118:PRO:O	2.21	0.41
1:F:283:GLU:OE2	1:F:320:VAL:HG13	2.21	0.41
1:E:593:GLY:O	1:F:592:ASP:N	2.53	0.41
1:C:348:ASN:OD1	1:C:349:ARG:HG3	2.21	0.41
1:F:631:PRO:HB3	1:F:766:ARG:HA	2.01	0.41
1:E:155:ARG:HH21	1:E:157:GLY:HA3	1.84	0.41
1:A:744:ARG:HE	1:F:761:THR:HG22	1.84	0.41
1:D:761:THR:HG22	1:E:744:ARG:HE	1.84	0.41
1:D:744:ARG:HA	1:D:744:ARG:HD2	1.76	0.41
1:E:348:ASN:OD1	1:E:349:ARG:HG3	2.21	0.41
1:F:219:MET:SD	1:F:241:ILE:HD12	2.61	0.41
1:B:28:VAL:HG13	1:B:89:ARG:HH22	1.84	0.41
1:A:82:ILE:HA	1:A:82:ILE:HD12	1.88	0.41
1:E:59:LEU:HA	1:E:101:SER:O	2.21	0.41
1:C:336:LYS:CB	1:C:338:ARG:HG2	2.49	0.41
1:B:121:ASP:HB3	1:B:161:VAL:CG2	2.49	0.41
1:E:734:ASP:O	1:E:737:GLU:HB2	2.21	0.41
1:D:219:MET:SD	1:D:241:ILE:HD12	2.61	0.41
1:A:219:MET:SD	1:A:241:ILE:HD12	2.61	0.41
1:B:113:ARG:CG	1:B:182:ILE:HG21	2.51	0.41
1:D:24:ASN:HA	1:D:45:LYS:NZ	2.35	0.41
1:D:59:LEU:HA	1:D:101:SER:O	2.21	0.41
1:A:28:VAL:HG13	1:A:89:ARG:HH22	1.84	0.41
1:B:670:VAL:HG13	1:B:733:ARG:HH11	1.86	0.41
1:A:494:GLN:NE2	1:A:534:GLU:HG2	2.36	0.41
1:B:494:GLN:NE2	1:B:534:GLU:HG2	2.36	0.41
1:D:494:GLN:NE2	1:D:534:GLU:HG2	2.36	0.41
1:E:117:LEU:HD23	1:E:118:PRO:O	2.20	0.41
1:C:257:ALA:O	1:C:261:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ALA:O	1:A:261:GLU:HG2	2.21	0.41
1:B:283:GLU:OE2	1:B:320:VAL:HG13	2.21	0.41
1:F:348:ASN:OD1	1:F:349:ARG:HG3	2.21	0.41
1:B:113:ARG:HG2	1:B:114:ILE:N	2.35	0.41
1:C:113:ARG:CG	1:C:182:ILE:HG21	2.51	0.41
1:A:113:ARG:CG	1:A:182:ILE:HG21	2.51	0.41
1:F:115:HIS:CG	1:F:116:VAL:H	2.38	0.41
1:F:113:ARG:CG	1:F:182:ILE:HG21	2.51	0.41
2:F:901:AGS:H5'1	2:F:901:AGS:C8	2.44	0.41
1:C:24:ASN:HA	1:C:45:LYS:NZ	2.35	0.41
1:E:24:ASN:HA	1:E:45:LYS:NZ	2.35	0.41
1:E:64:ARG:HH12	1:E:260:ASN:CA	2.25	0.41
1:C:28:VAL:HG13	1:C:89:ARG:HH22	1.84	0.41
1:C:59:LEU:HA	1:C:101:SER:O	2.21	0.41
1:B:59:LEU:HA	1:B:101:SER:O	2.21	0.41
1:F:59:LEU:HA	1:F:101:SER:O	2.21	0.41
1:C:164:LYS:HG2	1:C:165:VAL:N	2.30	0.41
1:D:670:VAL:HG13	1:D:733:ARG:HH11	1.86	0.41
1:E:512:LYS:CG	1:E:512:LYS:O	2.68	0.41
1:A:512:LYS:O	1:A:512:LYS:CG	2.68	0.41
1:A:764:GLN:O	1:A:765:SER:C	2.60	0.41
1:B:257:ALA:O	1:B:261:GLU:HG2	2.21	0.41
1:E:283:GLU:OE2	1:E:320:VAL:HG13	2.20	0.41
1:A:592:ASP:CA	1:F:593:GLY:HA3	2.51	0.41
1:D:593:GLY:HA3	1:E:592:ASP:CA	2.51	0.41
1:C:283:GLU:OE2	1:C:320:VAL:HG13	2.21	0.41
1:C:761:THR:HG22	1:D:744:ARG:HE	1.85	0.41
1:C:219:MET:SD	1:C:241:ILE:HD12	2.61	0.41
1:A:761:THR:HG22	1:B:744:ARG:HE	1.85	0.41
1:D:348:ASN:OD1	1:D:349:ARG:HG3	2.21	0.41
1:E:144:ARG:HB2	1:E:176:VAL:HG22	2.03	0.41
1:F:60:LYS:O	1:F:100:ILE:HD12	2.21	0.41
1:C:476:TRP:HE3	1:C:486:LYS:HE2	1.84	0.41
1:C:121:ASP:HB3	1:C:161:VAL:CG2	2.49	0.41
1:E:166:VAL:HG23	1:E:167:GLU:N	2.36	0.41
1:B:166:VAL:HG23	1:B:167:GLU:N	2.36	0.41
1:A:348:ASN:OD1	1:A:349:ARG:HG3	2.21	0.41
1:E:219:MET:SD	1:E:241:ILE:HD12	2.61	0.41
1:B:734:ASP:O	1:B:737:GLU:HB2	2.21	0.41
1:F:144:ARG:HB2	1:F:176:VAL:HG22	2.03	0.40
1:A:250:GLY:N	2:A:901:AGS:O2B	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:512:LYS:CG	1:F:512:LYS:O	2.68	0.40
1:D:257:ALA:O	1:D:261:GLU:HG2	2.21	0.40
1:C:593:GLY:HA3	1:D:592:ASP:CA	2.52	0.40
1:D:283:GLU:OE2	1:D:320:VAL:HG13	2.21	0.40
1:D:767:GLY:O	1:D:768:PHE:CG	2.75	0.40
1:E:672:LEU:HA	1:E:672:LEU:HD23	1.78	0.40
1:A:41:LEU:HD23	1:A:72:LEU:CA	2.51	0.40
1:C:58:LEU:N	1:C:103:GLN:O	2.38	0.40
1:D:29:ASP:N	1:D:82:ILE:O	2.34	0.40
1:A:60:LYS:O	1:A:100:ILE:HD12	2.21	0.40
1:C:670:VAL:HG13	1:C:733:ARG:HH11	1.86	0.40
1:B:117:LEU:HA	1:B:118:PRO:HD3	1.82	0.40
1:D:764:GLN:O	1:D:765:SER:C	2.60	0.40
1:B:348:ASN:OD1	1:B:349:ARG:HG3	2.21	0.40
1:E:767:GLY:O	1:E:768:PHE:CG	2.75	0.40
1:D:734:ASP:O	1:D:737:GLU:HB2	2.21	0.40
1:C:41:LEU:HD23	1:C:72:LEU:CA	2.51	0.40
1:D:22:ARG:O	1:D:25:ARG:HB3	2.21	0.40
1:B:41:LEU:HD23	1:B:72:LEU:CA	2.51	0.40
1:D:60:LYS:O	1:D:100:ILE:HD12	2.21	0.40
1:E:30:GLU:O	1:E:83:ARG:HG3	2.21	0.40
2:C:902:AGS:O2G	2:C:902:AGS:O1B	2.39	0.40
1:E:127:THR:O	1:E:133:VAL:HG21	2.22	0.40
1:D:166:VAL:HG23	1:D:167:GLU:N	2.36	0.40
1:F:117:LEU:HD23	1:F:118:PRO:O	2.21	0.40
1:F:257:ALA:O	1:F:261:GLU:HG2	2.21	0.40
1:A:283:GLU:OE2	1:A:320:VAL:HG13	2.21	0.40
1:C:767:GLY:O	1:C:768:PHE:CG	2.75	0.40
1:B:219:MET:SD	1:B:241:ILE:HD12	2.61	0.40
1:C:22:ARG:O	1:C:25:ARG:HB3	2.21	0.40
1:F:41:LEU:HD23	1:F:72:LEU:CA	2.51	0.40
1:D:164:LYS:HB3	1:D:164:LYS:HE3	1.93	0.40
1:A:670:VAL:HG13	1:A:733:ARG:HH11	1.86	0.40
2:E:902:AGS:O1B	2:E:902:AGS:O2G	2.39	0.40
1:A:166:VAL:HG23	1:A:167:GLU:N	2.36	0.40
1:B:764:GLN:O	1:B:765:SER:C	2.60	0.40
1:C:764:GLN:O	1:C:765:SER:C	2.60	0.40
1:E:764:GLN:O	1:E:765:SER:C	2.60	0.40
1:A:317:HIS:NE2	1:F:317:HIS:CE1	2.89	0.40
1:A:767:GLY:O	1:A:768:PHE:CG	2.75	0.40
1:C:144:ARG:HB2	1:C:176:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:ARG:HG2	1:F:114:ILE:N	2.35	0.40
1:B:42:SER:HB2	1:B:45:LYS:CB	2.51	0.40
1:F:40:SER:CB	1:F:83:ARG:HB3	2.48	0.40
1:F:30:GLU:O	1:F:83:ARG:HG3	2.21	0.40
1:C:494:GLN:NE2	1:C:534:GLU:HG2	2.36	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 PDB entries followed by that with respect to all EM entries.

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	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
1	B	733/806 (91%)	671 (92%)	55 (8%)	7 (1%)	19	58
1	C	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
1	D	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
1	E	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
1	F	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
All	All	4398/4836 (91%)	4031 (92%)	325 (7%)	42 (1%)	24	58

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ALA
1	B	297	ALA
1	C	297	ALA
1	D	297	ALA
1	E	297	ALA
1	F	297	ALA
1	A	95	ARG

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Mol	Chain	Res	Type
1	A	116	VAL
1	B	95	ARG
1	B	116	VAL
1	C	95	ARG
1	C	116	VAL
1	D	95	ARG
1	D	116	VAL
1	E	95	ARG
1	E	116	VAL
1	F	95	ARG
1	F	116	VAL
1	A	158	MET
1	B	158	MET
1	C	158	MET
1	D	158	MET
1	E	158	MET
1	F	158	MET
1	A	764	GLN
1	B	764	GLN
1	C	764	GLN
1	D	764	GLN
1	E	764	GLN
1	F	764	GLN
1	A	21	ASN
1	B	21	ASN
1	C	21	ASN
1	D	21	ASN
1	E	21	ASN
1	F	21	ASN
1	A	27	ILE
1	B	27	ILE
1	C	27	ILE
1	D	27	ILE
1	E	27	ILE
1	F	27	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	B	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	C	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	D	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	E	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	F	626/678 (92%)	625 (100%)	1 (0%)	95	98
All	All	3756/4068 (92%)	3750 (100%)	6 (0%)	95	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	VAL
1	B	474	VAL
1	C	474	VAL
1	D	474	VAL
1	E	474	VAL
1	F	474	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	317	HIS
1	A	327	GLN
1	A	337	GLN
1	A	494	GLN
1	B	91	ASN
1	B	317	HIS
1	B	327	GLN
1	B	337	GLN
1	B	494	GLN
1	C	91	ASN
1	C	317	HIS
1	C	327	GLN
1	C	337	GLN
1	C	494	GLN
1	D	91	ASN
1	D	317	HIS

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Mol	Chain	Res	Type
1	D	327	GLN
1	D	337	GLN
1	D	494	GLN
1	E	91	ASN
1	E	317	HIS
1	E	327	GLN
1	E	337	GLN
1	E	494	GLN
1	F	91	ASN
1	F	317	HIS
1	F	327	GLN
1	F	337	GLN
1	F	494	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AGS	A	901	-	26,33,33	2.19	4 (15%)	24,52,52	1.76	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	A	902	-	26,33,33	2.19	4 (15%)	24,52,52	1.80	2 (8%)
2	AGS	B	901	-	26,33,33	2.19	4 (15%)	24,52,52	1.75	2 (8%)
2	AGS	B	902	-	26,33,33	2.19	4 (15%)	24,52,52	1.81	2 (8%)
2	AGS	C	901	-	26,33,33	2.20	4 (15%)	24,52,52	1.76	2 (8%)
2	AGS	C	902	-	26,33,33	2.20	4 (15%)	24,52,52	1.80	2 (8%)
2	AGS	D	901	-	26,33,33	2.19	4 (15%)	24,52,52	1.76	2 (8%)
2	AGS	D	902	-	26,33,33	2.20	4 (15%)	24,52,52	1.80	2 (8%)
2	AGS	E	901	-	26,33,33	2.20	4 (15%)	24,52,52	1.76	2 (8%)
2	AGS	E	902	-	26,33,33	2.20	4 (15%)	24,52,52	1.79	2 (8%)
2	AGS	F	901	-	26,33,33	2.19	4 (15%)	24,52,52	1.75	2 (8%)
2	AGS	F	902	-	26,33,33	2.19	4 (15%)	24,52,52	1.80	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	A	901	-	-	0/17/38/38	0/3/3/3
2	AGS	A	902	-	-	0/17/38/38	0/3/3/3
2	AGS	B	901	-	-	0/17/38/38	0/3/3/3
2	AGS	B	902	-	-	0/17/38/38	0/3/3/3
2	AGS	C	901	-	-	0/17/38/38	0/3/3/3
2	AGS	C	902	-	-	0/17/38/38	0/3/3/3
2	AGS	D	901	-	-	0/17/38/38	0/3/3/3
2	AGS	D	902	-	-	0/17/38/38	0/3/3/3
2	AGS	E	901	-	-	0/17/38/38	0/3/3/3
2	AGS	E	902	-	-	0/17/38/38	0/3/3/3
2	AGS	F	901	-	-	0/17/38/38	0/3/3/3
2	AGS	F	902	-	-	0/17/38/38	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	AGS	PG-O3G	-2.62	1.48	1.55
2	E	901	AGS	PG-O3G	-2.62	1.48	1.55
2	A	901	AGS	PG-O3G	-2.62	1.48	1.55
2	D	901	AGS	PG-O3G	-2.62	1.48	1.55
2	F	901	AGS	PG-O3G	-2.62	1.48	1.55
2	B	901	AGS	PG-O3G	-2.62	1.48	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	902	AGS	PG-O3G	-2.59	1.48	1.55
2	D	902	AGS	PG-O3G	-2.58	1.48	1.55
2	B	902	AGS	PG-O3G	-2.56	1.48	1.55
2	E	902	AGS	PG-O3G	-2.56	1.48	1.55
2	A	902	AGS	PG-O3G	-2.55	1.48	1.55
2	C	902	AGS	PG-O3G	-2.55	1.48	1.55
2	C	901	AGS	PG-O2G	2.18	1.61	1.55
2	E	901	AGS	PG-O2G	2.19	1.61	1.55
2	B	901	AGS	PG-O2G	2.19	1.61	1.55
2	A	901	AGS	PG-O2G	2.20	1.61	1.55
2	D	901	AGS	PG-O2G	2.20	1.61	1.55
2	F	901	AGS	PG-O2G	2.20	1.61	1.55
2	E	902	AGS	PG-O2G	2.25	1.61	1.55
2	A	902	AGS	PG-O2G	2.25	1.61	1.55
2	D	902	AGS	PG-O2G	2.25	1.61	1.55
2	F	902	AGS	PG-O2G	2.26	1.61	1.55
2	C	902	AGS	PG-O2G	2.26	1.61	1.55
2	B	902	AGS	PG-O2G	2.26	1.61	1.55
2	B	901	AGS	C5-C4	2.97	1.47	1.40
2	C	901	AGS	C5-C4	2.99	1.47	1.40
2	A	901	AGS	C5-C4	3.01	1.47	1.40
2	D	901	AGS	C5-C4	3.01	1.47	1.40
2	B	902	AGS	C5-C4	3.02	1.47	1.40
2	E	902	AGS	C5-C4	3.02	1.47	1.40
2	A	902	AGS	C5-C4	3.03	1.47	1.40
2	D	902	AGS	C5-C4	3.03	1.47	1.40
2	F	902	AGS	C5-C4	3.03	1.47	1.40
2	C	902	AGS	C5-C4	3.04	1.47	1.40
2	E	901	AGS	C5-C4	3.05	1.47	1.40
2	F	901	AGS	C5-C4	3.06	1.47	1.40
2	B	902	AGS	PG-S1G	9.55	2.07	1.90
2	B	901	AGS	PG-S1G	9.55	2.07	1.90
2	F	902	AGS	PG-S1G	9.56	2.07	1.90
2	F	901	AGS	PG-S1G	9.57	2.07	1.90
2	A	902	AGS	PG-S1G	9.58	2.07	1.90
2	A	901	AGS	PG-S1G	9.58	2.07	1.90
2	D	901	AGS	PG-S1G	9.58	2.07	1.90
2	E	901	AGS	PG-S1G	9.60	2.07	1.90
2	C	902	AGS	PG-S1G	9.61	2.07	1.90
2	C	901	AGS	PG-S1G	9.62	2.07	1.90
2	D	902	AGS	PG-S1G	9.63	2.07	1.90
2	E	902	AGS	PG-S1G	9.64	2.07	1.90

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	AGS	N3-C2-N1	-6.60	123.68	128.87
2	C	902	AGS	N3-C2-N1	-6.54	123.73	128.87
2	F	902	AGS	N3-C2-N1	-6.54	123.73	128.87
2	A	902	AGS	N3-C2-N1	-6.54	123.74	128.87
2	D	902	AGS	N3-C2-N1	-6.54	123.74	128.87
2	E	902	AGS	N3-C2-N1	-6.50	123.77	128.87
2	A	901	AGS	N3-C2-N1	-6.45	123.81	128.87
2	D	901	AGS	N3-C2-N1	-6.45	123.81	128.87
2	C	901	AGS	N3-C2-N1	-6.44	123.82	128.87
2	E	901	AGS	N3-C2-N1	-6.43	123.82	128.87
2	B	901	AGS	N3-C2-N1	-6.42	123.82	128.87
2	F	901	AGS	N3-C2-N1	-6.40	123.84	128.87
2	B	902	AGS	PB-O3B-PG	-3.32	120.67	132.71
2	E	902	AGS	PB-O3B-PG	-3.31	120.69	132.71
2	A	902	AGS	PB-O3B-PG	-3.31	120.71	132.71
2	D	902	AGS	PB-O3B-PG	-3.31	120.71	132.71
2	C	902	AGS	PB-O3B-PG	-3.31	120.72	132.71
2	F	902	AGS	PB-O3B-PG	-3.30	120.72	132.71
2	B	901	AGS	PB-O3B-PG	-2.87	122.29	132.71
2	F	901	AGS	PB-O3B-PG	-2.87	122.31	132.71
2	A	901	AGS	PB-O3B-PG	-2.86	122.33	132.71
2	D	901	AGS	PB-O3B-PG	-2.86	122.33	132.71
2	E	901	AGS	PB-O3B-PG	-2.86	122.35	132.71
2	C	901	AGS	PB-O3B-PG	-2.86	122.35	132.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	AGS	8	0
2	A	902	AGS	2	0
2	B	901	AGS	8	0
2	B	902	AGS	2	0
2	C	901	AGS	7	0
2	C	902	AGS	3	0
2	D	901	AGS	7	0
2	D	902	AGS	2	0
2	E	901	AGS	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	902	AGS	3	0
2	F	901	AGS	8	0
2	F	902	AGS	2	0

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.