



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 1L1F / pdb_0000111f
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

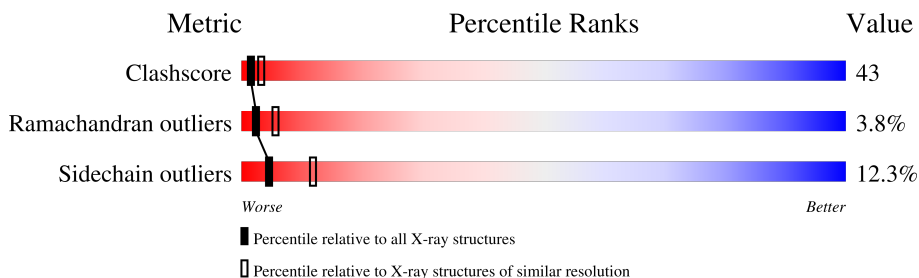
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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.

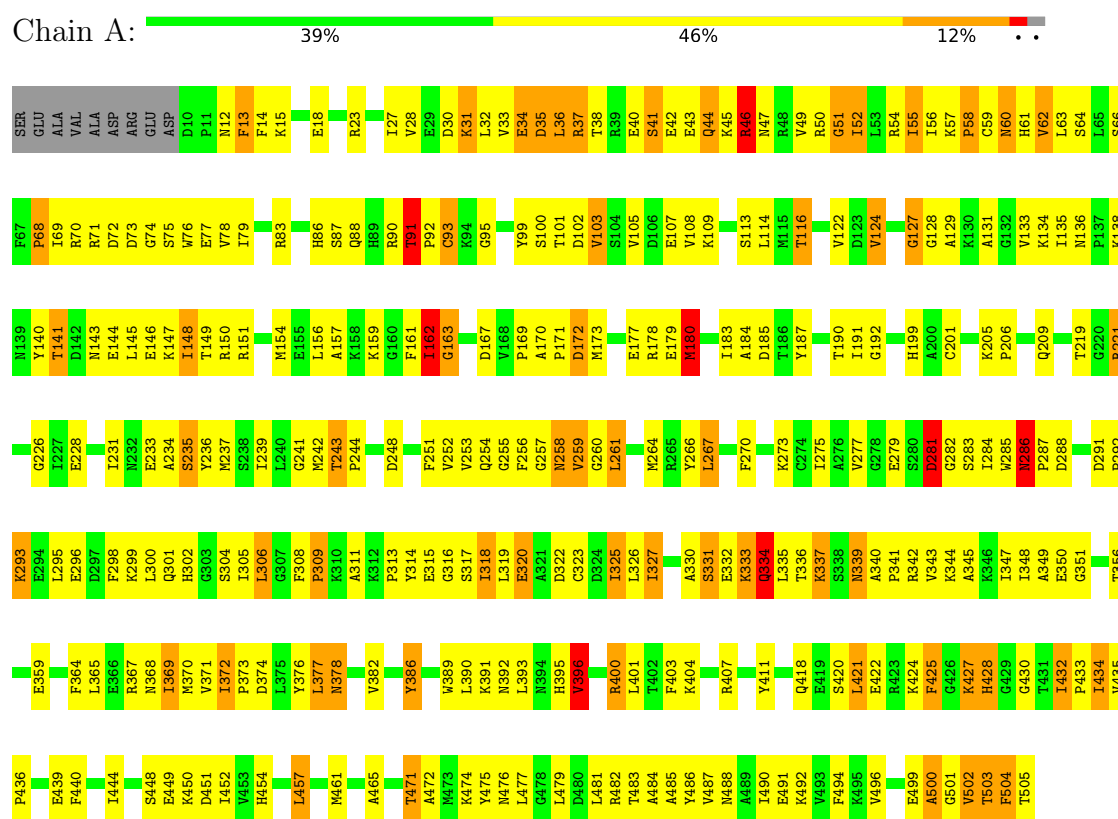
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	B	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	C	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	D	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	E	496	Total	C	N	O	S	0	0	0
	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

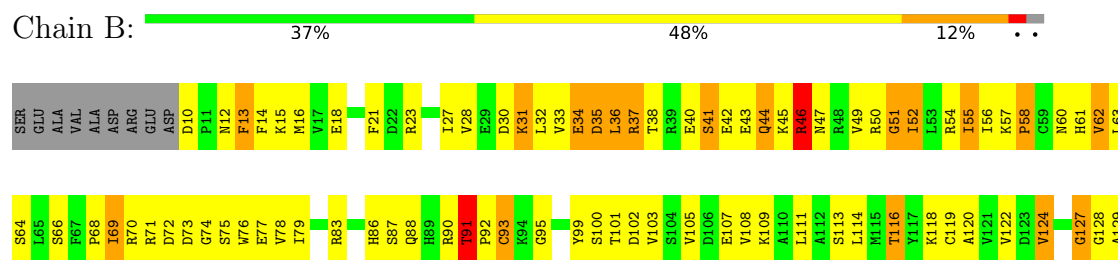
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

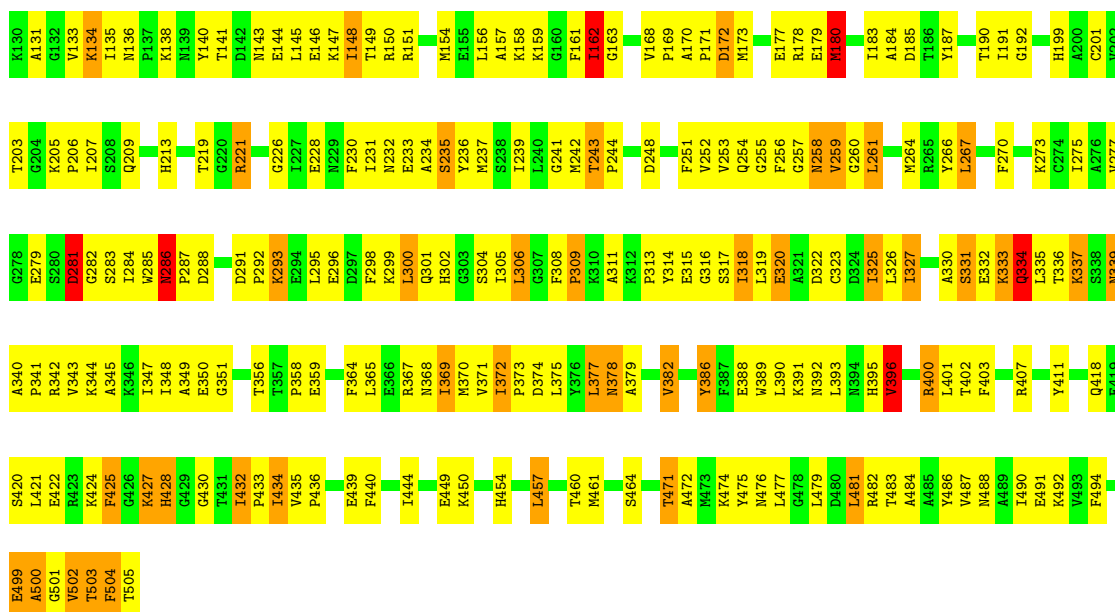
Note EDS was not executed.

• Molecule 1: Glutamate Dehydrogenase 1



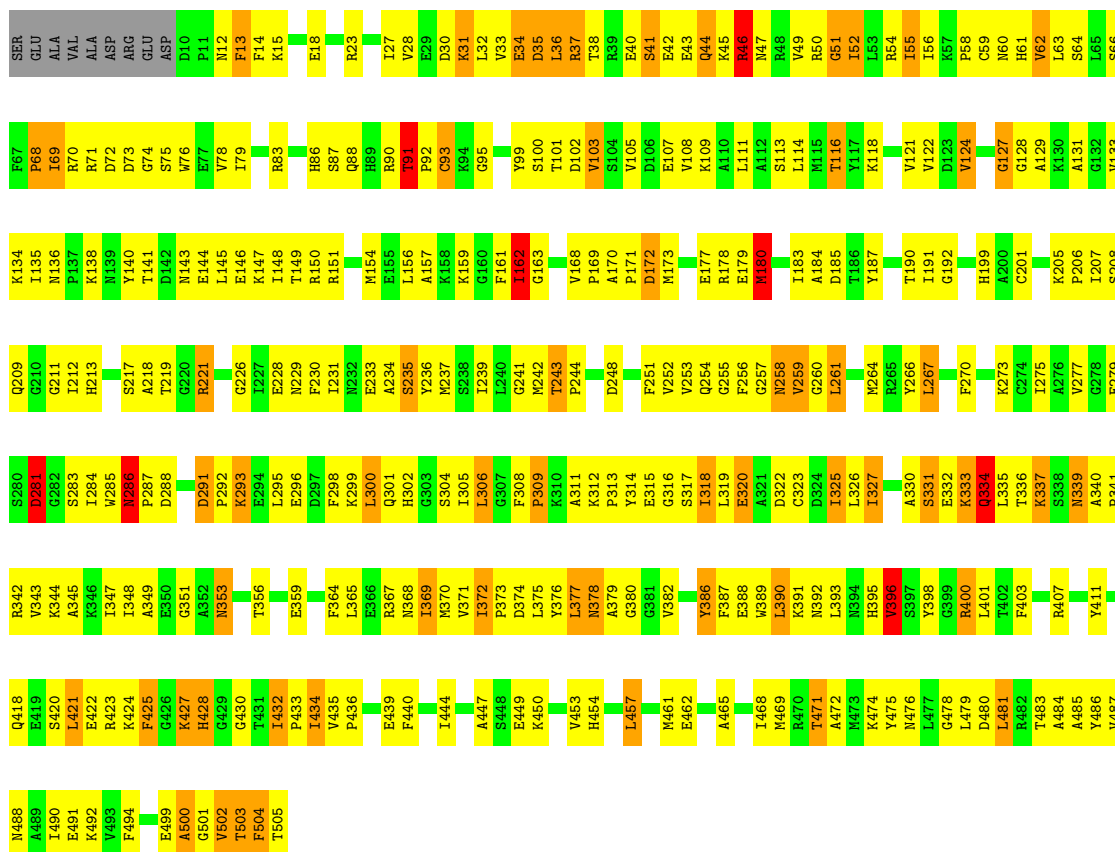
• Molecule 1: Glutamate Dehydrogenase 1



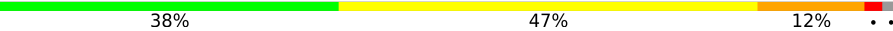


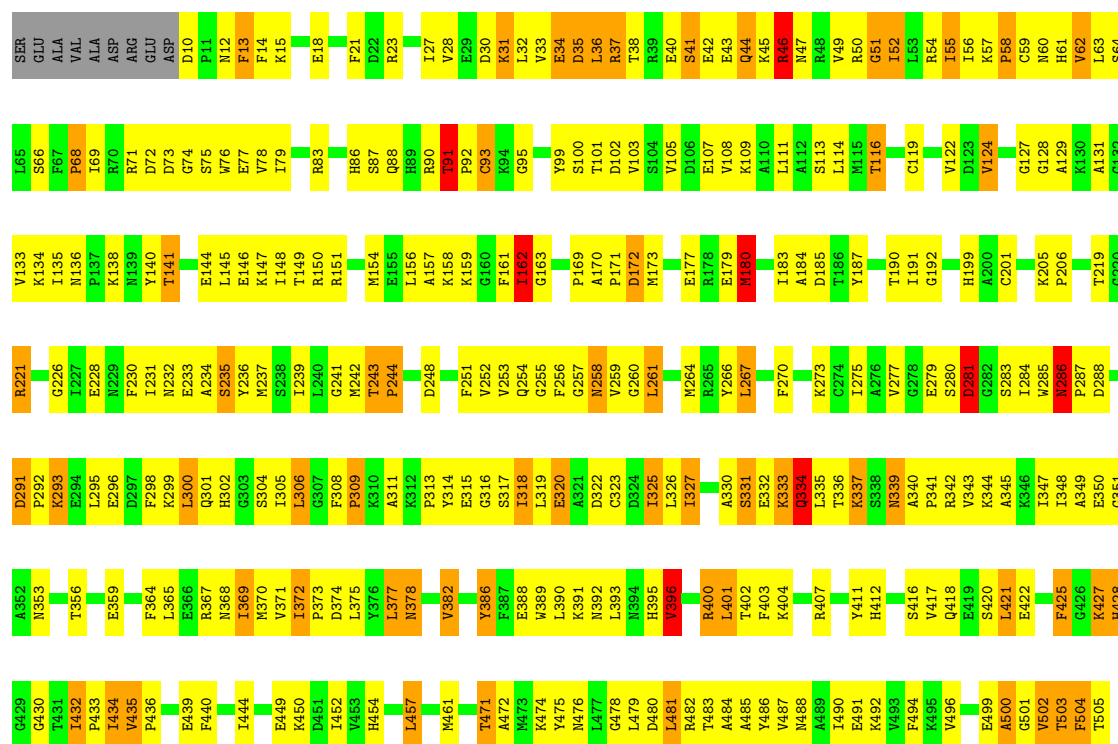
• Molecule 1: Glutamate Dehydrogenase 1

Chain C: 35% 49% 12% ..

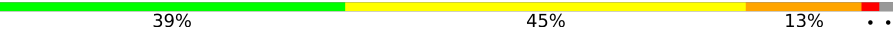


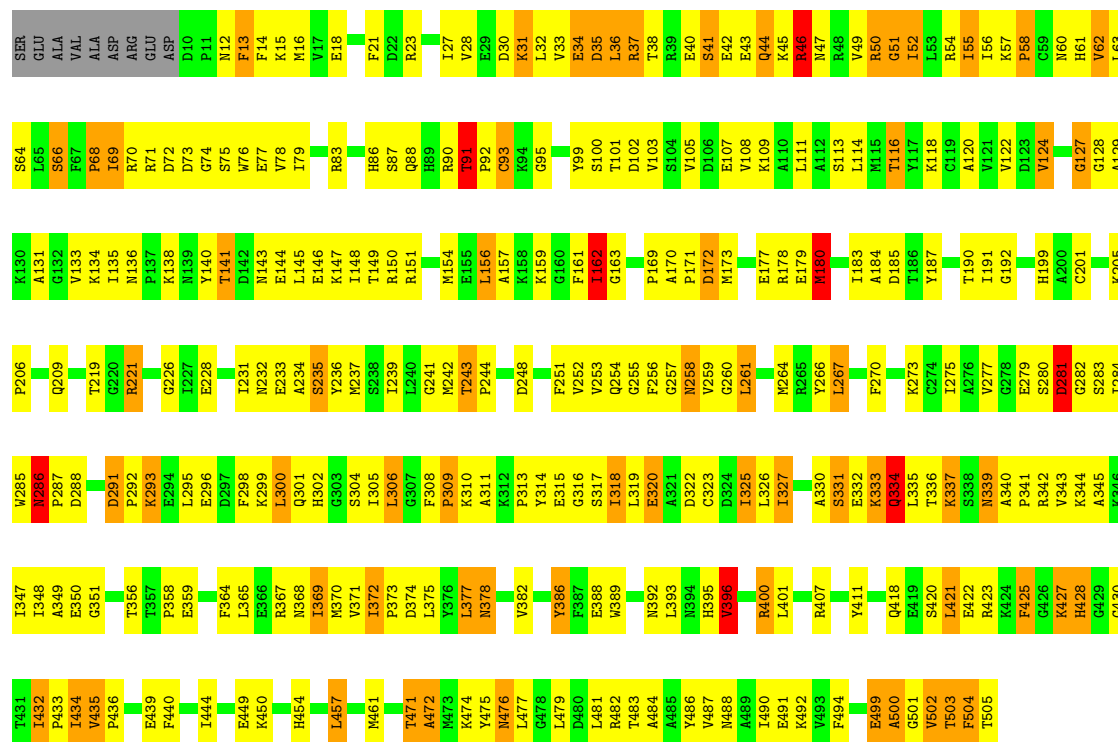
• Molecule 1: Glutamate Dehydrogenase 1

Chain D:  38% 47% 12% . .



• Molecule 1: Glutamate Dehydrogenase 1

Chain E:  39% 45% 13% . .



• Molecule 1: Glutamate Dehydrogenase 1

Chain F:  39% 47% 11% ..

P433	N353	K293	G226	P137	F67	SER
I434	E294	E294	I227	K138	P68	GLU
V435	T356	L295	E228	N139	I69	ALA
P436	E296	E296	N229	Y140	VAL	VAL
E439	E359	D297	F230	T141	R71	ALA
		F298	I231		D72	ASP
F440	F364	K299	N232	E144	D73	ARG
	L365	L300	E233	L145	G74	GLU
I444	E366	Q301	A234	E146	S75	ASP
A447	R367	H302	S235	K147	W76	D10
S448	N368	G303	Y236	T148	E77	P11
E449	I369	S304	M237	T149	V78	N12
K450	M370	I305	S238	R150	I79	F13
H454	V371	L306	I239	R151	F14	F14
	I372	G307	L240		R83	K15
L457	P373	F308	G241	M154		E18
	D374	P309	M242	E155	H86	
	L375	K310	T243	L156	S87	R23
	Y376	A311	P244	A157	Q88	
E462	L377	K312		K158	H89	
R463	N378	P313	D248	K159	R90	L27
S464	A379	Y314		G160	T91	V28
A465		E315	F251	F161	P92	E29
	V382	G316	V252	I162	C93	D30
		S317	V253	G163	K31	
M469	Y386	T318	Q254	R94	C95	L32
R470	L319	L318	G255	P169		V33
T471	E320	F256	D257	A170	Y99	E34
M473	K391	D322	N258	P171	S100	D35
K474	N392	C323	V259	D172	T101	L36
Y475	L393	D324	G260	M173	D102	R37
L477	N394	I325	L261		V103	T38
G478	H395	L326		E177	R39	R39
L479	Y386	P327	M264	A178	E105	E40
D480		R328	R265	E179	D106	S41
L481	R400	A329	V266	H180	E107	E42
R482	L401	A330	L267	I183	V108	E43
T483	T402	S331		A184	K109	Q44
A484	F403	E332	F270	D185	K45	
A485	K333	K333		T186	S113	R46
Y486	R407	Q334	K273	Y187	L114	N47
V487		L335	C274		M115	R48
M488	Y411	T336	I275	T190	T116	V49
A489		K337	A276	I191	Y117	R50
I490	Q418	S338	V277	G192	K118	G51
E491	E419	N339	G278		G122	L52
K492	S420	A340	E279	H199	V123	L53
V493	L421	P341	S260	A200	D123	R54
F494	E422	R342	D281	C201	V124	L55
	R423	V343	G282		I56	
E499	K424	K344	D283	K205	G127	R57
A500	F425	A345	I284	P206	A129	P58
G501	G426	K346	V285		K130	C59
V502	K427	I347	R286	Q209	H61	N60
T503	H428	T348	P287	T219	G132	V62
F504	G429	A349	D288	G220	V133	L63
T505	G430	E350		K134	I135	S64
		G351	D291	R221	L65	
	I432	A352	P292		N136	S66

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, α , β , γ	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		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 ²)	53.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.75	1/3958 (0.0%)	1.25	47/5340 (0.9%)
1	B	0.80	1/3958 (0.0%)	1.26	49/5340 (0.9%)
1	C	0.81	1/3958 (0.0%)	1.26	50/5340 (0.9%)
1	D	0.78	1/3958 (0.0%)	1.26	48/5340 (0.9%)
1	E	0.79	1/3958 (0.0%)	1.26	50/5340 (0.9%)
1	F	0.77	1/3958 (0.0%)	1.25	46/5340 (0.9%)
All	All	0.78	6/23748 (0.0%)	1.26	290/32040 (0.9%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	MET	SD-CE	-9.28	1.56	1.79
1	F	180	MET	SD-CE	-8.39	1.58	1.79
1	B	180	MET	SD-CE	-7.49	1.60	1.79
1	E	180	MET	SD-CE	-7.32	1.61	1.79
1	A	180	MET	SD-CE	-7.25	1.61	1.79
1	D	180	MET	SD-CE	-5.84	1.65	1.79

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	504	PHE	N-CA-C	-15.33	91.34	110.65
1	C	504	PHE	N-CA-C	-15.32	91.35	110.65
1	B	504	PHE	N-CA-C	-15.29	91.38	110.65
1	F	504	PHE	N-CA-C	-15.26	91.43	110.65
1	D	504	PHE	N-CA-C	-15.12	91.60	110.65
1	A	504	PHE	N-CA-C	-15.09	91.64	110.65
1	C	372	ILE	CA-C-N	12.61	132.76	119.90
1	C	372	ILE	C-N-CA	12.61	132.76	119.90
1	A	372	ILE	CA-C-N	12.40	132.54	119.90
1	A	372	ILE	C-N-CA	12.40	132.54	119.90
1	E	372	ILE	CA-C-N	12.39	132.54	119.90
1	E	372	ILE	C-N-CA	12.39	132.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	372	ILE	CA-C-N	12.34	132.49	119.90
1	D	372	ILE	C-N-CA	12.34	132.49	119.90
1	B	372	ILE	CA-C-N	12.32	132.47	119.90
1	B	372	ILE	C-N-CA	12.32	132.47	119.90
1	F	372	ILE	CA-C-N	12.26	132.41	119.90
1	F	372	ILE	C-N-CA	12.26	132.41	119.90
1	D	479	LEU	N-CA-C	-10.98	100.16	112.57
1	B	479	LEU	N-CA-C	-10.88	100.28	112.57
1	A	479	LEU	N-CA-C	-10.70	100.48	112.57
1	F	479	LEU	N-CA-C	-10.64	100.55	112.57
1	C	479	LEU	N-CA-C	-10.63	100.56	112.57
1	E	479	LEU	N-CA-C	-10.40	100.82	112.57
1	B	503	THR	N-CA-C	-10.00	101.64	114.04
1	E	503	THR	N-CA-C	-9.96	101.69	114.04
1	F	503	THR	N-CA-C	-9.92	101.74	114.04
1	C	503	THR	N-CA-C	-9.90	101.77	114.04
1	D	503	THR	N-CA-C	-9.81	101.87	114.04
1	A	503	THR	N-CA-C	-9.77	101.92	114.04
1	B	316	GLY	N-CA-C	-8.89	100.38	110.96
1	F	316	GLY	N-CA-C	-8.82	100.47	110.96
1	D	316	GLY	N-CA-C	-8.77	100.53	110.96
1	C	316	GLY	N-CA-C	-8.69	100.62	110.96
1	A	316	GLY	N-CA-C	-8.65	100.67	110.96
1	E	316	GLY	N-CA-C	-8.57	100.76	110.96
1	B	91	THR	N-CA-C	7.91	127.29	109.81
1	C	91	THR	N-CA-C	7.89	127.25	109.81
1	F	91	THR	N-CA-C	7.79	127.03	109.81
1	A	91	THR	N-CA-C	7.71	126.85	109.81
1	E	91	THR	N-CA-C	7.70	126.83	109.81
1	D	91	THR	N-CA-C	7.67	126.77	109.81
1	D	88	GLN	N-CA-C	-7.27	102.95	112.41
1	E	46	ARG	N-CA-C	-7.25	103.10	112.23
1	C	46	ARG	N-CA-C	-7.23	103.13	112.23
1	C	88	GLN	N-CA-C	-7.21	103.03	112.41
1	A	46	ARG	N-CA-C	-7.18	103.18	112.23
1	F	91	THR	CA-C-N	-7.08	111.77	119.98
1	F	91	THR	C-N-CA	-7.08	111.77	119.98
1	D	93	CYS	N-CA-C	-7.06	99.83	110.28
1	F	88	GLN	N-CA-C	-7.06	103.23	112.41
1	B	46	ARG	N-CA-C	-7.05	103.35	112.23
1	F	46	ARG	N-CA-C	-7.03	103.37	112.23
1	C	91	THR	CA-C-N	-7.01	111.85	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	THR	C-N-CA	-7.01	111.85	119.98
1	D	46	ARG	N-CA-C	-6.98	103.44	112.23
1	D	91	THR	CA-C-N	-6.96	111.91	119.98
1	D	91	THR	C-N-CA	-6.96	111.91	119.98
1	E	91	THR	CA-C-N	-6.93	111.95	119.98
1	E	91	THR	C-N-CA	-6.93	111.95	119.98
1	F	377	LEU	N-CA-C	6.86	119.63	111.33
1	A	91	THR	CA-C-N	-6.84	112.04	119.98
1	A	91	THR	C-N-CA	-6.84	112.04	119.98
1	B	91	THR	CA-C-N	-6.82	112.07	119.98
1	B	91	THR	C-N-CA	-6.82	112.07	119.98
1	A	377	LEU	N-CA-C	6.80	119.56	111.33
1	A	93	CYS	N-CA-C	-6.79	100.23	110.28
1	F	93	CYS	N-CA-C	-6.79	100.23	110.28
1	B	377	LEU	N-CA-C	6.78	119.54	111.33
1	B	93	CYS	N-CA-C	-6.78	100.25	110.28
1	E	88	GLN	N-CA-C	-6.73	103.66	112.41
1	A	396	VAL	CB-CA-C	-6.71	102.48	111.80
1	C	93	CYS	N-CA-C	-6.68	100.39	110.28
1	E	93	CYS	N-CA-C	-6.67	100.40	110.28
1	C	377	LEU	N-CA-C	6.67	119.40	111.33
1	E	377	LEU	N-CA-C	6.67	119.40	111.33
1	E	291	ASP	CA-C-N	6.64	126.15	119.24
1	E	291	ASP	C-N-CA	6.64	126.15	119.24
1	F	124	VAL	CA-C-N	6.61	128.10	119.84
1	F	124	VAL	C-N-CA	6.61	128.10	119.84
1	C	52	ILE	CB-CA-C	-6.56	103.58	111.97
1	D	377	LEU	N-CA-C	6.53	119.23	111.33
1	B	88	GLN	N-CA-C	-6.51	103.94	112.41
1	E	368	ASN	N-CA-C	6.51	120.39	111.54
1	D	124	VAL	CA-C-N	6.51	127.97	119.84
1	D	124	VAL	C-N-CA	6.51	127.97	119.84
1	C	396	VAL	CB-CA-C	-6.50	102.76	111.80
1	F	66	SER	N-CA-C	-6.50	97.21	107.93
1	F	396	VAL	CB-CA-C	-6.47	102.80	111.80
1	E	66	SER	N-CA-C	-6.46	97.27	107.93
1	A	88	GLN	N-CA-C	-6.43	104.05	112.41
1	A	369	ILE	N-CA-C	-6.42	99.34	108.58
1	D	66	SER	N-CA-C	-6.41	97.35	107.93
1	A	291	ASP	CA-C-N	6.40	125.89	119.24
1	A	291	ASP	C-N-CA	6.40	125.89	119.24
1	E	124	VAL	CA-C-N	6.39	127.82	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	124	VAL	C-N-CA	6.39	127.82	119.84
1	E	396	VAL	CB-CA-C	-6.37	102.95	111.80
1	C	172	ASP	N-CA-C	-6.35	99.41	109.07
1	C	66	SER	N-CA-C	-6.33	97.48	107.93
1	B	396	VAL	CB-CA-C	-6.33	103.00	111.80
1	B	291	ASP	CA-C-N	6.32	125.81	119.24
1	B	291	ASP	C-N-CA	6.32	125.81	119.24
1	D	396	VAL	CB-CA-C	-6.32	103.02	111.80
1	A	124	VAL	CA-C-N	6.32	127.74	119.84
1	A	124	VAL	C-N-CA	6.32	127.74	119.84
1	B	66	SER	N-CA-C	-6.32	97.51	107.93
1	C	291	ASP	CA-C-N	6.31	125.80	119.24
1	C	291	ASP	C-N-CA	6.31	125.80	119.24
1	A	66	SER	N-CA-C	-6.30	97.53	107.93
1	A	172	ASP	N-CA-C	-6.30	99.50	109.07
1	D	291	ASP	CA-C-N	6.30	125.79	119.24
1	D	291	ASP	C-N-CA	6.30	125.79	119.24
1	C	124	VAL	CA-C-N	6.28	127.69	119.84
1	C	124	VAL	C-N-CA	6.28	127.69	119.84
1	E	172	ASP	N-CA-C	-6.25	99.57	109.07
1	B	52	ILE	CB-CA-C	-6.23	104.00	111.97
1	B	368	ASN	N-CA-C	6.21	119.98	111.54
1	F	172	ASP	N-CA-C	-6.20	99.64	109.07
1	F	291	ASP	CA-C-N	6.20	125.68	119.24
1	F	291	ASP	C-N-CA	6.20	125.68	119.24
1	A	52	ILE	CB-CA-C	-6.17	104.07	111.97
1	D	172	ASP	N-CA-C	-6.17	99.70	109.07
1	A	368	ASN	N-CA-C	6.15	119.90	111.54
1	A	60	ASN	N-CA-C	6.14	121.45	111.37
1	C	368	ASN	N-CA-C	6.14	119.90	111.54
1	E	52	ILE	CB-CA-C	-6.12	104.14	111.97
1	D	368	ASN	N-CA-C	6.12	119.86	111.54
1	F	386	TYR	N-CA-C	-6.11	104.62	111.28
1	F	52	ILE	CB-CA-C	-6.11	104.06	111.88
1	C	386	TYR	N-CA-C	-6.11	104.62	111.28
1	B	172	ASP	N-CA-C	-6.10	99.80	109.07
1	D	52	ILE	CB-CA-C	-6.09	104.17	111.97
1	E	472	ALA	N-CA-C	-6.08	103.81	111.11
1	B	124	VAL	CA-C-N	6.08	127.44	119.84
1	B	124	VAL	C-N-CA	6.08	127.44	119.84
1	D	60	ASN	N-CA-C	6.06	121.30	111.37
1	B	472	ALA	N-CA-C	-6.05	103.84	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	368	ASN	N-CA-C	6.03	119.74	111.54
1	B	382	VAL	N-CA-C	-6.01	104.65	110.42
1	F	162	ILE	N-CA-C	5.97	121.75	109.34
1	F	60	ASN	N-CA-C	5.96	121.21	111.37
1	D	386	TYR	N-CA-C	-5.95	104.79	111.28
1	B	60	ASN	N-CA-C	5.92	121.08	111.37
1	E	369	ILE	N-CA-C	-5.92	99.17	108.23
1	C	60	ASN	N-CA-C	5.91	121.06	111.37
1	B	484	ALA	N-CA-C	-5.91	104.92	111.36
1	B	369	ILE	N-CA-C	-5.90	99.20	108.23
1	C	208	SER	O-C-N	5.89	130.27	122.43
1	D	472	ALA	N-CA-C	-5.88	104.05	111.11
1	F	472	ALA	N-CA-C	-5.87	104.06	111.11
1	C	58	PRO	N-CA-C	5.86	119.69	110.50
1	D	162	ILE	N-CA-C	5.85	121.50	109.34
1	B	58	PRO	N-CA-C	5.83	119.65	110.50
1	A	484	ALA	N-CA-C	-5.82	105.01	111.36
1	E	60	ASN	N-CA-C	5.82	120.92	111.37
1	D	163	GLY	CA-C-N	5.82	125.68	119.28
1	D	163	GLY	C-N-CA	5.82	125.68	119.28
1	C	472	ALA	N-CA-C	-5.82	104.13	111.11
1	A	472	ALA	N-CA-C	-5.81	104.14	111.11
1	C	286	ASN	CA-C-N	5.80	125.48	119.56
1	C	286	ASN	C-N-CA	5.80	125.48	119.56
1	B	162	ILE	N-CA-C	5.80	121.40	109.34
1	E	484	ALA	N-CA-C	-5.79	105.05	111.36
1	F	369	ILE	N-CA-C	-5.77	99.40	108.23
1	C	163	GLY	CA-C-N	5.77	125.63	119.28
1	C	163	GLY	C-N-CA	5.77	125.63	119.28
1	D	484	ALA	N-CA-C	-5.77	105.07	111.36
1	F	382	VAL	N-CA-C	-5.75	104.90	110.42
1	C	162	ILE	N-CA-C	5.74	121.29	109.34
1	C	484	ALA	N-CA-C	-5.74	105.10	111.36
1	B	90	ARG	N-CA-C	-5.74	98.74	108.26
1	C	90	ARG	N-CA-C	-5.73	98.74	108.26
1	F	286	ASN	CA-C-N	5.67	125.35	119.56
1	F	286	ASN	C-N-CA	5.67	125.35	119.56
1	D	369	ILE	N-CA-C	-5.66	99.57	108.23
1	D	382	VAL	N-CA-C	-5.65	104.99	110.42
1	B	286	ASN	CA-C-N	5.65	125.32	119.56
1	B	286	ASN	C-N-CA	5.65	125.32	119.56
1	E	162	ILE	N-CA-C	5.65	121.09	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	SER	N-CA-C	5.65	122.83	110.80
1	A	58	PRO	N-CA-C	5.63	119.30	110.80
1	C	382	VAL	N-CA-C	-5.63	105.02	110.42
1	A	286	ASN	CA-C-N	5.62	125.29	119.56
1	A	286	ASN	C-N-CA	5.62	125.29	119.56
1	D	286	ASN	CA-C-N	5.62	125.29	119.56
1	D	286	ASN	C-N-CA	5.62	125.29	119.56
1	D	58	PRO	N-CA-C	5.62	119.32	110.50
1	A	162	ILE	N-CA-C	5.62	121.02	109.34
1	A	331	SER	N-CA-C	5.60	122.73	110.80
1	C	369	ILE	N-CA-C	-5.55	99.73	108.23
1	F	351	GLY	N-CA-C	-5.55	105.53	113.86
1	A	386	TYR	N-CA-C	-5.54	105.24	111.28
1	E	331	SER	N-CA-C	5.53	122.59	110.80
1	E	51	GLY	N-CA-C	-5.53	106.91	113.99
1	B	51	GLY	N-CA-C	-5.52	106.92	113.99
1	E	90	ARG	N-CA-C	-5.52	99.09	108.26
1	A	127	GLY	N-CA-C	-5.50	104.27	113.02
1	F	127	GLY	N-CA-C	-5.50	104.27	113.02
1	D	331	SER	N-CA-C	5.49	122.50	110.80
1	B	386	TYR	N-CA-C	-5.49	105.30	111.28
1	F	484	ALA	N-CA-C	-5.48	105.39	111.36
1	F	331	SER	N-CA-C	5.47	122.45	110.80
1	E	163	GLY	CA-C-N	5.46	125.29	119.28
1	E	163	GLY	C-N-CA	5.46	125.29	119.28
1	A	382	VAL	N-CA-C	-5.46	105.18	110.42
1	E	386	TYR	N-CA-C	-5.46	105.33	111.28
1	C	178	ARG	N-CA-C	-5.45	104.98	111.03
1	F	163	GLY	CA-C-N	5.45	125.27	119.28
1	F	163	GLY	C-N-CA	5.45	125.27	119.28
1	C	127	GLY	N-CA-C	-5.44	104.37	113.02
1	E	286	ASN	CA-C-N	5.43	125.10	119.56
1	E	286	ASN	C-N-CA	5.43	125.10	119.56
1	B	331	SER	N-CA-C	5.42	122.35	110.80
1	E	58	PRO	N-CA-C	5.42	118.99	110.80
1	A	90	ARG	N-CA-C	-5.41	99.28	108.26
1	B	232	ASN	N-CA-C	-5.40	106.37	113.17
1	A	51	GLY	N-CA-C	-5.37	107.11	113.99
1	D	158	LYS	N-CA-C	5.37	118.93	112.38
1	B	127	GLY	N-CA-C	-5.36	104.50	113.02
1	E	69	ILE	N-CA-C	-5.35	100.76	108.42
1	B	309	PRO	N-CA-C	-5.35	102.79	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	127	GLY	N-CA-C	-5.34	104.52	113.02
1	F	69	ILE	N-CA-C	-5.34	100.79	108.42
1	B	334	GLN	N-CA-C	-5.33	106.46	113.12
1	D	90	ARG	N-CA-C	-5.32	99.43	108.26
1	C	241	GLY	N-CA-C	-5.31	106.91	115.08
1	F	90	ARG	N-CA-C	-5.31	99.45	108.26
1	D	417	VAL	N-CA-C	-5.30	105.55	110.53
1	F	51	GLY	N-CA-C	-5.30	107.21	113.99
1	A	477	LEU	N-CA-C	-5.29	103.40	110.55
1	B	69	ILE	N-CA-C	-5.29	100.85	108.42
1	C	51	GLY	N-CA-C	-5.29	107.22	113.99
1	E	351	GLY	N-CA-C	-5.29	105.93	113.86
1	C	334	GLN	N-CA-C	-5.29	106.51	113.12
1	E	178	ARG	N-CA-C	-5.28	105.17	111.03
1	A	163	GLY	CA-C-N	5.28	125.09	119.28
1	A	163	GLY	C-N-CA	5.28	125.09	119.28
1	D	309	PRO	N-CA-C	-5.28	102.91	111.14
1	A	351	GLY	N-CA-C	-5.28	105.95	113.86
1	E	477	LEU	N-CA-C	-5.28	103.43	110.55
1	A	309	PRO	N-CA-C	-5.27	102.92	111.14
1	D	351	GLY	N-CA-C	-5.27	105.96	113.86
1	C	103	VAL	N-CA-C	-5.27	102.05	109.63
1	A	148	ILE	CB-CA-C	-5.26	105.24	111.97
1	B	477	LEU	N-CA-C	-5.26	103.45	110.55
1	C	309	PRO	N-CA-C	-5.25	102.94	111.14
1	F	58	PRO	N-CA-C	5.25	119.11	110.55
1	A	241	GLY	N-CA-C	-5.24	107.01	115.08
1	F	309	PRO	N-CA-C	-5.24	102.97	111.14
1	E	50	ARG	N-CA-C	-5.22	106.97	113.19
1	A	178	ARG	N-CA-C	-5.22	105.23	111.03
1	C	69	ILE	N-CA-C	-5.22	100.96	108.42
1	E	309	PRO	N-CA-C	-5.21	103.01	111.14
1	B	163	GLY	CA-C-N	5.20	125.50	119.47
1	B	163	GLY	C-N-CA	5.20	125.50	119.47
1	B	55	ILE	CB-CA-C	-5.20	105.27	112.24
1	F	241	GLY	N-CA-C	-5.19	107.08	115.08
1	F	334	GLN	N-CA-C	-5.19	106.63	113.12
1	B	178	ARG	N-CA-C	-5.18	105.28	111.03
1	E	334	GLN	N-CA-C	-5.17	106.65	113.12
1	E	241	GLY	N-CA-C	-5.16	107.13	115.08
1	D	334	GLN	N-CA-C	-5.16	106.67	113.12
1	C	208	SER	CA-C-N	-5.14	114.58	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	SER	C-N-CA	-5.14	114.58	122.60
1	A	55	ILE	CB-CA-C	-5.13	105.36	112.24
1	C	390	LEU	N-CA-C	-5.13	105.68	111.28
1	D	435	VAL	CA-C-N	5.13	125.03	119.85
1	D	435	VAL	C-N-CA	5.13	125.03	119.85
1	D	232	ASN	N-CA-C	-5.13	106.70	113.17
1	D	51	GLY	N-CA-C	-5.13	107.42	113.99
1	E	55	ILE	CB-CA-C	-5.13	105.36	112.24
1	A	103	VAL	N-CA-C	-5.13	102.25	109.63
1	F	103	VAL	N-CA-C	-5.12	102.25	109.63
1	B	351	GLY	N-CA-C	-5.11	106.19	113.86
1	D	55	ILE	CB-CA-C	-5.10	105.41	112.24
1	C	351	GLY	N-CA-C	-5.09	106.22	113.86
1	B	148	ILE	CB-CA-C	-5.09	105.45	111.97
1	C	55	ILE	CB-CA-C	-5.08	105.43	112.24
1	A	334	GLN	N-CA-C	-5.08	106.77	113.12
1	D	241	GLY	N-CA-C	-5.06	107.28	115.08
1	F	55	ILE	CB-CA-C	-5.06	105.46	112.24
1	E	382	VAL	N-CA-C	-5.06	105.57	110.42
1	B	158	LYS	N-CA-C	5.05	118.54	112.38
1	E	435	VAL	CA-C-N	5.03	124.94	119.85
1	E	435	VAL	C-N-CA	5.03	124.94	119.85
1	E	232	ASN	N-CA-C	-5.02	106.85	113.17
1	F	477	LEU	N-CA-C	-5.02	103.78	110.55
1	B	241	GLY	N-CA-C	-5.01	107.37	115.08
1	D	244	PRO	N-CA-C	5.01	119.34	111.38

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	335	0
1	B	3874	0	3841	348	0
1	C	3874	0	3841	382	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3874	0	3841	349	0
1	E	3874	0	3841	358	0
1	F	3874	0	3841	345	0
All	All	23244	0	23046	1971	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 43.

All (1971) 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:C:61:HIS:HD2	1:F:159:LYS:HE3	1.33	0.93
1:E:41:SER:HA	1:E:46:ARG:HD2	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HE2	1:B:427:LYS:HA	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:159:LYS:HE3	1:F:61:HIS:CD2	2.11	0.86
1:C:327:ILE:HG22	1:C:349:ALA:HB3	1.54	0.86
1:A:427:LYS:HE2	1:A:427:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:HIS:CD2	1:B:116:THR:HG21	2.14	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: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
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:38:THR:HG23	1:A:41:SER:HB3	1.63	0.81
1:A:146:GLU:O	1:A:150:ARG:HG3	1.81	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:63:LEU:HD22	1:C:161:PHE:CD2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:GLU:O	1:C:150:ARG:HG3	1.82	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
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:HB3	1:A:71:ARG:HH11	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:HB3	1:D:71:ARG:HH11	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:HB3	1:B:71:ARG:HH11	1.51	0.75
1:C:71:ARG:HB3	1:C:71:ARG:HH11	1.51	0.75
1:C:285:TRP:CB	1:C:314:TYR:HB2	2.13	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:F:71:ARG:HB3	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
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:HD13	1:D:318:ILE:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:264:MET:HE3	1:B:292:PRO:HA	1.74	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:43:GLU:HB3	1:B:45:LYS:HG3	1.73	0.69
1:B:279:GLU:HG3	1:B:305:ILE:HG13	1.74	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:D:264:MET:HE3	1:D:292:PRO:HA	1.75	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:279:GLU:HG3	1:C:305:ILE:HG13	1.73	0.69
1:C:318:ILE:H	1:C:318:ILE:HD13	1.58	0.69
1:D:43:GLU:HB3	1:D:45:LYS:HG3	1.73	0.69
1:D:69:ILE:HA	1:D:151:ARG:NH1	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:264:MET:HE3	1:F:292:PRO:HA	1.75	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:E:264:MET:HE3	1:E:292:PRO:HA	1.75	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:A:264:MET:HE3	1:A:292:PRO:HA	1.75	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
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:HH11	1:F:400:ARG:HG3	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:C:230:PHE:CD2	1:C:469:MET:HE2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:221:ARG:HD2	1:F:454:HIS:CD2	2.31	0.66
1:F:298:PHE:CZ	1:F:302:HIS:HE1	2.14	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:27:ILE:HG22	1:E:475:TYR:CD1	2.31	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: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
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:C:264:MET:HE3	1:C:292:PRO:HA	1.79	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:71:ARG:HB3	1:E:71:ARG:NH1	2.11	0.65
1:E:264:MET:CE	1:E:292:PRO:HA	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:B:400:ARG:HG3	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:HB3	1:D:71:ARG:NH1	2.12	0.64
1:E:37:ARG:HH11	1:E:37:ARG:HB2	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
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:HH11	1:B:37:ARG:HB2	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:HG3	1:A:400:ARG:HH11	1.61	0.64
1:B:77:GLU:HA	1:D:54:ARG:HH12	1.59	0.64
1:B:277:VAL:HG21	1:B:295:LEU:CD2	2.28	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:C:423:ARG:HH21	1:E:435:VAL:HG13	1.63	0.64
1:D:325:ILE:HG22	1:D:347:ILE:CB	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:C:37:ARG:HH11	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:A:76:TRP:CD1	1:E:502:VAL:HG11	2.33	0.63
1:D:33:VAL:HG12	1:D:38:THR:OG1	1.99	0.63
1:D:37:ARG:HB2	1:D:37:ARG:HH11	1.63	0.63
1:E:277:VAL:HG21	1:E:295:LEU:CD2	2.28	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
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:HB2	1:F:37:ARG:HH11	1.64	0.62
1:A:154:MET:HE1	1:A:190:THR:HG21	1.81	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:C:207:ILE:C	1:C:209:GLN:H	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:LYS:NZ	1:E:388:GLU:OE1	2.33	0.61
1:F:32:LEU:HD11	1:F:494:PHE:CE2	2.35	0.61
1:F:135:ILE:HG13	1:F:140:TYR: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:C:337:LYS:HZ2	1:C:359:GLU:HG3	1.66	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:O	1:D:162:ILE:HD13	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:E:46:ARG:O	1:E:49:VAL:HG12	2.00	0.61
1:F:46:ARG:O	1:F: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:A:46:ARG:O	1:A:49:VAL:HG12	1.99	0.61
1:A:433:PRO:O	1:A:435:VAL:N	2.33	0.61
1:C:14:PHE:O	1:C:18:GLU:HB2	2.00	0.61
1:C:162:ILE:HD13	1:C:162:ILE:O	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:F:500:ALA:C	1:F:505:THR:HA	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:500:ALA:C	1:D:505:THR:HA	2.26	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:E:500:ALA:C	1:E:505:THR:HA	2.26	0.60
1:A:185:ASP:OD1	1:F:505:THR:HG23	2.01	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: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:500:ALA:C	1:A:505:THR:HA	2.27	0.60
1:A:502:VAL:HG11	1:E:76:TRP:HD1	1.64	0.60
1:B:10:ASP:HB2	1:B:333:LYS:CD	2.31	0.60
1:B:14:PHE:O	1:B:18:GLU:HB2	2.02	0.60
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:B:347:ILE:HG12	1:B:370:MET:HE2	1.83	0.60
1:D:52:ILE:O	1:D:56:ILE:HG13	2.02	0.60
1:D:154:MET:HE1	1:D:190:THR:HG21	1.83	0.60
1:D:343:VAL:HG21	1:D:364:PHE:CE1	2.36	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:C:347:ILE:HG12	1:C:370:MET:HE2	1.84	0.60
1:C:500:ALA:C	1:C:505:THR:HA	2.26	0.60
1:E:135:ILE:HG13	1:E:140:TYR:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:343:VAL:HG21	1:A:364:PHE:CE1	2.36	0.59
1:B:78:VAL:H	1:D:54:ARG:HH12	1.49	0.59
1:B:343:VAL:HG22	1:B:367:ARG:NH2	2.18	0.59
1:E:343:VAL:HG21	1:E:364:PHE:CE1	2.37	0.59
1:A:143:ASN:HD21	1:C:70:ARG:HH12	1.51	0.59
1:B:500:ALA:C	1:B:505:THR:HA	2.27	0.59
1:C:343:VAL:HG22	1:C:367:ARG:NH2	2.17	0.59
1:D:72:ASP:OD1	1:D:144:GLU:HG3	2.02	0.59
1:A:54:ARG:NH1	1:E:77:GLU:HA	2.17	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:154:MET:HE1	1:E:190:THR:HG21	1.85	0.59
1:E:343:VAL:HG22	1:E:367:ARG:NH2	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:154:MET:HE1	1:B:190:THR:HG21	1.84	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: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:C:154:MET:HE1	1:C:190:THR:HG21	1.84	0.59
1:D:69:ILE:HG22	1:D:151:ARG:HD2	1.84	0.59
1:A:347:ILE:HG12	1:A:370:MET:HE2	1.84	0.59
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:28:VAL:CG2	1:E:487:VAL:HG13	2.33	0.59
1:E:146:GLU:HG2	1:E:150:ARG:HD2	1.85	0.59
1:F:23:ARG:O	1:F:27:ILE:HG13	2.02	0.59
1:A:504:PHE:CE1	1:E:70:ARG:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:244:PRO:HB2	1:F:248:ASP:H	1.68	0.59
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:69:ILE:HG22	1:B:151:ARG:HD2	1.84	0.58
1:B:190:THR:HG22	1:B:191:ILE:N	2.18	0.58
1:C:207:ILE:C	1:C:209:GLN:N	2.61	0.58
1:D:12:ASN:OD1	1:D:15:LYS:HG2	2.03	0.58
1:D:93:CYS:HB3	1:D:129:ALA:HB2	1.85	0.58
1:D:146:GLU:HG2	1:D:150:ARG:HD2	1.84	0.58
1:A:483:THR:O	1:A:487:VAL:HG23	2.02	0.58
1:B:54:ARG:HH12	1:D:78:VAL:N	2.02	0.58
1:D:418:GLN:CB	1:D:433:PRO:HD2	2.32	0.58
1:F:343:VAL:HG21	1:F:364:PHE:CE1	2.37	0.58
1:A:70:ARG:HH12	1:C:143:ASN:HD21	1.51	0.58
1:A:308:PHE:HD2	1:A:311:ALA:HB2	1.68	0.58
1:C:345:ALA:O	1:C:369:ILE:HD12	2.03	0.58
1:C:502:VAL:HG11	1:F:76:TRP:CD1	2.39	0.58
1:E:91:THR:OG1	1:E:92:PRO:HD3	2.04	0.58
1:A:91:THR:OG1	1:A:92:PRO:HD3	2.04	0.58
1:A:386:TYR:OH	1:B:396:VAL:HG13	2.04	0.58
1:B:135:ILE:HG13	1:B:140:TYR:CE2	2.38	0.58
1:C:279:GLU:HG3	1:C:305:ILE:CG1	2.34	0.58
1:D:347:ILE:HG12	1:D:370:MET:HE2	1.84	0.58
1:D:435:VAL:HG13	1:E:423:ARG:HH21	1.68	0.58
1:A:343:VAL:HG22	1:A:367:ARG:NH2	2.18	0.58
1:A:345:ALA:O	1:A:369:ILE:HD12	2.02	0.58
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:F:154:MET:HE1	1:F:190:THR:HG21	1.86	0.58
1:B:54:ARG:NH1	1:D:77:GLU:HA	2.18	0.58
1:D:308:PHE:HD2	1:D:311:ALA:HB2	1.68	0.58
1:F:69:ILE:HG22	1:F:151:ARG:HD2	1.85	0.58
1:F:279:GLU:HG3	1:F:305:ILE:CG1	2.34	0.58
1:C:93:CYS:HB3	1:C:129:ALA:HB2	1.86	0.58
1:E:427:LYS:HA	1:E:427:LYS:CE	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ILE:HG22	1:A:434:ILE:HG12	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: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:72:ASP:OD1	1:E:144:GLU:HG3	2.02	0.57
1:E:244:PRO:HB2	1:E:248:ASP:H	1.69	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: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:B:252:VAL:HG11	1:B:318:ILE:HB	1.86	0.57
1:C:146:GLU:HG2	1:C:150:ARG:HD2	1.85	0.57
1:C:190:THR:HG22	1:C:191:ILE:N	2.19	0.57
1:C:213:HIS:O	1:C:453:VAL:HG21	2.04	0.57
1:F:347:ILE:HG12	1:F:370:MET:HE2	1.84	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:E:171:PRO:HG3	1:E:180:MET:SD	2.43	0.57
1:E:347:ILE:HG12	1:E:370:MET:HE2	1.85	0.57
1:A:12:ASN:OD1	1:A:15:LYS:HG2	2.03	0.57
1:B:76:TRP:CZ3	1:D:49:VAL:HA	2.40	0.57
1:B:154:MET:SD	1:B:190:THR:HG21	2.45	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
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:52:ILE:O	1:A:56:ILE:HG13	2.04	0.57
1:A:244:PRO:HB2	1:A:248:ASP:H	1.70	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:A:54:ARG:HH12	1:E:78:VAL:H	1.52	0.57
1:C:244:PRO:HB2	1:C:248:ASP:H	1.69	0.57
1:A:190:THR:HG22	1:A:191:ILE:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:205:LYS:HZ3	1:F:392:ASN:HD21	1.52	0.57
1:B:91:THR:CB	1:B:92:PRO:HD3	2.35	0.56
1:B:95:GLY:HA3	1:B:129:ALA:O	2.05	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:91:THR:CB	1:E:92:PRO:HD3	2.35	0.56
1:E:320:GLU:O	1:E:344:LYS:HG2	2.05	0.56
1:C:427:LYS:HA	1:C:427:LYS:CE	2.33	0.56
1:F:320:GLU:O	1:F:344:LYS:HG2	2.04	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: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
1:B:320:GLU:O	1:B:344:LYS:HG2	2.05	0.56
1:C:157:ALA:HA	1:C:162:ILE:HG22	1.87	0.56
1:D:304:SER:OG	1:D:306:LEU:HD13	2.06	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:F:375:LEU:HD23	1:F:485:ALA:HB1	1.87	0.56
1:A:337:LYS:HZ2	1:A:359:GLU:HG3	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:252:VAL:HG11	1:E:318:ILE:HB	1.87	0.56
1:E:293:LYS:O	1:E:296:GLU:HB3	2.06	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:C:503:THR:HG21	1:F:151:ARG:CD	2.35	0.56
1:D:154:MET:SD	1:D:190:THR:HG21	2.45	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:40:GLU:HG3	1:F:46:ARG:NH1	2.15	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:A:13:PHE:CD1	1:A:14:PHE:N	2.65	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
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: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: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:A:503:THR:HG21	1:E:151:ARG:NE	2.22	0.55
1:D:293:LYS:O	1:D:296:GLU:HB3	2.06	0.55
1:B:37:ARG:HB2	1:B:37:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:SER:OG	1:B:306:LEU:HD13	2.06	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: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:A:54:ARG:HH12	1:E:78:VAL:N	2.05	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
1:E:95:GLY:HA3	1:E:129:ALA:O	2.07	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:205:LYS:HZ3	1:F:392:ASN:ND2	2.04	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:B:499:GLU:HB2	1:F:209:GLN:NE2	2.23	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:37:ARG:HB2	1:E:37:ARG:NH1	2.21	0.54
1:E:273:LYS:HE2	1:E:288:ASP:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:337:LYS:HZ2	1:E:359:GLU:HG3	1.72	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:33:VAL:HG13	1:D:46:ARG:HB2	1.90	0.54
1:D:69:ILE:HA	1:D:151:ARG:CZ	2.37	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:B:499:GLU:HB2	1:F:209:GLN:HE21	1.73	0.54
1:C:154:MET:SD	1:C:190:THR:HG21	2.47	0.54
1:A:33:VAL:HG13	1:A:46:ARG:HB2	1.89	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
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:C:505:THR:C	1:D:150:ARG:HH22	2.15	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: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:337:LYS:NZ	1:C:359:GLU:HG3	2.22	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:A:503:THR:HG21	1:E:151:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:PHE:CE1	1:B:490:ILE:HD12	2.43	0.53
1:B:386:TYR:OH	1:F:396:VAL:HG13	2.08	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: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:243:THR:N	1:C:244:PRO:CD	2.69	0.53
1:E:41:SER:CA	1:E:46:ARG:HD2	2.32	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: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:F:427:LYS:HZ3	1:F:428:HIS:H	1.57	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
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:F:373:PRO:CG	1:F:481:LEU:HB3	2.39	0.53
1:A:391:LYS:NZ	1:A:449:GLU:OE1	2.41	0.52
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:78:VAL:H	1:F:54:ARG:HH12	1.57	0.52
1:C:122:VAL:CG1	1:C:379:ALA:CB	2.87	0.52
1:C:150:ARG:HH12	1:E:505:THR:C	2.17	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:A:105:VAL:O	1:A:109:LYS:HG3	2.08	0.52
1:B:99:TYR:HH	1:B:149:THR:HG22	1.70	0.52
1:B:273:LYS:HE2	1:B:288:ASP:O	2.09	0.52
1:C:95:GLY:HA3	1:C:129:ALA:O	2.10	0.52
1:C:116:THR:HG22	1:C:128:GLY:H	1.72	0.52
1:F:285:TRP:O	1:F:286:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:D:79:ILE:N	2.25	0.52
1:E:41:SER:HA	1:E:46:ARG:CD	2.34	0.52
1:E:255:GLY:HA3	1:E:330:ALA:HB2	1.91	0.52
1:F:62:VAL:HG11	1:F:109:LYS:NZ	2.24	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:B:332:GLU:HG2	1:B:333:LYS:HG2	1.91	0.52
1:C:257:GLY:O	1:C:258:ASN:C	2.53	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:A:79:ILE:HD12	1:A:79:ILE:N	2.25	0.52
1:B:92:PRO:HG2	1:B:389:TRP:CZ2	2.45	0.52
1:B:147:LYS:HD2	1:B:151:ARG:NH2	2.21	0.52
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:D:62:VAL:HG11	1:D:109:LYS:HZ3	1.75	0.52
1:F:92:PRO:HG2	1:F:389:TRP:CZ2	2.45	0.52
1:F:243:THR:HG23	1:F:243:THR:O	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:433:PRO:HA	1:E:420:SER:HB3	1.93	0.51
1:E:252:VAL:CG1	1:E:318:ILE:HB	2.41	0.51
1:F:428:HIS:N	1:F:428:HIS:CD2	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:40:GLU:HG3	1:D:46:ARG:NH1	2.16	0.51
1:D:62:VAL:HG11	1:D:109:LYS:NZ	2.25	0.51
1:D:504:PHE:HB3	1:E:146:GLU:OE1	2.09	0.51
1:C:243:THR:HG23	1:C:243:THR:O	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:B:285:TRP:O	1:B:286:ASN:HB2	2.10	0.51
1:C:256:PHE:HE2	1:C:264:MET:HE2	1.75	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:A:99:TYR:HH	1:A:149:THR:HG22	1.72	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:79:ILE:N	1:E:79:ILE:HD12	2.25	0.51
1:E:147:LYS:HD2	1:E:151:ARG:NH2	2.20	0.51
1:F:28:VAL:CG2	1:F:487:VAL:HG13	2.39	0.51
1:F:226:GLY:HA3	1:F:377:LEU:CD1	2.40	0.51
1:F:318:ILE:HD13	1:F:318:ILE:N	2.25	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:C:505:THR:C	1:D:150:ARG:HH12	2.19	0.51
1:D:41:SER:CA	1:D:46:ARG:HD2	2.31	0.51
1:D:308:PHE:O	1:D:311:ALA:HB3	2.09	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:A:150:ARG:HH12	1:F:505:THR:C	2.19	0.51
1:B:40:GLU:HG3	1:B:46:ARG:NH1	2.17	0.51
1:B:266:TYR:O	1:B:270:PHE:HD2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PHE:O	1:B:311:ALA:HB3	2.09	0.51
1:C:252:VAL:CG1	1:C:318:ILE:HB	2.40	0.51
1:D:257:GLY:O	1:D:258:ASN:C	2.54	0.51
1:F:337:LYS:HZ2	1:F:359:GLU:HG3	1.75	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:C:78:VAL:N	1:F:54:ARG:HH12	2.08	0.51
1:C:273:LYS:HE2	1:C:288:ASP:C	2.36	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:A:425:PHE:CD1	1:A:427:LYS:HB2	2.44	0.51
1:B:54:ARG:HH12	1:D:77:GLU:HA	1.75	0.51
1:B:257:GLY:O	1:B:258:ASN:C	2.54	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:E:73:ASP:O	1:E:75:SER:N	2.42	0.51
1:E:285:TRP:O	1:E:286:ASN:HB2	2.10	0.51
1:F:95:GLY:HA3	1:F:129:ALA:O	2.11	0.51
1:F:266:TYR:O	1:F:270:PHE:HD2	1.94	0.51
1:A:298:PHE:HE1	1:A:309:PRO:HD3	1.76	0.50
1:B:505:THR:N	1:F:150:ARG:HH12	2.08	0.50
1:C:30:ASP:O	1:C:34:GLU:HG2	2.11	0.50
1:C:118:LYS:HZ3	1:C:353:ASN:HD21	1.59	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:40:GLU:O	1:D:42:GLU:N	2.44	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: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:40:GLU:O	1:B:42:GLU:N	2.44	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:C:40:GLU:O	1:C:42:GLU:N	2.44	0.50
1:E:38:THR:CG2	1:E:41:SER:HB3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:VAL:HG11	1:E:109:LYS:HZ3	1.77	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:99:TYR:HH	1:E:149:THR:HG22	1.72	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:F:256:PHE:HE2	1:F:264:MET:HE2	1.76	0.50
1:A:78:VAL:N	1:E:54:ARG:HH12	2.10	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: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:273:LYS:HE2	1:D:288:ASP:C	2.37	0.50
1:D:428:HIS:N	1:D:428:HIS:CD2	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:390:LEU:HD13	1:D:396:VAL:HG21	1.93	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: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
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:273:LYS:HE2	1:A:288:ASP:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:PHE:CD1	1:D:427:LYS:HB2	2.44	0.50
1:E:226:GLY:HA3	1:E:377:LEU:CD1	2.42	0.50
1:E:347:ILE:HA	1:E:370:MET:O	2.12	0.50
1:C:213:HIS:HB2	1:C:449:GLU:HB3	1.93	0.49
1:C:421:LEU:HD21	1:E:421:LEU:HD21	1.93	0.49
1:C:504:PHE:CE1	1:F:70:ARG:HB3	2.47	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:A:40:GLU:HG3	1:A:46:ARG:NH1	2.15	0.49
1:A:427:LYS:HZ3	1:A:428:HIS:H	1.58	0.49
1:B:256:PHE:HE2	1:B:264:MET:HE2	1.77	0.49
1:B:471:THR:HA	1:B:474:LYS:HB3	1.93	0.49
1:D:318:ILE:HD13	1:D:318:ILE:N	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:79:ILE:HD12	1:F:79:ILE:N	2.27	0.49
1:F:332:GLU:HG2	1:F:333:LYS:HG2	1.93	0.49
1:B:243:THR:HG23	1:B:243:THR:O	2.11	0.49
1:C:78:VAL:HG23	1:C:78:VAL:O	2.13	0.49
1:C:206:PRO:HB2	1:C:209:GLN:CG	2.43	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:79:ILE:HD12	1:C:79:ILE:N	2.27	0.49
1:C:298:PHE:HE1	1:C:309:PRO:HD3	1.78	0.49
1:D:221:ARG:HD2	1:D:454:HIS:NE2	2.27	0.49
1:F:273:LYS:HE2	1:F:288:ASP:C	2.37	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:474:LYS:HD3	1:F:475:TYR:CE2	2.47	0.49
1:A:31:LYS:HD2	1:A:474:LYS:HZ3	1.76	0.49
1:A:40:GLU:O	1:A:42:GLU:N	2.45	0.49
1:B:76:TRP:HB2	1:D:51:GLY:HA3	1.95	0.49
1:B:502:VAL:N	1:B:505:THR:HB	2.28	0.49
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:256:PHE:HE2	1:D:264:MET:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:GLU:HG2	1:D:333:LYS:HG2	1.92	0.49
1:E:257:GLY:O	1:E:258:ASN:C	2.55	0.49
1:E:332:GLU:HG2	1:E:333:LYS:HG2	1.93	0.49
1:F:87:SER:O	1:F:127:GLY:HA3	2.12	0.49
1:F:347:ILE:HA	1:F:370:MET:O	2.13	0.49
1:A:147:LYS:HD2	1:A:151:ARG:NH2	2.20	0.49
1:A:226:GLY:HA3	1:A:377:LEU:CD1	2.42	0.49
1:A:256:PHE:HE2	1:A:264:MET:HE2	1.78	0.49
1:A:257:GLY:O	1:A:258:ASN:C	2.55	0.49
1:A:347:ILE:HA	1:A:370:MET:O	2.13	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:37:ARG:NH2	1:E:49:VAL:HG11	2.28	0.49
1:E:136:ASN:OD1	1:E:138:LYS:HB2	2.13	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:F:502:VAL:C	1:F:505:THR:HB	2.38	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:C	1:D:505:THR:HB	2.38	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:69:ILE:HG12	1:C:79:ILE:CD1	2.43	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: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:28:VAL:HG22	1:C:487:VAL:HG13	1.94	0.49
1:C:122:VAL:HG23	1:C:124:VAL:HG23	1.94	0.49
1:F:230:PHE:CD2	1:F:469:MET:HE2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:TRP:CD1	1:F:502:VAL:HG11	2.46	0.49
1:C:122:VAL:HG11	1:C:379:ALA:HB1	1.94	0.49
1:C:400:ARG:HG3	1:C:400:ARG:NH1	2.28	0.49
1:D:13:PHE:CE2	1:D:107:GLU:HG3	2.48	0.49
1:F:257:GLY:O	1:F:258:ASN:C	2.55	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:A:390:LEU:O	1:A:391:LYS:C	2.56	0.48
1:B:13:PHE:CE2	1:B:107:GLU:HG3	2.48	0.48
1:B:273:LYS:HE2	1:B:288:ASP:C	2.38	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:E:273:LYS:HE2	1:E:288:ASP:C	2.38	0.48
1:E:502:VAL:C	1:E:505:THR:HB	2.38	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:F:433:PRO:C	1:F:435:VAL:N	2.70	0.48
1:C:420:SER:HB2	1:E:433:PRO:HA	1.94	0.48
1:D:116:THR:HG22	1:D:128:GLY:H	1.78	0.48
1:E:256:PHE:HE2	1:E:264:MET:HE2	1.78	0.48
1:F:91:THR:HB	1:F:92:PRO:HD3	1.95	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:A:243:THR:H	1:A:244:PRO:HD3	1.74	0.48
1:A:502:VAL:C	1:A:505:THR:HB	2.38	0.48
1:C:78:VAL:HG13	1:F:54:ARG:NH1	2.28	0.48
1:C:118:LYS:HZ1	1:C:353:ASN:HD21	1.60	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:D:78:VAL:HG23	1:D:78:VAL:O	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:B:502:VAL:C	1:B:505:THR:HB	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:LYS:HZ2	1:D:359:GLU:HG3	1.78	0.48
1:E:319:LEU:HD12	1:E:319:LEU:N	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: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: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
1:C:187:TYR:CE2	1:C:192:GLY:HA3	2.49	0.48
1:D:298:PHE:CE1	1:D:309:PRO:HD3	2.48	0.48
1:E:78:VAL:O	1:E:78:VAL:HG23	2.12	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: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:E:261:LEU:C	1:E:261:LEU:HD12	2.39	0.48
1:A:41:SER:CA	1:A:46:ARG:HD2	2.32	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: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:D:427:LYS:HZ3	1:D:428:HIS:H	1.61	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:76:TRP:HD1	1:E:502:VAL:HG11	1.76	0.48
1:A:242:MET:O	1:A:243:THR:HG22	2.13	0.48
1:A:319:LEU:HD12	1:A:319:LEU:N	2.29	0.48
1:B:33:VAL:O	1:B:38:THR:N	2.47	0.48
1:D:350:GLU:CD	1:D:482:ARG:HH22	2.21	0.48
1:E:91:THR:HB	1:E:92:PRO:HD3	1.96	0.48
1:E:235:SER:O	1:E:239:ILE:HG12	2.14	0.48
1:F:38:THR:CG2	1:F:41:SER:HB3	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:502:VAL:C	1:C:505:THR:HB	2.38	0.48
1:D:100:SER:O	1:D:103:VAL:HG22	2.14	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:B:54:ARG:HH12	1:D:78:VAL:H	1.60	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: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
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:E:433:PRO:C	1:E:435:VAL:N	2.71	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:390:LEU:O	1:D:391:LYS:C	2.57	0.47
1:D:488:ASN:HD21	1:D:492:LYS:NZ	2.12	0.47
1:E:116:THR:HG22	1:E:128:GLY:H	1.79	0.47
1:E:122:VAL:HG23	1:E:124:VAL:HG23	1.96	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:C:503:THR:HG21	1:F:151:ARG:HD3	1.96	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: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:F:319:LEU:HD12	1:F:319:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:MET:HE2	1:C:242:MET:HA	1.97	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: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:A:100:SER:O	1:A:103:VAL:HG22	2.15	0.47
1:A:404:LYS:HZ2	1:A:407:ARG:NE	2.12	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
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:91:THR:HB	1:D:92:PRO:HD3	1.97	0.47
1:F:449:GLU:O	1:F:450:LYS:C	2.58	0.47
1:A:233:GLU:CG	1:A:236:TYR:HD1	2.27	0.47
1:A:261:LEU:C	1:A:261:LEU:HD12	2.39	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:C:347:ILE:HA	1:C:370:MET:O	2.14	0.47
1:D:13:PHE:CE1	1:D:107:GLU:HA	2.50	0.47
1:D:92:PRO:HG2	1:D:389:TRP:CZ2	2.50	0.47
1:D:261:LEU:C	1:D:261:LEU:HD12	2.40	0.47
1:E:21:PHE:CE1	1:E:490:ILE:HD12	2.49	0.47
1:E:177:GLU:HB2	1:E:206:PRO:HG3	1.97	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:E:449:GLU:O	1:E:450:LYS:C	2.57	0.47
1:F:251:PHE:HB3	1:F:325:ILE:CG1	2.41	0.47
1:F:261:LEU:C	1:F:261:LEU:HD12	2.40	0.47
1:F:327:ILE:CG2	1:F:349:ALA:HB3	2.33	0.47
1:A:54:ARG:HH12	1:E:77:GLU:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:120:ALA:O	1:E:492:LYS:NZ	2.48	0.47
1:E:187:TYR:CE2	1:E:192:GLY:HA3	2.50	0.47
1:B:339:ASN:HD22	1:B:339:ASN:N	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:154:MET:CE	1:D:190:THR:HG21	2.45	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:B:261:LEU:C	1:B:261:LEU:HD12	2.40	0.47
1:C:421:LEU:HD12	1:C:421:LEU:HA	1.74	0.47
1:C:433:PRO:C	1:C:435:VAL:N	2.73	0.47
1:D:33:VAL:O	1:D:38:THR:N	2.48	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:F:298:PHE:CE1	1:F:302:HIS:HE1	2.33	0.47
1:F:390:LEU:O	1:F:391:LYS:C	2.57	0.47
1:A:41:SER:HA	1:A:46:ARG:CD	2.35	0.46
1:C:38:THR:CG2	1:C:41:SER:HB3	2.40	0.46
1:C:54:ARG:NH1	1:F:77:GLU:HA	2.30	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:D:425:PHE:HD1	1:D:427:LYS:CB	2.27	0.46
1:A:184:ALA:HA	1:A:201:CYS:SG	2.55	0.46
1:B:69:ILE:HG12	1:B:79:ILE:CD1	2.46	0.46
1:B:233:GLU:HG2	1:B:236:TYR:HD1	1.80	0.46
1:B:505:THR:C	1:F:150:ARG:HH12	2.24	0.46
1:C:423:ARG:NH2	1:E:435:VAL:HG13	2.27	0.46
1:D:339:ASN:ND2	1:D:339:ASN:H	2.13	0.46
1:D:418:GLN:OE1	1:D:434:ILE:HG23	2.16	0.46
1:E:242:MET:HE2	1:E:242:MET:HA	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:GLN:HE21	1:C:334:GLN:HA	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:78:VAL:HG23	1:F:78:VAL:O	2.14	0.46
1:F:251:PHE:CE2	1:F:264:MET:HA	2.50	0.46
1:F:257:GLY:O	1:F:260:GLY:N	2.48	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: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: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:242:MET:HE2	1:B:242:MET:HA	1.97	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:261:LEU:C	1:C:261:LEU:HD12	2.40	0.46
1:C:487:VAL:O	1:C:491:GLU:HG3	2.15	0.46
1:D:427:LYS:HA	1:D:427:LYS:CE	2.32	0.46
1:E:298:PHE:CE1	1:E:309:PRO:HD3	2.49	0.46
1:F:334:GLN:HA	1:F:334:GLN:HE21	1.81	0.46
1:A:439:GLU:CD	1:A:439:GLU:H	2.22	0.46
1:B:257:GLY:O	1:B:260:GLY:N	2.48	0.46
1:B:327:ILE:CG2	1:B:349:ALA:HB3	2.34	0.46
1:B:418:GLN:OE1	1:B:434:ILE:HG23	2.16	0.46
1:B:427:LYS:HG3	1:B:430:GLY:H	1.81	0.46
1:C:51:GLY:O	1:C:55:ILE:HG13	2.15	0.46
1:C:233:GLU:CG	1:C:236:TYR:HD1	2.28	0.46
1:D:242:MET:HA	1:D:242:MET:HE2	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:435:VAL:CG1	1:E:423:ARG:HH21	2.28	0.46
1:E:285:TRP:CD1	1:E:287:PRO:HD3	2.50	0.46
1:F:37:ARG:NH2	1:F:49:VAL:HG11	2.29	0.46
1:F:100:SER:O	1:F:103:VAL:HG22	2.15	0.46
1:F:242:MET:HE2	1:F:242:MET:HA	1.97	0.46
1:A:206:PRO:HD2	1:A:209:GLN:HB2	1.98	0.46
1:A:242:MET:HA	1:A:242:MET:HE2	1.97	0.46
1:A:421:LEU:HA	1:A:421:LEU:HD12	1.73	0.46
1:B:13:PHE:CE1	1:B:107:GLU:HA	2.51	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:154:MET:CE	1:C:190:THR:HG21	2.45	0.46
1:C:427:LYS:HG3	1:C:430:GLY:H	1.81	0.46
1:C:439:GLU:H	1:C:439:GLU:CD	2.24	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:ND2	1:F:339:ASN:H	2.14	0.46
1:A:70:ARG:HB3	1:E:504:PHE:CE1	2.50	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:B:350:GLU:CD	1:B:482:ARG:HH22	2.24	0.46
1:C:12:ASN:ND2	1:C:14:PHE:HB3	2.30	0.46
1:C:49:VAL:HA	1:F:76:TRP:CZ3	2.50	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:HD22	1:E:339:ASN:N	2.13	0.46
1:F:439:GLU:H	1:F:439:GLU:CD	2.24	0.46
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:317:SER:C	1:B:319:LEU:N	2.73	0.46
1:B:339:ASN:HD22	1:B:339:ASN:H	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:ILE:O	1:E:184:ALA:C	2.59	0.46
1:E:374:ASP:O	1:E:378:ASN:ND2	2.49	0.46
1:F:91:THR:CB	1:F:92:PRO:CD	2.93	0.46
1:F:228:GLU:O	1:F:231:ILE:HG22	2.15	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:A:433:PRO:C	1:A:435:VAL:N	2.73	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:C:449:GLU:O	1:C:450:LYS:C	2.57	0.45
1:D:69:ILE:HG12	1:D:79:ILE:CD1	2.46	0.45
1:D:298:PHE:CE1	1:D:302:HIS:HE1	2.33	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:51:GLY:O	1:F:55:ILE:HG13	2.16	0.45
1:F:122:VAL:HG11	1:F:379:ALA:HB3	1.98	0.45
1:F:233:GLU:CG	1:F:236:TYR:HD1	2.28	0.45
1:B:118:LYS:NZ	1:B:378:ASN:ND2	2.64	0.45
1:B:177:GLU:HB2	1:B:206:PRO:HG3	1.99	0.45
1:B:337:LYS:HZ2	1:B:359:GLU:HG3	1.80	0.45
1:B:339:ASN:ND2	1:B:339:ASN:H	2.13	0.45
1:B:372:ILE:HA	1:B:373:PRO:HD3	1.62	0.45
1:B:449:GLU:O	1:B:450:LYS:C	2.60	0.45
1:C:251:PHE:CE2	1:C:264:MET:HA	2.51	0.45
1:C:420:SER:HB3	1:E:433:PRO:HA	1.95	0.45
1:D:233:GLU:CG	1:D:236:TYR:HD1	2.29	0.45
1:D:404:LYS:HZ2	1:D:407:ARG:NE	2.13	0.45
1:D:502:VAL:HG23	1:D:503:THR:N	2.28	0.45
1:A:38:THR:CG2	1:A:41:SER:HB3	2.41	0.45
1:A:504:PHE:CE1	1:E:70:ARG:CB	2.99	0.45
1:B:70:ARG:HH12	1:E:143:ASN:HD21	1.65	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: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:12:ASN:ND2	1:B:14:PHE:HB3	2.32	0.45
1:B:120:ALA:O	1:B:492:LYS:NZ	2.49	0.45
1:C:386:TYR:OH	1:D:396:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:VAL:HG12	1:D:135:ILE:HB	1.98	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:A:12:ASN:ND2	1:A:14:PHE:HB3	2.31	0.45
1:A:334:GLN:HA	1:A:334:GLN:HE21	1.82	0.45
1:A:339:ASN:ND2	1:A:339:ASN:H	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:HD13	1:B:318:ILE:N	2.24	0.45
1:B:334:GLN:HA	1:B:334:GLN:HE21	1.80	0.45
1:B:433:PRO:C	1:B:435:VAL:N	2.73	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:E:154:MET:CE	1:E:190:THR:HG21	2.45	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:B:113:SER:O	1:B:114:LEU:C	2.58	0.45
1:D:350:GLU:OE1	1:D:482:ARG:NH2	2.50	0.45
1:E:334:GLN:HA	1:E:334:GLN:HE21	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:D:449:GLU:O	1:D:450:LYS:C	2.60	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:THR:CB	1:E:92:PRO:CD	2.94	0.45
1:A:91:THR:CB	1:A:92:PRO:CD	2.95	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: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:150:ARG:NH2	1:E:505:THR:HG23	2.32	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:E:317:SER:C	1:E:319:LEU:N	2.74	0.45
1:F:177:GLU:HB2	1:F:206:PRO:HG3	1.99	0.45
1:F:298:PHE:CE1	1:F:308:PHE:HA	2.52	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:D:433:PRO:C	1:D:435:VAL:N	2.72	0.44
1:E:400:ARG:HG3	1:E:400:ARG:NH1	2.28	0.44
1:F:33:VAL:O	1:F:38:THR:N	2.48	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:A:51:GLY:O	1:A:55:ILE:HG13	2.17	0.44
1:A:151:ARG:CZ	1:E:503:THR:HG21	2.48	0.44
1:A:433:PRO:HA	1:B:420:SER:CB	2.47	0.44
1:B:118:LYS:HZ1	1:B:378:ASN:HD21	1.65	0.44
1:B:136:ASN:OD1	1:B:138:LYS:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PHE:HA	1:A:325:ILE:O	2.17	0.44
1:A:339:ASN:HD22	1:A:339:ASN:H	1.65	0.44
1:C:172:ASP:O	1:C:173:MET:C	2.60	0.44
1:C:322:ASP:OD1	1:C:344:LYS:HB3	2.17	0.44
1:C:339:ASN:HD22	1:C:339:ASN:N	2.15	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:320:GLU:HG3	1:D:342:ARG:HG2	1.98	0.44
1:D:339:ASN:HD22	1:D:339:ASN:N	2.14	0.44
1:D:501:GLY:N	1:D:505:THR:HA	2.32	0.44
1:E:16:MET:SD	1:E:358:PRO:HD3	2.57	0.44
1:E:133:VAL:HG12	1:E:135:ILE:HB	1.99	0.44
1:E:318:ILE:HD13	1:E:318:ILE:N	2.25	0.44
1:E:322:ASP:OD1	1:E:344:LYS:HB3	2.18	0.44
1:F:251:PHE:CE1	1:F:267:LEU:HB3	2.52	0.44
1:F:317:SER:C	1:F:319:LEU:N	2.74	0.44
1:A:427:LYS:HG3	1:A:430:GLY:H	1.81	0.44
1:B:37:ARG:NH2	1:B:49:VAL:HG11	2.29	0.44
1:B:183:ILE:O	1:B:184:ALA:C	2.61	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:C:91:THR:CB	1:C:92:PRO:CD	2.94	0.44
1:C:113:SER:O	1:C:114:LEU:C	2.61	0.44
1:D:251:PHE:CE2	1:D:264:MET:HA	2.52	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:170:ALA:CA	1:C:180:MET:HE2	2.48	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:49:VAL:C	1:D:51:GLY:H	2.26	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
1:B:252:VAL:HG23	1:B:323:CYS:SG	2.58	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:HA	1:D:421:LEU:HD12	1.73	0.44
1:B:44:GLN:C	1:B:46:ARG:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLU:C	1:D:54:ARG:HH12	2.25	0.44
1:C:31:LYS:HA	1:C:34:GLU:HG2	2.00	0.44
1:C:49:VAL:C	1:C:51:GLY:H	2.25	0.44
1:D:400:ARG:HG3	1:D:400:ARG:NH1	2.31	0.44
1:E:100:SER:O	1:E:103:VAL:HG22	2.17	0.44
1:E:172:ASP:O	1:E:173:MET:C	2.61	0.44
1:E:501:GLY:N	1:E:505:THR:HA	2.32	0.44
1:F:47:ASN:HD21	1:F:50:ARG:NH1	2.16	0.44
1:A:47:ASN:HD21	1:A:50:ARG:NH1	2.16	0.44
1:A:60:ASN:HA	1:E:66:SER:OG	2.18	0.44
1:A:254:GLN:HE21	1:A:330:ALA:HB3	1.82	0.44
1:A:449:GLU:O	1:A:450:LYS:C	2.59	0.44
1:B:27:ILE:CG2	1:B:475:TYR:CD1	2.99	0.44
1:B:298:PHE:CE1	1:B:308:PHE:HA	2.53	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:350:GLU:CD	1:E:482:ARG:HH22	2.26	0.44
1:F:49:VAL:C	1:F:51:GLY:H	2.25	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: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:49:VAL:C	1:E:51:GLY:H	2.25	0.44
1:E:251:PHE:CE2	1:E:264:MET:HA	2.53	0.44
1:A:172:ASP:O	1:A:173:MET:C	2.61	0.43
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:31:LYS:HD3	1:B:35:ASP:OD2	2.18	0.43
1:B:172:ASP:O	1:B:173:MET:C	2.60	0.43
1:B:323:CYS:O	1:B:345:ALA:HA	2.18	0.43
1:C:301:GLN:O	1:C:301:GLN:HG2	2.18	0.43
1:D:44:GLN:C	1:D:46:ARG:H	2.26	0.43
1:D:251:PHE:CE1	1:D:267:LEU:HB3	2.53	0.43
1:D:439:GLU:CD	1:D:439:GLU:H	2.25	0.43
1:E:488:ASN:HD21	1:E:492:LYS:HZ1	1.66	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: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:C:317:SER:C	1:C:319:LEU:N	2.75	0.43
1:D:51:GLY:O	1:D:55:ILE:HG13	2.18	0.43
1:D:183:ILE:O	1:D:184:ALA:C	2.61	0.43
1:D:298:PHE:CE1	1:D:308:PHE:HA	2.52	0.43
1:D:334:GLN:HA	1:D:334:GLN:HE21	1.82	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:49:VAL:C	1:B:51:GLY:H	2.26	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:21:PHE:CE1	1:D:490:ILE:HD12	2.54	0.43
1:D:47:ASN:HD21	1:D:50:ARG:NH1	2.16	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:E:69:ILE:HD13	1:E:148:ILE:CG1	2.49	0.43
1:E:113:SER:O	1:E:114:LEU:C	2.60	0.43
1:E:339:ASN:H	1:E:339:ASN:HD22	1.65	0.43
1:E:439:GLU:H	1:E:439:GLU:CD	2.25	0.43
1:F:172:ASP:O	1:F:173:MET:C	2.59	0.43
1:F:184:ALA:HA	1:F:201:CYS:SG	2.58	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:264:MET:HE3	1:B:292:PRO:CA	2.46	0.43
1:B:400:ARG:HG3	1:B:400:ARG:NH1	2.30	0.43
1:C:44:GLN:C	1:C:46:ARG:H	2.26	0.43
1:D:323:CYS:O	1:D:345:ALA:HA	2.18	0.43
1:D:505:THR:C	1:E:150:ARG:HH12	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:CD	1:A:482:ARG:HH22	2.27	0.43
1:C:54:ARG:NH1	1:F:78:VAL:HG13	2.34	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:47:ASN:HD21	1:E:50:ARG:NH1	2.17	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
1:E:422:GLU:HB3	1:E:427:LYS:HB3	2.00	0.43
1:F:28:VAL:HG22	1:F:487:VAL:HG13	2.00	0.43
1:F:44:GLN:C	1:F:46:ARG:H	2.26	0.43
1:F:68:PRO:HA	1:F:78:VAL:HA	2.01	0.43
1:A:28:VAL:HG22	1:A:487:VAL:HG13	1.99	0.43
1:A:183:ILE:O	1:A:184:ALA:C	2.61	0.43
1:A:228:GLU:HA	1:A:231:ILE:HG22	2.00	0.43
1:A:317:SER:C	1:A:319:LEU:N	2.74	0.43
1:A:501:GLY:N	1:A:505:THR:HA	2.33	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: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:C:183:ILE:O	1:C:184:ALA:C	2.60	0.43
1:C:502:VAL:HG23	1:C:504:PHE:CD1	2.54	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:376:TYR:OH	1:A:465:ALA:HB2	2.18	0.43
1:A:436:PRO:HB3	1:A:440:PHE:CD1	2.53	0.43
1:A:496:VAL:O	1:B:209:GLN:NE2	2.47	0.43
1:B:51:GLY:O	1:B:55:ILE:HG13	2.19	0.43
1:B:143:ASN:HD21	1:E:70:ARG:HH12	1.67	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:D:264:MET:HE3	1:D:292:PRO:CA	2.47	0.43
1:E:42:GLU:C	1:E:44:GLN:H	2.27	0.43
1:E:325:ILE:HG22	1:E:347:ILE:CG2	2.48	0.43
1:F:325:ILE:HG22	1:F:347:ILE:CG2	2.49	0.43
1:A:151:ARG:NH2	1:E:504:PHE:CZ	2.86	0.43
1:A:284:ILE:HD13	1:A:308:PHE:HB3	2.00	0.43
1:A:299:LYS:O	1:A:299:LYS:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:GLU:HB3	1:B:427:LYS:HB3	2.01	0.43
1:B:494:PHE:CD2	1:B:494:PHE:C	2.97	0.43
1:C:504:PHE:HZ	1:F:151:ARG:NH2	2.10	0.43
1:D:69:ILE:HD13	1:D:148:ILE:CG1	2.49	0.43
1:E:291:ASP:HA	1:E:292:PRO:HD3	1.89	0.43
1:F:183:ILE:O	1:F:184:ALA:C	2.62	0.43
1:A:502:VAL:HG23	1:A:503:THR:N	2.28	0.43
1:A:503:THR:HG21	1:E:151:ARG:CD	2.48	0.43
1:A:504:PHE:HE1	1:E:70:ARG:CB	2.32	0.43
1:B:439:GLU:CD	1:B:439:GLU:H	2.26	0.43
1:C:32:LEU:HD21	1:C:494:PHE:CD1	2.54	0.43
1:C:36:LEU:HD11	1:C:474:LYS:HZ1	1.84	0.43
1:C:40:GLU:O	1:C:42:GLU:HG3	2.19	0.43
1:D:57:LYS:HB3	1:D:58:PRO:HD3	2.01	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:F:305:ILE:HG13	1:F:305:ILE:H	1.67	0.43
1:A:42:GLU:C	1:A:44:GLN:H	2.27	0.43
1:A:494:PHE:CD2	1:A:494:PHE:C	2.97	0.43
1:B:111:LEU:HA	1:B:111:LEU:HD23	1.83	0.43
1:B:170:ALA:CA	1:B:180:MET:HE2	2.49	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:D:172:ASP:O	1:D:173:MET:C	2.62	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:122:VAL:HA	1:B:464:SER:OG	2.19	0.42
1:B:305:ILE:HG13	1:B:305:ILE:H	1.68	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:47:ASN:O	1:D:50:ARG:HG2	2.19	0.42
1:D:144:GLU:O	1:D:148:ILE:HG13	2.19	0.42
1:D:170:ALA:CA	1:D:180:MET:HE2	2.49	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:HG13	1:F:435:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:HA	1:A:78:VAL:HA	2.00	0.42
1:A:77:GLU:HA	1:E:54:ARG:NH1	2.33	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
1:F:373:PRO:HD3	1:F:481:LEU:HB3	2.01	0.42
1:A:31:LYS:HA	1:A:34:GLU:HG2	2.01	0.42
1:A:57:LYS:HB3	1:A:58:PRO:HD3	2.00	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: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:B:144:GLU:O	1:B:148:ILE:HG13	2.19	0.42
1:C:69:ILE:HG23	1:C:79:ILE:HD13	2.00	0.42
1:C:111:LEU:HA	1:C:111:LEU:HD23	1.82	0.42
1:C:299:LYS:O	1:C:299:LYS:HG3	2.18	0.42
1:C:494:PHE:CD2	1:C:494:PHE:C	2.98	0.42
1:D:91:THR:CB	1:D:92:PRO:CD	2.94	0.42
1:D:435:VAL:HG13	1:D:435:VAL:O	2.20	0.42
1:E:349:ALA:HB1	1:E:377:LEU:CD2	2.49	0.42
1:F:31:LYS:HD3	1:F:35:ASP:OD2	2.19	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: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:32:LEU:HA	1:C:36:LEU:HD13	2.02	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:436:PRO:HB3	1:C:440:PHE:CD1	2.54	0.42
1:D:31:LYS:HA	1:D:34:GLU:HG2	2.02	0.42
1:D:349:ALA:HB1	1:D:377:LEU:CD2	2.50	0.42
1:D:502:VAL:HG23	1:D:504:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:425:PHE:C	1:E:427:LYS:H	2.28	0.42
1:F:40:GLU:O	1:F:42:GLU:HG3	2.20	0.42
1:F:299:LYS:O	1:F:299:LYS:HG3	2.19	0.42
1:F:424:LYS:HE3	1:F:424:LYS:HB3	1.87	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
1:C:380:GLY:HA2	1:C:457:LEU:HD21	2.00	0.42
1:C:457:LEU:CD2	1:C:461:MET:HG2	2.50	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:50:ARG:O	1:F:50:ARG:HG3	2.20	0.42
1:F:62:VAL:HG11	1:F:109:LYS:HZ3	1.84	0.42
1:F:502:VAL:HG23	1:F:504:PHE:CD1	2.54	0.42
1:A:72:ASP:CG	1:A:141:THR:HG21	2.44	0.42
1:A:150:ARG:HH22	1:F:505:THR:C	2.27	0.42
1:A:424:LYS:HE3	1:A:424:LYS:HB3	1.88	0.42
1:B:47:ASN:O	1:B:50:ARG:HG2	2.20	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:A:44:GLN:C	1:A:46:ARG:H	2.27	0.42
1:A:49:VAL:C	1:A:51:GLY:H	2.27	0.42
1:A:502:VAL:HG23	1:A:504:PHE:CD1	2.54	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:68:PRO:HA	1:C:78:VAL:HA	2.01	0.42
1:C:121:VAL:HG21	1:C:375:LEU:HG	2.02	0.42
1:C:144:GLU:O	1:C:148:ILE:HG13	2.20	0.42
1:D:205:LYS:NZ	1:D:392:ASN:HD21	2.18	0.42
1:E:44:GLN:C	1:E:46:ARG:H	2.28	0.42
1:E:277:VAL:HG21	1:E:295:LEU:HD22	1.99	0.42
1:E:421:LEU:HD12	1:E:421:LEU:HA	1.76	0.42
1:F:254:GLN:HE21	1:F:330:ALA:HB3	1.85	0.42
1:F:264:MET:HE3	1:F:292:PRO:CA	2.48	0.42
1:A:78:VAL:O	1:A:78:VAL:CG2	2.68	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:B:42:GLU:C	1:B:44:GLN:H	2.28	0.42
1:B:228:GLU:HA	1:B:231:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:VAL:HA	1:C:108:VAL:HG22	2.02	0.42
1:E:33:VAL:O	1:E:34:GLU:O	2.38	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: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: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:31:LYS:HD3	1:D:35:ASP:OD2	2.19	0.42
1:D:43:GLU:C	1:D:45:LYS:N	2.78	0.42
1:D:317:SER:C	1:D:319:LEU:N	2.73	0.42
1:D:319:LEU:HD23	1:D:335:LEU:HD23	2.02	0.42
1:E:136:ASN:OD1	1:E:136:ASN:C	2.63	0.42
1:F:105:VAL:HA	1:F:108:VAL:HG22	2.02	0.42
1:F:425:PHE:C	1:F:427:LYS:H	2.28	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:433:PRO:HA	1:F:420:SER:HB3	2.02	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: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:E:433:PRO:C	1:E:435:VAL:H	2.28	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:92:PRO:HG2	1:C:389:TRP:CZ2	2.55	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:D:86:HIS:HD2	1:D:87:SER:HB2	1.85	0.41
1:D:494:PHE:CD2	1:D:494:PHE:C	2.98	0.41
1:F:113:SER:O	1:F:114:LEU:C	2.63	0.41
1:F:136:ASN:OD1	1:F:136:ASN:C	2.63	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:A:113:SER:O	1:A:114:LEU:C	2.63	0.41
1:B:47:ASN:HD21	1:B:50:ARG:NH1	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ARG:NH1	1:D:78:VAL:HG13	2.35	0.41
1:B:118:LYS:HG3	1:B:375:LEU:O	2.20	0.41
1:B:425:PHE:C	1:B:427:LYS:H	2.28	0.41
1:D:40:GLU:O	1:D:42:GLU:HG3	2.20	0.41
1:D:136:ASN:OD1	1:D:136:ASN:C	2.63	0.41
1:E:31:LYS:HA	1:E:34:GLU:HG2	2.01	0.41
1:E:92:PRO:HG2	1:E:389:TRP:CZ2	2.55	0.41
1:E:502:VAL:HG23	1:E:503:THR:N	2.28	0.41
1:F:32:LEU:HA	1:F:36:LEU:HD13	2.02	0.41
1:A:47:ASN:O	1:A:50:ARG:HG2	2.20	0.41
1:A:284:ILE:CG2	1:A:311:ALA:HB1	2.48	0.41
1:B:57:LYS:HB3	1:B:58:PRO:HD3	2.01	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: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:312:LYS:O	1:C:314:TYR:N	2.53	0.41
1:D:425:PHE:C	1:D:427:LYS:H	2.29	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:E:251:PHE:CE1	1:E:267:LEU:HB3	2.55	0.41
1:E:318:ILE:H	1:E:318:ILE:CD1	2.29	0.41
1:F:433:PRO:C	1:F:435:VAL:H	2.27	0.41
1:C:228:GLU:HA	1:C:231:ILE:HG22	2.02	0.41
1:C:425:PHE:C	1:C:427:LYS:H	2.29	0.41
1:D:113:SER:O	1:D:114:LEU:C	2.63	0.41
1:D:301:GLN:O	1:D:301:GLN:HG2	2.19	0.41
1:E:32:LEU:HA	1:E:36:LEU:HD13	2.02	0.41
1:E:43:GLU:C	1:E:45:LYS:N	2.77	0.41
1:E:149:THR:HG21	1:E:179:GLU:HG3	2.02	0.41
1:E:301:GLN:O	1:E:301:GLN:HG2	2.20	0.41
1:A:32:LEU:HA	1:A:36:LEU:HD13	2.02	0.41
1:A:62:VAL:HG11	1:A:109:LYS:HZ2	1.84	0.41
1:A:86:HIS:HD2	1:A:87:SER:HB2	1.84	0.41
1:B:40:GLU:O	1:B:42:GLU:HG3	2.21	0.41
1:B:118:LYS:HG3	1:B:379:ALA:HB2	2.02	0.41
1:B:134:LYS:HE3	1:B:134:LYS:HB2	1.94	0.41
1:B:390:LEU:O	1:B:391:LYS:C	2.60	0.41
1:D:402:THR:O	1:D:403:PHE:C	2.64	0.41
1:F:33:VAL:O	1:F:34:GLU:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ALA:CA	1:A:180:MET:HE2	2.50	0.41
1:A:400:ARG:HG3	1:A:400:ARG:NH1	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:47:ASN:O	1:C:50:ARG:HG2	2.21	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:D:12:ASN:HD21	1:D:14:PHE:HB3	1.86	0.41
1:D:505:THR:C	1:E:150:ARG:HH22	2.29	0.41
1:E:57:LYS:HB3	1:E:58:PRO:HD3	2.02	0.41
1:E:118:LYS:HG3	1:E:375:LEU:O	2.21	0.41
1:E:281:ASP:HB2	1:E:282:GLY:H	1.56	0.41
1:E:474:LYS:HD3	1:E:475:TYR:HE2	1.83	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:A:136:ASN:OD1	1:A:136:ASN:C	2.63	0.41
1:B:119:CYS:SG	1:B:382:VAL:HG11	2.60	0.41
1:B:349:ALA:HB1	1:B:377:LEU:CD2	2.51	0.41
1:C:33:VAL:O	1:C:34:GLU:O	2.38	0.41
1:C:217:SER:O	1:C:218:ALA:C	2.64	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:D:86:HIS:CG	1:D:116:THR:HG21	2.55	0.41
1:F:72:ASP:CG	1:F:141:THR:HG21	2.46	0.41
1:F:339:ASN:H	1:F:339:ASN:HD22	1.66	0.41
1:A:69:ILE:HG23	1:A:79:ILE:HD13	2.02	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:B:136:ASN:OD1	1:B:136:ASN:C	2.63	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:212:ILE:HD11	1:C:398:TYR:CE1	2.56	0.41
1:C:377:LEU:HD12	1:C:377:LEU:HA	1.93	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:72:ASP:CG	1:E:141:THR:HG21	2.46	0.41
1:F:42:GLU:C	1:F:44:GLN:H	2.28	0.41
1:F:47:ASN:O	1:F:50:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:494:PHE:CD2	1:F:494:PHE:C	2.98	0.41
1:A:144:GLU:O	1:A:148:ILE:HG13	2.21	0.41
1:B:205:LYS:HZ3	1:B:392:ASN:HD21	1.69	0.41
1:B:233:GLU:HG2	1:B:236:TYR:CD1	2.56	0.41
1:B:318:ILE:H	1:B:318:ILE:CD1	2.28	0.41
1:B:424:LYS:O	1:B:425:PHE:HB2	2.21	0.41
1:C:42:GLU:C	1:C:44:GLN:H	2.28	0.41
1:C:221:ARG:CD	1:C:454:HIS:CG	3.04	0.41
1:C:237:MET:HE2	1:C:237:MET:N	2.36	0.41
1:C:424:LYS:HE3	1:C:424:LYS:HB3	1.87	0.41
1:C:485:ALA:O	1:C:488:ASN:HB3	2.21	0.41
1:D:42:GLU:C	1:D:44:GLN:H	2.28	0.41
1:D:284:ILE:CG2	1:D:285:TRP:N	2.83	0.41
1:D:478:GLY:C	1:D:480:ASP:H	2.28	0.41
1:D:485:ALA:O	1:D:488:ASN:HB3	2.21	0.41
1:E:40:GLU:O	1:E:42:GLU:HG3	2.20	0.41
1:E:50:ARG:O	1:E:50:ARG:HG3	2.21	0.41
1:E:156:LEU:HB3	1:E:162:ILE:HB	2.03	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:O	1:A:301:GLN:HG2	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:31:LYS:HB2	1:C:475:TYR:HE1	1.86	0.41
1:C:136:ASN:OD1	1:C:138:LYS:N	2.51	0.41
1:C:478:GLY:C	1:C:480:ASP:H	2.27	0.41
1:D:38:THR:CG2	1:D:41:SER:HB3	2.40	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: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:170:ALA:CA	1:F:180:MET:HE2	2.50	0.41
1:F:285:TRP:NE1	1:F:287:PRO:HG3	2.36	0.41
1:F:463:ARG:HE	1:F:463:ARG:HB3	1.72	0.41
1:A:70:ARG:CB	1:E:504:PHE:CE1	3.04	0.40
1:A:319:LEU:H	1:A:319:LEU:CD1	2.34	0.40
1:C:23:ARG:NE	1:C:27:ILE:HD11	2.30	0.40
1:C:243:THR:O	1:C:243:THR:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ARG:NE	1:D:27:ILE:HD11	2.30	0.40
1:D:72:ASP:CG	1:D:141:THR:HG21	2.45	0.40
1:D:119:CYS:SG	1:D:382:VAL:HG11	2.61	0.40
1:D:319:LEU:CD1	1:D:319:LEU:H	2.33	0.40
1:E:170:ALA:CA	1:E:180:MET:HE2	2.52	0.40
1:E:372:ILE:HA	1:E:373:PRO:HD3	1.64	0.40
1:E:494:PHE:CD2	1:E:494:PHE:C	2.98	0.40
1:F:43:GLU:C	1:F:45:LYS:N	2.78	0.40
1:F:69:ILE:HG21	1:F:148:ILE:HG12	2.03	0.40
1:F:91:THR:HB	1:F:92:PRO:CD	2.51	0.40
1:F:190:THR:HG22	1:F:191:ILE:HG12	2.03	0.40
1:A:425:PHE:C	1:A:427:LYS:H	2.29	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:C:233:GLU:HG2	1:C:236:TYR:CD1	2.55	0.40
1:C:504:PHE:CE1	1:F:70:ARG:CB	3.05	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:A:40:GLU:O	1:A:42:GLU:HG3	2.20	0.40
1:A:163:GLY:O	1:A:167:ASP:O	2.39	0.40
1:B:284:ILE:CG2	1:B:311:ALA:HB1	2.47	0.40
1:C:69:ILE:HG12	1:C:79:ILE:HD11	2.03	0.40
1:C:136:ASN:OD1	1:C:136:ASN:C	2.64	0.40
1:C:205:LYS:HD2	1:C:209:GLN:O	2.21	0.40
1:D:68:PRO:HA	1:D:78:VAL:HA	2.03	0.40
1:D:500:ALA:HB1	1:D:505:THR:OXT	2.21	0.40
1:E:309:PRO:O	1:E:310:LYS:HB2	2.22	0.40
1:E:319:LEU:CD1	1:E:319:LEU:H	2.34	0.40
1:F:63:LEU:HD22	1:F:161:PHE:CE2	2.55	0.40
1:A:264:MET:HE3	1:A:292:PRO:CA	2.47	0.40
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:91:THR:O	1:B:92:PRO:C	2.63	0.40
1:B:505:THR:C	1:F:150:ARG:HH22	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:391:LYS:NZ	1:F:449:GLU:OE1	2.50	0.40
1:A:50:ARG:O	1:A:50:ARG:HG3	2.22	0.40
1:A:69:ILE:HG12	1:A:79:ILE:HD11	2.04	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:B:243:THR:O	1:B:243:THR:CG2	2.70	0.40
1:B:257:GLY:O	1:B:259:VAL:N	2.55	0.40
1:B:402:THR:O	1:B:403:PHE:C	2.64	0.40
1:C:43:GLU:C	1:C:45:LYS:N	2.78	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
1:F:478:GLY:C	1:F:480:ASP:H	2.29	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%)	2	5
1	B	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	2	5
1	C	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	2	5
1	D	494/505 (98%)	426 (86%)	49 (10%)	19 (4%)	2	5
1	E	494/505 (98%)	425 (86%)	50 (10%)	19 (4%)	2	5
1	F	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	2	5
All	All	2964/3030 (98%)	2563 (86%)	287 (10%)	114 (4%)	2	5

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	362 (88%)	51 (12%)	4	12
1	B	413/420 (98%)	363 (88%)	50 (12%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	413/420 (98%)	361 (87%)	52 (13%)	4	11
1	D	413/420 (98%)	361 (87%)	52 (13%)	4	11
1	E	413/420 (98%)	363 (88%)	50 (12%)	5	12
1	F	413/420 (98%)	363 (88%)	50 (12%)	5	12
All	All	2478/2520 (98%)	2173 (88%)	305 (12%)	4	12

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	31	LYS
1	A	36	LEU
1	A	37	ARG
1	A	44	GLN
1	A	46	ARG
1	A	59	CYS
1	A	62	VAL
1	A	64	SER
1	A	68	PRO
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	221	ARG
1	A	235	SER
1	A	243	THR
1	A	253	VAL
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
1	A	318	ILE
1	A	320	GLU
1	A	325	ILE

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Mol	Chain	Res	Type
1	A	326	LEU
1	A	327	ILE
1	A	334	GLN
1	A	337	LYS
1	A	339	ASN
1	A	365	LEU
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	B	13	PHE
1	B	31	LYS
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	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	221	ARG
1	B	235	SER
1	B	243	THR
1	B	253	VAL
1	B	259	VAL
1	B	261	LEU
1	B	267	LEU

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Mol	Chain	Res	Type
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	327	ILE
1	B	334	GLN
1	B	337	LYS
1	B	339	ASN
1	B	365	LEU
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	457	LEU
1	B	471	THR
1	B	476	ASN
1	B	481	LEU
1	B	499	GLU
1	C	13	PHE
1	C	31	LYS
1	C	36	LEU
1	C	37	ARG
1	C	44	GLN
1	C	46	ARG
1	C	59	CYS
1	C	62	VAL
1	C	64	SER
1	C	68	PRO
1	C	101	THR
1	C	116	THR
1	C	141	THR
1	C	156	LEU
1	C	162	ILE

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Mol	Chain	Res	Type
1	C	180	MET
1	C	219	THR
1	C	221	ARG
1	C	235	SER
1	C	243	THR
1	C	253	VAL
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	327	ILE
1	C	334	GLN
1	C	337	LYS
1	C	339	ASN
1	C	353	ASN
1	C	365	LEU
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	D	13	PHE
1	D	31	LYS
1	D	36	LEU
1	D	37	ARG
1	D	44	GLN

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Mol	Chain	Res	Type
1	D	46	ARG
1	D	59	CYS
1	D	62	VAL
1	D	64	SER
1	D	68	PRO
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	221	ARG
1	D	235	SER
1	D	243	THR
1	D	253	VAL
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	327	ILE
1	D	334	GLN
1	D	337	LYS
1	D	339	ASN
1	D	353	ASN
1	D	365	LEU
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

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Mol	Chain	Res	Type
1	D	457	LEU
1	D	471	THR
1	D	476	ASN
1	D	481	LEU
1	D	499	GLU
1	E	13	PHE
1	E	31	LYS
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	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	221	ARG
1	E	235	SER
1	E	243	THR
1	E	253	VAL
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	327	ILE
1	E	334	GLN
1	E	337	LYS
1	E	339	ASN
1	E	365	LEU

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Mol	Chain	Res	Type
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
1	E	471	THR
1	E	476	ASN
1	E	481	LEU
1	E	499	GLU
1	F	13	PHE
1	F	31	LYS
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	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	221	ARG
1	F	235	SER
1	F	243	THR
1	F	253	VAL
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

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Mol	Chain	Res	Type
1	F	320	GLU
1	F	325	ILE
1	F	326	LEU
1	F	327	ILE
1	F	334	GLN
1	F	337	LYS
1	F	339	ASN
1	F	365	LEU
1	F	378	ASN
1	F	396	VAL
1	F	400	ARG
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	60	ASN
1	A	61	HIS
1	A	86	HIS
1	A	143	ASN
1	A	209	GLN
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	467	GLN
1	A	476	ASN
1	A	488	ASN

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Mol	Chain	Res	Type
1	A	498	ASN
1	B	47	ASN
1	B	60	ASN
1	B	61	HIS
1	B	86	HIS
1	B	143	ASN
1	B	268	HIS
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
1	C	47	ASN
1	C	60	ASN
1	C	61	HIS
1	C	86	HIS
1	C	143	ASN
1	C	268	HIS
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	467	GLN
1	C	488	ASN
1	C	498	ASN
1	D	47	ASN
1	D	60	ASN
1	D	61	HIS
1	D	86	HIS
1	D	143	ASN
1	D	268	HIS
1	D	302	HIS
1	D	339	ASN

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Mol	Chain	Res	Type
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	467	GLN
1	D	488	ASN
1	D	498	ASN
1	E	47	ASN
1	E	60	ASN
1	E	61	HIS
1	E	86	HIS
1	E	143	ASN
1	E	209	GLN
1	E	268	HIS
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	467	GLN
1	E	488	ASN
1	E	498	ASN
1	F	47	ASN
1	F	60	ASN
1	F	61	HIS
1	F	86	HIS
1	F	143	ASN
1	F	209	GLN
1	F	268	HIS
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

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Mol	Chain	Res	Type
1	F	467	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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.