



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:41 am GMT

PDB ID : 1L1F  
Title : Structure of human glutamate dehydrogenase-apo form  
Authors : Smith, T.J.; Schmidt, T.; Fang, J.; Wu, J.; Siuzdak, G.; Stanley, C.A.  
Deposited on : 2002-02-15  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

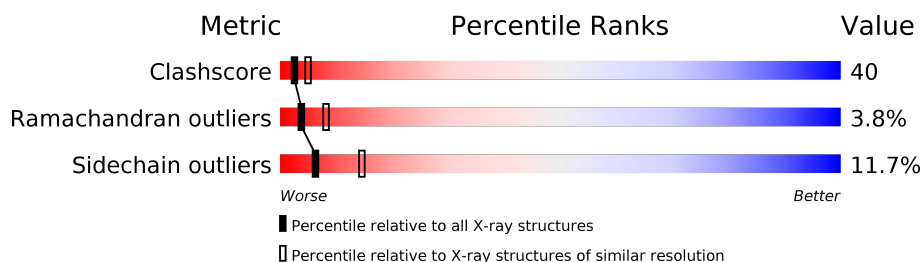
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	505	
1	B	505	
1	C	505	
1	D	505	
1	E	505	
1	F	505	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23244 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate Dehydrogenase 1.

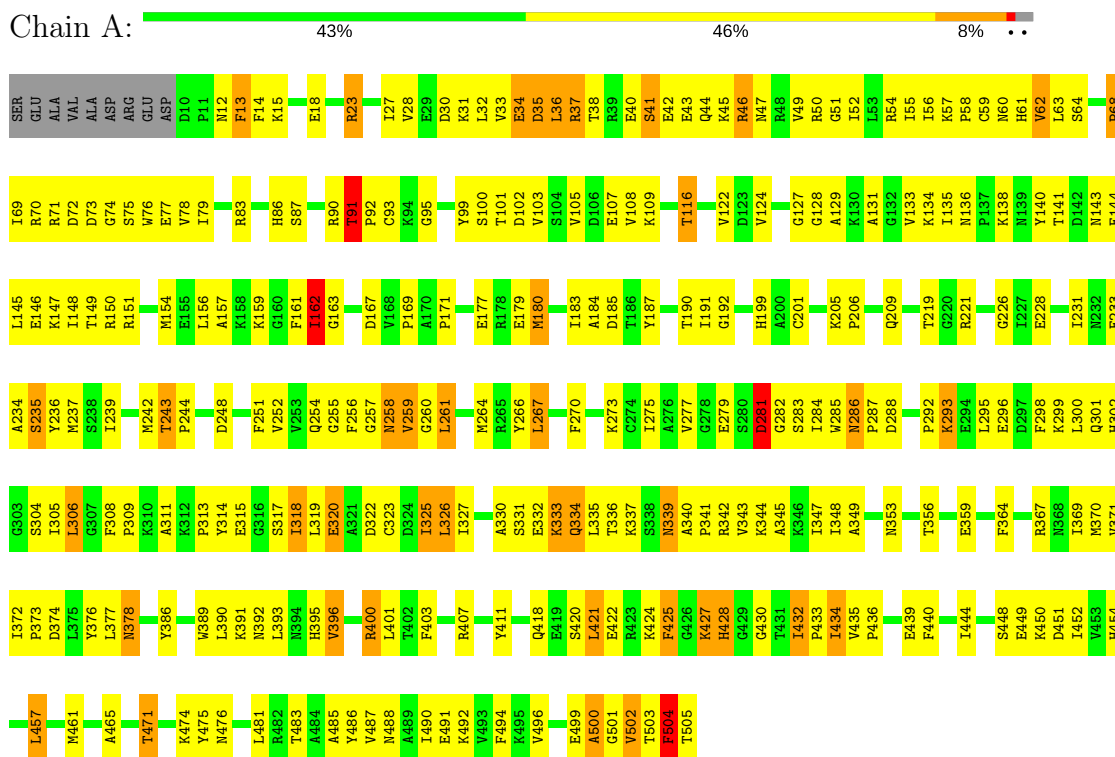
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	B	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	C	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	D	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	E	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	F	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			

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

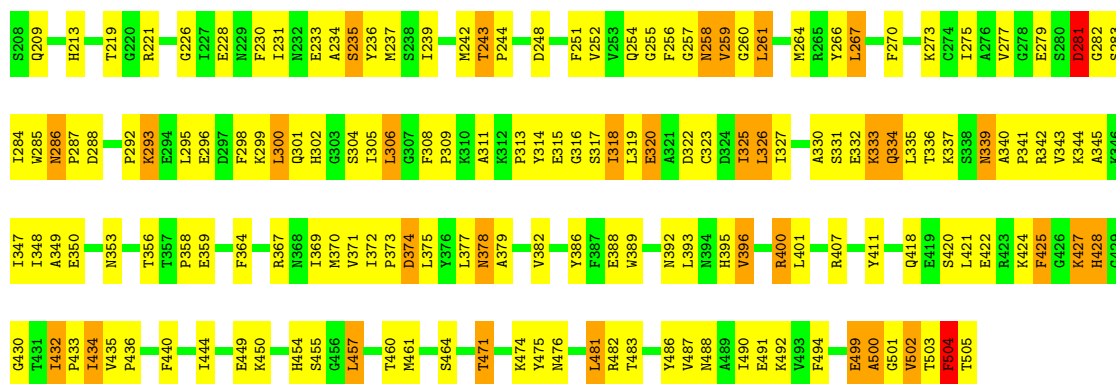
Note EDS was not executed.

#### • Molecule 1: Glutamate Dehydrogenase 1



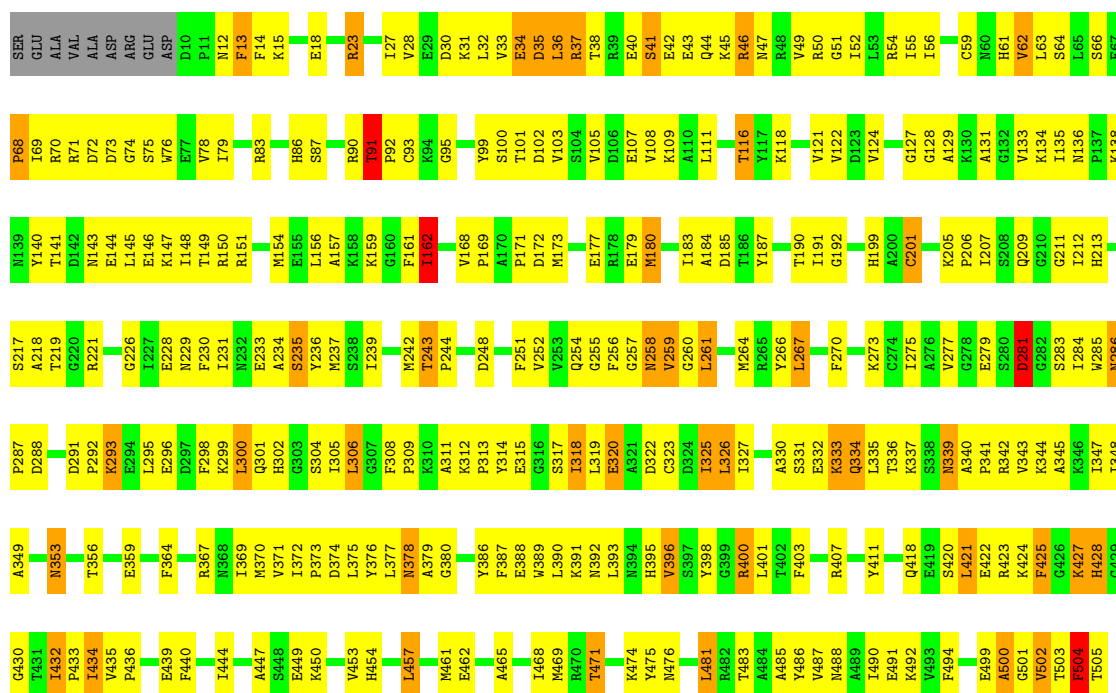
#### • Molecule 1: Glutamate Dehydrogenase 1





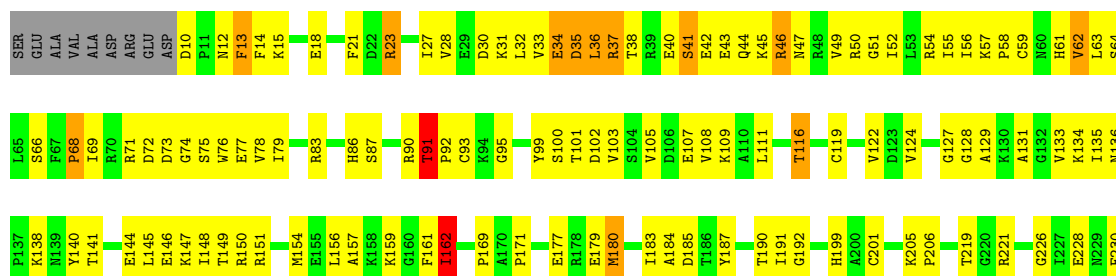
• Molecule 1: Glutamate Dehydrogenase 1

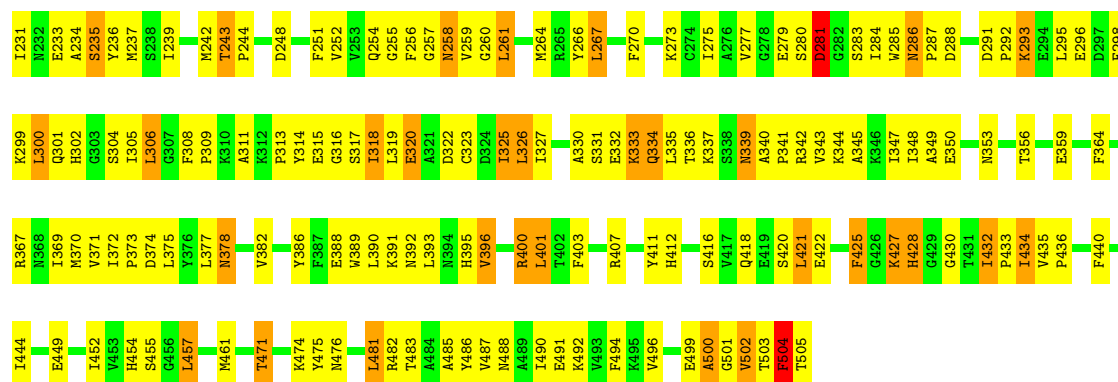
Chain C: 40% 49% 9% ..



• Molecule 1: Glutamate Dehydrogenase 1

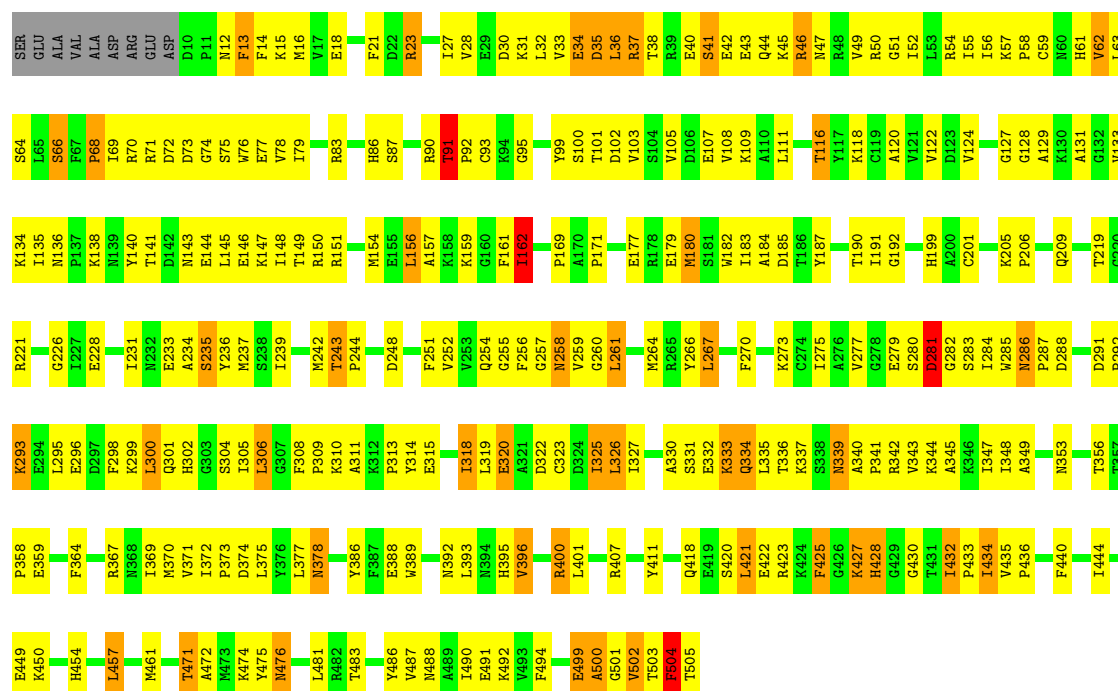
Chain D: 43% 46% 9% ..





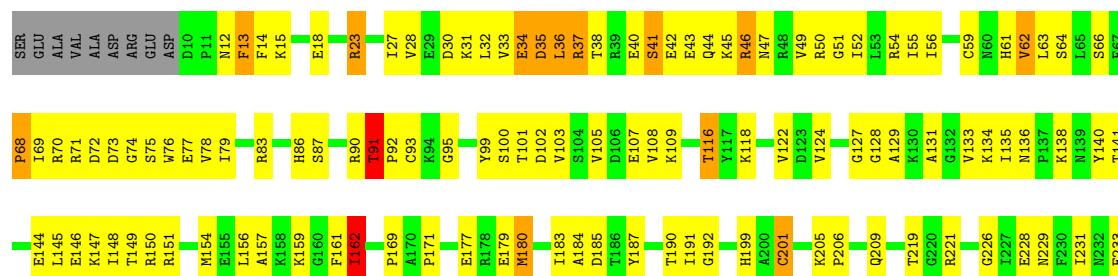
• Molecule 1: Glutamate Dehydrogenase 1

Chain E: 43% 45% 9% ..



• Molecule 1: Glutamate Dehydrogenase 1

Chain F: 43% 46% 8% ..



A234	A235	A236	A237	A238	A239	A240	A241	A242	A243	A244	A245	A246	A247	A248	A249	A250	A251	A252	A253	A254	A255	A256	A257	A258	A259	A260	A261	A262	A263	A264	A265	A266	A267	A268	A269	A270	A271	A272	A273	A274	A275	A276	A277	A278	A279	A280	A281	A282	A283	A284	A285	A286	A287	A288	A289	A290	A291	A292	A293	A294	A295	A296	A297	A298	A299	A300	A301	A302
G303	S304	I305	L306	G307	F308	P309	K310	A311	K312	P313	Y314	E315	G316	S317	I318	L319	E320	A321	D322	C323	I324	I325	L326	I327	P328	A329	A330	S331	E332	K333	Q334	L335	T336	K337	S338	N339	A340	P341	R342	V343	K344	A345	K346	I347	I348	A349	D348	N353	P352	T356	E359	F364	R367	N368	I369	M370												
V371	I372	D373	L374	Y375	R376	L377	N378	A379	Y386	K389	L390	K391	N392	L393	N394	H395	V396	R400	L401	T402	F403	R407	Y411	Q418	E419	S420	L421	E422	R423	K424	F425	G426	K427	H428	G429	G430	T431	I432	P433	I434	V435	P436	E439	F440	I444	A447	S448	E449	K450																			
H454	L457	E462	R463	S464	A465	T471	K474	Y475	N476	L481	R482	T483	A484	A485	Y486	V487	N488	A489	I490	E491	K492	F494	E499	A500	G501	V502	T503	F504	T505																																							

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.80Å 98.80Å 124.20Å 86.26° 70.28° 60.34°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	O	Depositor
R, $R_{free}$	0.262 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.62	1/3958 (0.0%)	0.82	3/5340 (0.1%)
1	B	0.63	1/3958 (0.0%)	0.82	5/5340 (0.1%)
1	C	0.65	2/3958 (0.1%)	0.82	4/5340 (0.1%)
1	D	0.62	1/3958 (0.0%)	0.82	5/5340 (0.1%)
1	E	0.62	1/3958 (0.0%)	0.82	4/5340 (0.1%)
1	F	0.62	2/3958 (0.1%)	0.82	5/5340 (0.1%)
All	All	0.63	8/23748 (0.0%)	0.82	26/32040 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	CYS	CB-SG	8.91	1.97	1.82
1	C	59	CYS	CB-SG	8.33	1.96	1.82
1	A	59	CYS	CB-SG	7.79	1.95	1.82
1	B	59	CYS	CB-SG	7.48	1.95	1.82
1	F	201	CYS	CB-SG	-7.10	1.70	1.82
1	E	59	CYS	CB-SG	6.18	1.92	1.82
1	C	201	CYS	CB-SG	-6.09	1.71	1.82
1	F	59	CYS	CB-SG	5.80	1.92	1.82

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	504	PHE	N-CA-C	-7.28	91.34	111.00
1	C	504	PHE	N-CA-C	-7.28	91.35	111.00
1	B	504	PHE	N-CA-C	-7.27	91.38	111.00
1	F	504	PHE	N-CA-C	-7.25	91.43	111.00
1	D	504	PHE	N-CA-C	-7.19	91.60	111.00
1	A	504	PHE	N-CA-C	-7.17	91.64	111.00
1	D	326	LEU	CA-CB-CG	6.70	130.71	115.30
1	C	326	LEU	CA-CB-CG	6.64	130.58	115.30
1	E	326	LEU	CA-CB-CG	6.63	130.55	115.30
1	F	326	LEU	CA-CB-CG	6.63	130.54	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	LEU	CA-CB-CG	6.60	130.47	115.30
1	B	326	LEU	CA-CB-CG	6.58	130.43	115.30
1	B	91	THR	N-CA-C	6.03	127.29	111.00
1	C	91	THR	N-CA-C	6.02	127.25	111.00
1	F	91	THR	N-CA-C	5.93	127.03	111.00
1	A	91	THR	N-CA-C	5.87	126.85	111.00
1	E	91	THR	N-CA-C	5.86	126.83	111.00
1	D	91	THR	N-CA-C	5.84	126.77	111.00
1	F	66	SER	N-CA-C	-5.11	97.21	111.00
1	B	316	GLY	N-CA-C	-5.09	100.38	113.10
1	E	66	SER	N-CA-C	-5.08	97.27	111.00
1	D	66	SER	N-CA-C	-5.06	97.35	111.00
1	F	316	GLY	N-CA-C	-5.05	100.47	113.10
1	B	374	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	316	GLY	N-CA-C	-5.03	100.53	113.10
1	C	66	SER	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	3874	0	3841	316	0
1	B	3874	0	3841	333	0
1	C	3874	0	3841	366	0
1	D	3874	0	3841	326	0
1	E	3874	0	3841	341	0
1	F	3874	0	3841	324	0
All	All	23244	0	23046	1865	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 40.

All (1865) 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:C:285:TRP:HB2	1:C:314:TYR:HB2	1.31	1.13
1:E:285:TRP:HB2	1:E:314:TYR:HB2	1.30	1.12
1:F:285:TRP:HB2	1:F:314:TYR:HB2	1.29	1.09
1:A:285:TRP:HB2	1:A:314:TYR:HB2	1.30	1.08
1:B:285:TRP:HB2	1:B:314:TYR:HB2	1.29	1.08
1:D:285:TRP:HB2	1:D:314:TYR:HB2	1.29	1.06
1:C:427:LYS:HD3	1:C:430:GLY:HA3	1.45	0.99
1:E:427:LYS:HD3	1:E:430:GLY:HA3	1.45	0.98
1:A:99:TYR:OH	1:A:149:THR:HG22	1.63	0.98
1:F:427:LYS:HD3	1:F:430:GLY:HA3	1.46	0.98
1:A:427:LYS:HD3	1:A:430:GLY:HA3	1.46	0.97
1:D:427:LYS:HD3	1:D:430:GLY:HA3	1.47	0.96
1:C:99:TYR:OH	1:C:149:THR:HG22	1.65	0.95
1:B:427:LYS:HD3	1:B:430:GLY:HA3	1.46	0.94
1:E:99:TYR:OH	1:E:149:THR:HG22	1.69	0.93
1:B:99:TYR:OH	1:B:149:THR:HG22	1.68	0.93
1:F:99:TYR:OH	1:F:149:THR:HG22	1.68	0.93
1:E:41:SER:HA	1:E:46:ARG:HD2	1.50	0.93
1:C:61:HIS:HD2	1:F:159:LYS:HE3	1.33	0.93
1:A:40:GLU:HG3	1:A:46:ARG:HH12	1.35	0.92
1:D:41:SER:HA	1:D:46:ARG:HD2	1.50	0.92
1:F:41:SER:HA	1:F:46:ARG:HD2	1.50	0.92
1:B:41:SER:HA	1:B:46:ARG:HD2	1.51	0.92
1:C:159:LYS:HE3	1:F:61:HIS:HD2	1.35	0.92
1:F:40:GLU:HG3	1:F:46:ARG:HH12	1.35	0.92
1:E:327:ILE:HG22	1:E:349:ALA:HB3	1.53	0.91
1:C:40:GLU:HG3	1:C:46:ARG:HH12	1.35	0.91
1:A:327:ILE:HG22	1:A:349:ALA:HB3	1.53	0.91
1:C:41:SER:HA	1:C:46:ARG:HD2	1.50	0.91
1:B:327:ILE:HG22	1:B:349:ALA:HB3	1.53	0.91
1:A:41:SER:HA	1:A:46:ARG:HD2	1.51	0.90
1:D:99:TYR:OH	1:D:149:THR:HG22	1.67	0.90
1:E:40:GLU:HG3	1:E:46:ARG:HH12	1.36	0.90
1:E:83:ARG:HD2	1:E:131:ALA:HB2	1.54	0.90
1:A:83:ARG:HD2	1:A:131:ALA:HB2	1.53	0.89
1:B:40:GLU:HG3	1:B:46:ARG:HH12	1.36	0.89
1:F:83:ARG:HD2	1:F:131:ALA:HB2	1.53	0.89
1:C:83:ARG:HD2	1:C:131:ALA:HB2	1.55	0.89
1:F:327:ILE:HG22	1:F:349:ALA:HB3	1.53	0.89
1:D:327:ILE:HG22	1:D:349:ALA:HB3	1.53	0.89
1:D:40:GLU:HG3	1:D:46:ARG:HH12	1.35	0.89
1:E:427:LYS:HA	1:E:427:LYS:HE2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:427:LYS:HE2	1:F:427:LYS:HA	1.55	0.88
1:D:83:ARG:HD2	1:D:131:ALA:HB2	1.54	0.88
1:C:427:LYS:HE2	1:C:427:LYS:HA	1.54	0.88
1:B:83:ARG:HD2	1:B:131:ALA:HB2	1.54	0.87
1:D:427:LYS:HE2	1:D:427:LYS:HA	1.54	0.87
1:D:325:ILE:HG22	1:D:347:ILE:HB	1.56	0.87
1:B:427:LYS:HA	1:B:427:LYS:HE2	1.55	0.87
1:B:61:HIS:HD2	1:D:159:LYS:HE3	1.39	0.87
1:F:325:ILE:HG22	1:F:347:ILE:HB	1.56	0.87
1:A:325:ILE:HG22	1:A:347:ILE:HB	1.56	0.86
1:C:325:ILE:HG22	1:C:347:ILE:HB	1.57	0.86
1:C:327:ILE:HG22	1:C:349:ALA:HB3	1.54	0.86
1:C:159:LYS:HE3	1:F:61:HIS:CD2	2.11	0.86
1:A:427:LYS:HA	1:A:427:LYS:HE2	1.55	0.86
1:A:159:LYS:HE3	1:E:61:HIS:HD2	1.41	0.85
1:E:325:ILE:HG22	1:E:347:ILE:HB	1.56	0.85
1:D:145:LEU:O	1:D:149:THR:HG23	1.76	0.85
1:C:145:LEU:O	1:C:149:THR:HG23	1.77	0.85
1:B:418:GLN:HB2	1:B:433:PRO:HD2	1.60	0.84
1:C:61:HIS:CD2	1:F:159:LYS:HE3	2.11	0.84
1:F:145:LEU:O	1:F:149:THR:HG23	1.76	0.84
1:B:159:LYS:HE3	1:D:61:HIS:HD2	1.40	0.84
1:D:146:GLU:O	1:D:150:ARG:HG3	1.77	0.84
1:C:376:TYR:OH	1:C:465:ALA:HB2	1.77	0.83
1:C:13:PHE:HD1	1:C:14:PHE:N	1.77	0.82
1:E:486:TYR:O	1:E:490:ILE:HG12	1.79	0.82
1:D:147:LYS:HD2	1:D:151:ARG:HH21	1.44	0.82
1:E:146:GLU:O	1:E:150:ARG:HG3	1.79	0.82
1:E:418:GLN:HB2	1:E:433:PRO:HD2	1.61	0.82
1:A:418:GLN:HB2	1:A:433:PRO:HD2	1.62	0.82
1:F:13:PHE:HD1	1:F:14:PHE:N	1.77	0.82
1:B:13:PHE:HD1	1:B:14:PHE:N	1.78	0.82
1:E:147:LYS:HD2	1:E:151:ARG:HH21	1.45	0.82
1:A:145:LEU:O	1:A:149:THR:HG23	1.80	0.82
1:B:147:LYS:HD2	1:B:151:ARG:HH21	1.45	0.82
1:B:325:ILE:HG22	1:B:347:ILE:HB	1.58	0.82
1:B:86:HIS:CD2	1:B:116:THR:HG21	2.14	0.82
1:D:13:PHE:HD1	1:D:14:PHE:N	1.77	0.82
1:C:229:ASN:OD1	1:C:462:GLU:HG3	1.78	0.82
1:D:486:TYR:O	1:D:490:ILE:HG12	1.79	0.82
1:E:13:PHE:HD1	1:E:14:PHE:N	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:HIS:CD2	1:E:116:THR:HG21	2.14	0.82
1:F:147:LYS:HD2	1:F:151:ARG:HH21	1.45	0.81
1:F:486:TYR:O	1:F:490:ILE:HG12	1.80	0.81
1:B:145:LEU:O	1:B:149:THR:HG23	1.79	0.81
1:C:38:THR:HG23	1:C:41:SER:HB3	1.62	0.81
1:E:145:LEU:O	1:E:149:THR:HG23	1.79	0.81
1:A:13:PHE:HD1	1:A:14:PHE:N	1.77	0.81
1:E:38:THR:HG23	1:E:41:SER:HB3	1.62	0.81
1:F:146:GLU:O	1:F:150:ARG:HG3	1.79	0.81
1:A:146:GLU:O	1:A:150:ARG:HG3	1.81	0.81
1:A:38:THR:HG23	1:A:41:SER:HB3	1.63	0.81
1:D:418:GLN:HB2	1:D:433:PRO:HD2	1.61	0.81
1:A:86:HIS:CD2	1:A:116:THR:HG21	2.16	0.81
1:A:486:TYR:O	1:A:490:ILE:HG12	1.80	0.81
1:F:38:THR:HG23	1:F:41:SER:HB3	1.63	0.81
1:C:116:THR:HG22	1:C:128:GLY:HA3	1.63	0.81
1:A:61:HIS:HD2	1:E:159:LYS:HE3	1.47	0.80
1:C:486:TYR:O	1:C:490:ILE:HG12	1.81	0.80
1:B:486:TYR:O	1:B:490:ILE:HG12	1.81	0.80
1:D:38:THR:HG23	1:D:41:SER:HB3	1.63	0.80
1:C:147:LYS:HD2	1:C:151:ARG:HH21	1.45	0.80
1:D:86:HIS:CD2	1:D:116:THR:HG21	2.17	0.80
1:F:63:LEU:HD22	1:F:161:PHE:CD2	2.16	0.80
1:F:418:GLN:HB2	1:F:433:PRO:HD2	1.63	0.80
1:F:86:HIS:CD2	1:F:116:THR:HG21	2.16	0.80
1:A:147:LYS:HD2	1:A:151:ARG:HH21	1.45	0.80
1:A:116:THR:HG22	1:A:128:GLY:HA3	1.64	0.80
1:B:146:GLU:O	1:B:150:ARG:HG3	1.82	0.80
1:C:146:GLU:O	1:C:150:ARG:HG3	1.82	0.80
1:C:63:LEU:HD22	1:C:161:PHE:CD2	2.17	0.80
1:B:285:TRP:CB	1:B:314:TYR:HB2	2.11	0.79
1:B:38:THR:HG23	1:B:41:SER:HB3	1.63	0.79
1:D:285:TRP:CB	1:D:314:TYR:HB2	2.12	0.79
1:E:63:LEU:HD22	1:E:161:PHE:CD2	2.17	0.79
1:B:77:GLU:HA	1:D:54:ARG:NH1	1.97	0.79
1:D:505:THR:HG23	1:E:185:ASP:OD1	1.82	0.79
1:F:221:ARG:HD2	1:F:454:HIS:NE2	1.97	0.79
1:C:86:HIS:CD2	1:C:116:THR:HG21	2.16	0.79
1:E:285:TRP:CB	1:E:314:TYR:HB2	2.12	0.79
1:A:281:ASP:HB2	1:A:306:LEU:HD11	1.64	0.79
1:C:281:ASP:HB2	1:C:306:LEU:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ASP:HB2	1:D:306:LEU:HD11	1.64	0.79
1:B:281:ASP:HB2	1:B:306:LEU:HD11	1.64	0.78
1:D:63:LEU:HD22	1:D:161:PHE:CD2	2.19	0.78
1:A:13:PHE:HD1	1:A:14:PHE:H	1.32	0.78
1:F:116:THR:HG22	1:F:128:GLY:HA3	1.66	0.78
1:F:281:ASP:HB2	1:F:306:LEU:HD11	1.65	0.78
1:B:63:LEU:HD22	1:B:161:PHE:CD2	2.18	0.78
1:C:418:GLN:HB2	1:C:433:PRO:HD2	1.64	0.78
1:B:61:HIS:CD2	1:D:159:LYS:HE3	2.19	0.77
1:C:221:ARG:HD2	1:C:454:HIS:CD2	2.20	0.77
1:D:116:THR:HG22	1:D:128:GLY:HA3	1.66	0.77
1:A:71:ARG:HH11	1:A:71:ARG:HB3	1.50	0.77
1:D:13:PHE:HD1	1:D:14:PHE:H	1.32	0.77
1:B:13:PHE:HD1	1:B:14:PHE:H	1.32	0.77
1:A:285:TRP:CB	1:A:314:TYR:HB2	2.13	0.77
1:A:63:LEU:HD22	1:A:161:PHE:CD2	2.21	0.76
1:E:116:THR:HG22	1:E:128:GLY:HA3	1.67	0.76
1:D:71:ARG:HH11	1:D:71:ARG:HB3	1.51	0.76
1:E:71:ARG:HB3	1:E:71:ARG:HH11	1.50	0.76
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.67	0.76
1:B:116:THR:HG22	1:B:128:GLY:HA3	1.65	0.76
1:C:504:PHE:CZ	1:F:151:ARG:NH2	2.52	0.76
1:E:281:ASP:HB2	1:E:306:LEU:HD11	1.64	0.76
1:B:340:ALA:HB3	1:B:341:PRO:HD3	1.66	0.76
1:F:13:PHE:HD1	1:F:14:PHE:H	1.31	0.76
1:A:159:LYS:HE3	1:E:61:HIS:CD2	2.20	0.75
1:B:71:ARG:HH11	1:B:71:ARG:HB3	1.51	0.75
1:C:285:TRP:CB	1:C:314:TYR:HB2	2.13	0.75
1:C:71:ARG:HB3	1:C:71:ARG:HH11	1.51	0.75
1:E:13:PHE:HD1	1:E:14:PHE:H	1.32	0.75
1:B:159:LYS:HE3	1:D:61:HIS:CD2	2.22	0.75
1:D:340:ALA:HB3	1:D:341:PRO:HD3	1.68	0.75
1:E:221:ARG:HD2	1:E:454:HIS:NE2	2.01	0.75
1:F:434:ILE:O	1:F:436:PRO:HD3	1.87	0.74
1:A:340:ALA:HB3	1:A:341:PRO:HD3	1.69	0.74
1:F:285:TRP:CB	1:F:314:TYR:HB2	2.12	0.74
1:C:13:PHE:HD1	1:C:14:PHE:H	1.32	0.74
1:F:71:ARG:HB3	1:F:71:ARG:HH11	1.52	0.74
1:C:434:ILE:O	1:C:436:PRO:HD3	1.88	0.74
1:A:434:ILE:O	1:A:436:PRO:HD3	1.87	0.74
1:F:340:ALA:HB3	1:F:341:PRO:HD3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:VAL:HG11	1:E:76:TRP:CD1	2.23	0.74
1:C:340:ALA:HB3	1:C:341:PRO:HD3	1.69	0.73
1:E:243:THR:N	1:E:244:PRO:HD3	2.03	0.73
1:A:251:PHE:HB3	1:A:325:ILE:HG13	1.69	0.73
1:B:284:ILE:HG23	1:B:311:ALA:HB1	1.71	0.73
1:B:251:PHE:HB3	1:B:325:ILE:HG13	1.69	0.73
1:B:434:ILE:O	1:B:436:PRO:HD3	1.89	0.73
1:C:420:SER:CB	1:E:433:PRO:HA	2.19	0.73
1:D:434:ILE:O	1:D:436:PRO:HD3	1.89	0.73
1:E:251:PHE:HB3	1:E:325:ILE:HG13	1.70	0.73
1:E:434:ILE:O	1:E:436:PRO:HD3	1.88	0.73
1:D:23:ARG:HE	1:D:27:ILE:HD11	1.54	0.73
1:D:318:ILE:H	1:D:318:ILE:HD13	1.54	0.73
1:C:23:ARG:HE	1:C:27:ILE:HD11	1.54	0.72
1:D:190:THR:HG23	1:F:190:THR:HG23	1.71	0.72
1:E:318:ILE:HD13	1:E:318:ILE:H	1.54	0.72
1:A:190:THR:HG23	1:C:190:THR:HG23	1.69	0.72
1:D:251:PHE:HB3	1:D:325:ILE:HG13	1.70	0.72
1:D:284:ILE:HG23	1:D:311:ALA:HB1	1.70	0.72
1:C:284:ILE:HG23	1:C:311:ALA:HB1	1.71	0.72
1:A:318:ILE:H	1:A:318:ILE:HD13	1.55	0.72
1:F:43:GLU:HB3	1:F:45:LYS:HG3	1.72	0.72
1:F:318:ILE:H	1:F:318:ILE:HD13	1.55	0.72
1:B:318:ILE:HD13	1:B:318:ILE:H	1.53	0.72
1:E:284:ILE:HG23	1:E:311:ALA:HB1	1.71	0.72
1:D:243:THR:N	1:D:244:PRO:HD3	2.05	0.71
1:B:502:VAL:HG23	1:B:503:THR:H	1.56	0.71
1:E:502:VAL:HG23	1:E:503:THR:H	1.56	0.71
1:F:243:THR:N	1:F:244:PRO:HD3	2.05	0.71
1:F:251:PHE:HB3	1:F:325:ILE:HG13	1.70	0.71
1:B:505:THR:HG23	1:F:185:ASP:OD1	1.90	0.71
1:A:279:GLU:HG3	1:A:305:ILE:HG13	1.73	0.71
1:B:27:ILE:HG22	1:B:475:TYR:CD1	2.24	0.71
1:E:69:ILE:HA	1:E:151:ARG:NH1	2.06	0.71
1:B:23:ARG:HE	1:B:27:ILE:HD11	1.56	0.71
1:E:43:GLU:HB3	1:E:45:LYS:HG3	1.72	0.71
1:A:23:ARG:HE	1:A:27:ILE:HD11	1.56	0.71
1:F:502:VAL:HG23	1:F:503:THR:H	1.55	0.71
1:B:190:THR:HG23	1:E:190:THR:HG23	1.73	0.71
1:B:243:THR:N	1:B:244:PRO:HD3	2.04	0.71
1:C:118:LYS:NZ	1:C:353:ASN:HD21	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:VAL:HG23	1:D:503:THR:H	1.55	0.71
1:C:243:THR:N	1:C:244:PRO:HD3	2.05	0.71
1:A:502:VAL:HG23	1:A:503:THR:H	1.55	0.71
1:A:43:GLU:HB3	1:A:45:LYS:HG3	1.73	0.70
1:C:43:GLU:HB3	1:C:45:LYS:HG3	1.73	0.70
1:A:243:THR:N	1:A:244:PRO:HD3	2.05	0.70
1:F:69:ILE:HA	1:F:151:ARG:NH1	2.07	0.70
1:C:221:ARG:HD2	1:C:454:HIS:NE2	2.06	0.70
1:C:251:PHE:HB3	1:C:325:ILE:HG13	1.73	0.70
1:D:279:GLU:HG3	1:D:305:ILE:HG13	1.72	0.70
1:A:284:ILE:HG23	1:A:311:ALA:HB1	1.72	0.70
1:F:23:ARG:HE	1:F:27:ILE:HD11	1.56	0.70
1:C:502:VAL:HG23	1:C:503:THR:H	1.56	0.69
1:F:284:ILE:HG23	1:F:311:ALA:HB1	1.73	0.69
1:B:279:GLU:HG3	1:B:305:ILE:HG13	1.74	0.69
1:B:43:GLU:HB3	1:B:45:LYS:HG3	1.73	0.69
1:E:23:ARG:HE	1:E:27:ILE:HD11	1.56	0.69
1:F:425:PHE:HD1	1:F:427:LYS:HB2	1.57	0.69
1:B:69:ILE:HA	1:B:151:ARG:NH1	2.07	0.69
1:A:61:HIS:CD2	1:E:159:LYS:HE3	2.28	0.69
1:B:78:VAL:N	1:D:54:ARG:HH12	1.91	0.69
1:F:285:TRP:HB2	1:F:314:TYR:CB	2.17	0.69
1:A:179:GLU:O	1:A:183:ILE:HG13	1.92	0.69
1:C:318:ILE:HD13	1:C:318:ILE:H	1.58	0.69
1:D:43:GLU:HB3	1:D:45:LYS:HG3	1.73	0.69
1:C:279:GLU:HG3	1:C:305:ILE:HG13	1.73	0.69
1:D:69:ILE:HA	1:D:151:ARG:NH1	2.08	0.69
1:F:229:ASN:OD1	1:F:462:GLU:HG3	1.93	0.69
1:B:343:VAL:HG21	1:B:364:PHE:HE1	1.58	0.69
1:D:28:VAL:CG2	1:D:487:VAL:HG13	2.23	0.69
1:E:279:GLU:HG3	1:E:305:ILE:HG13	1.73	0.69
1:C:116:THR:HG22	1:C:128:GLY:CA	2.22	0.68
1:D:179:GLU:O	1:D:183:ILE:HG13	1.94	0.68
1:D:336:THR:H	1:D:339:ASN:HD21	1.41	0.68
1:A:69:ILE:HA	1:A:151:ARG:NH1	2.07	0.68
1:C:400:ARG:HH11	1:C:400:ARG:HG3	1.58	0.68
1:C:69:ILE:HA	1:C:151:ARG:NH1	2.07	0.68
1:F:279:GLU:HG3	1:F:305:ILE:HG13	1.73	0.68
1:C:205:LYS:NZ	1:C:392:ASN:HD21	1.92	0.68
1:C:231:ILE:HD12	1:C:237:MET:SD	2.33	0.68
1:C:425:PHE:HD1	1:C:427:LYS:HB2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:ARG:HH11	1:E:400:ARG:HG3	1.59	0.68
1:F:336:THR:H	1:F:339:ASN:HD21	1.41	0.68
1:F:343:VAL:HG21	1:F:364:PHE:HE1	1.59	0.68
1:C:336:THR:H	1:C:339:ASN:HD21	1.41	0.68
1:D:231:ILE:HD12	1:D:237:MET:SD	2.33	0.68
1:A:336:THR:H	1:A:339:ASN:HD21	1.42	0.68
1:D:343:VAL:HG21	1:D:364:PHE:HE1	1.58	0.68
1:F:400:ARG:HG3	1:F:400:ARG:HH11	1.60	0.67
1:E:147:LYS:O	1:E:151:ARG:HG3	1.94	0.67
1:A:116:THR:HG22	1:A:128:GLY:CA	2.25	0.67
1:C:375:LEU:HD23	1:C:485:ALA:HB1	1.77	0.67
1:D:147:LYS:O	1:D:151:ARG:HG3	1.93	0.67
1:A:343:VAL:HG21	1:A:364:PHE:HE1	1.59	0.67
1:B:179:GLU:O	1:B:183:ILE:HG13	1.94	0.67
1:A:231:ILE:HD12	1:A:237:MET:SD	2.35	0.67
1:C:147:LYS:O	1:C:151:ARG:HG3	1.95	0.67
1:F:407:ARG:O	1:F:411:TYR:HD2	1.78	0.67
1:C:343:VAL:HG21	1:C:364:PHE:HE1	1.60	0.67
1:C:373:PRO:CG	1:C:481:LEU:HB3	2.25	0.67
1:E:62:VAL:HG21	1:E:105:VAL:HG13	1.77	0.67
1:A:71:ARG:HB3	1:A:71:ARG:NH1	2.11	0.67
1:B:231:ILE:HD12	1:B:237:MET:SD	2.35	0.67
1:E:179:GLU:O	1:E:183:ILE:HG13	1.94	0.66
1:D:298:PHE:CZ	1:D:302:HIS:HE1	2.13	0.66
1:C:122:VAL:HG11	1:C:379:ALA:CB	2.24	0.66
1:F:298:PHE:CZ	1:F:302:HIS:HE1	2.14	0.66
1:F:221:ARG:HD2	1:F:454:HIS:CD2	2.31	0.66
1:D:285:TRP:HB2	1:D:314:TYR:CB	2.17	0.66
1:A:407:ARG:O	1:A:411:TYR:HD2	1.79	0.66
1:E:336:THR:H	1:E:339:ASN:HD21	1.43	0.66
1:B:407:ARG:O	1:B:411:TYR:HD2	1.79	0.66
1:C:298:PHE:CZ	1:C:302:HIS:HE1	2.14	0.66
1:F:147:LYS:O	1:F:151:ARG:HG3	1.95	0.66
1:A:147:LYS:O	1:A:151:ARG:HG3	1.95	0.66
1:B:147:LYS:O	1:B:151:ARG:HG3	1.95	0.66
1:E:298:PHE:CZ	1:E:302:HIS:HE1	2.13	0.66
1:E:425:PHE:HD1	1:E:427:LYS:HB2	1.60	0.66
1:E:27:ILE:HG22	1:E:475:TYR:CD1	2.31	0.66
1:A:298:PHE:CZ	1:A:302:HIS:HE1	2.14	0.66
1:C:285:TRP:HB2	1:C:314:TYR:CB	2.18	0.66
1:E:285:TRP:HB2	1:E:314:TYR:CB	2.18	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:VAL:HG21	1:E:364:PHE:HE1	1.59	0.66
1:F:433:PRO:O	1:F:435:VAL:N	2.29	0.65
1:B:298:PHE:CZ	1:B:302:HIS:HE1	2.13	0.65
1:B:336:THR:H	1:B:339:ASN:HD21	1.42	0.65
1:F:231:ILE:HD12	1:F:237:MET:SD	2.36	0.65
1:B:116:THR:HG22	1:B:128:GLY:CA	2.26	0.65
1:B:264:MET:CE	1:B:292:PRO:HA	2.26	0.65
1:C:277:VAL:HG21	1:C:295:LEU:CD2	2.26	0.65
1:D:425:PHE:HD1	1:D:427:LYS:HB2	1.60	0.65
1:D:433:PRO:HA	1:E:420:SER:CB	2.25	0.65
1:C:122:VAL:HG11	1:C:379:ALA:HB3	1.77	0.65
1:D:264:MET:CE	1:D:292:PRO:HA	2.26	0.65
1:D:277:VAL:HG21	1:D:295:LEU:CD2	2.27	0.65
1:F:179:GLU:O	1:F:183:ILE:HG13	1.96	0.65
1:A:277:VAL:HG21	1:A:295:LEU:CD2	2.27	0.65
1:A:425:PHE:HD1	1:A:427:LYS:HB2	1.60	0.65
1:E:264:MET:CE	1:E:292:PRO:HA	2.25	0.65
1:E:71:ARG:HB3	1:E:71:ARG:NH1	2.11	0.65
1:B:71:ARG:HB3	1:B:71:ARG:NH1	2.12	0.65
1:C:54:ARG:HH12	1:F:78:VAL:H	1.42	0.65
1:C:54:ARG:HH12	1:F:78:VAL:N	1.95	0.65
1:B:425:PHE:HD1	1:B:427:LYS:HB2	1.60	0.65
1:D:407:ARG:O	1:D:411:TYR:HD2	1.78	0.65
1:C:62:VAL:HG21	1:C:105:VAL:HG13	1.78	0.65
1:A:264:MET:CE	1:A:292:PRO:HA	2.27	0.65
1:B:400:ARG:HG3	1:B:400:ARG:HH11	1.61	0.65
1:F:277:VAL:HG21	1:F:295:LEU:CD2	2.27	0.65
1:B:62:VAL:HG21	1:B:105:VAL:HG13	1.78	0.65
1:C:427:LYS:CD	1:C:430:GLY:HA3	2.25	0.65
1:F:264:MET:CE	1:F:292:PRO:HA	2.27	0.65
1:B:285:TRP:HB2	1:B:314:TYR:CB	2.17	0.64
1:D:71:ARG:NH1	1:D:71:ARG:HB3	2.12	0.64
1:E:37:ARG:HB2	1:E:37:ARG:HH11	1.62	0.64
1:B:162:ILE:O	1:B:162:ILE:HD13	1.97	0.64
1:A:37:ARG:HB2	1:A:37:ARG:HH11	1.63	0.64
1:C:393:LEU:O	1:C:395:HIS:CD2	2.50	0.64
1:D:62:VAL:HG21	1:D:105:VAL:HG13	1.79	0.64
1:E:231:ILE:HD12	1:E:237:MET:SD	2.36	0.64
1:F:62:VAL:HG21	1:F:105:VAL:HG13	1.79	0.64
1:A:62:VAL:HG21	1:A:105:VAL:HG13	1.79	0.64
1:D:116:THR:HG22	1:D:128:GLY:CA	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:PRO:HG3	1:D:180:MET:SD	2.38	0.64
1:F:71:ARG:HB3	1:F:71:ARG:NH1	2.12	0.64
1:B:37:ARG:HB2	1:B:37:ARG:HH11	1.63	0.64
1:A:285:TRP:HB2	1:A:314:TYR:CB	2.18	0.64
1:A:275:ILE:HG13	1:A:287:PRO:HA	1.80	0.64
1:B:33:VAL:HG12	1:B:38:THR:OG1	1.98	0.64
1:C:33:VAL:HG12	1:C:38:THR:OG1	1.98	0.64
1:C:407:ARG:O	1:C:411:TYR:HD2	1.80	0.64
1:E:162:ILE:O	1:E:162:ILE:HD13	1.98	0.64
1:E:433:PRO:O	1:E:435:VAL:N	2.31	0.64
1:F:116:THR:HG22	1:F:128:GLY:CA	2.27	0.64
1:A:400:ARG:HH11	1:A:400:ARG:HG3	1.61	0.64
1:B:277:VAL:HG21	1:B:295:LEU:CD2	2.28	0.64
1:B:77:GLU:HA	1:D:54:ARG:HH12	1.59	0.64
1:C:71:ARG:HB3	1:C:71:ARG:NH1	2.11	0.64
1:E:407:ARG:O	1:E:411:TYR:HD2	1.80	0.64
1:B:28:VAL:CG2	1:B:487:VAL:HG13	2.27	0.64
1:A:427:LYS:CD	1:A:430:GLY:HA3	2.26	0.64
1:D:325:ILE:HG22	1:D:347:ILE:CB	2.28	0.64
1:C:423:ARG:HH21	1:E:435:VAL:HG13	1.63	0.64
1:C:32:LEU:HD11	1:C:494:PHE:CE2	2.33	0.63
1:D:46:ARG:O	1:D:49:VAL:HG12	1.99	0.63
1:E:33:VAL:HG12	1:E:38:THR:OG1	1.98	0.63
1:B:52:ILE:O	1:B:56:ILE:HG13	1.98	0.63
1:D:275:ILE:HG13	1:D:287:PRO:HA	1.80	0.63
1:F:33:VAL:HG12	1:F:38:THR:OG1	1.98	0.63
1:A:33:VAL:HG12	1:A:38:THR:OG1	1.98	0.63
1:C:37:ARG:HH11	1:C:37:ARG:HB2	1.63	0.63
1:D:400:ARG:HG3	1:D:400:ARG:HH11	1.63	0.63
1:B:275:ILE:HG13	1:B:287:PRO:HA	1.80	0.63
1:C:179:GLU:O	1:C:183:ILE:HG13	1.99	0.63
1:C:264:MET:CE	1:C:292:PRO:HA	2.28	0.63
1:C:335:LEU:HD13	1:C:348:ILE:HD13	1.81	0.63
1:E:275:ILE:HG13	1:E:287:PRO:HA	1.81	0.63
1:D:33:VAL:HG12	1:D:38:THR:OG1	1.99	0.63
1:D:37:ARG:HH11	1:D:37:ARG:HB2	1.63	0.63
1:E:277:VAL:HG21	1:E:295:LEU:CD2	2.28	0.63
1:A:76:TRP:CD1	1:E:502:VAL:HG11	2.33	0.63
1:E:116:THR:HG22	1:E:128:GLY:CA	2.28	0.63
1:B:427:LYS:CD	1:B:430:GLY:HA3	2.25	0.63
1:D:393:LEU:O	1:D:395:HIS:CD2	2.52	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:LEU:HD11	1:E:494:PHE:CE2	2.34	0.63
1:E:325:ILE:HG22	1:E:347:ILE:CB	2.29	0.63
1:F:427:LYS:CD	1:F:430:GLY:HA3	2.25	0.62
1:D:433:PRO:O	1:D:435:VAL:N	2.32	0.62
1:A:335:LEU:HD13	1:A:348:ILE:HD13	1.81	0.62
1:C:46:ARG:O	1:C:49:VAL:HG12	1.99	0.62
1:E:427:LYS:CD	1:E:430:GLY:HA3	2.25	0.62
1:F:376:TYR:OH	1:F:465:ALA:HB2	1.99	0.62
1:B:49:VAL:O	1:B:52:ILE:HG12	2.00	0.62
1:C:72:ASP:OD1	1:C:144:GLU:HG3	1.99	0.62
1:F:37:ARG:HH11	1:F:37:ARG:HB2	1.64	0.62
1:B:32:LEU:HD11	1:B:494:PHE:CE2	2.35	0.62
1:B:46:ARG:O	1:B:49:VAL:HG12	2.00	0.62
1:F:49:VAL:O	1:F:52:ILE:HG12	1.99	0.62
1:A:171:PRO:HG3	1:A:180:MET:SD	2.40	0.62
1:C:52:ILE:O	1:C:56:ILE:HG13	2.00	0.62
1:C:433:PRO:O	1:C:435:VAL:N	2.33	0.62
1:D:427:LYS:CD	1:D:430:GLY:HA3	2.27	0.62
1:A:28:VAL:CG2	1:A:487:VAL:HG13	2.30	0.61
1:C:206:PRO:HB2	1:C:209:GLN:HG2	1.81	0.61
1:E:205:LYS:NZ	1:E:388:GLU:OE1	2.33	0.61
1:F:135:ILE:HG13	1:F:140:TYR:CE2	2.35	0.61
1:F:32:LEU:HD11	1:F:494:PHE:CE2	2.35	0.61
1:F:335:LEU:HD13	1:F:348:ILE:HD13	1.81	0.61
1:A:505:THR:HG23	1:B:185:ASP:OD1	2.00	0.61
1:B:433:PRO:O	1:B:435:VAL:N	2.33	0.61
1:E:49:VAL:O	1:E:52:ILE:HG12	2.00	0.61
1:F:205:LYS:NZ	1:F:392:ASN:HD21	1.98	0.61
1:B:221:ARG:HD2	1:B:454:HIS:NE2	2.15	0.61
1:D:162:ILE:HD13	1:D:162:ILE:O	2.00	0.61
1:D:335:LEU:HD13	1:D:348:ILE:HD13	1.82	0.61
1:A:162:ILE:O	1:A:162:ILE:HD13	2.00	0.61
1:B:345:ALA:O	1:B:369:ILE:HD12	2.00	0.61
1:E:37:ARG:HH21	1:E:49:VAL:HG11	1.65	0.61
1:B:95:GLY:O	1:B:169:PRO:HA	2.01	0.61
1:C:256:PHE:HE2	1:C:264:MET:HE2	1.65	0.61
1:E:46:ARG:O	1:E:49:VAL:HG12	2.00	0.61
1:F:275:ILE:HG13	1:F:287:PRO:HA	1.81	0.61
1:F:325:ILE:HG22	1:F:347:ILE:CB	2.29	0.61
1:F:345:ALA:O	1:F:369:ILE:HD12	2.00	0.61
1:F:46:ARG:O	1:F:49:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:O	1:A:435:VAL:N	2.33	0.61
1:A:46:ARG:O	1:A:49:VAL:HG12	1.99	0.61
1:C:14:PHE:O	1:C:18:GLU:HB2	2.00	0.61
1:C:162:ILE:O	1:C:162:ILE:HD13	2.00	0.61
1:C:135:ILE:HG13	1:C:140:TYR:CE2	2.36	0.61
1:D:32:LEU:HD11	1:D:494:PHE:CE2	2.36	0.61
1:D:49:VAL:O	1:D:52:ILE:HG12	2.00	0.61
1:A:95:GLY:O	1:A:169:PRO:HA	2.01	0.61
1:A:325:ILE:HG22	1:A:347:ILE:CB	2.29	0.61
1:B:13:PHE:CD1	1:B:14:PHE:N	2.66	0.61
1:F:72:ASP:OD1	1:F:144:GLU:HG3	2.00	0.61
1:A:32:LEU:HD11	1:A:494:PHE:CE2	2.35	0.61
1:B:393:LEU:O	1:B:395:HIS:CD2	2.54	0.61
1:C:151:ARG:NH2	1:F:504:PHE:CZ	2.69	0.61
1:A:49:VAL:O	1:A:52:ILE:HG12	2.00	0.60
1:B:72:ASP:OD1	1:B:144:GLU:HG3	2.01	0.60
1:D:345:ALA:O	1:D:369:ILE:HD12	2.01	0.60
1:D:505:THR:N	1:E:150:ARG:HH12	1.99	0.60
1:F:393:LEU:O	1:F:395:HIS:CD2	2.54	0.60
1:B:37:ARG:HH21	1:B:49:VAL:HG11	1.66	0.60
1:D:14:PHE:O	1:D:18:GLU:HB2	2.01	0.60
1:D:343:VAL:HG22	1:D:367:ARG:NH2	2.16	0.60
1:E:256:PHE:HE2	1:E:264:MET:HE2	1.66	0.60
1:C:95:GLY:O	1:C:169:PRO:HA	2.02	0.60
1:D:483:THR:O	1:D:487:VAL:HG23	2.01	0.60
1:E:335:LEU:HD13	1:E:348:ILE:HD13	1.83	0.60
1:B:335:LEU:HD13	1:B:348:ILE:HD13	1.81	0.60
1:C:49:VAL:O	1:C:52:ILE:HG12	2.00	0.60
1:C:185:ASP:OD1	1:E:505:THR:HG23	2.02	0.60
1:F:37:ARG:HH21	1:F:49:VAL:HG11	1.65	0.60
1:A:185:ASP:OD1	1:F:505:THR:HG23	2.01	0.60
1:A:37:ARG:HH21	1:A:49:VAL:HG11	1.66	0.60
1:B:325:ILE:HG22	1:B:347:ILE:CB	2.30	0.60
1:E:345:ALA:O	1:E:369:ILE:HD12	2.01	0.60
1:D:13:PHE:CD1	1:D:14:PHE:N	2.65	0.60
1:D:95:GLY:O	1:D:169:PRO:HA	2.02	0.60
1:E:95:GLY:O	1:E:169:PRO:HA	2.02	0.60
1:A:393:LEU:O	1:A:395:HIS:CD2	2.54	0.60
1:A:502:VAL:HG11	1:E:76:TRP:HD1	1.64	0.60
1:B:14:PHE:O	1:B:18:GLU:HB2	2.02	0.60
1:B:10:ASP:HB2	1:B:333:LYS:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ILE:HG13	1:C:287:PRO:HA	1.83	0.60
1:E:13:PHE:CD1	1:E:14:PHE:N	2.66	0.60
1:E:52:ILE:O	1:E:56:ILE:HG13	2.01	0.60
1:F:14:PHE:O	1:F:18:GLU:HB2	2.00	0.60
1:F:162:ILE:O	1:F:162:ILE:HD13	2.00	0.60
1:A:14:PHE:O	1:A:18:GLU:HB2	2.01	0.60
1:D:343:VAL:HG21	1:D:364:PHE:CE1	2.36	0.60
1:D:52:ILE:O	1:D:56:ILE:HG13	2.02	0.60
1:E:14:PHE:O	1:E:18:GLU:HB2	2.01	0.60
1:C:69:ILE:HG22	1:C:151:ARG:HD2	1.84	0.60
1:C:217:SER:OG	1:C:454:HIS:NE2	2.35	0.60
1:C:335:LEU:HB2	1:C:356:THR:HG22	1.84	0.60
1:E:135:ILE:HG13	1:E:140:TYR:CE2	2.37	0.60
1:F:52:ILE:O	1:F:56:ILE:HG13	2.02	0.60
1:B:418:GLN:CB	1:B:433:PRO:HD2	2.31	0.60
1:E:418:GLN:CB	1:E:433:PRO:HD2	2.32	0.60
1:F:256:PHE:HE2	1:F:264:MET:HE2	1.66	0.60
1:A:343:VAL:HG21	1:A:364:PHE:CE1	2.36	0.59
1:B:343:VAL:HG22	1:B:367:ARG:NH2	2.18	0.59
1:B:78:VAL:H	1:D:54:ARG:HH12	1.49	0.59
1:E:343:VAL:HG21	1:E:364:PHE:CE1	2.37	0.59
1:C:343:VAL:HG22	1:C:367:ARG:NH2	2.17	0.59
1:A:143:ASN:HD21	1:C:70:ARG:HH12	1.51	0.59
1:D:72:ASP:OD1	1:D:144:GLU:HG3	2.02	0.59
1:C:308:PHE:HD2	1:C:311:ALA:HB2	1.67	0.59
1:D:335:LEU:HB2	1:D:356:THR:HG22	1.84	0.59
1:E:343:VAL:HG22	1:E:367:ARG:NH2	2.17	0.59
1:A:54:ARG:NH1	1:E:77:GLU:HA	2.17	0.59
1:F:12:ASN:OD1	1:F:15:LYS:HG2	2.02	0.59
1:F:483:THR:O	1:F:487:VAL:HG23	2.03	0.59
1:A:72:ASP:OD1	1:A:144:GLU:HG3	2.03	0.59
1:B:335:LEU:HB2	1:B:356:THR:HG22	1.85	0.59
1:C:37:ARG:HH21	1:C:49:VAL:HG11	1.66	0.59
1:E:474:LYS:HD3	1:E:475:TYR:CE2	2.38	0.59
1:B:256:PHE:HE2	1:B:264:MET:HE2	1.67	0.59
1:C:325:ILE:HG22	1:C:347:ILE:CB	2.30	0.59
1:D:135:ILE:HG13	1:D:140:TYR:CE2	2.38	0.59
1:D:279:GLU:HG3	1:D:305:ILE:CG1	2.32	0.59
1:E:69:ILE:HG22	1:E:151:ARG:HD2	1.84	0.59
1:F:146:GLU:HG2	1:F:150:ARG:HD2	1.85	0.59
1:D:69:ILE:HG22	1:D:151:ARG:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ASN:OD1	1:C:15:LYS:HG2	2.03	0.59
1:F:335:LEU:HB2	1:F:356:THR:HG22	1.84	0.59
1:F:343:VAL:HG22	1:F:367:ARG:NH2	2.18	0.59
1:B:244:PRO:HB2	1:B:248:ASP:H	1.68	0.59
1:E:335:LEU:HB2	1:E:356:THR:HG22	1.85	0.59
1:F:13:PHE:CD1	1:F:14:PHE:N	2.65	0.59
1:E:146:GLU:HG2	1:E:150:ARG:HD2	1.85	0.59
1:E:28:VAL:CG2	1:E:487:VAL:HG13	2.33	0.59
1:F:23:ARG:O	1:F:27:ILE:HG13	2.02	0.59
1:A:264:MET:HE3	1:A:292:PRO:HA	1.84	0.59
1:B:12:ASN:OD1	1:B:15:LYS:HG2	2.03	0.59
1:B:343:VAL:HG21	1:B:364:PHE:CE1	2.36	0.59
1:E:12:ASN:OD1	1:E:15:LYS:HG2	2.03	0.59
1:A:504:PHE:CE1	1:E:70:ARG:HB3	2.38	0.59
1:F:244:PRO:HB2	1:F:248:ASP:H	1.68	0.59
1:D:256:PHE:HE2	1:D:264:MET:HE2	1.68	0.58
1:D:37:ARG:HH21	1:D:49:VAL:HG11	1.66	0.58
1:F:91:THR:OG1	1:F:92:PRO:HD3	2.03	0.58
1:A:69:ILE:HG22	1:A:151:ARG:HD2	1.85	0.58
1:B:190:THR:HG22	1:B:191:ILE:N	2.18	0.58
1:B:69:ILE:HG22	1:B:151:ARG:HD2	1.84	0.58
1:D:93:CYS:HB3	1:D:129:ALA:HB2	1.85	0.58
1:D:12:ASN:OD1	1:D:15:LYS:HG2	2.03	0.58
1:D:146:GLU:HG2	1:D:150:ARG:HD2	1.84	0.58
1:D:264:MET:HE3	1:D:292:PRO:HA	1.85	0.58
1:A:483:THR:O	1:A:487:VAL:HG23	2.02	0.58
1:D:418:GLN:CB	1:D:433:PRO:HD2	2.32	0.58
1:B:54:ARG:HH12	1:D:78:VAL:N	2.02	0.58
1:F:343:VAL:HG21	1:F:364:PHE:CE1	2.37	0.58
1:A:308:PHE:HD2	1:A:311:ALA:HB2	1.68	0.58
1:A:70:ARG:HH12	1:C:143:ASN:HD21	1.51	0.58
1:C:345:ALA:O	1:C:369:ILE:HD12	2.03	0.58
1:E:91:THR:OG1	1:E:92:PRO:HD3	2.04	0.58
1:C:502:VAL:HG11	1:F:76:TRP:CD1	2.39	0.58
1:A:91:THR:OG1	1:A:92:PRO:HD3	2.04	0.58
1:B:135:ILE:HG13	1:B:140:TYR:CE2	2.38	0.58
1:A:386:TYR:OH	1:B:396:VAL:HG13	2.04	0.58
1:C:279:GLU:HG3	1:C:305:ILE:CG1	2.34	0.58
1:D:435:VAL:HG13	1:E:423:ARG:HH21	1.68	0.58
1:A:345:ALA:O	1:A:369:ILE:HD12	2.02	0.58
1:A:343:VAL:HG22	1:A:367:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:PHE:CD1	1:C:14:PHE:N	2.65	0.58
1:F:91:THR:CB	1:F:92:PRO:HD3	2.34	0.58
1:D:308:PHE:HD2	1:D:311:ALA:HB2	1.68	0.58
1:D:427:LYS:HZ3	1:D:428:HIS:H	1.52	0.58
1:B:54:ARG:NH1	1:D:77:GLU:HA	2.18	0.58
1:F:279:GLU:HG3	1:F:305:ILE:CG1	2.34	0.58
1:F:69:ILE:HG22	1:F:151:ARG:HD2	1.85	0.58
1:C:190:THR:HG22	1:C:191:ILE:N	2.19	0.58
1:C:93:CYS:HB3	1:C:129:ALA:HB2	1.86	0.58
1:E:427:LYS:CE	1:E:427:LYS:HA	2.32	0.58
1:C:91:THR:OG1	1:C:92:PRO:HD3	2.04	0.58
1:A:146:GLU:HG2	1:A:150:ARG:HD2	1.86	0.58
1:A:432:ILE:HG22	1:A:434:ILE:HG12	1.86	0.58
1:B:264:MET:HE3	1:B:292:PRO:HA	1.86	0.58
1:E:190:THR:HG22	1:E:191:ILE:N	2.19	0.58
1:F:308:PHE:HD2	1:F:311:ALA:HB2	1.68	0.58
1:A:157:ALA:HA	1:A:162:ILE:HG22	1.86	0.57
1:A:418:GLN:CB	1:A:433:PRO:HD2	2.32	0.57
1:B:433:PRO:HA	1:F:420:SER:CB	2.34	0.57
1:C:207:ILE:C	1:C:209:GLN:H	2.06	0.57
1:C:293:LYS:O	1:C:296:GLU:HB3	2.04	0.57
1:C:343:VAL:HG21	1:C:364:PHE:CE1	2.37	0.57
1:E:244:PRO:HB2	1:E:248:ASP:H	1.69	0.57
1:E:72:ASP:OD1	1:E:144:GLU:HG3	2.02	0.57
1:A:293:LYS:O	1:A:296:GLU:HB3	2.04	0.57
1:A:335:LEU:HB2	1:A:356:THR:HG22	1.86	0.57
1:B:252:VAL:HG11	1:B:318:ILE:HB	1.86	0.57
1:B:10:ASP:HB2	1:B:333:LYS:HD3	1.86	0.57
1:B:93:CYS:HB3	1:B:129:ALA:HB2	1.85	0.57
1:C:146:GLU:HG2	1:C:150:ARG:HD2	1.85	0.57
1:C:213:HIS:O	1:C:453:VAL:HG21	2.04	0.57
1:F:418:GLN:CB	1:F:433:PRO:HD2	2.33	0.57
1:C:171:PRO:HG3	1:C:180:MET:SD	2.44	0.57
1:C:230:PHE:CD2	1:C:469:MET:HE2	2.39	0.57
1:E:171:PRO:HG3	1:E:180:MET:SD	2.43	0.57
1:A:12:ASN:OD1	1:A:15:LYS:HG2	2.03	0.57
1:B:154:MET:SD	1:B:190:THR:HG21	2.45	0.57
1:B:76:TRP:CZ3	1:D:49:VAL:HA	2.40	0.57
1:C:252:VAL:HG11	1:C:318:ILE:HB	1.87	0.57
1:D:91:THR:OG1	1:D:92:PRO:HD3	2.04	0.57
1:E:154:MET:SD	1:E:190:THR:HG21	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ALA:HA	1:E:162:ILE:HG22	1.86	0.57
1:A:504:PHE:CZ	1:E:151:ARG:NH2	2.73	0.57
1:B:28:VAL:HG23	1:B:487:VAL:HG13	1.85	0.57
1:D:105:VAL:O	1:D:109:LYS:HG3	2.04	0.57
1:E:69:ILE:HA	1:E:151:ARG:CZ	2.35	0.57
1:A:244:PRO:HB2	1:A:248:ASP:H	1.70	0.57
1:A:52:ILE:O	1:A:56:ILE:HG13	2.04	0.57
1:C:320:GLU:O	1:C:344:LYS:HG2	2.05	0.57
1:F:171:PRO:HG3	1:F:180:MET:SD	2.45	0.57
1:C:244:PRO:HB2	1:C:248:ASP:H	1.69	0.57
1:A:54:ARG:HH12	1:E:78:VAL:H	1.52	0.57
1:A:190:THR:HG22	1:A:191:ILE:N	2.20	0.57
1:A:221:ARG:HD2	1:A:454:HIS:NE2	2.19	0.57
1:A:252:VAL:HG11	1:A:318:ILE:HB	1.87	0.57
1:C:396:VAL:HG13	1:E:386:TYR:OH	2.05	0.57
1:F:105:VAL:O	1:F:109:LYS:HG3	2.04	0.57
1:F:157:ALA:HA	1:F:162:ILE:HG22	1.87	0.57
1:F:252:VAL:HG11	1:F:318:ILE:HB	1.86	0.57
1:B:279:GLU:HG3	1:B:305:ILE:CG1	2.34	0.57
1:B:308:PHE:HD2	1:B:311:ALA:HB2	1.69	0.57
1:C:205:LYS:HZ3	1:C:392:ASN:ND2	2.03	0.57
1:E:279:GLU:HG3	1:E:305:ILE:CG1	2.34	0.57
1:F:95:GLY:O	1:F:169:PRO:HA	2.04	0.57
1:A:427:LYS:HA	1:A:427:LYS:CE	2.33	0.57
1:B:293:LYS:O	1:B:296:GLU:HB3	2.05	0.57
1:C:91:THR:CB	1:C:92:PRO:HD3	2.35	0.57
1:D:157:ALA:HA	1:D:162:ILE:HG22	1.86	0.57
1:D:244:PRO:HB2	1:D:248:ASP:H	1.68	0.57
1:F:264:MET:HE3	1:F:292:PRO:HA	1.87	0.57
1:B:95:GLY:HA3	1:B:129:ALA:O	2.05	0.56
1:B:91:THR:CB	1:B:92:PRO:HD3	2.35	0.56
1:C:23:ARG:O	1:C:27:ILE:HG13	2.05	0.56
1:D:190:THR:HG22	1:D:191:ILE:N	2.20	0.56
1:D:320:GLU:O	1:D:344:LYS:HG2	2.05	0.56
1:E:320:GLU:O	1:E:344:LYS:HG2	2.05	0.56
1:E:91:THR:CB	1:E:92:PRO:HD3	2.35	0.56
1:A:256:PHE:HE2	1:A:264:MET:HE2	1.70	0.56
1:C:427:LYS:CE	1:C:427:LYS:HA	2.33	0.56
1:F:320:GLU:O	1:F:344:LYS:HG2	2.04	0.56
1:B:23:ARG:O	1:B:27:ILE:HG13	2.05	0.56
1:B:254:GLN:OE1	1:B:334:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ALA:HA	1:C:162:ILE:HG22	1.87	0.56
1:E:393:LEU:O	1:E:395:HIS:CD2	2.58	0.56
1:E:432:ILE:HG22	1:E:434:ILE:HG12	1.88	0.56
1:F:93:CYS:HB3	1:F:129:ALA:HB2	1.87	0.56
1:A:135:ILE:HG13	1:A:140:TYR:CE2	2.39	0.56
1:A:320:GLU:O	1:A:344:LYS:HG2	2.04	0.56
1:B:320:GLU:O	1:B:344:LYS:HG2	2.05	0.56
1:D:304:SER:OG	1:D:306:LEU:HD13	2.06	0.56
1:F:375:LEU:HD23	1:F:485:ALA:HB1	1.87	0.56
1:B:205:LYS:NZ	1:B:388:GLU:OE1	2.35	0.56
1:E:254:GLN:OE1	1:E:334:GLN:HG2	2.05	0.56
1:F:293:LYS:O	1:F:296:GLU:HB3	2.05	0.56
1:F:500:ALA:C	1:F:505:THR:HA	2.26	0.56
1:A:91:THR:CB	1:A:92:PRO:HD3	2.36	0.56
1:B:76:TRP:CD1	1:D:502:VAL:HG11	2.41	0.56
1:E:293:LYS:O	1:E:296:GLU:HB3	2.06	0.56
1:E:252:VAL:HG11	1:E:318:ILE:HB	1.87	0.56
1:A:99:TYR:HH	1:A:149:THR:HG22	1.66	0.56
1:A:69:ILE:HA	1:A:151:ARG:CZ	2.36	0.56
1:B:91:THR:OG1	1:B:92:PRO:HD3	2.06	0.56
1:D:154:MET:SD	1:D:190:THR:HG21	2.45	0.56
1:D:500:ALA:C	1:D:505:THR:HA	2.26	0.56
1:C:503:THR:HG21	1:F:151:ARG:CD	2.35	0.56
1:A:279:GLU:HG3	1:A:305:ILE:CG1	2.33	0.56
1:D:27:ILE:HG22	1:D:475:TYR:CD1	2.41	0.56
1:D:496:VAL:O	1:E:209:GLN:NE2	2.39	0.56
1:F:69:ILE:HA	1:F:151:ARG:CZ	2.35	0.56
1:F:206:PRO:HD2	1:F:209:GLN:HB2	1.88	0.56
1:F:40:GLU:HG3	1:F:46:ARG:NH1	2.15	0.56
1:A:13:PHE:CD1	1:A:14:PHE:N	2.65	0.56
1:E:500:ALA:C	1:E:505:THR:HA	2.26	0.56
1:B:62:VAL:HG11	1:B:109:LYS:NZ	2.21	0.56
1:C:304:SER:OG	1:C:306:LEU:HD13	2.06	0.56
1:D:252:VAL:HG11	1:D:318:ILE:HB	1.88	0.56
1:B:171:PRO:HG3	1:B:180:MET:SD	2.45	0.55
1:E:23:ARG:O	1:E:27:ILE:HG13	2.06	0.55
1:F:221:ARG:CD	1:F:454:HIS:CD2	2.90	0.55
1:B:146:GLU:HG2	1:B:150:ARG:HD2	1.87	0.55
1:B:157:ALA:HA	1:B:162:ILE:HG22	1.87	0.55
1:B:483:THR:O	1:B:487:VAL:HG23	2.06	0.55
1:D:28:VAL:HG23	1:D:487:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:THR:CB	1:D:92:PRO:HD3	2.35	0.55
1:E:304:SER:OG	1:E:306:LEU:HD13	2.06	0.55
1:F:41:SER:CA	1:F:46:ARG:HD2	2.31	0.55
1:A:500:ALA:C	1:A:505:THR:HA	2.27	0.55
1:B:243:THR:N	1:B:244:PRO:CD	2.68	0.55
1:D:432:ILE:HG22	1:D:434:ILE:HG12	1.88	0.55
1:F:243:THR:N	1:F:244:PRO:CD	2.69	0.55
1:A:254:GLN:OE1	1:A:334:GLN:HG2	2.06	0.55
1:B:77:GLU:CA	1:D:54:ARG:NH1	2.68	0.55
1:C:483:THR:O	1:C:487:VAL:HG23	2.06	0.55
1:C:500:ALA:C	1:C:505:THR:HA	2.26	0.55
1:D:254:GLN:OE1	1:D:334:GLN:HG2	2.07	0.55
1:E:308:PHE:HD2	1:E:311:ALA:HB2	1.71	0.55
1:F:190:THR:HG22	1:F:191:ILE:N	2.20	0.55
1:F:304:SER:OG	1:F:306:LEU:HD13	2.06	0.55
1:D:293:LYS:O	1:D:296:GLU:HB3	2.06	0.55
1:A:503:THR:HG21	1:E:151:ARG:NE	2.22	0.55
1:B:304:SER:OG	1:B:306:LEU:HD13	2.06	0.55
1:B:37:ARG:NH1	1:B:37:ARG:HB2	2.22	0.55
1:B:488:ASN:HD21	1:B:492:LYS:HZ2	1.53	0.55
1:C:33:VAL:HG13	1:C:46:ARG:HB2	1.89	0.55
1:C:69:ILE:HA	1:C:151:ARG:CZ	2.36	0.55
1:D:386:TYR:OH	1:E:396:VAL:HG13	2.07	0.55
1:A:93:CYS:HB3	1:A:129:ALA:HB2	1.89	0.55
1:A:251:PHE:CB	1:A:325:ILE:HG13	2.37	0.55
1:A:304:SER:OG	1:A:306:LEU:HD13	2.06	0.55
1:C:116:THR:HG22	1:C:128:GLY:N	2.21	0.55
1:C:221:ARG:CD	1:C:454:HIS:CD2	2.89	0.55
1:F:154:MET:SD	1:F:190:THR:HG21	2.47	0.55
1:F:273:LYS:HE2	1:F:288:ASP:O	2.07	0.55
1:A:154:MET:SD	1:A:190:THR:HG21	2.47	0.55
1:B:500:ALA:C	1:B:505:THR:HA	2.27	0.55
1:B:77:GLU:CA	1:D:54:ARG:HH12	2.19	0.55
1:D:10:ASP:HB2	1:D:333:LYS:CD	2.36	0.55
1:D:505:THR:HG23	1:E:150:ARG:NH2	2.22	0.55
1:E:483:THR:O	1:E:487:VAL:HG23	2.07	0.55
1:F:33:VAL:HG13	1:F:46:ARG:HB2	1.89	0.55
1:B:16:MET:HG2	1:B:358:PRO:CG	2.37	0.55
1:A:37:ARG:HB2	1:A:37:ARG:NH1	2.21	0.55
1:B:69:ILE:HA	1:B:151:ARG:CZ	2.36	0.55
1:C:273:LYS:HE2	1:C:288:ASP:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:GLY:HA3	1:E:129:ALA:O	2.07	0.55
1:A:54:ARG:HH12	1:E:78:VAL:N	2.05	0.55
1:A:337:LYS:NZ	1:A:359:GLU:HG3	2.22	0.54
1:C:41:SER:CA	1:C:46:ARG:HD2	2.32	0.54
1:D:273:LYS:HE2	1:D:288:ASP:O	2.07	0.54
1:D:337:LYS:NZ	1:D:359:GLU:HG3	2.22	0.54
1:F:337:LYS:NZ	1:F:359:GLU:HG3	2.22	0.54
1:A:13:PHE:CZ	1:A:107:GLU:HA	2.42	0.54
1:A:87:SER:O	1:A:127:GLY:HA3	2.07	0.54
1:D:37:ARG:HB2	1:D:37:ARG:NH1	2.22	0.54
1:B:105:VAL:O	1:B:109:LYS:HG3	2.07	0.54
1:C:254:GLN:OE1	1:C:334:GLN:HG2	2.07	0.54
1:F:254:GLN:OE1	1:F:334:GLN:HG2	2.07	0.54
1:B:432:ILE:HG22	1:B:434:ILE:HG12	1.89	0.54
1:C:37:ARG:HB2	1:C:37:ARG:NH1	2.21	0.54
1:D:23:ARG:O	1:D:27:ILE:HG13	2.06	0.54
1:E:273:LYS:HE2	1:E:288:ASP:O	2.08	0.54
1:E:37:ARG:HB2	1:E:37:ARG:NH1	2.21	0.54
1:B:499:GLU:HB2	1:F:209:GLN:NE2	2.23	0.54
1:A:62:VAL:HG11	1:A:109:LYS:NZ	2.23	0.54
1:A:95:GLY:HA3	1:A:129:ALA:O	2.08	0.54
1:C:388:GLU:O	1:C:391:LYS:N	2.40	0.54
1:C:432:ILE:HG22	1:C:434:ILE:HG12	1.88	0.54
1:E:93:CYS:HB3	1:E:129:ALA:HB2	1.89	0.54
1:A:273:LYS:HE2	1:A:288:ASP:O	2.08	0.54
1:D:427:LYS:NZ	1:D:428:HIS:H	2.05	0.54
1:E:62:VAL:HG11	1:E:109:LYS:NZ	2.23	0.54
1:E:337:LYS:NZ	1:E:359:GLU:HG3	2.23	0.54
1:A:427:LYS:NZ	1:A:428:HIS:H	2.05	0.54
1:C:418:GLN:CB	1:C:433:PRO:HD2	2.34	0.54
1:C:403:PHE:CD2	1:C:447:ALA:HB1	2.43	0.54
1:C:503:THR:HG21	1:F:151:ARG:NE	2.23	0.54
1:D:69:ILE:HA	1:D:151:ARG:CZ	2.37	0.54
1:D:33:VAL:HG13	1:D:46:ARG:HB2	1.90	0.54
1:E:221:ARG:HD2	1:E:454:HIS:CD2	2.43	0.54
1:F:37:ARG:HB2	1:F:37:ARG:NH1	2.22	0.54
1:B:251:PHE:CB	1:B:325:ILE:HG13	2.38	0.54
1:C:154:MET:SD	1:C:190:THR:HG21	2.47	0.54
1:B:499:GLU:HB2	1:F:209:GLN:HE21	1.73	0.54
1:A:308:PHE:O	1:A:311:ALA:HB3	2.08	0.54
1:A:440:PHE:O	1:A:444:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:HG13	1:A:46:ARG:HB2	1.89	0.54
1:C:105:VAL:O	1:C:109:LYS:HG3	2.08	0.54
1:C:427:LYS:NZ	1:C:428:HIS:H	2.06	0.54
1:D:13:PHE:CZ	1:D:107:GLU:HA	2.43	0.54
1:D:255:GLY:HA3	1:D:330:ALA:HB2	1.90	0.54
1:C:337:LYS:NZ	1:C:359:GLU:HG3	2.22	0.53
1:C:28:VAL:CG2	1:C:487:VAL:HG13	2.38	0.53
1:B:33:VAL:HG13	1:B:46:ARG:HB2	1.89	0.53
1:B:474:LYS:HD3	1:B:475:TYR:CE2	2.43	0.53
1:C:264:MET:HE3	1:C:292:PRO:HA	1.91	0.53
1:A:23:ARG:O	1:A:27:ILE:HG13	2.08	0.53
1:B:13:PHE:CZ	1:B:107:GLU:HA	2.43	0.53
1:B:337:LYS:NZ	1:B:359:GLU:HG3	2.23	0.53
1:B:205:LYS:NZ	1:B:392:ASN:HD21	2.07	0.53
1:B:427:LYS:NZ	1:B:428:HIS:H	2.07	0.53
1:C:13:PHE:CZ	1:C:107:GLU:HA	2.44	0.53
1:F:432:ILE:HG22	1:F:434:ILE:HG12	1.89	0.53
1:B:21:PHE:CE1	1:B:490:ILE:HD12	2.43	0.53
1:C:423:ARG:HH21	1:E:435:VAL:CG1	2.20	0.53
1:E:105:VAL:O	1:E:109:LYS:HG3	2.09	0.53
1:A:503:THR:HG21	1:E:151:ARG:CZ	2.39	0.53
1:B:386:TYR:OH	1:F:396:VAL:HG13	2.08	0.53
1:B:335:LEU:HD12	1:B:356:THR:HG22	1.91	0.53
1:B:502:VAL:HG11	1:D:76:TRP:CD1	2.43	0.53
1:C:118:LYS:HZ1	1:C:353:ASN:HD21	1.55	0.53
1:C:207:ILE:C	1:C:209:GLN:N	2.61	0.53
1:C:243:THR:N	1:C:244:PRO:CD	2.69	0.53
1:E:427:LYS:NZ	1:E:428:HIS:H	2.06	0.53
1:E:427:LYS:HZ3	1:E:428:HIS:H	1.57	0.53
1:E:440:PHE:O	1:E:444:ILE:HG13	2.08	0.53
1:E:41:SER:CA	1:E:46:ARG:HD2	2.32	0.53
1:F:251:PHE:CB	1:F:325:ILE:HG13	2.38	0.53
1:B:243:THR:H	1:B:244:PRO:HD3	1.74	0.53
1:D:318:ILE:HG12	1:D:319:LEU:HD12	1.91	0.53
1:F:308:PHE:O	1:F:311:ALA:HB3	2.07	0.53
1:A:252:VAL:CG1	1:A:318:ILE:HB	2.39	0.53
1:B:255:GLY:HA3	1:B:330:ALA:HB2	1.90	0.53
1:E:33:VAL:HG13	1:E:46:ARG:HB2	1.89	0.53
1:E:205:LYS:NZ	1:E:392:ASN:HD21	2.06	0.53
1:A:243:THR:N	1:A:244:PRO:CD	2.69	0.53
1:B:427:LYS:HA	1:B:427:LYS:CE	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LYS:HD2	1:C:151:ARG:NH2	2.21	0.53
1:C:205:LYS:NZ	1:C:392:ASN:ND2	2.55	0.53
1:E:264:MET:HE3	1:E:292:PRO:HA	1.90	0.53
1:F:373:PRO:CG	1:F:481:LEU:HB3	2.39	0.53
1:D:251:PHE:CB	1:D:325:ILE:HG13	2.38	0.52
1:F:147:LYS:HD2	1:F:151:ARG:NH2	2.21	0.52
1:B:347:ILE:HA	1:B:370:MET:O	2.09	0.52
1:C:122:VAL:CG1	1:C:379:ALA:CB	2.87	0.52
1:C:205:LYS:HZ3	1:C:392:ASN:HD21	1.53	0.52
1:F:255:GLY:HA3	1:F:330:ALA:HB2	1.91	0.52
1:F:427:LYS:NZ	1:F:428:HIS:H	2.06	0.52
1:C:78:VAL:H	1:F:54:ARG:HH12	1.57	0.52
1:A:105:VAL:O	1:A:109:LYS:HG3	2.08	0.52
1:B:273:LYS:HE2	1:B:288:ASP:O	2.09	0.52
1:C:116:THR:HG22	1:C:128:GLY:H	1.72	0.52
1:C:95:GLY:HA3	1:C:129:ALA:O	2.10	0.52
1:F:285:TRP:O	1:F:286:ASN:HB2	2.10	0.52
1:B:285:TRP:O	1:B:286:ASN:HB2	2.10	0.52
1:C:308:PHE:O	1:C:311:ALA:HB3	2.09	0.52
1:D:87:SER:O	1:D:127:GLY:HA3	2.08	0.52
1:D:336:THR:H	1:D:339:ASN:ND2	2.07	0.52
1:A:116:THR:HG22	1:A:128:GLY:N	2.25	0.52
1:C:62:VAL:HG11	1:C:109:LYS:NZ	2.24	0.52
1:A:73:ASP:O	1:A:75:SER:N	2.43	0.52
1:C:336:THR:H	1:C:339:ASN:ND2	2.07	0.52
1:D:79:ILE:N	1:D:79:ILE:HD12	2.25	0.52
1:E:255:GLY:HA3	1:E:330:ALA:HB2	1.91	0.52
1:E:41:SER:HA	1:E:46:ARG:CD	2.34	0.52
1:F:62:VAL:HG11	1:F:109:LYS:NZ	2.24	0.52
1:B:332:GLU:HG2	1:B:333:LYS:HG2	1.91	0.52
1:B:30:ASP:O	1:B:34:GLU:HG2	2.10	0.52
1:B:73:ASP:O	1:B:75:SER:N	2.43	0.52
1:C:428:HIS:N	1:C:428:HIS:CD2	2.78	0.52
1:D:41:SER:HA	1:D:46:ARG:CD	2.34	0.52
1:D:73:ASP:O	1:D:75:SER:N	2.43	0.52
1:E:87:SER:O	1:E:127:GLY:HA3	2.09	0.52
1:E:335:LEU:HD12	1:E:356:THR:HG22	1.91	0.52
1:E:205:LYS:HZ3	1:E:392:ASN:HD21	1.57	0.52
1:A:79:ILE:N	1:A:79:ILE:HD12	2.25	0.52
1:B:147:LYS:HD2	1:B:151:ARG:NH2	2.21	0.52
1:B:92:PRO:HG2	1:B:389:TRP:CZ2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:440:PHE:O	1:F:444:ILE:HG13	2.09	0.52
1:A:255:GLY:HA3	1:A:330:ALA:HB2	1.91	0.52
1:B:41:SER:CA	1:B:46:ARG:HD2	2.32	0.52
1:C:255:GLY:HA3	1:C:330:ALA:HB2	1.92	0.52
1:E:13:PHE:CZ	1:E:107:GLU:HA	2.44	0.52
1:E:327:ILE:CG2	1:E:349:ALA:HB3	2.35	0.52
1:E:425:PHE:CD1	1:E:427:LYS:HB2	2.44	0.52
1:F:243:THR:O	1:F:243:THR:HG23	2.10	0.52
1:F:92:PRO:HG2	1:F:389:TRP:CZ2	2.45	0.52
1:B:79:ILE:N	1:B:79:ILE:HD12	2.25	0.51
1:E:243:THR:H	1:E:244:PRO:HD3	1.74	0.51
1:F:13:PHE:CZ	1:F:107:GLU:HA	2.44	0.51
1:F:252:VAL:CG1	1:F:318:ILE:HB	2.39	0.51
1:A:122:VAL:HG23	1:A:124:VAL:HG23	1.92	0.51
1:A:322:ASP:HA	1:A:344:LYS:HB2	1.93	0.51
1:B:252:VAL:CG1	1:B:318:ILE:HB	2.40	0.51
1:B:322:ASP:HA	1:B:344:LYS:HB2	1.92	0.51
1:C:376:TYR:HB2	1:C:468:ILE:CD1	2.40	0.51
1:D:95:GLY:HA3	1:D:129:ALA:O	2.09	0.51
1:E:252:VAL:CG1	1:E:318:ILE:HB	2.41	0.51
1:D:433:PRO:HA	1:E:420:SER:HB3	1.93	0.51
1:F:428:HIS:CD2	1:F:428:HIS:N	2.78	0.51
1:A:78:VAL:HG23	1:A:78:VAL:O	2.11	0.51
1:B:226:GLY:HA3	1:B:377:LEU:CD1	2.40	0.51
1:B:318:ILE:HG12	1:B:319:LEU:HD12	1.92	0.51
1:D:62:VAL:HG11	1:D:109:LYS:NZ	2.25	0.51
1:D:40:GLU:HG3	1:D:46:ARG:NH1	2.16	0.51
1:D:504:PHE:HB3	1:E:146:GLU:OE1	2.09	0.51
1:F:427:LYS:HZ3	1:F:428:HIS:H	1.58	0.51
1:C:243:THR:O	1:C:243:THR:HG23	2.09	0.51
1:C:318:ILE:HG12	1:C:319:LEU:HD12	1.92	0.51
1:C:471:THR:HA	1:C:474:LYS:HB3	1.92	0.51
1:E:308:PHE:O	1:E:311:ALA:HB3	2.10	0.51
1:A:348:ILE:HB	1:A:371:VAL:HG22	1.92	0.51
1:A:428:HIS:N	1:A:428:HIS:CD2	2.78	0.51
1:A:471:THR:HA	1:A:474:LYS:HB3	1.93	0.51
1:D:474:LYS:HD3	1:D:475:TYR:CE2	2.45	0.51
1:D:487:VAL:O	1:D:491:GLU:HG3	2.11	0.51
1:D:99:TYR:HH	1:D:149:THR:HG22	1.72	0.51
1:D:348:ILE:HB	1:D:371:VAL:HG22	1.92	0.51
1:E:147:LYS:HD2	1:E:151:ARG:NH2	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ILE:HD12	1:E:79:ILE:N	2.25	0.51
1:F:28:VAL:CG2	1:F:487:VAL:HG13	2.39	0.51
1:F:318:ILE:N	1:F:318:ILE:HD13	2.25	0.51
1:F:226:GLY:HA3	1:F:377:LEU:CD1	2.40	0.51
1:A:285:TRP:O	1:A:286:ASN:HB2	2.11	0.51
1:C:221:ARG:HD2	1:C:454:HIS:CE1	2.45	0.51
1:C:251:PHE:CB	1:C:325:ILE:HG13	2.41	0.51
1:D:308:PHE:O	1:D:311:ALA:HB3	2.09	0.51
1:D:41:SER:CA	1:D:46:ARG:HD2	2.31	0.51
1:E:243:THR:HG23	1:E:243:THR:O	2.11	0.51
1:A:92:PRO:HG2	1:A:389:TRP:CZ2	2.46	0.51
1:B:266:TYR:O	1:B:270:PHE:HD2	1.94	0.51
1:B:308:PHE:O	1:B:311:ALA:HB3	2.09	0.51
1:B:40:GLU:HG3	1:B:46:ARG:NH1	2.17	0.51
1:C:252:VAL:CG1	1:C:318:ILE:HB	2.40	0.51
1:F:471:THR:HA	1:F:474:LYS:HB3	1.93	0.51
1:A:116:THR:HG22	1:A:128:GLY:H	1.76	0.51
1:B:87:SER:O	1:B:127:GLY:HA3	2.11	0.51
1:B:440:PHE:O	1:B:444:ILE:HG13	2.10	0.51
1:C:41:SER:HA	1:C:46:ARG:CD	2.34	0.51
1:D:335:LEU:HD12	1:D:356:THR:HG22	1.92	0.51
1:F:40:GLU:O	1:F:42:GLU:N	2.44	0.51
1:C:78:VAL:N	1:F:54:ARG:HH12	2.08	0.51
1:A:425:PHE:CD1	1:A:427:LYS:HB2	2.44	0.51
1:C:226:GLY:HA3	1:C:377:LEU:CD1	2.41	0.51
1:C:425:PHE:CD1	1:C:427:LYS:HB2	2.43	0.51
1:D:62:VAL:HG11	1:D:109:LYS:HZ3	1.76	0.51
1:B:54:ARG:HH12	1:D:77:GLU:HA	1.75	0.51
1:E:285:TRP:O	1:E:286:ASN:HB2	2.10	0.51
1:E:73:ASP:O	1:E:75:SER:N	2.42	0.51
1:F:266:TYR:O	1:F:270:PHE:HD2	1.94	0.51
1:F:95:GLY:HA3	1:F:129:ALA:O	2.11	0.51
1:A:298:PHE:HE1	1:A:309:PRO:HD3	1.76	0.50
1:C:30:ASP:O	1:C:34:GLU:HG2	2.11	0.50
1:B:505:THR:N	1:F:150:ARG:HH12	2.08	0.50
1:F:30:ASP:O	1:F:34:GLU:HG2	2.11	0.50
1:B:348:ILE:HB	1:B:371:VAL:HG22	1.93	0.50
1:C:73:ASP:O	1:C:75:SER:N	2.45	0.50
1:D:243:THR:O	1:D:243:THR:HG23	2.12	0.50
1:D:252:VAL:CG1	1:D:318:ILE:HB	2.41	0.50
1:D:40:GLU:O	1:D:42:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:PHE:CB	1:E:325:ILE:HG13	2.39	0.50
1:F:73:ASP:O	1:F:75:SER:N	2.44	0.50
1:A:243:THR:O	1:A:243:THR:HG23	2.12	0.50
1:B:116:THR:HG22	1:B:128:GLY:N	2.25	0.50
1:B:116:THR:HG22	1:B:128:GLY:H	1.77	0.50
1:B:425:PHE:CD1	1:B:427:LYS:HB2	2.44	0.50
1:B:40:GLU:O	1:B:42:GLU:N	2.44	0.50
1:C:40:GLU:O	1:C:42:GLU:N	2.44	0.50
1:D:488:ASN:HD21	1:D:492:LYS:HZ2	1.59	0.50
1:E:38:THR:CG2	1:E:41:SER:HB3	2.40	0.50
1:A:298:PHE:CE1	1:A:309:PRO:HD3	2.47	0.50
1:A:332:GLU:HG2	1:A:333:LYS:HG2	1.92	0.50
1:A:474:LYS:HD3	1:A:475:TYR:CE2	2.46	0.50
1:C:243:THR:H	1:C:244:PRO:HD3	1.74	0.50
1:C:332:GLU:HG2	1:C:333:LYS:HG2	1.93	0.50
1:C:372:ILE:HA	1:C:481:LEU:HD23	1.93	0.50
1:C:376:TYR:HB2	1:C:468:ILE:HD11	1.92	0.50
1:C:502:VAL:HG11	1:F:76:TRP:HD1	1.77	0.50
1:D:285:TRP:O	1:D:286:ASN:HB2	2.10	0.50
1:D:471:THR:HA	1:D:474:LYS:HB3	1.93	0.50
1:E:243:THR:N	1:E:244:PRO:CD	2.67	0.50
1:E:266:TYR:O	1:E:270:PHE:HD2	1.95	0.50
1:C:335:LEU:HD12	1:C:356:THR:HG22	1.94	0.50
1:D:30:ASP:O	1:D:34:GLU:HG2	2.11	0.50
1:D:440:PHE:O	1:D:444:ILE:HG13	2.11	0.50
1:E:318:ILE:HG12	1:E:319:LEU:HD12	1.92	0.50
1:E:428:HIS:CD2	1:E:428:HIS:N	2.78	0.50
1:A:78:VAL:N	1:E:54:ARG:HH12	2.10	0.50
1:F:335:LEU:HD12	1:F:356:THR:HG22	1.94	0.50
1:A:318:ILE:HG12	1:A:319:LEU:HD12	1.92	0.50
1:D:428:HIS:CD2	1:D:428:HIS:N	2.79	0.50
1:B:105:VAL:HG12	1:B:109:LYS:HE2	1.94	0.50
1:C:285:TRP:O	1:C:286:ASN:HB2	2.12	0.50
1:C:420:SER:HB3	1:E:432:ILE:O	2.12	0.50
1:D:122:VAL:HG23	1:D:124:VAL:HG23	1.94	0.50
1:C:390:LEU:HD13	1:D:396:VAL:HG21	1.93	0.50
1:F:318:ILE:HG12	1:F:319:LEU:HD12	1.93	0.50
1:A:343:VAL:CG2	1:A:364:PHE:HE1	2.25	0.50
1:B:428:HIS:CD2	1:B:428:HIS:N	2.79	0.50
1:C:440:PHE:O	1:C:444:ILE:HG13	2.11	0.50
1:D:347:ILE:HA	1:D:370:MET:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:VAL:HG23	1:E:487:VAL:HG13	1.94	0.50
1:F:348:ILE:HB	1:F:371:VAL:HG22	1.93	0.50
1:A:335:LEU:HD12	1:A:356:THR:HG22	1.93	0.50
1:B:435:VAL:HG13	1:F:423:ARG:HH21	1.75	0.50
1:C:348:ILE:HB	1:C:371:VAL:HG22	1.93	0.50
1:D:425:PHE:CD1	1:D:427:LYS:HB2	2.44	0.50
1:E:347:ILE:HA	1:E:370:MET:O	2.12	0.50
1:E:226:GLY:HA3	1:E:377:LEU:CD1	2.42	0.50
1:E:488:ASN:HD21	1:E:492:LYS:HZ2	1.60	0.50
1:C:421:LEU:HD21	1:E:421:LEU:HD21	1.93	0.49
1:C:213:HIS:HB2	1:C:449:GLU:HB3	1.93	0.49
1:D:319:LEU:HD12	1:D:319:LEU:N	2.27	0.49
1:D:327:ILE:CG2	1:D:349:ALA:HB3	2.34	0.49
1:E:322:ASP:HA	1:E:344:LYS:HB2	1.93	0.49
1:F:116:THR:HG22	1:F:128:GLY:N	2.27	0.49
1:F:322:ASP:HA	1:F:344:LYS:HB2	1.93	0.49
1:C:504:PHE:CE1	1:F:70:ARG:HB3	2.47	0.49
1:A:40:GLU:HG3	1:A:46:ARG:NH1	2.15	0.49
1:B:471:THR:HA	1:B:474:LYS:HB3	1.93	0.49
1:D:318:ILE:N	1:D:318:ILE:HD13	2.25	0.49
1:D:391:LYS:NZ	1:D:449:GLU:OE1	2.43	0.49
1:E:40:GLU:O	1:E:42:GLU:N	2.45	0.49
1:E:471:THR:HA	1:E:474:LYS:HB3	1.93	0.49
1:F:332:GLU:HG2	1:F:333:LYS:HG2	1.93	0.49
1:F:79:ILE:HD12	1:F:79:ILE:N	2.27	0.49
1:B:243:THR:HG23	1:B:243:THR:O	2.11	0.49
1:C:206:PRO:HB2	1:C:209:GLN:CG	2.43	0.49
1:C:78:VAL:O	1:C:78:VAL:HG23	2.13	0.49
1:D:266:TYR:O	1:D:270:PHE:HD2	1.95	0.49
1:E:30:ASP:O	1:E:34:GLU:HG2	2.12	0.49
1:A:336:THR:H	1:A:339:ASN:ND2	2.08	0.49
1:C:298:PHE:HE1	1:C:309:PRO:HD3	1.78	0.49
1:C:79:ILE:N	1:C:79:ILE:HD12	2.27	0.49
1:D:221:ARG:HD2	1:D:454:HIS:NE2	2.27	0.49
1:F:298:PHE:CE1	1:F:309:PRO:HD3	2.48	0.49
1:F:336:THR:H	1:F:339:ASN:ND2	2.08	0.49
1:F:337:LYS:HZ2	1:F:359:GLU:HG3	1.77	0.49
1:F:474:LYS:HD3	1:F:475:TYR:CE2	2.47	0.49
1:A:40:GLU:O	1:A:42:GLU:N	2.45	0.49
1:B:502:VAL:N	1:B:505:THR:HB	2.28	0.49
1:B:76:TRP:HB2	1:D:51:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:VAL:CG1	1:C:379:ALA:HB3	2.41	0.49
1:C:242:MET:O	1:C:243:THR:HG22	2.13	0.49
1:D:332:GLU:HG2	1:D:333:LYS:HG2	1.92	0.49
1:E:332:GLU:HG2	1:E:333:LYS:HG2	1.93	0.49
1:F:347:ILE:HA	1:F:370:MET:O	2.13	0.49
1:F:87:SER:O	1:F:127:GLY:HA3	2.12	0.49
1:A:147:LYS:HD2	1:A:151:ARG:NH2	2.20	0.49
1:A:347:ILE:HA	1:A:370:MET:O	2.13	0.49
1:A:226:GLY:HA3	1:A:377:LEU:CD1	2.42	0.49
1:B:336:THR:H	1:B:339:ASN:ND2	2.09	0.49
1:B:375:LEU:HD22	1:B:486:TYR:CE2	2.47	0.49
1:D:505:THR:HG23	1:E:150:ARG:HH22	1.77	0.49
1:E:136:ASN:OD1	1:E:138:LYS:HB2	2.13	0.49
1:E:37:ARG:NH2	1:E:49:VAL:HG11	2.28	0.49
1:F:105:VAL:HG12	1:F:109:LYS:HE2	1.95	0.49
1:F:487:VAL:O	1:F:491:GLU:HG3	2.12	0.49
1:A:30:ASP:O	1:A:34:GLU:HG2	2.13	0.49
1:B:16:MET:SD	1:B:358:PRO:HD3	2.52	0.49
1:C:105:VAL:HG12	1:C:109:LYS:HE2	1.95	0.49
1:C:376:TYR:CZ	1:C:465:ALA:HB2	2.47	0.49
1:D:116:THR:HG22	1:D:128:GLY:N	2.27	0.49
1:D:502:VAL:N	1:D:505:THR:HB	2.28	0.49
1:E:116:THR:HG22	1:E:128:GLY:N	2.27	0.49
1:E:348:ILE:HB	1:E:371:VAL:HG22	1.94	0.49
1:A:199:HIS:O	1:A:205:LYS:HE2	2.13	0.49
1:C:228:GLU:O	1:C:231:ILE:HG22	2.13	0.49
1:C:488:ASN:HD21	1:C:492:LYS:NZ	2.11	0.49
1:C:505:THR:C	1:D:150:ARG:HH22	2.15	0.49
1:C:69:ILE:HG12	1:C:79:ILE:CD1	2.43	0.49
1:D:243:THR:H	1:D:244:PRO:HD3	1.75	0.49
1:D:322:ASP:HA	1:D:344:LYS:HB2	1.93	0.49
1:E:13:PHE:CE2	1:E:107:GLU:HG3	2.48	0.49
1:A:69:ILE:HG12	1:A:79:ILE:CD1	2.43	0.49
1:C:122:VAL:HG23	1:C:124:VAL:HG23	1.94	0.49
1:C:28:VAL:HG22	1:C:487:VAL:HG13	1.94	0.49
1:F:242:MET:O	1:F:243:THR:HG22	2.12	0.49
1:A:266:TYR:O	1:A:270:PHE:HD2	1.95	0.49
1:B:91:THR:HB	1:B:92:PRO:HD3	1.95	0.49
1:C:122:VAL:HG11	1:C:379:ALA:HB1	1.94	0.49
1:C:400:ARG:NH1	1:C:400:ARG:HG3	2.28	0.49
1:C:76:TRP:CD1	1:F:502:VAL:HG11	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:PHE:CE2	1:D:107:GLU:HG3	2.48	0.49
1:F:285:TRP:CD1	1:F:287:PRO:HD3	2.48	0.49
1:A:233:GLU:HG2	1:A:236:TYR:HD1	1.78	0.48
1:B:13:PHE:CE2	1:B:107:GLU:HG3	2.48	0.48
1:B:343:VAL:CG2	1:B:364:PHE:HE1	2.25	0.48
1:B:487:VAL:O	1:B:491:GLU:HG3	2.13	0.48
1:D:505:THR:N	1:E:150:ARG:NH1	2.60	0.48
1:F:252:VAL:HG23	1:F:323:CYS:SG	2.53	0.48
1:F:425:PHE:CD1	1:F:427:LYS:HB2	2.42	0.48
1:D:116:THR:HG22	1:D:128:GLY:H	1.78	0.48
1:C:420:SER:HB2	1:E:433:PRO:HA	1.94	0.48
1:F:235:SER:O	1:F:239:ILE:HG12	2.13	0.48
1:F:343:VAL:CG2	1:F:364:PHE:HE1	2.25	0.48
1:F:427:LYS:HA	1:F:427:LYS:CE	2.33	0.48
1:F:91:THR:HB	1:F:92:PRO:HD3	1.95	0.48
1:A:243:THR:H	1:A:244:PRO:HD3	1.74	0.48
1:C:136:ASN:OD1	1:C:138:LYS:HB2	2.13	0.48
1:C:266:TYR:O	1:C:270:PHE:HD2	1.96	0.48
1:C:425:PHE:HD1	1:C:427:LYS:CB	2.26	0.48
1:C:78:VAL:HG13	1:F:54:ARG:NH1	2.28	0.48
1:D:78:VAL:O	1:D:78:VAL:HG23	2.12	0.48
1:F:13:PHE:CE2	1:F:107:GLU:HG3	2.49	0.48
1:A:13:PHE:CE2	1:A:107:GLU:HG3	2.48	0.48
1:A:488:ASN:HD21	1:A:492:LYS:NZ	2.12	0.48
1:B:427:LYS:HZ3	1:B:428:HIS:H	1.59	0.48
1:C:252:VAL:HG23	1:C:323:CYS:SG	2.53	0.48
1:C:322:ASP:HA	1:C:344:LYS:HB2	1.93	0.48
1:D:298:PHE:HE1	1:D:309:PRO:HD3	1.77	0.48
1:E:319:LEU:N	1:E:319:LEU:HD12	2.28	0.48
1:F:425:PHE:HD1	1:F:427:LYS:CB	2.25	0.48
1:A:187:TYR:CE2	1:A:192:GLY:HA3	2.48	0.48
1:E:221:ARG:CD	1:E:454:HIS:CD2	2.96	0.48
1:E:242:MET:O	1:E:243:THR:HG22	2.14	0.48
1:F:122:VAL:HG23	1:F:124:VAL:HG23	1.95	0.48
1:A:427:LYS:HZ3	1:A:428:HIS:H	1.60	0.48
1:A:49:VAL:HA	1:E:76:TRP:CZ3	2.48	0.48
1:A:78:VAL:H	1:E:54:ARG:HH12	1.61	0.48
1:C:13:PHE:CE2	1:C:107:GLU:HG3	2.48	0.48
1:C:187:TYR:CE2	1:C:192:GLY:HA3	2.49	0.48
1:C:40:GLU:HG3	1:C:46:ARG:NH1	2.15	0.48
1:C:87:SER:O	1:C:127:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:PHE:CE1	1:D:309:PRO:HD3	2.48	0.48
1:E:233:GLU:HG2	1:E:236:TYR:HD1	1.79	0.48
1:E:343:VAL:CG2	1:E:364:PHE:HE1	2.26	0.48
1:E:487:VAL:O	1:E:491:GLU:HG3	2.14	0.48
1:E:78:VAL:O	1:E:78:VAL:HG23	2.12	0.48
1:F:502:VAL:N	1:F:505:THR:HB	2.28	0.48
1:A:283:SER:HB2	1:A:314:TYR:O	2.13	0.48
1:B:319:LEU:HD12	1:B:319:LEU:N	2.29	0.48
1:C:298:PHE:CE1	1:C:309:PRO:HD3	2.48	0.48
1:C:502:VAL:N	1:C:505:THR:HB	2.28	0.48
1:D:37:ARG:NH2	1:D:49:VAL:HG11	2.29	0.48
1:A:154:MET:CE	1:A:190:THR:HG21	2.44	0.48
1:A:327:ILE:CG2	1:A:349:ALA:HB3	2.34	0.48
1:A:41:SER:CA	1:A:46:ARG:HD2	2.32	0.48
1:B:78:VAL:HG23	1:B:78:VAL:O	2.14	0.48
1:C:283:SER:HB2	1:C:314:TYR:O	2.14	0.48
1:F:118:LYS:NZ	1:F:353:ASN:HD21	2.12	0.48
1:F:298:PHE:HE1	1:F:309:PRO:HD3	1.77	0.48
1:A:242:MET:O	1:A:243:THR:HG22	2.13	0.48
1:A:319:LEU:N	1:A:319:LEU:HD12	2.29	0.48
1:B:33:VAL:O	1:B:38:THR:N	2.47	0.48
1:E:235:SER:O	1:E:239:ILE:HG12	2.14	0.48
1:A:76:TRP:HD1	1:E:502:VAL:HG11	1.76	0.48
1:E:91:THR:HB	1:E:92:PRO:HD3	1.96	0.48
1:F:38:THR:CG2	1:F:41:SER:HB3	2.41	0.48
1:A:502:VAL:N	1:A:505:THR:HB	2.28	0.48
1:B:242:MET:O	1:B:243:THR:HG22	2.13	0.48
1:D:100:SER:O	1:D:103:VAL:HG22	2.14	0.48
1:C:150:ARG:HH12	1:E:505:THR:C	2.17	0.48
1:E:502:VAL:N	1:E:505:THR:HB	2.28	0.48
1:F:283:SER:HB2	1:F:314:TYR:O	2.13	0.48
1:F:488:ASN:HD21	1:F:492:LYS:NZ	2.12	0.48
1:A:235:SER:O	1:A:239:ILE:HG12	2.14	0.47
1:A:391:LYS:NZ	1:A:449:GLU:OE1	2.41	0.47
1:B:230:PHE:CE2	1:B:481:LEU:HD21	2.49	0.47
1:C:37:ARG:NH2	1:C:49:VAL:HG11	2.29	0.47
1:D:205:LYS:NZ	1:D:388:GLU:OE1	2.43	0.47
1:B:54:ARG:HH12	1:D:78:VAL:H	1.60	0.47
1:E:336:THR:H	1:E:339:ASN:ND2	2.09	0.47
1:A:251:PHE:HB3	1:A:325:ILE:CG1	2.41	0.47
1:A:318:ILE:HD13	1:A:318:ILE:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:SER:O	1:C:103:VAL:HG22	2.15	0.47
1:C:211:GLY:O	1:C:391:LYS:NZ	2.42	0.47
1:C:217:SER:OG	1:C:454:HIS:CE1	2.67	0.47
1:D:343:VAL:CG2	1:D:364:PHE:HE1	2.25	0.47
1:A:257:GLY:O	1:A:260:GLY:N	2.48	0.47
1:C:427:LYS:HZ3	1:C:428:HIS:H	1.60	0.47
1:D:136:ASN:OD1	1:D:138:LYS:HB2	2.14	0.47
1:D:488:ASN:HD21	1:D:492:LYS:NZ	2.12	0.47
1:E:122:VAL:HG23	1:E:124:VAL:HG23	1.96	0.47
1:E:116:THR:HG22	1:E:128:GLY:H	1.79	0.47
1:F:116:THR:HG22	1:F:128:GLY:H	1.79	0.47
1:F:372:ILE:HA	1:F:373:PRO:HD3	1.64	0.47
1:A:285:TRP:CD1	1:A:287:PRO:HD3	2.49	0.47
1:B:187:TYR:CE2	1:B:192:GLY:HA3	2.49	0.47
1:B:235:SER:O	1:B:239:ILE:HG12	2.14	0.47
1:B:283:SER:HB2	1:B:314:TYR:O	2.14	0.47
1:B:285:TRP:CD1	1:B:287:PRO:HD3	2.50	0.47
1:C:343:VAL:CG2	1:C:364:PHE:HE1	2.26	0.47
1:D:226:GLY:HA3	1:D:377:LEU:CD1	2.44	0.47
1:E:69:ILE:HG12	1:E:79:ILE:CD1	2.44	0.47
1:C:503:THR:HG21	1:F:151:ARG:HD3	1.96	0.47
1:F:319:LEU:HD12	1:F:319:LEU:N	2.29	0.47
1:F:41:SER:HA	1:F:46:ARG:CD	2.33	0.47
1:F:69:ILE:HG12	1:F:79:ILE:CD1	2.44	0.47
1:A:251:PHE:CE2	1:A:264:MET:HA	2.50	0.47
1:A:432:ILE:HG22	1:A:434:ILE:CG1	2.43	0.47
1:A:487:VAL:O	1:A:491:GLU:HG3	2.14	0.47
1:C:257:GLY:O	1:C:258:ASN:C	2.53	0.47
1:C:319:LEU:HD12	1:C:319:LEU:N	2.30	0.47
1:C:373:PRO:HD3	1:C:481:LEU:HB3	1.96	0.47
1:D:105:VAL:HG12	1:D:109:LYS:HE2	1.96	0.47
1:D:184:ALA:HA	1:D:201:CYS:SG	2.54	0.47
1:E:233:GLU:CG	1:E:236:TYR:HD1	2.27	0.47
1:E:298:PHE:HE1	1:E:309:PRO:HD3	1.78	0.47
1:F:221:ARG:HD2	1:F:454:HIS:CE1	2.48	0.47
1:F:418:GLN:OE1	1:F:434:ILE:HG23	2.15	0.47
1:A:100:SER:O	1:A:103:VAL:HG22	2.15	0.47
1:A:33:VAL:O	1:A:38:THR:N	2.47	0.47
1:A:37:ARG:NH2	1:A:49:VAL:HG11	2.30	0.47
1:B:122:VAL:HG23	1:B:124:VAL:HG23	1.97	0.47
1:B:298:PHE:HE1	1:B:309:PRO:HD3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:PHE:CE1	1:B:302:HIS:HE1	2.33	0.47
1:B:298:PHE:CE1	1:B:309:PRO:HD3	2.49	0.47
1:C:235:SER:O	1:C:239:ILE:HG12	2.14	0.47
1:D:154:MET:CE	1:D:190:THR:HG21	2.45	0.47
1:D:91:THR:HB	1:D:92:PRO:HD3	1.97	0.47
1:A:233:GLU:CG	1:A:236:TYR:HD1	2.27	0.47
1:C:347:ILE:HA	1:C:370:MET:O	2.14	0.47
1:D:92:PRO:HG2	1:D:389:TRP:CZ2	2.50	0.47
1:E:298:PHE:CE1	1:E:302:HIS:HE1	2.33	0.47
1:E:432:ILE:HG22	1:E:434:ILE:CG1	2.45	0.47
1:F:327:ILE:CG2	1:F:349:ALA:HB3	2.33	0.47
1:B:136:ASN:OD1	1:B:138:LYS:HB2	2.14	0.47
1:C:285:TRP:CD1	1:C:287:PRO:HD3	2.50	0.47
1:C:327:ILE:CG2	1:C:349:ALA:HB3	2.36	0.47
1:D:13:PHE:CE1	1:D:107:GLU:HA	2.50	0.47
1:E:177:GLU:HB2	1:E:206:PRO:HG3	1.97	0.47
1:E:21:PHE:CE1	1:E:490:ILE:HD12	2.49	0.47
1:F:251:PHE:HB3	1:F:325:ILE:CG1	2.41	0.47
1:A:228:GLU:O	1:A:231:ILE:HG22	2.15	0.47
1:C:33:VAL:O	1:C:38:THR:N	2.47	0.47
1:D:242:MET:O	1:D:243:THR:HG22	2.14	0.47
1:D:257:GLY:O	1:D:260:GLY:N	2.48	0.47
1:E:187:TYR:CE2	1:E:192:GLY:HA3	2.50	0.47
1:A:54:ARG:HH12	1:E:77:GLU:HA	1.80	0.47
1:B:339:ASN:N	1:B:339:ASN:HD22	2.13	0.47
1:B:374:ASP:O	1:B:378:ASN:ND2	2.48	0.47
1:C:91:THR:HB	1:C:92:PRO:HD3	1.97	0.47
1:D:432:ILE:HG22	1:D:434:ILE:CG1	2.45	0.47
1:E:105:VAL:HG12	1:E:109:LYS:HE2	1.97	0.47
1:F:243:THR:H	1:F:244:PRO:HD3	1.75	0.47
1:C:421:LEU:HA	1:C:421:LEU:HD12	1.74	0.47
1:D:187:TYR:CE2	1:D:192:GLY:HA3	2.50	0.47
1:D:283:SER:HB2	1:D:314:TYR:O	2.14	0.47
1:D:33:VAL:O	1:D:38:THR:N	2.48	0.47
1:F:298:PHE:CE1	1:F:302:HIS:HE1	2.33	0.47
1:A:41:SER:HA	1:A:46:ARG:CD	2.35	0.46
1:C:154:MET:CE	1:C:190:THR:HG21	2.45	0.46
1:C:233:GLU:HG2	1:C:236:TYR:HD1	1.80	0.46
1:C:373:PRO:CD	1:C:481:LEU:HB3	2.46	0.46
1:C:38:THR:CG2	1:C:41:SER:HB3	2.40	0.46
1:D:425:PHE:HD1	1:D:427:LYS:CB	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ARG:NH1	1:F:77:GLU:HA	2.30	0.46
1:A:184:ALA:HA	1:A:201:CYS:SG	2.55	0.46
1:B:233:GLU:HG2	1:B:236:TYR:HD1	1.80	0.46
1:B:69:ILE:HG12	1:B:79:ILE:CD1	2.46	0.46
1:C:423:ARG:NH2	1:E:435:VAL:HG13	2.27	0.46
1:D:339:ASN:H	1:D:339:ASN:ND2	2.13	0.46
1:D:418:GLN:OE1	1:D:434:ILE:HG23	2.16	0.46
1:E:154:MET:CE	1:E:190:THR:HG21	2.45	0.46
1:E:320:GLU:HG3	1:E:342:ARG:HG2	1.98	0.46
1:F:233:GLU:HG2	1:F:236:TYR:HD1	1.80	0.46
1:A:13:PHE:CE1	1:A:107:GLU:HA	2.50	0.46
1:A:177:GLU:HB2	1:A:206:PRO:HG3	1.97	0.46
1:B:41:SER:HA	1:B:46:ARG:CD	2.34	0.46
1:C:298:PHE:CE1	1:C:302:HIS:HE1	2.33	0.46
1:C:334:GLN:HA	1:C:334:GLN:HE21	1.80	0.46
1:C:374:ASP:O	1:C:378:ASN:ND2	2.48	0.46
1:C:388:GLU:O	1:C:391:LYS:HB3	2.15	0.46
1:E:283:SER:HB2	1:E:314:TYR:O	2.15	0.46
1:E:488:ASN:HD21	1:E:492:LYS:NZ	2.13	0.46
1:F:257:GLY:O	1:F:260:GLY:N	2.48	0.46
1:F:251:PHE:CE2	1:F:264:MET:HA	2.50	0.46
1:F:78:VAL:O	1:F:78:VAL:HG23	2.14	0.46
1:A:425:PHE:HD1	1:A:427:LYS:CB	2.28	0.46
1:C:184:ALA:HA	1:C:201:CYS:SG	2.56	0.46
1:C:505:THR:C	1:D:150:ARG:HH12	2.19	0.46
1:D:252:VAL:HG23	1:D:323:CYS:SG	2.56	0.46
1:E:13:PHE:CE1	1:E:107:GLU:HA	2.51	0.46
1:E:33:VAL:O	1:E:38:THR:N	2.47	0.46
1:F:133:VAL:HG12	1:F:135:ILE:HB	1.98	0.46
1:A:150:ARG:HH12	1:F:505:THR:C	2.19	0.46
1:A:298:PHE:CE1	1:A:302:HIS:HE1	2.34	0.46
1:B:190:THR:HG22	1:B:191:ILE:HG12	1.98	0.46
1:B:502:VAL:HG23	1:B:503:THR:N	2.28	0.46
1:B:505:THR:HG23	1:F:150:ARG:NH2	2.31	0.46
1:C:13:PHE:CE1	1:C:107:GLU:HA	2.51	0.46
1:C:487:VAL:O	1:C:491:GLU:HG3	2.15	0.46
1:D:257:GLY:O	1:D:258:ASN:C	2.54	0.46
1:D:427:LYS:CE	1:D:427:LYS:HA	2.32	0.46
1:E:298:PHE:CE1	1:E:309:PRO:HD3	2.49	0.46
1:F:334:GLN:HE21	1:F:334:GLN:HA	1.81	0.46
1:B:257:GLY:O	1:B:260:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ILE:CG2	1:B:349:ALA:HB3	2.34	0.46
1:B:427:LYS:HG3	1:B:430:GLY:H	1.81	0.46
1:B:418:GLN:OE1	1:B:434:ILE:HG23	2.16	0.46
1:C:233:GLU:CG	1:C:236:TYR:HD1	2.28	0.46
1:C:51:GLY:O	1:C:55:ILE:HG13	2.15	0.46
1:D:285:TRP:CD1	1:D:287:PRO:HD3	2.50	0.46
1:D:421:LEU:HD23	1:E:421:LEU:HD11	1.96	0.46
1:E:120:ALA:O	1:E:492:LYS:NZ	2.48	0.46
1:D:435:VAL:HG13	1:E:423:ARG:NH2	2.31	0.46
1:F:432:ILE:HG22	1:F:434:ILE:CG1	2.46	0.46
1:B:154:MET:CE	1:B:190:THR:HG21	2.45	0.46
1:B:322:ASP:OD1	1:B:344:LYS:HB3	2.16	0.46
1:B:432:ILE:HG22	1:B:434:ILE:CG1	2.45	0.46
1:C:150:ARG:HH12	1:E:505:THR:N	2.13	0.46
1:C:257:GLY:O	1:C:260:GLY:N	2.49	0.46
1:C:418:GLN:OE1	1:C:434:ILE:HG23	2.15	0.46
1:E:285:TRP:CD1	1:E:287:PRO:HD3	2.50	0.46
1:D:435:VAL:CG1	1:E:423:ARG:HH21	2.28	0.46
1:F:100:SER:O	1:F:103:VAL:HG22	2.15	0.46
1:F:37:ARG:NH2	1:F:49:VAL:HG11	2.29	0.46
1:A:206:PRO:HD2	1:A:209:GLN:HB2	1.98	0.46
1:A:421:LEU:HD12	1:A:421:LEU:HA	1.73	0.46
1:B:13:PHE:CE1	1:B:107:GLU:HA	2.51	0.46
1:B:257:GLY:O	1:B:258:ASN:C	2.54	0.46
1:B:91:THR:CB	1:B:92:PRO:CD	2.94	0.46
1:C:133:VAL:HG12	1:C:135:ILE:HB	1.98	0.46
1:C:427:LYS:HG3	1:C:430:GLY:H	1.81	0.46
1:D:233:GLU:HG2	1:D:236:TYR:HD1	1.80	0.46
1:E:339:ASN:ND2	1:E:339:ASN:H	2.14	0.46
1:F:136:ASN:OD1	1:F:138:LYS:HB2	2.15	0.46
1:F:187:TYR:CE2	1:F:192:GLY:HA3	2.51	0.46
1:F:339:ASN:H	1:F:339:ASN:ND2	2.14	0.46
1:A:91:THR:HB	1:A:92:PRO:HD3	1.97	0.46
1:B:184:ALA:HA	1:B:201:CYS:SG	2.56	0.46
1:B:320:GLU:HG3	1:B:342:ARG:HG2	1.98	0.46
1:C:12:ASN:ND2	1:C:14:PHE:HB3	2.30	0.46
1:C:432:ILE:HG22	1:C:434:ILE:CG1	2.45	0.46
1:D:277:VAL:HG21	1:D:295:LEU:HD22	1.98	0.46
1:E:339:ASN:N	1:E:339:ASN:HD22	2.13	0.46
1:A:70:ARG:HB3	1:E:504:PHE:CE1	2.50	0.46
1:C:49:VAL:HA	1:F:76:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:OD1	1:A:138:LYS:HB2	2.15	0.46
1:A:252:VAL:HG23	1:A:323:CYS:SG	2.56	0.46
1:A:374:ASP:O	1:A:378:ASN:ND2	2.48	0.46
1:B:339:ASN:HD22	1:B:339:ASN:H	1.64	0.46
1:C:273:LYS:HE2	1:C:288:ASP:C	2.36	0.46
1:C:308:PHE:CD2	1:C:311:ALA:HB2	2.49	0.46
1:C:320:GLU:HG3	1:C:342:ARG:HG2	1.98	0.46
1:C:421:LEU:HD11	1:E:421:LEU:HD23	1.97	0.46
1:E:12:ASN:ND2	1:E:14:PHE:HB3	2.31	0.46
1:E:374:ASP:O	1:E:378:ASN:ND2	2.49	0.46
1:F:228:GLU:O	1:F:231:ILE:HG22	2.15	0.46
1:F:91:THR:CB	1:F:92:PRO:CD	2.93	0.46
1:A:339:ASN:HD22	1:A:339:ASN:N	2.14	0.45
1:A:372:ILE:HA	1:A:373:PRO:HD3	1.63	0.45
1:B:100:SER:O	1:B:103:VAL:HG22	2.17	0.45
1:B:133:VAL:HG12	1:B:135:ILE:HB	1.98	0.45
1:C:373:PRO:HG3	1:C:481:LEU:HB3	1.96	0.45
1:D:298:PHE:CE1	1:D:302:HIS:HE1	2.33	0.45
1:D:69:ILE:HG12	1:D:79:ILE:CD1	2.46	0.45
1:E:298:PHE:CE1	1:E:308:PHE:HA	2.52	0.45
1:F:12:ASN:ND2	1:F:14:PHE:HB3	2.31	0.45
1:F:233:GLU:CG	1:F:236:TYR:HD1	2.28	0.45
1:F:122:VAL:HG11	1:F:379:ALA:HB3	1.98	0.45
1:F:51:GLY:O	1:F:55:ILE:HG13	2.16	0.45
1:B:177:GLU:HB2	1:B:206:PRO:HG3	1.99	0.45
1:B:339:ASN:H	1:B:339:ASN:ND2	2.13	0.45
1:B:372:ILE:HA	1:B:373:PRO:HD3	1.62	0.45
1:B:118:LYS:NZ	1:B:378:ASN:ND2	2.64	0.45
1:C:251:PHE:CE2	1:C:264:MET:HA	2.51	0.45
1:D:233:GLU:CG	1:D:236:TYR:HD1	2.29	0.45
1:D:502:VAL:HG23	1:D:503:THR:N	2.28	0.45
1:E:149:THR:HG1	1:E:182:TRP:HE3	1.64	0.45
1:C:420:SER:HB3	1:E:433:PRO:HA	1.95	0.45
1:A:38:THR:CG2	1:A:41:SER:HB3	2.41	0.45
1:B:70:ARG:HH12	1:E:143:ASN:HD21	1.65	0.45
1:C:118:LYS:HZ3	1:C:353:ASN:HD21	1.64	0.45
1:D:235:SER:O	1:D:239:ILE:HG12	2.15	0.45
1:E:252:VAL:HG23	1:E:323:CYS:SG	2.57	0.45
1:E:257:GLY:O	1:E:260:GLY:N	2.49	0.45
1:E:427:LYS:HG3	1:E:430:GLY:H	1.81	0.45
1:A:504:PHE:CE1	1:E:70:ARG:CB	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:PHE:CE1	1:F:107:GLU:HA	2.51	0.45
1:A:28:VAL:HG23	1:A:487:VAL:HG13	1.98	0.45
1:B:120:ALA:O	1:B:492:LYS:NZ	2.49	0.45
1:B:12:ASN:ND2	1:B:14:PHE:HB3	2.32	0.45
1:D:133:VAL:HG12	1:D:135:ILE:HB	1.98	0.45
1:D:273:LYS:HE2	1:D:288:ASP:C	2.37	0.45
1:C:386:TYR:OH	1:D:396:VAL:HG13	2.16	0.45
1:D:496:VAL:HA	1:E:209:GLN:NE2	2.31	0.45
1:F:320:GLU:HG3	1:F:342:ARG:HG2	1.99	0.45
1:F:36:LEU:HD11	1:F:474:LYS:HZ1	1.81	0.45
1:A:12:ASN:ND2	1:A:14:PHE:HB3	2.31	0.45
1:A:180:MET:HE3	1:A:183:ILE:HD12	1.99	0.45
1:A:273:LYS:HE2	1:A:288:ASP:C	2.37	0.45
1:A:334:GLN:HA	1:A:334:GLN:HE21	1.82	0.45
1:A:339:ASN:H	1:A:339:ASN:ND2	2.14	0.45
1:E:251:PHE:HB3	1:E:325:ILE:CG1	2.42	0.45
1:F:277:VAL:HG21	1:F:295:LEU:HD22	1.99	0.45
1:F:322:ASP:OD1	1:F:344:LYS:HB3	2.16	0.45
1:A:320:GLU:HG3	1:A:342:ARG:HG2	1.99	0.45
1:B:318:ILE:N	1:B:318:ILE:HD13	2.24	0.45
1:B:334:GLN:HE21	1:B:334:GLN:HA	1.80	0.45
1:C:298:PHE:CE1	1:C:308:PHE:HA	2.52	0.45
1:C:318:ILE:HD13	1:C:318:ILE:N	2.29	0.45
1:C:474:LYS:HD3	1:C:475:TYR:CE2	2.51	0.45
1:D:251:PHE:HA	1:D:325:ILE:O	2.17	0.45
1:D:375:LEU:HD22	1:D:486:TYR:CE2	2.52	0.45
1:E:40:GLU:HG3	1:E:46:ARG:NH1	2.16	0.45
1:F:427:LYS:HG3	1:F:430:GLY:H	1.81	0.45
1:A:133:VAL:HG12	1:A:135:ILE:HB	1.98	0.45
1:D:350:GLU:OE1	1:D:482:ARG:NH2	2.50	0.45
1:E:334:GLN:HE21	1:E:334:GLN:HA	1.81	0.45
1:E:425:PHE:HD1	1:E:427:LYS:CB	2.27	0.45
1:F:308:PHE:CD2	1:F:311:ALA:HB2	2.50	0.45
1:F:374:ASP:O	1:F:378:ASN:ND2	2.50	0.45
1:B:251:PHE:CE2	1:B:264:MET:HA	2.52	0.45
1:C:209:GLN:NE2	1:E:499:GLU:HB2	2.31	0.45
1:D:12:ASN:ND2	1:D:14:PHE:HB3	2.31	0.45
1:D:243:THR:N	1:D:244:PRO:CD	2.69	0.45
1:D:372:ILE:HA	1:D:373:PRO:HD3	1.62	0.45
1:E:418:GLN:OE1	1:E:434:ILE:HG23	2.16	0.45
1:F:226:GLY:HA3	1:F:377:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:ASP:HB2	1:F:282:GLY:H	1.56	0.45
1:F:501:GLY:N	1:F:505:THR:HA	2.32	0.45
1:B:488:ASN:HD21	1:B:492:LYS:NZ	2.15	0.45
1:C:226:GLY:HA3	1:C:377:LEU:HD12	1.99	0.45
1:D:374:ASP:O	1:D:378:ASN:ND2	2.50	0.45
1:E:91:THR:CB	1:E:92:PRO:CD	2.94	0.45
1:A:136:ASN:OD1	1:A:138:LYS:N	2.50	0.45
1:A:322:ASP:OD1	1:A:344:LYS:HB3	2.17	0.45
1:A:91:THR:CB	1:A:92:PRO:CD	2.95	0.45
1:B:233:GLU:CG	1:B:236:TYR:HD1	2.29	0.45
1:B:350:GLU:OE1	1:B:482:ARG:NH2	2.50	0.45
1:C:502:VAL:HG23	1:C:503:THR:N	2.28	0.45
1:D:199:HIS:O	1:D:205:LYS:HE2	2.16	0.45
1:D:228:GLU:O	1:D:231:ILE:HG22	2.17	0.45
1:D:325:ILE:HG22	1:D:347:ILE:CG2	2.47	0.45
1:D:339:ASN:H	1:D:339:ASN:HD22	1.65	0.45
1:D:425:PHE:CD1	1:D:427:LYS:HD2	2.52	0.45
1:D:427:LYS:HG3	1:D:430:GLY:H	1.82	0.45
1:E:228:GLU:O	1:E:231:ILE:HG22	2.17	0.45
1:C:150:ARG:NH2	1:E:505:THR:HG23	2.32	0.45
1:F:177:GLU:HB2	1:F:206:PRO:HG3	1.99	0.45
1:F:273:LYS:HE2	1:F:288:ASP:C	2.37	0.45
1:F:298:PHE:CE1	1:F:308:PHE:HA	2.52	0.45
1:F:205:LYS:HZ3	1:F:392:ASN:HD21	1.64	0.45
1:F:400:ARG:HG3	1:F:400:ARG:NH1	2.29	0.45
1:F:425:PHE:CD1	1:F:427:LYS:HD2	2.51	0.45
1:A:298:PHE:CE1	1:A:308:PHE:HA	2.51	0.44
1:A:396:VAL:HG13	1:F:386:TYR:OH	2.17	0.44
1:B:251:PHE:HA	1:B:325:ILE:O	2.17	0.44
1:C:339:ASN:ND2	1:C:339:ASN:H	2.15	0.44
1:D:299:LYS:O	1:D:299:LYS:HG3	2.17	0.44
1:D:322:ASP:OD1	1:D:344:LYS:HB3	2.16	0.44
1:E:257:GLY:O	1:E:258:ASN:C	2.55	0.44
1:E:400:ARG:HG3	1:E:400:ARG:NH1	2.28	0.44
1:F:154:MET:CE	1:F:190:THR:HG21	2.47	0.44
1:F:339:ASN:N	1:F:339:ASN:HD22	2.14	0.44
1:F:33:VAL:O	1:F:38:THR:N	2.48	0.44
1:A:151:ARG:CZ	1:E:503:THR:HG21	2.48	0.44
1:A:257:GLY:O	1:A:258:ASN:C	2.55	0.44
1:A:51:GLY:O	1:A:55:ILE:HG13	2.17	0.44
1:B:118:LYS:HZ1	1:B:378:ASN:HD21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASN:OD1	1:B:138:LYS:N	2.50	0.44
1:A:433:PRO:HA	1:B:420:SER:CB	2.47	0.44
1:B:425:PHE:CD1	1:B:427:LYS:HD2	2.52	0.44
1:C:277:VAL:HG21	1:C:295:LEU:HD22	1.98	0.44
1:D:28:VAL:HG22	1:D:487:VAL:HG13	1.99	0.44
1:E:86:HIS:HD2	1:E:116:THR:HG21	1.78	0.44
1:F:364:PHE:HB3	1:F:369:ILE:HB	1.98	0.44
1:F:502:VAL:C	1:F:505:THR:HB	2.38	0.44
1:A:251:PHE:HA	1:A:325:ILE:O	2.17	0.44
1:A:339:ASN:H	1:A:339:ASN:HD22	1.65	0.44
1:A:337:LYS:HZ2	1:A:359:GLU:HG3	1.83	0.44
1:C:339:ASN:N	1:C:339:ASN:HD22	2.15	0.44
1:C:322:ASP:OD1	1:C:344:LYS:HB3	2.17	0.44
1:C:440:PHE:CG	1:D:412:HIS:HB3	2.52	0.44
1:C:501:GLY:N	1:C:505:THR:HA	2.32	0.44
1:D:339:ASN:HD22	1:D:339:ASN:N	2.14	0.44
1:D:320:GLU:HG3	1:D:342:ARG:HG2	1.98	0.44
1:D:501:GLY:N	1:D:505:THR:HA	2.32	0.44
1:D:502:VAL:C	1:D:505:THR:HB	2.38	0.44
1:E:133:VAL:HG12	1:E:135:ILE:HB	1.99	0.44
1:E:318:ILE:N	1:E:318:ILE:HD13	2.25	0.44
1:E:322:ASP:OD1	1:E:344:LYS:HB3	2.18	0.44
1:E:16:MET:SD	1:E:358:PRO:HD3	2.57	0.44
1:F:251:PHE:CE1	1:F:267:LEU:HB3	2.52	0.44
1:A:427:LYS:HG3	1:A:430:GLY:H	1.81	0.44
1:B:251:PHE:HB3	1:B:325:ILE:CG1	2.41	0.44
1:B:325:ILE:HG22	1:B:347:ILE:CG2	2.48	0.44
1:B:37:ARG:NH2	1:B:49:VAL:HG11	2.29	0.44
1:C:91:THR:CB	1:C:92:PRO:CD	2.94	0.44
1:D:251:PHE:CE2	1:D:264:MET:HA	2.52	0.44
1:D:337:LYS:HZ2	1:D:359:GLU:HG3	1.83	0.44
1:E:425:PHE:CD1	1:E:427:LYS:HD2	2.52	0.44
1:A:277:VAL:HG21	1:A:295:LEU:HD22	1.98	0.44
1:B:205:LYS:HG3	1:B:388:GLU:OE1	2.18	0.44
1:C:180:MET:HE3	1:C:183:ILE:HD12	2.00	0.44
1:C:425:PHE:CD1	1:C:427:LYS:HD2	2.53	0.44
1:C:505:THR:HG23	1:D:185:ASP:OD1	2.17	0.44
1:D:308:PHE:CD2	1:D:311:ALA:HB2	2.50	0.44
1:E:136:ASN:OD1	1:E:138:LYS:N	2.50	0.44
1:F:199:HIS:O	1:F:205:LYS:HE2	2.18	0.44
1:A:105:VAL:HG12	1:A:109:LYS:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG23	1:B:323:CYS:SG	2.58	0.44
1:B:502:VAL:C	1:B:505:THR:HB	2.37	0.44
1:C:69:ILE:HD13	1:C:148:ILE:CG1	2.47	0.44
1:D:111:LEU:HA	1:D:111:LEU:HD23	1.81	0.44
1:D:147:LYS:HD2	1:D:151:ARG:NH2	2.20	0.44
1:D:421:LEU:HD12	1:D:421:LEU:HA	1.73	0.44
1:A:390:LEU:O	1:A:391:LYS:C	2.56	0.44
1:B:273:LYS:HE2	1:B:288:ASP:C	2.38	0.44
1:C:31:LYS:HA	1:C:34:GLU:HG2	2.00	0.44
1:D:400:ARG:NH1	1:D:400:ARG:HG3	2.31	0.44
1:E:100:SER:O	1:E:103:VAL:HG22	2.17	0.44
1:E:502:VAL:C	1:E:505:THR:HB	2.38	0.44
1:E:501:GLY:N	1:E:505:THR:HA	2.32	0.44
1:F:257:GLY:O	1:F:258:ASN:C	2.55	0.44
1:F:47:ASN:HD21	1:F:50:ARG:NH1	2.16	0.44
1:A:254:GLN:HE21	1:A:330:ALA:HB3	1.82	0.44
1:A:47:ASN:HD21	1:A:50:ARG:NH1	2.16	0.44
1:B:298:PHE:CE1	1:B:308:PHE:HA	2.53	0.44
1:B:27:ILE:CG2	1:B:475:TYR:CD1	2.99	0.44
1:C:284:ILE:CG2	1:C:285:TRP:N	2.81	0.44
1:D:177:GLU:HB2	1:D:206:PRO:HG3	2.00	0.44
1:D:251:PHE:HB3	1:D:325:ILE:CG1	2.42	0.44
1:E:184:ALA:HA	1:E:201:CYS:SG	2.58	0.44
1:E:273:LYS:HE2	1:E:288:ASP:C	2.38	0.44
1:A:60:ASN:HA	1:E:66:SER:OG	2.18	0.44
1:F:205:LYS:NZ	1:F:392:ASN:ND2	2.63	0.44
1:A:418:GLN:OE1	1:A:434:ILE:HG23	2.17	0.44
1:A:502:VAL:C	1:A:505:THR:HB	2.38	0.44
1:B:226:GLY:HA3	1:B:377:LEU:HD12	1.99	0.44
1:C:372:ILE:HA	1:C:373:PRO:HD3	1.64	0.44
1:E:251:PHE:CE2	1:E:264:MET:HA	2.53	0.44
1:A:190:THR:HG22	1:A:191:ILE:HG12	2.00	0.43
1:A:226:GLY:HA3	1:A:377:LEU:HD12	1.98	0.43
1:A:457:LEU:CD2	1:A:461:MET:HG2	2.48	0.43
1:B:16:MET:HG2	1:B:358:PRO:HG2	2.00	0.43
1:B:323:CYS:O	1:B:345:ALA:HA	2.18	0.43
1:B:31:LYS:HD3	1:B:35:ASP:OD2	2.18	0.43
1:C:301:GLN:O	1:C:301:GLN:HG2	2.18	0.43
1:D:251:PHE:CE1	1:D:267:LEU:HB3	2.53	0.43
1:F:69:ILE:HD13	1:F:148:ILE:CG1	2.48	0.43
1:F:284:ILE:HD13	1:F:308:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:GLN:O	1:F:301:GLN:HG2	2.18	0.43
1:F:488:ASN:HD21	1:F:492:LYS:HZ1	1.66	0.43
1:B:151:ARG:NH2	1:D:504:PHE:CZ	2.86	0.43
1:B:436:PRO:HB3	1:B:440:PHE:CD1	2.54	0.43
1:C:199:HIS:O	1:C:205:LYS:HE2	2.18	0.43
1:C:291:ASP:HA	1:C:292:PRO:HD3	1.88	0.43
1:C:300:LEU:HD22	1:C:300:LEU:HA	1.87	0.43
1:D:298:PHE:CE1	1:D:308:PHE:HA	2.52	0.43
1:D:334:GLN:HE21	1:D:334:GLN:HA	1.82	0.43
1:D:51:GLY:O	1:D:55:ILE:HG13	2.18	0.43
1:E:299:LYS:O	1:E:299:LYS:HG3	2.17	0.43
1:F:502:VAL:HG23	1:F:503:THR:N	2.28	0.43
1:B:228:GLU:O	1:B:231:ILE:HG22	2.18	0.43
1:B:301:GLN:O	1:B:301:GLN:HG2	2.18	0.43
1:C:284:ILE:HD13	1:C:308:PHE:HB3	2.01	0.43
1:C:503:THR:HG21	1:F:151:ARG:CZ	2.48	0.43
1:D:254:GLN:HE21	1:D:330:ALA:HB3	1.83	0.43
1:D:364:PHE:HB3	1:D:369:ILE:HB	2.00	0.43
1:D:47:ASN:HD21	1:D:50:ARG:NH1	2.16	0.43
1:D:21:PHE:CE1	1:D:490:ILE:HD12	2.54	0.43
1:E:69:ILE:HD13	1:E:148:ILE:CG1	2.49	0.43
1:E:339:ASN:H	1:E:339:ASN:HD22	1.65	0.43
1:F:184:ALA:HA	1:F:201:CYS:SG	2.58	0.43
1:F:433:PRO:C	1:F:435:VAL:N	2.70	0.43
1:F:403:PHE:CD2	1:F:447:ALA:HB1	2.53	0.43
1:A:205:LYS:NZ	1:A:392:ASN:HD21	2.17	0.43
1:A:425:PHE:CD1	1:A:427:LYS:HD2	2.54	0.43
1:B:31:LYS:HA	1:B:34:GLU:HG2	2.00	0.43
1:B:400:ARG:HG3	1:B:400:ARG:NH1	2.30	0.43
1:D:323:CYS:O	1:D:345:ALA:HA	2.18	0.43
1:E:180:MET:HE3	1:E:183:ILE:HD12	2.00	0.43
1:E:190:THR:HG22	1:E:191:ILE:HG12	2.00	0.43
1:E:226:GLY:HA3	1:E:377:LEU:HD12	1.99	0.43
1:A:69:ILE:HD13	1:A:148:ILE:CG1	2.49	0.43
1:A:284:ILE:CG2	1:A:285:TRP:N	2.82	0.43
1:A:501:GLY:N	1:A:505:THR:HA	2.33	0.43
1:D:228:GLU:HA	1:D:231:ILE:HG22	2.01	0.43
1:D:284:ILE:HD13	1:D:308:PHE:HB3	2.01	0.43
1:D:403:PHE:CE2	1:D:452:ILE:HD11	2.53	0.43
1:E:199:HIS:O	1:E:205:LYS:HE2	2.18	0.43
1:E:364:PHE:HB3	1:E:369:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:GLU:HB3	1:E:427:LYS:HB3	2.00	0.43
1:E:47:ASN:HD21	1:E:50:ARG:NH1	2.17	0.43
1:F:28:VAL:HG22	1:F:487:VAL:HG13	2.00	0.43
1:F:68:PRO:HA	1:F:78:VAL:HA	2.01	0.43
1:C:54:ARG:NH1	1:F:78:VAL:HG13	2.34	0.43
1:A:228:GLU:HA	1:A:231:ILE:HG22	2.00	0.43
1:A:28:VAL:HG22	1:A:487:VAL:HG13	1.99	0.43
1:B:69:ILE:HD13	1:B:148:ILE:CG1	2.48	0.43
1:B:284:ILE:HD13	1:B:308:PHE:HB3	2.00	0.43
1:C:502:VAL:C	1:C:505:THR:HB	2.38	0.43
1:C:502:VAL:HG23	1:C:504:PHE:CD1	2.54	0.43
1:C:47:ASN:HD21	1:C:50:ARG:NH1	2.17	0.43
1:C:62:VAL:HG11	1:C:109:LYS:HZ3	1.83	0.43
1:D:350:GLU:CD	1:D:482:ARG:HH22	2.21	0.43
1:E:308:PHE:CD2	1:E:311:ALA:HB2	2.53	0.43
1:F:251:PHE:HA	1:F:325:ILE:O	2.19	0.43
1:F:284:ILE:CG2	1:F:285:TRP:N	2.82	0.43
1:A:325:ILE:HG22	1:A:347:ILE:CG2	2.48	0.43
1:A:436:PRO:HB3	1:A:440:PHE:CD1	2.53	0.43
1:A:376:TYR:OH	1:A:465:ALA:HB2	2.18	0.43
1:A:496:VAL:O	1:B:209:GLN:NE2	2.47	0.43
1:B:299:LYS:HG3	1:B:299:LYS:O	2.17	0.43
1:B:425:PHE:HD1	1:B:427:LYS:CB	2.27	0.43
1:B:51:GLY:O	1:B:55:ILE:HG13	2.19	0.43
1:E:325:ILE:HG22	1:E:347:ILE:CG2	2.48	0.43
1:B:143:ASN:HD21	1:E:70:ARG:HH12	1.67	0.43
1:F:180:MET:HE3	1:F:183:ILE:HD12	1.99	0.43
1:F:325:ILE:HG22	1:F:347:ILE:CG2	2.49	0.43
1:A:284:ILE:HD13	1:A:308:PHE:HB3	2.00	0.43
1:A:299:LYS:HG3	1:A:299:LYS:O	2.17	0.43
1:B:422:GLU:HB3	1:B:427:LYS:HB3	2.01	0.43
1:C:31:LYS:HD2	1:C:474:LYS:HZ1	1.84	0.43
1:D:69:ILE:HD13	1:D:148:ILE:CG1	2.49	0.43
1:E:261:LEU:HD12	1:E:261:LEU:C	2.39	0.43
1:E:291:ASP:HA	1:E:292:PRO:HD3	1.89	0.43
1:E:433:PRO:C	1:E:435:VAL:N	2.71	0.43
1:A:151:ARG:NH2	1:E:504:PHE:CZ	2.86	0.43
1:C:504:PHE:HZ	1:F:151:ARG:NH2	2.10	0.43
1:A:502:VAL:HG23	1:A:503:THR:N	2.28	0.43
1:A:504:PHE:HE1	1:E:70:ARG:CB	2.32	0.43
1:C:32:LEU:HD21	1:C:494:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLU:O	1:C:42:GLU:HG3	2.19	0.43
1:D:136:ASN:OD1	1:D:138:LYS:N	2.51	0.43
1:D:421:LEU:HD21	1:E:421:LEU:HD21	2.00	0.43
1:D:422:GLU:HB3	1:D:427:LYS:HB3	2.01	0.43
1:D:57:LYS:HB3	1:D:58:PRO:HD3	2.01	0.43
1:A:503:THR:HG21	1:E:151:ARG:CD	2.48	0.43
1:F:305:ILE:H	1:F:305:ILE:HG13	1.67	0.43
1:A:261:LEU:HD12	1:A:261:LEU:C	2.39	0.43
1:A:439:GLU:H	1:A:439:GLU:CD	2.22	0.43
1:B:111:LEU:HA	1:B:111:LEU:HD23	1.83	0.43
1:B:180:MET:HE3	1:B:183:ILE:HD12	2.00	0.43
1:B:203:THR:HA	1:B:388:GLU:OE1	2.19	0.43
1:B:501:GLY:N	1:B:505:THR:HA	2.33	0.43
1:C:177:GLU:HB2	1:C:206:PRO:HG3	2.01	0.43
1:C:325:ILE:HG22	1:C:347:ILE:CG2	2.49	0.43
1:C:387:PHE:CD1	1:D:401:LEU:HD21	2.54	0.43
1:E:375:LEU:HD22	1:E:486:TYR:CE2	2.54	0.43
1:F:31:LYS:HA	1:F:34:GLU:HG2	2.01	0.43
1:A:233:GLU:HG2	1:A:236:TYR:CD1	2.54	0.42
1:B:305:ILE:H	1:B:305:ILE:HG13	1.68	0.42
1:B:122:VAL:HA	1:B:464:SER:OG	2.19	0.42
1:C:206:PRO:HD2	1:C:209:GLN:HB2	1.99	0.42
1:C:364:PHE:HB3	1:C:369:ILE:HB	2.00	0.42
1:D:144:GLU:O	1:D:148:ILE:HG13	2.19	0.42
1:D:390:LEU:O	1:D:391:LYS:C	2.57	0.42
1:D:47:ASN:O	1:D:50:ARG:HG2	2.19	0.42
1:E:251:PHE:HA	1:E:325:ILE:O	2.18	0.42
1:E:284:ILE:CG2	1:E:285:TRP:N	2.81	0.42
1:F:435:VAL:O	1:F:435:VAL:HG13	2.19	0.42
1:A:68:PRO:HA	1:A:78:VAL:HA	2.00	0.42
1:B:199:HIS:O	1:B:205:LYS:HE2	2.19	0.42
1:B:308:PHE:CD2	1:B:311:ALA:HB2	2.51	0.42
1:B:502:VAL:HG23	1:B:504:PHE:CD1	2.54	0.42
1:C:436:PRO:HA	1:D:416:SER:OG	2.19	0.42
1:D:105:VAL:HA	1:D:108:VAL:HG22	2.01	0.42
1:D:190:THR:HG22	1:D:191:ILE:HG12	2.01	0.42
1:D:300:LEU:HD22	1:D:300:LEU:HA	1.88	0.42
1:D:391:LYS:HD2	1:D:449:GLU:OE2	2.19	0.42
1:E:105:VAL:HA	1:E:108:VAL:HG22	2.01	0.42
1:E:300:LEU:HD22	1:E:300:LEU:HA	1.88	0.42
1:E:502:VAL:HG23	1:E:504:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:HA	1:E:54:ARG:NH1	2.33	0.42
1:F:373:PRO:HD3	1:F:481:LEU:HB3	2.01	0.42
1:A:209:GLN:NE2	1:F:499:GLU:HB2	2.35	0.42
1:A:251:PHE:CE1	1:A:267:LEU:HB3	2.55	0.42
1:A:31:LYS:HA	1:A:34:GLU:HG2	2.01	0.42
1:A:323:CYS:O	1:A:345:ALA:HA	2.19	0.42
1:A:403:PHE:CE2	1:A:452:ILE:HD11	2.53	0.42
1:A:57:LYS:HB3	1:A:58:PRO:HD3	2.00	0.42
1:B:144:GLU:O	1:B:148:ILE:HG13	2.19	0.42
1:B:205:LYS:HZ3	1:B:392:ASN:HD21	1.67	0.42
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.82	0.42
1:C:299:LYS:O	1:C:299:LYS:HG3	2.18	0.42
1:C:69:ILE:HG23	1:C:79:ILE:HD13	2.00	0.42
1:D:435:VAL:HG13	1:D:435:VAL:O	2.20	0.42
1:D:91:THR:CB	1:D:92:PRO:CD	2.94	0.42
1:E:349:ALA:HB1	1:E:377:LEU:CD2	2.49	0.42
1:F:136:ASN:OD1	1:F:138:LYS:N	2.52	0.42
1:F:323:CYS:O	1:F:345:ALA:HA	2.18	0.42
1:F:31:LYS:HD3	1:F:35:ASP:OD2	2.19	0.42
1:F:449:GLU:O	1:F:450:LYS:C	2.58	0.42
1:A:105:VAL:HA	1:A:108:VAL:HG22	2.01	0.42
1:A:448:SER:O	1:A:451:ASP:HB2	2.19	0.42
1:B:86:HIS:CG	1:B:116:THR:HG21	2.53	0.42
1:C:251:PHE:HA	1:C:325:ILE:O	2.20	0.42
1:C:254:GLN:HE21	1:C:330:ALA:HB3	1.84	0.42
1:C:32:LEU:HA	1:C:36:LEU:HD13	2.02	0.42
1:C:436:PRO:HB3	1:C:440:PHE:CD1	2.54	0.42
1:D:261:LEU:HD12	1:D:261:LEU:C	2.40	0.42
1:D:349:ALA:HB1	1:D:377:LEU:CD2	2.50	0.42
1:D:31:LYS:HA	1:D:34:GLU:HG2	2.02	0.42
1:D:502:VAL:HG23	1:D:504:PHE:CD1	2.54	0.42
1:E:233:GLU:HG2	1:E:236:TYR:CD1	2.54	0.42
1:E:254:GLN:HE21	1:E:330:ALA:HB3	1.84	0.42
1:E:284:ILE:HD13	1:E:308:PHE:HB3	2.01	0.42
1:E:449:GLU:O	1:E:450:LYS:C	2.57	0.42
1:F:261:LEU:C	1:F:261:LEU:HD12	2.40	0.42
1:F:299:LYS:HG3	1:F:299:LYS:O	2.19	0.42
1:F:424:LYS:HE3	1:F:424:LYS:HB3	1.87	0.42
1:F:40:GLU:O	1:F:42:GLU:HG3	2.20	0.42
1:F:485:ALA:O	1:F:488:ASN:HB3	2.20	0.42
1:C:251:PHE:CE1	1:C:267:LEU:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:LEU:CD2	1:C:461:MET:HG2	2.50	0.42
1:C:380:GLY:HA2	1:C:457:LEU:HD21	2.00	0.42
1:D:436:PRO:HB3	1:D:440:PHE:CD1	2.55	0.42
1:E:457:LEU:CD2	1:E:461:MET:HG2	2.50	0.42
1:F:502:VAL:HG23	1:F:504:PHE:CD1	2.54	0.42
1:F:50:ARG:O	1:F:50:ARG:HG3	2.20	0.42
1:A:424:LYS:HB3	1:A:424:LYS:HE3	1.88	0.42
1:B:277:VAL:HG21	1:B:295:LEU:HD22	1.99	0.42
1:B:457:LEU:CD2	1:B:461:MET:HG2	2.49	0.42
1:B:47:ASN:O	1:B:50:ARG:HG2	2.20	0.42
1:B:62:VAL:HG11	1:B:109:LYS:HZ2	1.84	0.42
1:A:502:VAL:HG23	1:A:504:PHE:CD1	2.54	0.42
1:B:99:TYR:HH	1:B:149:THR:HG22	1.81	0.42
1:B:284:ILE:CG2	1:B:285:TRP:N	2.82	0.42
1:B:364:PHE:HB3	1:B:369:ILE:HB	2.01	0.42
1:C:144:GLU:O	1:C:148:ILE:HG13	2.20	0.42
1:C:121:VAL:HG21	1:C:375:LEU:HG	2.02	0.42
1:C:68:PRO:HA	1:C:78:VAL:HA	2.01	0.42
1:D:205:LYS:NZ	1:D:392:ASN:HD21	2.18	0.42
1:E:277:VAL:HG21	1:E:295:LEU:HD22	1.99	0.42
1:E:421:LEU:HA	1:E:421:LEU:HD12	1.76	0.42
1:F:254:GLN:HE21	1:F:330:ALA:HB3	1.85	0.42
1:A:78:VAL:CG2	1:A:78:VAL:O	2.68	0.42
1:B:228:GLU:HA	1:B:231:ILE:HG22	2.01	0.42
1:B:261:LEU:HD12	1:B:261:LEU:C	2.40	0.42
1:B:32:LEU:HA	1:B:36:LEU:HD13	2.02	0.42
1:B:38:THR:CG2	1:B:41:SER:HB3	2.40	0.42
1:C:105:VAL:HA	1:C:108:VAL:HG22	2.02	0.42
1:C:433:PRO:C	1:C:435:VAL:N	2.73	0.42
1:E:111:LEU:HA	1:E:111:LEU:HD23	1.82	0.42
1:E:323:CYS:O	1:E:345:ALA:HA	2.19	0.42
1:E:33:VAL:O	1:E:34:GLU:O	2.38	0.42
1:E:436:PRO:HB3	1:E:440:PHE:CD1	2.55	0.42
1:F:144:GLU:O	1:F:148:ILE:HG13	2.20	0.42
1:F:390:LEU:O	1:F:391:LYS:C	2.57	0.42
1:A:364:PHE:HB3	1:A:369:ILE:HB	2.00	0.42
1:B:254:GLN:HE21	1:B:330:ALA:HB3	1.83	0.42
1:B:424:LYS:HE3	1:B:424:LYS:HB3	1.87	0.42
1:C:323:CYS:O	1:C:345:ALA:HA	2.19	0.42
1:C:380:GLY:CA	1:C:457:LEU:HD21	2.50	0.42
1:D:319:LEU:HD23	1:D:335:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LYS:HD3	1:D:35:ASP:OD2	2.19	0.42
1:E:205:LYS:HZ3	1:E:392:ASN:ND2	2.17	0.42
1:F:105:VAL:HA	1:F:108:VAL:HG22	2.02	0.42
1:A:420:SER:CB	1:F:433:PRO:HA	2.50	0.42
1:B:118:LYS:HD3	1:B:379:ALA:HA	2.02	0.42
1:B:122:VAL:HB	1:B:460:THR:CG2	2.50	0.42
1:B:317:SER:C	1:B:319:LEU:N	2.73	0.42
1:B:433:PRO:HA	1:F:420:SER:HB3	2.02	0.42
1:B:505:THR:C	1:F:150:ARG:HH12	2.24	0.42
1:C:31:LYS:HD3	1:C:35:ASP:OD2	2.19	0.42
1:D:318:ILE:H	1:D:318:ILE:CD1	2.29	0.42
1:B:504:PHE:HB3	1:F:146:GLU:OE1	2.19	0.42
1:B:505:THR:N	1:F:150:ARG:NH1	2.68	0.42
1:F:436:PRO:HB3	1:F:440:PHE:CD1	2.55	0.42
1:B:281:ASP:HB2	1:B:282:GLY:H	1.56	0.41
1:C:190:THR:HG22	1:C:191:ILE:HG12	2.00	0.41
1:C:251:PHE:HB3	1:C:325:ILE:CG1	2.44	0.41
1:C:339:ASN:H	1:C:339:ASN:HD22	1.67	0.41
1:C:92:PRO:HG2	1:C:389:TRP:CZ2	2.55	0.41
1:D:317:SER:C	1:D:319:LEU:N	2.73	0.41
1:D:86:HIS:HD2	1:D:87:SER:HB2	1.85	0.41
1:F:150:ARG:NH2	1:F:185:ASP:OD1	2.53	0.41
1:A:31:LYS:HD3	1:A:35:ASP:OD2	2.19	0.41
1:B:118:LYS:HG3	1:B:375:LEU:O	2.20	0.41
1:B:47:ASN:HD21	1:B:50:ARG:NH1	2.17	0.41
1:D:301:GLN:HG2	1:D:301:GLN:O	2.19	0.41
1:D:40:GLU:O	1:D:42:GLU:HG3	2.20	0.41
1:B:54:ARG:NH1	1:D:78:VAL:HG13	2.35	0.41
1:E:31:LYS:HA	1:E:34:GLU:HG2	2.01	0.41
1:E:502:VAL:HG23	1:E:503:THR:N	2.28	0.41
1:E:92:PRO:HG2	1:E:389:TRP:CZ2	2.55	0.41
1:F:32:LEU:HA	1:F:36:LEU:HD13	2.02	0.41
1:A:284:ILE:CG2	1:A:311:ALA:HB1	2.48	0.41
1:A:47:ASN:O	1:A:50:ARG:HG2	2.20	0.41
1:B:105:VAL:HA	1:B:108:VAL:HG22	2.02	0.41
1:B:319:LEU:HD23	1:B:335:LEU:HD23	2.03	0.41
1:B:57:LYS:HB3	1:B:58:PRO:HD3	2.01	0.41
1:C:218:ALA:O	1:C:457:LEU:HD11	2.20	0.41
1:C:257:GLY:O	1:C:259:VAL:N	2.53	0.41
1:C:261:LEU:HD12	1:C:261:LEU:C	2.40	0.41
1:C:312:LYS:O	1:C:314:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:PHE:CE1	1:E:267:LEU:HB3	2.55	0.41
1:E:318:ILE:CD1	1:E:318:ILE:H	2.29	0.41
1:E:337:LYS:HZ2	1:E:359:GLU:HG3	1.85	0.41
1:E:31:LYS:HD3	1:E:35:ASP:OD2	2.19	0.41
1:E:51:GLY:O	1:E:55:ILE:HG13	2.19	0.41
1:E:68:PRO:HA	1:E:78:VAL:HA	2.02	0.41
1:C:228:GLU:HA	1:C:231:ILE:HG22	2.02	0.41
1:C:439:GLU:CD	1:C:439:GLU:H	2.24	0.41
1:E:149:THR:HG21	1:E:179:GLU:HG3	2.02	0.41
1:E:301:GLN:HG2	1:E:301:GLN:O	2.20	0.41
1:E:32:LEU:HA	1:E:36:LEU:HD13	2.02	0.41
1:A:32:LEU:HA	1:A:36:LEU:HD13	2.02	0.41
1:A:86:HIS:HD2	1:A:87:SER:HB2	1.84	0.41
1:B:134:LYS:HB2	1:B:134:LYS:HE3	1.94	0.41
1:B:118:LYS:HG3	1:B:379:ALA:HB2	2.02	0.41
1:B:40:GLU:O	1:B:42:GLU:HG3	2.21	0.41
1:F:33:VAL:O	1:F:34:GLU:O	2.39	0.41
1:A:400:ARG:NH1	1:A:400:ARG:HG3	2.30	0.41
1:A:435:VAL:O	1:A:435:VAL:HG13	2.20	0.41
1:B:207:ILE:HG21	1:B:213:HIS:NE2	2.36	0.41
1:C:349:ALA:HB1	1:C:377:LEU:CD2	2.51	0.41
1:C:422:GLU:HB3	1:C:427:LYS:HB3	2.02	0.41
1:C:47:ASN:O	1:C:50:ARG:HG2	2.21	0.41
1:D:12:ASN:HD21	1:D:14:PHE:HB3	1.86	0.41
1:E:281:ASP:HB2	1:E:282:GLY:H	1.56	0.41
1:E:118:LYS:HG3	1:E:375:LEU:O	2.21	0.41
1:E:474:LYS:HD3	1:E:475:TYR:HE2	1.83	0.41
1:E:57:LYS:HB3	1:E:58:PRO:HD3	2.02	0.41
1:F:228:GLU:HA	1:F:231:ILE:HG22	2.01	0.41
1:F:254:GLN:HB3	1:F:328:PRO:HA	2.03	0.41
1:F:319:LEU:HD23	1:F:335:LEU:HD23	2.03	0.41
1:A:12:ASN:HD21	1:A:14:PHE:HB3	1.86	0.41
1:B:349:ALA:HB1	1:B:377:LEU:CD2	2.51	0.41
1:B:350:GLU:CD	1:B:482:ARG:HH22	2.24	0.41
1:B:119:CYS:SG	1:B:382:VAL:HG11	2.60	0.41
1:C:33:VAL:O	1:C:34:GLU:O	2.38	0.41
1:D:86:HIS:CG	1:D:116:THR:HG21	2.55	0.41
1:D:32:LEU:HA	1:D:36:LEU:HD13	2.03	0.41
1:D:78:VAL:O	1:D:78:VAL:CG2	2.69	0.41
1:E:62:VAL:HG11	1:E:109:LYS:HZ3	1.85	0.41
1:F:339:ASN:H	1:F:339:ASN:HD22	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:GLU:H	1:F:439:GLU:CD	2.24	0.41
1:A:308:PHE:CD2	1:A:311:ALA:HB2	2.50	0.41
1:A:349:ALA:HB1	1:A:377:LEU:CD2	2.51	0.41
1:A:69:ILE:HG23	1:A:79:ILE:HD13	2.02	0.41
1:B:300:LEU:HD22	1:B:300:LEU:HA	1.88	0.41
1:C:168:VAL:HA	1:C:201:CYS:O	2.21	0.41
1:C:377:LEU:HD12	1:C:377:LEU:HA	1.93	0.41
1:C:212:ILE:HD11	1:C:398:TYR:CE1	2.56	0.41
1:C:435:VAL:HG13	1:C:435:VAL:O	2.21	0.41
1:D:291:ASP:HA	1:D:292:PRO:HD3	1.89	0.41
1:D:457:LEU:CD2	1:D:461:MET:HG2	2.51	0.41
1:E:183:ILE:O	1:E:184:ALA:C	2.59	0.41
1:F:47:ASN:O	1:F:50:ARG:HG2	2.21	0.41
1:A:433:PRO:C	1:A:435:VAL:N	2.73	0.41
1:B:149:THR:HG1	1:B:182:TRP:HE3	1.67	0.41
1:B:318:ILE:CD1	1:B:318:ILE:H	2.28	0.41
1:C:424:LYS:HB3	1:C:424:LYS:HE3	1.87	0.41
1:C:449:GLU:O	1:C:450:LYS:C	2.57	0.41
1:C:485:ALA:O	1:C:488:ASN:HB3	2.21	0.41
1:D:284:ILE:CG2	1:D:285:TRP:N	2.83	0.41
1:D:485:ALA:O	1:D:488:ASN:HB3	2.21	0.41
1:A:144:GLU:O	1:A:148:ILE:HG13	2.21	0.41
1:B:233:GLU:HG2	1:B:236:TYR:CD1	2.56	0.41
1:B:424:LYS:O	1:B:425:PHE:HB2	2.21	0.41
1:B:449:GLU:O	1:B:450:LYS:C	2.60	0.41
1:C:221:ARG:CD	1:C:454:HIS:CG	3.04	0.41
1:E:156:LEU:HB3	1:E:162:ILE:HB	2.03	0.41
1:E:40:GLU:O	1:E:42:GLU:HG3	2.20	0.41
1:E:50:ARG:HG3	1:E:50:ARG:O	2.21	0.41
1:F:69:ILE:HG23	1:F:79:ILE:HD13	2.03	0.41
1:A:105:VAL:HG12	1:A:109:LYS:HG3	2.03	0.41
1:A:150:ARG:HH12	1:F:505:THR:N	2.19	0.41
1:A:281:ASP:HB2	1:A:282:GLY:H	1.56	0.41
1:A:301:GLN:HG2	1:A:301:GLN:O	2.20	0.41
1:B:168:VAL:HA	1:B:201:CYS:O	2.21	0.41
1:B:319:LEU:CD1	1:B:319:LEU:H	2.34	0.41
1:C:136:ASN:OD1	1:C:138:LYS:N	2.51	0.41
1:C:31:LYS:HB2	1:C:475:TYR:HE1	1.86	0.41
1:D:177:GLU:HA	1:D:180:MET:HB2	2.03	0.41
1:D:230:PHE:CE2	1:D:481:LEU:HD21	2.55	0.41
1:D:38:THR:CG2	1:D:41:SER:HB3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ARG:NH2	1:E:185:ASP:OD1	2.54	0.41
1:E:228:GLU:HA	1:E:231:ILE:HG22	2.02	0.41
1:E:472:ALA:O	1:E:476:ASN:N	2.54	0.41
1:F:285:TRP:NE1	1:F:287:PRO:HG3	2.36	0.41
1:F:463:ARG:HB3	1:F:463:ARG:HE	1.72	0.41
1:A:317:SER:C	1:A:319:LEU:N	2.74	0.40
1:A:319:LEU:H	1:A:319:LEU:CD1	2.34	0.40
1:C:243:THR:O	1:C:243:THR:CG2	2.69	0.40
1:C:23:ARG:NE	1:C:27:ILE:HD11	2.30	0.40
1:C:317:SER:C	1:C:319:LEU:N	2.75	0.40
1:D:23:ARG:NE	1:D:27:ILE:HD11	2.30	0.40
1:D:319:LEU:H	1:D:319:LEU:CD1	2.33	0.40
1:D:119:CYS:SG	1:D:382:VAL:HG11	2.61	0.40
1:D:433:PRO:C	1:D:435:VAL:N	2.72	0.40
1:E:372:ILE:HA	1:E:373:PRO:HD3	1.64	0.40
1:A:70:ARG:CB	1:E:504:PHE:CE1	3.04	0.40
1:F:69:ILE:HG21	1:F:148:ILE:HG12	2.03	0.40
1:F:190:THR:HG22	1:F:191:ILE:HG12	2.03	0.40
1:F:91:THR:HB	1:F:92:PRO:CD	2.51	0.40
1:A:449:GLU:O	1:A:450:LYS:C	2.59	0.40
1:B:150:ARG:NH2	1:B:185:ASP:OD1	2.54	0.40
1:B:251:PHE:CE1	1:B:267:LEU:HB3	2.56	0.40
1:B:337:LYS:HZ2	1:B:359:GLU:HG3	1.84	0.40
1:C:233:GLU:HG2	1:C:236:TYR:CD1	2.55	0.40
1:D:105:VAL:HG12	1:D:109:LYS:HG3	2.03	0.40
1:D:226:GLY:HA3	1:D:377:LEU:HD12	2.01	0.40
1:E:285:TRP:NE1	1:E:287:PRO:HG3	2.37	0.40
1:F:12:ASN:HD21	1:F:14:PHE:HB3	1.86	0.40
1:C:504:PHE:CE1	1:F:70:ARG:CB	3.05	0.40
1:A:163:GLY:O	1:A:167:ASP:O	2.39	0.40
1:A:40:GLU:O	1:A:42:GLU:HG3	2.20	0.40
1:B:284:ILE:CG2	1:B:311:ALA:HB1	2.47	0.40
1:B:433:PRO:C	1:B:435:VAL:N	2.73	0.40
1:C:172:ASP:O	1:C:173:MET:C	2.60	0.40
1:C:205:LYS:HD2	1:C:209:GLN:O	2.21	0.40
1:C:69:ILE:HG12	1:C:79:ILE:HD11	2.03	0.40
1:D:500:ALA:HB1	1:D:505:THR:OXT	2.21	0.40
1:D:68:PRO:HA	1:D:78:VAL:HA	2.03	0.40
1:E:309:PRO:O	1:E:310:LYS:HB2	2.22	0.40
1:E:319:LEU:H	1:E:319:LEU:CD1	2.34	0.40
1:F:63:LEU:HD22	1:F:161:PHE:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TRP:NE1	1:A:287:PRO:HG3	2.36	0.40
1:A:422:GLU:HB3	1:A:427:LYS:HB3	2.03	0.40
1:A:485:ALA:O	1:A:488:ASN:HB3	2.21	0.40
1:B:113:SER:O	1:B:114:LEU:C	2.58	0.40
1:C:12:ASN:HD21	1:C:14:PHE:HB3	1.86	0.40
1:C:433:PRO:HA	1:D:420:SER:CB	2.51	0.40
1:E:279:GLU:HB3	1:E:280:SER:H	1.73	0.40
1:F:233:GLU:HG2	1:F:236:TYR:CD1	2.56	0.40
1:F:391:LYS:NZ	1:F:449:GLU:OE1	2.50	0.40
1:A:257:GLY:O	1:A:259:VAL:N	2.54	0.40
1:A:284:ILE:CD1	1:A:308:PHE:HB3	2.51	0.40
1:A:50:ARG:HG3	1:A:50:ARG:O	2.22	0.40
1:A:69:ILE:HG12	1:A:79:ILE:HD11	2.04	0.40
1:B:243:THR:CG2	1:B:243:THR:O	2.70	0.40
1:B:257:GLY:O	1:B:259:VAL:N	2.55	0.40
1:D:279:GLU:HB3	1:D:280:SER:H	1.74	0.40
1:E:284:ILE:CG2	1:E:311:ALA:HB1	2.47	0.40
1:F:105:VAL:HG12	1:F:109:LYS:HG3	2.03	0.40
1:F:312:LYS:O	1:F:314:TYR:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	4	8
1	B	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	4	8
1	C	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	4	8
1	D	494/505 (98%)	426 (86%)	49 (10%)	19 (4%)	4	8
1	E	494/505 (98%)	425 (86%)	50 (10%)	19 (4%)	4	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	4	8
All	All	2964/3030 (98%)	2563 (86%)	287 (10%)	114 (4%)	4	8

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	41	SER
1	A	91	THR
1	A	102	ASP
1	A	258	ASN
1	A	331	SER
1	B	34	GLU
1	B	41	SER
1	B	91	THR
1	B	102	ASP
1	B	258	ASN
1	B	331	SER
1	C	34	GLU
1	C	41	SER
1	C	91	THR
1	C	102	ASP
1	C	258	ASN
1	C	331	SER
1	D	34	GLU
1	D	41	SER
1	D	91	THR
1	D	102	ASP
1	D	258	ASN
1	D	331	SER
1	E	34	GLU
1	E	41	SER
1	E	91	THR
1	E	102	ASP
1	E	258	ASN
1	E	331	SER
1	F	34	GLU
1	F	41	SER
1	F	91	THR
1	F	102	ASP
1	F	258	ASN
1	F	331	SER

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Mol	Chain	Res	Type
1	A	74	GLY
1	A	333	LYS
1	A	434	ILE
1	B	74	GLY
1	B	333	LYS
1	B	434	ILE
1	C	74	GLY
1	C	333	LYS
1	C	434	ILE
1	D	74	GLY
1	D	333	LYS
1	D	434	ILE
1	E	74	GLY
1	E	333	LYS
1	E	434	ILE
1	F	74	GLY
1	F	333	LYS
1	F	434	ILE
1	A	425	PHE
1	A	500	ALA
1	B	425	PHE
1	B	500	ALA
1	C	425	PHE
1	C	500	ALA
1	D	425	PHE
1	D	500	ALA
1	E	425	PHE
1	E	500	ALA
1	F	425	PHE
1	F	500	ALA
1	A	35	ASP
1	A	134	LYS
1	A	234	ALA
1	B	35	ASP
1	B	134	LYS
1	B	234	ALA
1	C	35	ASP
1	C	134	LYS
1	C	234	ALA
1	D	35	ASP
1	D	234	ALA
1	E	35	ASP

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Mol	Chain	Res	Type
1	E	134	LYS
1	E	234	ALA
1	F	35	ASP
1	F	234	ALA
1	A	281	ASP
1	A	286	ASN
1	A	313	PRO
1	B	162	ILE
1	B	281	ASP
1	B	286	ASN
1	B	313	PRO
1	C	162	ILE
1	C	281	ASP
1	C	286	ASN
1	C	313	PRO
1	D	134	LYS
1	D	281	ASP
1	D	286	ASN
1	D	313	PRO
1	E	162	ILE
1	E	281	ASP
1	E	286	ASN
1	E	313	PRO
1	F	134	LYS
1	F	281	ASP
1	F	286	ASN
1	F	313	PRO
1	A	162	ILE
1	A	502	VAL
1	B	502	VAL
1	C	502	VAL
1	D	162	ILE
1	D	502	VAL
1	F	162	ILE
1	F	502	VAL
1	E	502	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/420 (98%)	365 (88%)	48 (12%)	6	15
1	B	413/420 (98%)	364 (88%)	49 (12%)	6	14
1	C	413/420 (98%)	365 (88%)	48 (12%)	6	15
1	D	413/420 (98%)	364 (88%)	49 (12%)	6	14
1	E	413/420 (98%)	365 (88%)	48 (12%)	6	15
1	F	413/420 (98%)	365 (88%)	48 (12%)	6	15
All	All	2478/2520 (98%)	2188 (88%)	290 (12%)	6	14

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	23	ARG
1	A	36	LEU
1	A	37	ARG
1	A	44	GLN
1	A	46	ARG
1	A	62	VAL
1	A	64	SER
1	A	68	PRO
1	A	90	ARG
1	A	101	THR
1	A	116	THR
1	A	141	THR
1	A	156	LEU
1	A	162	ILE
1	A	180	MET
1	A	219	THR
1	A	235	SER
1	A	243	THR
1	A	259	VAL
1	A	261	LEU
1	A	267	LEU
1	A	281	ASP
1	A	293	LYS
1	A	300	LEU
1	A	306	LEU
1	A	315	GLU

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Mol	Chain	Res	Type
1	A	318	ILE
1	A	320	GLU
1	A	325	ILE
1	A	326	LEU
1	A	334	GLN
1	A	339	ASN
1	A	353	ASN
1	A	378	ASN
1	A	396	VAL
1	A	400	ARG
1	A	401	LEU
1	A	421	LEU
1	A	427	LYS
1	A	428	HIS
1	A	432	ILE
1	A	457	LEU
1	A	471	THR
1	A	476	ASN
1	A	481	LEU
1	A	499	GLU
1	A	504	PHE
1	B	13	PHE
1	B	23	ARG
1	B	36	LEU
1	B	37	ARG
1	B	44	GLN
1	B	46	ARG
1	B	62	VAL
1	B	64	SER
1	B	68	PRO
1	B	90	ARG
1	B	101	THR
1	B	116	THR
1	B	141	THR
1	B	156	LEU
1	B	162	ILE
1	B	180	MET
1	B	219	THR
1	B	235	SER
1	B	243	THR
1	B	259	VAL
1	B	261	LEU

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Mol	Chain	Res	Type
1	B	267	LEU
1	B	281	ASP
1	B	293	LYS
1	B	300	LEU
1	B	306	LEU
1	B	315	GLU
1	B	318	ILE
1	B	320	GLU
1	B	325	ILE
1	B	326	LEU
1	B	334	GLN
1	B	339	ASN
1	B	353	ASN
1	B	378	ASN
1	B	396	VAL
1	B	400	ARG
1	B	401	LEU
1	B	421	LEU
1	B	427	LYS
1	B	428	HIS
1	B	432	ILE
1	B	455	SER
1	B	457	LEU
1	B	471	THR
1	B	476	ASN
1	B	481	LEU
1	B	499	GLU
1	B	504	PHE
1	C	13	PHE
1	C	23	ARG
1	C	36	LEU
1	C	37	ARG
1	C	44	GLN
1	C	46	ARG
1	C	62	VAL
1	C	64	SER
1	C	68	PRO
1	C	90	ARG
1	C	101	THR
1	C	116	THR
1	C	141	THR
1	C	156	LEU

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Mol	Chain	Res	Type
1	C	162	ILE
1	C	180	MET
1	C	219	THR
1	C	235	SER
1	C	243	THR
1	C	259	VAL
1	C	261	LEU
1	C	267	LEU
1	C	281	ASP
1	C	293	LYS
1	C	300	LEU
1	C	306	LEU
1	C	315	GLU
1	C	318	ILE
1	C	320	GLU
1	C	325	ILE
1	C	326	LEU
1	C	334	GLN
1	C	339	ASN
1	C	353	ASN
1	C	378	ASN
1	C	396	VAL
1	C	400	ARG
1	C	401	LEU
1	C	421	LEU
1	C	427	LYS
1	C	428	HIS
1	C	432	ILE
1	C	457	LEU
1	C	471	THR
1	C	476	ASN
1	C	481	LEU
1	C	499	GLU
1	C	504	PHE
1	D	13	PHE
1	D	23	ARG
1	D	36	LEU
1	D	37	ARG
1	D	44	GLN
1	D	46	ARG
1	D	62	VAL
1	D	64	SER

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Mol	Chain	Res	Type
1	D	68	PRO
1	D	90	ARG
1	D	101	THR
1	D	116	THR
1	D	141	THR
1	D	156	LEU
1	D	162	ILE
1	D	180	MET
1	D	219	THR
1	D	235	SER
1	D	243	THR
1	D	259	VAL
1	D	261	LEU
1	D	267	LEU
1	D	281	ASP
1	D	293	LYS
1	D	300	LEU
1	D	306	LEU
1	D	315	GLU
1	D	318	ILE
1	D	320	GLU
1	D	325	ILE
1	D	326	LEU
1	D	334	GLN
1	D	339	ASN
1	D	353	ASN
1	D	378	ASN
1	D	396	VAL
1	D	400	ARG
1	D	401	LEU
1	D	421	LEU
1	D	427	LYS
1	D	428	HIS
1	D	432	ILE
1	D	455	SER
1	D	457	LEU
1	D	471	THR
1	D	476	ASN
1	D	481	LEU
1	D	499	GLU
1	D	504	PHE
1	E	13	PHE

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Mol	Chain	Res	Type
1	E	23	ARG
1	E	36	LEU
1	E	37	ARG
1	E	44	GLN
1	E	46	ARG
1	E	62	VAL
1	E	64	SER
1	E	68	PRO
1	E	90	ARG
1	E	101	THR
1	E	116	THR
1	E	141	THR
1	E	156	LEU
1	E	162	ILE
1	E	180	MET
1	E	219	THR
1	E	235	SER
1	E	243	THR
1	E	259	VAL
1	E	261	LEU
1	E	267	LEU
1	E	281	ASP
1	E	293	LYS
1	E	300	LEU
1	E	306	LEU
1	E	315	GLU
1	E	318	ILE
1	E	320	GLU
1	E	325	ILE
1	E	326	LEU
1	E	334	GLN
1	E	339	ASN
1	E	353	ASN
1	E	378	ASN
1	E	396	VAL
1	E	400	ARG
1	E	401	LEU
1	E	421	LEU
1	E	427	LYS
1	E	428	HIS
1	E	432	ILE
1	E	457	LEU

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Mol	Chain	Res	Type
1	E	471	THR
1	E	476	ASN
1	E	481	LEU
1	E	499	GLU
1	E	504	PHE
1	F	13	PHE
1	F	23	ARG
1	F	36	LEU
1	F	37	ARG
1	F	44	GLN
1	F	46	ARG
1	F	62	VAL
1	F	64	SER
1	F	68	PRO
1	F	90	ARG
1	F	101	THR
1	F	116	THR
1	F	141	THR
1	F	156	LEU
1	F	162	ILE
1	F	180	MET
1	F	219	THR
1	F	235	SER
1	F	243	THR
1	F	259	VAL
1	F	261	LEU
1	F	267	LEU
1	F	281	ASP
1	F	293	LYS
1	F	300	LEU
1	F	306	LEU
1	F	315	GLU
1	F	318	ILE
1	F	320	GLU
1	F	325	ILE
1	F	326	LEU
1	F	334	GLN
1	F	339	ASN
1	F	353	ASN
1	F	378	ASN
1	F	396	VAL
1	F	400	ARG

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Mol	Chain	Res	Type
1	F	401	LEU
1	F	421	LEU
1	F	427	LYS
1	F	428	HIS
1	F	432	ILE
1	F	457	LEU
1	F	471	THR
1	F	476	ASN
1	F	481	LEU
1	F	499	GLU
1	F	504	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	86	HIS
1	A	143	ASN
1	A	302	HIS
1	A	339	ASN
1	A	353	ASN
1	A	378	ASN
1	A	392	ASN
1	A	395	HIS
1	A	410	ASN
1	A	428	HIS
1	A	488	ASN
1	A	498	ASN
1	B	47	ASN
1	B	61	HIS
1	B	86	HIS
1	B	143	ASN
1	B	302	HIS
1	B	339	ASN
1	B	353	ASN
1	B	378	ASN
1	B	392	ASN
1	B	395	HIS
1	B	410	ASN
1	B	428	HIS
1	B	488	ASN
1	B	498	ASN

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Mol	Chain	Res	Type
1	C	47	ASN
1	C	86	HIS
1	C	143	ASN
1	C	209	GLN
1	C	302	HIS
1	C	339	ASN
1	C	353	ASN
1	C	378	ASN
1	C	392	ASN
1	C	395	HIS
1	C	410	ASN
1	C	428	HIS
1	C	488	ASN
1	C	498	ASN
1	D	47	ASN
1	D	86	HIS
1	D	143	ASN
1	D	302	HIS
1	D	339	ASN
1	D	353	ASN
1	D	378	ASN
1	D	392	ASN
1	D	395	HIS
1	D	410	ASN
1	D	428	HIS
1	D	488	ASN
1	D	498	ASN
1	E	47	ASN
1	E	61	HIS
1	E	86	HIS
1	E	143	ASN
1	E	209	GLN
1	E	302	HIS
1	E	339	ASN
1	E	353	ASN
1	E	378	ASN
1	E	392	ASN
1	E	395	HIS
1	E	410	ASN
1	E	428	HIS
1	E	488	ASN
1	E	498	ASN

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Mol	Chain	Res	Type
1	F	47	ASN
1	F	61	HIS
1	F	86	HIS
1	F	143	ASN
1	F	209	GLN
1	F	302	HIS
1	F	339	ASN
1	F	353	ASN
1	F	378	ASN
1	F	392	ASN
1	F	395	HIS
1	F	410	ASN
1	F	428	HIS
1	F	488	ASN
1	F	498	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.