



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:16 PM BST

PDB ID : 5FTK  
EMDB ID: : EMD-3296  
Title : Cryo-EM structure of human p97 bound to ADP  
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 : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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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

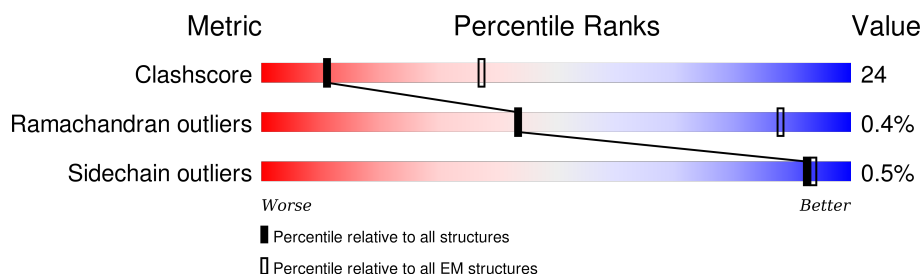
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.40 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	806	51% 37% • 10%
1	B	806	50% 38% • 10%
1	C	806	51% 38% • 10%
1	D	806	51% 38% • 10%
1	E	806	51% 38% • 10%
1	F	806	51% 38% • 10%

## 2 Entry composition [i](#)

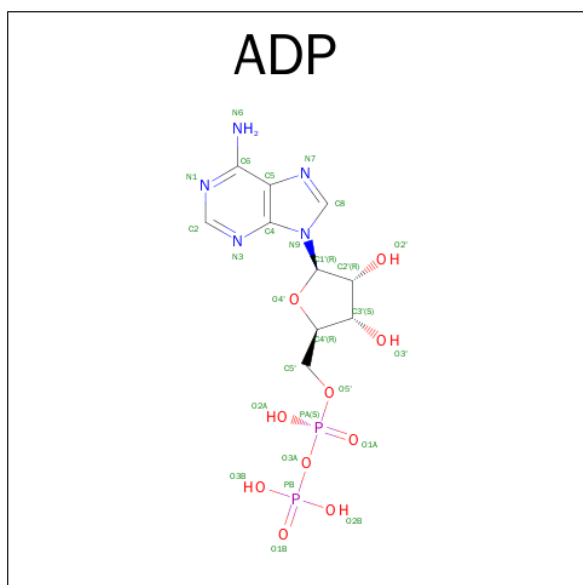
There are 3 unique types of molecules in this entry. The entry contains 34374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	B	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	C	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	D	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	E	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	F	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	D	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	D	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	F	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	F	1	Total	C	N	O	P	0
			54	20	10	20	4	

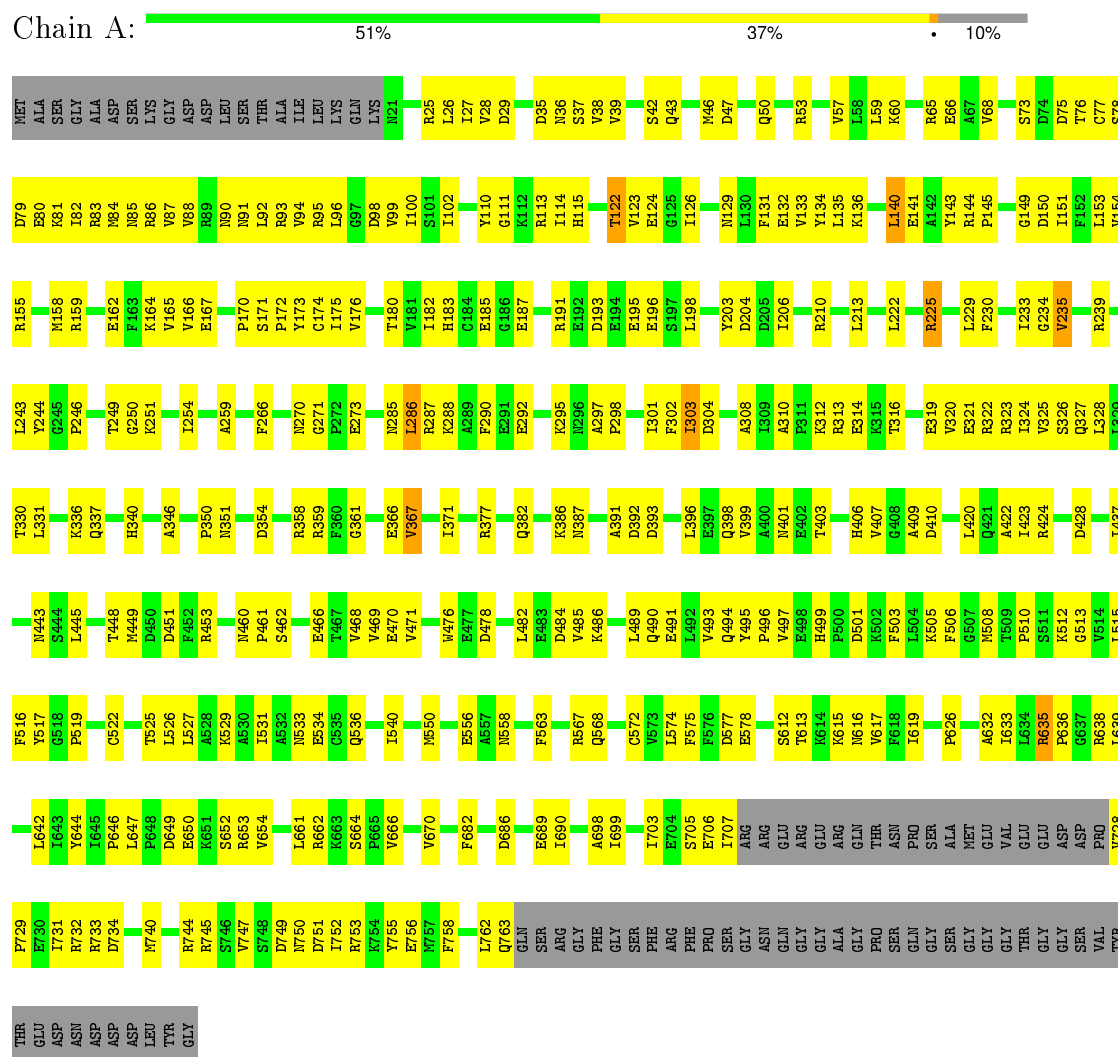
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	16	Total	O	0
			16	16	
3	B	16	Total	O	0
			16	16	
3	C	16	Total	O	0
			16	16	
3	D	16	Total	O	0
			16	16	
3	E	16	Total	O	0
			16	16	
3	F	16	Total	O	0
			16	16	

### 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

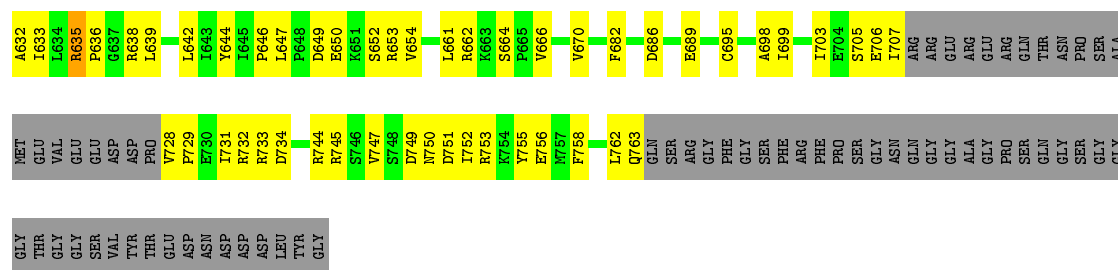


D79	F152	L243	L329	M427	T509	I619	SER	GLY
E80	L153	L243	T330	D428	P510	PE26	ALA	SER
R81	V154	Y244	L331	L429	G513	PE26	MET	GLY
I82	R155	P246	K336	I437	G514	A632	GLY	GLY
R83	M158	T249	Q337	M443	L514	A632	VAL	GLY
M84	R159	K250	K337	S444	F516	L634	GLY	THR
N85	E162	K251	H340	S445	G517	R635	GLY	GLY
R86	F163	L254	A346	T448	P519	R635	ASP	GLY
V87	K164	P170	A346	T448	C522	L638	PRD	SER
V88	V165	S171	P350	M449	G522	L638	VAL	TYR
N90	V166	P172	N351	D450	T525	L642	TYR	THR
N91	E167	P266	D354	D451	L526	L643	GLY	GLY
L92	P170	N270	R358	F452	L527	Y644	ASP	ASP
R93	S171	G271	R359	R453	A528	PE46	ASP	ASN
R95	P172	P272	P360	L456	K529	L647	ASP	ASP
L96	Y173	E273	G361	M460	A530	PE48	ASP	ASP
G97	C174	N285	E366	P461	I531	D649	LEU	TYR
D98	Y175	L286	V367	S462	A532	E550	TYR	GLY
V99	V176	K287	E367	R466	N533	S652	GLY	GLY
I100	T180	R288	I371	T467	E534	R653	ASP	GLY
I102	L181	K288	E377	V468	C535	V654	THR	GLY
Y110	L182	L289	R377	V469	Q536		GLY	GLY
G111	H183	F290	R377	E470	I540	L661	GLY	GLY
R112	C184	E291	Q382	V471	M550	R662	GLY	GLY
R113	E185	E292	K386	M476	E556	R662	GLY	GLY
I114	G186	K295	N387	E477	A557	V670	GLY	GLY
H115	E187	N296	A391	D478	N558	F757	GLY	GLY
Y116	R191	P298	D392	L482	R560	F758	GLY	GLY
L117	E192	I301	D393	E483	F563	L762	GLY	GLY
P118	E194	F302	L396	D484	Q568	Q763	GLY	GLY
T122	E195	I303	E397	V485	R567	GLN	GLY	GLY
V123	E196	D304	V399	K486	Q568	SER	GLY	GLY
E124	S197	A308	V399	L489	C572	ARG	GLY	GLY
G125	L198	Y203	A400	E491	L573	GLY	GLY	GLY
I126	Y203	D204	M401	E491	L574	GLY	GLY	GLY
N129	D204	E205	E402	L492	F575	GLY	GLY	GLY
L130	E132	I206	T403	V493	F576	GLY	GLY	GLY
F131	R210	E314	H406	Q494	E704	GLY	GLY	GLY
V133	R210	E314	V407	Y495	S705	GLY	GLY	GLY
Y134	L222	T316	G408	P496	E706	GLY	GLY	GLY
L135	R225	E319	E409	V497	I707	GLY	GLY	GLY
K136	R225	V320	D410	E499	ARG	GLY	GLY	GLY
L140	E141	E321	L414	F500	ARG	GLY	GLY	GLY
E141	L229	R322	L414	S612	GLY	GLY	GLY	GLY
Y143	F230	R322	L420	T613	GLY	GLY	GLY	GLY
R144	I233	R322	L420	K614	GLY	GLY	GLY	GLY
P145	G234	V325	Q421	K615	GLY	GLY	GLY	GLY
G149	V235	Q327	A422	N616	GLY	GLY	GLY	GLY
I151	R239	L328	R424	V617	GLY	GLY	GLY	GLY
				F618	GLY	GLY	GLY	GLY

● Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain C:  51% 38% 10%

MET	D79	D150	Q327	L429	G513	
ALA	E80	I151	L328		V514	
SER	R81	F152	L329	T437	L515	
GLY	I82	L153	T330		F516	
ALA	R83	V154	L331	V441	Y517	
ASP	M84	R155	K336	M442	G518	
SER	N85	R159	Q337	M443	P519	
LYS	R86			S444		
GLY	V87			L445		
ASP	V88					
ASP	R89	E162	H340	T448	C522	
ASP	V90	F163	A346	M449	T525	
LEU	N91	K164	Y450	D451	L526	
SER	L92	V165	P350	D451	L527	
THR	R93	E167	N351	R453	A528	
ASP	V94		D354	K529	K530	
ASP	R95			M460	I531	
ASP	L96			P461	A532	
LEU	G97			S462	C535	
GLN	D98			E466	Q536	
LYS	V99			V468	I540	
LYS	I100			V469	M550	
	S101			E470	E556	
	I102			V471	A557	
					N558	
	Y110				R560	
	G111				F563	
	R112				R567	
	H183				Q568	
	G184				C572	
	E185				V573	
	H115				L574	
	Y116				F576	
	L117				D577	
	P118				E578	
	I119				E607	
	D120				S612	
	D121				T613	
	T122				K614	
	V123				N616	
	E124				V617	
	G125				F618	
	I126				I619	
	N129				P626	
	L130					
	F131					
	E132					
	V133					
	Y134					
	L135					
	K136					
	L140					
	E141					
	L229					
	F230					
	I233					
	G234					
	V235					
	S326					







ASP	ASP	PRO	V728	P729	E730	I731	R732	R733	D734	M740	R744	R745	S746	V747	S748	D749	N750	D751	I752	R753	K754	V755	E756	R757	F758	L762	O763	G1N	SER	SER	ARG	GLY	PHE	PHE	GLY	SER	SER	PHE	ARG	PHE	PRO	SER	GLY	ASN	GLN	GLY	GLY	ALA	GLY	PRO	SER	SER	GLN	GLY	SER	GLY	GLY	GLY	GLY	THR	GLY
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GLY	SER	VAL	TYR	THR	GLU	ASP	ASN	ASP	ASP	ASP	ASP	LEU	TYR	GLY
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## 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, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	215000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.51	0/5751	0.70	3/7767 (0.0%)
1	B	0.51	0/5751	0.70	3/7767 (0.0%)
1	C	0.51	0/5751	0.70	3/7767 (0.0%)
1	D	0.51	0/5751	0.70	3/7767 (0.0%)
1	E	0.51	0/5751	0.70	3/7767 (0.0%)
1	F	0.51	0/5751	0.70	3/7767 (0.0%)
All	All	0.51	0/34506	0.70	18/46602 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
All	All	0	18

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	THR	N-CA-C	6.01	127.22	111.00
1	F	122	THR	N-CA-C	6.00	127.20	111.00
1	D	122	THR	N-CA-C	6.00	127.19	111.00
1	A	122	THR	N-CA-C	5.99	127.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	THR	N-CA-C	5.99	127.17	111.00
1	B	122	THR	N-CA-C	5.98	127.15	111.00
1	B	303	ILE	CG1-CB-CG2	-5.36	99.62	111.40
1	F	303	ILE	CG1-CB-CG2	-5.35	99.63	111.40
1	C	303	ILE	CG1-CB-CG2	-5.35	99.63	111.40
1	D	303	ILE	CG1-CB-CG2	-5.35	99.64	111.40
1	E	303	ILE	CG1-CB-CG2	-5.34	99.64	111.40
1	A	303	ILE	CG1-CB-CG2	-5.34	99.65	111.40
1	E	140	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	140	LEU	CA-CB-CG	5.32	127.53	115.30
1	F	140	LEU	CA-CB-CG	5.32	127.53	115.30
1	D	140	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	140	LEU	CA-CB-CG	5.31	127.50	115.30
1	B	140	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ARG	Peptide
1	A	225	ARG	Sidechain
1	A	635	ARG	Sidechain
1	B	210	ARG	Peptide
1	B	225	ARG	Sidechain
1	B	635	ARG	Sidechain
1	C	210	ARG	Peptide
1	C	225	ARG	Sidechain
1	C	635	ARG	Sidechain
1	D	210	ARG	Peptide
1	D	225	ARG	Sidechain
1	D	635	ARG	Sidechain
1	E	210	ARG	Peptide
1	E	225	ARG	Sidechain
1	E	635	ARG	Sidechain
1	F	210	ARG	Peptide
1	F	225	ARG	Sidechain
1	F	635	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5659	0	5731	282	0
1	B	5659	0	5731	284	0
1	C	5659	0	5731	281	0
1	D	5659	0	5731	289	0
1	E	5659	0	5731	288	0
1	F	5659	0	5731	286	0
2	A	54	0	24	3	0
2	B	54	0	24	3	0
2	C	54	0	24	3	0
2	D	54	0	24	3	0
2	E	54	0	24	3	0
2	F	54	0	24	3	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
3	E	16	0	0	0	0
3	F	16	0	0	0	0
All	All	34374	0	34530	1630	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 24.

All (1630) 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:87:VAL:HG12	1:B:198:LEU:HD21	1.44	0.99
1:A:87:VAL:HG12	1:A:198:LEU:HD21	1.44	0.99
1:E:87:VAL:HG12	1:E:198:LEU:HD21	1.44	0.98
1:D:87:VAL:HG12	1:D:198:LEU:HD21	1.44	0.97
1:C:87:VAL:HG12	1:C:198:LEU:HD21	1.44	0.96
1:F:87:VAL:HG12	1:F:198:LEU:HD21	1.44	0.96
1:A:286:LEU:HD13	1:A:324:ILE:HD11	1.53	0.91
1:D:286:LEU:HD13	1:D:324:ILE:HD11	1.53	0.91
1:C:286:LEU:HD13	1:C:324:ILE:HD11	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:HD13	1:B:324:ILE:HD11	1.53	0.90
1:F:286:LEU:HD13	1:F:324:ILE:HD11	1.53	0.90
1:E:286:LEU:HD13	1:E:324:ILE:HD11	1.53	0.90
1:E:132:GLU:HA	1:E:136:LYS:HD3	1.56	0.87
1:D:132:GLU:HA	1:D:136:LYS:HD3	1.56	0.87
1:F:132:GLU:HA	1:F:136:LYS:HD3	1.56	0.87
1:D:87:VAL:CG1	1:D:198:LEU:HD21	2.05	0.86
1:B:87:VAL:CG1	1:B:198:LEU:HD21	2.05	0.86
1:C:132:GLU:HA	1:C:136:LYS:HD3	1.56	0.86
1:E:87:VAL:CG1	1:E:198:LEU:HD21	2.05	0.85
1:A:132:GLU:HA	1:A:136:LYS:HD3	1.56	0.85
1:C:87:VAL:CG1	1:C:198:LEU:HD21	2.05	0.85
1:A:87:VAL:CG1	1:A:198:LEU:HD21	2.05	0.85
1:B:132:GLU:HA	1:B:136:LYS:HD3	1.55	0.85
1:F:87:VAL:CG1	1:F:198:LEU:HD21	2.05	0.85
1:B:36:ASN:HA	1:B:85:ASN:HD21	1.44	0.83
1:C:36:ASN:HA	1:C:85:ASN:HD21	1.44	0.82
1:D:297:ALA:HB1	1:D:340:HIS:HB2	1.62	0.82
1:E:297:ALA:HB1	1:E:340:HIS:HB2	1.62	0.82
1:C:297:ALA:HB1	1:C:340:HIS:HB2	1.62	0.82
1:A:290:PHE:CD1	1:A:301:ILE:HD13	2.15	0.81
1:F:290:PHE:CD1	1:F:301:ILE:HD13	2.15	0.81
1:E:290:PHE:CD1	1:E:301:ILE:HD13	2.15	0.81
1:B:297:ALA:HB1	1:B:340:HIS:HB2	1.62	0.81
1:A:36:ASN:HA	1:A:85:ASN:HD21	1.44	0.81
1:E:36:ASN:HA	1:E:85:ASN:HD21	1.44	0.81
1:B:290:PHE:CD1	1:B:301:ILE:HD13	2.15	0.81
1:A:297:ALA:HB1	1:A:340:HIS:HB2	1.62	0.81
1:D:290:PHE:CD1	1:D:301:ILE:HD13	2.15	0.81
1:F:297:ALA:HB1	1:F:340:HIS:HB2	1.62	0.80
1:D:36:ASN:HA	1:D:85:ASN:HD21	1.44	0.80
1:C:290:PHE:CD1	1:C:301:ILE:HD13	2.15	0.80
1:F:36:ASN:HA	1:F:85:ASN:HD21	1.44	0.80
1:B:87:VAL:HG12	1:B:198:LEU:CD2	2.13	0.79
1:A:87:VAL:HG12	1:A:198:LEU:CD2	2.13	0.79
1:F:87:VAL:HG12	1:F:198:LEU:CD2	2.13	0.78
1:F:290:PHE:CD1	1:F:301:ILE:CD1	2.67	0.78
1:E:290:PHE:CD1	1:E:301:ILE:CD1	2.67	0.78
1:D:302:PHE:CE2	1:D:304:ASP:HB3	2.19	0.78
1:E:87:VAL:HG12	1:E:198:LEU:CD2	2.13	0.78
1:D:290:PHE:CD1	1:D:301:ILE:CD1	2.67	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:VAL:HG12	1:D:198:LEU:CD2	2.13	0.78
1:A:290:PHE:CD1	1:A:301:ILE:CD1	2.67	0.78
1:E:302:PHE:CE2	1:E:304:ASP:HB3	2.19	0.78
1:C:302:PHE:CE2	1:C:304:ASP:HB3	2.19	0.77
1:A:302:PHE:CE2	1:A:304:ASP:HB3	2.19	0.77
1:C:87:VAL:HG12	1:C:198:LEU:CD2	2.13	0.77
1:F:302:PHE:CE2	1:F:304:ASP:HB3	2.19	0.77
1:C:290:PHE:CD1	1:C:301:ILE:CD1	2.67	0.77
1:B:290:PHE:CD1	1:B:301:ILE:CD1	2.67	0.77
1:B:302:PHE:CE2	1:B:304:ASP:HB3	2.19	0.77
1:D:53:ARG:NH2	1:D:73:SER:OG	2.22	0.73
1:B:53:ARG:NH2	1:B:73:SER:OG	2.22	0.73
1:C:53:ARG:NH2	1:C:73:SER:OG	2.22	0.73
1:A:53:ARG:NH2	1:A:73:SER:OG	2.22	0.72
1:F:53:ARG:NH2	1:F:73:SER:OG	2.22	0.72
1:F:95:ARG:NH2	1:F:196:GLU:OE2	2.23	0.72
1:B:124:GLU:O	1:B:159:ARG:NH1	2.23	0.72
1:E:53:ARG:NH2	1:E:73:SER:OG	2.22	0.72
1:E:95:ARG:NH2	1:E:196:GLU:OE2	2.23	0.72
1:D:95:ARG:NH2	1:D:196:GLU:OE2	2.23	0.72
1:B:95:ARG:NH2	1:B:196:GLU:OE2	2.23	0.71
1:F:682:PHE:HB3	1:F:686:ASP:HB2	1.73	0.71
1:A:95:ARG:NH2	1:A:196:GLU:OE2	2.23	0.71
1:C:682:PHE:HB3	1:C:686:ASP:HB2	1.73	0.71
1:E:682:PHE:HB3	1:E:686:ASP:HB2	1.73	0.71
1:C:95:ARG:NH2	1:C:196:GLU:OE2	2.23	0.71
1:D:682:PHE:HB3	1:D:686:ASP:HB2	1.73	0.71
1:E:124:GLU:O	1:E:159:ARG:NH1	2.23	0.71
1:A:682:PHE:HB3	1:A:686:ASP:HB2	1.73	0.71
1:B:682:PHE:HB3	1:B:686:ASP:HB2	1.73	0.71
1:B:763:GLN:HG3	1:C:744:ARG:NH2	2.06	0.70
1:A:124:GLU:O	1:A:159:ARG:NH1	2.23	0.70
1:E:763:GLN:HG3	1:F:744:ARG:NH2	2.07	0.70
1:E:650:GLU:OE1	1:E:650:GLU:N	2.24	0.70
1:D:650:GLU:OE1	1:D:650:GLU:N	2.24	0.70
1:C:650:GLU:N	1:C:650:GLU:OE1	2.24	0.70
1:D:124:GLU:O	1:D:159:ARG:NH1	2.23	0.69
1:D:763:GLN:HG3	1:E:744:ARG:NH2	2.07	0.69
1:C:124:GLU:O	1:C:159:ARG:NH1	2.23	0.69
1:A:763:GLN:HG3	1:B:744:ARG:NH2	2.08	0.69
1:D:36:ASN:O	1:D:144:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:763:GLN:HG3	1:D:744:ARG:NH2	2.08	0.69
1:A:744:ARG:NH2	1:F:763:GLN:HG3	2.08	0.69
1:B:650:GLU:OE1	1:B:650:GLU:N	2.24	0.69
1:B:469:VAL:HG22	1:B:540:ILE:HG12	1.75	0.69
1:E:36:ASN:O	1:E:144:ARG:NH1	2.26	0.69
1:A:36:ASN:O	1:A:144:ARG:NH1	2.26	0.69
1:A:469:VAL:HG22	1:A:540:ILE:HG12	1.75	0.68
1:E:91:ASN:OD1	1:E:92:LEU:N	2.27	0.68
1:B:36:ASN:O	1:B:144:ARG:NH1	2.26	0.68
1:F:650:GLU:OE1	1:F:650:GLU:N	2.24	0.68
1:F:36:ASN:O	1:F:144:ARG:NH1	2.26	0.68
1:E:270:ASN:OD1	1:E:273:GLU:HG3	1.94	0.68
1:C:469:VAL:HG22	1:C:540:ILE:HG12	1.75	0.68
1:D:91:ASN:OD1	1:D:92:LEU:N	2.27	0.68
1:E:191:ARG:HH21	1:E:195:GLU:HG3	1.59	0.68
1:E:469:VAL:HG22	1:E:540:ILE:HG12	1.75	0.68
1:A:682:PHE:CD1	1:A:745:ARG:HB3	2.29	0.68
1:B:91:ASN:OD1	1:B:92:LEU:N	2.27	0.68
1:F:91:ASN:OD1	1:F:92:LEU:N	2.27	0.68
1:F:682:PHE:CD1	1:F:745:ARG:HB3	2.29	0.67
1:B:682:PHE:CD1	1:B:745:ARG:HB3	2.29	0.67
1:C:270:ASN:OD1	1:C:273:GLU:HG3	1.94	0.67
1:C:36:ASN:O	1:C:144:ARG:NH1	2.26	0.67
1:C:91:ASN:OD1	1:C:92:LEU:N	2.27	0.67
1:C:682:PHE:CD1	1:C:745:ARG:HB3	2.29	0.67
1:F:469:VAL:HG22	1:F:540:ILE:HG12	1.75	0.67
1:B:270:ASN:OD1	1:B:273:GLU:HG3	1.94	0.67
1:D:682:PHE:CD1	1:D:745:ARG:HB3	2.29	0.67
1:D:469:VAL:HG22	1:D:540:ILE:HG12	1.75	0.67
1:A:91:ASN:OD1	1:A:92:LEU:N	2.27	0.67
1:A:270:ASN:OD1	1:A:273:GLU:HG3	1.94	0.67
1:A:191:ARG:HH21	1:A:195:GLU:HG3	1.59	0.67
1:B:503:PHE:HD1	1:C:699:ILE:HD13	1.59	0.67
1:A:650:GLU:OE1	1:A:650:GLU:N	2.24	0.67
1:B:191:ARG:HH21	1:B:195:GLU:HG3	1.59	0.67
1:F:124:GLU:O	1:F:159:ARG:NH1	2.23	0.67
1:D:270:ASN:OD1	1:D:273:GLU:HG3	1.94	0.67
1:E:682:PHE:CD1	1:E:745:ARG:HB3	2.29	0.67
1:D:191:ARG:HH21	1:D:195:GLU:HG3	1.59	0.66
1:F:270:ASN:OD1	1:F:273:GLU:HG3	1.94	0.66
1:F:191:ARG:HH21	1:F:195:GLU:HG3	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:VAL:HG23	1:D:98:ASP:HB2	1.78	0.66
1:A:94:VAL:HG23	1:A:98:ASP:HB2	1.78	0.66
1:C:191:ARG:HH21	1:C:195:GLU:HG3	1.59	0.66
1:A:649:ASP:O	1:A:653:ARG:N	2.26	0.66
1:F:94:VAL:HG23	1:F:98:ASP:HB2	1.78	0.66
1:E:423:ILE:HG12	1:E:445:LEU:HD11	1.78	0.66
1:C:94:VAL:HG23	1:C:98:ASP:HB2	1.78	0.66
1:E:94:VAL:HG23	1:E:98:ASP:HB2	1.78	0.66
1:D:423:ILE:HG12	1:D:445:LEU:HD11	1.78	0.66
1:E:503:PHE:HD1	1:F:699:ILE:HD13	1.60	0.65
1:F:131:PHE:HD1	1:F:135:LEU:HD22	1.61	0.65
1:F:649:ASP:O	1:F:653:ARG:N	2.26	0.65
1:B:460:ASN:O	1:B:462:SER:N	2.28	0.65
1:B:251:LYS:HE2	1:B:346:ALA:HB1	1.78	0.65
1:B:94:VAL:HG23	1:B:98:ASP:HB2	1.78	0.65
1:A:699:ILE:HD13	1:F:503:PHE:HD1	1.62	0.65
1:B:423:ILE:HG12	1:B:445:LEU:HD11	1.78	0.65
1:D:503:PHE:HD1	1:E:699:ILE:HD13	1.61	0.65
1:E:131:PHE:HD1	1:E:135:LEU:HD22	1.61	0.65
1:F:423:ILE:HG12	1:F:445:LEU:HD11	1.78	0.65
1:E:251:LYS:HE2	1:E:346:ALA:HB1	1.78	0.65
1:F:290:PHE:CD2	1:F:331:LEU:HD13	2.31	0.65
1:A:503:PHE:HD1	1:B:699:ILE:HD13	1.61	0.65
1:B:131:PHE:HD1	1:B:135:LEU:HD22	1.61	0.65
1:C:251:LYS:HE2	1:C:346:ALA:HB1	1.78	0.65
1:D:251:LYS:HE2	1:D:346:ALA:HB1	1.79	0.65
1:A:290:PHE:CD2	1:A:331:LEU:HD13	2.31	0.65
1:E:290:PHE:CD2	1:E:331:LEU:HD13	2.31	0.65
1:A:423:ILE:HG12	1:A:445:LEU:HD11	1.78	0.65
1:D:131:PHE:HD1	1:D:135:LEU:HD22	1.61	0.65
1:E:377:ARG:HD2	1:E:403:THR:HG23	1.79	0.65
1:A:377:ARG:HD2	1:A:403:THR:HG23	1.79	0.65
1:F:377:ARG:HD2	1:F:403:THR:HG23	1.79	0.65
1:D:290:PHE:CD2	1:D:331:LEU:HD13	2.31	0.64
1:C:290:PHE:CD2	1:C:331:LEU:HD13	2.31	0.64
1:C:503:PHE:HD1	1:D:699:ILE:HD13	1.60	0.64
1:D:290:PHE:HD2	1:D:331:LEU:HD13	1.63	0.64
1:C:290:PHE:HD2	1:C:331:LEU:HD13	1.63	0.64
1:B:377:ARG:HD2	1:B:403:THR:HG23	1.79	0.64
1:F:251:LYS:HE2	1:F:346:ALA:HB1	1.78	0.64
1:C:423:ILE:HG12	1:C:445:LEU:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:PHE:CD2	1:B:331:LEU:HD13	2.31	0.64
1:B:290:PHE:HD2	1:B:331:LEU:HD13	1.63	0.64
1:F:90:ASN:O	1:F:93:ARG:NH1	2.28	0.64
1:D:377:ARG:HD2	1:D:403:THR:HG23	1.79	0.64
1:E:290:PHE:HD2	1:E:331:LEU:HD13	1.63	0.64
1:C:377:ARG:HD2	1:C:403:THR:HG23	1.79	0.64
1:D:350:PRO:O	1:D:358:ARG:NH2	2.31	0.64
1:F:350:PRO:O	1:F:358:ARG:NH2	2.31	0.64
1:A:251:LYS:HE2	1:A:346:ALA:HB1	1.78	0.64
1:E:491:GLU:HG2	1:E:495:TYR:CE2	2.33	0.63
1:F:491:GLU:HG2	1:F:495:TYR:CE2	2.33	0.63
1:A:90:ASN:O	1:A:93:ARG:NH1	2.28	0.63
1:A:131:PHE:HD1	1:A:135:LEU:HD22	1.61	0.63
1:B:491:GLU:HG2	1:B:495:TYR:CE2	2.33	0.63
1:A:290:PHE:HD2	1:A:331:LEU:HD13	1.63	0.63
1:C:491:GLU:HG2	1:C:495:TYR:CE2	2.33	0.63
1:D:491:GLU:HG2	1:D:495:TYR:CE2	2.33	0.63
1:C:350:PRO:O	1:C:358:ARG:NH2	2.31	0.63
1:A:350:PRO:O	1:A:358:ARG:NH2	2.31	0.63
1:E:350:PRO:O	1:E:358:ARG:NH2	2.31	0.63
1:C:131:PHE:HD1	1:C:135:LEU:HD22	1.61	0.63
1:B:350:PRO:O	1:B:358:ARG:NH2	2.31	0.63
1:D:649:ASP:O	1:D:653:ARG:N	2.26	0.63
1:F:290:PHE:HD2	1:F:331:LEU:HD13	1.63	0.63
1:A:491:GLU:HG2	1:A:495:TYR:CE2	2.33	0.63
1:F:460:ASN:O	1:F:462:SER:N	2.28	0.62
1:B:90:ASN:O	1:B:93:ARG:NH1	2.28	0.62
1:D:460:ASN:O	1:D:462:SER:N	2.28	0.62
1:C:476:TRP:NE1	1:C:534:GLU:OE1	2.31	0.62
1:E:90:ASN:O	1:E:93:ARG:NH1	2.28	0.62
1:A:460:ASN:O	1:A:462:SER:N	2.28	0.62
1:A:476:TRP:NE1	1:A:534:GLU:OE1	2.31	0.62
1:B:496:PRO:HG3	1:B:503:PHE:HE2	1.65	0.61
1:E:496:PRO:HG3	1:E:503:PHE:HE2	1.65	0.61
1:E:460:ASN:N	1:E:460:ASN:OD1	2.33	0.61
1:D:460:ASN:OD1	1:D:460:ASN:N	2.33	0.61
1:F:496:PRO:HG3	1:F:503:PHE:HE2	1.65	0.61
1:E:460:ASN:O	1:E:462:SER:N	2.28	0.61
1:E:649:ASP:O	1:E:653:ARG:N	2.26	0.61
1:C:649:ASP:O	1:C:653:ARG:N	2.26	0.61
1:A:496:PRO:HG3	1:A:503:PHE:HE2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LYS:HB2	1:C:325:VAL:HG21	1.83	0.61
1:D:312:LYS:HB2	1:D:325:VAL:HG21	1.83	0.61
1:F:476:TRP:NE1	1:F:534:GLU:OE1	2.31	0.61
1:D:496:PRO:HG3	1:D:503:PHE:HE2	1.65	0.61
1:C:496:PRO:HG3	1:C:503:PHE:HE2	1.65	0.61
1:B:460:ASN:OD1	1:B:460:ASN:N	2.33	0.61
1:A:460:ASN:N	1:A:460:ASN:OD1	2.33	0.60
1:C:460:ASN:N	1:C:460:ASN:OD1	2.33	0.60
1:C:460:ASN:O	1:C:462:SER:N	2.28	0.60
1:C:230:PHE:HA	1:C:233:ILE:HG22	1.84	0.60
1:D:310:ALA:HA	1:D:325:VAL:HG12	1.83	0.60
1:B:476:TRP:NE1	1:B:534:GLU:OE1	2.31	0.60
1:B:312:LYS:HB2	1:B:325:VAL:HG21	1.83	0.60
1:D:230:PHE:HA	1:D:233:ILE:HG22	1.84	0.60
1:F:460:ASN:N	1:F:460:ASN:OD1	2.33	0.60
1:E:312:LYS:HB2	1:E:325:VAL:HG21	1.83	0.60
1:E:230:PHE:HA	1:E:233:ILE:HG22	1.84	0.60
1:E:155:ARG:HH12	1:E:386:LYS:HE2	1.67	0.60
1:C:90:ASN:O	1:C:93:ARG:NH1	2.28	0.60
1:D:155:ARG:HH12	1:D:386:LYS:HE2	1.67	0.60
1:D:90:ASN:O	1:D:93:ARG:NH1	2.28	0.60
1:D:526:LEU:HD11	2:D:900:ADP:H2'	1.84	0.60
1:F:155:ARG:HH12	1:F:386:LYS:HE2	1.67	0.60
1:E:476:TRP:NE1	1:E:534:GLU:OE1	2.31	0.60
1:A:310:ALA:HA	1:A:325:VAL:HG12	1.84	0.60
1:E:310:ALA:HA	1:E:325:VAL:HG12	1.83	0.59
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.84	0.59
1:C:526:LEU:HD11	2:C:900:ADP:H2'	1.84	0.59
1:A:312:LYS:HB2	1:A:325:VAL:HG21	1.83	0.59
1:E:526:LEU:HD11	2:E:900:ADP:H2'	1.84	0.59
1:F:310:ALA:HA	1:F:325:VAL:HG12	1.84	0.59
1:C:270:ASN:OD1	1:C:273:GLU:CG	2.51	0.59
1:C:310:ALA:HA	1:C:325:VAL:HG12	1.83	0.59
1:F:312:LYS:HB2	1:F:325:VAL:HG21	1.83	0.59
1:A:762:LEU:HD12	1:A:763:GLN:N	2.18	0.59
1:A:155:ARG:HH12	1:A:386:LYS:HE2	1.67	0.59
1:C:155:ARG:HH12	1:C:386:LYS:HE2	1.67	0.59
1:F:526:LEU:HD11	2:F:900:ADP:H2'	1.84	0.59
1:D:476:TRP:NE1	1:D:534:GLU:OE1	2.31	0.59
1:F:314:GLU:N	1:F:314:GLU:OE1	2.28	0.59
1:F:230:PHE:HA	1:F:233:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:VAL:HB	1:B:733:ARG:HA	1.85	0.59
1:D:270:ASN:OD1	1:D:273:GLU:CG	2.51	0.59
1:B:155:ARG:HH12	1:B:386:LYS:HE2	1.67	0.59
1:E:666:VAL:HA	1:E:731:ILE:HG21	1.85	0.59
1:D:762:LEU:HD12	1:D:763:GLN:N	2.18	0.59
1:E:650:GLU:HA	1:E:653:ARG:HB2	1.85	0.59
1:B:270:ASN:OD1	1:B:273:GLU:CG	2.51	0.59
1:E:222:LEU:HG	1:E:230:PHE:HE1	1.68	0.59
1:B:143:TYR:HD1	1:B:176:VAL:O	1.86	0.59
1:B:526:LEU:HD11	2:B:900:ADP:H2'	1.84	0.59
1:C:143:TYR:HD1	1:C:176:VAL:O	1.86	0.59
1:E:762:LEU:HD12	1:E:763:GLN:N	2.18	0.58
1:B:762:LEU:HD12	1:B:763:GLN:N	2.18	0.58
1:D:650:GLU:HA	1:D:653:ARG:HB2	1.85	0.58
1:B:649:ASP:O	1:B:653:ARG:N	2.26	0.58
1:C:666:VAL:HA	1:C:731:ILE:HG21	1.85	0.58
1:A:222:LEU:HG	1:A:230:PHE:HE1	1.68	0.58
1:D:143:TYR:HD1	1:D:176:VAL:O	1.86	0.58
1:E:670:VAL:HB	1:E:733:ARG:HA	1.85	0.58
1:F:762:LEU:HD12	1:F:763:GLN:N	2.18	0.58
1:B:310:ALA:HA	1:B:325:VAL:HG12	1.83	0.58
1:B:525:THR:HG22	1:B:529:LYS:HE2	1.85	0.58
1:C:60:LYS:HA	1:C:66:GLU:HG3	1.86	0.58
1:A:526:LEU:HD11	2:A:900:ADP:H2'	1.84	0.58
1:A:143:TYR:HD1	1:A:176:VAL:O	1.86	0.58
1:F:513:GLY:HA3	1:F:639:LEU:HA	1.85	0.58
1:C:762:LEU:HD12	1:C:763:GLN:N	2.18	0.58
1:C:650:GLU:HA	1:C:653:ARG:HB2	1.85	0.58
1:F:222:LEU:HG	1:F:230:PHE:HE1	1.68	0.58
1:A:230:PHE:HA	1:A:233:ILE:HG22	1.84	0.58
1:B:250:GLY:O	1:B:254:ILE:HG12	2.04	0.58
1:E:707:ILE:O	1:E:707:ILE:HG22	2.04	0.58
1:A:314:GLU:N	1:A:314:GLU:OE1	2.28	0.58
1:D:513:GLY:HA3	1:D:639:LEU:HA	1.85	0.58
1:C:222:LEU:HG	1:C:230:PHE:HE1	1.68	0.58
1:E:143:TYR:HD1	1:E:176:VAL:O	1.86	0.58
1:F:250:GLY:O	1:F:254:ILE:HG12	2.04	0.58
1:F:143:TYR:HD1	1:F:176:VAL:O	1.86	0.58
1:D:60:LYS:HA	1:D:66:GLU:HG3	1.86	0.58
1:B:666:VAL:HA	1:B:731:ILE:HG21	1.85	0.58
1:A:670:VAL:HB	1:A:733:ARG:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:ARG:HH21	1:D:612:SER:H	1.51	0.58
1:D:707:ILE:O	1:D:707:ILE:HG22	2.04	0.58
1:D:525:THR:HG22	1:D:529:LYS:HE2	1.85	0.58
1:E:513:GLY:HA3	1:E:639:LEU:HA	1.85	0.58
1:F:707:ILE:O	1:F:707:ILE:HG22	2.04	0.58
1:B:650:GLU:HA	1:B:653:ARG:HB2	1.85	0.58
1:F:650:GLU:HA	1:F:653:ARG:HB2	1.85	0.58
1:E:270:ASN:OD1	1:E:273:GLU:CG	2.51	0.58
1:C:420:LEU:O	1:C:424:ARG:HG3	2.03	0.58
1:F:666:VAL:HA	1:F:731:ILE:HG21	1.85	0.58
1:A:707:ILE:O	1:A:707:ILE:HG22	2.04	0.58
1:F:316:THR:O	1:F:322:ARG:NH2	2.37	0.58
1:F:525:THR:HG22	1:F:529:LYS:HE2	1.85	0.58
1:A:525:THR:HG22	1:A:529:LYS:HE2	1.85	0.58
1:C:513:GLY:HA3	1:C:639:LEU:HA	1.85	0.58
1:A:270:ASN:OD1	1:A:273:GLU:CG	2.51	0.58
1:A:250:GLY:O	1:A:254:ILE:HG12	2.04	0.58
1:C:567:ARG:HH21	1:C:612:SER:H	1.51	0.58
1:B:707:ILE:O	1:B:707:ILE:HG22	2.04	0.58
1:C:250:GLY:O	1:C:254:ILE:HG12	2.04	0.58
1:F:670:VAL:HB	1:F:733:ARG:HA	1.85	0.58
1:E:316:THR:O	1:E:322:ARG:NH2	2.37	0.57
1:B:222:LEU:HG	1:B:230:PHE:HE1	1.68	0.57
1:C:670:VAL:HB	1:C:733:ARG:HA	1.85	0.57
1:A:567:ARG:HH21	1:A:612:SER:H	1.51	0.57
1:D:43:GLN:O	1:D:46:MET:HG2	2.04	0.57
1:E:420:LEU:O	1:E:424:ARG:HG3	2.03	0.57
1:F:270:ASN:OD1	1:F:273:GLU:CG	2.51	0.57
1:C:525:THR:HG22	1:C:529:LYS:HE2	1.85	0.57
1:C:575:PHE:CE2	1:C:577:ASP:HB2	2.39	0.57
1:D:575:PHE:CE2	1:D:577:ASP:HB2	2.40	0.57
1:E:567:ARG:HH21	1:E:612:SER:H	1.51	0.57
1:E:575:PHE:CE2	1:E:577:ASP:HB2	2.39	0.57
1:F:43:GLN:O	1:F:46:MET:HG2	2.04	0.57
1:C:707:ILE:HG22	1:C:707:ILE:O	2.04	0.57
1:A:316:THR:O	1:A:322:ARG:NH2	2.37	0.57
1:E:525:THR:HG22	1:E:529:LYS:HE2	1.85	0.57
1:A:43:GLN:O	1:A:46:MET:HG2	2.04	0.57
1:D:222:LEU:HG	1:D:230:PHE:HE1	1.68	0.57
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.45	0.57
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:LEU:O	1:D:424:ARG:HG3	2.03	0.57
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.45	0.57
1:D:670:VAL:HB	1:D:733:ARG:HA	1.85	0.57
1:B:420:LEU:O	1:B:424:ARG:HG3	2.04	0.57
1:D:290:PHE:HD1	1:D:301:ILE:CD1	2.18	0.57
1:B:316:THR:O	1:B:322:ARG:NH2	2.37	0.57
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.45	0.57
1:D:666:VAL:HA	1:D:731:ILE:HG21	1.85	0.57
1:B:60:LYS:HA	1:B:66:GLU:HG3	1.86	0.57
1:F:420:LEU:O	1:F:424:ARG:HG3	2.04	0.57
1:A:650:GLU:HA	1:A:653:ARG:HB2	1.85	0.57
1:A:494:GLN:O	1:A:497:VAL:HG22	2.05	0.57
1:A:319:GLU:HG3	1:A:323:ARG:HG3	1.87	0.57
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.45	0.57
1:E:250:GLY:O	1:E:254:ILE:HG12	2.04	0.57
1:D:250:GLY:O	1:D:254:ILE:HG12	2.04	0.57
1:C:290:PHE:HD1	1:C:301:ILE:CD1	2.18	0.57
1:D:222:LEU:HG	1:D:230:PHE:CE1	2.40	0.57
1:F:567:ARG:HH21	1:F:612:SER:H	1.51	0.57
1:A:420:LEU:O	1:A:424:ARG:HG3	2.04	0.57
1:B:575:PHE:CE2	1:B:577:ASP:HB2	2.39	0.57
1:F:575:PHE:CE2	1:F:577:ASP:HB2	2.40	0.57
1:F:60:LYS:HA	1:F:66:GLU:HG3	1.86	0.57
1:F:494:GLN:O	1:F:497:VAL:HG22	2.05	0.57
1:C:222:LEU:HG	1:C:230:PHE:CE1	2.40	0.57
1:C:43:GLN:O	1:C:46:MET:HG2	2.04	0.57
1:C:145:PRO:HB3	1:C:175:ILE:HD13	1.87	0.57
1:C:314:GLU:N	1:C:314:GLU:OE1	2.28	0.57
1:C:316:THR:O	1:C:322:ARG:NH2	2.37	0.56
1:D:316:THR:O	1:D:322:ARG:NH2	2.37	0.56
1:E:155:ARG:NH1	1:E:386:LYS:HE2	2.20	0.56
1:F:155:ARG:NH1	1:F:386:LYS:HE2	2.20	0.56
1:A:222:LEU:HG	1:A:230:PHE:CE1	2.40	0.56
1:C:752:ILE:O	1:C:756:GLU:N	2.29	0.56
1:B:319:GLU:HG3	1:B:323:ARG:HG3	1.87	0.56
1:E:43:GLN:O	1:E:46:MET:HG2	2.04	0.56
1:A:749:ASP:HA	1:A:752:ILE:HD13	1.87	0.56
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.45	0.56
1:A:60:LYS:HA	1:A:66:GLU:HG3	1.86	0.56
1:A:666:VAL:HA	1:A:731:ILE:HG21	1.85	0.56
1:C:319:GLU:HG3	1:C:323:ARG:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PRO:HB3	1:B:175:ILE:HD13	1.87	0.56
1:B:567:ARG:HH21	1:B:612:SER:H	1.51	0.56
1:D:77:CYS:HB3	1:D:83:ARG:HE	1.70	0.56
1:C:494:GLN:O	1:C:497:VAL:HG22	2.05	0.56
1:B:494:GLN:O	1:B:497:VAL:HG22	2.05	0.56
1:B:222:LEU:HG	1:B:230:PHE:CE1	2.40	0.56
1:F:222:LEU:HG	1:F:230:PHE:CE1	2.40	0.56
1:D:732:ARG:NE	1:D:734:ASP:OD1	2.39	0.56
1:B:749:ASP:HA	1:B:752:ILE:HD13	1.87	0.56
1:F:732:ARG:NE	1:F:734:ASP:OD1	2.39	0.56
1:A:513:GLY:HA3	1:A:639:LEU:HA	1.85	0.56
1:E:314:GLU:N	1:E:314:GLU:OE1	2.28	0.56
1:B:513:GLY:HA3	1:B:639:LEU:HA	1.85	0.56
1:F:319:GLU:HG3	1:F:323:ARG:HG3	1.87	0.56
1:A:575:PHE:CE2	1:A:577:ASP:HB2	2.39	0.56
1:D:749:ASP:HA	1:D:752:ILE:HD13	1.87	0.56
1:E:60:LYS:HA	1:E:66:GLU:HG3	1.86	0.56
1:E:222:LEU:HG	1:E:230:PHE:CE1	2.40	0.56
1:A:732:ARG:NE	1:A:734:ASP:OD1	2.39	0.56
1:A:155:ARG:NH1	1:A:386:LYS:HE2	2.20	0.56
1:D:494:GLN:O	1:D:497:VAL:HG22	2.05	0.56
1:E:661:LEU:HD13	1:E:666:VAL:HG21	1.88	0.56
1:B:43:GLN:O	1:B:46:MET:HG2	2.04	0.56
1:A:145:PRO:HB3	1:A:175:ILE:HD13	1.87	0.56
1:A:466:GLU:OE1	1:A:466:GLU:N	2.39	0.56
1:D:155:ARG:NH1	1:D:386:LYS:HE2	2.20	0.56
1:D:752:ILE:O	1:D:756:GLU:N	2.29	0.56
1:E:732:ARG:NE	1:E:734:ASP:OD1	2.39	0.56
1:F:466:GLU:N	1:F:466:GLU:OE1	2.39	0.56
1:E:752:ILE:O	1:E:756:GLU:N	2.28	0.56
1:C:732:ARG:NE	1:C:734:ASP:OD1	2.39	0.56
1:B:290:PHE:HD1	1:B:301:ILE:CD1	2.18	0.56
1:B:155:ARG:NH1	1:B:386:LYS:HE2	2.20	0.56
1:F:661:LEU:HD13	1:F:666:VAL:HG21	1.88	0.56
1:A:661:LEU:HD13	1:A:666:VAL:HG21	1.88	0.56
1:E:271:GLY:HA3	1:E:308:ALA:HB3	1.88	0.56
1:E:494:GLN:O	1:E:497:VAL:HG22	2.05	0.56
1:D:661:LEU:HD13	1:D:666:VAL:HG21	1.88	0.56
1:F:749:ASP:HA	1:F:752:ILE:HD13	1.87	0.56
1:C:155:ARG:NH1	1:C:386:LYS:HE2	2.20	0.56
1:D:145:PRO:HB3	1:D:175:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:GLU:HG3	1:D:323:ARG:HG3	1.87	0.56
1:B:466:GLU:OE1	1:B:466:GLU:N	2.39	0.56
1:B:661:LEU:HD13	1:B:666:VAL:HG21	1.88	0.55
1:F:75:ASP:OD1	1:F:76:THR:N	2.39	0.55
1:E:503:PHE:HA	1:F:699:ILE:HD13	1.88	0.55
1:C:75:ASP:OD1	1:C:76:THR:N	2.39	0.55
1:B:732:ARG:NE	1:B:734:ASP:OD1	2.39	0.55
1:F:37:SER:OG	1:F:144:ARG:HD2	2.07	0.55
1:E:290:PHE:HD1	1:E:301:ILE:CD1	2.18	0.55
1:A:77:CYS:HB3	1:A:83:ARG:HE	1.70	0.55
1:A:75:ASP:OD1	1:A:76:THR:N	2.39	0.55
1:B:271:GLY:HA3	1:B:308:ALA:HB3	1.88	0.55
1:E:466:GLU:OE1	1:E:466:GLU:N	2.39	0.55
1:A:37:SER:OG	1:A:144:ARG:HD2	2.07	0.55
1:E:37:SER:OG	1:E:144:ARG:HD2	2.07	0.55
1:D:39:VAL:HG12	1:D:84:MET:HB3	1.89	0.55
1:B:77:CYS:HB3	1:B:83:ARG:HE	1.70	0.55
1:B:503:PHE:HA	1:C:699:ILE:HD13	1.87	0.55
1:E:75:ASP:OD1	1:E:76:THR:N	2.39	0.55
1:F:145:PRO:HB3	1:F:175:ILE:HD13	1.87	0.55
1:E:39:VAL:HG12	1:E:84:MET:HB3	1.89	0.55
1:F:39:VAL:HG12	1:F:84:MET:HB3	1.89	0.55
1:C:77:CYS:HB3	1:C:83:ARG:HE	1.70	0.55
1:C:749:ASP:HA	1:C:752:ILE:HD13	1.87	0.55
1:E:145:PRO:HB3	1:E:175:ILE:HD13	1.87	0.55
1:C:466:GLU:N	1:C:466:GLU:OE1	2.39	0.55
1:E:319:GLU:HG3	1:E:323:ARG:HG3	1.87	0.55
1:B:314:GLU:N	1:B:314:GLU:OE1	2.28	0.55
1:E:77:CYS:HB3	1:E:83:ARG:HE	1.70	0.55
1:F:77:CYS:HB3	1:F:83:ARG:HE	1.70	0.55
1:D:75:ASP:OD1	1:D:76:THR:N	2.39	0.55
1:E:749:ASP:HA	1:E:752:ILE:HD13	1.87	0.55
1:B:501:ASP:O	1:B:505:LYS:HG3	2.07	0.55
1:C:501:ASP:O	1:C:505:LYS:HG3	2.07	0.55
1:D:503:PHE:HA	1:E:699:ILE:HD13	1.88	0.55
1:A:501:ASP:O	1:A:505:LYS:HG3	2.07	0.55
1:F:244:TYR:HE1	1:F:366:GLU:HG2	1.72	0.55
1:E:172:PRO:HG2	1:E:173:TYR:CD2	2.42	0.55
1:D:466:GLU:OE1	1:D:466:GLU:N	2.39	0.55
1:C:493:VAL:HG11	1:C:531:ILE:CG1	2.37	0.55
1:A:271:GLY:HA3	1:A:308:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:752:ILE:O	1:F:756:GLU:N	2.29	0.55
1:C:271:GLY:HA3	1:C:308:ALA:HB3	1.88	0.55
1:E:493:VAL:HG11	1:E:531:ILE:CG1	2.37	0.55
1:B:37:SER:OG	1:B:144:ARG:HD2	2.07	0.55
1:B:503:PHE:CE1	1:C:699:ILE:HG21	2.42	0.55
1:C:661:LEU:HD13	1:C:666:VAL:HG21	1.88	0.55
1:B:75:ASP:OD1	1:B:76:THR:N	2.39	0.55
1:F:172:PRO:HG2	1:F:173:TYR:CD2	2.42	0.55
1:B:88:VAL:O	1:B:92:LEU:HD13	2.07	0.54
1:A:88:VAL:O	1:A:92:LEU:HD13	2.07	0.54
1:D:515:LEU:HB3	1:D:642:LEU:HD23	1.89	0.54
1:D:493:VAL:HG11	1:D:531:ILE:CG1	2.37	0.54
1:F:501:ASP:O	1:F:505:LYS:HG3	2.07	0.54
1:D:88:VAL:O	1:D:92:LEU:HD13	2.07	0.54
1:A:699:ILE:HD13	1:F:503:PHE:HA	1.88	0.54
1:C:503:PHE:HA	1:D:699:ILE:HD13	1.88	0.54
1:C:503:PHE:CE1	1:D:699:ILE:HG21	2.43	0.54
1:D:647:LEU:HD21	1:D:747:VAL:HG21	1.90	0.54
1:D:271:GLY:HA3	1:D:308:ALA:HB3	1.88	0.54
1:F:493:VAL:HG11	1:F:531:ILE:CG1	2.37	0.54
1:B:493:VAL:HG11	1:B:531:ILE:CG1	2.37	0.54
1:E:244:TYR:HE1	1:E:366:GLU:HG2	1.72	0.54
1:C:88:VAL:O	1:C:92:LEU:HD13	2.07	0.54
1:A:752:ILE:O	1:A:756:GLU:N	2.29	0.54
1:D:172:PRO:HG2	1:D:173:TYR:CD2	2.42	0.54
1:D:501:ASP:O	1:D:505:LYS:HG3	2.07	0.54
1:F:88:VAL:O	1:F:92:LEU:HD13	2.07	0.54
1:C:39:VAL:HG12	1:C:84:MET:HB3	1.89	0.54
1:C:172:PRO:HG2	1:C:173:TYR:CD2	2.42	0.54
1:A:493:VAL:HG11	1:A:531:ILE:CG1	2.37	0.54
1:D:314:GLU:N	1:D:314:GLU:OE1	2.28	0.54
1:E:88:VAL:O	1:E:92:LEU:HD13	2.07	0.54
1:F:27:ILE:HG13	1:F:99:VAL:HG22	1.90	0.54
1:C:244:TYR:HE1	1:C:366:GLU:HG2	1.72	0.54
1:B:172:PRO:HG2	1:B:173:TYR:CD2	2.42	0.54
1:E:503:PHE:CE1	1:F:699:ILE:HG21	2.43	0.54
1:D:503:PHE:CE1	1:E:699:ILE:HG21	2.43	0.54
1:D:484:ASP:OD1	1:D:485:VAL:N	2.40	0.54
1:A:515:LEU:HB3	1:A:642:LEU:HD23	1.89	0.54
1:B:484:ASP:OD1	1:B:485:VAL:N	2.40	0.54
1:A:39:VAL:HG12	1:A:84:MET:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:515:LEU:HB3	1:F:642:LEU:HD23	1.89	0.54
1:F:647:LEU:HD21	1:F:747:VAL:HG21	1.90	0.54
1:A:244:TYR:HE1	1:A:366:GLU:HG2	1.72	0.54
1:F:484:ASP:OD1	1:F:485:VAL:N	2.40	0.54
1:F:271:GLY:HA3	1:F:308:ALA:HB3	1.88	0.54
1:C:84:MET:HB2	1:C:88:VAL:HG11	1.90	0.54
1:A:503:PHE:CE1	1:B:699:ILE:HG21	2.43	0.54
1:A:172:PRO:HG2	1:A:173:TYR:CD2	2.42	0.54
1:C:515:LEU:HB3	1:C:642:LEU:HD23	1.89	0.54
1:E:27:ILE:HG13	1:E:99:VAL:HG22	1.90	0.54
1:E:501:ASP:O	1:E:505:LYS:HG3	2.07	0.54
1:A:290:PHE:HD1	1:A:301:ILE:CD1	2.18	0.53
1:D:84:MET:HB2	1:D:88:VAL:HG11	1.90	0.53
1:E:515:LEU:HB3	1:E:642:LEU:HD23	1.89	0.53
1:D:37:SER:OG	1:D:144:ARG:HD2	2.07	0.53
1:C:35:ASP:HB2	1:C:144:ARG:HH22	1.74	0.53
1:F:35:ASP:HB2	1:F:144:ARG:HH22	1.73	0.53
1:F:26:LEU:HD23	1:F:82:ILE:HG13	1.91	0.53
1:D:244:TYR:HE1	1:D:366:GLU:HG2	1.72	0.53
1:A:26:LEU:HD23	1:A:82:ILE:HG13	1.91	0.53
1:A:27:ILE:HG13	1:A:99:VAL:HG22	1.90	0.53
1:B:489:LEU:O	1:B:493:VAL:HG12	2.09	0.53
1:C:647:LEU:HD21	1:C:747:VAL:HG21	1.90	0.53
1:E:287:ARG:HB3	1:E:327:GLN:NE2	2.24	0.53
1:F:84:MET:HB2	1:F:88:VAL:HG11	1.90	0.53
1:C:489:LEU:O	1:C:493:VAL:HG12	2.09	0.53
1:A:484:ASP:OD1	1:A:485:VAL:N	2.40	0.53
1:F:287:ARG:HB3	1:F:327:GLN:NE2	2.24	0.53
1:D:287:ARG:HB3	1:D:327:GLN:NE2	2.24	0.53
1:A:406:HIS:HE1	1:A:460:ASN:ND2	2.06	0.53
1:F:406:HIS:HE1	1:F:460:ASN:ND2	2.06	0.53
1:A:489:LEU:O	1:A:493:VAL:HG12	2.09	0.53
1:C:484:ASP:OD1	1:C:485:VAL:N	2.40	0.53
1:E:133:VAL:HG21	1:E:443:ASN:CG	2.29	0.53
1:E:36:ASN:ND2	1:E:153:LEU:O	2.42	0.53
1:C:37:SER:OG	1:C:144:ARG:HD2	2.07	0.53
1:B:39:VAL:HG12	1:B:84:MET:HB3	1.89	0.53
1:A:84:MET:HB2	1:A:88:VAL:HG11	1.90	0.53
1:B:406:HIS:HE1	1:B:460:ASN:ND2	2.06	0.53
1:B:26:LEU:HD23	1:B:82:ILE:HG13	1.91	0.53
1:E:647:LEU:HD21	1:E:747:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:ASP:OD1	1:E:485:VAL:N	2.40	0.53
1:A:647:LEU:HD21	1:A:747:VAL:HG21	1.90	0.53
1:C:287:ARG:HB3	1:C:327:GLN:NE2	2.24	0.53
1:C:649:ASP:N	1:C:652:SER:OG	2.42	0.53
1:B:244:TYR:HE1	1:B:366:GLU:HG2	1.72	0.53
1:A:35:ASP:HB2	1:A:144:ARG:HH22	1.74	0.53
1:C:26:LEU:HD23	1:C:82:ILE:HG13	1.91	0.53
1:B:133:VAL:HG21	1:B:443:ASN:OD1	2.09	0.53
1:B:647:LEU:HD21	1:B:747:VAL:HG21	1.90	0.53
1:A:133:VAL:HG21	1:A:443:ASN:OD1	2.09	0.53
1:B:35:ASP:HB2	1:B:144:ARG:HH22	1.74	0.53
1:C:36:ASN:ND2	1:C:153:LEU:O	2.42	0.53
1:A:287:ARG:HB3	1:A:327:GLN:NE2	2.24	0.53
1:F:489:LEU:O	1:F:493:VAL:HG12	2.09	0.53
1:C:133:VAL:HG21	1:C:443:ASN:OD1	2.09	0.53
1:B:515:LEU:HB3	1:B:642:LEU:HD23	1.89	0.53
1:A:36:ASN:ND2	1:A:153:LEU:O	2.42	0.53
1:D:27:ILE:HG13	1:D:99:VAL:HG22	1.90	0.53
1:E:26:LEU:HD23	1:E:82:ILE:HG13	1.90	0.53
1:D:489:LEU:O	1:D:493:VAL:HG12	2.09	0.53
1:F:246:PRO:HG2	1:F:249:THR:HG21	1.91	0.53
1:D:35:ASP:HB2	1:D:144:ARG:HH22	1.74	0.52
1:C:406:HIS:HE1	1:C:460:ASN:ND2	2.06	0.52
1:E:489:LEU:O	1:E:493:VAL:HG12	2.09	0.52
1:C:246:PRO:HG2	1:C:249:THR:HG21	1.91	0.52
1:D:649:ASP:N	1:D:652:SER:OG	2.42	0.52
1:D:124:GLU:O	1:D:126:ILE:N	2.42	0.52
1:E:84:MET:HB2	1:E:88:VAL:HG11	1.90	0.52
1:F:124:GLU:O	1:F:126:ILE:N	2.42	0.52
1:B:27:ILE:HG13	1:B:99:VAL:HG22	1.90	0.52
1:E:406:HIS:HE1	1:E:460:ASN:ND2	2.06	0.52
1:D:406:HIS:HE1	1:D:460:ASN:ND2	2.06	0.52
1:A:246:PRO:HG2	1:A:249:THR:HG21	1.91	0.52
1:B:246:PRO:HG2	1:B:249:THR:HG21	1.91	0.52
1:E:246:PRO:HG2	1:E:249:THR:HG21	1.91	0.52
1:B:36:ASN:ND2	1:B:153:LEU:O	2.42	0.52
1:C:649:ASP:O	1:C:652:SER:N	2.43	0.52
1:F:25:ARG:HB3	1:F:99:VAL:CG1	2.40	0.52
1:A:699:ILE:HG21	1:F:503:PHE:CE1	2.44	0.52
1:D:110:TYR:CD1	1:D:175:ILE:HB	2.45	0.52
1:E:110:TYR:CD1	1:E:175:ILE:HB	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ARG:NE	1:C:183:HIS:H	2.07	0.52
1:F:133:VAL:HG21	1:F:443:ASN:CG	2.29	0.52
1:C:96:LEU:O	1:C:225:ARG:NH2	2.43	0.52
1:B:649:ASP:O	1:B:652:SER:N	2.43	0.52
1:B:133:VAL:HG21	1:B:443:ASN:CG	2.29	0.52
1:C:133:VAL:HG21	1:C:443:ASN:CG	2.29	0.52
1:D:133:VAL:HG21	1:D:443:ASN:CG	2.29	0.52
1:D:96:LEU:O	1:D:225:ARG:NH2	2.43	0.52
1:D:246:PRO:HG2	1:D:249:THR:HG21	1.91	0.52
1:B:124:GLU:O	1:B:126:ILE:N	2.42	0.52
1:A:124:GLU:O	1:A:126:ILE:N	2.42	0.52
1:C:124:GLU:O	1:C:126:ILE:N	2.43	0.52
1:B:649:ASP:N	1:B:652:SER:OG	2.42	0.52
1:B:84:MET:HB2	1:B:88:VAL:HG11	1.90	0.52
1:D:26:LEU:HD23	1:D:82:ILE:HG13	1.91	0.52
1:C:25:ARG:HB3	1:C:99:VAL:CG1	2.40	0.52
1:C:27:ILE:HG13	1:C:99:VAL:HG22	1.90	0.52
1:E:25:ARG:HB3	1:E:99:VAL:CG1	2.40	0.52
1:F:110:TYR:CD1	1:F:175:ILE:HB	2.45	0.52
1:A:133:VAL:HG21	1:A:443:ASN:CG	2.29	0.52
1:B:96:LEU:O	1:B:225:ARG:NH2	2.43	0.52
1:E:96:LEU:O	1:E:225:ARG:NH2	2.43	0.52
1:D:25:ARG:HB3	1:D:99:VAL:CG1	2.40	0.52
1:A:503:PHE:HA	1:B:699:ILE:HD13	1.90	0.52
1:C:110:TYR:CD1	1:C:175:ILE:HB	2.45	0.52
1:A:113:ARG:NE	1:A:183:HIS:H	2.07	0.52
1:E:124:GLU:O	1:E:126:ILE:N	2.42	0.52
1:E:650:GLU:O	1:E:654:VAL:HG23	2.10	0.52
1:A:25:ARG:HB3	1:A:99:VAL:CG1	2.40	0.52
1:B:460:ASN:C	1:B:462:SER:H	2.13	0.52
1:D:133:VAL:HG21	1:D:443:ASN:OD1	2.09	0.52
1:B:499:HIS:CE1	1:C:703:ILE:HG23	2.45	0.52
1:B:113:ARG:NE	1:B:183:HIS:H	2.07	0.52
1:F:96:LEU:O	1:F:225:ARG:NH2	2.43	0.52
1:A:96:LEU:O	1:A:225:ARG:NH2	2.43	0.52
1:E:35:ASP:HB2	1:E:144:ARG:HH22	1.74	0.52
1:B:287:ARG:HB3	1:B:327:GLN:NE2	2.24	0.52
1:D:649:ASP:O	1:D:652:SER:N	2.43	0.52
1:C:650:GLU:O	1:C:654:VAL:HG23	2.10	0.52
1:A:650:GLU:O	1:A:654:VAL:HG23	2.10	0.52
1:C:482:LEU:HD13	1:C:527:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ASN:ND2	1:D:153:LEU:O	2.42	0.52
1:F:36:ASN:ND2	1:F:153:LEU:O	2.42	0.52
1:E:649:ASP:O	1:E:652:SER:N	2.43	0.52
1:F:649:ASP:O	1:F:652:SER:N	2.43	0.52
1:E:406:HIS:ND1	1:E:410:ASP:HB3	2.26	0.52
1:F:113:ARG:NE	1:F:183:HIS:H	2.07	0.51
1:B:482:LEU:HD13	1:B:527:LEU:HD11	1.92	0.51
1:E:113:ARG:NE	1:E:183:HIS:H	2.07	0.51
1:F:290:PHE:HD1	1:F:301:ILE:CD1	2.18	0.51
1:D:650:GLU:O	1:D:654:VAL:HG23	2.10	0.51
1:A:649:ASP:O	1:A:652:SER:N	2.43	0.51
1:F:406:HIS:ND1	1:F:410:ASP:HB3	2.25	0.51
1:C:460:ASN:C	1:C:462:SER:H	2.13	0.51
1:A:158:MET:N	1:A:387:ASN:O	2.38	0.51
1:F:650:GLU:O	1:F:654:VAL:HG23	2.10	0.51
1:B:25:ARG:HB3	1:B:99:VAL:CG1	2.40	0.51
1:A:110:TYR:CD1	1:A:175:ILE:HB	2.45	0.51
1:A:515:LEU:HB3	1:A:642:LEU:CD2	2.40	0.51
1:E:133:VAL:HG21	1:E:443:ASN:OD1	2.09	0.51
1:D:113:ARG:NE	1:D:183:HIS:H	2.07	0.51
1:E:649:ASP:N	1:E:652:SER:OG	2.42	0.51
1:B:506:PHE:O	1:C:664:SER:HB3	2.10	0.51
1:B:28:VAL:HG21	1:B:94:VAL:HG21	1.92	0.51
1:D:406:HIS:ND1	1:D:410:ASP:HB3	2.25	0.51
1:B:650:GLU:O	1:B:654:VAL:HG23	2.10	0.51
1:C:28:VAL:HG21	1:C:94:VAL:HG21	1.92	0.51
1:D:503:PHE:CD1	1:E:699:ILE:HG21	2.46	0.51
1:B:110:TYR:CD1	1:B:175:ILE:HB	2.45	0.51
1:B:515:LEU:HB3	1:B:642:LEU:CD2	2.40	0.51
1:F:133:VAL:HG21	1:F:443:ASN:OD1	2.09	0.51
1:D:158:MET:N	1:D:387:ASN:O	2.38	0.51
1:A:649:ASP:N	1:A:652:SER:OG	2.42	0.51
1:D:460:ASN:C	1:D:462:SER:H	2.13	0.51
1:D:515:LEU:HB3	1:D:642:LEU:CD2	2.40	0.51
1:C:515:LEU:HB3	1:C:642:LEU:CD2	2.40	0.51
1:C:303:ILE:HG22	1:C:303:ILE:O	2.11	0.51
1:E:303:ILE:O	1:E:303:ILE:HG22	2.11	0.51
1:D:482:LEU:HD13	1:D:527:LEU:HD11	1.92	0.51
1:B:752:ILE:O	1:B:756:GLU:N	2.29	0.51
1:A:517:TYR:HE1	1:A:642:LEU:HB3	1.76	0.51
1:F:515:LEU:HB3	1:F:642:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:499:HIS:CE1	1:F:703:ILE:HG23	2.46	0.51
1:B:140:LEU:HG	1:B:141:GLU:OE1	2.11	0.51
1:E:158:MET:N	1:E:387:ASN:O	2.38	0.51
1:F:28:VAL:HG21	1:F:94:VAL:HG21	1.92	0.51
1:A:406:HIS:ND1	1:A:410:ASP:HB3	2.26	0.51
1:A:140:LEU:HG	1:A:141:GLU:OE1	2.11	0.51
1:F:140:LEU:HG	1:F:141:GLU:OE1	2.11	0.51
1:B:303:ILE:HG22	1:B:303:ILE:O	2.11	0.51
1:D:303:ILE:O	1:D:303:ILE:HG22	2.11	0.51
1:F:158:MET:N	1:F:387:ASN:O	2.38	0.51
1:A:699:ILE:HG13	1:F:506:PHE:CD2	2.46	0.51
1:C:406:HIS:ND1	1:C:410:ASP:HB3	2.26	0.51
1:E:140:LEU:HG	1:E:141:GLU:OE1	2.11	0.51
1:F:649:ASP:N	1:F:652:SER:OG	2.42	0.50
1:B:503:PHE:CD1	1:C:699:ILE:HG21	2.45	0.50
1:C:503:PHE:CD1	1:D:699:ILE:HG21	2.46	0.50
1:A:482:LEU:HD13	1:A:527:LEU:HD11	1.92	0.50
1:E:482:LEU:HD13	1:E:527:LEU:HD11	1.92	0.50
1:A:303:ILE:HG22	1:A:303:ILE:O	2.11	0.50
1:A:28:VAL:HG21	1:A:94:VAL:HG21	1.92	0.50
1:E:503:PHE:CD1	1:F:699:ILE:HG21	2.46	0.50
1:D:506:PHE:O	1:E:664:SER:HB3	2.11	0.50
1:F:517:TYR:HE1	1:F:642:LEU:HB3	1.76	0.50
1:C:122:THR:N	1:C:123:VAL:HB	2.27	0.50
1:B:359:ARG:NH2	2:C:807:ADP:O1A	2.44	0.50
1:C:359:ARG:NH2	2:D:807:ADP:O1A	2.44	0.50
1:D:359:ARG:NH2	2:E:807:ADP:O1A	2.44	0.50
1:B:406:HIS:ND1	1:B:410:ASP:HB3	2.26	0.50
1:A:326:SER:O	1:A:328:LEU:N	2.44	0.50
1:F:482:LEU:HD13	1:F:527:LEU:HD11	1.92	0.50
1:E:359:ARG:NH2	2:F:807:ADP:O1A	2.44	0.50
1:C:635:ARG:NH1	1:D:578:GLU:OE2	2.45	0.50
1:E:506:PHE:O	1:F:664:SER:HB3	2.11	0.50
1:E:391:ALA:HB3	1:E:448:THR:HA	1.94	0.50
1:F:632:ALA:HA	1:F:635:ARG:NE	2.27	0.50
1:E:28:VAL:HG21	1:E:94:VAL:HG21	1.92	0.50
1:E:515:LEU:HB3	1:E:642:LEU:CD2	2.40	0.50
1:C:499:HIS:CE1	1:D:703:ILE:HG23	2.47	0.50
1:B:122:THR:N	1:B:123:VAL:HB	2.27	0.50
1:D:499:HIS:CE1	1:E:703:ILE:HG23	2.46	0.50
1:A:632:ALA:HA	1:A:635:ARG:NE	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:ARG:NH1	1:C:578:GLU:OE2	2.45	0.50
1:F:122:THR:N	1:F:123:VAL:HB	2.26	0.50
1:B:290:PHE:CD1	1:B:301:ILE:HD12	2.47	0.50
1:A:371:ILE:HD11	1:A:466:GLU:OE2	2.12	0.50
1:B:371:ILE:HD11	1:B:466:GLU:OE2	2.12	0.50
1:B:517:TYR:HE1	1:B:642:LEU:HB3	1.76	0.50
1:E:632:ALA:HA	1:E:635:ARG:NE	2.27	0.50
1:A:468:VAL:HG22	1:A:470:GLU:OE1	2.12	0.50
1:A:503:PHE:CD1	1:B:699:ILE:HG21	2.47	0.50
1:D:185:GLU:HB3	1:D:187:GLU:OE1	2.12	0.50
1:D:122:THR:N	1:D:123:VAL:HB	2.26	0.50
1:D:140:LEU:HG	1:D:141:GLU:OE1	2.11	0.50
1:B:468:VAL:HG22	1:B:470:GLU:OE1	2.12	0.50
1:B:326:SER:O	1:B:328:LEU:N	2.44	0.49
1:C:158:MET:N	1:C:387:ASN:O	2.38	0.49
1:C:468:VAL:HG22	1:C:470:GLU:OE1	2.12	0.49
1:A:699:ILE:HG21	1:F:503:PHE:CD1	2.47	0.49
1:C:749:ASP:HA	1:C:752:ILE:CD1	2.43	0.49
1:F:185:GLU:HB3	1:F:187:GLU:OE1	2.12	0.49
1:C:140:LEU:HG	1:C:141:GLU:OE1	2.11	0.49
1:E:122:THR:N	1:E:123:VAL:HB	2.27	0.49
1:F:303:ILE:O	1:F:303:ILE:HG22	2.11	0.49
1:A:290:PHE:CD1	1:A:301:ILE:HD12	2.47	0.49
1:D:28:VAL:HG21	1:D:94:VAL:HG21	1.92	0.49
1:E:460:ASN:C	1:E:462:SER:H	2.13	0.49
1:C:506:PHE:O	1:D:664:SER:HB3	2.11	0.49
1:E:749:ASP:HA	1:E:752:ILE:CD1	2.42	0.49
1:E:185:GLU:HB3	1:E:187:GLU:OE1	2.12	0.49
2:A:807:ADP:O1A	1:F:359:ARG:NH2	2.45	0.49
1:F:170:PRO:HG2	1:F:174:CYS:SG	2.52	0.49
1:C:170:PRO:HG2	1:C:174:CYS:SG	2.52	0.49
1:F:287:ARG:HB3	1:F:327:GLN:HE21	1.77	0.49
1:C:290:PHE:CD1	1:C:301:ILE:HD12	2.47	0.49
1:B:749:ASP:HA	1:B:752:ILE:CD1	2.43	0.49
1:A:635:ARG:NH1	1:B:578:GLU:OE2	2.45	0.49
1:F:468:VAL:HG22	1:F:470:GLU:OE1	2.12	0.49
1:D:749:ASP:HA	1:D:752:ILE:CD1	2.42	0.49
1:F:371:ILE:HD11	1:F:466:GLU:OE2	2.12	0.49
1:E:517:TYR:HE1	1:E:642:LEU:HB3	1.76	0.49
1:D:632:ALA:HA	1:D:635:ARG:NE	2.27	0.49
1:C:259:ALA:HB1	1:C:266:PHE:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:ALA:HB1	1:E:266:PHE:HB2	1.95	0.49
1:A:749:ASP:HA	1:A:752:ILE:CD1	2.43	0.49
1:B:632:ALA:HA	1:B:635:ARG:NE	2.27	0.49
1:B:391:ALA:HB3	1:B:448:THR:HA	1.94	0.49
1:F:391:ALA:HB3	1:F:448:THR:HA	1.94	0.49
1:A:751:ASP:O	1:A:755:TYR:N	2.35	0.49
1:D:170:PRO:HG2	1:D:174:CYS:SG	2.52	0.49
1:D:287:ARG:HB3	1:D:327:GLN:HE21	1.77	0.49
1:E:371:ILE:HD11	1:E:466:GLU:OE2	2.12	0.49
1:B:185:GLU:HB3	1:B:187:GLU:OE1	2.12	0.49
1:E:635:ARG:NH1	1:F:578:GLU:OE2	2.45	0.49
1:D:635:ARG:NH1	1:E:578:GLU:OE2	2.45	0.49
1:A:391:ALA:HB3	1:A:448:THR:HA	1.94	0.49
1:C:326:SER:O	1:C:328:LEU:N	2.44	0.49
1:D:468:VAL:HG22	1:D:470:GLU:OE1	2.12	0.49
1:A:506:PHE:O	1:B:664:SER:HB3	2.12	0.49
1:F:749:ASP:HA	1:F:752:ILE:CD1	2.43	0.49
1:D:371:ILE:HD11	1:D:466:GLU:OE2	2.12	0.49
1:C:185:GLU:HB3	1:C:187:GLU:OE1	2.12	0.49
1:A:185:GLU:HB3	1:A:187:GLU:OE1	2.12	0.49
1:F:644:TYR:CE2	1:F:646:PRO:HB3	2.48	0.49
1:A:122:THR:N	1:A:123:VAL:HB	2.26	0.49
1:D:259:ALA:HB1	1:D:266:PHE:HB2	1.95	0.49
1:A:398:GLN:HA	1:A:401:ASN:OD1	2.13	0.49
1:F:290:PHE:CD1	1:F:301:ILE:HD12	2.46	0.49
1:C:287:ARG:HB3	1:C:327:GLN:HE21	1.77	0.49
1:C:371:ILE:HD11	1:C:466:GLU:OE2	2.12	0.49
1:E:644:TYR:CE2	1:E:646:PRO:HB3	2.48	0.49
1:E:468:VAL:HG22	1:E:470:GLU:OE1	2.12	0.49
1:A:170:PRO:HG2	1:A:174:CYS:SG	2.52	0.49
1:A:644:TYR:CE2	1:A:646:PRO:HB3	2.48	0.49
1:E:398:GLN:HA	1:E:401:ASN:OD1	2.13	0.49
1:E:287:ARG:HB3	1:E:327:GLN:HE21	1.77	0.49
1:F:503:PHE:CE2	1:F:510:PRO:HB3	2.48	0.49
1:E:244:TYR:CE1	1:E:366:GLU:HG2	2.48	0.49
1:C:517:TYR:HE1	1:C:642:LEU:HB3	1.76	0.49
1:C:632:ALA:HA	1:C:635:ARG:NE	2.27	0.49
1:D:644:TYR:CE2	1:D:646:PRO:HB3	2.48	0.49
1:C:391:ALA:HB3	1:C:448:THR:HA	1.94	0.49
1:D:751:ASP:O	1:D:755:TYR:N	2.35	0.49
1:E:170:PRO:HG2	1:E:174:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLU:HA	1:B:295:LYS:NZ	2.28	0.49
1:F:326:SER:O	1:F:328:LEU:N	2.44	0.49
1:A:664:SER:HB3	1:F:506:PHE:O	2.12	0.49
1:D:506:PHE:CD2	1:E:699:ILE:HG13	2.48	0.49
1:F:259:ALA:HB1	1:F:266:PHE:HB2	1.95	0.49
1:A:499:HIS:CE1	1:B:703:ILE:HG23	2.47	0.49
1:B:259:ALA:HB1	1:B:266:PHE:HB2	1.95	0.49
1:A:292:GLU:HA	1:A:295:LYS:NZ	2.28	0.49
1:A:287:ARG:HB3	1:A:327:GLN:HE21	1.77	0.48
1:B:287:ARG:HB3	1:B:327:GLN:HE21	1.77	0.48
1:A:113:ARG:CZ	1:A:182:ILE:HG13	2.43	0.48
1:C:398:GLN:HA	1:C:401:ASN:OD1	2.13	0.48
1:D:57:VAL:O	1:D:68:VAL:HA	2.13	0.48
1:D:391:ALA:HB3	1:D:448:THR:HA	1.94	0.48
1:E:57:VAL:O	1:E:68:VAL:HA	2.13	0.48
1:B:57:VAL:O	1:B:68:VAL:HA	2.13	0.48
1:E:43:GLN:OE1	1:E:43:GLN:N	2.43	0.48
1:F:244:TYR:CE1	1:F:366:GLU:HG2	2.48	0.48
1:D:517:TYR:HE1	1:D:642:LEU:HB3	1.76	0.48
1:D:244:TYR:CE1	1:D:366:GLU:HG2	2.48	0.48
1:D:113:ARG:CZ	1:D:182:ILE:HG13	2.43	0.48
1:A:578:GLU:OE2	1:F:635:ARG:NH1	2.45	0.48
1:A:506:PHE:CD2	1:B:699:ILE:HG13	2.49	0.48
1:B:113:ARG:CZ	1:B:182:ILE:HG13	2.43	0.48
1:B:398:GLN:HA	1:B:401:ASN:OD1	2.13	0.48
1:A:259:ALA:HB1	1:A:266:PHE:HB2	1.95	0.48
1:E:506:PHE:CD2	1:F:699:ILE:HG13	2.48	0.48
1:E:503:PHE:CE2	1:E:510:PRO:HB3	2.48	0.48
1:A:503:PHE:CE2	1:A:510:PRO:HB3	2.48	0.48
1:C:503:PHE:CE2	1:C:510:PRO:HB3	2.48	0.48
1:C:244:TYR:CE1	1:C:366:GLU:HG2	2.48	0.48
1:A:359:ARG:NH2	2:B:807:ADP:O1A	2.46	0.48
1:B:170:PRO:HG2	1:B:174:CYS:SG	2.52	0.48
1:D:326:SER:O	1:D:328:LEU:N	2.44	0.48
1:F:172:PRO:HG2	1:F:173:TYR:HD2	1.78	0.48
1:C:115:HIS:HE1	1:C:185:GLU:HG3	1.79	0.48
1:B:644:TYR:CE2	1:B:646:PRO:HB3	2.48	0.48
1:B:503:PHE:CE2	1:B:510:PRO:HB3	2.48	0.48
1:F:115:HIS:HE1	1:F:185:GLU:HG3	1.79	0.48
1:F:113:ARG:CZ	1:F:182:ILE:HG13	2.43	0.48
1:D:292:GLU:HA	1:D:295:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:ASP:HB2	1:F:144:ARG:NH2	2.29	0.48
1:A:686:ASP:O	1:A:689:GLU:HB3	2.14	0.48
1:B:686:ASP:O	1:B:689:GLU:HB3	2.14	0.48
1:C:501:ASP:OD1	1:C:501:ASP:N	2.47	0.48
1:E:115:HIS:HE1	1:E:185:GLU:HG3	1.78	0.48
1:C:644:TYR:CE2	1:C:646:PRO:HB3	2.48	0.48
1:F:292:GLU:HA	1:F:295:LYS:NZ	2.28	0.48
1:A:703:ILE:HG23	1:F:499:HIS:CE1	2.47	0.48
1:A:478:ASP:OD1	1:A:662:ARG:NH2	2.47	0.48
1:A:35:ASP:HB2	1:A:144:ARG:NH2	2.29	0.48
1:D:503:PHE:CE2	1:D:510:PRO:HB3	2.48	0.48
1:F:460:ASN:C	1:F:462:SER:H	2.13	0.48
1:C:506:PHE:CD2	1:D:699:ILE:HG13	2.48	0.48
1:A:172:PRO:HG2	1:A:173:TYR:HD2	1.78	0.48
1:B:244:TYR:CE1	1:B:366:GLU:HG2	2.48	0.48
1:A:115:HIS:HE1	1:A:185:GLU:HG3	1.79	0.48
1:D:115:HIS:HE1	1:D:185:GLU:HG3	1.78	0.48
1:C:478:ASP:OD1	1:C:662:ARG:NH2	2.47	0.48
1:E:292:GLU:HA	1:E:295:LYS:NZ	2.28	0.48
1:E:35:ASP:HB2	1:E:144:ARG:NH2	2.29	0.48
1:D:290:PHE:CD1	1:D:301:ILE:HD12	2.46	0.48
1:E:686:ASP:O	1:E:689:GLU:HB3	2.14	0.48
1:F:635:ARG:O	1:F:638:ARG:HB2	2.14	0.48
1:E:635:ARG:O	1:E:638:ARG:HB2	2.14	0.48
1:D:398:GLN:HA	1:D:401:ASN:OD1	2.13	0.48
1:E:290:PHE:CD1	1:E:301:ILE:HD12	2.47	0.48
1:D:615:LYS:O	1:D:616:ASN:HB2	2.14	0.48
1:E:172:PRO:HG2	1:E:173:TYR:HD2	1.78	0.48
1:E:113:ARG:CZ	1:E:182:ILE:HG13	2.43	0.48
1:A:635:ARG:O	1:A:638:ARG:HB2	2.14	0.48
1:F:57:VAL:O	1:F:68:VAL:HA	2.13	0.48
1:F:398:GLN:HA	1:F:401:ASN:OD1	2.13	0.48
1:B:35:ASP:HB2	1:B:144:ARG:NH2	2.29	0.47
1:F:686:ASP:O	1:F:689:GLU:HB3	2.14	0.47
1:B:501:ASP:N	1:B:501:ASP:OD1	2.47	0.47
1:C:292:GLU:HA	1:C:295:LYS:NZ	2.28	0.47
1:D:35:ASP:HB2	1:D:144:ARG:NH2	2.29	0.47
1:C:113:ARG:CZ	1:C:182:ILE:HG13	2.43	0.47
1:C:57:VAL:O	1:C:68:VAL:HA	2.13	0.47
1:B:506:PHE:CD2	1:C:699:ILE:HG13	2.49	0.47
1:B:172:PRO:HG2	1:B:173:TYR:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:ASP:OD1	1:D:662:ARG:NH2	2.47	0.47
1:E:478:ASP:OD1	1:E:662:ARG:NH2	2.47	0.47
1:A:244:TYR:CE1	1:A:366:GLU:HG2	2.48	0.47
1:B:635:ARG:O	1:B:638:ARG:HB2	2.14	0.47
1:D:635:ARG:O	1:D:638:ARG:HB2	2.14	0.47
1:D:321:GLU:O	1:D:324:ILE:HG22	2.15	0.47
1:E:326:SER:O	1:E:328:LEU:N	2.44	0.47
1:C:686:ASP:O	1:C:689:GLU:HB3	2.14	0.47
1:E:615:LYS:O	1:E:616:ASN:HB2	2.14	0.47
1:A:732:ARG:HE	1:A:734:ASP:CG	2.18	0.47
1:E:732:ARG:HE	1:E:734:ASP:CG	2.18	0.47
1:C:732:ARG:HE	1:C:734:ASP:CG	2.18	0.47
1:D:501:ASP:N	1:D:501:ASP:OD1	2.47	0.47
1:B:115:HIS:HE1	1:B:185:GLU:HG3	1.79	0.47
1:F:449:MET:HG3	1:F:453:ARG:NE	2.30	0.47
1:A:449:MET:HG3	1:A:453:ARG:NE	2.30	0.47
1:A:321:GLU:O	1:A:324:ILE:HG22	2.15	0.47
1:D:698:ALA:HB2	1:D:731:ILE:HD12	1.96	0.47
1:D:172:PRO:HG2	1:D:173:TYR:HD2	1.78	0.47
1:E:751:ASP:O	1:E:755:TYR:N	2.35	0.47
1:A:57:VAL:O	1:A:68:VAL:HA	2.13	0.47
1:B:478:ASP:OD1	1:B:662:ARG:NH2	2.47	0.47
1:D:327:GLN:HA	1:D:330:THR:OG1	2.15	0.47
1:C:327:GLN:HA	1:C:330:THR:OG1	2.15	0.47
1:D:686:ASP:O	1:D:689:GLU:HB3	2.14	0.47
1:B:503:PHE:CD1	1:C:699:ILE:HD13	2.45	0.47
1:D:525:THR:HB	2:D:900:ADP:O1A	2.15	0.47
1:C:525:THR:HB	2:C:900:ADP:O1A	2.15	0.47
1:C:615:LYS:O	1:C:616:ASN:HB2	2.14	0.47
1:A:698:ALA:HB2	1:A:731:ILE:HD12	1.96	0.47
1:D:635:ARG:H	1:D:635:ARG:HG3	1.54	0.47
1:C:705:SER:HA	1:C:706:GLU:HA	1.67	0.47
1:B:449:MET:HG3	1:B:453:ARG:NE	2.30	0.47
1:A:556:GLU:OE1	1:A:556:GLU:N	2.48	0.47
1:E:744:ARG:HD3	1:E:745:ARG:H	1.80	0.47
1:A:615:LYS:O	1:A:616:ASN:HB2	2.14	0.47
1:F:732:ARG:HE	1:F:734:ASP:CG	2.18	0.47
1:D:396:LEU:HA	1:D:399:VAL:HB	1.97	0.47
1:D:117:LEU:HA	1:D:118:PRO:HD3	1.78	0.47
1:D:572:CYS:SG	1:D:617:VAL:HG22	2.55	0.47
1:F:512:LYS:HD3	1:F:512:LYS:HA	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:PHE:CD1	1:D:699:ILE:HD13	2.46	0.47
1:C:312:LYS:HD2	1:C:313:ARG:H	1.80	0.47
1:E:501:ASP:N	1:E:501:ASP:OD1	2.47	0.47
1:E:396:LEU:HA	1:E:399:VAL:HB	1.97	0.47
1:F:478:ASP:OD1	1:F:662:ARG:NH2	2.47	0.47
1:D:626:PRO:HB2	1:D:758:PHE:CZ	2.50	0.47
1:C:744:ARG:HD3	1:C:745:ARG:H	1.80	0.47
1:C:762:LEU:HD12	1:C:763:GLN:CA	2.45	0.47
1:B:77:CYS:CB	1:B:83:ARG:HE	2.28	0.47
1:D:312:LYS:HD2	1:D:313:ARG:H	1.80	0.47
1:A:525:THR:HB	2:A:900:ADP:O1A	2.15	0.47
1:B:244:TYR:OH	1:B:568:GLN:HG2	2.15	0.47
1:C:572:CYS:SG	1:C:617:VAL:HG22	2.55	0.47
1:E:449:MET:HG3	1:E:453:ARG:NE	2.30	0.47
1:A:626:PRO:HB2	1:A:758:PHE:CZ	2.50	0.47
1:D:556:GLU:OE1	1:D:556:GLU:N	2.48	0.47
1:D:449:MET:HG3	1:D:453:ARG:NE	2.30	0.47
1:C:321:GLU:O	1:C:324:ILE:HG22	2.15	0.46
1:B:321:GLU:O	1:B:324:ILE:HG22	2.15	0.46
1:C:77:CYS:CB	1:C:83:ARG:HE	2.28	0.46
1:B:698:ALA:HB2	1:B:731:ILE:HD12	1.96	0.46
1:F:615:LYS:O	1:F:616:ASN:HB2	2.14	0.46
1:E:556:GLU:OE1	1:E:556:GLU:N	2.48	0.46
1:B:556:GLU:N	1:B:556:GLU:OE1	2.48	0.46
1:E:327:GLN:HA	1:E:330:THR:OG1	2.15	0.46
1:D:327:GLN:O	1:D:331:LEU:HG	2.15	0.46
1:F:77:CYS:CB	1:F:83:ARG:HE	2.28	0.46
1:A:77:CYS:CB	1:A:83:ARG:HE	2.28	0.46
1:A:312:LYS:HD2	1:A:313:ARG:H	1.80	0.46
1:E:698:ALA:HB2	1:E:731:ILE:HD12	1.96	0.46
1:B:615:LYS:O	1:B:616:ASN:HB2	2.14	0.46
1:B:732:ARG:HE	1:B:734:ASP:CG	2.18	0.46
1:B:572:CYS:SG	1:B:617:VAL:HG22	2.55	0.46
1:C:626:PRO:HB2	1:C:758:PHE:CZ	2.50	0.46
1:F:321:GLU:O	1:F:324:ILE:HG22	2.15	0.46
1:D:77:CYS:CB	1:D:83:ARG:HE	2.28	0.46
1:C:403:THR:O	1:C:406:HIS:CD2	2.69	0.46
1:F:396:LEU:HA	1:F:399:VAL:HB	1.97	0.46
1:C:556:GLU:N	1:C:556:GLU:OE1	2.48	0.46
1:D:403:THR:O	1:D:406:HIS:CD2	2.69	0.46
1:A:155:ARG:HH12	1:A:386:LYS:CE	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:THR:HB	2:F:900:ADP:O1A	2.15	0.46
1:C:698:ALA:HB2	1:C:731:ILE:HD12	1.96	0.46
1:A:43:GLN:N	1:A:43:GLN:OE1	2.43	0.46
1:D:732:ARG:HE	1:D:734:ASP:CG	2.18	0.46
1:C:635:ARG:O	1:C:638:ARG:HB2	2.14	0.46
1:F:556:GLU:N	1:F:556:GLU:OE1	2.48	0.46
1:C:35:ASP:HB2	1:C:144:ARG:NH2	2.29	0.46
1:E:77:CYS:CB	1:E:83:ARG:HE	2.28	0.46
1:E:525:THR:HB	2:E:900:ADP:O1A	2.15	0.46
1:C:244:TYR:OH	1:C:568:GLN:HG2	2.16	0.46
1:A:705:SER:HA	1:A:706:GLU:HA	1.67	0.46
1:F:626:PRO:HB2	1:F:758:PHE:CZ	2.50	0.46
1:C:449:MET:HG3	1:C:453:ARG:NE	2.30	0.46
1:C:327:GLN:O	1:C:331:LEU:HG	2.16	0.46
1:F:762:LEU:HD12	1:F:763:GLN:CA	2.45	0.46
1:B:403:THR:O	1:B:406:HIS:CD2	2.69	0.46
1:F:155:ARG:HH12	1:F:386:LYS:CE	2.28	0.46
1:B:155:ARG:HH12	1:B:386:LYS:CE	2.28	0.46
1:E:626:PRO:HB2	1:E:758:PHE:CZ	2.50	0.46
1:E:321:GLU:O	1:E:324:ILE:HG22	2.15	0.46
1:F:327:GLN:O	1:F:331:LEU:HG	2.16	0.46
1:A:403:THR:O	1:A:406:HIS:CD2	2.69	0.46
1:A:460:ASN:C	1:A:462:SER:H	2.13	0.46
1:E:155:ARG:HH12	1:E:386:LYS:CE	2.28	0.46
1:C:172:PRO:HG2	1:C:173:TYR:HD2	1.78	0.46
1:F:572:CYS:SG	1:F:617:VAL:HG22	2.55	0.46
1:E:572:CYS:SG	1:E:617:VAL:HG22	2.55	0.46
1:A:327:GLN:O	1:A:331:LEU:HG	2.15	0.46
1:F:327:GLN:HA	1:F:330:THR:OG1	2.15	0.46
1:B:327:GLN:O	1:B:331:LEU:HG	2.15	0.46
1:E:762:LEU:HD12	1:E:763:GLN:CA	2.45	0.46
1:A:762:LEU:HD12	1:A:763:GLN:CA	2.45	0.46
1:B:496:PRO:HG3	1:B:503:PHE:CE2	2.50	0.46
1:D:155:ARG:HH12	1:D:386:LYS:CE	2.28	0.46
1:F:244:TYR:OH	1:F:568:GLN:HG2	2.15	0.46
1:B:626:PRO:HB2	1:B:758:PHE:CZ	2.50	0.46
1:A:699:ILE:HD13	1:F:503:PHE:CD1	2.48	0.46
1:A:503:PHE:CD1	1:B:699:ILE:HD13	2.47	0.46
1:E:403:THR:O	1:E:406:HIS:CD2	2.69	0.46
1:B:312:LYS:HD2	1:B:313:ARG:H	1.80	0.46
1:F:501:ASP:OD1	1:F:501:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:TYR:OH	1:E:568:GLN:HG2	2.16	0.46
1:D:244:TYR:OH	1:D:568:GLN:HG2	2.16	0.46
1:F:113:ARG:CZ	1:F:183:HIS:H	2.29	0.46
1:D:512:LYS:HD3	1:D:512:LYS:HA	1.68	0.46
1:B:327:GLN:HA	1:B:330:THR:OG1	2.15	0.46
1:D:762:LEU:HD12	1:D:763:GLN:CA	2.45	0.46
1:B:744:ARG:HD3	1:B:745:ARG:H	1.80	0.46
1:F:312:LYS:HD2	1:F:313:ARG:H	1.80	0.46
1:C:155:ARG:HH12	1:C:386:LYS:CE	2.28	0.46
1:A:113:ARG:CZ	1:A:183:HIS:H	2.29	0.46
1:C:396:LEU:HA	1:C:399:VAL:HB	1.97	0.46
1:B:229:LEU:HA	1:C:437:ILE:HD12	1.98	0.46
1:F:744:ARG:HD3	1:F:745:ARG:H	1.80	0.45
1:B:525:THR:HB	2:B:900:ADP:O1A	2.15	0.45
1:F:698:ALA:HB2	1:F:731:ILE:HD12	1.96	0.45
1:E:113:ARG:CZ	1:E:183:HIS:H	2.29	0.45
1:B:303:ILE:HD13	1:B:303:ILE:HG21	1.74	0.45
1:A:572:CYS:SG	1:A:617:VAL:HG22	2.55	0.45
1:A:574:LEU:HD23	1:A:619:ILE:HD12	1.98	0.45
1:F:129:ASN:HD21	1:F:132:GLU:CD	2.20	0.45
1:E:327:GLN:O	1:E:331:LEU:HG	2.15	0.45
1:B:158:MET:N	1:B:387:ASN:O	2.39	0.45
1:B:762:LEU:HD12	1:B:763:GLN:CA	2.45	0.45
1:F:403:THR:O	1:F:406:HIS:CD2	2.69	0.45
1:F:312:LYS:HB3	1:F:354:ASP:HB2	1.99	0.45
1:A:244:TYR:OH	1:A:568:GLN:HG2	2.16	0.45
1:B:113:ARG:CZ	1:B:183:HIS:H	2.29	0.45
1:E:229:LEU:HA	1:F:437:ILE:HD12	1.98	0.45
1:E:129:ASN:HD21	1:E:132:GLU:CD	2.20	0.45
1:D:744:ARG:HD3	1:D:745:ARG:H	1.80	0.45
1:D:312:LYS:HB3	1:D:354:ASP:HB2	1.99	0.45
1:E:312:LYS:HD2	1:E:313:ARG:H	1.80	0.45
1:F:43:GLN:N	1:F:43:GLN:OE1	2.43	0.45
1:B:43:GLN:N	1:B:43:GLN:OE1	2.43	0.45
1:F:574:LEU:HD23	1:F:619:ILE:HD12	1.98	0.45
1:A:396:LEU:HA	1:A:399:VAL:HB	1.97	0.45
1:A:327:GLN:HA	1:A:330:THR:OG1	2.15	0.45
1:A:744:ARG:HD3	1:A:745:ARG:H	1.80	0.45
1:A:486:LYS:O	1:A:490:GLN:HG3	2.17	0.45
1:E:486:LYS:O	1:E:490:GLN:HG3	2.16	0.45
1:C:751:ASP:O	1:C:755:TYR:N	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:LEU:HD23	1:B:619:ILE:HD12	1.98	0.45
1:D:229:LEU:HA	1:E:437:ILE:HD12	1.98	0.45
1:D:129:ASN:HD21	1:D:132:GLU:CD	2.20	0.45
1:D:27:ILE:HD12	1:D:80:GLU:HB3	1.99	0.45
1:E:27:ILE:HD12	1:E:80:GLU:HB3	1.99	0.45
1:A:501:ASP:OD1	1:A:501:ASP:N	2.47	0.45
1:D:113:ARG:CZ	1:D:183:HIS:H	2.29	0.45
1:C:243:LEU:HD23	1:C:367:VAL:HG13	1.99	0.45
1:B:533:ASN:OD1	1:B:536:GLN:NE2	2.50	0.45
1:E:533:ASN:OD1	1:E:536:GLN:NE2	2.50	0.45
1:E:503:PHE:CD1	1:F:699:ILE:HD13	2.46	0.45
1:C:113:ARG:CZ	1:C:183:HIS:H	2.29	0.45
1:B:486:LYS:O	1:B:490:GLN:HG3	2.16	0.45
1:E:312:LYS:HB3	1:E:354:ASP:HB2	1.99	0.45
1:D:489:LEU:HD21	1:D:516:PHE:CZ	2.52	0.45
1:D:134:TYR:O	1:D:154:VAL:HG11	2.17	0.45
1:B:499:HIS:ND1	1:C:703:ILE:HG23	2.32	0.45
1:D:533:ASN:OD1	1:D:536:GLN:NE2	2.50	0.45
1:C:42:SER:HA	1:C:77:CYS:SG	2.57	0.45
1:F:27:ILE:HD12	1:F:80:GLU:HB3	1.99	0.45
1:A:312:LYS:HB3	1:A:354:ASP:HB2	1.99	0.45
1:B:243:LEU:HD23	1:B:367:VAL:HG13	1.99	0.45
1:B:396:LEU:HA	1:B:399:VAL:HB	1.97	0.45
1:B:159:ARG:N	1:B:387:ASN:HB3	2.32	0.45
1:E:42:SER:HA	1:E:77:CYS:SG	2.57	0.45
1:C:312:LYS:HB3	1:C:354:ASP:HB2	1.99	0.45
1:C:489:LEU:HD21	1:C:516:PHE:CZ	2.52	0.45
1:D:203:TYR:HA	1:D:206:ILE:HD12	1.99	0.45
1:E:574:LEU:HD23	1:E:619:ILE:HD12	1.98	0.45
1:D:243:LEU:HD23	1:D:367:VAL:HG13	1.99	0.45
1:B:129:ASN:HD21	1:B:132:GLU:CD	2.20	0.45
1:A:159:ARG:N	1:A:387:ASN:HB3	2.32	0.45
1:A:496:PRO:HG3	1:A:503:PHE:CE2	2.50	0.45
1:E:134:TYR:O	1:E:154:VAL:HG11	2.17	0.45
1:B:111:GLY:HA2	1:B:170:PRO:CG	2.47	0.45
1:F:149:GLY:H	1:F:165:VAL:HG13	1.82	0.45
1:B:151:ILE:HG22	1:B:162:GLU:HG3	1.99	0.45
1:E:580:ASP:OD1	1:E:580:ASP:N	2.49	0.45
1:C:27:ILE:HD12	1:C:80:GLU:HB3	1.99	0.44
1:E:26:LEU:HD11	1:E:80:GLU:HA	2.00	0.44
1:F:486:LYS:O	1:F:490:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:MET:SD	1:D:558:ASN:HB2	2.57	0.44
1:B:550:MET:SD	1:B:558:ASN:HB2	2.57	0.44
1:E:151:ILE:HG22	1:E:162:GLU:HG3	1.99	0.44
1:C:129:ASN:HD21	1:C:132:GLU:CD	2.20	0.44
1:A:42:SER:HA	1:A:77:CYS:SG	2.57	0.44
1:F:159:ARG:N	1:F:387:ASN:HB3	2.32	0.44
1:C:486:LYS:O	1:C:490:GLN:HG3	2.17	0.44
1:D:486:LYS:O	1:D:490:GLN:HG3	2.17	0.44
1:A:234:GLY:O	1:A:235:VAL:HB	2.17	0.44
1:E:489:LEU:HD21	1:E:516:PHE:CZ	2.52	0.44
1:C:111:GLY:HA2	1:C:170:PRO:CG	2.47	0.44
1:F:533:ASN:OD1	1:F:536:GLN:NE2	2.50	0.44
1:A:151:ILE:HG22	1:A:162:GLU:HG3	1.99	0.44
1:D:151:ILE:HG22	1:D:162:GLU:HG3	1.99	0.44
1:E:149:GLY:H	1:E:165:VAL:HG13	1.82	0.44
1:A:229:LEU:HA	1:B:437:ILE:HD12	1.98	0.44
1:E:159:ARG:N	1:E:387:ASN:HB3	2.32	0.44
1:C:134:TYR:O	1:C:154:VAL:HG11	2.17	0.44
1:D:111:GLY:HA2	1:D:170:PRO:CG	2.47	0.44
1:A:111:GLY:HA2	1:A:170:PRO:CG	2.47	0.44
1:A:533:ASN:OD1	1:A:536:GLN:NE2	2.50	0.44
1:E:392:ASP:OD1	1:E:393:ASP:N	2.51	0.44
1:F:392:ASP:OD1	1:F:393:ASP:N	2.51	0.44
1:C:574:LEU:HD23	1:C:619:ILE:HD12	1.98	0.44
1:D:499:HIS:ND1	1:E:703:ILE:HG23	2.33	0.44
1:C:550:MET:SD	1:C:558:ASN:HB2	2.57	0.44
1:B:751:ASP:O	1:B:755:TYR:N	2.35	0.44
1:A:149:GLY:H	1:A:165:VAL:HG13	1.82	0.44
1:F:550:MET:SD	1:F:558:ASN:HB2	2.57	0.44
1:E:203:TYR:HA	1:E:206:ILE:HD12	1.99	0.44
1:C:151:ILE:HG22	1:C:162:GLU:HG3	1.99	0.44
1:F:151:ILE:HG22	1:F:162:GLU:HG3	1.99	0.44
1:F:42:SER:HA	1:F:77:CYS:SG	2.57	0.44
1:A:26:LEU:HD11	1:A:80:GLU:HA	2.00	0.44
1:E:234:GLY:O	1:E:235:VAL:HB	2.17	0.44
1:F:113:ARG:NH2	1:F:183:HIS:H	2.15	0.44
1:D:633:ILE:O	1:D:638:ARG:HB3	2.18	0.44
1:C:117:LEU:HA	1:C:118:PRO:HD3	1.78	0.44
1:F:285:ASN:HD22	1:F:288:LYS:NZ	2.16	0.44
1:A:285:ASN:HD22	1:A:288:LYS:NZ	2.16	0.44
1:E:512:LYS:HD3	1:E:512:LYS:HA	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASN:HD21	1:A:132:GLU:CD	2.20	0.44
1:D:297:ALA:HA	1:D:298:PRO:C	2.38	0.44
1:A:699:ILE:HG13	1:F:506:PHE:HD2	1.81	0.44
1:D:312:LYS:HB3	1:D:354:ASP:CG	2.38	0.44
1:C:234:GLY:O	1:C:235:VAL:HB	2.17	0.44
1:B:312:LYS:HB3	1:B:354:ASP:HB2	1.99	0.44
1:B:234:GLY:O	1:B:235:VAL:HB	2.17	0.44
1:A:43:GLN:CD	1:A:75:ASP:HA	2.38	0.44
1:C:320:VAL:HA	1:C:323:ARG:HD2	2.00	0.44
1:F:134:TYR:O	1:F:154:VAL:HG11	2.17	0.44
1:E:499:HIS:ND1	1:F:703:ILE:HG23	2.33	0.44
1:E:111:GLY:HA2	1:E:170:PRO:CG	2.48	0.44
1:A:336:LYS:O	1:A:337:GLN:HB2	2.18	0.44
1:D:574:LEU:HD23	1:D:619:ILE:HD12	1.98	0.44
1:A:392:ASP:OD1	1:A:393:ASP:N	2.51	0.44
1:E:243:LEU:HD23	1:E:367:VAL:HG13	1.99	0.44
1:D:193:ASP:N	1:D:193:ASP:OD1	2.51	0.44
1:B:203:TYR:HA	1:B:206:ILE:HD12	1.99	0.44
1:F:297:ALA:HA	1:F:298:PRO:C	2.38	0.44
1:C:159:ARG:N	1:C:387:ASN:HB3	2.32	0.44
1:B:42:SER:HA	1:B:77:CYS:SG	2.57	0.44
1:D:506:PHE:HD2	1:E:699:ILE:HG13	1.82	0.44
1:B:312:LYS:HB3	1:B:354:ASP:CG	2.38	0.44
1:B:489:LEU:HD21	1:B:516:PHE:CZ	2.52	0.44
1:A:134:TYR:O	1:A:154:VAL:HG11	2.17	0.44
1:B:113:ARG:NH2	1:B:183:HIS:H	2.15	0.44
1:E:183:HIS:NE2	1:E:185:GLU:OE2	2.51	0.44
1:E:633:ILE:O	1:E:638:ARG:HB3	2.18	0.44
1:D:59:LEU:HD23	1:D:102:ILE:HA	2.00	0.44
1:C:336:LYS:O	1:C:337:GLN:HB2	2.18	0.44
1:A:550:MET:SD	1:A:558:ASN:HB2	2.57	0.44
1:C:149:GLY:H	1:C:165:VAL:HG13	1.82	0.44
1:A:203:TYR:HA	1:A:206:ILE:HD12	1.99	0.44
1:A:193:ASP:N	1:A:193:ASP:OD1	2.51	0.44
1:E:297:ALA:HA	1:E:298:PRO:C	2.38	0.44
1:D:159:ARG:N	1:D:387:ASN:HB3	2.32	0.44
1:E:42:SER:HB2	1:E:78:SER:O	2.18	0.44
1:A:27:ILE:HD12	1:A:80:GLU:HB3	1.99	0.44
1:B:27:ILE:HD12	1:B:80:GLU:HB3	1.99	0.44
1:D:234:GLY:O	1:D:235:VAL:HB	2.17	0.44
1:F:234:GLY:O	1:F:235:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:GLN:OE1	1:C:43:GLN:N	2.43	0.44
1:F:183:HIS:NE2	1:F:185:GLU:OE2	2.51	0.44
1:D:183:HIS:NE2	1:D:185:GLU:OE2	2.51	0.44
1:C:633:ILE:O	1:C:638:ARG:HB3	2.18	0.44
1:A:243:LEU:HD23	1:A:367:VAL:HG13	1.99	0.44
1:E:550:MET:SD	1:E:558:ASN:HB2	2.57	0.44
1:A:437:ILE:HD12	1:F:229:LEU:HA	1.99	0.44
1:C:59:LEU:HD23	1:C:102:ILE:HA	2.00	0.44
1:D:153:LEU:HD13	1:D:198:LEU:HD23	2.00	0.44
1:C:297:ALA:HA	1:C:298:PRO:C	2.38	0.44
1:E:59:LEU:HD23	1:E:102:ILE:HA	2.00	0.44
1:E:506:PHE:HD2	1:F:699:ILE:HG13	1.83	0.44
1:F:496:PRO:HG3	1:F:503:PHE:CE2	2.50	0.44
1:C:312:LYS:HB3	1:C:354:ASP:CG	2.38	0.44
1:B:43:GLN:CD	1:B:75:ASP:HA	2.38	0.44
1:B:171:SER:HB3	1:B:172:PRO:HA	2.00	0.44
1:B:134:TYR:O	1:B:154:VAL:HG11	2.17	0.44
1:E:113:ARG:NH2	1:E:183:HIS:H	2.15	0.44
1:F:111:GLY:HA2	1:F:170:PRO:CG	2.47	0.44
1:E:285:ASN:HD22	1:E:288:LYS:NZ	2.16	0.44
1:B:149:GLY:H	1:B:165:VAL:HG13	1.82	0.44
1:D:120:ASP:HB3	1:D:121:ASP:H	1.52	0.44
1:D:336:LYS:O	1:D:337:GLN:HB2	2.18	0.44
1:E:312:LYS:HB3	1:E:354:ASP:CG	2.38	0.43
1:D:43:GLN:N	1:D:43:GLN:OE1	2.43	0.43
1:F:489:LEU:HD21	1:F:516:PHE:CZ	2.52	0.43
1:C:171:SER:HB3	1:C:172:PRO:HA	2.00	0.43
1:C:499:HIS:ND1	1:D:703:ILE:HG23	2.33	0.43
1:C:285:ASN:HD22	1:C:288:LYS:NZ	2.16	0.43
1:F:203:TYR:HA	1:F:206:ILE:HD12	1.99	0.43
1:B:285:ASN:HD22	1:B:288:LYS:NZ	2.16	0.43
1:C:229:LEU:HA	1:D:437:ILE:HD12	1.98	0.43
1:B:193:ASP:OD1	1:B:193:ASP:N	2.51	0.43
1:D:42:SER:HA	1:D:77:CYS:SG	2.57	0.43
1:F:42:SER:CB	1:F:79:ASP:HA	2.48	0.43
1:D:43:GLN:CD	1:D:75:ASP:HA	2.38	0.43
1:E:133:VAL:HG13	1:E:134:TYR:CD2	2.54	0.43
1:C:183:HIS:NE2	1:C:185:GLU:OE2	2.51	0.43
1:A:113:ARG:NH2	1:A:183:HIS:H	2.15	0.43
1:C:635:ARG:HG3	1:C:635:ARG:H	1.54	0.43
1:D:285:ASN:HD22	1:D:288:LYS:NZ	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ASP:OD1	1:C:393:ASP:N	2.51	0.43
1:B:29:ASP:HB2	1:B:81:LYS:HB3	2.01	0.43
1:F:243:LEU:HD23	1:F:367:VAL:HG13	1.99	0.43
1:C:533:ASN:OD1	1:C:536:GLN:NE2	2.50	0.43
1:C:42:SER:CB	1:C:79:ASP:HA	2.48	0.43
1:A:506:PHE:HD2	1:B:699:ILE:HG13	1.83	0.43
1:C:233:ILE:HG23	1:C:235:VAL:HG12	2.01	0.43
1:C:113:ARG:NH2	1:C:183:HIS:H	2.15	0.43
1:C:393:ASP:N	1:C:393:ASP:OD1	2.51	0.43
1:B:690:ILE:HD13	1:B:740:MET:HE1	2.00	0.43
1:B:392:ASP:OD1	1:B:393:ASP:N	2.51	0.43
1:E:336:LYS:O	1:E:337:GLN:HB2	2.18	0.43
1:B:153:LEU:HD13	1:B:198:LEU:HD23	2.00	0.43
1:F:42:SER:HB2	1:F:78:SER:O	2.18	0.43
1:C:42:SER:HB2	1:C:78:SER:O	2.18	0.43
1:B:26:LEU:HD11	1:B:80:GLU:HA	2.00	0.43
1:D:503:PHE:CD1	1:E:699:ILE:HD13	2.46	0.43
1:D:377:ARG:CD	1:D:403:THR:HG23	2.48	0.43
1:A:350:PRO:CB	1:A:358:ARG:HH22	2.32	0.43
1:C:476:TRP:CZ3	1:C:486:LYS:HG2	2.54	0.43
1:F:43:GLN:CD	1:F:75:ASP:HA	2.38	0.43
1:E:320:VAL:HA	1:E:323:ARG:HD2	2.00	0.43
1:B:297:ALA:HA	1:B:298:PRO:C	2.38	0.43
1:E:42:SER:CB	1:E:79:ASP:HA	2.48	0.43
1:A:42:SER:CB	1:A:79:ASP:HA	2.49	0.43
1:B:506:PHE:HD2	1:C:699:ILE:HG13	1.84	0.43
1:E:496:PRO:HG3	1:E:503:PHE:CE2	2.50	0.43
1:F:312:LYS:HB3	1:F:354:ASP:CG	2.38	0.43
1:A:171:SER:HB3	1:A:172:PRO:HA	2.00	0.43
1:F:133:VAL:HG13	1:F:134:TYR:CD2	2.54	0.43
1:A:183:HIS:NE2	1:A:185:GLU:OE2	2.51	0.43
1:D:113:ARG:NH2	1:D:183:HIS:H	2.15	0.43
1:F:633:ILE:O	1:F:638:ARG:HB3	2.18	0.43
1:B:633:ILE:O	1:B:638:ARG:HB3	2.18	0.43
1:F:295:LYS:HE2	1:F:295:LYS:HB2	1.76	0.43
1:C:203:TYR:HA	1:C:206:ILE:HD12	1.99	0.43
1:D:393:ASP:N	1:D:393:ASP:OD1	2.51	0.43
1:C:29:ASP:HB2	1:C:81:LYS:HB3	2.01	0.43
1:A:29:ASP:HB2	1:A:81:LYS:HB3	2.01	0.43
1:F:290:PHE:HD1	1:F:301:ILE:HD12	1.82	0.43
1:A:297:ALA:HA	1:A:298:PRO:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD23	1:B:102:ILE:HA	2.00	0.43
1:F:59:LEU:HD23	1:F:102:ILE:HA	2.00	0.43
1:C:377:ARG:CD	1:C:403:THR:HG23	2.48	0.43
1:E:233:ILE:HG23	1:E:235:VAL:HG12	2.01	0.43
1:F:29:ASP:HB2	1:F:81:LYS:HB3	2.01	0.43
1:F:193:ASP:N	1:F:193:ASP:OD1	2.51	0.43
1:D:26:LEU:HD11	1:D:80:GLU:HA	2.00	0.43
1:F:26:LEU:HD11	1:F:80:GLU:HA	2.00	0.43
1:C:26:LEU:HD11	1:C:80:GLU:HA	2.00	0.43
1:F:233:ILE:HG23	1:F:235:VAL:HG12	2.01	0.43
1:B:493:VAL:HG11	1:B:531:ILE:HG12	2.01	0.43
1:B:183:HIS:NE2	1:B:185:GLU:OE2	2.51	0.43
1:B:150:ASP:O	1:B:164:LYS:HA	2.19	0.43
1:F:351:ASN:N	1:F:351:ASN:OD1	2.52	0.43
1:C:153:LEU:HD13	1:C:198:LEU:HD23	2.00	0.43
1:D:350:PRO:CB	1:D:358:ARG:HH22	2.32	0.43
1:C:350:PRO:CB	1:C:358:ARG:HH22	2.32	0.43
1:E:350:PRO:CB	1:E:358:ARG:HH22	2.32	0.43
1:A:312:LYS:HB3	1:A:354:ASP:CG	2.38	0.43
1:D:476:TRP:CZ3	1:D:486:LYS:HG2	2.54	0.43
1:A:489:LEU:HD21	1:A:516:PHE:CZ	2.52	0.43
1:C:133:VAL:HG13	1:C:134:TYR:CD2	2.54	0.43
1:A:633:ILE:O	1:A:638:ARG:HB3	2.18	0.43
1:F:150:ASP:O	1:F:164:LYS:HA	2.19	0.43
1:D:149:GLY:H	1:D:165:VAL:HG13	1.82	0.43
1:C:193:ASP:N	1:C:193:ASP:OD1	2.51	0.43
1:B:351:ASN:N	1:B:351:ASN:OD1	2.52	0.43
1:E:191:ARG:HH21	1:E:195:GLU:CG	2.31	0.43
1:B:42:SER:HB2	1:B:78:SER:O	2.18	0.43
1:A:406:HIS:CE1	1:A:460:ASN:ND2	2.87	0.43
1:C:406:HIS:CE1	1:C:460:ASN:ND2	2.87	0.43
1:B:476:TRP:CZ3	1:B:486:LYS:HG2	2.54	0.43
1:B:133:VAL:HG13	1:B:134:TYR:CD2	2.54	0.43
1:B:705:SER:HA	1:B:706:GLU:HA	1.67	0.43
1:E:29:ASP:HB2	1:E:81:LYS:HB3	2.01	0.43
1:A:407:VAL:HG23	1:A:409:ALA:H	1.84	0.43
1:A:153:LEU:HD13	1:A:198:LEU:HD23	2.00	0.43
1:A:290:PHE:HD1	1:A:301:ILE:HD12	1.82	0.43
1:E:290:PHE:HD1	1:E:301:ILE:HD12	1.82	0.43
1:D:42:SER:HB2	1:D:78:SER:O	2.18	0.43
1:D:42:SER:CB	1:D:79:ASP:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HB3	1:B:100:ILE:HD12	2.01	0.43
1:D:27:ILE:HG22	1:D:28:VAL:N	2.34	0.43
1:F:476:TRP:CZ3	1:F:486:LYS:HG2	2.54	0.43
1:F:171:SER:HB3	1:F:172:PRO:HA	2.00	0.43
1:A:115:HIS:HB3	1:A:167:GLU:HB3	2.01	0.43
1:C:59:LEU:HB3	1:C:100:ILE:HD12	2.01	0.43
1:B:393:ASP:OD1	1:B:393:ASP:N	2.51	0.43
1:B:407:VAL:HG23	1:B:409:ALA:H	1.84	0.43
1:B:336:LYS:O	1:B:337:GLN:HB2	2.18	0.43
1:E:120:ASP:HB3	1:E:121:ASP:H	1.52	0.43
1:D:150:ASP:O	1:D:164:LYS:HA	2.19	0.43
1:E:150:ASP:O	1:E:164:LYS:HA	2.19	0.43
1:F:336:LYS:O	1:F:337:GLN:HB2	2.18	0.43
1:B:42:SER:CB	1:B:79:ASP:HA	2.48	0.42
1:A:27:ILE:HG22	1:A:28:VAL:N	2.34	0.42
1:E:377:ARG:CD	1:E:403:THR:HG23	2.48	0.42
1:A:403:THR:O	1:A:406:HIS:HD2	2.02	0.42
1:C:506:PHE:HD2	1:D:699:ILE:HG13	1.83	0.42
1:B:350:PRO:CB	1:B:358:ARG:HH22	2.32	0.42
1:C:43:GLN:CD	1:C:75:ASP:HA	2.38	0.42
1:F:285:ASN:HA	1:F:288:LYS:HE3	2.01	0.42
1:A:285:ASN:HA	1:A:288:LYS:HE3	2.01	0.42
1:D:392:ASP:OD1	1:D:393:ASP:N	2.51	0.42
1:F:705:SER:HA	1:F:706:GLU:HA	1.67	0.42
1:F:690:ILE:HD13	1:F:740:MET:HE1	2.00	0.42
1:B:27:ILE:HG22	1:B:28:VAL:N	2.34	0.42
1:F:406:HIS:CE1	1:F:460:ASN:ND2	2.87	0.42
1:D:233:ILE:HG23	1:D:235:VAL:HG12	2.01	0.42
1:B:320:VAL:HA	1:B:323:ARG:HD2	2.00	0.42
1:E:43:GLN:CD	1:E:75:ASP:HA	2.38	0.42
1:D:171:SER:HB3	1:D:172:PRO:HA	2.00	0.42
1:A:493:VAL:HG11	1:A:531:ILE:HG12	2.00	0.42
1:A:133:VAL:HG13	1:A:134:TYR:CD2	2.54	0.42
1:A:246:PRO:HG2	1:A:249:THR:CG2	2.49	0.42
1:C:113:ARG:HE	1:C:183:HIS:H	1.68	0.42
1:D:115:HIS:HB3	1:D:167:GLU:HB3	2.01	0.42
1:A:703:ILE:HG23	1:F:499:HIS:ND1	2.34	0.42
1:A:150:ASP:O	1:A:164:LYS:HA	2.19	0.42
1:D:422:ALA:HB2	1:D:451:ASP:OD2	2.20	0.42
1:A:42:SER:HB2	1:A:78:SER:O	2.18	0.42
1:B:403:THR:O	1:B:406:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:HIS:NE2	1:B:461:PRO:HG3	2.35	0.42
1:C:406:HIS:NE2	1:C:461:PRO:HG3	2.35	0.42
1:A:312:LYS:HD2	1:A:313:ARG:N	2.35	0.42
1:F:320:VAL:HA	1:F:323:ARG:HD2	2.00	0.42
1:D:320:VAL:HA	1:D:323:ARG:HD2	2.00	0.42
1:D:133:VAL:HG13	1:D:134:TYR:CD2	2.54	0.42
1:B:115:HIS:HB3	1:B:167:GLU:HB3	2.01	0.42
1:A:499:HIS:ND1	1:B:703:ILE:HG23	2.34	0.42
1:C:151:ILE:O	1:C:162:GLU:HB2	2.20	0.42
1:B:285:ASN:HA	1:B:288:LYS:HE3	2.01	0.42
1:D:86:ARG:HD2	1:D:204:ASP:OD1	2.20	0.42
1:C:422:ALA:HB2	1:C:451:ASP:OD2	2.20	0.42
1:A:326:SER:O	1:A:327:GLN:HB3	2.19	0.42
1:C:326:SER:O	1:C:327:GLN:HB3	2.19	0.42
1:E:39:VAL:HA	1:E:83:ARG:O	2.19	0.42
1:B:39:VAL:HA	1:B:83:ARG:O	2.19	0.42
1:A:39:VAL:HA	1:A:83:ARG:O	2.19	0.42
1:D:25:ARG:HB3	1:D:99:VAL:HG11	2.02	0.42
1:F:25:ARG:HB3	1:F:99:VAL:HG11	2.02	0.42
1:F:350:PRO:CB	1:F:358:ARG:HH22	2.32	0.42
1:C:493:VAL:HG11	1:C:531:ILE:HG12	2.01	0.42
1:C:115:HIS:HD2	1:C:166:VAL:CG2	2.33	0.42
1:D:246:PRO:HG2	1:D:249:THR:CG2	2.49	0.42
1:D:151:ILE:O	1:D:162:GLU:HB2	2.20	0.42
1:E:285:ASN:HA	1:E:288:LYS:HE3	2.01	0.42
1:C:285:ASN:HA	1:C:288:LYS:HE3	2.01	0.42
1:E:86:ARG:HD2	1:E:204:ASP:OD1	2.20	0.42
1:E:407:VAL:HG23	1:E:409:ALA:H	1.84	0.42
1:A:59:LEU:HD23	1:A:102:ILE:HA	2.00	0.42
1:E:351:ASN:N	1:E:351:ASN:OD1	2.52	0.42
1:F:153:LEU:HD13	1:F:198:LEU:HD23	2.00	0.42
1:F:27:ILE:HG22	1:F:28:VAL:N	2.34	0.42
1:C:27:ILE:HG22	1:C:28:VAL:N	2.34	0.42
1:D:496:PRO:HG3	1:D:503:PHE:CE2	2.50	0.42
1:E:403:THR:O	1:E:406:HIS:HD2	2.02	0.42
1:D:406:HIS:NE2	1:D:461:PRO:HG3	2.35	0.42
1:B:312:LYS:HD2	1:B:313:ARG:N	2.35	0.42
1:F:312:LYS:HD2	1:F:313:ARG:N	2.35	0.42
1:A:320:VAL:HA	1:A:323:ARG:HD2	2.00	0.42
1:F:246:PRO:HG2	1:F:249:THR:CG2	2.49	0.42
1:B:115:HIS:HD2	1:B:166:VAL:CG2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:ARG:HE	1:F:183:HIS:H	1.67	0.42
1:E:113:ARG:HE	1:E:183:HIS:H	1.68	0.42
1:D:285:ASN:HA	1:D:288:LYS:HE3	2.01	0.42
1:D:29:ASP:HB2	1:D:81:LYS:HB3	2.01	0.42
1:C:86:ARG:HD2	1:C:204:ASP:OD1	2.20	0.42
1:A:351:ASN:OD1	1:A:351:ASN:N	2.52	0.42
1:F:326:SER:O	1:F:327:GLN:HB3	2.19	0.42
1:E:25:ARG:HB3	1:E:99:VAL:HG11	2.02	0.42
1:B:406:HIS:CE1	1:B:460:ASN:ND2	2.87	0.42
1:F:406:HIS:NE2	1:F:461:PRO:HG3	2.35	0.42
1:E:476:TRP:CZ3	1:E:486:LYS:HG2	2.54	0.42
1:B:233:ILE:HG23	1:B:235:VAL:HG12	2.01	0.42
1:F:316:THR:HG23	1:F:322:ARG:CZ	2.50	0.42
1:C:246:PRO:HG2	1:C:249:THR:CG2	2.49	0.42
1:C:115:HIS:HB3	1:C:167:GLU:HB3	2.01	0.42
1:D:113:ARG:HE	1:D:183:HIS:H	1.68	0.42
1:E:422:ALA:HB2	1:E:451:ASP:OD2	2.20	0.42
1:B:422:ALA:HB2	1:B:451:ASP:OD2	2.20	0.42
1:F:38:VAL:HG23	1:F:144:ARG:HH12	1.85	0.42
1:D:290:PHE:HD1	1:D:301:ILE:HD12	1.82	0.42
1:E:27:ILE:HG22	1:E:28:VAL:N	2.34	0.42
1:B:377:ARG:CD	1:B:403:THR:HG23	2.48	0.42
1:E:406:HIS:CE1	1:E:460:ASN:ND2	2.87	0.42
1:C:403:THR:O	1:C:406:HIS:HD2	2.02	0.42
1:A:476:TRP:CZ3	1:A:486:LYS:HG2	2.54	0.42
1:B:113:ARG:HE	1:B:183:HIS:H	1.68	0.42
1:D:115:HIS:HD2	1:D:166:VAL:CG2	2.33	0.42
1:B:151:ILE:O	1:B:162:GLU:HB2	2.20	0.42
1:C:150:ASP:O	1:C:164:LYS:HA	2.19	0.42
1:F:86:ARG:HD2	1:F:204:ASP:OD1	2.20	0.42
1:D:351:ASN:N	1:D:351:ASN:OD1	2.52	0.42
1:C:38:VAL:HG23	1:C:144:ARG:HH12	1.85	0.42
1:E:312:LYS:HD2	1:E:313:ARG:N	2.35	0.42
1:E:171:SER:HB3	1:E:172:PRO:HA	2.00	0.42
1:D:493:VAL:HG11	1:D:531:ILE:HG12	2.01	0.42
1:D:295:LYS:HE2	1:D:295:LYS:HB2	1.76	0.42
1:E:151:ILE:O	1:E:162:GLU:HB2	2.20	0.42
1:C:407:VAL:HG23	1:C:409:ALA:H	1.84	0.42
1:A:508:MET:HB3	1:A:508:MET:HE2	1.96	0.42
1:A:38:VAL:HG23	1:A:144:ARG:HH12	1.85	0.42
1:D:326:SER:O	1:D:327:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:VAL:HA	1:F:83:ARG:O	2.19	0.42
1:A:406:HIS:NE2	1:A:461:PRO:HG3	2.35	0.42
1:C:312:LYS:HD2	1:C:313:ARG:N	2.35	0.42
1:C:316:THR:HG23	1:C:322:ARG:CZ	2.50	0.42
1:D:312:LYS:HD2	1:D:313:ARG:N	2.35	0.42
1:C:567:ARG:HG3	1:C:615:LYS:HD3	2.02	0.42
1:C:752:ILE:O	1:C:756:GLU:HG2	2.20	0.42
1:B:752:ILE:O	1:B:756:GLU:HG2	2.20	0.42
1:F:752:ILE:O	1:F:756:GLU:HG2	2.20	0.42
1:E:96:LEU:HA	1:E:96:LEU:HD23	1.87	0.42
1:B:728:VAL:N	1:B:729:PRO:HD3	2.35	0.42
1:C:728:VAL:N	1:C:729:PRO:HD3	2.35	0.42
1:C:508:MET:HB3	1:C:508:MET:HE2	1.93	0.42
1:E:153:LEU:HD13	1:E:198:LEU:HD23	2.00	0.42
1:D:322:ARG:HA	1:D:325:VAL:HG22	2.02	0.42
1:A:233:ILE:HG23	1:A:235:VAL:HG12	2.01	0.42
1:A:567:ARG:HG3	1:A:615:LYS:HD3	2.02	0.42
1:A:752:ILE:O	1:A:756:GLU:HG2	2.20	0.42
1:B:246:PRO:HG2	1:B:249:THR:CG2	2.49	0.42
1:A:113:ARG:HE	1:A:183:HIS:H	1.68	0.42
1:A:151:ILE:O	1:A:162:GLU:HB2	2.20	0.42
1:B:86:ARG:HD2	1:B:204:ASP:OD1	2.20	0.42
1:A:422:ALA:HB2	1:A:451:ASP:OD2	2.20	0.42
1:D:407:VAL:HG23	1:D:409:ALA:H	1.84	0.42
1:F:422:ALA:HB2	1:F:451:ASP:OD2	2.20	0.42
1:A:682:PHE:CE1	1:A:745:ARG:HB3	2.56	0.41
1:A:312:LYS:C	1:A:313:ARG:HG3	2.40	0.41
1:F:312:LYS:C	1:F:313:ARG:HG3	2.40	0.41
1:D:567:ARG:HG3	1:D:615:LYS:HD3	2.02	0.41
1:F:567:ARG:HG3	1:F:615:LYS:HD3	2.02	0.41
1:C:351:ASN:N	1:C:351:ASN:OD1	2.52	0.41
1:A:86:ARG:HD2	1:A:204:ASP:OD1	2.20	0.41
1:A:25:ARG:HB3	1:A:99:VAL:HG11	2.02	0.41
1:A:377:ARG:CD	1:A:403:THR:HG23	2.48	0.41
1:F:377:ARG:CD	1:F:403:THR:HG23	2.48	0.41
1:D:316:THR:HG23	1:D:322:ARG:CZ	2.50	0.41
1:C:65:ARG:NH2	1:C:93:ARG:CZ	2.84	0.41
1:B:567:ARG:HG3	1:B:615:LYS:HD3	2.02	0.41
1:E:115:HIS:HB3	1:E:167:GLU:HB3	2.01	0.41
1:E:295:LYS:HB2	1:E:295:LYS:HE2	1.76	0.41
1:F:393:ASP:N	1:F:393:ASP:OD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:ILE:O	1:F:162:GLU:HB2	2.20	0.41
1:D:750:ASN:HA	1:D:753:ARG:NH2	2.36	0.41
1:E:750:ASN:HA	1:E:753:ARG:NH2	2.35	0.41
1:E:193:ASP:OD1	1:E:193:ASP:N	2.51	0.41
1:C:290:PHE:HD1	1:C:301:ILE:HD12	1.82	0.41
1:B:682:PHE:CE1	1:B:745:ARG:HB3	2.55	0.41
1:F:59:LEU:HB3	1:F:100:ILE:HD12	2.01	0.41
1:D:191:ARG:HH21	1:D:195:GLU:CG	2.31	0.41
1:E:406:HIS:NE2	1:E:461:PRO:HG3	2.35	0.41
1:A:65:ARG:NH2	1:A:93:ARG:CZ	2.84	0.41
1:C:322:ARG:HA	1:C:325:VAL:HG22	2.02	0.41
1:E:312:LYS:C	1:E:313:ARG:HG3	2.40	0.41
1:A:316:THR:HG23	1:A:322:ARG:CZ	2.50	0.41
1:E:115:HIS:HD2	1:E:166:VAL:CG2	2.33	0.41
1:E:393:ASP:OD1	1:E:393:ASP:N	2.51	0.41
1:C:471:VAL:HG11	1:C:536:GLN:OE1	2.21	0.41
1:A:59:LEU:HB3	1:A:100:ILE:HD12	2.01	0.41
1:E:690:ILE:HD13	1:E:740:MET:HE1	2.01	0.41
1:A:728:VAL:N	1:A:729:PRO:HD3	2.35	0.41
1:D:728:VAL:N	1:D:729:PRO:HD3	2.35	0.41
1:B:290:PHE:HD1	1:B:301:ILE:HD12	1.82	0.41
1:E:59:LEU:HB3	1:E:100:ILE:HD12	2.01	0.41
1:B:65:ARG:NH2	1:B:93:ARG:CZ	2.84	0.41
1:B:312:LYS:C	1:B:313:ARG:HG3	2.40	0.41
1:E:322:ARG:HA	1:E:325:VAL:HG22	2.02	0.41
1:F:115:HIS:HB3	1:F:167:GLU:HB3	2.01	0.41
1:D:471:VAL:HG11	1:D:536:GLN:OE1	2.21	0.41
1:F:471:VAL:HG11	1:F:536:GLN:OE1	2.21	0.41
1:A:393:ASP:OD1	1:A:393:ASP:N	2.51	0.41
1:C:750:ASN:HA	1:C:753:ARG:NH2	2.36	0.41
1:F:47:ASP:HA	1:F:50:GLN:HA	2.03	0.41
1:F:751:ASP:O	1:F:755:TYR:N	2.35	0.41
1:B:117:LEU:HA	1:B:118:PRO:HD3	1.78	0.41
1:E:326:SER:O	1:E:327:GLN:HB3	2.19	0.41
1:F:682:PHE:CE1	1:F:745:ARG:HB3	2.55	0.41
1:D:403:THR:O	1:D:406:HIS:HD2	2.02	0.41
1:E:316:THR:HG23	1:E:322:ARG:CZ	2.50	0.41
1:F:322:ARG:HA	1:F:325:VAL:HG22	2.02	0.41
1:E:567:ARG:HG3	1:E:615:LYS:HD3	2.02	0.41
1:A:295:LYS:HB2	1:A:295:LYS:HE2	1.76	0.41
1:D:690:ILE:HD13	1:D:740:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:750:ASN:HA	1:B:753:ARG:NH2	2.35	0.41
1:F:750:ASN:HA	1:F:753:ARG:NH2	2.36	0.41
1:F:120:ASP:HB3	1:F:121:ASP:H	1.52	0.41
1:F:508:MET:HB3	1:F:508:MET:HE2	1.96	0.41
1:F:41:LEU:HD23	1:F:41:LEU:HA	1.87	0.41
1:B:326:SER:O	1:B:327:GLN:HB3	2.19	0.41
1:C:39:VAL:HA	1:C:83:ARG:O	2.19	0.41
1:F:65:ARG:NH2	1:F:93:ARG:CZ	2.84	0.41
1:D:406:HIS:CE1	1:D:460:ASN:ND2	2.87	0.41
1:C:312:LYS:C	1:C:313:ARG:HG3	2.40	0.41
1:B:316:THR:HG23	1:B:322:ARG:CZ	2.50	0.41
1:D:752:ILE:O	1:D:756:GLU:HG2	2.20	0.41
1:D:59:LEU:HB3	1:D:100:ILE:HD12	2.01	0.41
1:F:728:VAL:N	1:F:729:PRO:HD3	2.35	0.41
1:A:750:ASN:HA	1:A:753:ARG:NH2	2.36	0.41
1:F:407:VAL:HG23	1:F:409:ALA:H	1.84	0.41
1:E:38:VAL:HG23	1:E:144:ARG:HH12	1.85	0.41
1:D:39:VAL:HA	1:D:83:ARG:O	2.19	0.41
1:D:26:LEU:HA	1:D:26:LEU:HD12	1.91	0.41
1:F:615:LYS:O	1:F:615:LYS:HG2	2.21	0.41
1:E:493:VAL:HG11	1:E:531:ILE:HG12	2.01	0.41
1:A:635:ARG:HA	1:A:636:PRO:HD3	1.85	0.41
1:B:471:VAL:HG11	1:B:536:GLN:OE1	2.21	0.41
1:A:512:LYS:HD3	1:A:512:LYS:HA	1.68	0.41
1:D:38:VAL:HG23	1:D:144:ARG:HH12	1.85	0.41
1:A:468:VAL:HG22	1:A:469:VAL:N	2.36	0.41
1:C:490:GLN:O	1:C:494:GLN:HB2	2.21	0.41
1:D:151:ILE:HD12	1:D:151:ILE:HG23	1.83	0.41
1:A:690:ILE:HD13	1:A:740:MET:HE1	2.02	0.41
1:E:728:VAL:N	1:E:729:PRO:HD3	2.35	0.41
1:E:47:ASP:HA	1:E:50:GLN:HA	2.03	0.41
1:E:427:MET:SD	1:E:441:VAL:HG22	2.61	0.41
1:B:580:ASP:OD1	1:B:580:ASP:N	2.49	0.41
1:F:663:LYS:HB2	1:F:663:LYS:HE2	1.91	0.41
1:B:38:VAL:HG23	1:B:144:ARG:HH12	1.85	0.41
1:A:326:SER:C	1:A:328:LEU:H	2.24	0.41
1:C:682:PHE:CE1	1:C:745:ARG:HB3	2.56	0.41
1:E:682:PHE:CE1	1:E:745:ARG:HB3	2.56	0.41
1:D:468:VAL:HG22	1:D:469:VAL:N	2.36	0.41
1:B:26:LEU:HA	1:B:26:LEU:HD12	1.91	0.41
1:E:65:ARG:NH2	1:E:93:ARG:CZ	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLN:O	1:A:494:GLN:HB2	2.21	0.41
1:F:482:LEU:O	1:F:486:LYS:HG3	2.21	0.41
1:F:490:GLN:O	1:F:494:GLN:HB2	2.21	0.41
1:B:490:GLN:O	1:B:494:GLN:HB2	2.21	0.41
1:D:65:ARG:NH2	1:D:93:ARG:CZ	2.84	0.41
1:A:322:ARG:HA	1:A:325:VAL:HG22	2.02	0.41
1:D:615:LYS:O	1:D:615:LYS:HG2	2.21	0.41
1:B:666:VAL:HA	1:B:731:ILE:CG2	2.51	0.41
1:E:615:LYS:HG2	1:E:615:LYS:O	2.21	0.41
1:E:246:PRO:HG2	1:E:249:THR:CG2	2.49	0.41
1:A:115:HIS:HD2	1:A:166:VAL:CG2	2.33	0.41
1:F:115:HIS:HD2	1:F:166:VAL:CG2	2.33	0.41
1:B:295:LYS:HE2	1:B:295:LYS:HB2	1.76	0.41
1:E:114:ILE:HD12	1:E:165:VAL:HG21	2.03	0.41
1:B:114:ILE:HD12	1:B:165:VAL:HG21	2.03	0.41
1:D:114:ILE:HD12	1:D:165:VAL:HG21	2.03	0.41
1:A:47:ASP:HA	1:A:50:GLN:HA	2.03	0.41
1:B:25:ARG:HB3	1:B:99:VAL:HG11	2.02	0.41
1:F:403:THR:O	1:F:406:HIS:HD2	2.02	0.41
1:E:482:LEU:O	1:E:486:LYS:HG3	2.21	0.41
1:A:113:ARG:H	1:A:180:THR:HB	1.86	0.41
1:E:471:VAL:HG11	1:E:536:GLN:OE1	2.21	0.41
1:F:114:ILE:HD12	1:F:165:VAL:HG21	2.03	0.41
1:A:114:ILE:HD12	1:A:165:VAL:HG21	2.03	0.41
1:E:427:MET:O	1:E:429:LEU:N	2.54	0.41
1:C:427:MET:SD	1:C:441:VAL:HG22	2.61	0.41
1:F:28:VAL:CG2	1:F:94:VAL:HG21	2.51	0.40
1:A:482:LEU:O	1:A:486:LYS:HG3	2.21	0.40
1:B:312:LYS:O	1:B:313:ARG:HG3	2.22	0.40
1:A:615:LYS:HG2	1:A:615:LYS:O	2.21	0.40
1:E:752:ILE:O	1:E:756:GLU:HG2	2.20	0.40
1:D:560:ARG:HG2	1:D:607:GLU:OE2	2.21	0.40
1:C:120:ASP:HB3	1:C:121:ASP:H	1.52	0.40
1:E:560:ARG:HG2	1:E:607:GLU:OE2	2.21	0.40
1:D:427:MET:SD	1:D:441:VAL:HG22	2.61	0.40
1:F:673:GLU:N	1:F:673:GLU:OE1	2.43	0.40
1:F:427:MET:O	1:F:429:LEU:N	2.54	0.40
1:C:468:VAL:HG22	1:C:469:VAL:N	2.36	0.40
1:F:468:VAL:HG22	1:F:469:VAL:N	2.36	0.40
1:E:28:VAL:CG2	1:E:94:VAL:HG21	2.51	0.40
1:C:496:PRO:HG3	1:C:503:PHE:CE2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:LYS:O	1:D:313:ARG:HG3	2.21	0.40
1:D:382:GLN:O	1:D:386:LYS:HG3	2.22	0.40
1:E:490:GLN:O	1:E:494:GLN:HB2	2.21	0.40
1:A:382:GLN:O	1:A:386:LYS:HG3	2.22	0.40
1:C:113:ARG:H	1:C:180:THR:HB	1.86	0.40
1:F:113:ARG:H	1:F:180:THR:HB	1.86	0.40
1:D:113:ARG:H	1:D:180:THR:HB	1.86	0.40
1:D:303:ILE:HG21	1:D:303:ILE:HD13	1.74	0.40
1:D:427:MET:O	1:D:429:LEU:N	2.55	0.40
1:B:508:MET:SD	1:C:695:CYS:HB3	2.61	0.40
1:A:239:ARG:HD2	1:A:361:GLY:HA2	2.04	0.40
1:F:117:LEU:HA	1:F:118:PRO:HD3	1.78	0.40
1:F:48:GLU:OE1	1:F:48:GLU:N	2.48	0.40
1:D:682:PHE:CE1	1:D:745:ARG:HB3	2.56	0.40
1:B:92:LEU:HD23	1:B:100:ILE:HG21	2.03	0.40
1:F:92:LEU:HD23	1:F:100:ILE:HG21	2.03	0.40
1:E:503:PHE:HA	1:F:699:ILE:CD1	2.52	0.40
1:C:312:LYS:O	1:C:313:ARG:HG3	2.21	0.40
1:B:322:ARG:HA	1:B:325:VAL:HG22	2.03	0.40
1:E:312:LYS:O	1:E:313:ARG:HG3	2.21	0.40
1:D:490:GLN:O	1:D:494:GLN:HB2	2.21	0.40
1:B:113:ARG:HD3	1:B:181:VAL:O	2.21	0.40
1:C:635:ARG:HA	1:C:636:PRO:HD3	1.85	0.40
1:C:259:ALA:CB	1:C:266:PHE:HB2	2.51	0.40
1:C:29:ASP:CB	1:C:81:LYS:HB3	2.52	0.40
1:F:29:ASP:CB	1:F:81:LYS:HB3	2.52	0.40
1:E:239:ARG:HD2	1:E:361:GLY:HA2	2.04	0.40
1:C:239:ARG:HD2	1:C:361:GLY:HA2	2.03	0.40
1:E:41:LEU:HA	1:E:41:LEU:HD23	1.87	0.40
1:D:239:ARG:HD2	1:D:361:GLY:HA2	2.04	0.40
1:D:28:VAL:CG2	1:D:94:VAL:HG21	2.51	0.40
1:D:312:LYS:C	1:D:313:ARG:HG3	2.40	0.40
1:A:312:LYS:O	1:A:313:ARG:HG3	2.21	0.40
1:D:259:ALA:CB	1:D:266:PHE:HB2	2.51	0.40
1:A:471:VAL:HG11	1:A:536:GLN:OE1	2.21	0.40
1:E:29:ASP:CB	1:E:81:LYS:HB3	2.52	0.40
1:C:427:MET:O	1:C:429:LEU:N	2.55	0.40
1:F:427:MET:SD	1:F:441:VAL:HG22	2.61	0.40
1:B:427:MET:O	1:B:429:LEU:N	2.54	0.40
1:C:560:ARG:HG2	1:C:607:GLU:OE2	2.21	0.40
1:B:239:ARG:HD2	1:B:361:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LEU:HD11	1:B:456:LEU:HD12	2.04	0.40
1:D:306:LEU:HD23	1:D:353:ILE:HG21	2.04	0.40
1:B:47:ASP:HA	1:B:50:GLN:HA	2.03	0.40
1:C:47:ASP:HA	1:C:50:GLN:HA	2.02	0.40
1:E:92:LEU:HD23	1:E:100:ILE:HG21	2.04	0.40
1:A:28:VAL:CG2	1:A:94:VAL:HG21	2.51	0.40
1:D:482:LEU:O	1:D:486:LYS:HG3	2.21	0.40
1:B:382:GLN:O	1:B:386:LYS:HG3	2.22	0.40
1:E:666:VAL:HA	1:E:731:ILE:CG2	2.51	0.40
1:E:489:LEU:HD21	1:E:516:PHE:CE1	2.56	0.40
1:F:489:LEU:HD21	1:F:516:PHE:CE1	2.56	0.40
1:B:113:ARG:H	1:B:180:THR:HB	1.86	0.40
1:C:303:ILE:HG21	1:C:303:ILE:HD13	1.74	0.40
1:E:259:ALA:CB	1:E:266:PHE:HB2	2.52	0.40
1:C:295:LYS:HB2	1:C:295:LYS:HE2	1.76	0.40
1:A:29:ASP:CB	1:A:81:LYS:HB3	2.52	0.40
1:B:508:MET:HE2	1:B:508:MET:HB3	1.95	0.40
1:E:306:LEU:HD23	1:E:353:ILE:HG21	2.04	0.40
1:B:560:ARG:HG2	1:B:607:GLU:OE2	2.21	0.40
1:A:213:LEU:HD12	1:A:213:LEU:HA	1.91	0.40
1:D:41:LEU:HA	1:D:41:LEU:HD23	1.87	0.40
1:D:48:GLU:N	1:D:48:GLU:OE1	2.48	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	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
1	B	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
1	C	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
1	E	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
1	F	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
All	All	4314/4836 (89%)	4032 (94%)	264 (6%)	18 (0%)	43	56

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	VAL
1	B	235	VAL
1	C	235	VAL
1	D	235	VAL
1	E	235	VAL
1	F	235	VAL
1	A	428	ASP
1	B	428	ASP
1	C	428	ASP
1	D	428	ASP
1	E	428	ASP
1	F	428	ASP
1	A	613	THR
1	B	613	THR
1	C	613	THR
1	D	613	THR
1	E	613	THR
1	F	613	THR

### 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	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	B	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	C	615/678 (91%)	612 (100%)	3 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	E	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	F	615/678 (91%)	612 (100%)	3 (0%)	92	97
All	All	3690/4068 (91%)	3672 (100%)	18 (0%)	92	97

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	LEU
1	A	367	VAL
1	A	563	PHE
1	B	286	LEU
1	B	367	VAL
1	B	563	PHE
1	C	286	LEU
1	C	367	VAL
1	C	563	PHE
1	D	286	LEU
1	D	367	VAL
1	D	563	PHE
1	E	286	LEU
1	E	367	VAL
1	E	563	PHE
1	F	286	LEU
1	F	367	VAL
1	F	563	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	103	GLN
1	A	129	ASN
1	A	285	ASN
1	A	406	HIS
1	A	443	ASN
1	A	558	ASN
1	B	50	GLN
1	B	103	GLN
1	B	129	ASN

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Mol	Chain	Res	Type
1	B	285	ASN
1	B	406	HIS
1	B	443	ASN
1	B	558	ASN
1	C	50	GLN
1	C	103	GLN
1	C	129	ASN
1	C	285	ASN
1	C	337	GLN
1	C	406	HIS
1	C	443	ASN
1	C	558	ASN
1	D	50	GLN
1	D	103	GLN
1	D	129	ASN
1	D	285	ASN
1	D	337	GLN
1	D	406	HIS
1	D	443	ASN
1	D	558	ASN
1	E	50	GLN
1	E	103	GLN
1	E	129	ASN
1	E	285	ASN
1	E	337	GLN
1	E	406	HIS
1	E	443	ASN
1	E	558	ASN
1	F	50	GLN
1	F	103	GLN
1	F	129	ASN
1	F	285	ASN
1	F	406	HIS
1	F	443	ASN
1	F	558	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	ADP	A	807	-	24,29,29	1.00	1 (4%)	23,45,45	1.90	2 (8%)
2	ADP	A	900	-	24,29,29	0.98	1 (4%)	23,45,45	1.92	4 (17%)
2	ADP	B	807	-	24,29,29	0.99	1 (4%)	23,45,45	1.89	2 (8%)
2	ADP	B	900	-	24,29,29	0.99	1 (4%)	23,45,45	1.93	4 (17%)
2	ADP	C	807	-	24,29,29	1.00	1 (4%)	23,45,45	1.89	2 (8%)
2	ADP	C	900	-	24,29,29	0.98	1 (4%)	23,45,45	1.93	4 (17%)
2	ADP	D	807	-	24,29,29	1.00	1 (4%)	23,45,45	1.91	2 (8%)
2	ADP	D	900	-	24,29,29	0.98	1 (4%)	23,45,45	1.93	4 (17%)
2	ADP	E	807	-	24,29,29	0.99	1 (4%)	23,45,45	1.89	2 (8%)
2	ADP	E	900	-	24,29,29	0.99	1 (4%)	23,45,45	1.92	4 (17%)
2	ADP	F	807	-	24,29,29	1.00	1 (4%)	23,45,45	1.91	2 (8%)
2	ADP	F	900	-	24,29,29	0.99	1 (4%)	23,45,45	1.92	4 (17%)

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	ADP	A	807	-	-	0/12/32/32	0/3/3/3
2	ADP	A	900	-	-	0/12/32/32	0/3/3/3
2	ADP	B	807	-	-	0/12/32/32	0/3/3/3
2	ADP	B	900	-	-	0/12/32/32	0/3/3/3
2	ADP	C	807	-	-	0/12/32/32	0/3/3/3
2	ADP	C	900	-	-	0/12/32/32	0/3/3/3
2	ADP	D	807	-	-	0/12/32/32	0/3/3/3
2	ADP	D	900	-	-	0/12/32/32	0/3/3/3
2	ADP	E	807	-	-	0/12/32/32	0/3/3/3
2	ADP	E	900	-	-	0/12/32/32	0/3/3/3
2	ADP	F	807	-	-	0/12/32/32	0/3/3/3
2	ADP	F	900	-	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	807	ADP	C5-C4	2.21	1.45	1.40
2	E	807	ADP	C5-C4	2.21	1.45	1.40
2	B	807	ADP	C5-C4	2.21	1.45	1.40
2	F	807	ADP	C5-C4	2.22	1.45	1.40
2	A	807	ADP	C5-C4	2.23	1.45	1.40
2	D	807	ADP	C5-C4	2.25	1.45	1.40
2	D	900	ADP	C5-C4	2.36	1.45	1.40
2	E	900	ADP	C5-C4	2.37	1.45	1.40
2	C	900	ADP	C5-C4	2.38	1.45	1.40
2	A	900	ADP	C5-C4	2.38	1.45	1.40
2	B	900	ADP	C5-C4	2.40	1.45	1.40
2	F	900	ADP	C5-C4	2.41	1.45	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	807	ADP	N3-C2-N1	-7.14	123.26	128.87
2	D	807	ADP	N3-C2-N1	-7.14	123.26	128.87
2	A	807	ADP	N3-C2-N1	-7.09	123.30	128.87
2	E	807	ADP	N3-C2-N1	-7.07	123.32	128.87
2	C	807	ADP	N3-C2-N1	-7.07	123.32	128.87
2	B	807	ADP	N3-C2-N1	-7.05	123.33	128.87
2	B	900	ADP	N3-C2-N1	-6.45	123.80	128.87
2	D	900	ADP	N3-C2-N1	-6.45	123.80	128.87
2	C	900	ADP	N3-C2-N1	-6.42	123.83	128.87
2	A	900	ADP	N3-C2-N1	-6.41	123.84	128.87
2	E	900	ADP	N3-C2-N1	-6.38	123.86	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	900	ADP	N3-C2-N1	-6.37	123.86	128.87
2	C	900	ADP	C2'-C1'-N9	-3.42	104.31	113.47
2	B	900	ADP	C2'-C1'-N9	-3.42	104.32	113.47
2	A	900	ADP	C2'-C1'-N9	-3.41	104.33	113.47
2	D	900	ADP	C2'-C1'-N9	-3.41	104.34	113.47
2	E	900	ADP	C2'-C1'-N9	-3.41	104.35	113.47
2	F	900	ADP	C2'-C1'-N9	-3.40	104.36	113.47
2	C	807	ADP	C4'-O4'-C1'	2.18	111.95	109.64
2	C	900	ADP	O3B-PB-O2B	2.22	115.58	107.44
2	B	900	ADP	O3B-PB-O2B	2.22	115.58	107.44
2	D	807	ADP	C4'-O4'-C1'	2.22	112.00	109.64
2	A	807	ADP	C4'-O4'-C1'	2.22	112.00	109.64
2	A	900	ADP	O3B-PB-O2B	2.22	115.60	107.44
2	B	807	ADP	C4'-O4'-C1'	2.22	112.00	109.64
2	F	900	ADP	O3B-PB-O2B	2.23	115.62	107.44
2	E	807	ADP	C4'-O4'-C1'	2.23	112.00	109.64
2	E	900	ADP	O3B-PB-O2B	2.23	115.62	107.44
2	D	900	ADP	O3B-PB-O2B	2.23	115.64	107.44
2	F	807	ADP	C4'-O4'-C1'	2.25	112.03	109.64
2	B	900	ADP	C4'-O4'-C1'	2.60	112.40	109.64
2	E	900	ADP	C4'-O4'-C1'	2.60	112.40	109.64
2	D	900	ADP	C4'-O4'-C1'	2.60	112.40	109.64
2	F	900	ADP	C4'-O4'-C1'	2.61	112.41	109.64
2	A	900	ADP	C4'-O4'-C1'	2.61	112.41	109.64
2	C	900	ADP	C4'-O4'-C1'	2.62	112.42	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	807	ADP	1	0
2	A	900	ADP	2	0
2	B	807	ADP	1	0
2	B	900	ADP	2	0
2	C	807	ADP	1	0
2	C	900	ADP	2	0
2	D	807	ADP	1	0
2	D	900	ADP	2	0
2	E	807	ADP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	900	ADP	2	0
2	F	807	ADP	1	0
2	F	900	ADP	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.