



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:54 PM GMT

PDB ID : 1HMY
Title : THE STRUCTURE OF UNLIGANDED REVERSE TRANSCRIPTASE
FROM THE HUMAN IMMUNODEFICIENCY VIRUS TYPE 1
Authors : Rodgers, D.W.; Gamblin, S.J.; Harris, B.A.; Ray, S.; Culp, J.S.; Hellmig, B.;
Woolf, D.J.; Debouck, C.; Harrison, S.C.
Deposited on : 1994-12-15
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

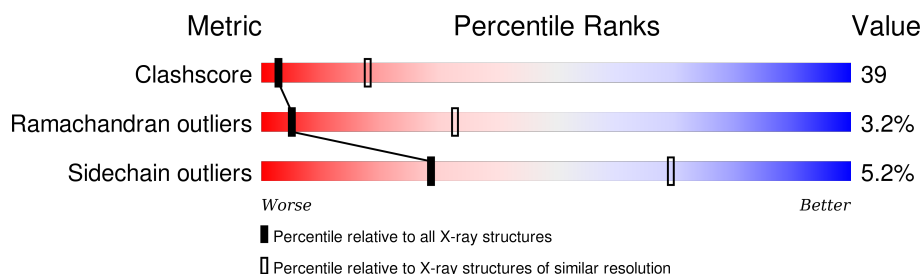
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)


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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
1	C	560	
1	E	560	
1	G	560	
2	B	440	
2	D	440	
2	F	440	

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Mol	Chain	Length	Quality of chain
2	H	440	 A horizontal bar chart showing the quality of chain H. The bar is divided into four segments: green (39%), yellow (45%), orange (10%), and red (6%). The percentages 39%, 45%, and 10% are labeled below the bar. The red segment is the smallest and is followed by a small gap and then the 10% label.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29596 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 HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			
1	C	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			
1	E	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			
1	G	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			
2	D	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			
2	F	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			
2	H	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			

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

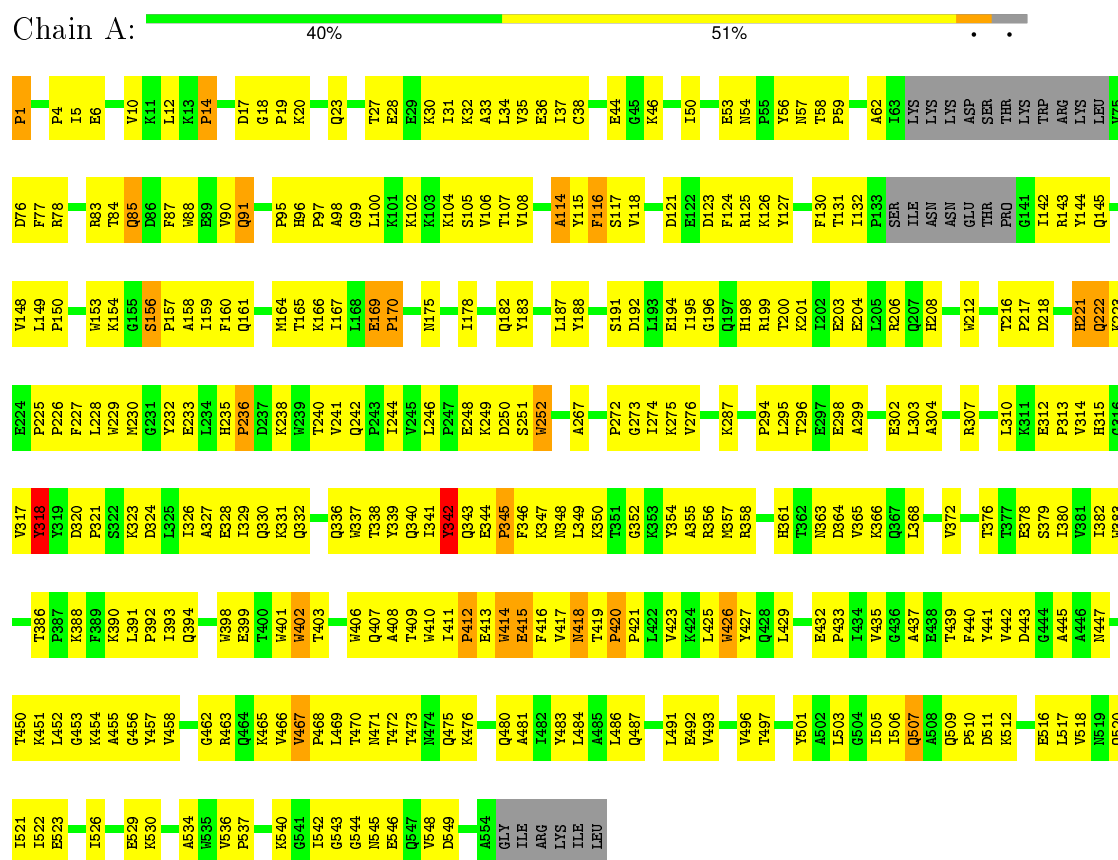
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

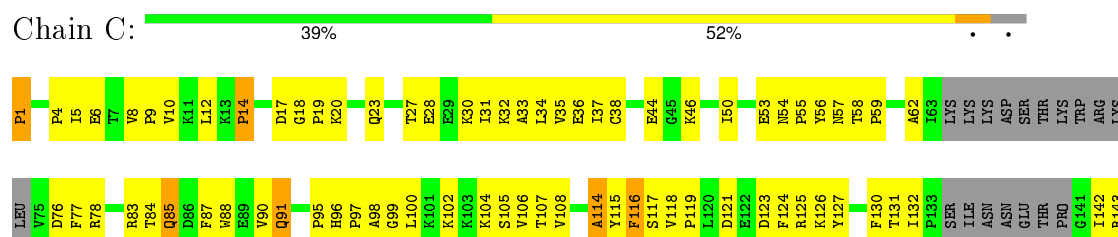
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

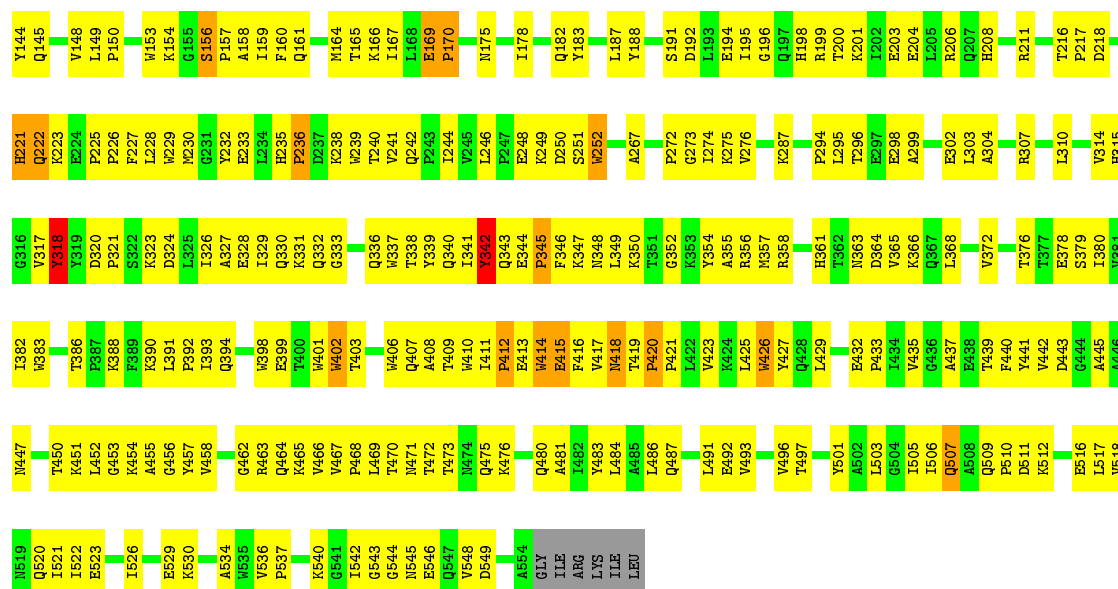
Note EDS was not executed.

• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)



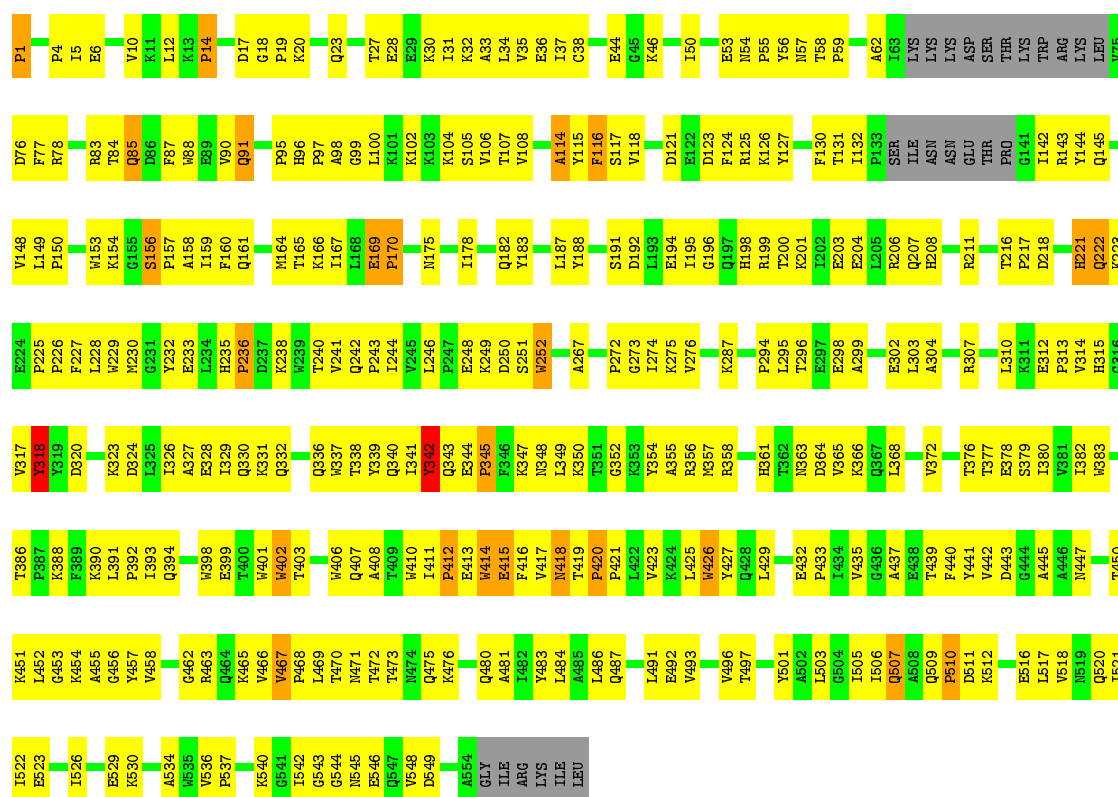
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)





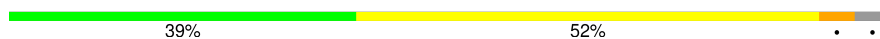
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

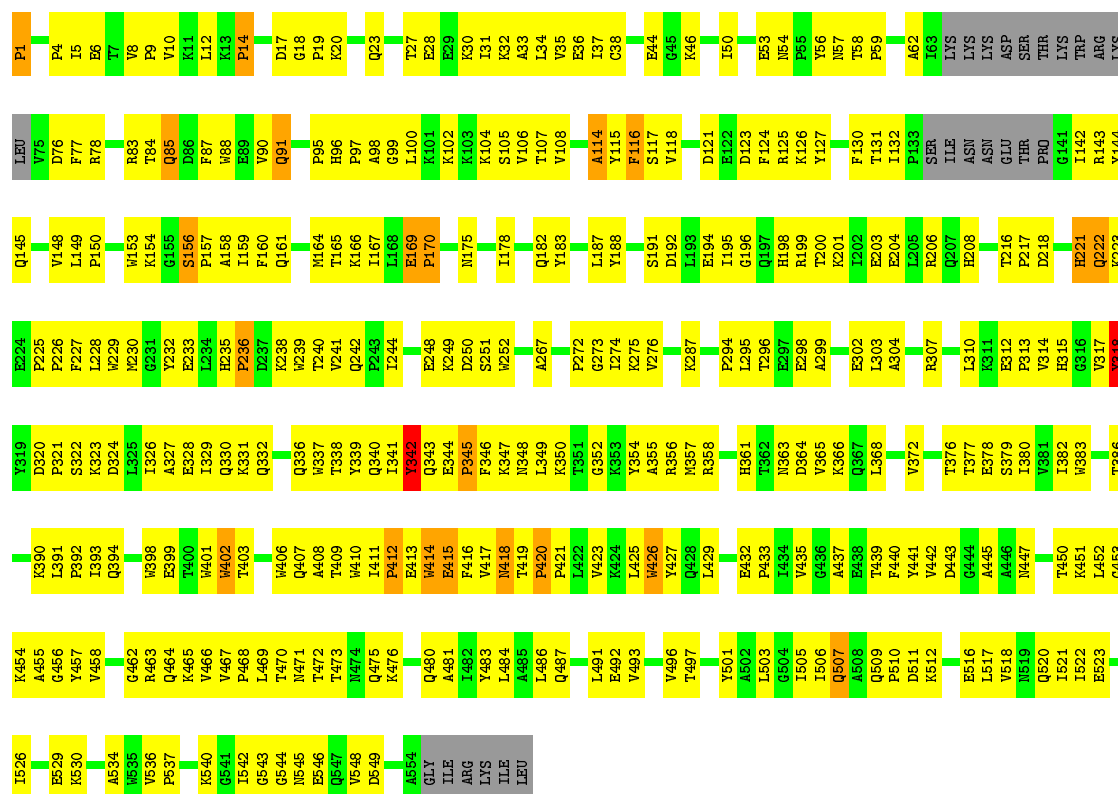
Chain E:



- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

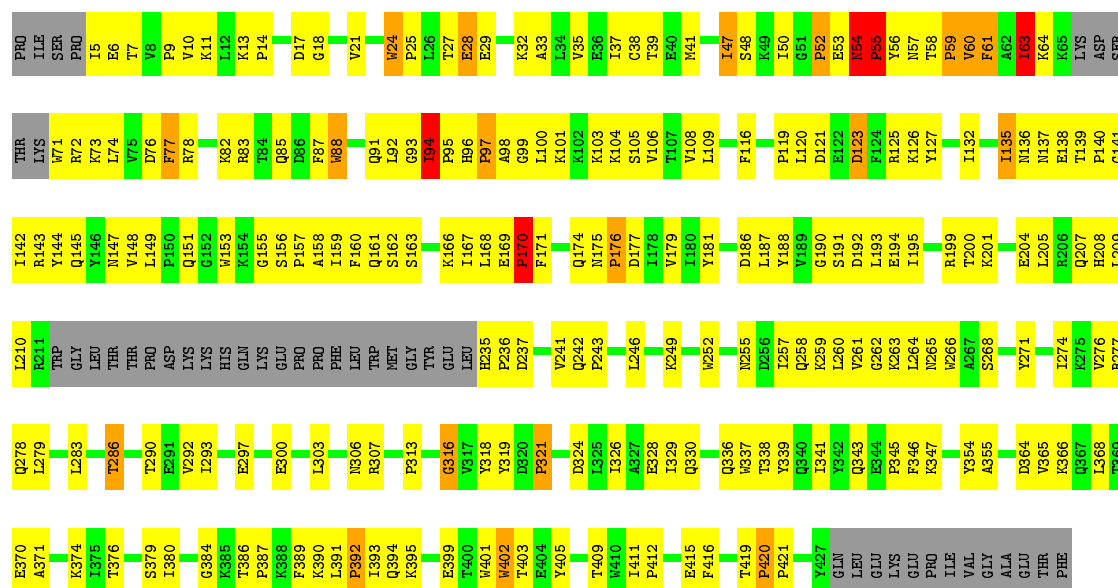
Chain G:





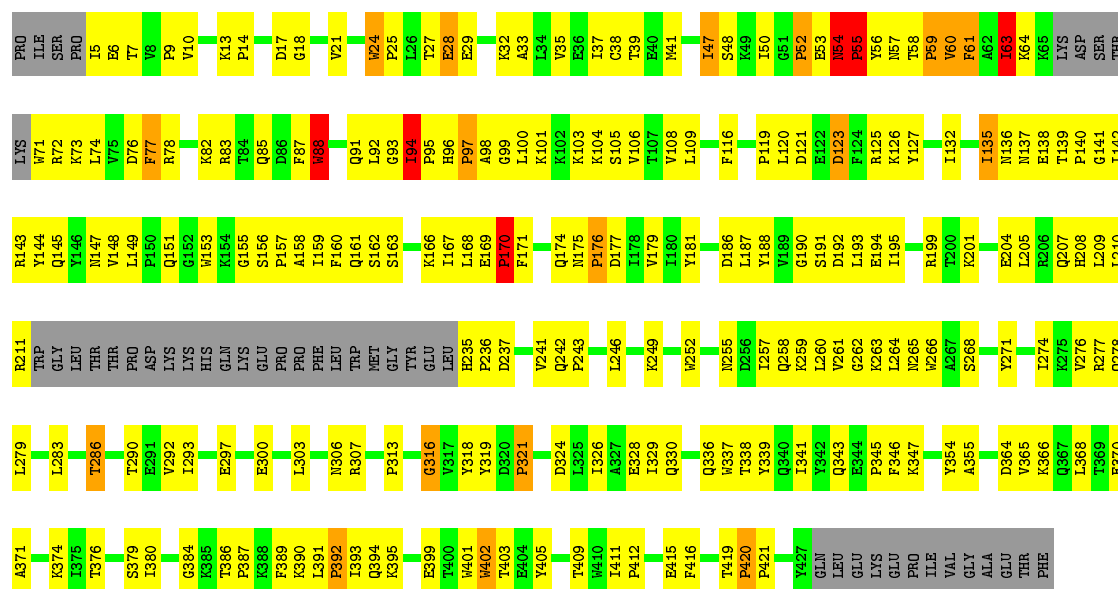
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain B: 39% 45% 10%



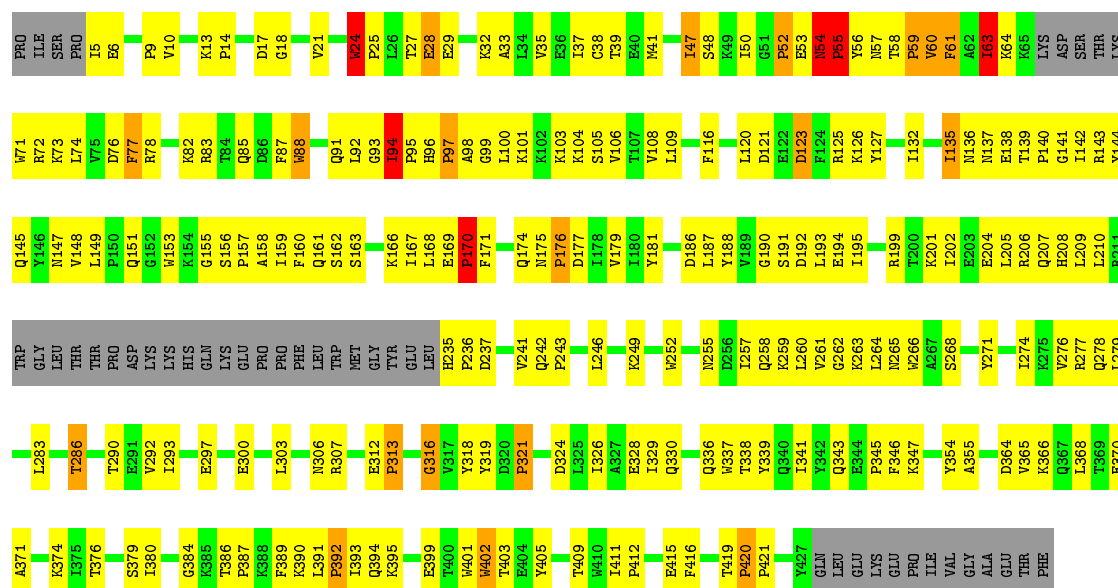
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain D: 40% 45% 10%



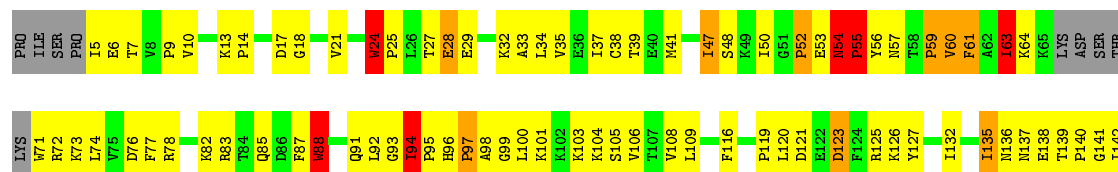
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain F: 40% 45% 10%



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain H: 39% 45% 10%



A371	L279	R211	R143
K374	L283	TRP	Y144
T376	T286	GLY	Q145
S379	T290	LEU	Y146
I380	E291	THR	N147
K384	V292	PRO	V148
T386	I293	ASP	L149
P387	E297	LYS	F150
K388	E300	HIS	Q151
F389	L303	GLN	G152
K390	N306	LYS	W153
L391	R307	GLN	K154
P392	P313	LYS	G155
I393	G316	GLU	S156
Q394	V317	PRO	P157
K395	Y318	PRO	A158
E399	Y319	PHE	I159
T400	D320	LEU	F160
W401	P321	TRP	Q161
W402	D324	MET	S162
T403	L325	GLY	S163
E404	I326	TYR	K166
Y405	A327	LEU	I167
T409	E328	H235	L168
W410	I329	P236	E169
I411	Q330	D237	F170
P412	Q336	V241	F171
E415	W337	Q242	Q174
F416	T338	P243	N175
T419	Y339	P246	P176
P420	I341	L246	D177
P421	Q340	K249	I178
Y427	Y342	W252	V179
GLN	Q343	N255	I180
LEU	E344	D256	Y181
GLU	P345	I257	D186
LYS	F346	Q258	L187
GLU	K347	K259	Y188
PRO	Y354	L260	V189
ILE	A355	V261	G190
VAL	D364	K262	S191
GLY	V365	L264	D192
ALA	K366	N265	L193
GLU	Q367	W266	E194
THR	L368	A267	I195
PHE	T369	S268	R199
	E370	Y271	T200
		I274	K201
		K275	E204
		V276	L205
		R277	Q206
		Q278	Q207
			H208
			L209
			L210

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.70 Å 162.80 Å 331.80 Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.254 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29596	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.71	1/4307 (0.0%)	0.98	5/5865 (0.1%)
1	C	0.71	1/4307 (0.0%)	0.98	4/5865 (0.1%)
1	E	0.71	1/4307 (0.0%)	0.98	5/5865 (0.1%)
1	G	0.71	1/4307 (0.0%)	0.98	4/5865 (0.1%)
2	B	0.74	0/3285	1.02	5/4466 (0.1%)
2	D	0.74	0/3285	1.02	5/4466 (0.1%)
2	F	0.74	1/3285 (0.0%)	1.02	5/4466 (0.1%)
2	H	0.74	1/3285 (0.0%)	1.02	5/4466 (0.1%)
All	All	0.72	6/30368 (0.0%)	0.99	38/41324 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	E	0	2
1	G	0	2
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	GLN	C-O	5.35	1.33	1.23
1	A	222	GLN	C-O	5.33	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	222	GLN	C-O	5.32	1.33	1.23
1	E	222	GLN	C-O	5.32	1.33	1.23
2	F	24	TRP	CB-CG	-5.02	1.41	1.50
2	H	24	TRP	CB-CG	-5.01	1.41	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	94	ILE	C-N-CD	7.79	144.77	128.40
2	F	94	ILE	C-N-CD	7.77	144.72	128.40
2	B	94	ILE	C-N-CD	7.77	144.71	128.40
2	D	94	ILE	C-N-CD	7.76	144.69	128.40
2	D	54	ASN	C-N-CD	-7.01	105.17	120.60
2	H	54	ASN	C-N-CD	-7.01	105.18	120.60
2	B	54	ASN	C-N-CD	-7.01	105.18	120.60
2	F	54	ASN	C-N-CD	-7.00	105.20	120.60
2	H	60	VAL	CB-CA-C	-6.46	99.12	111.40
2	F	60	VAL	CB-CA-C	-6.45	99.14	111.40
2	B	60	VAL	CB-CA-C	-6.45	99.15	111.40
2	D	60	VAL	CB-CA-C	-6.44	99.17	111.40
1	A	221	HIS	C-N-CA	6.11	136.97	121.70
1	E	221	HIS	C-N-CA	6.11	136.96	121.70
1	G	221	HIS	C-N-CA	6.10	136.95	121.70
1	C	221	HIS	C-N-CA	6.10	136.95	121.70
2	F	47	ILE	CB-CA-C	-5.61	100.39	111.60
1	G	294	PRO	N-CA-CB	5.60	110.02	103.30
2	H	47	ILE	CB-CA-C	-5.59	100.43	111.60
2	B	47	ILE	CB-CA-C	-5.58	100.43	111.60
2	D	47	ILE	CB-CA-C	-5.58	100.44	111.60
1	E	294	PRO	N-CA-CB	5.57	109.99	103.30
1	A	294	PRO	N-CA-CB	5.57	109.98	103.30
1	C	294	PRO	N-CA-CB	5.56	109.98	103.30
1	A	272	PRO	N-CA-CB	5.54	109.94	103.30
1	E	272	PRO	N-CA-CB	5.54	109.94	103.30
1	C	272	PRO	N-CA-CB	5.53	109.93	103.30
1	G	272	PRO	N-CA-CB	5.51	109.91	103.30
1	A	222	GLN	CA-C-N	5.42	129.11	117.20
1	C	222	GLN	CA-C-N	5.41	129.11	117.20
1	E	222	GLN	CA-C-N	5.40	129.09	117.20
1	G	222	GLN	CA-C-N	5.40	129.08	117.20
2	D	63	ILE	N-CA-C	-5.15	97.09	111.00
2	F	63	ILE	N-CA-C	-5.14	97.12	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	ILE	N-CA-C	-5.13	97.14	111.00
2	H	63	ILE	N-CA-C	-5.13	97.15	111.00
1	A	467	VAL	CB-CA-C	-5.00	101.89	111.40
1	E	467	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	TYR	Sidechain
1	A	342	TYR	Sidechain
2	B	61	PHE	Sidechain
1	C	318	TYR	Sidechain
1	C	342	TYR	Sidechain
2	D	61	PHE	Sidechain
1	E	318	TYR	Sidechain
1	E	342	TYR	Sidechain
2	F	61	PHE	Sidechain
1	G	318	TYR	Sidechain
1	G	342	TYR	Sidechain
2	H	61	PHE	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4200	0	4064	338	2
1	C	4200	0	4064	405	24
1	E	4200	0	4064	342	2
1	G	4200	0	4064	401	8
2	B	3198	0	3184	242	4
2	D	3198	0	3184	241	8
2	F	3198	0	3184	245	0
2	H	3198	0	3184	242	20
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
All	All	29596	0	28992	2306	34

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

All (2306) 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:345:PRO:HG3	1:G:326:ILE:CD1	1.22	1.68
1:C:346:PHE:CD1	1:G:390:LYS:CE	1.87	1.58
1:C:345:PRO:CG	1:G:326:ILE:CD1	1.79	1.54
1:C:346:PHE:CD1	1:G:390:LYS:HE3	0.98	1.51
1:C:346:PHE:CE1	1:G:390:LYS:HG3	1.60	1.36
1:C:346:PHE:HB2	1:G:390:LYS:NZ	1.46	1.28
1:C:417:VAL:HG11	1:G:346:PHE:CE2	1.67	1.27
1:C:417:VAL:CG1	1:G:346:PHE:CE2	2.19	1.25
1:C:345:PRO:CG	1:G:326:ILE:HD12	1.49	1.21
1:C:345:PRO:CG	1:G:326:ILE:HD13	1.56	1.12
1:C:345:PRO:HG2	1:G:326:ILE:CD1	1.70	1.11
1:C:346:PHE:CE1	1:G:390:LYS:HE3	1.89	1.07
1:C:345:PRO:HG2	1:G:326:ILE:HD13	1.23	1.07
1:E:393:ILE:HG23	1:E:414:TRP:CH2	1.93	1.04
1:C:393:ILE:HG23	1:C:414:TRP:CH2	1.93	1.03
1:G:393:ILE:HG23	1:G:414:TRP:CH2	1.93	1.03
1:A:393:ILE:HG23	1:A:414:TRP:CH2	1.93	1.02
2:B:264:LEU:HD22	2:B:274:ILE:HD11	1.42	1.02
2:D:264:LEU:HD22	2:D:274:ILE:HD11	1.42	1.02
2:H:264:LEU:HD22	2:H:274:ILE:HD11	1.42	1.02
2:F:264:LEU:HD22	2:F:274:ILE:HD11	1.42	1.02
1:G:540:LYS:HZ1	2:H:265:ASN:HB2	1.24	1.01
1:C:346:PHE:CZ	1:G:390:LYS:HG3	1.95	1.00
1:C:346:PHE:CB	1:G:390:LYS:NZ	2.24	1.00
1:C:417:VAL:HG13	1:G:346:PHE:CE2	1.97	1.00
1:C:376:THR:HG23	1:C:386:THR:HG23	1.43	0.99
1:A:376:THR:HG23	1:A:386:THR:HG23	1.43	0.99
1:C:346:PHE:CG	1:G:390:LYS:CE	2.47	0.98
1:C:346:PHE:CE1	1:G:390:LYS:CG	2.46	0.98
1:A:540:LYS:HZ1	2:B:265:ASN:HB2	1.30	0.97
1:G:376:THR:HG23	1:G:386:THR:HG23	1.43	0.97
1:C:346:PHE:HB2	1:G:390:LYS:HZ2	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:376:THR:HG23	1:E:386:THR:HG23	1.43	0.97
1:G:420:PRO:HG2	1:G:421:PRO:HD2	1.47	0.95
2:H:103:LYS:HZ2	2:H:179:VAL:H	1.15	0.94
1:C:417:VAL:HG13	1:G:346:PHE:CD2	2.02	0.94
2:D:103:LYS:HZ2	2:D:179:VAL:H	1.15	0.94
1:E:420:PRO:HG2	1:E:421:PRO:HD2	1.47	0.94
1:C:342:TYR:OH	1:G:345:PRO:HG3	1.68	0.94
2:B:103:LYS:HZ2	2:B:179:VAL:H	1.15	0.93
1:C:420:PRO:HG2	1:C:421:PRO:HD2	1.47	0.93
1:A:420:PRO:HG2	1:A:421:PRO:HD2	1.47	0.93
1:C:417:VAL:HG11	1:G:346:PHE:CZ	2.03	0.92
1:C:346:PHE:CE1	1:G:342:TYR:OH	2.22	0.92
2:F:50:ILE:HG21	2:F:145:GLN:HB2	1.49	0.92
2:H:50:ILE:HG21	2:H:145:GLN:HB2	1.49	0.92
2:D:50:ILE:HG21	2:D:145:GLN:HB2	1.49	0.91
1:A:540:LYS:NZ	2:B:265:ASN:HB2	1.86	0.91
1:G:540:LYS:NZ	2:H:265:ASN:HB2	1.86	0.91
2:B:50:ILE:HG21	2:B:145:GLN:HB2	1.49	0.91
1:C:540:LYS:NZ	2:D:265:ASN:HB2	1.86	0.91
1:C:346:PHE:HE1	1:G:342:TYR:OH	1.53	0.90
1:C:346:PHE:HB2	1:G:390:LYS:HZ1	1.10	0.90
1:C:346:PHE:CB	1:G:390:LYS:HZ2	1.83	0.90
2:H:260:LEU:HD21	2:H:303:LEU:HD21	1.53	0.90
1:E:540:LYS:NZ	2:F:265:ASN:HB2	1.86	0.89
1:C:107:THR:HG23	1:C:198:HIS:HE1	1.38	0.89
1:A:107:THR:HG23	1:A:198:HIS:HE1	1.38	0.89
1:G:107:THR:HG23	1:G:198:HIS:HE1	1.38	0.89
2:D:260:LEU:HD21	2:D:303:LEU:HD21	1.54	0.89
2:F:103:LYS:HZ2	2:F:179:VAL:H	1.19	0.88
2:B:260:LEU:HD21	2:B:303:LEU:HD21	1.54	0.88
1:E:107:THR:HG23	1:E:198:HIS:HE1	1.38	0.88
2:F:260:LEU:HD21	2:F:303:LEU:HD21	1.54	0.87
2:F:104:LYS:HB3	2:F:192:ASP:HA	1.55	0.87
2:H:104:LYS:HB3	2:H:192:ASP:HA	1.55	0.86
1:C:346:PHE:CD1	1:G:390:LYS:CD	2.57	0.86
1:C:540:LYS:HZ1	2:D:265:ASN:HB2	1.40	0.86
1:G:244:ILE:HD12	1:G:267:ALA:HB2	1.56	0.86
1:C:244:ILE:HD12	1:C:267:ALA:HB2	1.56	0.86
2:H:171:PHE:HE2	2:H:204:GLU:HB2	1.41	0.86
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.58	0.86
1:C:317:VAL:HG21	1:C:347:LYS:HB3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:PHE:HE2	2:F:204:GLU:HB2	1.41	0.86
1:G:317:VAL:HG21	1:G:347:LYS:HB3	1.58	0.85
2:D:104:LYS:HB3	2:D:192:ASP:HA	1.55	0.85
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.55	0.85
1:E:317:VAL:HG21	1:E:347:LYS:HB3	1.58	0.85
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.56	0.84
2:F:365:VAL:HG11	2:F:401:TRP:HB2	1.59	0.84
1:E:244:ILE:HD12	1:E:267:ALA:HB2	1.56	0.84
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.59	0.84
1:C:417:VAL:CG1	1:G:346:PHE:CD2	2.59	0.84
1:E:391:LEU:HB2	1:E:414:TRP:CZ3	2.13	0.84
1:C:342:TYR:OH	1:G:345:PRO:CB	2.26	0.84
1:E:540:LYS:HZ1	2:F:265:ASN:HB2	1.37	0.83
2:D:171:PHE:HE2	2:D:204:GLU:HB2	1.41	0.83
2:B:171:PHE:HE2	2:B:204:GLU:HB2	1.41	0.83
1:G:391:LEU:HB2	1:G:414:TRP:CZ3	2.13	0.83
1:A:391:LEU:HB2	1:A:414:TRP:CZ3	2.13	0.83
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.59	0.83
2:H:365:VAL:HG11	2:H:401:TRP:HB2	1.59	0.82
2:B:24:TRP:CH2	2:B:61:PHE:CD1	2.68	0.82
1:C:391:LEU:HB2	1:C:414:TRP:CZ3	2.13	0.82
2:D:24:TRP:CH2	2:D:61:PHE:CD1	2.68	0.82
1:C:342:TYR:OH	1:G:345:PRO:CG	2.26	0.82
2:H:61:PHE:CZ	2:H:74:LEU:HD23	2.14	0.82
2:D:61:PHE:CZ	2:D:74:LEU:HD23	2.14	0.82
2:F:61:PHE:CZ	2:F:74:LEU:HD23	2.14	0.82
1:G:326:ILE:HB	1:G:342:TYR:CE1	2.15	0.82
1:C:326:ILE:HB	1:C:342:TYR:CE1	2.15	0.82
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.15	0.82
2:F:33:ALA:O	2:F:37:ILE:HG13	1.80	0.82
2:D:33:ALA:O	2:D:37:ILE:HG13	1.80	0.82
2:B:33:ALA:O	2:B:37:ILE:HG13	1.80	0.81
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.14	0.81
2:H:24:TRP:CH2	2:H:61:PHE:CD1	2.68	0.81
2:H:24:TRP:HH2	2:H:61:PHE:CE1	1.99	0.81
2:H:33:ALA:O	2:H:37:ILE:HG13	1.80	0.81
1:E:107:THR:HG23	1:E:198:HIS:CE1	2.16	0.81
1:E:326:ILE:HB	1:E:342:TYR:CE1	2.15	0.81
2:F:157:PRO:HG2	2:F:158:ALA:H	1.46	0.81
2:F:24:TRP:HH2	2:F:61:PHE:CE1	1.99	0.81
2:F:24:TRP:CH2	2:F:61:PHE:CD1	2.68	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:THR:HG23	1:G:198:HIS:CE1	2.16	0.80
2:H:157:PRO:HG2	2:H:158:ALA:H	1.46	0.80
1:A:107:THR:HG23	1:A:198:HIS:CE1	2.16	0.80
1:E:91:GLN:HE21	1:E:91:GLN:HA	1.47	0.80
1:G:91:GLN:HE21	1:G:91:GLN:HA	1.47	0.80
2:D:24:TRP:HH2	2:D:61:PHE:CE1	1.99	0.80
1:C:91:GLN:HE21	1:C:91:GLN:HA	1.47	0.80
1:C:107:THR:HG23	1:C:198:HIS:CE1	2.16	0.79
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.18	0.79
2:B:24:TRP:HH2	2:B:61:PHE:CE1	1.99	0.79
1:G:393:ILE:HB	1:G:423:VAL:CG2	2.12	0.79
2:D:249:LYS:HB2	2:D:252:TRP:CE2	2.18	0.79
1:C:393:ILE:HB	1:C:423:VAL:CG2	2.12	0.79
1:A:91:GLN:HA	1:A:91:GLN:HE21	1.47	0.79
1:A:391:LEU:HB2	1:A:414:TRP:HZ3	1.48	0.79
1:G:361:HIS:CD2	1:G:518:VAL:HG11	2.18	0.78
2:D:157:PRO:HG2	2:D:158:ALA:H	1.46	0.78
1:E:393:ILE:HB	1:E:423:VAL:CG2	2.12	0.78
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.12	0.78
2:B:157:PRO:HG2	2:B:158:ALA:H	1.46	0.78
2:H:249:LYS:HB2	2:H:252:TRP:CE2	2.18	0.78
1:C:391:LEU:HB2	1:C:414:TRP:HZ3	1.48	0.78
2:F:420:PRO:HB2	2:F:421:PRO:HD2	1.66	0.78
2:F:249:LYS:HB2	2:F:252:TRP:CE2	2.18	0.78
1:A:361:HIS:HD2	1:A:518:VAL:HG11	1.49	0.77
1:C:346:PHE:CG	1:G:390:LYS:NZ	2.52	0.77
1:E:361:HIS:CD2	1:E:518:VAL:HG11	2.18	0.77
1:G:361:HIS:HD2	1:G:518:VAL:HG11	1.49	0.77
1:A:361:HIS:CD2	1:A:518:VAL:HG11	2.18	0.77
1:C:361:HIS:HD2	1:C:518:VAL:HG11	1.49	0.77
1:C:361:HIS:CD2	1:C:518:VAL:HG11	2.18	0.77
2:B:420:PRO:HB2	2:B:421:PRO:HD2	1.66	0.76
1:G:391:LEU:HB2	1:G:414:TRP:HZ3	1.48	0.76
2:H:420:PRO:HB2	2:H:421:PRO:HD2	1.66	0.76
1:E:354:TYR:OH	1:E:356:ARG:HD3	1.85	0.76
2:D:420:PRO:HB2	2:D:421:PRO:HD2	1.66	0.76
1:A:85:GLN:O	1:A:85:GLN:HG2	1.86	0.75
2:D:24:TRP:HH2	2:D:61:PHE:CD1	2.05	0.75
1:G:354:TYR:OH	1:G:356:ARG:HD3	1.85	0.75
1:E:85:GLN:HG2	1:E:85:GLN:O	1.86	0.75
1:C:354:TYR:OH	1:C:356:ARG:HD3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:THR:HG22	1:C:143:ARG:HG3	1.69	0.74
1:C:249:LYS:HE2	1:C:251:SER:HB3	1.69	0.74
1:E:391:LEU:HB2	1:E:414:TRP:HZ3	1.48	0.74
2:F:24:TRP:HH2	2:F:61:PHE:CD1	2.05	0.74
2:F:17:ASP:O	2:F:83:ARG:HD3	1.87	0.74
1:C:10:VAL:HG21	1:C:153:TRP:HH2	1.52	0.74
1:G:131:THR:HG22	1:G:143:ARG:HG3	1.69	0.74
1:C:342:TYR:CZ	1:G:345:PRO:HG3	2.22	0.74
1:E:361:HIS:HD2	1:E:518:VAL:HG11	1.49	0.74
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.52	0.74
1:A:354:TYR:OH	1:A:356:ARG:HD3	1.85	0.74
1:C:85:GLN:HG2	1:C:85:GLN:O	1.86	0.74
1:A:249:LYS:HE2	1:A:251:SER:HB3	1.69	0.74
2:B:24:TRP:HH2	2:B:61:PHE:CD1	2.05	0.74
1:E:10:VAL:HG21	1:E:153:TRP:HH2	1.52	0.74
1:A:131:THR:HG22	1:A:143:ARG:HG3	1.69	0.74
1:G:10:VAL:HG21	1:G:153:TRP:HH2	1.52	0.74
1:G:85:GLN:O	1:G:85:GLN:HG2	1.86	0.74
1:G:249:LYS:HE2	1:G:251:SER:HB3	1.69	0.74
2:H:17:ASP:O	2:H:83:ARG:HD3	1.87	0.74
1:E:391:LEU:HD12	1:E:414:TRP:CE3	2.23	0.73
1:E:249:LYS:HE2	1:E:251:SER:HB3	1.69	0.73
2:D:103:LYS:NZ	2:D:179:VAL:HG23	2.04	0.73
2:F:103:LYS:NZ	2:F:179:VAL:HG23	2.04	0.73
2:B:17:ASP:O	2:B:83:ARG:HD3	1.87	0.73
2:B:50:ILE:CG2	2:B:145:GLN:HB2	2.18	0.73
2:H:103:LYS:HZ2	2:H:179:VAL:N	1.86	0.73
2:B:63:ILE:HG23	2:B:72:ARG:HB3	1.70	0.73
2:B:103:LYS:NZ	2:B:179:VAL:HG23	2.04	0.73
1:G:391:LEU:HD12	1:G:414:TRP:CE3	2.24	0.73
1:E:90:VAL:HG12	2:F:141:GLY:H	1.53	0.73
2:D:17:ASP:O	2:D:83:ARG:HD3	1.87	0.73
2:H:103:LYS:NZ	2:H:179:VAL:HG23	2.04	0.73
2:D:103:LYS:HZ2	2:D:179:VAL:N	1.86	0.73
2:H:24:TRP:HH2	2:H:61:PHE:CD1	2.04	0.73
1:C:90:VAL:HG12	2:D:141:GLY:H	1.53	0.73
1:E:131:THR:HG22	1:E:143:ARG:HG3	1.69	0.73
1:G:90:VAL:HG12	2:H:141:GLY:H	1.53	0.73
2:D:63:ILE:HG23	2:D:72:ARG:HB3	1.70	0.73
2:H:171:PHE:HB2	2:H:208:HIS:CE1	2.24	0.72
1:E:442:VAL:CG1	1:E:481:ALA:HB1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.24	0.72
2:F:103:LYS:HZ2	2:F:179:VAL:N	1.86	0.72
1:G:157:PRO:HG2	1:G:158:ALA:H	1.54	0.72
1:C:157:PRO:HG2	1:C:158:ALA:H	1.54	0.72
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.72	0.72
2:H:246:LEU:HD11	2:H:264:LEU:HD21	1.72	0.72
2:F:50:ILE:CG2	2:F:145:GLN:HB2	2.18	0.72
2:D:171:PHE:HB2	2:D:208:HIS:CE1	2.25	0.72
2:B:171:PHE:HB2	2:B:208:HIS:CE1	2.24	0.72
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.72	0.72
1:A:90:VAL:HG12	2:B:141:GLY:H	1.53	0.72
1:C:391:LEU:HD12	1:C:414:TRP:CE3	2.23	0.72
1:A:393:ILE:O	1:A:414:TRP:HH2	1.73	0.72
1:E:157:PRO:HG2	1:E:158:ALA:H	1.54	0.72
1:C:393:ILE:O	1:C:414:TRP:HH2	1.73	0.72
2:F:171:PHE:HB2	2:F:208:HIS:CE1	2.25	0.72
1:G:442:VAL:CG1	1:G:481:ALA:HB1	2.19	0.72
2:D:50:ILE:CG2	2:D:145:GLN:HB2	2.18	0.72
1:C:442:VAL:CG1	1:C:481:ALA:HB1	2.19	0.72
2:F:92:LEU:HG	2:F:158:ALA:HB2	1.72	0.71
2:F:63:ILE:HG23	2:F:72:ARG:HB3	1.70	0.71
1:E:518:VAL:O	1:E:522:ILE:HG13	1.90	0.71
1:G:518:VAL:O	1:G:522:ILE:HG13	1.90	0.71
1:A:518:VAL:O	1:A:522:ILE:HG13	1.90	0.71
1:E:341:ILE:HD12	1:E:383:TRP:HE1	1.55	0.71
1:C:341:ILE:HD12	1:C:383:TRP:HE1	1.55	0.71
1:A:157:PRO:HG2	1:A:158:ALA:H	1.54	0.71
2:H:63:ILE:HG23	2:H:72:ARG:HB3	1.70	0.71
1:G:393:ILE:O	1:G:414:TRP:HH2	1.73	0.71
2:H:47:ILE:HG22	2:H:48:SER:H	1.56	0.71
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.19	0.71
1:E:393:ILE:O	1:E:414:TRP:HH2	1.73	0.71
2:F:246:LEU:HD11	2:F:264:LEU:HD21	1.72	0.71
1:C:518:VAL:O	1:C:522:ILE:HG13	1.90	0.71
2:B:47:ILE:HG22	2:B:48:SER:H	1.56	0.71
2:H:50:ILE:CG2	2:H:145:GLN:HB2	2.18	0.71
2:D:47:ILE:HG22	2:D:48:SER:H	1.56	0.71
1:A:341:ILE:HD12	1:A:383:TRP:HE1	1.55	0.70
1:A:225:PRO:HG2	1:A:226:PRO:HD3	1.73	0.70
2:H:92:LEU:HG	2:H:158:ALA:HB2	1.72	0.70
1:C:225:PRO:HG2	1:C:226:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:341:ILE:HD12	1:G:383:TRP:HE1	1.55	0.70
2:D:92:LEU:HG	2:D:158:ALA:HB2	1.72	0.70
2:F:47:ILE:HG22	2:F:48:SER:H	1.56	0.70
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.27	0.70
1:E:114:ALA:HB1	1:E:160:PHE:CZ	2.27	0.70
1:C:345:PRO:HG3	1:G:326:ILE:HD12	0.70	0.70
1:G:114:ALA:HB1	1:G:160:PHE:CZ	2.27	0.70
2:H:136:ASN:HB3	2:H:138:GLU:HG3	1.73	0.70
2:D:168:LEU:HD21	2:D:209:LEU:HD21	1.74	0.70
2:F:59:PRO:HG2	2:F:76:ASP:HB3	1.74	0.70
1:E:225:PRO:HG2	1:E:226:PRO:HD3	1.73	0.69
1:G:416:PHE:CD1	1:G:417:VAL:N	2.60	0.69
2:B:103:LYS:HZ2	2:B:179:VAL:N	1.86	0.69
2:B:92:LEU:HG	2:B:158:ALA:HB2	1.72	0.69
2:H:168:LEU:HD21	2:H:209:LEU:HD21	1.74	0.69
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.74	0.69
1:G:31:ILE:O	1:G:35:VAL:HG23	1.92	0.69
1:E:416:PHE:CD1	1:E:417:VAL:N	2.60	0.69
1:G:6:GLU:CD	1:G:6:GLU:H	1.95	0.69
1:E:233:GLU:OE2	1:E:242:GLN:HG3	1.93	0.69
1:C:31:ILE:O	1:C:35:VAL:HG23	1.92	0.69
1:C:6:GLU:CD	1:C:6:GLU:H	1.95	0.69
1:A:419:THR:HG23	1:A:420:PRO:HD2	1.74	0.69
1:A:416:PHE:CD1	1:A:417:VAL:N	2.60	0.69
1:G:233:GLU:OE2	1:G:242:GLN:HG3	1.93	0.69
1:C:426:TRP:CE3	1:C:426:TRP:HA	2.28	0.69
1:A:6:GLU:H	1:A:6:GLU:CD	1.95	0.69
1:G:225:PRO:HG2	1:G:226:PRO:HD3	1.73	0.69
1:C:416:PHE:CD1	1:C:417:VAL:N	2.60	0.69
1:C:419:THR:HG23	1:C:420:PRO:HD2	1.74	0.69
1:G:130:PHE:CZ	1:G:144:TYR:HB2	2.28	0.69
1:E:442:VAL:HG12	1:E:481:ALA:HB1	1.75	0.69
1:A:442:VAL:HG12	1:A:481:ALA:HB1	1.75	0.69
2:H:316:GLY:O	2:H:318:TYR:HD1	1.76	0.69
1:C:233:GLU:OE2	1:C:242:GLN:HG3	1.93	0.69
1:E:6:GLU:H	1:E:6:GLU:CD	1.95	0.69
2:D:136:ASN:HB3	2:D:138:GLU:HG3	1.74	0.69
2:D:59:PRO:HG2	2:D:76:ASP:HB3	1.74	0.69
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.27	0.69
1:A:31:ILE:O	1:A:35:VAL:HG23	1.92	0.69
1:G:426:TRP:CE3	1:G:426:TRP:HA	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:316:GLY:O	2:F:318:TYR:HD1	1.76	0.69
1:E:426:TRP:CE3	1:E:426:TRP:HA	2.28	0.69
1:C:99:GLY:HA2	1:C:383:TRP:CZ3	2.28	0.69
1:C:221:HIS:O	1:C:223:LYS:N	2.26	0.69
1:A:99:GLY:HA2	1:A:383:TRP:CZ3	2.28	0.68
2:B:136:ASN:HB3	2:B:138:GLU:HG3	1.74	0.68
2:F:72:ARG:HH12	2:F:409:THR:HG22	1.58	0.68
2:B:316:GLY:O	2:B:318:TYR:HD1	1.76	0.68
1:E:221:HIS:O	1:E:223:LYS:N	2.26	0.68
2:H:59:PRO:HG2	2:H:76:ASP:HB3	1.74	0.68
1:G:221:HIS:O	1:G:223:LYS:N	2.26	0.68
2:B:168:LEU:HD21	2:B:209:LEU:HD21	1.74	0.68
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.28	0.68
1:G:442:VAL:HG12	1:G:481:ALA:HB1	1.75	0.68
1:A:426:TRP:HA	1:A:426:TRP:CE3	2.28	0.68
1:A:221:HIS:O	1:A:223:LYS:N	2.27	0.68
2:H:163:SER:O	2:H:167:ILE:HG13	1.94	0.68
2:D:316:GLY:O	2:D:318:TYR:HD1	1.76	0.68
2:F:104:LYS:HA	2:F:237:ASP:OD2	1.94	0.68
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.28	0.68
1:A:233:GLU:OE2	1:A:242:GLN:HG3	1.93	0.68
2:F:163:SER:O	2:F:167:ILE:HG13	1.93	0.68
2:H:104:LYS:HA	2:H:237:ASP:OD2	1.94	0.68
2:B:72:ARG:HH12	2:B:409:THR:HG22	1.58	0.68
1:E:130:PHE:CZ	1:E:144:TYR:HB2	2.28	0.68
1:C:442:VAL:HG12	1:C:481:ALA:HB1	1.75	0.68
1:G:99:GLY:HA2	1:G:383:TRP:CZ3	2.28	0.68
1:E:31:ILE:O	1:E:35:VAL:HG23	1.92	0.68
2:H:72:ARG:HH12	2:H:409:THR:HG22	1.58	0.68
1:E:100:LEU:O	1:E:318:TYR:HB3	1.94	0.68
1:G:420:PRO:HG2	1:G:421:PRO:CD	2.22	0.68
2:D:157:PRO:HG2	2:D:158:ALA:N	2.08	0.68
1:E:99:GLY:HA2	1:E:383:TRP:CZ3	2.28	0.68
2:B:163:SER:O	2:B:167:ILE:HG13	1.94	0.68
2:F:168:LEU:HD21	2:F:209:LEU:HD21	1.74	0.68
2:F:136:ASN:HB3	2:F:138:GLU:HG3	1.74	0.68
2:D:97:PRO:HG2	2:D:181:TYR:HB2	1.76	0.68
1:E:419:THR:HG23	1:E:420:PRO:HD2	1.74	0.68
2:D:72:ARG:HH12	2:D:409:THR:HG22	1.58	0.68
2:D:163:SER:O	2:D:167:ILE:HG13	1.94	0.68
2:H:97:PRO:HG2	2:H:181:TYR:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:123:ASP:HA	2:F:126:LYS:NZ	2.09	0.68
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.94	0.68
1:E:98:ALA:CB	1:E:383:TRP:HH2	2.07	0.68
1:C:345:PRO:CD	1:G:326:ILE:HD12	2.24	0.67
2:D:104:LYS:HA	2:D:237:ASP:OD2	1.94	0.67
2:B:157:PRO:HG2	2:B:158:ALA:N	2.08	0.67
1:C:100:LEU:O	1:C:318:TYR:HB3	1.94	0.67
1:C:346:PHE:CD1	1:G:390:LYS:NZ	2.62	0.67
1:G:419:THR:HG23	1:G:420:PRO:HD2	1.74	0.67
2:H:157:PRO:HG2	2:H:158:ALA:N	2.08	0.67
1:E:378:GLU:O	1:E:382:ILE:HG13	1.95	0.67
1:G:100:LEU:O	1:G:318:TYR:HB3	1.94	0.67
1:A:426:TRP:HA	1:A:426:TRP:HE3	1.59	0.67
2:B:97:PRO:HG2	2:B:181:TYR:HB2	1.76	0.67
2:B:123:ASP:HA	2:B:126:LYS:NZ	2.10	0.67
1:E:244:ILE:CD1	1:E:267:ALA:HB2	2.25	0.67
2:F:94:ILE:HG22	2:F:95:PRO:CD	2.24	0.67
1:A:100:LEU:O	1:A:318:TYR:HB3	1.94	0.67
1:G:393:ILE:O	1:G:414:TRP:CH2	2.48	0.67
1:G:378:GLU:O	1:G:382:ILE:HG13	1.95	0.67
2:F:97:PRO:HG2	2:F:181:TYR:HB2	1.76	0.67
2:D:123:ASP:HA	2:D:126:LYS:NZ	2.10	0.67
1:A:378:GLU:O	1:A:382:ILE:HG13	1.95	0.67
2:H:123:ASP:HA	2:H:126:LYS:NZ	2.10	0.67
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.25	0.67
1:G:98:ALA:CB	1:G:383:TRP:HH2	2.07	0.67
2:F:153:TRP:CZ3	2:F:155:GLY:HA3	2.30	0.67
1:G:244:ILE:CD1	1:G:267:ALA:HB2	2.25	0.67
1:C:426:TRP:HE3	1:C:426:TRP:HA	1.59	0.67
1:C:457:TYR:CE1	1:C:465:LYS:HB3	2.30	0.67
2:D:94:ILE:HG22	2:D:95:PRO:CD	2.25	0.67
2:B:153:TRP:CZ3	2:B:155:GLY:HA3	2.30	0.66
1:A:98:ALA:CB	1:A:383:TRP:HH2	2.07	0.66
2:H:94:ILE:HG22	2:H:95:PRO:CD	2.25	0.66
1:G:457:TYR:CE1	1:G:465:LYS:HB3	2.31	0.66
1:E:426:TRP:HA	1:E:426:TRP:HE3	1.59	0.66
1:C:378:GLU:O	1:C:382:ILE:HG13	1.95	0.66
1:E:393:ILE:O	1:E:414:TRP:CH2	2.48	0.66
1:E:420:PRO:HG2	1:E:421:PRO:CD	2.22	0.66
1:G:167:ILE:O	1:G:208:HIS:HE1	1.78	0.66
2:F:109:LEU:HD12	2:F:187:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:ALA:O	1:G:37:ILE:HG13	1.95	0.66
1:A:457:TYR:CE1	1:A:465:LYS:HB3	2.31	0.66
2:F:21:VAL:CG1	2:F:59:PRO:HD3	2.26	0.66
2:H:21:VAL:CG1	2:H:59:PRO:HD3	2.26	0.66
1:E:167:ILE:O	1:E:208:HIS:HE1	1.78	0.66
2:D:153:TRP:CZ3	2:D:155:GLY:HA3	2.30	0.66
1:E:457:TYR:CE1	1:E:465:LYS:HB3	2.31	0.66
2:B:94:ILE:HG22	2:B:95:PRO:CD	2.25	0.66
1:E:149:LEU:HD22	1:E:156:SER:HA	1.78	0.66
1:C:393:ILE:O	1:C:414:TRP:CH2	2.48	0.66
2:H:153:TRP:CZ3	2:H:155:GLY:HA3	2.30	0.66
1:C:98:ALA:CB	1:C:383:TRP:HH2	2.07	0.66
2:H:109:LEU:HD12	2:H:187:LEU:HD23	1.77	0.66
1:C:537:PRO:HG2	2:D:262:GLY:HA2	1.78	0.66
2:B:21:VAL:CG1	2:B:59:PRO:HD3	2.26	0.66
1:G:165:THR:HG21	2:H:140:PRO:HG2	1.77	0.66
1:A:165:THR:HG21	2:B:140:PRO:HG2	1.77	0.66
1:G:149:LEU:HD22	1:G:156:SER:HA	1.78	0.66
2:B:151:GLN:HA	2:B:151:GLN:HE21	1.61	0.66
2:F:151:GLN:HA	2:F:151:GLN:HE21	1.61	0.66
1:A:393:ILE:O	1:A:414:TRP:CH2	2.48	0.65
2:D:21:VAL:CG1	2:D:59:PRO:HD3	2.26	0.65
1:A:33:ALA:O	1:A:37:ILE:HG13	1.95	0.65
1:C:165:THR:HG21	2:D:140:PRO:HG2	1.77	0.65
1:C:167:ILE:O	1:C:208:HIS:HE1	1.78	0.65
1:E:33:ALA:O	1:E:37:ILE:HG13	1.95	0.65
1:A:537:PRO:HG2	2:B:262:GLY:HA2	1.78	0.65
2:B:103:LYS:NZ	2:B:179:VAL:H	1.93	0.65
2:B:61:PHE:CE2	2:B:74:LEU:HD23	2.31	0.65
1:A:167:ILE:O	1:A:208:HIS:HE1	1.78	0.65
1:A:27:THR:OG1	1:A:30:LYS:HG3	1.97	0.65
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.78	0.65
2:D:169:GLU:HB3	2:D:170:PRO:HD3	1.78	0.65
1:G:27:THR:OG1	1:G:30:LYS:HG3	1.97	0.65
2:D:151:GLN:HE21	2:D:151:GLN:HA	1.61	0.65
2:F:61:PHE:CE2	2:F:74:LEU:HD23	2.31	0.65
2:D:109:LEU:HD12	2:D:187:LEU:HD23	1.77	0.65
2:D:303:LEU:O	2:D:307:ARG:HG3	1.97	0.65
2:H:303:LEU:O	2:H:307:ARG:HG3	1.97	0.65
1:C:420:PRO:HG2	1:C:421:PRO:CD	2.22	0.65
1:E:27:THR:OG1	1:E:30:LYS:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:THR:OG1	1:C:30:LYS:HG3	1.97	0.65
1:C:33:ALA:O	1:C:37:ILE:HG13	1.95	0.65
2:H:151:GLN:HA	2:H:151:GLN:HE21	1.61	0.65
1:G:406:TRP:CE3	1:G:407:GLN:HG3	2.32	0.65
1:G:328:GLU:O	1:G:339:TYR:HA	1.97	0.65
1:G:537:PRO:HG2	2:H:262:GLY:HA2	1.78	0.65
1:E:537:PRO:HG2	2:F:262:GLY:HA2	1.78	0.65
2:H:104:LYS:NZ	2:H:194:GLU:HA	2.12	0.65
2:H:61:PHE:CE2	2:H:74:LEU:HD23	2.31	0.65
1:G:426:TRP:HE3	1:G:426:TRP:HA	1.59	0.65
1:E:248:GLU:HG3	1:E:307:ARG:HH21	1.62	0.65
2:B:303:LEU:O	2:B:307:ARG:HG3	1.97	0.65
2:F:103:LYS:NZ	2:F:179:VAL:H	1.93	0.65
2:D:61:PHE:CE2	2:D:74:LEU:HD23	2.31	0.65
1:G:248:GLU:HG3	1:G:307:ARG:HH21	1.62	0.65
1:A:406:TRP:CE3	1:A:407:GLN:HG3	2.32	0.65
2:F:28:GLU:HG3	2:F:135:ILE:CD1	2.27	0.65
1:A:149:LEU:HD22	1:A:156:SER:HA	1.78	0.65
1:A:328:GLU:O	1:A:339:TYR:HA	1.97	0.65
1:C:406:TRP:CE3	1:C:407:GLN:HG3	2.32	0.65
2:B:109:LEU:HD12	2:B:187:LEU:HD23	1.77	0.65
2:F:303:LEU:O	2:F:307:ARG:HG3	1.97	0.65
2:H:28:GLU:HG3	2:H:135:ILE:CD1	2.27	0.65
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.27	0.65
1:A:248:GLU:HG3	1:A:307:ARG:HH21	1.62	0.65
1:C:328:GLU:O	1:C:339:TYR:HA	1.97	0.65
1:E:406:TRP:CE3	1:E:407:GLN:HG3	2.32	0.65
2:D:28:GLU:HG3	2:D:135:ILE:CD1	2.27	0.64
1:C:248:GLU:HG3	1:C:307:ARG:HH21	1.62	0.64
1:G:537:PRO:HD2	1:G:542:ILE:CD1	2.27	0.64
1:E:328:GLU:O	1:E:339:TYR:HA	1.97	0.64
1:C:376:THR:HG23	1:C:386:THR:CG2	2.25	0.64
1:C:244:ILE:CD1	1:C:267:ALA:HB2	2.25	0.64
1:C:149:LEU:HD22	1:C:156:SER:HA	1.78	0.64
1:E:165:THR:HG21	2:F:140:PRO:HG2	1.77	0.64
1:C:393:ILE:HG23	1:C:414:TRP:HH2	1.58	0.64
2:B:264:LEU:CD2	2:B:274:ILE:HD11	2.24	0.64
1:E:537:PRO:HD2	1:E:542:ILE:CD1	2.27	0.64
2:B:24:TRP:CZ3	2:B:61:PHE:HB3	2.32	0.64
2:D:24:TRP:CZ3	2:D:61:PHE:HB3	2.32	0.64
2:D:149:LEU:HD22	2:D:156:SER:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:PRO:HD2	1:C:542:ILE:CD1	2.27	0.64
2:F:246:LEU:HB2	2:F:307:ARG:NH1	2.13	0.64
2:F:104:LYS:NZ	2:F:194:GLU:HA	2.12	0.64
2:D:104:LYS:NZ	2:D:194:GLU:HA	2.12	0.64
2:B:104:LYS:NZ	2:B:194:GLU:HA	2.12	0.64
2:F:24:TRP:CZ3	2:F:61:PHE:HB3	2.32	0.64
2:B:246:LEU:CD1	2:B:264:LEU:HD21	2.27	0.64
2:H:246:LEU:CD1	2:H:264:LEU:HD21	2.27	0.64
2:H:246:LEU:HB2	2:H:307:ARG:NH1	2.13	0.64
2:D:103:LYS:NZ	2:D:179:VAL:H	1.93	0.64
2:H:126:LYS:HA	2:H:145:GLN:NE2	2.13	0.64
2:F:157:PRO:HG2	2:F:158:ALA:N	2.08	0.64
2:D:264:LEU:CD2	2:D:274:ILE:HD11	2.24	0.64
2:B:149:LEU:HD22	2:B:156:SER:HA	1.79	0.64
1:A:393:ILE:HG23	1:A:414:TRP:HH2	1.58	0.64
2:B:246:LEU:HB2	2:B:307:ARG:NH1	2.13	0.64
2:H:264:LEU:CD2	2:H:274:ILE:HD11	2.24	0.64
2:F:246:LEU:CD1	2:F:264:LEU:HD21	2.27	0.64
1:G:376:THR:HG23	1:G:386:THR:CG2	2.25	0.64
1:A:420:PRO:HG2	1:A:421:PRO:CD	2.22	0.64
2:H:169:GLU:HB3	2:H:170:PRO:HD3	1.78	0.64
2:D:246:LEU:HB2	2:D:307:ARG:NH1	2.13	0.63
1:A:376:THR:HG23	1:A:386:THR:CG2	2.25	0.63
2:B:94:ILE:HG22	2:B:95:PRO:HD3	1.81	0.63
2:F:169:GLU:HB3	2:F:170:PRO:HD3	1.78	0.63
2:D:94:ILE:HG22	2:D:95:PRO:HD3	1.81	0.63
1:G:28:GLU:O	1:G:32:LYS:HG3	1.98	0.63
1:E:28:GLU:O	1:E:32:LYS:HG3	1.98	0.63
2:D:246:LEU:CD1	2:D:264:LEU:HD21	2.27	0.63
2:B:126:LYS:HA	2:B:145:GLN:NE2	2.13	0.63
2:H:63:ILE:HG12	2:H:64:LYS:N	2.14	0.63
1:E:376:THR:HG23	1:E:386:THR:CG2	2.25	0.63
1:C:342:TYR:CE1	1:G:345:PRO:HG3	2.33	0.63
2:F:126:LYS:HA	2:F:145:GLN:NE2	2.13	0.63
1:C:393:ILE:HB	1:C:423:VAL:HG21	1.79	0.63
1:A:537:PRO:HD2	1:A:542:ILE:CD1	2.27	0.63
2:H:94:ILE:HG22	2:H:95:PRO:HD3	1.81	0.63
2:F:264:LEU:CD2	2:F:274:ILE:HD11	2.24	0.63
2:H:24:TRP:CZ3	2:H:61:PHE:HB3	2.32	0.63
1:A:393:ILE:HB	1:A:423:VAL:HG21	1.79	0.63
1:E:206:ARG:HH22	1:E:218:ASP:HA	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:103:LYS:NZ	2:H:179:VAL:H	1.93	0.63
2:D:126:LYS:HA	2:D:145:GLN:NE2	2.13	0.63
2:F:63:ILE:HG12	2:F:64:LYS:N	2.14	0.63
1:A:206:ARG:HH22	1:A:218:ASP:HA	1.64	0.63
1:C:540:LYS:HZ3	2:D:261:VAL:CG1	2.12	0.63
2:F:94:ILE:HG22	2:F:95:PRO:HD3	1.81	0.63
1:A:28:GLU:O	1:A:32:LYS:HG3	1.98	0.63
2:H:149:LEU:HD22	2:H:156:SER:HA	1.79	0.62
2:F:21:VAL:HG11	2:F:59:PRO:HD3	1.80	0.62
2:B:21:VAL:HG11	2:B:59:PRO:HD3	1.80	0.62
1:A:238:LYS:HE2	1:A:240:THR:CG2	2.29	0.62
1:C:238:LYS:HE2	1:C:240:THR:CG2	2.29	0.62
2:H:21:VAL:HG11	2:H:59:PRO:HD3	1.80	0.62
2:B:63:ILE:HG12	2:B:64:LYS:N	2.14	0.62
1:E:393:ILE:HB	1:E:423:VAL:HG21	1.80	0.62
2:D:63:ILE:HG12	2:D:64:LYS:N	2.14	0.62
2:D:21:VAL:HG11	2:D:59:PRO:HD3	1.80	0.62
1:C:28:GLU:O	1:C:32:LYS:HG3	1.98	0.62
1:G:206:ARG:HH22	1:G:218:ASP:HA	1.64	0.62
2:F:125:ARG:NH1	2:F:147:ASN:HA	2.15	0.62
1:C:346:PHE:HD1	1:G:390:LYS:HE3	0.80	0.62
2:F:149:LEU:HD22	2:F:156:SER:HA	1.79	0.62
2:B:125:ARG:NH1	2:B:147:ASN:HA	2.15	0.62
2:D:125:ARG:NH1	2:D:147:ASN:HA	2.15	0.62
1:E:206:ARG:HG3	1:E:216:THR:OG1	2.00	0.62
1:C:206:ARG:HG3	1:C:216:THR:OG1	2.00	0.62
1:C:206:ARG:HH22	1:C:218:ASP:HA	1.64	0.62
1:G:339:TYR:CE1	1:G:352:GLY:HA3	2.35	0.62
1:C:249:LYS:HG2	1:C:250:ASP:N	2.15	0.62
1:E:491:LEU:HB3	1:E:529:GLU:CB	2.30	0.62
1:A:491:LEU:HB3	1:A:529:GLU:CB	2.30	0.62
1:A:206:ARG:HG3	1:A:216:THR:OG1	2.00	0.62
2:D:376:THR:HG22	2:D:389:PHE:CE1	2.35	0.62
2:H:125:ARG:NH1	2:H:147:ASN:HA	2.15	0.62
2:F:376:THR:HG22	2:F:389:PHE:CE1	2.35	0.62
1:C:491:LEU:HB3	1:C:529:GLU:CB	2.30	0.62
1:G:249:LYS:HG2	1:G:250:ASP:N	2.15	0.61
1:G:238:LYS:HE2	1:G:240:THR:CG2	2.29	0.61
2:B:47:ILE:HG21	2:B:144:TYR:HB3	1.82	0.61
2:F:47:ILE:HG21	2:F:144:TYR:HB3	1.82	0.61
2:F:257:ILE:HB	2:F:283:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:TYR:OH	2:D:374:LYS:HG2	2.00	0.61
1:E:393:ILE:HG23	1:E:414:TRP:HH2	1.58	0.61
1:G:393:ILE:HB	1:G:423:VAL:HG21	1.79	0.61
1:A:249:LYS:HG2	1:A:250:ASP:N	2.15	0.61
1:C:339:TYR:CE1	1:C:352:GLY:HA3	2.35	0.61
1:C:104:LYS:HB2	1:C:192:ASP:HA	1.82	0.61
2:B:354:TYR:OH	2:B:374:LYS:HG2	2.00	0.61
1:E:238:LYS:HE2	1:E:240:THR:CG2	2.29	0.61
2:H:376:THR:HG22	2:H:389:PHE:CE1	2.35	0.61
1:G:435:VAL:HG22	2:H:290:THR:HG21	1.83	0.61
1:G:104:LYS:HB2	1:G:192:ASP:HA	1.82	0.61
2:D:87:PHE:CE2	2:D:155:GLY:HA2	2.36	0.61
1:G:206:ARG:HG3	1:G:216:THR:OG1	2.00	0.61
2:B:376:THR:HG22	2:B:389:PHE:CE1	2.35	0.61
1:E:376:THR:O	1:E:380:ILE:HG13	2.01	0.61
2:F:87:PHE:CE2	2:F:155:GLY:HA2	2.36	0.61
2:H:87:PHE:CE2	2:H:155:GLY:HA2	2.36	0.61
1:E:104:LYS:HB2	1:E:192:ASP:HA	1.82	0.61
2:H:354:TYR:OH	2:H:374:LYS:HG2	2.00	0.61
1:C:225:PRO:HG2	1:C:226:PRO:CD	2.31	0.61
1:C:435:VAL:HG22	2:D:290:THR:HG21	1.83	0.61
1:E:435:VAL:HG22	2:F:290:THR:HG21	1.83	0.61
1:A:376:THR:O	1:A:380:ILE:HG13	2.01	0.61
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.36	0.61
1:E:249:LYS:HG2	1:E:250:ASP:N	2.15	0.61
2:H:47:ILE:HG21	2:H:144:TYR:HB3	1.82	0.61
1:A:225:PRO:HG2	1:A:226:PRO:CD	2.31	0.61
1:A:339:TYR:CE1	1:A:352:GLY:HA3	2.35	0.61
1:E:339:TYR:CE1	1:E:352:GLY:HA3	2.35	0.61
1:E:88:TRP:CH2	2:F:57:ASN:HB3	2.36	0.61
1:E:225:PRO:HG2	1:E:226:PRO:CD	2.31	0.61
1:E:238:LYS:HE2	1:E:240:THR:HG22	1.83	0.61
1:G:491:LEU:HB3	1:G:529:GLU:CB	2.30	0.61
1:G:225:PRO:HG2	1:G:226:PRO:CD	2.31	0.60
1:G:238:LYS:HE2	1:G:240:THR:HG22	1.83	0.60
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.83	0.60
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.82	0.60
1:G:393:ILE:HG23	1:G:414:TRP:HH2	1.58	0.60
1:G:376:THR:O	1:G:380:ILE:HG13	2.01	0.60
2:F:354:TYR:OH	2:F:374:LYS:HG2	2.00	0.60
1:E:326:ILE:HB	1:E:342:TYR:HE1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:509:GLN:N	1:E:510:PRO:HD3	2.17	0.60
2:D:47:ILE:HG21	2:D:144:TYR:HB3	1.82	0.60
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.82	0.60
2:D:257:ILE:HB	2:D:283:LEU:HD21	1.82	0.60
1:C:376:THR:O	1:C:380:ILE:HG13	2.01	0.60
2:F:151:GLN:HA	2:F:151:GLN:NE2	2.17	0.60
2:H:151:GLN:HA	2:H:151:GLN:NE2	2.17	0.60
1:G:88:TRP:CH2	2:H:57:ASN:HB3	2.36	0.60
1:E:540:LYS:HZ3	2:F:261:VAL:CG1	2.14	0.60
2:D:171:PHE:CE2	2:D:204:GLU:HB2	2.31	0.60
2:H:47:ILE:CG2	2:H:144:TYR:HB3	2.31	0.60
2:B:47:ILE:CG2	2:B:144:TYR:HB3	2.31	0.60
1:C:88:TRP:CH2	2:D:57:ASN:HB3	2.36	0.60
2:H:257:ILE:HB	2:H:283:LEU:HD21	1.82	0.60
2:D:47:ILE:CG2	2:D:144:TYR:HB3	2.31	0.60
1:A:88:TRP:CH2	2:B:57:ASN:HB3	2.36	0.60
1:C:326:ILE:HB	1:C:342:TYR:HE1	1.66	0.60
2:F:47:ILE:CG2	2:F:144:TYR:HB3	2.31	0.60
1:C:160:PHE:CE1	1:C:164:MET:HG2	2.37	0.60
2:B:328:GLU:O	2:B:339:TYR:HA	2.02	0.60
2:D:328:GLU:O	2:D:339:TYR:HA	2.02	0.60
1:C:323:LYS:HE2	1:G:322:SER:O	2.01	0.60
1:C:363:ASN:OD1	1:C:364:ASP:N	2.35	0.60
1:G:509:GLN:N	1:G:510:PRO:HD3	2.17	0.60
1:A:160:PHE:CE1	1:A:164:MET:HG2	2.37	0.60
1:A:238:LYS:HE3	1:A:315:HIS:CD2	2.36	0.60
1:C:238:LYS:HE2	1:C:240:THR:HG22	1.83	0.60
2:H:328:GLU:O	2:H:339:TYR:HA	2.02	0.60
1:A:509:GLN:N	1:A:510:PRO:HD3	2.17	0.59
1:C:238:LYS:HE3	1:C:315:HIS:CD2	2.37	0.59
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.84	0.59
1:A:326:ILE:HB	1:A:342:TYR:HE1	1.66	0.59
1:C:509:GLN:N	1:C:510:PRO:HD3	2.16	0.59
1:A:238:LYS:HE2	1:A:240:THR:HG22	1.83	0.59
1:E:160:PHE:CE1	1:E:164:MET:HG2	2.37	0.59
1:C:235:HIS:HB3	1:C:236:PRO:HD2	1.84	0.59
1:G:363:ASN:OD1	1:G:364:ASP:N	2.35	0.59
1:A:392:PRO:O	1:A:423:VAL:HG22	2.03	0.59
1:G:160:PHE:CE1	1:G:164:MET:HG2	2.37	0.59
1:E:238:LYS:HE3	1:E:315:HIS:CD2	2.36	0.59
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.84	0.59
1:G:238:LYS:HE3	1:G:315:HIS:CD2	2.36	0.59
1:E:363:ASN:OD1	1:E:364:ASP:N	2.35	0.59
1:A:363:ASN:OD1	1:A:364:ASP:N	2.35	0.59
1:G:326:ILE:HB	1:G:342:TYR:HE1	1.66	0.59
1:C:392:PRO:O	1:C:423:VAL:HG22	2.03	0.59
2:B:106:VAL:HA	2:B:190:GLY:HA2	1.85	0.59
2:F:328:GLU:O	2:F:339:TYR:HA	2.02	0.59
1:E:392:PRO:O	1:E:423:VAL:HG22	2.03	0.59
2:F:104:LYS:HZ2	2:F:194:GLU:HA	1.68	0.59
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.38	0.59
2:D:151:GLN:NE2	2:D:151:GLN:HA	2.17	0.59
1:E:161:GLN:O	1:E:165:THR:HG23	2.03	0.59
2:F:153:TRP:CH2	2:F:155:GLY:HA3	2.38	0.59
1:G:161:GLN:O	1:G:165:THR:HG23	2.03	0.59
2:D:106:VAL:HA	2:D:190:GLY:HA2	1.85	0.59
1:G:295:LEU:CB	1:G:299:ALA:HB2	2.33	0.59
1:A:161:GLN:O	1:A:165:THR:HG23	2.03	0.59
1:C:161:GLN:O	1:C:165:THR:HG23	2.03	0.59
1:E:295:LEU:CB	1:E:299:ALA:HB2	2.33	0.59
1:E:235:HIS:HB3	1:E:236:PRO:HD2	1.84	0.59
1:E:492:GLU:HG2	1:E:530:LYS:HB2	1.84	0.58
1:G:492:GLU:HG2	1:G:530:LYS:HB2	1.84	0.58
2:D:153:TRP:CH2	2:D:155:GLY:HA3	2.38	0.58
2:B:151:GLN:HA	2:B:151:GLN:NE2	2.17	0.58
2:B:171:PHE:CE2	2:B:204:GLU:HB2	2.31	0.58
1:C:346:PHE:CZ	1:G:390:LYS:CG	2.80	0.58
2:B:103:LYS:HZ1	2:B:179:VAL:HG23	1.67	0.58
1:G:167:ILE:O	1:G:170:PRO:HD2	2.04	0.58
1:E:17:ASP:O	1:E:83:ARG:HD3	2.03	0.58
1:E:167:ILE:O	1:E:170:PRO:HD2	2.03	0.58
1:G:235:HIS:HB3	1:G:236:PRO:HD2	1.84	0.58
1:C:523:GLU:O	1:C:526:ILE:HG12	2.04	0.58
1:A:295:LEU:CB	1:A:299:ALA:HB2	2.33	0.58
1:C:295:LEU:CB	1:C:299:ALA:HB2	2.33	0.58
1:E:393:ILE:HB	1:E:423:VAL:HG22	1.86	0.58
1:C:17:ASP:O	1:C:83:ARG:HD3	2.03	0.58
2:H:106:VAL:HA	2:H:190:GLY:HA2	1.85	0.58
2:H:171:PHE:CE2	2:H:204:GLU:HB2	2.31	0.58
1:G:523:GLU:O	1:G:526:ILE:HG12	2.04	0.58
1:C:411:ILE:HG22	1:C:412:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:O	1:A:83:ARG:HD3	2.03	0.58
2:D:103:LYS:HZ1	2:D:179:VAL:HG23	1.69	0.58
2:H:153:TRP:CH2	2:H:155:GLY:HA3	2.38	0.58
1:A:303:LEU:O	1:A:307:ARG:HG3	2.04	0.58
1:A:523:GLU:O	1:A:526:ILE:HG12	2.04	0.58
2:F:106:VAL:HA	2:F:190:GLY:HA2	1.84	0.58
2:H:55:PRO:HG2	2:H:56:TYR:N	2.19	0.58
2:F:395:LYS:HG3	2:F:416:PHE:CE2	2.39	0.58
2:F:55:PRO:HG2	2:F:56:TYR:N	2.19	0.58
2:F:171:PHE:CE2	2:F:204:GLU:HB2	2.31	0.57
1:A:411:ILE:HG22	1:A:412:PRO:HD2	1.86	0.57
2:D:10:VAL:CG1	2:D:159:ILE:HD11	2.34	0.57
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.39	0.57
1:G:392:PRO:O	1:G:423:VAL:HG22	2.03	0.57
1:E:406:TRP:CZ3	1:E:407:GLN:HG3	2.39	0.57
2:H:395:LYS:HG3	2:H:416:PHE:CE2	2.39	0.57
1:A:167:ILE:O	1:A:170:PRO:HD2	2.03	0.57
1:G:303:LEU:O	1:G:307:ARG:HG3	2.04	0.57
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.40	0.57
2:D:395:LYS:HG3	2:D:416:PHE:CE2	2.39	0.57
1:E:429:LEU:HD11	1:E:506:ILE:HG22	1.87	0.57
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.86	0.57
1:E:441:TYR:HE2	1:E:543:GLY:O	1.88	0.57
2:H:10:VAL:CG1	2:H:159:ILE:HD11	2.35	0.57
2:B:10:VAL:CG1	2:B:159:ILE:HD11	2.35	0.57
1:A:229:TRP:CH2	1:A:230:MET:HE1	2.39	0.57
1:C:167:ILE:O	1:C:170:PRO:HD2	2.03	0.57
1:E:87:PHE:CE2	1:E:159:ILE:HD11	2.40	0.57
2:B:5:ILE:HG22	2:B:6:GLU:N	2.20	0.57
1:E:418:ASN:HD22	1:E:418:ASN:C	2.08	0.57
2:D:28:GLU:HG2	2:D:32:LYS:NZ	2.19	0.57
2:F:28:GLU:HG2	2:F:32:LYS:NZ	2.19	0.57
1:C:320:ASP:OD2	1:C:323:LYS:HG3	2.05	0.57
1:E:232:TYR:HD1	1:E:241:VAL:HG22	1.70	0.57
1:C:406:TRP:CZ3	1:C:407:GLN:HG3	2.39	0.57
1:C:303:LEU:O	1:C:307:ARG:HG3	2.04	0.57
2:H:395:LYS:O	2:H:399:GLU:HG3	2.05	0.57
1:G:418:ASN:C	1:G:418:ASN:HD22	2.08	0.57
1:G:393:ILE:HB	1:G:423:VAL:HG22	1.86	0.57
1:G:406:TRP:CZ3	1:G:407:GLN:HG3	2.40	0.57
2:F:54:ASN:HD21	2:F:56:TYR:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ASN:HD21	2:D:56:TYR:HB2	1.70	0.57
1:E:523:GLU:O	1:E:526:ILE:HG12	2.04	0.57
2:B:54:ASN:HD21	2:B:56:TYR:HB2	1.70	0.57
1:G:458:VAL:HG23	1:G:548:VAL:HG22	1.87	0.57
2:D:5:ILE:HG22	2:D:6:GLU:N	2.20	0.57
1:G:17:ASP:O	1:G:83:ARG:HD3	2.03	0.57
2:F:5:ILE:HG22	2:F:6:GLU:N	2.20	0.57
1:E:320:ASP:OD2	1:E:323:LYS:HG3	2.05	0.57
1:E:56:TYR:O	1:E:143:ARG:NH2	2.38	0.57
2:H:28:GLU:HG2	2:H:32:LYS:NZ	2.19	0.57
1:C:229:TRP:CH2	1:C:230:MET:HE1	2.39	0.57
2:F:395:LYS:O	2:F:399:GLU:HG3	2.05	0.57
1:A:418:ASN:C	1:A:418:ASN:HD22	2.08	0.57
1:C:393:ILE:HB	1:C:423:VAL:HG22	1.86	0.56
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.05	0.56
1:E:411:ILE:HG22	1:E:412:PRO:HD2	1.86	0.56
1:E:98:ALA:HB1	1:E:383:TRP:HH2	1.70	0.56
2:B:54:ASN:C	2:B:54:ASN:HD22	2.08	0.56
2:H:379:SER:OG	2:H:387:PRO:HD3	2.05	0.56
1:C:346:PHE:CG	1:G:390:LYS:CD	2.87	0.56
1:G:441:TYR:HE2	1:G:543:GLY:O	1.88	0.56
2:B:28:GLU:HG2	2:B:32:LYS:NZ	2.19	0.56
1:G:429:LEU:HD11	1:G:506:ILE:HG22	1.87	0.56
1:C:418:ASN:C	1:C:418:ASN:HD22	2.08	0.56
1:A:458:VAL:HG23	1:A:548:VAL:HG22	1.87	0.56
2:B:271:TYR:O	2:B:274:ILE:HG22	2.06	0.56
2:D:271:TYR:O	2:D:274:ILE:HG22	2.06	0.56
1:G:411:ILE:HG22	1:G:412:PRO:HD2	1.86	0.56
2:B:61:PHE:CE2	2:B:403:THR:HG22	2.41	0.56
2:H:61:PHE:CE2	2:H:403:THR:HG22	2.41	0.56
1:A:98:ALA:HB1	1:A:383:TRP:HH2	1.70	0.56
2:H:139:THR:HG22	2:H:140:PRO:O	2.06	0.56
2:H:54:ASN:HD22	2:H:54:ASN:C	2.08	0.56
2:F:54:ASN:HD22	2:F:54:ASN:C	2.08	0.56
2:D:395:LYS:O	2:D:399:GLU:HG3	2.05	0.56
2:D:55:PRO:HG2	2:D:56:TYR:N	2.19	0.56
2:D:54:ASN:C	2:D:54:ASN:HD22	2.08	0.56
1:A:87:PHE:CE2	1:A:159:ILE:HD11	2.40	0.56
2:F:379:SER:OG	2:F:387:PRO:HD3	2.05	0.56
2:H:5:ILE:HG22	2:H:6:GLU:N	2.20	0.56
1:C:87:PHE:CE2	1:C:159:ILE:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:LEU:O	1:C:521:ILE:HG13	2.06	0.56
1:C:329:ILE:HD12	1:C:391:LEU:CD2	2.36	0.56
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.36	0.56
1:G:320:ASP:OD2	1:G:323:LYS:HG3	2.05	0.56
2:B:105:SER:HB3	2:B:235:HIS:CE1	2.41	0.56
1:G:56:TYR:O	1:G:143:ARG:NH2	2.38	0.56
2:B:55:PRO:HG2	2:B:56:TYR:N	2.19	0.56
1:A:517:LEU:O	1:A:521:ILE:HG13	2.06	0.56
1:A:453:GLY:O	1:A:469:LEU:HB2	2.06	0.56
1:G:87:PHE:CE2	1:G:159:ILE:HD11	2.40	0.56
2:F:105:SER:HB3	2:F:235:HIS:CE1	2.41	0.56
2:D:105:SER:HB3	2:D:235:HIS:CE1	2.41	0.56
2:D:61:PHE:CE2	2:D:403:THR:HG22	2.41	0.56
1:E:303:LEU:O	1:E:307:ARG:HG3	2.04	0.56
2:B:395:LYS:O	2:B:399:GLU:HG3	2.05	0.56
1:G:517:LEU:O	1:G:521:ILE:HG13	2.06	0.56
1:G:453:GLY:O	1:G:469:LEU:HB2	2.06	0.56
2:H:271:TYR:O	2:H:274:ILE:HG22	2.06	0.56
2:F:10:VAL:CG1	2:F:159:ILE:HD11	2.35	0.56
1:C:98:ALA:HB1	1:C:383:TRP:HH2	1.71	0.56
1:G:98:ALA:HB1	1:G:383:TRP:HH2	1.70	0.56
1:A:441:TYR:HE2	1:A:543:GLY:O	1.88	0.56
1:C:441:TYR:HE2	1:C:543:GLY:O	1.88	0.56
2:F:139:THR:HG22	2:F:140:PRO:O	2.06	0.56
2:F:125:ARG:HH11	2:F:125:ARG:HG2	1.71	0.56
2:H:54:ASN:HD21	2:H:56:TYR:HB2	1.70	0.56
1:C:458:VAL:HG23	1:C:548:VAL:HG22	1.86	0.56
1:A:56:TYR:O	1:A:143:ARG:NH2	2.38	0.56
1:A:248:GLU:HG3	1:A:307:ARG:NH2	2.20	0.56
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.87	0.56
1:C:453:GLY:O	1:C:469:LEU:HB2	2.06	0.56
1:G:491:LEU:HB3	1:G:529:GLU:HB3	1.88	0.56
1:E:458:VAL:HG23	1:E:548:VAL:HG22	1.87	0.56
2:F:271:TYR:O	2:F:274:ILE:HG22	2.06	0.56
1:C:56:TYR:O	1:C:143:ARG:NH2	2.38	0.56
1:C:429:LEU:HD11	1:C:506:ILE:HG22	1.87	0.56
2:B:379:SER:OG	2:B:387:PRO:HD3	2.05	0.56
1:A:232:TYR:HD1	1:A:241:VAL:HG22	1.70	0.55
1:G:232:TYR:HD1	1:G:241:VAL:HG22	1.70	0.55
2:D:139:THR:HG22	2:D:140:PRO:O	2.06	0.55
1:G:248:GLU:HG3	1:G:307:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLU:HG3	1:C:307:ARG:NH2	2.20	0.55
1:E:453:GLY:O	1:E:469:LEU:HB2	2.06	0.55
2:H:105:SER:HB3	2:H:235:HIS:CE1	2.41	0.55
2:F:72:ARG:HH12	2:F:409:THR:HA	1.71	0.55
2:H:72:ARG:HH12	2:H:409:THR:HA	1.71	0.55
1:E:248:GLU:HG3	1:E:307:ARG:NH2	2.20	0.55
2:H:125:ARG:HG2	2:H:125:ARG:HH11	1.71	0.55
1:G:298:GLU:O	1:G:302:GLU:HG3	2.06	0.55
1:E:298:GLU:O	1:E:302:GLU:HG3	2.06	0.55
1:E:337:TRP:HZ3	1:E:368:LEU:HD13	1.72	0.55
1:G:337:TRP:HZ3	1:G:368:LEU:HD13	1.72	0.55
1:A:337:TRP:HZ3	1:A:368:LEU:HD13	1.72	0.55
1:A:540:LYS:HZ3	2:B:261:VAL:CG1	2.19	0.55
1:E:439:THR:HG22	1:E:441:TYR:CE1	2.42	0.55
2:D:72:ARG:HH12	2:D:409:THR:HA	1.71	0.55
1:G:98:ALA:HB1	1:G:349:LEU:HB3	1.89	0.55
2:B:139:THR:HG22	2:B:140:PRO:O	2.06	0.55
2:F:376:THR:HB	2:F:386:THR:HG22	1.88	0.55
1:G:329:ILE:HD12	1:G:391:LEU:CD2	2.36	0.55
1:C:439:THR:HG22	1:C:441:TYR:CE1	2.42	0.55
2:F:97:PRO:O	2:F:98:ALA:HB3	2.07	0.55
2:F:61:PHE:CE2	2:F:403:THR:HG22	2.41	0.55
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.89	0.55
1:E:28:GLU:HB3	1:E:32:LYS:HE3	1.88	0.55
2:B:125:ARG:HG2	2:B:125:ARG:HH11	1.71	0.55
2:H:368:LEU:O	2:H:371:ALA:HB3	2.07	0.55
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.42	0.55
2:B:97:PRO:O	2:B:98:ALA:HB3	2.07	0.55
1:G:28:GLU:HB3	1:G:32:LYS:HE3	1.88	0.55
1:C:298:GLU:O	1:C:302:GLU:HG3	2.06	0.55
2:H:366:LYS:O	2:H:370:GLU:HG3	2.07	0.55
1:C:337:TRP:HZ3	1:C:368:LEU:HD13	1.72	0.55
1:G:537:PRO:HD2	1:G:542:ILE:HD11	1.88	0.55
1:G:323:LYS:HD3	1:G:344:GLU:OE2	2.07	0.55
1:E:323:LYS:HD3	1:E:344:GLU:OE2	2.07	0.55
2:B:201:LYS:HD3	2:B:204:GLU:OE1	2.07	0.55
2:H:61:PHE:CZ	2:H:402:TRP:CZ2	2.95	0.55
2:B:72:ARG:HH12	2:B:409:THR:HA	1.71	0.55
1:C:232:TYR:HD1	1:C:241:VAL:HG22	1.70	0.55
1:C:98:ALA:HB1	1:C:349:LEU:HB3	1.89	0.55
2:D:379:SER:OG	2:D:387:PRO:HD3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:LYS:O	2:D:236:PRO:HB2	2.07	0.55
2:B:101:LYS:O	2:B:236:PRO:HB2	2.07	0.55
1:A:298:GLU:O	1:A:302:GLU:HG3	2.06	0.55
1:E:517:LEU:O	1:E:521:ILE:HG13	2.06	0.55
1:G:439:THR:HG22	1:G:441:TYR:CE1	2.42	0.55
1:E:537:PRO:HD2	1:E:542:ILE:HD11	1.88	0.55
2:H:201:LYS:HD3	2:H:204:GLU:OE1	2.07	0.55
2:B:104:LYS:HZ3	2:B:194:GLU:HA	1.72	0.55
2:D:201:LYS:HD3	2:D:204:GLU:OE1	2.07	0.55
1:E:98:ALA:HB1	1:E:349:LEU:HB3	1.89	0.55
1:G:229:TRP:CH2	1:G:230:MET:HE1	2.42	0.55
1:E:491:LEU:HB3	1:E:529:GLU:HB3	1.88	0.55
1:A:401:TRP:HB2	1:A:425:LEU:HD21	1.89	0.55
1:C:332:GLN:O	1:C:332:GLN:HG2	2.07	0.55
1:C:346:PHE:CE1	1:G:390:LYS:CD	2.86	0.55
1:C:491:LEU:HB3	1:C:529:GLU:HB3	1.88	0.55
1:C:496:VAL:HG22	1:C:534:ALA:HB3	1.89	0.55
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.89	0.55
1:A:332:GLN:O	1:A:332:GLN:HG2	2.07	0.55
1:E:329:ILE:HD12	1:E:391:LEU:CD2	2.36	0.54
1:C:323:LYS:HD3	1:C:344:GLU:OE2	2.07	0.54
1:A:99:GLY:HA2	1:A:383:TRP:HZ3	1.72	0.54
1:C:229:TRP:CZ3	1:C:230:MET:HE1	2.43	0.54
2:D:125:ARG:HH11	2:D:125:ARG:HG2	1.71	0.54
1:G:5:ILE:HD11	1:G:166:LYS:HD2	1.89	0.54
2:B:366:LYS:O	2:B:370:GLU:HG3	2.07	0.54
1:A:463:ARG:HG3	1:A:463:ARG:HH11	1.72	0.54
2:H:97:PRO:O	2:H:98:ALA:HB3	2.07	0.54
2:D:104:LYS:HZ3	2:D:194:GLU:HA	1.72	0.54
2:B:376:THR:HB	2:B:386:THR:HG22	1.88	0.54
2:D:27:THR:O	2:D:29:GLU:N	2.41	0.54
1:G:201:LYS:HD3	1:G:204:GLU:OE2	2.07	0.54
1:A:201:LYS:HD3	1:A:204:GLU:OE2	2.07	0.54
1:E:332:GLN:O	1:E:332:GLN:HG2	2.07	0.54
1:E:342:TYR:HB3	1:E:348:ASN:HB3	1.89	0.54
2:F:318:TYR:HE1	2:F:347:LYS:HD3	1.73	0.54
1:A:491:LEU:HB3	1:A:529:GLU:HB3	1.88	0.54
1:A:200:THR:O	1:A:203:GLU:HB3	2.07	0.54
1:C:5:ILE:HD11	1:C:166:LYS:HD2	1.89	0.54
1:A:537:PRO:CG	2:B:262:GLY:HA2	2.38	0.54
2:D:303:LEU:HD13	2:D:307:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:PRO:O	2:D:98:ALA:HB3	2.07	0.54
1:G:131:THR:HA	1:G:142:ILE:O	2.07	0.54
1:C:99:GLY:HA2	1:C:383:TRP:HZ3	1.72	0.54
2:B:318:TYR:HE1	2:B:347:LYS:HD3	1.73	0.54
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.43	0.54
1:A:126:LYS:HA	1:A:145:GLN:HE21	1.73	0.54
1:A:537:PRO:HD2	1:A:542:ILE:HD11	1.88	0.54
1:C:537:PRO:CG	2:D:262:GLY:HA2	2.38	0.54
2:F:303:LEU:HD13	2:F:307:ARG:NH2	2.23	0.54
1:E:131:THR:HA	1:E:142:ILE:O	2.07	0.54
1:G:99:GLY:HA2	1:G:383:TRP:HZ3	1.72	0.54
1:E:229:TRP:CH2	1:E:230:MET:HE1	2.42	0.54
2:F:366:LYS:O	2:F:370:GLU:HG3	2.07	0.54
2:B:27:THR:O	2:B:29:GLU:N	2.41	0.54
1:G:200:THR:O	1:G:203:GLU:HB3	2.07	0.54
1:C:463:ARG:HH11	1:C:463:ARG:HG3	1.72	0.54
1:G:332:GLN:O	1:G:332:GLN:HG2	2.07	0.54
1:C:346:PHE:HD1	1:G:390:LYS:CE	1.66	0.54
2:B:303:LEU:HD13	2:B:307:ARG:NH2	2.23	0.54
2:H:303:LEU:HD13	2:H:307:ARG:NH2	2.23	0.54
1:C:342:TYR:HB3	1:C:348:ASN:HB3	1.89	0.54
1:A:323:LYS:HD3	1:A:344:GLU:OE2	2.07	0.54
1:C:98:ALA:O	1:C:383:TRP:HZ3	1.91	0.54
1:A:98:ALA:O	1:A:383:TRP:HZ3	1.91	0.54
1:G:97:PRO:HD3	1:G:232:TYR:CZ	2.43	0.54
2:D:318:TYR:HE1	2:D:347:LYS:HD3	1.72	0.54
2:F:93:GLY:O	2:F:94:ILE:O	2.26	0.54
2:B:93:GLY:O	2:B:94:ILE:O	2.26	0.54
2:F:27:THR:O	2:F:29:GLU:N	2.41	0.54
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.89	0.54
2:F:97:PRO:C	2:F:99:GLY:H	2.11	0.54
2:F:61:PHE:CZ	2:F:402:TRP:CZ2	2.95	0.54
1:C:200:THR:O	1:C:203:GLU:HB3	2.07	0.54
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.43	0.54
1:E:200:THR:O	1:E:203:GLU:HB3	2.07	0.54
1:C:401:TRP:HB2	1:C:425:LEU:HD21	1.89	0.54
1:G:496:VAL:HG22	1:G:534:ALA:HB3	1.89	0.54
1:E:401:TRP:HB2	1:E:425:LEU:HD21	1.89	0.54
2:D:366:LYS:O	2:D:370:GLU:HG3	2.07	0.54
1:G:463:ARG:HH11	1:G:463:ARG:HG3	1.72	0.54
2:F:392:PRO:O	2:F:392:PRO:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:PHE:CZ	2:D:402:TRP:CZ2	2.95	0.54
1:A:341:ILE:HD11	1:A:350:LYS:HB3	1.90	0.54
1:G:341:ILE:HD11	1:G:350:LYS:HB3	1.90	0.54
2:D:376:THR:HB	2:D:386:THR:HG22	1.88	0.54
2:H:376:THR:HB	2:H:386:THR:HG22	1.88	0.54
2:F:368:LEU:O	2:F:371:ALA:HB3	2.07	0.54
1:C:201:LYS:HD3	1:C:204:GLU:OE2	2.07	0.54
2:D:392:PRO:O	2:D:392:PRO:HG2	2.08	0.54
2:H:97:PRO:C	2:H:99:GLY:H	2.11	0.54
2:B:61:PHE:CZ	2:B:402:TRP:CZ2	2.95	0.54
1:A:131:THR:HA	1:A:142:ILE:O	2.07	0.54
2:H:318:TYR:HE1	2:H:347:LYS:HD3	1.73	0.54
1:E:126:LYS:HA	1:E:145:GLN:HE21	1.73	0.54
2:B:365:VAL:HG12	2:B:405:TYR:CE2	2.43	0.54
1:C:341:ILE:HD11	1:C:350:LYS:HB3	1.90	0.54
1:C:182:GLN:HG2	1:C:183:TYR:N	2.23	0.54
1:A:28:GLU:HB3	1:A:32:LYS:HE3	1.88	0.54
1:C:28:GLU:HB3	1:C:32:LYS:HE3	1.88	0.54
1:C:126:LYS:HA	1:C:145:GLN:HE21	1.72	0.54
2:H:27:THR:O	2:H:29:GLU:N	2.41	0.54
2:H:103:LYS:HZ1	2:H:179:VAL:HG23	1.70	0.53
1:G:98:ALA:O	1:G:383:TRP:HZ3	1.91	0.53
1:G:402:TRP:CE3	1:G:402:TRP:C	2.82	0.53
2:D:368:LEU:O	2:D:371:ALA:HB3	2.07	0.53
1:G:441:TYR:CD2	1:G:544:GLY:HA3	2.44	0.53
1:E:537:PRO:CG	2:F:262:GLY:HA2	2.38	0.53
1:E:97:PRO:HD3	1:E:232:TYR:CZ	2.43	0.53
1:C:97:PRO:HD3	1:C:232:TYR:CZ	2.43	0.53
1:A:182:GLN:HG2	1:A:183:TYR:N	2.23	0.53
1:A:229:TRP:CZ3	1:A:230:MET:HE1	2.43	0.53
2:D:93:GLY:O	2:D:94:ILE:O	2.26	0.53
1:C:402:TRP:CE3	1:C:402:TRP:C	2.82	0.53
2:F:101:LYS:O	2:F:236:PRO:HB2	2.07	0.53
2:B:368:LEU:O	2:B:371:ALA:HB3	2.07	0.53
1:E:463:ARG:HG3	1:E:463:ARG:HH11	1.72	0.53
1:G:475:GLN:HB3	1:G:501:TYR:CE2	2.43	0.53
1:G:537:PRO:CG	2:H:262:GLY:HA2	2.38	0.53
2:H:365:VAL:HG12	2:H:405:TYR:CE2	2.43	0.53
2:F:153:TRP:CE3	2:F:155:GLY:HA3	2.43	0.53
1:E:341:ILE:HD11	1:E:350:LYS:HB3	1.90	0.53
1:G:401:TRP:HB2	1:G:425:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:101:LYS:O	2:H:236:PRO:HB2	2.07	0.53
1:E:496:VAL:HG22	1:E:534:ALA:HB3	1.89	0.53
1:C:537:PRO:HD2	1:C:542:ILE:HD11	1.88	0.53
2:D:103:LYS:NZ	2:D:179:VAL:N	2.55	0.53
2:D:153:TRP:CE3	2:D:155:GLY:HA3	2.43	0.53
1:C:131:THR:HA	1:C:142:ILE:O	2.07	0.53
1:A:341:ILE:HD12	1:A:383:TRP:NE1	2.23	0.53
1:A:402:TRP:CE3	1:A:402:TRP:C	2.82	0.53
1:G:342:TYR:HB3	1:G:348:ASN:HB3	1.89	0.53
2:D:268:SER:HA	2:D:274:ILE:HG22	1.90	0.53
2:B:103:LYS:NZ	2:B:179:VAL:N	2.55	0.53
2:F:201:LYS:HD3	2:F:204:GLU:OE1	2.07	0.53
1:A:97:PRO:HD3	1:A:232:TYR:CZ	2.43	0.53
2:B:392:PRO:O	2:B:392:PRO:HG2	2.08	0.53
2:F:365:VAL:HG12	2:F:405:TYR:CE2	2.43	0.53
2:H:153:TRP:CE3	2:H:155:GLY:HA3	2.43	0.53
1:C:341:ILE:HD12	1:C:383:TRP:NE1	2.23	0.53
1:E:201:LYS:HD3	1:E:204:GLU:OE2	2.07	0.53
1:C:346:PHE:CG	1:G:390:LYS:HD2	2.44	0.53
2:F:268:SER:HA	2:F:274:ILE:HG22	1.90	0.53
1:A:342:TYR:HB3	1:A:348:ASN:HB3	1.89	0.53
1:G:126:LYS:HA	1:G:145:GLN:HE21	1.73	0.53
1:E:196:GLY:O	1:E:199:ARG:HB3	2.09	0.53
1:C:196:GLY:O	1:C:199:ARG:HB3	2.09	0.53
1:E:475:GLN:HB3	1:E:501:TYR:CE2	2.43	0.53
1:A:106:VAL:O	1:A:227:PHE:CZ	2.62	0.53
1:C:345:PRO:CG	1:G:326:ILE:HD11	2.19	0.53
2:F:264:LEU:HB2	2:F:276:VAL:CG1	2.39	0.53
2:D:365:VAL:HG12	2:D:405:TYR:CE2	2.43	0.53
2:B:153:TRP:CE3	2:B:155:GLY:HA3	2.43	0.53
2:H:93:GLY:O	2:H:94:ILE:O	2.26	0.53
1:A:465:LYS:O	1:A:466:VAL:HG23	2.08	0.53
1:E:5:ILE:HD11	1:E:166:LYS:HD2	1.89	0.53
1:E:408:ALA:HB1	2:F:364:ASP:HB3	1.91	0.53
1:C:106:VAL:O	1:C:227:PHE:CZ	2.62	0.53
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.44	0.53
1:E:441:TYR:CD2	1:E:544:GLY:HA3	2.44	0.53
1:G:372:VAL:HG11	1:G:411:ILE:HG23	1.91	0.53
1:E:99:GLY:HA2	1:E:383:TRP:HZ3	1.72	0.53
2:H:13:LYS:HB3	2:H:14:PRO:HD2	1.91	0.53
1:E:106:VAL:O	1:E:227:PHE:CZ	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:VAL:CG2	1:G:346:PHE:CG	2.92	0.52
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.44	0.52
2:D:264:LEU:HB2	2:D:276:VAL:CG1	2.39	0.52
1:G:491:LEU:HB3	1:G:529:GLU:HB2	1.91	0.52
1:G:196:GLY:O	1:G:199:ARG:HB3	2.09	0.52
1:G:408:ALA:HB1	2:H:364:ASP:HB3	1.91	0.52
2:B:264:LEU:HB2	2:B:276:VAL:CG1	2.39	0.52
2:H:268:SER:HA	2:H:274:ILE:HG22	1.90	0.52
1:C:105:SER:HB3	1:C:198:HIS:CG	2.45	0.52
1:A:105:SER:HB3	1:A:198:HIS:CG	2.44	0.52
1:E:98:ALA:O	1:E:383:TRP:HZ3	1.91	0.52
1:A:157:PRO:HG2	1:A:158:ALA:N	2.24	0.52
1:G:465:LYS:O	1:G:466:VAL:HG23	2.08	0.52
1:E:465:LYS:O	1:E:466:VAL:HG23	2.08	0.52
1:C:408:ALA:HB1	2:D:364:ASP:HB3	1.91	0.52
1:E:402:TRP:C	1:E:402:TRP:CE3	2.82	0.52
1:A:196:GLY:O	1:A:199:ARG:HB3	2.09	0.52
2:H:392:PRO:O	2:H:392:PRO:HG2	2.08	0.52
1:G:414:TRP:CE3	1:G:415:GLU:N	2.78	0.52
1:A:540:LYS:CE	2:B:265:ASN:HB2	2.40	0.52
2:D:246:LEU:HB2	2:D:307:ARG:HH12	1.75	0.52
1:G:105:SER:HB3	1:G:198:HIS:CG	2.44	0.52
2:B:72:ARG:NH1	2:B:409:THR:HG22	2.25	0.52
1:G:182:GLN:HG2	1:G:183:TYR:N	2.23	0.52
1:C:414:TRP:CE3	1:C:415:GLU:N	2.78	0.52
2:B:246:LEU:HB2	2:B:307:ARG:HH12	1.75	0.52
2:B:268:SER:HA	2:B:274:ILE:HG22	1.90	0.52
2:H:264:LEU:HB2	2:H:276:VAL:CG1	2.39	0.52
1:E:540:LYS:CE	2:F:265:ASN:HB2	2.40	0.52
1:C:372:VAL:HG11	1:C:411:ILE:HG23	1.91	0.52
1:E:157:PRO:HG2	1:E:158:ALA:N	2.24	0.52
1:C:126:LYS:HA	1:C:145:GLN:NE2	2.25	0.52
1:A:452:LEU:HD22	1:A:470:THR:HG22	1.92	0.52
2:D:35:VAL:O	2:D:39:THR:HG23	2.10	0.52
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.91	0.52
2:F:329:ILE:HA	2:F:338:THR:O	2.10	0.52
2:D:97:PRO:C	2:D:99:GLY:H	2.11	0.52
1:C:326:ILE:HG21	1:G:345:PRO:HG3	1.91	0.52
1:C:465:LYS:O	1:C:466:VAL:HG23	2.08	0.52
1:A:402:TRP:CE3	1:A:403:THR:HA	2.45	0.52
1:E:452:LEU:HD22	1:E:470:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:454:LYS:HA	1:G:467:VAL:O	2.10	0.52
2:B:35:VAL:O	2:B:39:THR:HG23	2.10	0.52
1:G:106:VAL:O	1:G:227:PHE:CZ	2.62	0.52
1:E:414:TRP:CE3	1:E:415:GLU:N	2.78	0.52
1:A:126:LYS:HA	1:A:145:GLN:NE2	2.25	0.52
1:G:126:LYS:HA	1:G:145:GLN:NE2	2.25	0.52
2:F:326:ILE:O	2:F:341:ILE:HA	2.10	0.52
2:H:35:VAL:O	2:H:39:THR:HG23	2.10	0.52
1:A:441:TYR:CE2	1:A:543:GLY:O	2.63	0.52
1:E:441:TYR:CE2	1:E:543:GLY:O	2.63	0.52
2:B:97:PRO:C	2:B:99:GLY:H	2.11	0.52
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.91	0.52
1:G:91:GLN:HE21	1:G:91:GLN:CA	2.22	0.52
2:H:329:ILE:HA	2:H:338:THR:O	2.10	0.52
1:C:441:TYR:CE2	1:C:543:GLY:O	2.63	0.52
2:F:103:LYS:NZ	2:F:179:VAL:N	2.55	0.52
1:C:249:LYS:HG2	1:C:250:ASP:H	1.75	0.52
1:E:491:LEU:HB3	1:E:529:GLU:HB2	1.91	0.52
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.91	0.52
1:A:402:TRP:O	1:A:402:TRP:HE3	1.93	0.52
2:F:13:LYS:HB3	2:F:14:PRO:HD2	1.91	0.52
1:E:454:LYS:HA	1:E:467:VAL:O	2.10	0.52
1:A:324:ASP:O	1:A:343:GLN:HG2	2.09	0.52
1:G:341:ILE:HD12	1:G:383:TRP:NE1	2.23	0.52
1:C:491:LEU:HB3	1:C:529:GLU:HB2	1.91	0.52
2:F:35:VAL:O	2:F:39:THR:HG23	2.10	0.52
2:F:9:PRO:HA	2:F:121:ASP:OD2	2.10	0.52
2:D:13:LYS:HB3	2:D:14:PRO:HD2	1.91	0.52
1:C:326:ILE:CB	1:C:342:TYR:CE1	2.92	0.51
1:E:324:ASP:O	1:E:343:GLN:HG2	2.09	0.51
1:E:361:HIS:CD2	1:E:505:ILE:CG2	2.93	0.51
1:C:157:PRO:HG2	1:C:158:ALA:N	2.24	0.51
1:E:182:GLN:HG2	1:E:183:TYR:N	2.23	0.51
2:H:376:THR:HG22	2:H:389:PHE:CZ	2.45	0.51
1:E:126:LYS:HA	1:E:145:GLN:NE2	2.25	0.51
1:C:402:TRP:CE3	1:C:403:THR:HA	2.45	0.51
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.10	0.51
2:B:13:LYS:HB3	2:B:14:PRO:HD2	1.91	0.51
1:C:540:LYS:CE	2:D:265:ASN:HB2	2.40	0.51
1:C:540:LYS:HZ3	2:D:261:VAL:HG12	1.74	0.51
2:H:103:LYS:NZ	2:H:179:VAL:N	2.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:104:LYS:HZ1	2:H:194:GLU:HA	1.74	0.51
1:G:410:TRP:CH2	1:G:412:PRO:HA	2.46	0.51
1:A:249:LYS:HG2	1:A:250:ASP:H	1.75	0.51
1:A:118:VAL:HG12	1:A:118:VAL:O	2.10	0.51
2:D:376:THR:HG22	2:D:389:PHE:CZ	2.45	0.51
1:C:402:TRP:HE3	1:C:402:TRP:O	1.93	0.51
2:H:326:ILE:O	2:H:341:ILE:HA	2.10	0.51
1:C:452:LEU:HD22	1:C:470:THR:HG22	1.92	0.51
1:G:542:ILE:O	1:G:545:ASN:HB3	2.11	0.51
1:G:540:LYS:CE	2:H:265:ASN:HB2	2.40	0.51
2:D:97:PRO:HB3	2:D:179:VAL:HG11	1.93	0.51
1:E:105:SER:HB3	1:E:198:HIS:CG	2.45	0.51
1:E:410:TRP:CH2	1:E:412:PRO:HA	2.46	0.51
2:H:24:TRP:CH2	2:H:61:PHE:CE1	2.88	0.51
1:G:157:PRO:HG2	1:G:158:ALA:N	2.24	0.51
1:E:341:ILE:HD12	1:E:383:TRP:NE1	2.23	0.51
1:G:206:ARG:NH2	1:G:218:ASP:HA	2.25	0.51
2:B:376:THR:HG22	2:B:389:PHE:CZ	2.45	0.51
1:A:454:LYS:HA	1:A:467:VAL:O	2.10	0.51
1:G:441:TYR:CE2	1:G:543:GLY:O	2.63	0.51
2:H:246:LEU:HB2	2:H:307:ARG:HH12	1.75	0.51
1:E:372:VAL:HG11	1:E:411:ILE:HG23	1.91	0.51
1:E:326:ILE:CB	1:E:342:TYR:CE1	2.92	0.51
1:E:249:LYS:HG2	1:E:250:ASP:H	1.75	0.51
1:C:118:VAL:HG12	1:C:118:VAL:O	2.10	0.51
1:G:402:TRP:CE3	1:G:403:THR:HA	2.45	0.51
2:B:329:ILE:HA	2:B:338:THR:O	2.10	0.51
1:C:324:ASP:O	1:C:343:GLN:HG2	2.09	0.51
1:C:391:LEU:HD12	1:C:414:TRP:CZ3	2.46	0.51
1:G:118:VAL:HG12	1:G:118:VAL:O	2.10	0.51
2:H:54:ASN:ND2	2:H:56:TYR:HB2	2.25	0.51
2:D:54:ASN:ND2	2:D:56:TYR:HB2	2.25	0.51
1:G:391:LEU:HD12	1:G:414:TRP:CZ3	2.46	0.51
1:A:391:LEU:HD12	1:A:414:TRP:CZ3	2.46	0.51
1:E:91:GLN:HE21	1:E:91:GLN:CA	2.21	0.51
2:D:10:VAL:HG21	2:D:153:TRP:CH2	2.46	0.51
1:A:361:HIS:CD2	1:A:505:ILE:CG2	2.93	0.51
2:D:9:PRO:HA	2:D:121:ASP:OD2	2.10	0.51
2:B:10:VAL:HG21	2:B:153:TRP:CH2	2.46	0.51
1:G:160:PHE:CZ	1:G:164:MET:HG2	2.46	0.51
1:E:402:TRP:CE3	1:E:403:THR:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:LYS:O	1:C:471:ASN:HA	2.11	0.51
2:D:326:ILE:O	2:D:341:ILE:HA	2.10	0.51
1:C:542:ILE:O	1:C:545:ASN:HB3	2.11	0.51
1:G:540:LYS:HZ3	2:H:261:VAL:CG1	2.24	0.51
1:C:342:TYR:OH	1:G:345:PRO:HB3	2.08	0.51
1:A:326:ILE:CB	1:A:342:TYR:CE1	2.92	0.51
2:H:10:VAL:HG21	2:H:153:TRP:CH2	2.46	0.51
2:D:10:VAL:HG21	2:D:153:TRP:HH2	1.76	0.51
2:B:10:VAL:HG21	2:B:153:TRP:HH2	1.76	0.51
2:F:376:THR:HG22	2:F:389:PHE:CZ	2.45	0.51
1:C:454:LYS:HA	1:C:467:VAL:O	2.10	0.51
2:B:97:PRO:HB3	2:B:179:VAL:HG11	1.93	0.51
2:F:194:GLU:HG2	2:F:195:ILE:N	2.26	0.51
2:H:10:VAL:HG21	2:H:153:TRP:HH2	1.76	0.51
1:C:164:MET:HE2	1:C:187:LEU:HD21	1.93	0.51
1:E:118:VAL:O	1:E:118:VAL:HG12	2.10	0.51
2:F:54:ASN:ND2	2:F:56:TYR:HB2	2.25	0.51
1:G:452:LEU:HD22	1:G:470:THR:HG22	1.92	0.51
1:C:12:LEU:HD11	1:C:127:TYR:CE1	2.46	0.51
2:H:9:PRO:HA	2:H:121:ASP:OD2	2.10	0.51
1:G:326:ILE:CG2	1:G:342:TYR:CE1	2.94	0.51
1:E:540:LYS:NZ	2:F:276:VAL:HG21	2.26	0.51
1:C:410:TRP:CH2	1:C:412:PRO:HA	2.46	0.51
1:E:361:HIS:NE2	1:E:518:VAL:HG21	2.26	0.51
1:C:160:PHE:CZ	1:C:164:MET:HG2	2.46	0.51
1:C:206:ARG:NH2	1:C:218:ASP:HA	2.25	0.51
1:A:451:LYS:O	1:A:471:ASN:HA	2.11	0.51
1:G:451:LYS:O	1:G:471:ASN:HA	2.11	0.51
2:B:326:ILE:O	2:B:341:ILE:HA	2.10	0.51
1:E:391:LEU:HD12	1:E:414:TRP:CZ3	2.46	0.50
1:E:542:ILE:O	1:E:545:ASN:HB3	2.11	0.50
1:C:326:ILE:CG2	1:C:342:TYR:CE1	2.94	0.50
2:D:24:TRP:HZ3	2:D:61:PHE:HB3	1.77	0.50
1:G:361:HIS:NE2	1:G:518:VAL:HG21	2.26	0.50
1:A:363:ASN:ND2	1:A:365:VAL:HB	2.26	0.50
1:E:402:TRP:O	1:E:402:TRP:HE3	1.93	0.50
2:D:329:ILE:HA	2:D:338:THR:O	2.10	0.50
1:A:414:TRP:CE3	1:A:415:GLU:N	2.78	0.50
1:C:540:LYS:HZ3	2:D:261:VAL:HG13	1.76	0.50
1:G:361:HIS:CD2	1:G:505:ILE:CG2	2.93	0.50
1:C:361:HIS:CD2	1:C:505:ILE:CG2	2.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:ARG:NH1	2:H:409:THR:HA	2.26	0.50
1:C:363:ASN:ND2	1:C:365:VAL:HB	2.26	0.50
2:B:54:ASN:ND2	2:B:56:TYR:HB2	2.25	0.50
1:G:402:TRP:HE3	1:G:402:TRP:O	1.93	0.50
1:C:417:VAL:CG1	1:G:346:PHE:HE2	2.12	0.50
2:H:97:PRO:HB3	2:H:179:VAL:HG11	1.93	0.50
1:G:244:ILE:HB	1:G:310:LEU:HD22	1.94	0.50
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.46	0.50
1:G:90:VAL:HG12	2:H:141:GLY:N	2.24	0.50
1:G:132:ILE:HD11	1:G:144:TYR:HE2	1.77	0.50
1:G:249:LYS:HG2	1:G:250:ASP:H	1.75	0.50
1:E:160:PHE:CZ	1:E:164:MET:HG2	2.46	0.50
1:A:240:THR:HG22	1:A:315:HIS:CB	2.42	0.50
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.46	0.50
1:C:417:VAL:HG22	1:G:346:PHE:CG	2.47	0.50
1:A:542:ILE:O	1:A:545:ASN:HB3	2.11	0.50
1:E:540:LYS:NZ	2:F:261:VAL:O	2.45	0.50
1:C:419:THR:CG2	1:C:420:PRO:HD2	2.41	0.50
1:A:419:THR:CG2	1:A:420:PRO:HD2	2.41	0.50
1:A:90:VAL:HG12	1:A:90:VAL:O	2.12	0.50
1:A:160:PHE:CZ	1:A:164:MET:HG2	2.46	0.50
1:A:194:GLU:O	1:A:196:GLY:N	2.45	0.50
1:C:468:PRO:HG2	1:C:468:PRO:O	2.12	0.50
1:G:324:ASP:O	1:G:343:GLN:HG2	2.09	0.50
1:E:244:ILE:HB	1:E:310:LEU:HD22	1.94	0.50
1:A:345:PRO:HG3	1:E:326:ILE:HD13	1.94	0.50
2:F:10:VAL:HG21	2:F:153:TRP:HH2	1.76	0.50
1:A:361:HIS:NE2	1:A:518:VAL:HG21	2.26	0.50
1:C:361:HIS:NE2	1:C:518:VAL:HG21	2.26	0.50
1:G:318:TYR:HD1	1:G:318:TYR:N	2.10	0.50
2:B:27:THR:C	2:B:29:GLU:H	2.15	0.50
1:E:451:LYS:O	1:E:471:ASN:HA	2.11	0.50
1:A:540:LYS:NZ	2:B:276:VAL:HG21	2.26	0.50
1:A:244:ILE:HB	1:A:310:LEU:HD22	1.94	0.50
1:A:326:ILE:CG2	1:A:342:TYR:CE1	2.94	0.50
2:F:72:ARG:NH1	2:F:409:THR:HG22	2.25	0.50
1:G:229:TRP:O	1:G:230:MET:HB2	2.12	0.50
1:A:328:GLU:HG2	1:A:330:GLN:HE21	1.77	0.50
1:C:240:THR:HG22	1:C:315:HIS:CB	2.42	0.50
1:E:194:GLU:O	1:E:196:GLY:N	2.45	0.50
1:G:540:LYS:NZ	2:H:276:VAL:HG21	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:194:GLU:HG2	2:H:195:ILE:N	2.26	0.50
2:D:61:PHE:CZ	2:D:402:TRP:HZ2	2.30	0.50
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.25	0.50
1:C:540:LYS:NZ	2:D:261:VAL:O	2.45	0.50
2:F:246:LEU:HB2	2:F:307:ARG:HH12	1.75	0.50
1:C:342:TYR:CZ	1:G:345:PRO:CG	2.92	0.50
2:H:61:PHE:CZ	2:H:402:TRP:HZ2	2.30	0.50
1:E:90:VAL:HG12	1:E:90:VAL:O	2.12	0.50
2:B:156:SER:N	2:B:157:PRO:HD2	2.27	0.50
1:E:363:ASN:ND2	1:E:365:VAL:HB	2.27	0.50
1:C:194:GLU:O	1:C:196:GLY:N	2.45	0.50
1:G:468:PRO:HG2	1:G:468:PRO:O	2.12	0.50
1:E:399:GLU:HG2	1:E:399:GLU:O	2.12	0.50
1:A:540:LYS:NZ	2:B:261:VAL:O	2.45	0.50
1:G:540:LYS:NZ	2:H:261:VAL:O	2.45	0.50
2:D:194:GLU:HG2	2:D:195:ILE:N	2.26	0.50
1:E:344:GLU:HB2	1:E:347:LYS:HB2	1.94	0.50
2:F:72:ARG:NH1	2:F:409:THR:HA	2.26	0.50
1:C:328:GLU:HG2	1:C:330:GLN:HE21	1.76	0.50
1:G:12:LEU:HD11	1:G:127:TYR:CE1	2.46	0.50
1:E:12:LEU:HD11	1:E:127:TYR:CE1	2.46	0.50
1:G:399:GLU:O	1:G:399:GLU:HG2	2.12	0.50
1:G:328:GLU:HG2	1:G:330:GLN:HE21	1.76	0.49
1:G:394:GLN:HG2	1:G:416:PHE:CE2	2.47	0.49
1:C:244:ILE:HB	1:C:310:LEU:HD22	1.94	0.49
2:B:61:PHE:CZ	2:B:402:TRP:HZ2	2.30	0.49
2:F:24:TRP:CH2	2:F:61:PHE:CE1	2.88	0.49
1:G:90:VAL:HG12	1:G:90:VAL:O	2.12	0.49
2:B:72:ARG:NH1	2:B:409:THR:HA	2.26	0.49
2:H:27:THR:C	2:H:29:GLU:H	2.15	0.49
1:G:194:GLU:O	1:G:196:GLY:N	2.45	0.49
2:F:10:VAL:HG21	2:F:153:TRP:CH2	2.46	0.49
2:F:156:SER:N	2:F:157:PRO:HD2	2.27	0.49
1:C:90:VAL:O	1:C:90:VAL:HG12	2.12	0.49
1:E:206:ARG:NH2	1:E:218:ASP:HA	2.25	0.49
1:E:240:THR:HG22	1:E:315:HIS:CB	2.42	0.49
2:D:27:THR:C	2:D:29:GLU:H	2.15	0.49
1:G:447:ASN:HB3	1:G:450:THR:OG1	2.12	0.49
1:C:345:PRO:HG3	1:G:326:ILE:HD13	1.34	0.49
2:B:194:GLU:HG2	2:B:195:ILE:N	2.26	0.49
1:A:90:VAL:O	1:A:91:GLN:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ILE:HD11	1:C:144:TYR:HE2	1.77	0.49
1:G:183:TYR:CD2	1:G:230:MET:HG2	2.47	0.49
1:C:169:GLU:HB3	1:C:170:PRO:HD3	1.95	0.49
1:G:240:THR:HG22	1:G:315:HIS:CB	2.42	0.49
2:B:54:ASN:HD22	2:B:56:TYR:H	1.60	0.49
1:A:468:PRO:O	1:A:468:PRO:HG2	2.12	0.49
1:C:394:GLN:HG2	1:C:416:PHE:CE2	2.47	0.49
1:C:540:LYS:NZ	2:D:276:VAL:HG21	2.26	0.49
2:F:97:PRO:HB3	2:F:179:VAL:HG11	1.93	0.49
1:E:326:ILE:CG2	1:E:342:TYR:CE1	2.94	0.49
1:C:229:TRP:O	1:C:230:MET:HB2	2.12	0.49
1:G:363:ASN:ND2	1:G:365:VAL:HB	2.27	0.49
2:B:24:TRP:CZ3	2:B:61:PHE:CG	3.00	0.49
2:F:61:PHE:CZ	2:F:402:TRP:HZ2	2.30	0.49
1:E:90:VAL:HG12	2:F:141:GLY:N	2.25	0.49
1:C:90:VAL:O	1:C:91:GLN:NE2	2.45	0.49
2:D:156:SER:N	2:D:157:PRO:HD2	2.27	0.49
1:E:318:TYR:N	1:E:318:TYR:HD1	2.10	0.49
2:F:27:THR:C	2:F:29:GLU:H	2.15	0.49
1:E:468:PRO:O	1:E:468:PRO:HG2	2.12	0.49
1:E:191:SER:OG	1:E:198:HIS:CD2	2.66	0.49
2:F:24:TRP:CZ3	2:F:61:PHE:CG	3.00	0.49
1:C:90:VAL:HG12	2:D:141:GLY:N	2.24	0.49
1:E:132:ILE:HD11	1:E:144:TYR:HE2	1.77	0.49
2:D:72:ARG:NH1	2:D:409:THR:HA	2.26	0.49
2:H:72:ARG:NH1	2:H:409:THR:HG22	2.25	0.49
2:B:142:ILE:HG22	2:B:144:TYR:CE1	2.48	0.49
1:G:164:MET:HE2	1:G:187:LEU:HD21	1.95	0.49
1:C:318:TYR:N	1:C:318:TYR:HD1	2.10	0.49
2:F:54:ASN:HD22	2:F:56:TYR:H	1.60	0.49
2:F:27:THR:C	2:F:29:GLU:N	2.66	0.49
2:H:156:SER:N	2:H:157:PRO:HD2	2.27	0.49
1:G:473:THR:OG1	1:G:476:LYS:HG2	2.13	0.49
1:C:346:PHE:HZ	1:G:328:GLU:OE1	1.96	0.49
1:E:540:LYS:HZ3	2:F:261:VAL:HG13	1.76	0.49
2:D:24:TRP:CZ3	2:D:61:PHE:CG	3.00	0.49
1:A:132:ILE:HD11	1:A:144:TYR:HE2	1.77	0.49
1:A:164:MET:HE2	1:A:187:LEU:HD21	1.95	0.49
1:E:183:TYR:CD2	1:E:230:MET:HG2	2.47	0.49
1:A:394:GLN:HG2	1:A:416:PHE:CE2	2.47	0.49
1:G:169:GLU:HB3	1:G:170:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:VAL:HG12	2:D:188:TYR:CD2	2.48	0.49
1:E:328:GLU:HG2	1:E:330:GLN:HE21	1.77	0.49
2:H:27:THR:C	2:H:29:GLU:N	2.66	0.49
1:G:344:GLU:HB2	1:G:347:LYS:HB2	1.94	0.49
1:A:191:SER:OG	1:A:198:HIS:CD2	2.66	0.49
2:F:207:GLN:O	2:F:210:LEU:N	2.46	0.49
2:D:72:ARG:NH1	2:D:409:THR:HG22	2.25	0.49
1:E:394:GLN:HG2	1:E:416:PHE:CE2	2.47	0.49
1:A:318:TYR:N	1:A:318:TYR:HD1	2.10	0.49
2:H:108:VAL:HG12	2:H:188:TYR:CD2	2.48	0.49
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.95	0.49
1:A:46:LYS:HD2	1:A:116:PHE:HB3	1.94	0.49
2:D:27:THR:C	2:D:29:GLU:N	2.66	0.49
1:E:447:ASN:HB3	1:E:450:THR:OG1	2.12	0.49
2:H:207:GLN:O	2:H:210:LEU:N	2.46	0.49
1:G:356:ARG:HH21	1:G:358:ARG:NH1	2.11	0.49
2:H:142:ILE:HG22	2:H:144:TYR:CE1	2.48	0.49
1:A:229:TRP:O	1:A:230:MET:HB2	2.12	0.49
1:E:229:TRP:O	1:E:230:MET:HB2	2.12	0.49
1:C:46:LYS:HD2	1:C:116:PHE:HB3	1.94	0.49
1:A:342:TYR:CD1	1:A:342:TYR:C	2.87	0.48
2:D:142:ILE:HG22	2:D:144:TYR:CE1	2.48	0.48
1:C:183:TYR:CD2	1:C:230:MET:HG2	2.47	0.48
2:B:108:VAL:HG12	2:B:188:TYR:CD2	2.48	0.48
2:H:395:LYS:HG3	2:H:416:PHE:HE2	1.78	0.48
1:E:473:THR:OG1	1:E:476:LYS:HG2	2.13	0.48
1:G:326:ILE:CB	1:G:342:TYR:CE1	2.92	0.48
1:C:416:PHE:HD1	1:C:417:VAL:H	1.61	0.48
1:A:337:TRP:N	1:A:337:TRP:CD1	2.81	0.48
1:G:191:SER:OG	1:G:198:HIS:CD2	2.66	0.48
1:A:344:GLU:HB2	1:A:347:LYS:HB2	1.94	0.48
1:G:90:VAL:O	1:G:91:GLN:NE2	2.45	0.48
2:B:97:PRO:HD3	2:B:181:TYR:CD1	2.49	0.48
2:F:103:LYS:HZ2	2:F:179:VAL:HG23	1.74	0.48
1:C:344:GLU:HB2	1:C:347:LYS:HB2	1.94	0.48
1:C:10:VAL:HA	1:C:85:GLN:OE1	2.13	0.48
2:F:142:ILE:HG22	2:F:144:TYR:CE1	2.48	0.48
2:F:108:VAL:HG12	2:F:188:TYR:CD2	2.48	0.48
1:A:88:TRP:CZ2	2:B:57:ASN:CB	2.96	0.48
2:D:54:ASN:HD22	2:D:56:TYR:H	1.60	0.48
1:E:452:LEU:HD23	1:E:471:ASN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:452:LEU:HD23	1:G:471:ASN:H	1.78	0.48
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.12	0.48
1:G:342:TYR:C	1:G:342:TYR:CD1	2.87	0.48
1:G:416:PHE:HD1	1:G:417:VAL:H	1.61	0.48
2:D:97:PRO:HD3	2:D:181:TYR:CD1	2.49	0.48
1:C:191:SER:OG	1:C:198:HIS:CD2	2.66	0.48
1:E:342:TYR:CD1	1:E:342:TYR:C	2.87	0.48
2:D:153:TRP:CE3	2:D:156:SER:N	2.82	0.48
2:B:153:TRP:CE3	2:B:156:SER:N	2.82	0.48
1:E:356:ARG:HH21	1:E:358:ARG:NH1	2.11	0.48
1:A:356:ARG:HH21	1:A:358:ARG:NH1	2.11	0.48
1:E:96:HIS:CG	1:E:97:PRO:HD2	2.49	0.48
1:A:98:ALA:O	1:A:383:TRP:CZ3	2.66	0.48
1:G:98:ALA:O	1:G:383:TRP:CZ3	2.66	0.48
1:A:452:LEU:HD23	1:A:471:ASN:H	1.78	0.48
1:G:511:ASP:O	1:G:512:LYS:HD3	2.14	0.48
2:B:241:VAL:HG12	2:B:242:GLN:N	2.28	0.48
2:D:241:VAL:HG12	2:D:242:GLN:N	2.28	0.48
1:C:447:ASN:HB3	1:C:450:THR:OG1	2.12	0.48
1:G:419:THR:CG2	1:G:420:PRO:HD2	2.42	0.48
2:D:24:TRP:CH2	2:D:61:PHE:CE1	2.88	0.48
2:H:24:TRP:CZ3	2:H:61:PHE:CG	3.00	0.48
2:H:153:TRP:CE3	2:H:156:SER:N	2.82	0.48
1:A:10:VAL:HA	1:A:85:GLN:OE1	2.13	0.48
1:E:98:ALA:O	1:E:383:TRP:CZ3	2.66	0.48
1:A:183:TYR:CD2	1:A:230:MET:HG2	2.47	0.48
1:E:164:MET:HE2	1:E:187:LEU:HD21	1.96	0.48
2:B:27:THR:C	2:B:29:GLU:N	2.66	0.48
2:F:268:SER:HA	2:F:274:ILE:CG2	2.43	0.48
1:C:342:TYR:C	1:C:342:TYR:CD1	2.87	0.48
1:G:510:PRO:O	1:G:522:ILE:HD13	2.14	0.48
1:E:510:PRO:O	1:E:522:ILE:HD13	2.14	0.48
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.14	0.48
1:E:46:LYS:HD2	1:E:116:PHE:HB3	1.94	0.48
1:C:452:LEU:HD23	1:C:471:ASN:H	1.78	0.48
1:C:399:GLU:HG2	1:C:399:GLU:O	2.12	0.48
2:D:268:SER:HA	2:D:274:ILE:CG2	2.43	0.48
2:F:153:TRP:CE3	2:F:156:SER:N	2.82	0.48
1:A:90:VAL:HG12	2:B:141:GLY:N	2.24	0.48
1:G:10:VAL:HA	1:G:85:GLN:OE1	2.13	0.48
1:E:108:VAL:HG22	1:E:188:TYR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:TRP:CZ2	2:F:57:ASN:CB	2.96	0.48
2:D:207:GLN:O	2:D:210:LEU:N	2.46	0.48
1:E:90:VAL:O	1:E:91:GLN:NE2	2.45	0.48
1:E:10:VAL:HA	1:E:85:GLN:OE1	2.13	0.48
1:A:164:MET:HG3	1:A:182:GLN:NE2	2.29	0.48
1:A:416:PHE:HD1	1:A:417:VAL:H	1.61	0.48
1:G:46:LYS:HD2	1:G:116:PHE:HB3	1.94	0.48
2:D:395:LYS:HG3	2:D:416:PHE:HE2	1.78	0.48
1:E:455:ALA:HB2	1:E:469:LEU:HD11	1.96	0.48
2:F:336:GLN:HG2	2:F:355:ALA:CB	2.44	0.48
1:A:473:THR:OG1	1:A:476:LYS:HG2	2.13	0.48
1:E:540:LYS:HZ3	2:F:261:VAL:HG12	1.77	0.48
2:B:207:GLN:O	2:B:210:LEU:N	2.46	0.48
1:G:76:ASP:OD1	1:G:78:ARG:HG3	2.14	0.48
1:E:76:ASP:OD1	1:E:78:ARG:HG3	2.14	0.48
1:C:98:ALA:O	1:C:383:TRP:CZ3	2.66	0.48
1:C:88:TRP:CZ2	2:D:57:ASN:CB	2.96	0.48
2:H:54:ASN:HD22	2:H:56:TYR:H	1.60	0.48
1:A:455:ALA:HB2	1:A:469:LEU:HD11	1.96	0.48
1:G:455:ALA:HB2	1:G:469:LEU:HD11	1.96	0.48
1:C:473:THR:OG1	1:C:476:LYS:HG2	2.13	0.48
1:C:511:ASP:O	1:C:512:LYS:HD3	2.14	0.48
1:E:511:ASP:O	1:E:512:LYS:HD3	2.14	0.48
2:F:241:VAL:HG12	2:F:242:GLN:N	2.28	0.48
1:G:132:ILE:HB	1:G:142:ILE:HG12	1.96	0.48
1:A:108:VAL:HG22	1:A:188:TYR:HA	1.96	0.48
1:G:164:MET:HG3	1:G:182:GLN:NE2	2.29	0.48
2:D:52:PRO:HD2	2:D:53:GLU:OE1	2.14	0.48
2:H:241:VAL:HG12	2:H:242:GLN:N	2.28	0.48
2:B:52:PRO:HD2	2:B:53:GLU:OE1	2.14	0.48
1:G:337:TRP:N	1:G:337:TRP:CD1	2.81	0.47
2:F:158:ALA:O	2:F:161:GLN:HB2	2.15	0.47
1:C:356:ARG:HH21	1:C:358:ARG:NH1	2.11	0.47
1:C:76:ASP:OD1	1:C:78:ARG:HG3	2.14	0.47
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.49	0.47
1:G:108:VAL:HG22	1:G:188:TYR:HA	1.96	0.47
1:C:108:VAL:HG22	1:C:188:TYR:HA	1.96	0.47
1:E:169:GLU:HB3	1:E:170:PRO:HD3	1.95	0.47
1:G:336:GLN:HG2	1:G:355:ALA:HB2	1.97	0.47
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.96	0.47
1:C:164:MET:HG3	1:C:182:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:HG2	1:A:399:GLU:O	2.12	0.47
2:B:268:SER:HA	2:B:274:ILE:CG2	2.43	0.47
2:F:97:PRO:HD3	2:F:181:TYR:CD1	2.49	0.47
2:F:24:TRP:HZ3	2:F:61:PHE:HB3	1.76	0.47
1:A:46:LYS:HG3	1:A:116:PHE:CD2	2.50	0.47
2:B:395:LYS:HG3	2:B:416:PHE:HE2	1.78	0.47
2:D:336:GLN:HG2	2:D:355:ALA:CB	2.44	0.47
1:C:390:LYS:HB3	1:C:417:VAL:HG21	1.96	0.47
1:E:336:GLN:HG2	1:E:355:ALA:HB2	1.97	0.47
1:E:419:THR:CG2	1:E:420:PRO:HD2	2.42	0.47
2:H:158:ALA:O	2:H:161:GLN:HB2	2.14	0.47
1:G:354:TYR:CZ	1:G:356:ARG:HD3	2.49	0.47
1:C:132:ILE:HB	1:C:142:ILE:HG12	1.96	0.47
1:A:354:TYR:CZ	1:A:356:ARG:HD3	2.49	0.47
1:E:102:LYS:CG	1:E:318:TYR:HB2	2.45	0.47
1:E:304:ALA:HA	1:E:307:ARG:HD2	1.96	0.47
1:C:46:LYS:HG3	1:C:116:PHE:CD2	2.50	0.47
1:G:88:TRP:CZ2	2:H:57:ASN:CB	2.96	0.47
1:A:511:ASP:O	1:A:512:LYS:HD3	2.14	0.47
2:H:336:GLN:HG2	2:H:355:ALA:CB	2.44	0.47
2:H:97:PRO:HD3	2:H:181:TYR:CD1	2.48	0.47
2:B:24:TRP:CH2	2:B:61:PHE:CE1	2.88	0.47
1:A:510:PRO:O	1:A:522:ILE:HD13	2.14	0.47
1:A:20:LYS:HG2	1:A:56:TYR:HA	1.96	0.47
1:A:23:GLN:HG2	1:A:59:PRO:HA	1.96	0.47
2:B:64:LYS:HB2	2:B:71:TRP:CE3	2.50	0.47
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.49	0.47
1:E:164:MET:HG3	1:E:182:GLN:NE2	2.29	0.47
1:E:318:TYR:N	1:E:318:TYR:CD1	2.82	0.47
1:A:304:ALA:HA	1:A:307:ARG:HD2	1.96	0.47
1:C:455:ALA:HB2	1:C:469:LEU:HD11	1.96	0.47
2:F:41:MET:HE1	2:F:73:LYS:HD2	1.95	0.47
2:H:268:SER:HA	2:H:274:ILE:CG2	2.43	0.47
2:H:24:TRP:HZ3	2:H:61:PHE:HB3	1.76	0.47
1:A:342:TYR:HB3	1:A:348:ASN:CB	2.44	0.47
1:C:354:TYR:CZ	1:C:356:ARG:HD3	2.49	0.47
1:C:23:GLN:HG2	1:C:59:PRO:HA	1.97	0.47
1:G:23:GLN:HG2	1:G:59:PRO:HA	1.97	0.47
2:F:64:LYS:HB2	2:F:71:TRP:CZ3	2.50	0.47
2:H:64:LYS:HB2	2:H:71:TRP:CZ3	2.50	0.47
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:LEU:HD21	1:C:233:GLU:HG2	1.96	0.47
1:A:228:LEU:HD21	1:A:233:GLU:HG2	1.96	0.47
1:A:318:TYR:N	1:A:318:TYR:CD1	2.82	0.47
1:G:46:LYS:HG3	1:G:116:PHE:CD2	2.50	0.47
2:H:56:TYR:O	2:H:143:ARG:NH2	2.48	0.47
2:F:56:TYR:O	2:F:143:ARG:NH2	2.48	0.47
1:G:326:ILE:HB	1:G:342:TYR:CD1	2.50	0.47
1:G:390:LYS:HB3	1:G:417:VAL:HG21	1.96	0.47
1:C:417:VAL:CG2	1:G:346:PHE:CD2	2.98	0.47
1:E:337:TRP:CD1	1:E:337:TRP:N	2.81	0.47
1:A:336:GLN:HG2	1:A:355:ALA:HB2	1.97	0.47
1:A:540:LYS:HZ3	2:B:261:VAL:HG13	1.78	0.47
1:C:326:ILE:HB	1:C:342:TYR:CD1	2.50	0.47
1:A:345:PRO:HG3	1:E:326:ILE:CD1	2.44	0.47
1:E:23:GLN:HG2	1:E:59:PRO:HA	1.97	0.47
1:E:132:ILE:HB	1:E:142:ILE:HG12	1.96	0.47
1:E:442:VAL:HG12	1:E:443:ASP:N	2.30	0.47
1:C:442:VAL:HG12	1:C:443:ASP:N	2.30	0.47
1:E:228:LEU:HD21	1:E:233:GLU:HG2	1.96	0.47
1:A:6:GLU:N	1:A:6:GLU:CD	2.66	0.47
1:G:102:LYS:CG	1:G:318:TYR:HB2	2.45	0.47
1:G:318:TYR:CD1	1:G:318:TYR:N	2.82	0.47
2:D:56:TYR:O	2:D:143:ARG:NH2	2.48	0.47
2:B:336:GLN:HG2	2:B:355:ALA:CB	2.44	0.47
2:H:52:PRO:HD2	2:H:53:GLU:OE1	2.14	0.47
2:B:158:ALA:O	2:B:161:GLN:HB2	2.15	0.47
1:E:354:TYR:CZ	1:E:356:ARG:HD3	2.49	0.47
1:G:78:ARG:NH1	1:G:287:LYS:O	2.39	0.47
1:E:20:LYS:HG2	1:E:56:TYR:HA	1.96	0.47
2:D:64:LYS:HB2	2:D:71:TRP:CZ3	2.50	0.47
1:A:442:VAL:HG12	1:A:443:ASP:N	2.30	0.47
1:G:228:LEU:HD21	1:G:233:GLU:HG2	1.96	0.47
1:C:391:LEU:HA	1:C:392:PRO:HD3	1.72	0.47
2:H:276:VAL:HG12	2:H:279:LEU:HD12	1.97	0.47
1:C:342:TYR:HB3	1:C:348:ASN:CB	2.44	0.47
1:C:191:SER:OG	1:C:198:HIS:HD2	1.98	0.47
2:F:24:TRP:HZ3	2:F:61:PHE:CB	2.28	0.47
1:C:20:LYS:HG2	1:C:56:TYR:HA	1.96	0.47
2:D:64:LYS:HB2	2:D:71:TRP:CE3	2.50	0.47
1:E:390:LYS:HB3	1:E:417:VAL:HG21	1.96	0.47
1:E:416:PHE:HD1	1:E:417:VAL:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:GLU:CD	1:C:6:GLU:N	2.66	0.47
1:C:318:TYR:CD1	1:C:318:TYR:N	2.82	0.47
1:C:121:ASP:O	1:C:125:ARG:HG3	2.15	0.47
1:C:336:GLN:HG2	1:C:355:ALA:HB2	1.97	0.47
1:E:537:PRO:HB2	1:E:540:LYS:HD2	1.97	0.47
1:A:326:ILE:HB	1:A:342:TYR:CD1	2.50	0.47
2:D:158:ALA:O	2:D:161:GLN:HB2	2.15	0.47
2:D:330:GLN:HG3	2:D:419:THR:HG21	1.96	0.47
2:B:64:LYS:HB2	2:B:71:TRP:CZ3	2.50	0.47
1:G:96:HIS:CG	1:G:97:PRO:HD2	2.49	0.47
1:A:102:LYS:CG	1:A:318:TYR:HB2	2.45	0.47
2:F:108:VAL:HA	2:F:187:LEU:O	2.15	0.47
1:A:33:ALA:O	1:A:36:GLU:HB3	2.15	0.47
2:F:52:PRO:HD2	2:F:53:GLU:OE1	2.14	0.47
1:A:191:SER:OG	1:A:198:HIS:HD2	1.98	0.46
1:C:510:PRO:O	1:C:522:ILE:HD13	2.14	0.46
1:G:442:VAL:HG12	1:G:443:ASP:N	2.30	0.46
2:F:135:ILE:H	2:F:135:ILE:HG12	1.38	0.46
1:G:33:ALA:O	1:G:36:GLU:HB3	2.15	0.46
2:D:108:VAL:HA	2:D:187:LEU:O	2.15	0.46
2:H:55:PRO:HG2	2:H:56:TYR:CD2	2.51	0.46
2:B:56:TYR:O	2:B:143:ARG:NH2	2.48	0.46
2:B:55:PRO:HG2	2:B:56:TYR:CD2	2.51	0.46
2:F:345:PRO:O	2:F:346:PHE:HB2	2.15	0.46
1:E:437:ALA:HB1	1:E:493:VAL:HA	1.97	0.46
1:C:346:PHE:CB	1:G:390:LYS:HZ1	1.98	0.46
2:F:64:LYS:HB2	2:F:71:TRP:CE3	2.50	0.46
1:G:248:GLU:CG	1:G:307:ARG:HH21	2.28	0.46
2:B:108:VAL:HA	2:B:187:LEU:O	2.15	0.46
1:C:304:ALA:HA	1:C:307:ARG:HD2	1.96	0.46
1:G:240:THR:HG22	1:G:315:HIS:HB3	1.97	0.46
2:D:55:PRO:HG2	2:D:56:TYR:CD2	2.51	0.46
1:A:121:ASP:O	1:A:125:ARG:HG3	2.15	0.46
1:G:121:ASP:O	1:G:125:ARG:HG3	2.15	0.46
1:G:342:TYR:HB3	1:G:348:ASN:CB	2.44	0.46
1:C:337:TRP:CD1	1:C:337:TRP:N	2.81	0.46
1:E:326:ILE:HB	1:E:342:TYR:CD1	2.50	0.46
2:H:108:VAL:HA	2:H:187:LEU:O	2.15	0.46
1:E:33:ALA:O	1:E:36:GLU:HB3	2.15	0.46
1:C:33:ALA:O	1:C:36:GLU:HB3	2.15	0.46
1:E:248:GLU:CG	1:E:307:ARG:HH21	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:O	1:A:507:GLN:HG2	2.16	0.46
1:C:503:LEU:O	1:C:507:GLN:HG2	2.16	0.46
2:B:276:VAL:HG12	2:B:279:LEU:HD12	1.98	0.46
1:G:191:SER:OG	1:G:198:HIS:HD2	1.99	0.46
1:A:398:TRP:CZ3	1:A:411:ILE:HD11	2.51	0.46
2:H:64:LYS:HB2	2:H:71:TRP:CE3	2.50	0.46
1:A:102:LYS:HG3	1:A:318:TYR:HB2	1.97	0.46
2:F:330:GLN:HG3	2:F:419:THR:HG21	1.96	0.46
2:F:259:LYS:HE3	2:F:263:LYS:NZ	2.30	0.46
1:A:537:PRO:HB2	1:A:540:LYS:HD2	1.97	0.46
2:D:24:TRP:HZ3	2:D:61:PHE:CB	2.28	0.46
1:G:229:TRP:CZ3	1:G:230:MET:HE1	2.51	0.46
1:E:115:TYR:CE2	1:E:156:SER:HB3	2.51	0.46
1:G:304:ALA:HA	1:G:307:ARG:HD2	1.96	0.46
1:G:451:LYS:O	1:G:452:LEU:HD23	2.15	0.46
2:H:330:GLN:HG3	2:H:419:THR:HG21	1.96	0.46
1:E:516:GLU:O	1:E:520:GLN:HG2	2.15	0.46
1:E:540:LYS:NZ	2:F:261:VAL:HG12	2.31	0.46
1:E:59:PRO:HG2	1:E:76:ASP:HB3	1.98	0.46
1:E:6:GLU:CD	1:E:6:GLU:N	2.66	0.46
1:A:118:VAL:C	1:A:148:VAL:HG13	2.36	0.46
1:E:240:THR:HG22	1:E:315:HIS:HB3	1.97	0.46
2:F:55:PRO:HG2	2:F:56:TYR:CD2	2.51	0.46
1:E:451:LYS:O	1:E:452:LEU:HD23	2.15	0.46
2:H:345:PRO:O	2:H:346:PHE:HB2	2.15	0.46
1:G:342:TYR:C	1:G:342:TYR:HD1	2.19	0.46
2:D:276:VAL:HG12	2:D:279:LEU:HD12	1.98	0.46
2:F:276:VAL:HG12	2:F:279:LEU:HD12	1.98	0.46
1:C:91:GLN:HE21	1:C:91:GLN:CA	2.21	0.46
1:G:59:PRO:HG2	1:G:76:ASP:HB3	1.98	0.46
1:C:102:LYS:CG	1:C:318:TYR:HB2	2.45	0.46
1:E:121:ASP:O	1:E:125:ARG:HG3	2.15	0.46
1:C:451:LYS:O	1:C:452:LEU:HD23	2.15	0.46
2:H:259:LYS:HE3	2:H:263:LYS:NZ	2.30	0.46
2:B:345:PRO:O	2:B:346:PHE:HB2	2.15	0.46
2:B:259:LYS:HE3	2:B:263:LYS:NZ	2.30	0.46
1:A:540:LYS:NZ	2:B:261:VAL:HG12	2.31	0.46
1:C:342:TYR:HD1	1:C:342:TYR:C	2.19	0.46
1:G:398:TRP:CZ3	1:G:411:ILE:HD11	2.51	0.46
1:E:342:TYR:HD1	1:E:342:TYR:C	2.19	0.46
2:H:10:VAL:HG11	2:H:153:TRP:HH2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ARG:HH22	2:B:409:THR:HB	1.81	0.46
1:C:241:VAL:HB	1:C:314:VAL:HG22	1.98	0.46
2:H:135:ILE:C	2:H:137:ASN:H	2.20	0.46
1:G:46:LYS:HG3	1:G:116:PHE:HD2	1.81	0.46
1:A:451:LYS:O	1:A:452:LEU:HD23	2.15	0.46
1:A:516:GLU:O	1:A:520:GLN:HG2	2.15	0.46
2:D:259:LYS:HE3	2:D:263:LYS:NZ	2.30	0.46
1:C:417:VAL:HG22	1:G:346:PHE:CD2	2.51	0.46
1:G:540:LYS:NZ	2:H:261:VAL:HG12	2.31	0.46
1:E:398:TRP:CZ3	1:E:411:ILE:HD11	2.51	0.46
2:B:365:VAL:HG12	2:B:405:TYR:HE2	1.80	0.46
1:A:342:TYR:HD1	1:A:342:TYR:C	2.19	0.46
1:A:91:GLN:CA	1:A:91:GLN:HE21	2.22	0.46
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.98	0.46
2:D:72:ARG:HH22	2:D:409:THR:HB	1.81	0.46
1:A:241:VAL:HB	1:A:314:VAL:HG22	1.98	0.46
1:E:102:LYS:HG3	1:E:318:TYR:HB2	1.97	0.46
1:G:102:LYS:HG3	1:G:318:TYR:HB2	1.97	0.46
1:E:46:LYS:HG3	1:E:116:PHE:CD2	2.50	0.46
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.51	0.46
1:C:118:VAL:C	1:C:148:VAL:HG13	2.36	0.46
1:C:148:VAL:HG12	1:C:149:LEU:N	2.31	0.46
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.64	0.46
1:C:175:ASN:ND2	1:C:201:LYS:NZ	2.64	0.46
2:B:297:GLU:HA	2:B:300:GLU:HB3	1.98	0.46
2:D:297:GLU:HA	2:D:300:GLU:HB3	1.98	0.46
1:C:537:PRO:HB2	1:C:540:LYS:HD2	1.97	0.46
2:F:103:LYS:HZ1	2:F:179:VAL:HG23	1.80	0.46
1:C:398:TRP:CZ3	1:C:411:ILE:HD11	2.51	0.46
1:G:20:LYS:HG2	1:G:56:TYR:HA	1.96	0.46
1:E:229:TRP:CZ3	1:E:230:MET:HE1	2.51	0.46
2:F:135:ILE:C	2:F:137:ASN:H	2.19	0.46
1:C:102:LYS:HG3	1:C:318:TYR:HB2	1.97	0.46
1:G:118:VAL:C	1:G:148:VAL:HG13	2.36	0.46
1:A:116:PHE:C	1:A:148:VAL:HG11	2.37	0.46
1:E:175:ASN:ND2	1:E:201:LYS:NZ	2.64	0.46
1:G:125:ARG:O	1:G:126:LYS:C	2.55	0.46
2:F:390:LYS:HA	2:F:415:GLU:O	2.17	0.46
2:H:171:PHE:HA	2:H:174:GLN:HB3	1.98	0.45
2:D:171:PHE:HA	2:D:174:GLN:HB3	1.98	0.45
2:B:24:TRP:HZ3	2:B:61:PHE:CB	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:TYR:HB3	1:E:348:ASN:CB	2.44	0.45
2:B:135:ILE:C	2:B:137:ASN:H	2.19	0.45
1:G:115:TYR:CE2	1:G:156:SER:HB3	2.51	0.45
1:E:125:ARG:O	1:E:126:LYS:C	2.55	0.45
2:B:390:LYS:HA	2:B:415:GLU:O	2.17	0.45
2:B:330:GLN:HG3	2:B:419:THR:HG21	1.96	0.45
2:F:96:HIS:CD2	2:F:384:GLY:HA3	2.51	0.45
2:D:345:PRO:O	2:D:346:PHE:HB2	2.15	0.45
1:G:540:LYS:HZ3	2:H:261:VAL:HG13	1.81	0.45
2:B:24:TRP:HZ3	2:B:61:PHE:HB3	1.76	0.45
1:G:6:GLU:CD	1:G:6:GLU:N	2.66	0.45
1:E:46:LYS:HG3	1:E:116:PHE:HD2	1.81	0.45
2:B:116:PHE:CZ	2:B:151:GLN:HG2	2.52	0.45
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.98	0.45
1:C:116:PHE:C	1:C:148:VAL:HG11	2.37	0.45
1:C:115:TYR:CE2	1:C:156:SER:HB3	2.51	0.45
1:G:516:GLU:O	1:G:520:GLN:HG2	2.15	0.45
1:C:437:ALA:HB1	1:C:493:VAL:HA	1.97	0.45
2:H:96:HIS:CD2	2:H:384:GLY:HA3	2.51	0.45
1:G:437:ALA:HB1	1:G:493:VAL:HA	1.97	0.45
1:A:437:ALA:HB1	1:A:493:VAL:HA	1.97	0.45
2:F:171:PHE:CZ	2:F:205:LEU:HB2	2.51	0.45
2:B:171:PHE:HA	2:B:174:GLN:HB3	1.98	0.45
1:E:361:HIS:CD2	1:E:505:ILE:HG23	2.52	0.45
1:C:59:PRO:HG2	1:C:76:ASP:HB3	1.98	0.45
1:E:118:VAL:C	1:E:148:VAL:HG13	2.36	0.45
1:G:115:TYR:O	1:G:117:SER:N	2.50	0.45
2:D:116:PHE:CZ	2:D:151:GLN:HG2	2.52	0.45
1:C:240:THR:HG22	1:C:315:HIS:HB3	1.97	0.45
1:A:445:ALA:O	1:A:453:GLY:HA3	2.16	0.45
1:G:175:ASN:ND2	1:G:201:LYS:NZ	2.64	0.45
1:C:345:PRO:HG2	1:G:326:ILE:HD11	1.84	0.45
1:G:326:ILE:CB	1:G:342:TYR:HE1	2.28	0.45
1:C:329:ILE:HA	1:C:338:THR:O	2.17	0.45
1:G:537:PRO:HB2	1:G:540:LYS:HD2	1.97	0.45
2:D:171:PHE:CZ	2:D:205:LEU:HB2	2.51	0.45
2:H:24:TRP:HZ3	2:H:61:PHE:CB	2.28	0.45
1:G:361:HIS:CD2	1:G:505:ILE:HG23	2.52	0.45
2:D:10:VAL:HG11	2:D:153:TRP:HH2	1.81	0.45
1:C:361:HIS:CD2	1:C:505:ILE:HG23	2.52	0.45
1:A:95:PRO:HG2	1:A:230:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HG22	1:A:315:HIS:HB3	1.97	0.45
1:G:445:ALA:O	1:G:453:GLY:HA3	2.16	0.45
1:C:445:ALA:O	1:C:453:GLY:HA3	2.16	0.45
2:D:96:HIS:CD2	2:D:384:GLY:HA3	2.51	0.45
2:B:96:HIS:CD2	2:B:384:GLY:HA3	2.51	0.45
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.51	0.45
2:F:10:VAL:HG11	2:F:153:TRP:HH2	1.81	0.45
1:A:361:HIS:CD2	1:A:505:ILE:HG23	2.52	0.45
2:F:116:PHE:CZ	2:F:151:GLN:HG2	2.52	0.45
2:H:116:PHE:CZ	2:H:151:GLN:HG2	2.52	0.45
1:C:115:TYR:O	1:C:117:SER:N	2.50	0.45
1:E:445:ALA:O	1:E:453:GLY:HA3	2.16	0.45
2:F:255:ASN:HA	2:F:258:GLN:HB2	1.98	0.45
2:D:390:LYS:HA	2:D:415:GLU:O	2.16	0.45
1:E:503:LEU:O	1:E:507:GLN:HG2	2.16	0.45
1:C:53:GLU:CD	1:C:53:GLU:H	2.20	0.45
1:G:53:GLU:CD	1:G:53:GLU:H	2.20	0.45
1:A:329:ILE:HA	1:A:338:THR:O	2.17	0.45
2:H:195:ILE:O	2:H:199:ARG:HG3	2.17	0.45
2:B:195:ILE:O	2:B:199:ARG:HG3	2.17	0.45
1:G:95:PRO:HG2	1:G:230:MET:CE	2.47	0.45
2:D:135:ILE:C	2:D:137:ASN:H	2.20	0.45
1:G:116:PHE:C	1:G:148:VAL:HG11	2.37	0.45
1:A:46:LYS:HG3	1:A:116:PHE:HD2	1.81	0.45
1:G:546:GLU:O	1:G:549:ASP:HB3	2.17	0.45
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.99	0.45
1:G:503:LEU:O	1:G:507:GLN:HG2	2.16	0.45
1:E:191:SER:OG	1:E:198:HIS:HD2	1.98	0.45
2:H:171:PHE:CZ	2:H:205:LEU:HB2	2.51	0.45
2:D:195:ILE:O	2:D:199:ARG:HG3	2.17	0.45
1:A:85:GLN:O	1:A:85:GLN:CG	2.55	0.45
1:G:241:VAL:HB	1:G:314:VAL:HG22	1.98	0.45
2:H:135:ILE:H	2:H:135:ILE:HG12	1.38	0.45
1:A:148:VAL:HG12	1:A:149:LEU:N	2.31	0.45
2:H:259:LYS:HE3	2:H:263:LYS:HZ1	1.81	0.45
1:G:327:ALA:HA	1:G:340:GLN:O	2.17	0.45
2:H:104:LYS:HZ3	2:H:194:GLU:HA	1.80	0.45
2:H:193:LEU:CD1	2:H:201:LYS:HG3	2.47	0.45
1:A:410:TRP:HZ3	2:B:401:TRP:CZ2	2.35	0.45
2:B:10:VAL:HG11	2:B:153:TRP:HH2	1.81	0.45
1:E:57:ASN:OD1	1:E:130:PHE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:PRO:HG2	1:E:230:MET:CE	2.47	0.45
1:C:248:GLU:CG	1:C:307:ARG:HH21	2.28	0.45
2:B:120:LEU:O	2:B:125:ARG:CZ	2.65	0.45
2:H:390:LYS:HG2	2:H:415:GLU:OE1	2.17	0.45
2:H:390:LYS:HA	2:H:415:GLU:O	2.16	0.45
1:C:516:GLU:O	1:C:520:GLN:HG2	2.15	0.45
2:F:297:GLU:HA	2:F:300:GLU:HB3	1.98	0.45
2:H:41:MET:HE1	2:H:73:LYS:HD2	1.98	0.45
2:B:207:GLN:O	2:B:208:HIS:C	2.56	0.45
1:C:410:TRP:HZ3	2:D:401:TRP:CZ2	2.35	0.45
2:D:365:VAL:HG12	2:D:405:TYR:HE2	1.80	0.45
1:C:78:ARG:NH1	1:C:287:LYS:O	2.39	0.45
1:G:57:ASN:OD1	1:G:130:PHE:HA	2.17	0.45
2:F:72:ARG:HH22	2:F:409:THR:HB	1.81	0.45
2:H:72:ARG:HH22	2:H:409:THR:HB	1.81	0.45
1:C:95:PRO:HG2	1:C:230:MET:CE	2.47	0.45
2:D:108:VAL:HG11	2:D:188:TYR:CE2	2.52	0.45
1:A:248:GLU:CG	1:A:307:ARG:HH21	2.28	0.45
2:D:376:THR:HG22	2:D:389:PHE:HE1	1.80	0.45
1:C:125:ARG:O	1:C:126:LYS:C	2.55	0.45
2:F:241:VAL:O	2:F:243:PRO:HD3	2.17	0.45
1:A:53:GLU:CD	1:A:53:GLU:H	2.20	0.45
1:G:329:ILE:HA	1:G:338:THR:O	2.17	0.45
1:C:326:ILE:CB	1:C:342:TYR:HE1	2.28	0.45
2:F:195:ILE:O	2:F:199:ARG:HG3	2.17	0.45
2:B:104:LYS:HZ1	2:B:194:GLU:HA	1.82	0.45
2:D:78:ARG:O	2:D:82:LYS:HG3	2.17	0.45
1:E:326:ILE:CB	1:E:342:TYR:HE1	2.28	0.45
1:E:442:VAL:HG12	1:E:481:ALA:CB	2.46	0.45
1:C:440:PHE:CE2	1:C:457:TYR:CE2	3.05	0.45
1:G:167:ILE:O	1:G:208:HIS:CE1	2.66	0.45
1:A:115:TYR:O	1:A:117:SER:N	2.50	0.45
1:C:46:LYS:HG3	1:C:116:PHE:HD2	1.81	0.45
2:D:120:LEU:O	2:D:125:ARG:CZ	2.65	0.45
1:E:54:ASN:HA	1:E:55:PRO:HD3	1.78	0.45
1:G:34:LEU:HD21	1:G:62:ALA:HB2	1.99	0.45
2:D:193:LEU:CD1	2:D:201:LYS:HG3	2.47	0.44
1:G:410:TRP:HZ3	2:H:401:TRP:CZ2	2.35	0.44
2:F:78:ARG:O	2:F:82:LYS:HG3	2.17	0.44
1:E:10:VAL:HG11	1:E:153:TRP:CZ2	2.52	0.44
1:C:10:VAL:HG11	1:C:153:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:CE2	1:A:457:TYR:CE2	3.05	0.44
2:B:108:VAL:HG11	2:B:188:TYR:CE2	2.52	0.44
2:F:120:LEU:O	2:F:125:ARG:CZ	2.65	0.44
2:H:241:VAL:O	2:H:243:PRO:HD3	2.17	0.44
1:A:546:GLU:O	1:A:549:ASP:HB3	2.17	0.44
1:E:329:ILE:HA	1:E:338:THR:O	2.17	0.44
1:A:439:THR:HG22	1:A:441:TYR:HE1	1.82	0.44
2:F:171:PHE:HA	2:F:174:GLN:HB3	1.98	0.44
2:B:193:LEU:CD1	2:B:201:LYS:HG3	2.47	0.44
1:A:78:ARG:NH1	1:A:287:LYS:O	2.39	0.44
1:A:57:ASN:OD1	1:A:130:PHE:HA	2.17	0.44
1:C:379:SER:HB3	1:C:383:TRP:HD1	1.83	0.44
1:A:379:SER:HB3	1:A:383:TRP:HD1	1.82	0.44
1:A:160:PHE:CZ	1:A:164:MET:CG	3.01	0.44
1:A:229:TRP:CH2	1:A:230:MET:CE	3.01	0.44
1:G:160:PHE:CZ	1:G:164:MET:CG	3.01	0.44
2:B:390:LYS:HG2	2:B:415:GLU:OE1	2.17	0.44
2:B:162:SER:O	2:B:166:LYS:HG2	2.17	0.44
2:F:292:VAL:HG12	2:F:293:ILE:N	2.33	0.44
2:D:255:ASN:HA	2:D:258:GLN:HB2	1.99	0.44
2:H:297:GLU:HA	2:H:300:GLU:HB3	1.98	0.44
1:C:540:LYS:NZ	2:D:261:VAL:HG12	2.31	0.44
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.52	0.44
2:F:390:LYS:HG2	2:F:415:GLU:OE1	2.17	0.44
1:E:546:GLU:O	1:E:549:ASP:HB3	2.17	0.44
1:C:546:GLU:O	1:C:549:ASP:HB3	2.17	0.44
2:F:100:LEU:HA	2:F:100:LEU:HD23	1.81	0.44
2:B:78:ARG:O	2:B:82:LYS:HG3	2.17	0.44
1:E:379:SER:HB3	1:E:383:TRP:HD1	1.83	0.44
2:F:108:VAL:HG11	2:F:188:TYR:CE2	2.53	0.44
1:E:115:TYR:O	1:E:117:SER:N	2.50	0.44
1:E:148:VAL:HG12	1:E:149:LEU:N	2.31	0.44
1:A:327:ALA:HA	1:A:340:GLN:O	2.17	0.44
1:E:327:ALA:HA	1:E:340:GLN:O	2.17	0.44
1:E:441:TYR:O	1:E:548:VAL:HG21	2.18	0.44
1:E:410:TRP:HZ3	2:F:401:TRP:CZ2	2.35	0.44
1:G:412:PRO:HG2	1:G:413:GLU:H	1.83	0.44
2:H:78:ARG:O	2:H:82:LYS:HG3	2.17	0.44
2:B:157:PRO:CG	2:B:158:ALA:N	2.79	0.44
1:C:57:ASN:OD1	1:C:130:PHE:HA	2.17	0.44
1:E:241:VAL:HB	1:E:314:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:PHE:CZ	1:E:164:MET:CG	3.01	0.44
1:E:116:PHE:C	1:E:148:VAL:HG11	2.37	0.44
1:C:451:LYS:O	1:C:471:ASN:N	2.51	0.44
1:G:451:LYS:O	1:G:471:ASN:N	2.51	0.44
1:C:327:ALA:HA	1:C:340:GLN:O	2.17	0.44
1:E:53:GLU:CD	1:E:53:GLU:H	2.20	0.44
2:D:104:LYS:HZ1	2:D:194:GLU:HA	1.82	0.44
2:D:157:PRO:CG	2:D:158:ALA:N	2.79	0.44
1:C:229:TRP:CH2	1:C:230:MET:CE	3.01	0.44
2:H:354:TYR:CE1	2:H:374:LYS:HD3	2.53	0.44
2:F:395:LYS:HG3	2:F:416:PHE:HE2	1.78	0.44
1:A:125:ARG:O	1:A:126:LYS:C	2.55	0.44
1:A:451:LYS:O	1:A:471:ASN:N	2.51	0.44
2:D:390:LYS:HG2	2:D:415:GLU:OE1	2.17	0.44
2:D:292:VAL:HG12	2:D:293:ILE:N	2.33	0.44
2:D:162:SER:O	2:D:166:LYS:HG2	2.17	0.44
2:H:292:VAL:HG12	2:H:293:ILE:N	2.33	0.44
2:B:292:VAL:HG12	2:B:293:ILE:N	2.33	0.44
1:C:417:VAL:HG21	1:G:346:PHE:CG	2.53	0.44
1:E:540:LYS:C	1:E:542:ILE:H	2.20	0.44
1:A:326:ILE:CB	1:A:342:TYR:HE1	2.28	0.44
2:D:47:ILE:HG22	2:D:48:SER:N	2.30	0.44
1:G:379:SER:HB3	1:G:383:TRP:HD1	1.83	0.44
1:G:229:TRP:CH2	1:G:230:MET:CE	3.01	0.44
1:G:95:PRO:HG2	1:G:230:MET:HE1	2.00	0.44
1:C:160:PHE:CZ	1:C:164:MET:CG	3.00	0.44
2:H:120:LEU:O	2:H:125:ARG:CZ	2.65	0.44
2:H:319:TYR:O	2:H:321:PRO:HD3	2.18	0.44
2:H:162:SER:O	2:H:166:LYS:HG2	2.17	0.44
2:B:255:ASN:HA	2:B:258:GLN:HB2	1.99	0.44
2:B:249:LYS:HB2	2:B:252:TRP:CZ2	2.52	0.44
2:D:249:LYS:HB2	2:D:252:TRP:CZ2	2.52	0.44
1:E:540:LYS:HB2	1:E:542:ILE:HG13	2.00	0.44
2:F:365:VAL:HG12	2:F:405:TYR:HE2	1.81	0.44
2:D:24:TRP:CZ3	2:D:61:PHE:CB	3.00	0.44
2:F:24:TRP:CZ3	2:F:61:PHE:CB	3.01	0.44
2:F:420:PRO:HB2	2:F:421:PRO:CD	2.42	0.44
1:G:10:VAL:HG11	1:G:153:TRP:CZ2	2.53	0.44
2:H:108:VAL:HG11	2:H:188:TYR:CE2	2.52	0.44
2:F:376:THR:HG22	2:F:389:PHE:HE1	1.80	0.44
2:B:354:TYR:CE1	2:B:374:LYS:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:255:ASN:HA	2:H:258:GLN:HB2	1.99	0.44
1:G:1:PRO:O	1:G:1:PRO:HG2	2.18	0.44
1:A:441:TYR:O	1:A:548:VAL:HG21	2.18	0.44
1:C:439:THR:HG22	1:C:441:TYR:HE1	1.82	0.44
1:E:114:ALA:HB1	1:E:160:PHE:CE1	2.52	0.44
1:E:440:PHE:CE2	1:E:457:TYR:CE2	3.05	0.44
1:E:88:TRP:CH2	2:F:57:ASN:CB	3.01	0.44
1:E:451:LYS:O	1:E:471:ASN:N	2.51	0.44
2:B:241:VAL:O	2:B:243:PRO:HD3	2.17	0.44
2:F:38:CYS:SG	2:F:132:ILE:HD11	2.58	0.44
2:D:286:THR:O	2:D:286:THR:HG22	2.18	0.44
2:B:286:THR:HG22	2:B:286:THR:O	2.18	0.44
1:C:336:GLN:C	1:C:337:TRP:CD1	2.92	0.43
1:G:336:GLN:C	1:G:337:TRP:CD1	2.92	0.43
1:G:441:TYR:O	1:G:548:VAL:HG21	2.18	0.43
1:E:543:GLY:C	1:E:545:ASN:H	2.22	0.43
1:E:412:PRO:HG2	1:E:413:GLU:H	1.83	0.43
1:G:440:PHE:CE2	1:G:457:TYR:CE2	3.05	0.43
2:B:376:THR:HG22	2:B:389:PHE:HE1	1.80	0.43
1:C:363:ASN:OD1	1:C:365:VAL:N	2.50	0.43
1:E:336:GLN:HG2	1:E:355:ALA:CB	2.48	0.43
1:C:441:TYR:O	1:C:548:VAL:HG21	2.18	0.43
1:G:543:GLY:C	1:G:545:ASN:H	2.22	0.43
2:H:207:GLN:O	2:H:208:HIS:C	2.56	0.43
1:G:132:ILE:HD11	1:G:144:TYR:CE2	2.54	0.43
2:F:286:THR:O	2:F:286:THR:HG22	2.18	0.43
2:H:286:THR:O	2:H:286:THR:HG22	2.18	0.43
1:E:368:LEU:HD11	1:E:391:LEU:HD22	2.00	0.43
1:A:536:VAL:HB	1:A:542:ILE:HD13	2.01	0.43
1:G:540:LYS:HZ3	2:H:276:VAL:HG21	1.83	0.43
1:E:536:VAL:HB	1:E:542:ILE:HD13	2.01	0.43
2:F:193:LEU:CD1	2:F:201:LYS:HG3	2.47	0.43
2:B:28:GLU:HG2	2:B:32:LYS:HZ2	1.84	0.43
1:G:148:VAL:HG12	1:G:149:LEU:N	2.31	0.43
1:C:167:ILE:O	1:C:208:HIS:CE1	2.66	0.43
2:F:354:TYR:CE1	2:F:374:LYS:HD3	2.53	0.43
2:D:319:TYR:O	2:D:321:PRO:HD3	2.18	0.43
2:D:100:LEU:HA	2:D:100:LEU:HD23	1.81	0.43
1:G:540:LYS:HB2	1:G:542:ILE:HG13	2.00	0.43
1:E:229:TRP:CH2	1:E:230:MET:CE	3.01	0.43
2:D:28:GLU:HG2	2:D:32:LYS:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:LYS:HE2	2:D:399:GLU:OE1	2.18	0.43
1:E:467:VAL:HG12	1:E:468:PRO:O	2.18	0.43
2:F:162:SER:O	2:F:166:LYS:HG2	2.17	0.43
2:B:324:ASP:O	2:B:343:GLN:HG2	2.19	0.43
1:E:34:LEU:HD21	1:E:62:ALA:HB2	1.99	0.43
2:H:38:CYS:SG	2:H:132:ILE:HD11	2.58	0.43
1:E:336:GLN:C	1:E:337:TRP:CD1	2.92	0.43
2:D:274:ILE:HG13	2:D:306:ASN:CG	2.39	0.43
1:G:540:LYS:C	1:G:542:ILE:H	2.20	0.43
1:C:320:ASP:HA	1:C:321:PRO:HD2	1.85	0.43
2:F:207:GLN:O	2:F:208:HIS:C	2.55	0.43
1:E:95:PRO:HG2	1:E:230:MET:HE1	2.00	0.43
1:G:88:TRP:CH2	2:H:57:ASN:CB	3.01	0.43
2:D:241:VAL:O	2:D:243:PRO:HD3	2.17	0.43
2:H:320:ASP:HA	2:H:321:PRO:HD3	1.84	0.43
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.43
2:H:324:ASP:O	2:H:343:GLN:HG2	2.19	0.43
2:F:312:GLU:HA	2:F:313:PRO:HD3	1.72	0.43
1:A:336:GLN:C	1:A:337:TRP:CD1	2.92	0.43
1:C:540:LYS:C	1:C:542:ILE:H	2.20	0.43
1:A:412:PRO:HG2	1:A:413:GLU:H	1.83	0.43
1:C:188:TYR:HB2	1:C:229:TRP:CD1	2.54	0.43
2:H:91:GLN:CD	2:H:94:ILE:HG23	2.39	0.43
1:A:88:TRP:CH2	2:B:57:ASN:CB	3.01	0.43
2:F:395:LYS:HE2	2:F:399:GLU:OE1	2.18	0.43
1:A:12:LEU:HD23	1:A:124:PHE:HE2	1.83	0.43
1:G:84:THR:CG2	1:G:154:LYS:HE2	2.49	0.43
2:F:324:ASP:O	2:F:343:GLN:HG2	2.19	0.43
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.58	0.43
1:E:391:LEU:HA	1:E:392:PRO:HD3	1.72	0.43
2:B:274:ILE:HG13	2:B:306:ASN:CG	2.39	0.43
1:C:412:PRO:HG2	1:C:413:GLU:H	1.83	0.43
2:H:420:PRO:HB2	2:H:421:PRO:CD	2.42	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.52	0.43
1:A:188:TYR:HB2	1:A:229:TRP:CD1	2.54	0.43
1:G:114:ALA:HB1	1:G:160:PHE:CE1	2.52	0.43
1:G:188:TYR:HB2	1:G:229:TRP:CD1	2.54	0.43
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.52	0.43
2:B:395:LYS:HE2	2:B:399:GLU:OE1	2.18	0.43
2:H:395:LYS:HE2	2:H:399:GLU:OE1	2.18	0.43
1:A:467:VAL:HG12	1:A:468:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:O	1:A:480:GLN:HG2	2.19	0.43
1:E:14:PRO:O	1:E:14:PRO:HG2	2.18	0.43
1:A:540:LYS:C	1:A:542:ILE:H	2.20	0.43
2:B:24:TRP:CZ3	2:B:61:PHE:CB	3.00	0.43
1:C:132:ILE:HD11	1:C:144:TYR:CE2	2.54	0.43
1:A:356:ARG:HH21	1:A:358:ARG:CZ	2.32	0.43
1:E:132:ILE:HD11	1:E:144:TYR:CE2	2.54	0.43
2:F:108:VAL:CG1	2:F:188:TYR:CE2	3.02	0.43
2:B:91:GLN:CD	2:B:94:ILE:HG23	2.39	0.43
2:H:108:VAL:CG1	2:H:188:TYR:CE2	3.02	0.43
2:D:108:VAL:CG1	2:D:188:TYR:CE2	3.02	0.43
2:D:354:TYR:CE1	2:D:374:LYS:HD3	2.53	0.43
1:A:50:ILE:HD13	1:A:145:GLN:HB2	2.01	0.43
1:C:12:LEU:HD23	1:C:124:PHE:HE2	1.83	0.43
1:G:476:LYS:O	1:G:480:GLN:HG2	2.19	0.43
2:D:324:ASP:O	2:D:343:GLN:HG2	2.19	0.43
2:F:319:TYR:O	2:F:321:PRO:HD3	2.18	0.43
1:A:84:THR:CG2	1:A:154:LYS:HE2	2.49	0.43
1:A:14:PRO:HG2	1:A:14:PRO:O	2.18	0.43
1:C:368:LEU:HD11	1:C:391:LEU:HD22	2.00	0.43
1:C:536:VAL:HB	1:C:542:ILE:HD13	2.01	0.43
1:G:536:VAL:HB	1:G:542:ILE:HD13	2.01	0.43
2:B:61:PHE:CZ	2:B:411:ILE:HD11	2.54	0.43
1:G:238:LYS:HE3	1:G:315:HIS:CG	2.54	0.43
1:C:50:ILE:HD13	1:C:145:GLN:HB2	2.01	0.43
1:C:467:VAL:HG12	1:C:468:PRO:O	2.18	0.43
2:B:160:PHE:CD1	2:B:160:PHE:O	2.72	0.43
1:G:336:GLN:HG2	1:G:355:ALA:CB	2.48	0.43
1:A:543:GLY:C	1:A:545:ASN:H	2.22	0.43
1:C:356:ARG:HH21	1:C:358:ARG:CZ	2.32	0.43
1:A:132:ILE:HD11	1:A:144:TYR:CE2	2.54	0.43
2:D:72:ARG:HH12	2:D:409:THR:CG2	2.29	0.43
1:E:188:TYR:HB2	1:E:229:TRP:CD1	2.54	0.43
2:F:91:GLN:CD	2:F:94:ILE:HG23	2.39	0.43
2:H:120:LEU:HB3	2:H:125:ARG:NH1	2.34	0.43
2:H:376:THR:HG22	2:H:389:PHE:HE1	1.80	0.43
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.58	0.43
1:E:1:PRO:O	1:E:1:PRO:HG2	2.18	0.43
1:A:336:GLN:HG2	1:A:355:ALA:CB	2.48	0.42
1:A:540:LYS:HB2	1:A:542:ILE:HG13	2.00	0.42
2:H:274:ILE:HG13	2:H:306:ASN:CG	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:PHE:CZ	2:D:411:ILE:HD11	2.54	0.42
1:G:356:ARG:HH21	1:G:358:ARG:CZ	2.32	0.42
1:E:238:LYS:HE3	1:E:315:HIS:CG	2.54	0.42
1:A:175:ASN:HB3	1:A:178:ILE:HD12	2.00	0.42
1:C:476:LYS:O	1:C:480:GLN:HG2	2.19	0.42
1:C:84:THR:CG2	1:C:154:LYS:HE2	2.49	0.42
2:D:160:PHE:CD1	2:D:160:PHE:O	2.72	0.42
2:B:78:ARG:HD3	2:B:411:ILE:O	2.20	0.42
2:D:78:ARG:HD3	2:D:411:ILE:O	2.20	0.42
2:F:61:PHE:CZ	2:F:411:ILE:HD11	2.54	0.42
1:A:90:VAL:CG1	2:B:141:GLY:H	2.29	0.42
1:G:104:LYS:N	1:G:192:ASP:OD1	2.52	0.42
1:E:363:ASN:OD1	1:E:365:VAL:N	2.50	0.42
1:G:175:ASN:HB3	1:G:178:ILE:HD12	2.00	0.42
1:E:175:ASN:CB	1:E:178:ILE:HD12	2.49	0.42
1:G:12:LEU:HD23	1:G:124:PHE:HE2	1.83	0.42
1:A:368:LEU:HD11	1:A:391:LEU:HD22	2.00	0.42
1:C:540:LYS:HB2	1:C:542:ILE:HG13	2.00	0.42
1:C:543:GLY:C	1:C:545:ASN:H	2.22	0.42
2:F:204:GLU:O	2:F:208:HIS:CD2	2.72	0.42
2:D:207:GLN:O	2:D:208:HIS:C	2.55	0.42
1:C:90:VAL:CG1	2:D:141:GLY:H	2.29	0.42
2:B:47:ILE:HG22	2:B:48:SER:N	2.30	0.42
2:F:316:GLY:O	2:F:318:TYR:CD1	2.66	0.42
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.85	0.42
1:G:467:VAL:HG12	1:G:468:PRO:O	2.18	0.42
1:C:345:PRO:HB3	1:G:342:TYR:CE1	2.54	0.42
2:B:262:GLY:O	2:B:265:ASN:HB3	2.20	0.42
2:H:249:LYS:HB2	2:H:252:TRP:CZ2	2.52	0.42
1:G:363:ASN:OD1	1:G:365:VAL:N	2.50	0.42
1:C:408:ALA:HB2	2:D:337:TRP:HH2	1.85	0.42
1:E:84:THR:CG2	1:E:154:LYS:HE2	2.49	0.42
1:G:14:PRO:O	1:G:14:PRO:HG2	2.18	0.42
1:C:336:GLN:HG2	1:C:355:ALA:CB	2.48	0.42
1:G:368:LEU:HD11	1:G:391:LEU:HD22	2.00	0.42
2:H:246:LEU:HD13	2:H:260:LEU:HD11	2.02	0.42
2:H:204:GLU:O	2:H:208:HIS:CD2	2.72	0.42
2:B:204:GLU:O	2:B:208:HIS:CD2	2.72	0.42
1:A:346:PHE:HE1	1:E:342:TYR:OH	2.02	0.42
1:A:23:GLN:NE2	1:A:131:THR:H	2.18	0.42
2:F:47:ILE:HG21	2:F:47:ILE:HD13	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:VAL:CG1	2:B:188:TYR:CE2	3.02	0.42
1:C:44:GLU:HB2	1:C:46:LYS:HG2	2.02	0.42
1:A:175:ASN:CB	1:A:178:ILE:HD12	2.49	0.42
1:G:50:ILE:HD13	1:G:145:GLN:HB2	2.01	0.42
1:G:432:GLU:HB3	1:G:433:PRO:HD2	2.01	0.42
1:E:483:TYR:O	1:E:486:LEU:HB2	2.20	0.42
2:B:41:MET:HE1	2:B:73:LYS:HD2	2.01	0.42
1:C:14:PRO:HG2	1:C:14:PRO:O	2.18	0.42
2:D:262:GLY:O	2:D:265:ASN:HB3	2.20	0.42
2:D:204:GLU:O	2:D:208:HIS:CD2	2.72	0.42
1:C:23:GLN:NE2	1:C:131:THR:H	2.18	0.42
1:G:23:GLN:NE2	1:G:131:THR:H	2.18	0.42
1:E:164:MET:HE1	1:E:187:LEU:HD11	2.01	0.42
1:G:363:ASN:HB3	1:G:366:LYS:HB2	2.02	0.42
1:C:175:ASN:HB3	1:C:178:ILE:HD12	2.00	0.42
1:E:175:ASN:HB3	1:E:178:ILE:HD12	2.00	0.42
1:C:1:PRO:O	1:C:1:PRO:HG2	2.18	0.42
2:F:160:PHE:CD1	2:F:160:PHE:O	2.72	0.42
2:F:278:GLN:HA	2:F:278:GLN:OE1	2.20	0.42
2:F:249:LYS:HB2	2:F:252:TRP:CZ2	2.52	0.42
2:F:262:GLY:O	2:F:265:ASN:HB3	2.20	0.42
2:F:274:ILE:HG13	2:F:306:ASN:CG	2.39	0.42
2:H:61:PHE:CZ	2:H:411:ILE:HD11	2.54	0.42
1:E:23:GLN:NE2	1:E:131:THR:H	2.18	0.42
1:C:96:HIS:ND1	1:C:98:ALA:HB3	2.35	0.42
2:H:72:ARG:HH12	2:H:409:THR:CG2	2.29	0.42
1:G:232:TYR:CD1	1:G:241:VAL:HG22	2.53	0.42
2:D:91:GLN:CD	2:D:94:ILE:HG23	2.39	0.42
1:C:238:LYS:HE3	1:C:315:HIS:CG	2.54	0.42
2:F:5:ILE:HG22	2:F:6:GLU:H	1.85	0.42
1:G:175:ASN:CB	1:G:178:ILE:HD12	2.50	0.42
1:C:175:ASN:CB	1:C:178:ILE:HD12	2.49	0.42
1:E:476:LYS:O	1:E:480:GLN:HG2	2.19	0.42
2:F:380:ILE:O	2:F:384:GLY:HA2	2.20	0.42
2:H:380:ILE:O	2:H:384:GLY:HA2	2.20	0.42
1:E:432:GLU:HB3	1:E:433:PRO:HD2	2.01	0.42
2:F:271:TYR:N	2:F:271:TYR:CD1	2.88	0.42
2:F:123:ASP:HA	2:F:126:LYS:HZ1	1.83	0.42
1:C:54:ASN:HA	1:C:55:PRO:HD3	1.77	0.42
2:H:47:ILE:HG22	2:H:48:SER:N	2.30	0.42
1:G:164:MET:HE1	1:G:187:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:LEU:HB3	2:F:125:ARG:NH1	2.34	0.42
1:C:104:LYS:N	1:C:192:ASP:OD1	2.52	0.42
1:A:104:LYS:N	1:A:192:ASP:OD1	2.52	0.42
1:C:483:TYR:O	1:C:486:LEU:HB2	2.20	0.42
1:A:483:TYR:O	1:A:486:LEU:HB2	2.20	0.42
1:A:540:LYS:HZ3	2:B:261:VAL:HG12	1.85	0.42
2:H:262:GLY:O	2:H:265:ASN:HB3	2.20	0.42
1:E:439:THR:HG22	1:E:441:TYR:HE1	1.82	0.42
1:C:421:PRO:HG2	1:C:421:PRO:O	2.20	0.42
2:B:420:PRO:HB2	2:B:421:PRO:CD	2.43	0.42
1:E:356:ARG:HH21	1:E:358:ARG:CZ	2.32	0.42
1:E:132:ILE:N	1:E:142:ILE:O	2.52	0.42
1:A:96:HIS:ND1	1:A:98:ALA:HB3	2.35	0.42
1:C:225:PRO:N	1:C:226:PRO:HD2	2.35	0.42
2:F:28:GLU:O	2:F:32:LYS:HG3	2.20	0.42
1:C:88:TRP:CH2	2:D:57:ASN:CB	3.01	0.42
1:C:363:ASN:HB3	1:C:366:LYS:HB2	2.02	0.42
1:G:53:GLU:CD	1:G:53:GLU:N	2.73	0.42
2:D:393:ILE:HG12	2:D:394:GLN:N	2.35	0.42
1:A:432:GLU:HB3	1:A:433:PRO:HD2	2.01	0.42
1:G:331:LYS:HG2	1:G:331:LYS:O	2.20	0.42
2:B:278:GLN:HA	2:B:278:GLN:OE1	2.20	0.42
1:A:1:PRO:O	1:A:1:PRO:HG2	2.18	0.42
2:H:271:TYR:N	2:H:271:TYR:CD1	2.88	0.42
1:C:342:TYR:CZ	1:G:345:PRO:HB3	2.54	0.42
1:C:96:HIS:CD2	1:C:97:PRO:HD2	2.55	0.42
1:G:96:HIS:ND1	1:G:98:ALA:HB3	2.35	0.42
2:H:109:LEU:O	2:H:186:ASP:HA	2.20	0.42
1:G:116:PHE:CD1	1:G:116:PHE:N	2.88	0.42
1:A:44:GLU:HB2	1:A:46:LYS:HG2	2.02	0.42
1:E:50:ILE:HD13	1:E:145:GLN:HB2	2.01	0.42
1:E:18:GLY:HA3	1:E:127:TYR:HD1	1.85	0.42
1:G:483:TYR:O	1:G:486:LEU:HB2	2.20	0.42
2:H:160:PHE:O	2:H:160:PHE:CD1	2.72	0.42
2:H:278:GLN:OE1	2:H:278:GLN:HA	2.20	0.42
1:A:312:GLU:HA	1:A:313:PRO:HD2	1.89	0.42
1:G:439:THR:CG2	1:G:441:TYR:HE1	2.33	0.41
2:H:365:VAL:HG12	2:H:405:TYR:HE2	1.81	0.41
2:B:24:TRP:HZ3	2:B:61:PHE:CG	2.38	0.41
2:H:78:ARG:HD3	2:H:411:ILE:O	2.20	0.41
1:G:38:CYS:HB3	1:G:144:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:TYR:CD1	1:C:241:VAL:HG22	2.53	0.41
1:G:96:HIS:CD2	1:G:97:PRO:HD2	2.55	0.41
2:D:28:GLU:O	2:D:32:LYS:HG3	2.20	0.41
2:D:120:LEU:HB3	2:D:125:ARG:NH1	2.34	0.41
2:B:395:LYS:O	2:B:399:GLU:N	2.48	0.41
1:G:201:LYS:HA	1:G:201:LYS:HD3	1.85	0.41
2:H:393:ILE:HG12	2:H:394:GLN:N	2.35	0.41
1:G:8:VAL:HA	1:G:9:PRO:HD2	1.78	0.41
1:A:427:TYR:CD1	1:A:427:TYR:N	2.88	0.41
1:G:439:THR:HG22	1:G:441:TYR:HE1	1.82	0.41
1:E:439:THR:CG2	1:E:441:TYR:HE1	2.33	0.41
2:F:246:LEU:HD13	2:F:260:LEU:HD11	2.02	0.41
1:G:320:ASP:HA	1:G:321:PRO:HD2	1.85	0.41
2:F:78:ARG:HD3	2:F:411:ILE:O	2.19	0.41
1:C:38:CYS:HB3	1:C:144:TYR:CE2	2.55	0.41
1:A:249:LYS:CG	1:A:250:ASP:N	2.83	0.41
1:E:96:HIS:ND1	1:E:98:ALA:HB3	2.35	0.41
2:B:28:GLU:O	2:B:32:LYS:HG3	2.20	0.41
1:G:116:PHE:HD1	1:G:116:PHE:N	2.18	0.41
2:B:120:LEU:HB3	2:B:125:ARG:NH1	2.34	0.41
1:G:18:GLY:HA3	1:G:127:TYR:HD1	1.85	0.41
2:H:336:GLN:HG2	2:H:355:ALA:HB1	2.02	0.41
2:B:380:ILE:O	2:B:384:GLY:HA2	2.20	0.41
1:G:77:PHE:CE2	1:G:150:PRO:HB3	2.55	0.41
1:E:77:PHE:CE2	1:E:150:PRO:HB3	2.55	0.41
2:F:18:GLY:HA3	2:F:127:TYR:CD1	2.56	0.41
1:C:427:TYR:N	1:C:427:TYR:CD1	2.88	0.41
1:E:427:TYR:CD1	1:E:427:TYR:N	2.88	0.41
1:A:421:PRO:HG2	1:A:421:PRO:O	2.20	0.41
2:B:72:ARG:HH12	2:B:409:THR:CG2	2.29	0.41
1:E:408:ALA:HB2	2:F:337:TRP:HH2	1.85	0.41
2:D:246:LEU:HD13	2:D:260:LEU:HD11	2.02	0.41
1:G:409:THR:O	1:G:410:TRP:HB2	2.21	0.41
2:D:24:TRP:HZ3	2:D:61:PHE:CG	2.38	0.41
2:H:10:VAL:HA	2:H:85:GLN:OE1	2.20	0.41
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.55	0.41
1:E:456:GLY:HA3	1:E:466:VAL:HA	2.02	0.41
1:E:116:PHE:N	1:E:116:PHE:HD1	2.18	0.41
1:C:116:PHE:HD1	1:C:116:PHE:N	2.18	0.41
1:A:363:ASN:HB3	1:A:366:LYS:HB2	2.02	0.41
1:C:53:GLU:N	1:C:53:GLU:CD	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:PHE:CE2	1:C:150:PRO:HB3	2.55	0.41
1:C:432:GLU:HB3	1:C:433:PRO:HD2	2.01	0.41
2:B:100:LEU:HD23	2:B:100:LEU:HA	1.81	0.41
1:G:427:TYR:CD1	1:G:427:TYR:N	2.88	0.41
1:G:421:PRO:O	1:G:421:PRO:HG2	2.20	0.41
1:G:344:GLU:HA	1:G:345:PRO:HD2	1.81	0.41
1:C:10:VAL:HG11	1:C:153:TRP:HZ2	1.86	0.41
1:E:249:LYS:CG	1:E:250:ASP:N	2.83	0.41
1:E:78:ARG:NH1	1:E:287:LYS:O	2.39	0.41
2:B:136:ASN:O	2:B:137:ASN:HB2	2.21	0.41
2:F:136:ASN:O	2:F:137:ASN:HB2	2.21	0.41
1:E:116:PHE:CD1	1:E:116:PHE:N	2.88	0.41
2:B:109:LEU:O	2:B:186:ASP:HA	2.20	0.41
1:A:238:LYS:HE3	1:A:315:HIS:CG	2.54	0.41
1:E:12:LEU:HD23	1:E:124:PHE:HE2	1.83	0.41
1:G:53:GLU:OE2	1:G:53:GLU:N	2.54	0.41
1:C:331:LYS:O	1:C:331:LYS:HG2	2.20	0.41
2:F:393:ILE:HG12	2:F:394:GLN:N	2.35	0.41
2:D:278:GLN:OE1	2:D:278:GLN:HA	2.20	0.41
2:F:193:LEU:HD12	2:F:201:LYS:HG3	2.03	0.41
2:F:153:TRP:CE3	2:F:155:GLY:CA	3.03	0.41
2:F:10:VAL:HA	2:F:85:GLN:OE1	2.20	0.41
1:C:349:LEU:HA	1:C:349:LEU:HD23	1.84	0.41
1:E:225:PRO:N	1:E:226:PRO:HD2	2.35	0.41
1:G:225:PRO:N	1:G:226:PRO:HD2	2.35	0.41
2:D:136:ASN:O	2:D:137:ASN:HB2	2.21	0.41
2:F:109:LEU:O	2:F:186:ASP:HA	2.20	0.41
1:G:44:GLU:HB2	1:G:46:LYS:HG2	2.02	0.41
2:B:391:LEU:HD12	2:B:416:PHE:HE1	1.86	0.41
2:D:395:LYS:O	2:D:399:GLU:N	2.48	0.41
1:G:408:ALA:HB2	2:H:337:TRP:HH2	1.85	0.41
1:C:53:GLU:OE2	1:C:53:GLU:N	2.54	0.41
1:E:53:GLU:CD	1:E:53:GLU:N	2.73	0.41
2:B:246:LEU:HD13	2:B:260:LEU:HD11	2.02	0.41
2:D:103:LYS:HB3	2:D:191:SER:O	2.21	0.41
2:F:104:LYS:O	2:F:235:HIS:CD2	2.74	0.41
1:C:409:THR:O	1:C:410:TRP:HB2	2.21	0.41
2:B:61:PHE:CD2	2:B:403:THR:HG22	2.56	0.41
2:D:61:PHE:CD2	2:D:403:THR:HG22	2.56	0.41
2:F:24:TRP:HZ3	2:F:61:PHE:CG	2.38	0.41
2:D:156:SER:HB2	2:D:157:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:VAL:HG11	1:E:153:TRP:HZ2	1.86	0.41
1:E:38:CYS:HB3	1:E:144:TYR:CE2	2.55	0.41
1:A:456:GLY:HA3	1:A:466:VAL:HA	2.02	0.41
2:B:108:VAL:CG1	2:B:188:TYR:CD2	3.04	0.41
1:G:418:ASN:C	1:G:418:ASN:ND2	2.74	0.41
1:A:18:GLY:HA3	1:A:127:TYR:HD1	1.85	0.41
1:E:472:THR:HB	1:E:476:LYS:HB2	2.03	0.41
2:D:336:GLN:HG2	2:D:355:ALA:HB1	2.02	0.41
2:D:380:ILE:O	2:D:384:GLY:HA2	2.20	0.41
2:B:393:ILE:HG12	2:B:394:GLN:N	2.35	0.41
1:G:391:LEU:HA	1:G:392:PRO:HD3	1.73	0.41
1:A:439:THR:CG2	1:A:441:TYR:HE1	2.33	0.41
2:H:61:PHE:CD2	2:H:403:THR:HG22	2.56	0.41
1:G:90:VAL:CG1	2:H:141:GLY:H	2.29	0.41
2:B:156:SER:HB2	2:B:157:PRO:CD	2.51	0.41
1:C:57:ASN:HB2	1:C:143:ARG:HH21	1.86	0.41
1:C:249:LYS:CG	1:C:250:ASP:N	2.83	0.41
1:C:442:VAL:CG1	1:C:481:ALA:CB	2.96	0.41
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.55	0.41
1:A:225:PRO:N	1:A:226:PRO:HD2	2.35	0.41
1:G:440:PHE:HD2	1:G:457:TYR:CD2	2.39	0.41
1:E:440:PHE:HD2	1:E:457:TYR:CD2	2.39	0.41
2:B:94:ILE:HG13	2:B:94:ILE:H	1.54	0.41
1:E:44:GLU:HB2	1:E:46:LYS:HG2	2.02	0.41
2:H:108:VAL:CG1	2:H:188:TYR:CD2	3.04	0.41
1:A:116:PHE:HD1	1:A:116:PHE:N	2.18	0.41
1:C:116:PHE:CD1	1:C:116:PHE:N	2.88	0.41
1:C:118:VAL:HA	1:C:119:PRO:HD2	1.71	0.41
1:E:53:GLU:N	1:E:53:GLU:OE2	2.54	0.41
2:H:175:ASN:O	2:H:177:ASP:N	2.54	0.41
2:F:202:ILE:O	2:F:206:ARG:N	2.54	0.41
2:D:18:GLY:HA3	2:D:127:TYR:CD1	2.56	0.41
2:B:58:THR:HG21	2:B:77:PHE:CD1	2.56	0.41
1:C:417:VAL:HG21	1:G:346:PHE:CD1	2.56	0.41
2:D:271:TYR:CD1	2:D:271:TYR:N	2.88	0.41
2:H:252:TRP:CH2	2:H:260:LEU:HD22	2.56	0.41
2:F:252:TRP:CH2	2:F:260:LEU:HD22	2.56	0.41
1:E:421:PRO:HG2	1:E:421:PRO:O	2.20	0.41
1:G:317:VAL:CG2	1:G:347:LYS:HB3	2.41	0.41
2:B:103:LYS:HB3	2:B:191:SER:O	2.21	0.41
1:C:420:PRO:CG	1:C:421:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:104:LYS:O	2:H:235:HIS:CD2	2.74	0.41
2:H:193:LEU:HD12	2:H:201:LYS:HG3	2.03	0.41
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.85	0.41
1:E:323:LYS:O	1:E:343:GLN:NE2	2.52	0.41
1:E:388:LYS:HA	1:E:413:GLU:HB2	2.03	0.41
1:A:388:LYS:HA	1:A:413:GLU:HB2	2.03	0.41
2:B:193:LEU:HD12	2:B:201:LYS:HG3	2.03	0.41
2:H:24:TRP:HZ3	2:H:61:PHE:CG	2.38	0.41
2:H:74:LEU:HA	2:H:74:LEU:HD12	1.83	0.41
2:H:153:TRP:CE3	2:H:155:GLY:CA	3.04	0.41
2:H:156:SER:HB2	2:H:157:PRO:CD	2.51	0.41
2:B:11:LYS:N	2:B:85:GLN:OE1	2.49	0.41
2:B:153:TRP:CE3	2:B:155:GLY:CA	3.03	0.41
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.86	0.41
1:G:132:ILE:CD1	1:G:144:TYR:HE2	2.33	0.41
1:A:57:ASN:HB2	1:A:143:ARG:HH21	1.86	0.41
1:A:132:ILE:CD1	1:A:144:TYR:HE2	2.34	0.41
1:A:54:ASN:O	1:A:143:ARG:NH1	2.54	0.41
2:D:63:ILE:HG12	2:D:64:LYS:H	1.86	0.41
1:E:96:HIS:CD2	1:E:97:PRO:HD2	2.55	0.41
2:H:136:ASN:O	2:H:137:ASN:HB2	2.21	0.41
1:A:116:PHE:CD1	1:A:116:PHE:N	2.88	0.41
1:C:116:PHE:HA	1:C:148:VAL:HG11	2.03	0.41
2:H:391:LEU:HD12	2:H:416:PHE:HE1	1.86	0.41
2:D:391:LEU:HD12	2:D:416:PHE:HE1	1.86	0.41
1:A:418:ASN:C	1:A:418:ASN:ND2	2.74	0.41
1:A:463:ARG:NH1	1:A:463:ARG:HG3	2.35	0.41
1:C:463:ARG:NH1	1:C:463:ARG:HG3	2.35	0.41
1:G:472:THR:HB	1:G:476:LYS:HB2	2.03	0.41
2:F:336:GLN:HG2	2:F:355:ALA:HB1	2.02	0.41
1:A:53:GLU:N	1:A:53:GLU:CD	2.73	0.41
1:A:53:GLU:N	1:A:53:GLU:OE2	2.54	0.41
1:C:484:LEU:O	1:C:487:GLN:N	2.54	0.41
1:A:77:PHE:CE2	1:A:150:PRO:HB3	2.55	0.41
2:H:18:GLY:HA3	2:H:127:TYR:CD1	2.56	0.41
2:B:175:ASN:O	2:B:177:ASP:N	2.54	0.41
1:A:484:LEU:O	1:A:487:GLN:N	2.54	0.41
2:H:100:LEU:HA	2:H:100:LEU:HD23	1.81	0.41
1:A:331:LYS:HG2	1:A:331:LYS:O	2.20	0.41
2:D:58:THR:HG21	2:D:77:PHE:CD1	2.56	0.41
1:E:484:LEU:O	1:E:487:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:TYR:N	2:B:271:TYR:CD1	2.88	0.41
1:C:439:THR:CG2	1:C:441:TYR:HE1	2.33	0.41
1:C:540:LYS:O	1:C:542:ILE:N	2.53	0.41
2:H:274:ILE:HG13	2:H:306:ASN:OD1	2.21	0.41
1:A:409:THR:O	1:A:410:TRP:HB2	2.21	0.41
2:B:37:ILE:H	2:B:37:ILE:HG13	1.69	0.41
2:F:156:SER:HB2	2:F:157:PRO:CD	2.51	0.41
2:B:10:VAL:HA	2:B:85:GLN:OE1	2.20	0.41
2:D:420:PRO:HB2	2:D:421:PRO:CD	2.43	0.41
1:C:54:ASN:O	1:C:143:ARG:NH1	2.54	0.41
1:E:116:PHE:HA	1:E:148:VAL:HG11	2.03	0.41
1:G:116:PHE:HA	1:G:148:VAL:HG11	2.03	0.41
1:E:363:ASN:HB3	1:E:366:LYS:HB2	2.02	0.41
2:B:336:GLN:HG2	2:B:355:ALA:HB1	2.02	0.41
2:H:52:PRO:HG2	2:H:53:GLU:N	2.36	0.41
2:D:175:ASN:O	2:D:177:ASP:N	2.54	0.41
2:F:175:ASN:O	2:F:177:ASP:N	2.54	0.41
2:H:34:LEU:HA	2:H:34:LEU:HD23	1.92	0.41
1:E:331:LYS:O	1:E:331:LYS:HG2	2.20	0.41
1:C:8:VAL:HA	1:C:9:PRO:HD2	1.78	0.41
2:D:274:ILE:HG13	2:D:306:ASN:OD1	2.21	0.40
1:G:536:VAL:HA	1:G:537:PRO:HD3	1.77	0.40
1:G:377:THR:O	1:G:380:ILE:N	2.54	0.40
2:B:104:LYS:O	2:B:235:HIS:CD2	2.74	0.40
2:F:61:PHE:CD2	2:F:403:THR:HG22	2.56	0.40
2:D:153:TRP:CE3	2:D:155:GLY:CA	3.03	0.40
1:A:164:MET:HE1	1:A:187:LEU:HD11	2.02	0.40
1:E:229:TRP:CE2	1:E:230:MET:HE3	2.56	0.40
1:C:456:GLY:HA3	1:C:466:VAL:HA	2.02	0.40
2:D:108:VAL:CG1	2:D:188:TYR:CD2	3.04	0.40
1:A:116:PHE:HA	1:A:148:VAL:HG11	2.03	0.40
1:C:418:ASN:C	1:C:418:ASN:ND2	2.74	0.40
1:C:18:GLY:HA3	1:C:127:TYR:HD1	1.85	0.40
2:F:259:LYS:HE3	2:F:263:LYS:HZ1	1.85	0.40
1:G:312:GLU:HA	1:G:313:PRO:HD2	1.89	0.40
2:D:419:THR:HA	2:D:420:PRO:HD2	1.96	0.40
1:A:132:ILE:N	1:A:142:ILE:O	2.52	0.40
2:F:63:ILE:HG12	2:F:64:LYS:H	1.86	0.40
1:E:232:TYR:CD1	1:E:241:VAL:HG22	2.53	0.40
2:H:47:ILE:HG21	2:H:47:ILE:HD13	1.82	0.40
1:G:349:LEU:HD23	1:G:349:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:TRP:CE2	1:G:230:MET:HE3	2.56	0.40
2:H:28:GLU:O	2:H:32:LYS:HG3	2.20	0.40
1:C:402:TRP:CE3	1:C:402:TRP:O	2.74	0.40
1:C:331:LYS:O	1:C:333:GLY:N	2.54	0.40
1:C:252:TRP:HA	1:C:252:TRP:CE3	2.56	0.40
2:F:274:ILE:HG13	2:F:306:ASN:OD1	2.21	0.40
1:E:377:THR:O	1:E:380:ILE:N	2.55	0.40
2:D:104:LYS:O	2:D:235:HIS:CD2	2.74	0.40
1:E:344:GLU:HA	1:E:345:PRO:HD2	1.82	0.40
1:E:326:ILE:CG2	1:E:342:TYR:HE1	2.35	0.40
2:F:72:ARG:HH12	2:F:409:THR:CA	2.35	0.40
1:A:232:TYR:CD1	1:A:241:VAL:HG22	2.53	0.40
1:G:456:GLY:HA3	1:G:466:VAL:HA	2.02	0.40
1:A:440:PHE:HD2	1:A:457:TYR:CD2	2.39	0.40
2:D:109:LEU:O	2:D:186:ASP:HA	2.20	0.40
1:A:246:LEU:O	1:A:307:ARG:NH1	2.54	0.40
1:A:402:TRP:CE3	1:A:402:TRP:O	2.74	0.40
1:G:452:LEU:HD22	1:G:470:THR:HA	2.04	0.40
1:E:252:TRP:HA	1:E:252:TRP:CE3	2.56	0.40
1:A:252:TRP:HA	1:A:252:TRP:CE3	2.56	0.40
2:D:252:TRP:CH2	2:D:260:LEU:HD22	2.56	0.40
2:F:103:LYS:HB3	2:F:191:SER:O	2.21	0.40
1:G:244:ILE:HD12	1:G:267:ALA:CB	2.40	0.40
2:D:193:LEU:HD12	2:D:201:LYS:HG3	2.03	0.40
1:C:388:LYS:HA	1:C:413:GLU:HB2	2.03	0.40
2:D:10:VAL:HA	2:D:85:GLN:OE1	2.20	0.40
1:C:132:ILE:CD1	1:C:144:TYR:HE2	2.33	0.40
1:G:10:VAL:HG11	1:G:153:TRP:HZ2	1.86	0.40
1:E:132:ILE:CD1	1:E:144:TYR:HE2	2.34	0.40
1:E:228:LEU:CD2	1:E:233:GLU:HG2	2.51	0.40
2:F:28:GLU:HG3	2:F:135:ILE:HD13	2.02	0.40
1:C:239:TRP:N	1:C:318:TYR:HE1	2.20	0.40
1:G:239:TRP:N	1:G:318:TYR:HE1	2.20	0.40
2:F:108:VAL:CG1	2:F:188:TYR:CD2	3.04	0.40
1:C:30:LYS:HB3	1:C:62:ALA:HB3	2.04	0.40
1:E:246:LEU:O	1:E:307:ARG:NH1	2.54	0.40
1:C:246:LEU:O	1:C:307:ARG:NH1	2.54	0.40
2:F:391:LEU:HD12	2:F:416:PHE:HE1	1.86	0.40
1:E:452:LEU:HD22	1:E:470:THR:HA	2.04	0.40
1:A:472:THR:HB	1:A:476:LYS:HB2	2.03	0.40
1:C:472:THR:HB	1:C:476:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:52:PRO:HG2	2:F:53:GLU:N	2.36	0.40
2:D:7:THR:HG22	2:D:119:PRO:HG2	2.04	0.40
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.56	0.40
2:F:58:THR:HG21	2:F:77:PHE:CD1	2.56	0.40
2:H:7:THR:HG22	2:H:119:PRO:HG2	2.03	0.40
1:E:243:PRO:HD3	1:E:313:PRO:HB3	2.04	0.40
1:E:312:GLU:HA	1:E:313:PRO:HD2	1.90	0.40
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.04	0.40
2:B:252:TRP:CH2	2:B:260:LEU:HD22	2.56	0.40
1:G:377:THR:OG1	1:G:378:GLU:N	2.55	0.40
2:H:103:LYS:HB3	2:H:191:SER:O	2.21	0.40
1:C:442:VAL:HG12	1:C:481:ALA:CB	2.46	0.40
2:B:316:GLY:O	2:B:318:TYR:CD1	2.65	0.40
1:E:104:LYS:N	1:E:192:ASP:OD1	2.52	0.40
2:H:395:LYS:HG2	2:H:399:GLU:OE1	2.21	0.40
1:C:201:LYS:HA	1:C:201:LYS:HD3	1.85	0.40
2:F:330:GLN:HB2	2:F:338:THR:OG1	2.22	0.40
2:D:41:MET:HE1	2:D:73:LYS:HD2	2.02	0.40
1:G:484:LEU:O	1:G:487:GLN:N	2.54	0.40

All (34) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASN:CA	2:H:88:TRP:CZ2[3_445]	0.68	1.52
1:C:53:GLU:O	2:H:88:TRP:NE1[3_445]	0.72	1.48
2:D:88:TRP:NE1	1:G:54:ASN:N[3_445]	0.91	1.29
1:C:53:GLU:O	2:H:88:TRP:CD1[3_445]	1.03	1.17
1:C:53:GLU:C	2:H:88:TRP:NE1[3_445]	1.08	1.12
2:B:200:THR:CG2	1:C:211:ARG:NH2[2_657]	1.33	0.87
1:C:54:ASN:N	2:H:88:TRP:CE2[3_445]	1.35	0.85
1:C:464:GLN:NE2	1:G:464:GLN:NE2[2_657]	1.36	0.84
1:C:54:ASN:CA	2:H:88:TRP:CE2[3_445]	1.39	0.81
2:B:200:THR:CG2	1:C:211:ARG:CZ[2_657]	1.45	0.75
2:D:88:TRP:NE1	1:G:54:ASN:CA[3_445]	1.49	0.71
2:B:200:THR:CG2	1:C:211:ARG:NE[2_657]	1.54	0.66
1:C:54:ASN:CB	2:H:88:TRP:CZ2[3_445]	1.55	0.65
1:C:54:ASN:N	2:H:88:TRP:CZ2[3_445]	1.58	0.62
2:D:88:TRP:CD1	1:G:53:GLU:C[3_445]	1.69	0.51
1:C:54:ASN:N	2:H:88:TRP:NE1[3_445]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:GLN:O	1:G:464:GLN:O[2_657]	1.73	0.47
1:C:53:GLU:C	2:H:88:TRP:CE2[3_445]	1.74	0.46
2:D:88:TRP:CD1	1:G:54:ASN:N[3_445]	1.77	0.43
1:C:53:GLU:C	2:H:88:TRP:CD1[3_445]	1.80	0.40
1:A:212:TRP:CZ2	2:H:211:ARG:NE[4_647]	1.90	0.30
2:D:88:TRP:NE1	1:G:53:GLU:C[3_445]	1.91	0.29
1:C:54:ASN:CA	2:H:88:TRP:CH2[3_445]	2.03	0.17
2:D:208:HIS:O	1:E:211:ARG:NE[2_657]	2.04	0.16
1:C:53:GLU:O	2:H:88:TRP:CE2[3_445]	2.04	0.16
2:B:200:THR:CB	1:C:211:ARG:NE[2_657]	2.09	0.11
2:D:211:ARG:O	1:E:207:GLN:OE1[2_657]	2.14	0.06
1:C:54:ASN:C	2:H:88:TRP:NE1[3_445]	2.14	0.06
1:A:212:TRP:CH2	2:H:211:ARG:CZ[4_647]	2.15	0.05
1:C:54:ASN:C	2:H:88:TRP:CZ2[3_445]	2.15	0.05
2:D:88:TRP:CE2	1:G:54:ASN:CA[3_445]	2.15	0.05
1:C:54:ASN:CB	2:H:88:TRP:CH2[3_445]	2.16	0.04
1:C:54:ASN:CA	2:H:88:TRP:NE1[3_445]	2.17	0.03
1:C:54:ASN:C	2:H:88:TRP:CE2[3_445]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	5	33
1	C	530/560 (95%)	438 (83%)	75 (14%)	17 (3%)	5	33
1	E	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	5	33
1	G	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	5	33
2	B	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	5	34
2	D	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	5	34
2	F	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	5	34
2	H	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3676/4000 (92%)	3035 (83%)	525 (14%)	116 (3%)	5	33

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	345	PRO
2	B	94	ILE
1	C	222	GLN
1	C	345	PRO
2	D	94	ILE
1	E	222	GLN
1	E	345	PRO
2	F	94	ILE
1	G	222	GLN
1	G	345	PRO
2	H	94	ILE
1	A	85	GLN
1	A	273	GLY
1	A	412	PRO
1	C	85	GLN
1	C	273	GLY
1	C	412	PRO
1	E	85	GLN
1	E	273	GLY
1	E	412	PRO
1	G	85	GLN
1	G	273	GLY
1	G	412	PRO
1	A	123	ASP
1	A	156	SER
1	A	296	THR
1	A	420	PRO
2	B	28	GLU
2	B	123	ASP
2	B	176	PRO
2	B	286	THR
1	C	123	ASP
1	C	156	SER
1	C	296	THR
1	C	420	PRO
2	D	28	GLU

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Mol	Chain	Res	Type
2	D	123	ASP
2	D	176	PRO
2	D	286	THR
1	E	123	ASP
1	E	156	SER
1	E	296	THR
1	E	420	PRO
2	F	28	GLU
2	F	123	ASP
2	F	176	PRO
2	F	286	THR
1	G	123	ASP
1	G	156	SER
1	G	296	THR
1	G	420	PRO
2	H	28	GLU
2	H	123	ASP
2	H	176	PRO
2	H	286	THR
1	A	114	ALA
1	A	116	PHE
1	A	195	ILE
1	A	274	ILE
1	A	275	LYS
2	B	277	ARG
2	B	316	GLY
1	C	114	ALA
1	C	116	PHE
1	C	195	ILE
1	C	274	ILE
1	C	275	LYS
2	D	277	ARG
2	D	316	GLY
1	E	114	ALA
1	E	116	PHE
1	E	195	ILE
1	E	274	ILE
1	E	275	LYS
2	F	277	ARG
2	F	316	GLY
1	G	114	ALA
1	G	116	PHE

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Mol	Chain	Res	Type
1	G	195	ILE
1	G	274	ILE
1	G	275	LYS
2	H	277	ARG
2	H	316	GLY
1	A	357	MET
2	B	77	PHE
2	B	88	TRP
1	C	357	MET
2	D	77	PHE
2	D	88	TRP
1	E	357	MET
2	F	77	PHE
2	F	88	TRP
1	G	276	VAL
1	G	357	MET
2	H	77	PHE
2	H	88	TRP
1	A	276	VAL
1	A	462	GLY
2	B	55	PRO
1	C	276	VAL
1	C	462	GLY
2	D	55	PRO
1	E	276	VAL
1	E	462	GLY
2	F	55	PRO
1	G	462	GLY
2	H	55	PRO
2	B	170	PRO
2	D	170	PRO
2	F	170	PRO
2	H	170	PRO
2	B	420	PRO
2	D	420	PRO
2	F	420	PRO
2	H	420	PRO

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	431/500 (86%)	411 (95%)	20 (5%)	33	74
1	C	431/500 (86%)	411 (95%)	20 (5%)	33	74
1	E	431/500 (86%)	410 (95%)	21 (5%)	31	72
1	G	431/500 (86%)	411 (95%)	20 (5%)	33	74
2	B	343/400 (86%)	323 (94%)	20 (6%)	25	66
2	D	343/400 (86%)	323 (94%)	20 (6%)	25	66
2	F	343/400 (86%)	323 (94%)	20 (6%)	25	66
2	H	343/400 (86%)	323 (94%)	20 (6%)	25	66
All	All	3096/3600 (86%)	2935 (95%)	161 (5%)	29	69

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	4	PRO
1	A	14	PRO
1	A	19	PRO
1	A	58	THR
1	A	91	GLN
1	A	169	GLU
1	A	170	PRO
1	A	217	PRO
1	A	236	PRO
1	A	252	TRP
1	A	318	TYR
1	A	342	TYR
1	A	402	TRP
1	A	414	TRP
1	A	415	GLU
1	A	418	ASN
1	A	426	TRP
1	A	497	THR
1	A	507	GLN
2	B	24	TRP
2	B	25	PRO
2	B	52	PRO

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Mol	Chain	Res	Type
2	B	54	ASN
2	B	55	PRO
2	B	59	PRO
2	B	60	VAL
2	B	63	ILE
2	B	88	TRP
2	B	97	PRO
2	B	135	ILE
2	B	148	VAL
2	B	170	PRO
2	B	176	PRO
2	B	266	TRP
2	B	313	PRO
2	B	321	PRO
2	B	392	PRO
2	B	402	TRP
2	B	412	PRO
1	C	1	PRO
1	C	4	PRO
1	C	14	PRO
1	C	19	PRO
1	C	58	THR
1	C	91	GLN
1	C	169	GLU
1	C	170	PRO
1	C	217	PRO
1	C	236	PRO
1	C	252	TRP
1	C	318	TYR
1	C	342	TYR
1	C	402	TRP
1	C	414	TRP
1	C	415	GLU
1	C	418	ASN
1	C	426	TRP
1	C	497	THR
1	C	507	GLN
2	D	24	TRP
2	D	25	PRO
2	D	52	PRO
2	D	54	ASN
2	D	55	PRO

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Mol	Chain	Res	Type
2	D	59	PRO
2	D	60	VAL
2	D	63	ILE
2	D	88	TRP
2	D	97	PRO
2	D	135	ILE
2	D	148	VAL
2	D	170	PRO
2	D	176	PRO
2	D	266	TRP
2	D	313	PRO
2	D	321	PRO
2	D	392	PRO
2	D	402	TRP
2	D	412	PRO
1	E	1	PRO
1	E	4	PRO
1	E	14	PRO
1	E	19	PRO
1	E	58	THR
1	E	91	GLN
1	E	169	GLU
1	E	170	PRO
1	E	217	PRO
1	E	236	PRO
1	E	252	TRP
1	E	318	TYR
1	E	342	TYR
1	E	402	TRP
1	E	414	TRP
1	E	415	GLU
1	E	418	ASN
1	E	426	TRP
1	E	497	THR
1	E	507	GLN
1	E	510	PRO
2	F	24	TRP
2	F	25	PRO
2	F	52	PRO
2	F	54	ASN
2	F	55	PRO
2	F	59	PRO

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Mol	Chain	Res	Type
2	F	60	VAL
2	F	63	ILE
2	F	88	TRP
2	F	97	PRO
2	F	135	ILE
2	F	148	VAL
2	F	170	PRO
2	F	176	PRO
2	F	266	TRP
2	F	313	PRO
2	F	321	PRO
2	F	392	PRO
2	F	402	TRP
2	F	412	PRO
1	G	1	PRO
1	G	4	PRO
1	G	14	PRO
1	G	19	PRO
1	G	58	THR
1	G	91	GLN
1	G	169	GLU
1	G	170	PRO
1	G	217	PRO
1	G	236	PRO
1	G	252	TRP
1	G	318	TYR
1	G	342	TYR
1	G	402	TRP
1	G	414	TRP
1	G	415	GLU
1	G	418	ASN
1	G	426	TRP
1	G	497	THR
1	G	507	GLN
2	H	24	TRP
2	H	25	PRO
2	H	52	PRO
2	H	54	ASN
2	H	55	PRO
2	H	59	PRO
2	H	60	VAL
2	H	63	ILE

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Mol	Chain	Res	Type
2	H	88	TRP
2	H	97	PRO
2	H	135	ILE
2	H	148	VAL
2	H	170	PRO
2	H	176	PRO
2	H	266	TRP
2	H	313	PRO
2	H	321	PRO
2	H	392	PRO
2	H	402	TRP
2	H	412	PRO

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

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	145	GLN
1	A	161	GLN
1	A	174	GLN
1	A	175	ASN
1	A	198	HIS
1	A	208	HIS
1	A	315	HIS
1	A	367	GLN
1	A	373	GLN
1	A	407	GLN
1	A	418	ASN
1	A	471	ASN
2	B	54	ASN
2	B	57	ASN
2	B	96	HIS
2	B	145	GLN
2	B	147	ASN
2	B	151	GLN
2	B	208	HIS
2	B	235	HIS
2	B	269	GLN
2	B	394	GLN
2	B	418	ASN
1	C	23	GLN

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Mol	Chain	Res	Type
1	C	91	GLN
1	C	145	GLN
1	C	161	GLN
1	C	174	GLN
1	C	175	ASN
1	C	198	HIS
1	C	208	HIS
1	C	315	HIS
1	C	367	GLN
1	C	373	GLN
1	C	407	GLN
1	C	418	ASN
1	C	471	ASN
2	D	54	ASN
2	D	57	ASN
2	D	96	HIS
2	D	145	GLN
2	D	147	ASN
2	D	151	GLN
2	D	208	HIS
2	D	235	HIS
2	D	269	GLN
2	D	394	GLN
2	D	418	ASN
1	E	23	GLN
1	E	91	GLN
1	E	145	GLN
1	E	161	GLN
1	E	174	GLN
1	E	175	ASN
1	E	198	HIS
1	E	208	HIS
1	E	315	HIS
1	E	367	GLN
1	E	373	GLN
1	E	407	GLN
1	E	418	ASN
1	E	471	ASN
2	F	54	ASN
2	F	57	ASN
2	F	96	HIS
2	F	145	GLN

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Mol	Chain	Res	Type
2	F	147	ASN
2	F	151	GLN
2	F	208	HIS
2	F	235	HIS
2	F	269	GLN
2	F	394	GLN
2	F	418	ASN
1	G	23	GLN
1	G	91	GLN
1	G	145	GLN
1	G	161	GLN
1	G	174	GLN
1	G	175	ASN
1	G	198	HIS
1	G	208	HIS
1	G	315	HIS
1	G	367	GLN
1	G	373	GLN
1	G	407	GLN
1	G	418	ASN
1	G	471	ASN
2	H	54	ASN
2	H	57	ASN
2	H	96	HIS
2	H	145	GLN
2	H	147	ASN
2	H	151	GLN
2	H	208	HIS
2	H	235	HIS
2	H	269	GLN
2	H	394	GLN
2	H	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.