



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 07:32 PM EST

PDB ID : 1HMV  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

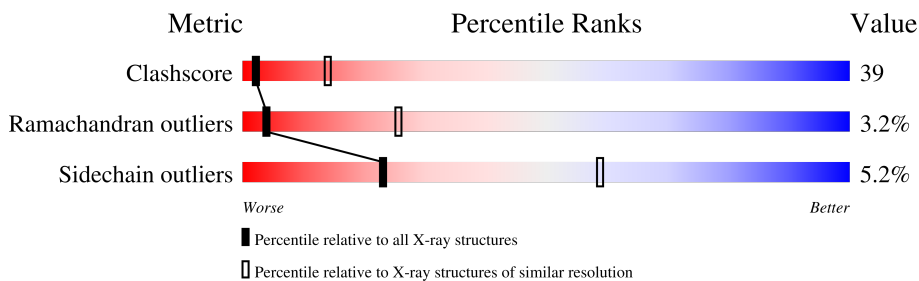
# 1 Overall quality at a glance

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	40% 51% . .
1	C	560	39% 52% . .
1	E	560	40% 51% . .
1	G	560	39% 52% . .
2	B	440	39% 45% . . 10%
2	D	440	40% 45% . . 10%
2	F	440	40% 45% . . 10%
2	H	440	39% 45% . . 10%

## 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
			Total	C	N	O	S			
1	A	536	4200	2711	698	784	7	0	0	0
1	C	536	4200	2711	698	784	7	0	0	0
1	E	536	4200	2711	698	784	7	0	0	0
1	G	536	4200	2711	698	784	7	0	0	0

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

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

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

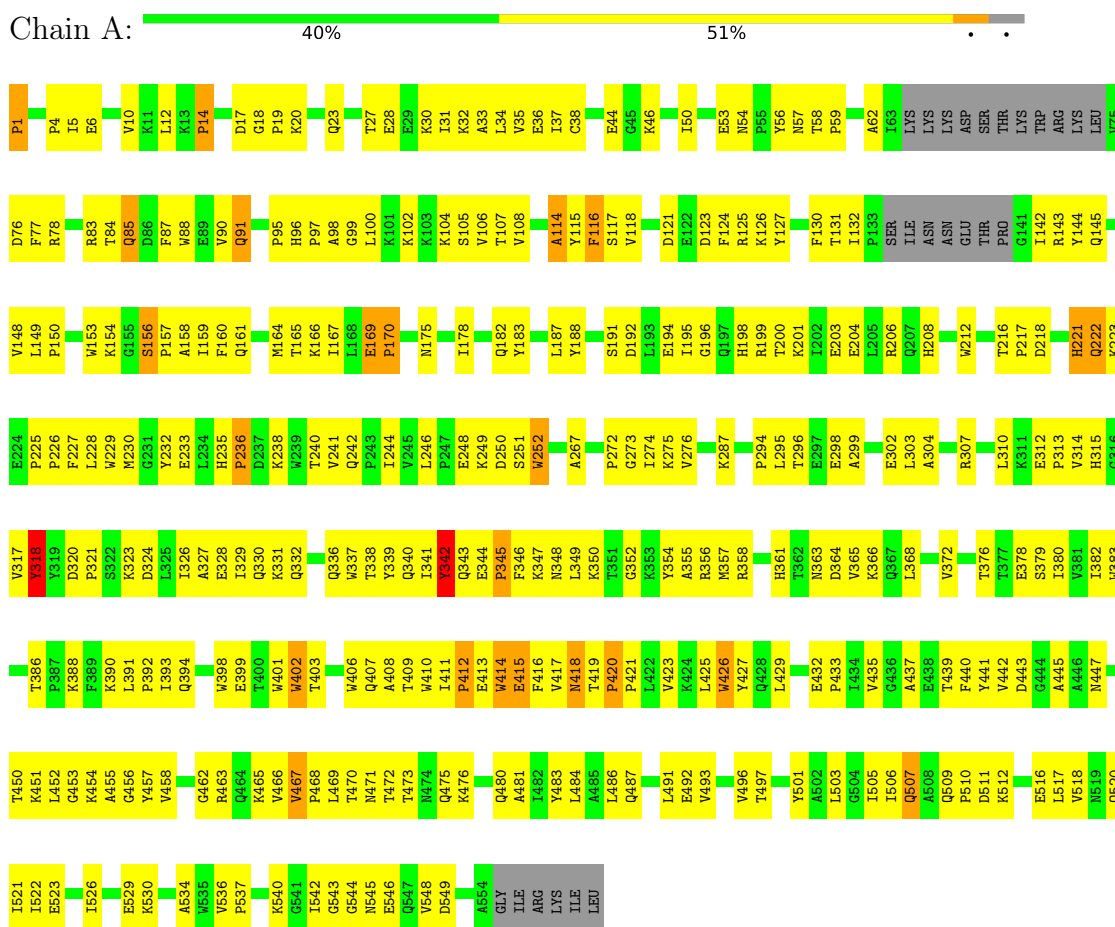
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0

### 3 Residue-property plots

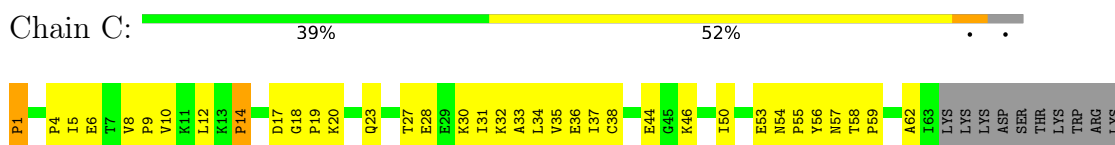
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

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



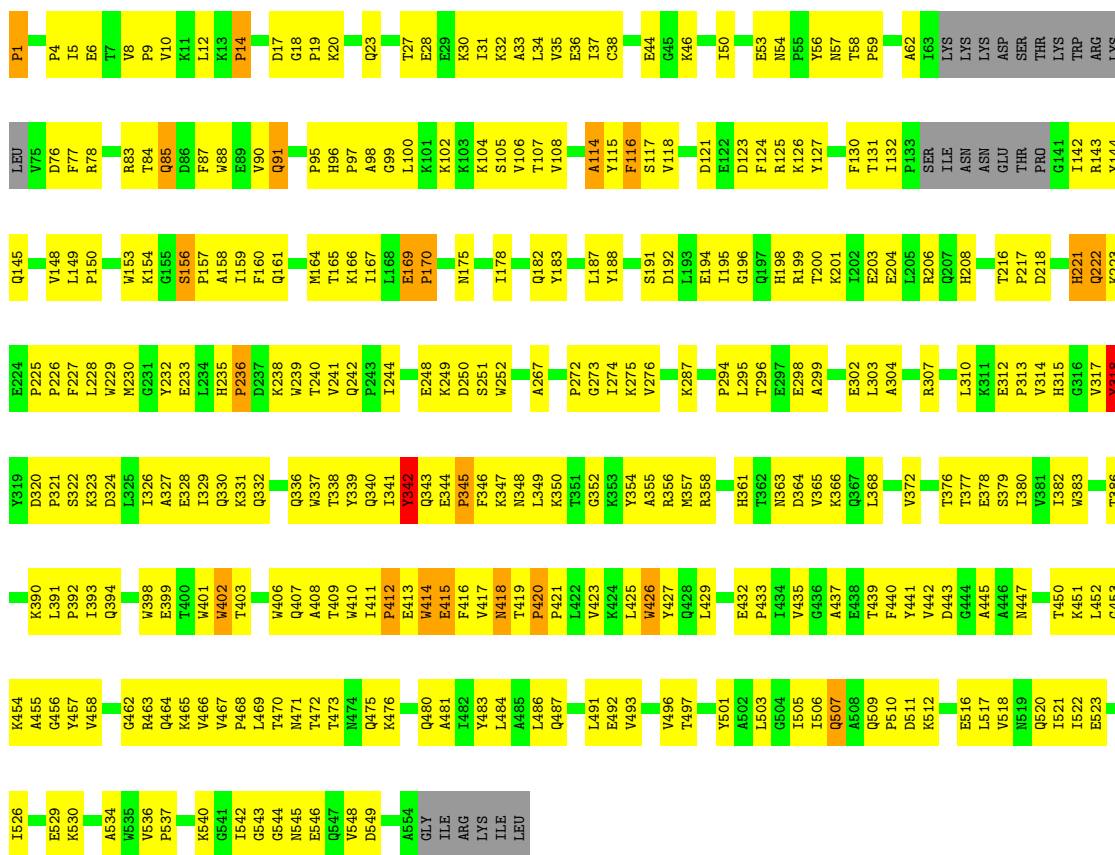
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)





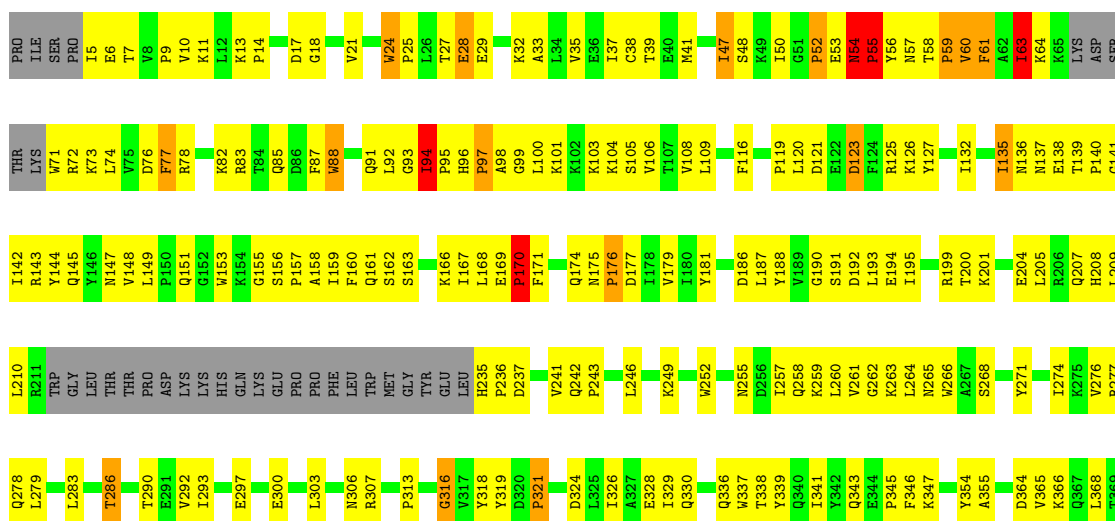
● Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

Chain G:  39% 52%



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

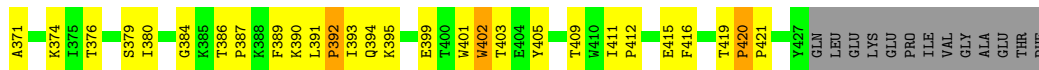
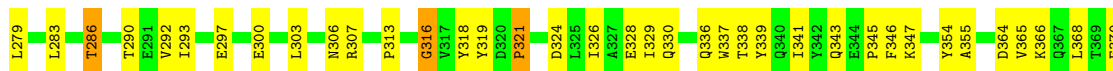
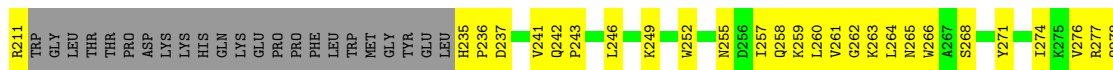
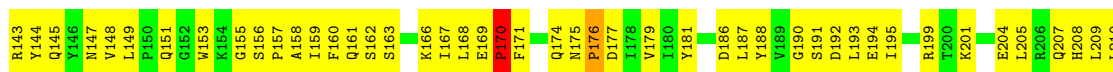
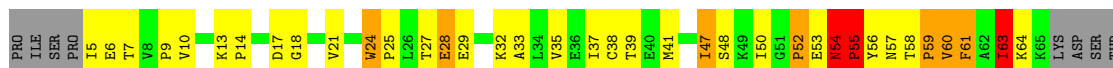
Chain B:  39% 45% 10%





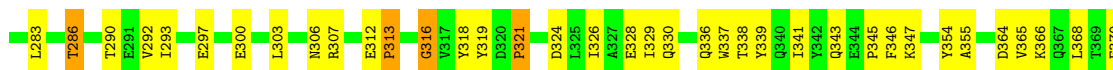
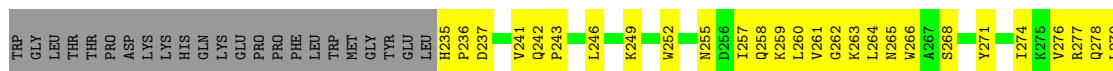
● Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

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%

PRO	ILE	SER	PRO	I5	E6	T7	F6	P9	V10	K13	P14	D17	G18	V21	K24	P25	L26	T27	E28	E29	K32	A33	L34	V35	F36	L37	C38	T39	E40	M41	I47	S48	K49	I50	G51	P52	E53	K64	P65	Y66	N57	T58	P59	V60	F61	A62	K64	K65	LYS	ASP	SER	THR		
LYS	W71	K72	K73	L74	V75	D76	F77	R78	K82	R83	T84	Q85	D86	F87	W88	G91	L92	G93	I94	P95	H96	P97	A98	G99	L100	K101	K102	K103	K104	S105	V106	T107	V108	L109	F116	P119	L120	D121	E122	D123	F124	R125	K126	Y127	I132	I135	N136	N137	E138	T139	P140	G141	SER	THR
R143	Y144	Q145	Y146	N147	V148	L149	P150	Q151	G152	W153	K154	G155	S156	P157	A158	I159	F160	O161	S162	S163	K166	I167	L168	E169	F170	F171	Q174	N175	P176	D177	I178	V179	I180	Y181	D186	L187	Y188	V189	G190	S191	D192	L193	E194	I195	R199	T200	K201	E204	L205	S206	Q207	H208	L209	L210
R211	TRP	GLY	LEU	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU	PRO	PRO	PHE	LEU	TRP	MET	GLY	TYR	H235	P236	D237	V241	Q242	P243	L246	K249	W252	N255	D256	L257	Q258	K259	L260	V261	G262	K263	L264	N265	W266	K267	S268	Y271	I274	K275	V276	R277	Q278				
L279	L283	L283	L283	T286	T290	E291	V292	L293	E297	E300	L303	N306	R307	F313	G316	V317	Y318	Y319	D320	P321	D324	L325	L326	A327	E328	I329	Q330	Q336	W337	T338	Y339	Q340	I341	Y342	Q343	E344	P345	F346	K347	Y354	A355	G364	V365	K366	Q367	L368	T369	E370						
A371	K374	L375	T376	S379	L380	G384	K385	T386	P387	K388	F389	K390	L391	P392	I393	Q394	K395	E399	W400	W401	W402	T403	E404	Y405	T409	W410	L411	P412	E415	F416	T419	P420	P421	Y427	GLN	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE							



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.70Å 162.80Å 331.80Å 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.	Xtrriage
Total number of atoms	29596	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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

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 [i](#)

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:CE1	1:G:390:LYS:CG	2.46	0.98
1:C:346:PHE:CG	1:G:390:LYS:CE	2.47	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:C:342:TYR:OH	1:G:345:PRO:HG3	1.68	0.94
1:E:420:PRO:HG2	1:E:421:PRO:HD2	1.47	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:HB2	1:G:390:LYS:HZ1	1.10	0.90
1:C:346:PHE:HE1	1:G:342:TYR:OH	1.53	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:A:107:THR:HG23	1:A:198:HIS:HE1	1.38	0.89
1:C:107:THR:HG23	1:C: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:104:LYS:HB3	2:F:192:ASP:HA	1.55	0.87
2:F:260:LEU:HD21	2:F:303:LEU:HD21	1.54	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:C:244:ILE:HD12	1:C:267:ALA:HB2	1.56	0.86
1:G:244:ILE:HD12	1:G: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
1:E:244:ILE:HD12	1:E:267:ALA:HB2	1.56	0.84
2:F:365:VAL:HG11	2:F:401:TRP:HB2	1.59	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
2:D:171:PHE:HE2	2:D:204:GLU:HB2	1.41	0.83
1:E:540:LYS:HZ1	2:F:265:ASN:HB2	1.37	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:C:326:ILE:HB	1:C:342:TYR:CE1	2.15	0.82
1:G:326:ILE:HB	1:G:342:TYR:CE1	2.15	0.82
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.15	0.82
2:D:33:ALA:O	2:D:37:ILE:HG13	1.80	0.82
2:F:33:ALA:O	2:F: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:HA	1:G:91:GLN:HE21	1.47	0.80
1:C:91:GLN:HA	1:C:91:GLN:HE21	1.47	0.80
2:D:24:TRP:HH2	2:D:61:PHE:CE1	1.99	0.80
1:C:107:THR:HG23	1:C:198:HIS:CE1	2.16	0.79
2:B:24:TRP:HH2	2:B:61:PHE:CE1	1.99	0.79
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.18	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:A:393:ILE:HB	1:A:423:VAL:CG2	2.12	0.78
1:E:393:ILE:HB	1:E: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:A:361:HIS:CD2	1:A:518:VAL:HG11	2.18	0.77
1:G:361:HIS:HD2	1:G:518:VAL:HG11	1.49	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:HG2	1:A:85:GLN:O	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:O	1:E:85:GLN:HG2	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
1:C:10:VAL:HG21	1:C:153:TRP:HH2	1.52	0.74
2:F:17:ASP:O	2:F:83:ARG:HD3	1.87	0.74
2:F:24:TRP:HH2	2:F:61:PHE:CD1	2.05	0.74
1:G:131:THR:HG22	1:G:143:ARG:HG3	1.69	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: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:C:85:GLN:O	1:C:85:GLN:HG2	1.86	0.74
1:A:249:LYS:HE2	1:A:251:SER:HB3	1.69	0.74
1:A:131:THR:HG22	1:A:143:ARG:HG3	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:G:10:VAL:HG21	1:G:153:TRP:HH2	1.52	0.74
1:G:85:GLN:HG2	1:G:85:GLN:O	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:249:LYS:HE2	1:E:251:SER:HB3	1.69	0.73
1:E:391:LEU:HD12	1:E:414:TRP:CE3	2.23	0.73
2:B:17:ASP:O	2:B:83:ARG:HD3	1.87	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:50:ILE:CG2	2:B:145:GLN:HB2	2.18	0.73
2:B:63:ILE:HG23	2:B:72:ARG:HB3	1.70	0.73
2:H:103:LYS:HZ2	2:H:179:VAL:N	1.86	0.73
2:B:103:LYS:NZ	2:B:179:VAL:HG23	2.04	0.73
2:D:17:ASP:O	2:D:83:ARG:HD3	1.87	0.73
1:E:90:VAL:HG12	2:F:141:GLY:H	1.53	0.73
1:G:391:LEU:HD12	1:G:414:TRP:CE3	2.24	0.73
2:D:103:LYS:HZ2	2:D:179:VAL:N	1.86	0.73
2:H:103:LYS:NZ	2:H:179:VAL:HG23	2.04	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
2:D:63:ILE:HG23	2:D:72:ARG:HB3	1.70	0.73
1:G:90:VAL:HG12	2:H:141:GLY:H	1.53	0.73
1:E:442:VAL:CG1	1:E:481:ALA:HB1	2.19	0.72
2:H:171:PHE:HB2	2:H:208:HIS:CE1	2.24	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
1:C:157:PRO:HG2	1:C:158:ALA:H	1.54	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
2:B:171:PHE:HB2	2:B:208:HIS:CE1	2.24	0.72
2:D:171:PHE:HB2	2:D:208:HIS:CE1	2.25	0.72
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.72	0.72
2:F:50:ILE:CG2	2:F:145:GLN:HB2	2.18	0.72
2:H:246:LEU:HD11	2:H:264:LEU:HD21	1.72	0.72
1:A:90:VAL:HG12	2:B:141:GLY:H	1.53	0.72
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.72	0.72
1:A:393:ILE:O	1:A:414:TRP:HH2	1.73	0.72
1:C:391:LEU:HD12	1:C:414:TRP:CE3	2.23	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
1:C:442:VAL:CG1	1:C:481:ALA:HB1	2.19	0.72
2:D:50:ILE:CG2	2:D:145:GLN:HB2	2.18	0.72
2:F:63:ILE:HG23	2:F:72:ARG:HB3	1.70	0.71
2:F:92:LEU:HG	2:F:158:ALA:HB2	1.72	0.71
1:E:518:VAL:O	1:E:522:ILE:HG13	1.90	0.71
1:A:518:VAL:O	1:A:522:ILE:HG13	1.90	0.71
1:C:341:ILE:HD12	1:C:383:TRP:HE1	1.55	0.71
1:E:341:ILE:HD12	1:E:383:TRP:HE1	1.55	0.71
1:G:518:VAL:O	1:G:522:ILE:HG13	1.90	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:A:442:VAL:CG1	1:A:481:ALA:HB1	2.19	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: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
2:B:47:ILE:HG22	2:B:48:SER:H	1.56	0.71
1:C:518:VAL:O	1:C:522:ILE:HG13	1.90	0.71
2:D:47:ILE:HG22	2:D:48:SER:H	1.56	0.71
2:H:50:ILE:CG2	2:H:145:GLN:HB2	2.18	0.71
1:A:225:PRO:HG2	1:A:226:PRO:HD3	1.73	0.70
1:A:341:ILE:HD12	1:A:383:TRP:HE1	1.55	0.70
1:C:225:PRO:HG2	1:C:226:PRO:HD3	1.73	0.70
1:G:341:ILE:HD12	1:G:383:TRP:HE1	1.55	0.70

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ALA:CB	1:E:383:TRP:HH2	2.07	0.68
2:F:123:ASP:HA	2:F:126:LYS:NZ	2.09	0.68
2:H:97:PRO:HG2	2:H:181:TYR:HB2	1.76	0.68
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: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
1:C:346:PHE:CD1	1:G:390:LYS:NZ	2.62	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: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:A:426:TRP:HA	1:A:426:TRP:HE3	1.59	0.67
1:A:100:LEU:O	1:A:318:TYR:HB3	1.94	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
2:F:97:PRO:HG2	2:F:181:TYR:HB2	1.76	0.67
1:G:378:GLU:O	1:G:382:ILE:HG13	1.95	0.67
1:G:393:ILE:O	1:G:414:TRP:CH2	2.48	0.67
1:A:378:GLU:O	1:A:382:ILE:HG13	1.95	0.67
2:D:123:ASP:HA	2:D: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:H:123:ASP:HA	2:H:126:LYS:NZ	2.10	0.67
2:F:153:TRP:CZ3	2:F:155:GLY:HA3	2.30	0.67
1:C:426:TRP:HA	1:C:426:TRP:HE3	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
1:G:244:ILE:CD1	1:G:267:ALA:HB2	2.25	0.67
1:A:98:ALA:CB	1:A:383:TRP:HH2	2.07	0.66
2:B:153:TRP:CZ3	2:B:155:GLY:HA3	2.30	0.66
1:G:457:TYR:CE1	1:G:465:LYS:HB3	2.31	0.66
2:H:94:ILE:HG22	2:H:95:PRO:CD	2.25	0.66
1:C:378:GLU:O	1:C:382:ILE:HG13	1.95	0.66
1:E:426:TRP:HA	1:E:426:TRP:HE3	1.59	0.66
1:A:457:TYR:CE1	1:A:465:LYS:HB3	2.31	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
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:G:167:ILE:O	1:G:208:HIS:HE1	1.78	0.66
1:E:167:ILE:O	1:E:208:HIS:HE1	1.78	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
2:B:94:ILE:HG22	2:B:95:PRO:CD	2.25	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
1:E:149:LEU:HD22	1:E:156:SER:HA	1.78	0.66
1:C:98:ALA:CB	1:C:383:TRP:HH2	2.07	0.66
1:C:393:ILE:O	1:C:414:TRP:CH2	2.48	0.66
2:H:109:LEU:HD12	2:H:187:LEU:HD23	1.77	0.66
2:H:153:TRP:CZ3	2:H:155:GLY:HA3	2.30	0.66
1:A:165:THR:HG21	2:B:140:PRO:HG2	1.77	0.66
2:B:21:VAL:CG1	2:B:59:PRO:HD3	2.26	0.66
1:C:537:PRO:HG2	2:D:262:GLY:HA2	1.78	0.66
1:G:165:THR:HG21	2:H:140:PRO:HG2	1.77	0.66
2:B:151:GLN:HE21	2:B:151:GLN:HA	1.61	0.66
2:F:151:GLN:HA	2:F:151:GLN:HE21	1.61	0.66
1:G:149:LEU:HD22	1:G:156:SER:HA	1.78	0.66
1:A:33:ALA:O	1:A:37:ILE:HG13	1.95	0.65
1:A:393:ILE:O	1:A:414:TRP:CH2	2.48	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
2:D:21:VAL:CG1	2:D:59:PRO:HD3	2.26	0.65
1:E:33:ALA:O	1:E:37:ILE:HG13	1.95	0.65
1:A:27:THR:OG1	1:A:30:LYS:HG3	1.97	0.65
1:A:167:ILE:O	1:A:208:HIS:HE1	1.78	0.65
1:A:537:PRO:HG2	2:B:262:GLY:HA2	1.78	0.65
2:B:61:PHE:CE2	2:B:74:LEU:HD23	2.31	0.65
2:B:103:LYS:NZ	2:B:179:VAL:H	1.93	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
2:D:151:GLN:HA	2:D:151:GLN:HE21	1.61	0.65
1:G:27:THR:OG1	1:G:30:LYS:HG3	1.97	0.65
2:D:109:LEU:HD12	2:D:187:LEU:HD23	1.77	0.65
2:F:61:PHE:CE2	2:F:74:LEU:HD23	2.31	0.65
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
1:C:420:PRO:HG2	1:C:421:PRO:CD	2.22	0.65
2:D:303:LEU:O	2:D:307:ARG:HG3	1.97	0.65

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:LYS:NZ	2:B:194:GLU:HA	2.12	0.64
1:C:537:PRO:HD2	1:C:542:ILE:CD1	2.27	0.64
2:D:104:LYS:NZ	2:D:194:GLU:HA	2.12	0.64
2:F:24:TRP:CZ3	2:F:61:PHE:HB3	2.32	0.64
2:F:104:LYS:NZ	2:F:194:GLU:HA	2.12	0.64
2:F:246:LEU:HB2	2:F:307:ARG:NH1	2.13	0.64
2:B:246:LEU:CD1	2:B:264:LEU:HD21	2.27	0.64
2:D:103:LYS:NZ	2:D:179:VAL:H	1.93	0.64
2:F:157:PRO:HG2	2:F:158:ALA:N	2.08	0.64
2:H:126:LYS:HA	2:H:145:GLN:NE2	2.13	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:B:149:LEU:HD22	2:B:156:SER:HA	1.79	0.64
2:D:264:LEU:CD2	2:D:274:ILE:HD11	2.24	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:A:420:PRO:HG2	1:A:421:PRO:CD	2.22	0.64
1:G:376:THR:HG23	1:G:386:THR:CG2	2.25	0.64
2:H:169:GLU:HB3	2:H:170:PRO:HD3	1.78	0.64
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:D:246:LEU:HB2	2:D:307:ARG:NH1	2.13	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:E:28:GLU:O	1:E:32:LYS:HG3	1.98	0.63
1:G:28:GLU:O	1:G:32:LYS:HG3	1.98	0.63
2:B:126:LYS:HA	2:B:145:GLN:NE2	2.13	0.63
2:D:246:LEU:CD1	2:D:264:LEU:HD21	2.27	0.63
2:H:63:ILE:HG12	2:H:64:LYS:N	2.14	0.63
1:C:342:TYR:CE1	1:G:345:PRO:HG3	2.33	0.63
1:E:376:THR:HG23	1:E:386:THR:CG2	2.25	0.63
2:F:126:LYS:HA	2:F:145:GLN:NE2	2.13	0.63
1:A:537:PRO:HD2	1:A:542:ILE:CD1	2.27	0.63
1:C:393:ILE:HB	1:C:423:VAL:HG21	1.79	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)
1:A:206:ARG:HH22	1:A:218:ASP:HA	1.64	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
2:H:103:LYS:NZ	2:H:179:VAL:H	1.93	0.63
1:A:28:GLU:O	1:A:32:LYS:HG3	1.98	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:238:LYS:HE2	1:A:240:THR:CG2	2.29	0.62
2:B:21:VAL:HG11	2:B:59:PRO:HD3	1.80	0.62
1:C:238:LYS:HE2	1:C:240:THR:CG2	2.29	0.62
2:F:21:VAL:HG11	2:F:59:PRO:HD3	1.80	0.62
2:H:149:LEU:HD22	2:H:156:SER:HA	1.79	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:C:28:GLU:O	1:C:32:LYS:HG3	1.98	0.62
2:D:21:VAL:HG11	2:D:59:PRO:HD3	1.80	0.62
2:D:63:ILE:HG12	2:D:64:LYS:N	2.14	0.62
1:E:393:ILE:HB	1:E:423:VAL:HG21	1.80	0.62
2:F:125:ARG:NH1	2:F:147:ASN:HA	2.15	0.62
1:G:206:ARG:HH22	1:G:218:ASP:HA	1.64	0.62
2:B:125:ARG:NH1	2:B:147:ASN:HA	2.15	0.62
1:C:346:PHE:HD1	1:G:390:LYS:HE3	0.80	0.62
2:D:125:ARG:NH1	2:D:147:ASN:HA	2.15	0.62
2:F:149:LEU:HD22	2:F:156:SER:HA	1.79	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:E:206:ARG:HG3	1:E:216:THR:OG1	2.00	0.62
1:A:491:LEU:HB3	1:A:529:GLU:CB	2.30	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:G:339:TYR:CE1	1:G:352:GLY:HA3	2.35	0.62
1:A:206:ARG:HG3	1:A:216:THR:OG1	2.00	0.62
1:C:491:LEU:HB3	1:C:529:GLU:CB	2.30	0.62
2:D:376:THR:HG22	2:D:389:PHE:CE1	2.35	0.62
2:F:376:THR:HG22	2:F:389:PHE:CE1	2.35	0.62
2:H:125:ARG:NH1	2:H:147:ASN:HA	2.15	0.62
1:G:238:LYS:HE2	1:G:240:THR:CG2	2.29	0.61
1:G:249:LYS:HG2	1:G:250:ASP:N	2.15	0.61
2:B:47:ILE:HG21	2:B:144:TYR:HB3	1.82	0.61
2:D:354:TYR:OH	2:D:374:LYS:HG2	2.00	0.61
2:F:47:ILE:HG21	2:F:144:TYR:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:257:ILE:HB	2:F:283:LEU:HD21	1.82	0.61
1:A:249:LYS:HG2	1:A:250:ASP:N	2.15	0.61
2:B:354:TYR:OH	2:B:374:LYS:HG2	2.00	0.61
1:C:104:LYS:HB2	1:C:192:ASP:HA	1.82	0.61
1:C:339:TYR:CE1	1:C:352:GLY:HA3	2.35	0.61
1:E:238:LYS:HE2	1:E:240:THR:CG2	2.29	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
2:H:376:THR:HG22	2:H:389:PHE:CE1	2.35	0.61
1:G:104:LYS:HB2	1:G:192:ASP:HA	1.82	0.61
1:G:435:VAL:HG22	2:H:290:THR:HG21	1.83	0.61
2:B:376:THR:HG22	2:B:389:PHE:CE1	2.35	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
1:E:104:LYS:HB2	1:E:192:ASP:HA	1.82	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
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: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: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:88:TRP:CH2	2:F:57:ASN:HB3	2.36	0.61
1:E:249:LYS:HG2	1:E:250:ASP:N	2.15	0.61
1:E:339:TYR:CE1	1:E:352:GLY:HA3	2.35	0.61
2:H:47:ILE:HG21	2:H:144:TYR:HB3	1.82	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:A:104:LYS:HB2	1:A:192:ASP:HA	1.82	0.60
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.83	0.60
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
2:F:354:TYR:OH	2:F:374:LYS:HG2	2.00	0.60
1:G:376:THR:O	1:G:380:ILE:HG13	2.01	0.60
1:G:393:ILE:HG23	1:G:414:TRP:HH2	1.58	0.60
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ILE:HG21	2:D:144:TYR:HB3	1.82	0.60
2:D:257:ILE:HB	2:D:283:LEU:HD21	1.82	0.60
1:E:326:ILE:HB	1:E:342:TYR:HE1	1.65	0.60
1:E:509:GLN:N	1:E:510:PRO:HD3	2.17	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
1:G:88:TRP:CH2	2:H:57:ASN:HB3	2.36	0.60
2:H:151:GLN:HA	2:H:151:GLN:NE2	2.17	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:D:171:PHE:CE2	2:D:204:GLU:HB2	2.31	0.60
1:E:540:LYS:HZ3	2:F:261:VAL:CG1	2.14	0.60
2:H:47:ILE:CG2	2:H:144:TYR:HB3	2.31	0.60
2:H:257:ILE:HB	2:H:283:LEU:HD21	1.82	0.60
1:A:88:TRP:CH2	2:B:57:ASN:HB3	2.36	0.60
2:D:47:ILE:CG2	2:D:144:TYR:HB3	2.31	0.60
2:B:328:GLU:O	2:B:339:TYR:HA	2.02	0.60
1:C:160:PHE:CE1	1:C:164:MET:HG2	2.37	0.60
1:C:326:ILE:HB	1:C:342:TYR:HE1	1.66	0.60
2:D:328:GLU:O	2:D:339:TYR:HA	2.02	0.60
2:F:47:ILE:CG2	2:F:144:TYR:HB3	2.31	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: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
1:G:509:GLN:N	1:G:510:PRO:HD3	2.17	0.60
2:H:328:GLU:O	2:H:339:TYR:HA	2.02	0.60
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.84	0.59
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:238:LYS:HE2	1:A:240:THR:HG22	1.83	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:C:235:HIS:HB3	1:C:236:PRO:HD2	1.84	0.59
1:E:160:PHE:CE1	1:E:164:MET:HG2	2.37	0.59
1:G:363:ASN:OD1	1:G:364:ASP:N	2.35	0.59
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.84	0.59
1:A:392:PRO:O	1:A:423:VAL:HG22	2.03	0.59
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.84	0.59
1:E:238:LYS:HE3	1:E:315:HIS:CD2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:PHE:CE1	1:G:164:MET:HG2	2.37	0.59
1:A:363:ASN:OD1	1:A:364:ASP:N	2.35	0.59
1:E:363:ASN:OD1	1:E:364:ASP:N	2.35	0.59
1:G:238:LYS:HE3	1:G:315:HIS:CD2	2.36	0.59
2:B:106:VAL:HA	2:B:190:GLY:HA2	1.85	0.59
1:C:392:PRO:O	1:C:423:VAL:HG22	2.03	0.59
2:F:328:GLU:O	2:F:339:TYR:HA	2.02	0.59
1:G:326:ILE:HB	1:G:342:TYR:HE1	1.66	0.59
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.38	0.59
2:D:151:GLN:HA	2:D:151:GLN:NE2	2.17	0.59
1:E:161:GLN:O	1:E:165:THR:HG23	2.03	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:D:106:VAL:HA	2:D:190:GLY:HA2	1.85	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
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:235:HIS:HB3	1:E:236:PRO:HD2	1.84	0.59
1:E:295:LEU:CB	1:E:299:ALA:HB2	2.33	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:B:151:GLN:HA	2:B:151:GLN:NE2	2.17	0.58
2:D:153:TRP:CH2	2:D:155:GLY:HA3	2.38	0.58
2:B:171:PHE:CE2	2:B:204:GLU:HB2	2.31	0.58
2:B:103:LYS:HZ1	2:B:179:VAL:HG23	1.67	0.58
1:C:346:PHE:CZ	1:G:390:LYS:CG	2.80	0.58
1:E:17:ASP:O	1:E:83:ARG:HD3	2.03	0.58
1:G:167:ILE:O	1:G:170:PRO:HD2	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:C:523:GLU:O	1:C:526:ILE:HG12	2.04	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:17:ASP:O	1:C:83:ARG:HD3	2.03	0.58
1:E:393:ILE:HB	1:E:423:VAL:HG22	1.86	0.58
2:H:106:VAL:HA	2:H:190:GLY:HA2	1.85	0.58
1:G:523:GLU:O	1:G:526:ILE:HG12	2.04	0.58
2:H:171:PHE:CE2	2:H:204:GLU:HB2	2.31	0.58
1:A:17:ASP:O	1:A:83:ARG:HD3	2.03	0.58

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:ASN:HD21	2:F:56:TYR:HB2	1.70	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:D:5:ILE:HG22	2:D:6:GLU:N	2.20	0.57
2:F:5:ILE:HG22	2:F:6:GLU:N	2.20	0.57
1:G:17:ASP:O	1:G:83:ARG:HD3	2.03	0.57
1:G:458:VAL:HG23	1:G:548:VAL:HG22	1.87	0.57
1:A:418:ASN:HD22	1:A:418:ASN:C	2.08	0.57
1:C:229:TRP:CH2	1:C:230:MET:HE1	2.39	0.57
1:E:56:TYR:O	1:E:143:ARG:NH2	2.38	0.57
1:E:320:ASP:OD2	1:E:323:LYS:HG3	2.05	0.57
2:F:395:LYS:O	2:F:399:GLU:HG3	2.05	0.57
2:H:28:GLU:HG2	2:H:32:LYS:NZ	2.19	0.57
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.05	0.56
2:B:54:ASN:C	2:B:54:ASN:HD22	2.08	0.56
1:C:393:ILE:HB	1:C:423:VAL:HG22	1.86	0.56
1:E:98:ALA:HB1	1:E:383:TRP:HH2	1.70	0.56
1:E:411:ILE:HG22	1:E:412:PRO:HD2	1.86	0.56
2:H:379:SER:OG	2:H:387:PRO:HD3	2.05	0.56
2:B:28:GLU:HG2	2:B:32:LYS:NZ	2.19	0.56
1:C:346:PHE:CG	1:G:390:LYS:CD	2.87	0.56
1:C:418:ASN:C	1:C:418:ASN:HD22	2.08	0.56
1:G:429:LEU:HD11	1:G:506:ILE:HG22	1.87	0.56
1:G:441:TYR:HE2	1:G:543:GLY:O	1.88	0.56
1:A:87:PHE:CE2	1:A:159:ILE:HD11	2.40	0.56
1:A:98:ALA:HB1	1:A:383:TRP:HH2	1.70	0.56
1:A:458:VAL:HG23	1:A:548:VAL:HG22	1.87	0.56
2:B:61:PHE:CE2	2:B:403:THR:HG22	2.41	0.56
2:B:271:TYR:O	2:B:274:ILE:HG22	2.06	0.56
1:C:87:PHE:CE2	1:C:159:ILE:HD11	2.40	0.56
1:C:517:LEU:O	1:C:521:ILE:HG13	2.06	0.56
2:D:54:ASN:C	2:D:54:ASN:HD22	2.08	0.56
2:D:55:PRO:HG2	2:D:56:TYR:N	2.19	0.56
2:D:271:TYR:O	2:D:274:ILE:HG22	2.06	0.56
2:D:395:LYS:O	2:D:399:GLU:HG3	2.05	0.56
2:F:54:ASN:HD22	2:F:54:ASN:C	2.08	0.56
2:F:379:SER:OG	2:F:387:PRO:HD3	2.05	0.56
1:G:411:ILE:HG22	1:G:412:PRO:HD2	1.86	0.56
2:H:5:ILE:HG22	2:H:6:GLU:N	2.20	0.56
2:H:54:ASN:C	2:H:54:ASN:HD22	2.08	0.56
2:H:61:PHE:CE2	2:H:403:THR:HG22	2.41	0.56

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:TYR:HD1	1:G:241:VAL:HG22	1.70	0.55
1:G:248:GLU:HG3	1:G:307:ARG:NH2	2.20	0.55
2:F:72:ARG:HH12	2:F:409:THR:HA	1.71	0.55
2:H:105:SER:HB3	2:H:235:HIS:CE1	2.41	0.55
1:E:248:GLU:HG3	1:E:307:ARG:NH2	2.20	0.55
1:E:298:GLU:O	1:E:302:GLU:HG3	2.06	0.55
1:G:298:GLU:O	1:G:302:GLU:HG3	2.06	0.55
2:H:72:ARG:HH12	2:H:409:THR:HA	1.71	0.55
2:H:125:ARG:HG2	2:H:125:ARG:HH11	1.71	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
2:B:139:THR:HG22	2:B:140:PRO:O	2.06	0.55
2:D:72:ARG:HH12	2:D:409:THR:HA	1.71	0.55
1:E:337:TRP:HZ3	1:E:368:LEU:HD13	1.72	0.55
1:E:439:THR:HG22	1:E:441:TYR:CE1	2.42	0.55
2:F:376:THR:HB	2:F:386:THR:HG22	1.88	0.55
1:G:98:ALA:HB1	1:G:349:LEU:HB3	1.89	0.55
1:G:337:TRP:HZ3	1:G:368:LEU:HD13	1.72	0.55
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.89	0.55
2:B:125:ARG:HG2	2:B:125:ARG:HH11	1.71	0.55
1:C:439:THR:HG22	1:C:441:TYR:CE1	2.42	0.55
1:E:28:GLU:HB3	1:E:32:LYS:HE3	1.88	0.55
2:F:61:PHE:CE2	2:F:403:THR:HG22	2.41	0.55
2:F:97:PRO:O	2:F:98:ALA:HB3	2.07	0.55
1:G:329:ILE:HD12	1:G:391:LEU:CD2	2.36	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:C:298:GLU:O	1:C:302:GLU:HG3	2.06	0.55
1:G:28:GLU:HB3	1:G:32:LYS:HE3	1.88	0.55
2:H:366:LYS:O	2:H:370:GLU:HG3	2.07	0.55
1:A:298:GLU:O	1:A:302:GLU:HG3	2.06	0.55
2:B:72:ARG:HH12	2:B:409:THR:HA	1.71	0.55
2:B:101:LYS:O	2:B:236:PRO:HB2	2.07	0.55
2:B:201:LYS:HD3	2:B:204:GLU:OE1	2.07	0.55
1:C:98:ALA:HB1	1:C:349:LEU:HB3	1.89	0.55
1:C:232:TYR:HD1	1:C:241:VAL:HG22	1.70	0.55
1:C:337:TRP:HZ3	1:C:368:LEU:HD13	1.72	0.55
2:D:101:LYS:O	2:D:236:PRO:HB2	2.07	0.55
2:D:379:SER:OG	2:D:387:PRO:HD3	2.05	0.55
1:E:323:LYS:HD3	1:E:344:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:LEU:O	1:E:521:ILE:HG13	2.06	0.55
1:G:323:LYS:HD3	1:G:344:GLU:OE2	2.07	0.55
1:G:537:PRO:HD2	1:G:542:ILE:HD11	1.88	0.55
2:H:61:PHE:CZ	2:H:402:TRP:CZ2	2.95	0.55
1:A:401:TRP:HB2	1:A:425:LEU:HD21	1.89	0.55
2:B:104:LYS:HZ3	2:B:194:GLU:HA	1.72	0.55
1:C:332:GLN:HG2	1:C:332:GLN:O	2.07	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:E:491:LEU:HB3	1:E:529:GLU:HB3	1.88	0.55
1:E:537:PRO:HD2	1:E:542:ILE:HD11	1.88	0.55
1:G:229:TRP:CH2	1:G:230:MET:HE1	2.42	0.55
1:G:439:THR:HG22	1:G:441:TYR:CE1	2.42	0.55
2:H:201:LYS:HD3	2:H:204:GLU:OE1	2.07	0.55
1:A:332:GLN:O	1:A:332:GLN:HG2	2.07	0.55
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.89	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:99:GLY:HA2	1:A:383:TRP:HZ3	1.72	0.54
1:A:463:ARG:HH11	1:A:463:ARG:HG3	1.72	0.54
2:B:366:LYS:O	2:B:370:GLU:HG3	2.07	0.54
1:C:229:TRP:CZ3	1:C:230:MET:HE1	2.43	0.54
1:C:323:LYS:HD3	1:C:344:GLU:OE2	2.07	0.54
2:D:125:ARG:HH11	2:D:125:ARG:HG2	1.71	0.54
1:E:329:ILE:HD12	1:E:391:LEU:CD2	2.36	0.54
1:G:5:ILE:HD11	1:G:166:LYS:HD2	1.89	0.54
1:A:201:LYS:HD3	1:A:204:GLU:OE2	2.07	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
2:D:104:LYS:HZ3	2:D:194:GLU:HA	1.72	0.54
1:E:332:GLN:O	1:E:332:GLN:HG2	2.07	0.54
1:G:201:LYS:HD3	1:G:204:GLU:OE2	2.07	0.54
2:H:97:PRO:O	2:H:98:ALA:HB3	2.07	0.54
1:A:200:THR:O	1:A:203:GLU:HB3	2.07	0.54
1:A:491:LEU:HB3	1:A:529:GLU:HB3	1.88	0.54
1:C:5:ILE:HD11	1:C:166:LYS:HD2	1.89	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:126:LYS:HA	1:A:145:GLN:HE21	1.73	0.54
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.43	0.54

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:HD11	1:A:350:LYS:HB3	1.90	0.54
1:C:201:LYS:HD3	1:C:204:GLU:OE2	2.07	0.54
2:D:61:PHE:CZ	2:D:402:TRP:CZ2	2.95	0.54
2:D:376:THR:HB	2:D:386:THR:HG22	1.88	0.54
2:D:392:PRO:HG2	2:D:392:PRO:O	2.08	0.54
2:F:368:LEU:O	2:F:371:ALA:HB3	2.07	0.54
1:G:341:ILE:HD11	1:G:350:LYS:HB3	1.90	0.54
2:H:376:THR:HB	2:H:386:THR:HG22	1.88	0.54
1:A:131:THR:HA	1:A:142:ILE:O	2.07	0.54
2:B:61:PHE:CZ	2:B:402:TRP:CZ2	2.95	0.54
1:E:126:LYS:HA	1:E:145:GLN:HE21	1.73	0.54
2:H:97:PRO:C	2:H:99:GLY:H	2.11	0.54
2:H:318:TYR:HE1	2:H:347:LYS:HD3	1.73	0.54
1:A:28:GLU:HB3	1:A:32:LYS:HE3	1.88	0.54
2:B:365:VAL:HG12	2:B:405:TYR:CE2	2.43	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
1:C:182:GLN:HG2	1:C:183:TYR:N	2.23	0.54
1:C:341:ILE:HD11	1:C:350:LYS:HB3	1.90	0.54
2:H:27:THR:O	2:H:29:GLU:N	2.41	0.54
2:D:368:LEU:O	2:D:371:ALA:HB3	2.07	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:H:103:LYS:HZ1	2:H:179:VAL:HG23	1.70	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:B:368:LEU:O	2:B:371:ALA:HB3	2.07	0.53
1:C:97:PRO:HD3	1:C:232:TYR:CZ	2.43	0.53
1:C:402:TRP:CE3	1:C:402:TRP:C	2.82	0.53
2:D:93:GLY:O	2:D:94:ILE:O	2.26	0.53
1:E:97:PRO:HD3	1:E:232:TYR:CZ	2.43	0.53
1:E:463:ARG:HH11	1:E:463:ARG:HG3	1.72	0.53
1:E:537:PRO:CG	2:F:262:GLY:HA2	2.38	0.53
2:F:101:LYS:O	2:F:236:PRO:HB2	2.07	0.53
1:G:441:TYR:CD2	1:G:544:GLY:HA3	2.44	0.53
1:G:475:GLN:HB3	1:G:501:TYR:CE2	2.43	0.53
1:E:341:ILE:HD11	1:E:350:LYS:HB3	1.90	0.53
1:E:496:VAL:HG22	1:E:534:ALA:HB3	1.89	0.53
2:F:153:TRP:CE3	2:F:155:GLY:HA3	2.43	0.53
1:G:401:TRP:HB2	1:G:425:LEU:HD21	1.89	0.53
1:G:537:PRO:CG	2:H:262:GLY:HA2	2.38	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
2:H:365:VAL:HG12	2:H:405:TYR:CE2	2.43	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:C:131:THR:HA	1:C:142:ILE:O	2.07	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:A:97:PRO:HD3	1:A:232:TYR:CZ	2.43	0.53
2:B:103:LYS:NZ	2:B:179:VAL:N	2.55	0.53
2:B:392:PRO:O	2:B:392:PRO:HG2	2.08	0.53
2:D:268:SER:HA	2:D:274:ILE:HG22	1.90	0.53
2:F:201:LYS:HD3	2:F:204:GLU:OE1	2.07	0.53
1:G:342:TYR:HB3	1:G:348:ASN:HB3	1.89	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
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:A:106:VAL:O	1:A:227:PHE:CZ	2.62	0.53
1:A:342:TYR:HB3	1:A:348:ASN:HB3	1.89	0.53
1:C:196:GLY:O	1:C:199:ARG:HB3	2.09	0.53
1:C:346:PHE:CG	1:G:390:LYS:HD2	2.44	0.53
1:E:196:GLY:O	1:E:199:ARG:HB3	2.09	0.53
1:E:475:GLN:HB3	1:E:501:TYR:CE2	2.43	0.53
2:F:268:SER:HA	2:F:274:ILE:HG22	1.90	0.53
1:G:126:LYS:HA	1:G:145:GLN:HE21	1.73	0.53
1:A:465:LYS:O	1:A:466:VAL:HG23	2.08	0.53
2:B:153:TRP:CE3	2:B:155:GLY:HA3	2.43	0.53
1:C:106:VAL:O	1:C:227:PHE:CZ	2.62	0.53
1:C:345:PRO:CG	1:G:326:ILE:HD11	2.19	0.53
2:D:365:VAL:HG12	2:D:405:TYR:CE2	2.43	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
2:F:264:LEU:HB2	2:F:276:VAL:CG1	2.39	0.53
2:H:93:GLY:O	2:H:94:ILE:O	2.26	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:E:99:GLY:HA2	1:E:383:TRP:HZ3	1.72	0.53
1:E:106:VAL:O	1:E:227:PHE:CZ	2.62	0.53
1:G:372:VAL:HG11	1:G:411:ILE:HG23	1.91	0.53
2:H:13:LYS:HB3	2:H:14:PRO:HD2	1.91	0.53

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:LEU:HD22	1:E:470:THR:HG22	1.92	0.52
1:G:106:VAL:O	1:G:227:PHE:CZ	2.62	0.52
1:G:454:LYS:HA	1:G:467:VAL:O	2.10	0.52
1:A:126:LYS:HA	1:A:145:GLN:NE2	2.25	0.52
1:E:414:TRP:CE3	1:E:415:GLU:N	2.78	0.52
2:F:326:ILE:O	2:F:341:ILE:HA	2.10	0.52
1:G:126:LYS:HA	1:G:145:GLN:NE2	2.25	0.52
2:H:35:VAL:O	2:H:39:THR:HG23	2.10	0.52
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.91	0.52
1:A:441:TYR:CE2	1:A:543:GLY:O	2.63	0.52
2:B:97:PRO:C	2:B:99:GLY:H	2.11	0.52
1:E:441:TYR:CE2	1:E:543:GLY:O	2.63	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:A:324:ASP:O	1:A:343:GLN:HG2	2.09	0.52
1:A:402:TRP:O	1:A:402:TRP:HE3	1.93	0.52
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.91	0.52
1:C:249:LYS:HG2	1:C:250:ASP:H	1.75	0.52
1:C:441:TYR:CE2	1:C:543:GLY:O	2.63	0.52
1:E:454:LYS:HA	1:E:467:VAL:O	2.10	0.52
1:E:491:LEU:HB3	1:E:529:GLU:HB2	1.91	0.52
2:F:13:LYS:HB3	2:F:14:PRO:HD2	1.91	0.52
2:F:103:LYS:NZ	2:F:179:VAL:N	2.55	0.52
1:C:491:LEU:HB3	1:C:529:GLU:HB2	1.91	0.52
2:D:13:LYS:HB3	2:D:14:PRO:HD2	1.91	0.52
2:F:9:PRO:HA	2:F:121:ASP:OD2	2.10	0.52
2:F:35:VAL:O	2:F:39:THR:HG23	2.10	0.52
1:G:341:ILE:HD12	1:G:383:TRP:NE1	2.23	0.52
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:157:PRO:HG2	1:C:158:ALA:N	2.24	0.51
1:C:326:ILE:CB	1:C:342:TYR:CE1	2.92	0.51
1:C:402:TRP:CE3	1:C:403:THR:HA	2.45	0.51
1:E:126:LYS:HA	1:E:145:GLN:NE2	2.25	0.51
1:E:182:GLN:HG2	1:E:183:TYR:N	2.23	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
2:H:376:THR:HG22	2:H:389:PHE:CZ	2.45	0.51
1:A:118:VAL:O	1:A:118:VAL:HG12	2.10	0.51
1:A:249:LYS:HG2	1:A:250:ASP:H	1.75	0.51
1:C:402:TRP:HE3	1:C:402:TRP:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:LEU:HD22	1:C:470:THR:HG22	1.92	0.51
1:C:540:LYS:HZ3	2:D:261:VAL:HG12	1.74	0.51
1:C:540:LYS:CE	2:D:265:ASN:HB2	2.40	0.51
2:D:376:THR:HG22	2:D:389:PHE:CZ	2.45	0.51
1:G:410:TRP:CH2	1:G:412:PRO:HA	2.46	0.51
2:H:103:LYS:NZ	2:H:179:VAL:N	2.55	0.51
2:H:104:LYS:HZ1	2:H:194:GLU:HA	1.74	0.51
2:H:326:ILE:O	2:H:341:ILE:HA	2.10	0.51
1:A:454:LYS:HA	1:A:467:VAL:O	2.10	0.51
2:B:376:THR:HG22	2:B:389:PHE:CZ	2.45	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:341:ILE:HD12	1:E:383:TRP:NE1	2.23	0.51
1:E:410:TRP:CH2	1:E:412:PRO:HA	2.46	0.51
1:G:157:PRO:HG2	1:G:158:ALA:N	2.24	0.51
1:G:206:ARG:NH2	1:G:218:ASP:HA	2.25	0.51
1:G:540:LYS:CE	2:H:265:ASN:HB2	2.40	0.51
1:G:542:ILE:O	1:G:545:ASN:HB3	2.11	0.51
2:H:24:TRP:CH2	2:H:61:PHE:CE1	2.88	0.51
2:B:329:ILE:HA	2:B:338:THR:O	2.10	0.51
1:C:118:VAL:O	1:C:118:VAL:HG12	2.10	0.51
1:C:324:ASP:O	1:C:343:GLN:HG2	2.09	0.51
1:E:249:LYS:HG2	1:E:250:ASP:H	1.75	0.51
1:E:326:ILE:CB	1:E:342:TYR:CE1	2.92	0.51
1:E:372:VAL:HG11	1:E:411:ILE:HG23	1.91	0.51
1:G:402:TRP:CE3	1:G:403:THR:HA	2.45	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:C:391:LEU:HD12	1:C:414:TRP:CZ3	2.46	0.51
2:D:54:ASN:ND2	2:D:56:TYR:HB2	2.25	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
1:A:361:HIS:CD2	1:A:505:ILE:CG2	2.93	0.51
1:A:391:LEU:HD12	1:A:414:TRP:CZ3	2.46	0.51
2:D:9:PRO:HA	2:D:121:ASP:OD2	2.10	0.51
2:D:10:VAL:HG21	2:D:153:TRP:CH2	2.46	0.51
1:E:91:GLN:HE21	1:E:91:GLN:CA	2.21	0.51
1:G:391:LEU:HD12	1:G:414:TRP:CZ3	2.46	0.51
2:B:10:VAL:HG21	2:B:153:TRP:CH2	2.46	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:TRP:CE3	1:E:403:THR:HA	2.45	0.51
1:G:160:PHE:CZ	1:G:164:MET:HG2	2.46	0.51
1:A:326:ILE:CB	1:A:342:TYR:CE1	2.92	0.51
2:B:10:VAL:HG21	2:B:153:TRP:HH2	1.76	0.51
1:C:342:TYR:OH	1:G:345:PRO:HB3	2.08	0.51
1:C:454:LYS:HA	1:C:467:VAL:O	2.10	0.51
1:C:542:ILE:O	1:C:545:ASN:HB3	2.11	0.51
2:D:10:VAL:HG21	2:D:153:TRP:HH2	1.76	0.51
2:F:376:THR:HG22	2:F:389:PHE:CZ	2.45	0.51
1:G:540:LYS:HZ3	2:H:261:VAL:CG1	2.24	0.51
2:H:10:VAL:HG21	2:H:153:TRP:CH2	2.46	0.51
2:B:97:PRO:HB3	2:B:179:VAL:HG11	1.93	0.51
1:C:12:LEU:HD11	1:C:127:TYR:CE1	2.46	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
2:F:194:GLU:HG2	2:F:195:ILE:N	2.26	0.51
1:G:452:LEU:HD22	1:G:470:THR:HG22	1.92	0.51
2:H:9:PRO:HA	2:H:121:ASP:OD2	2.10	0.51
2:H:10:VAL:HG21	2:H:153:TRP:HH2	1.76	0.51
1:A:451:LYS:O	1:A:471:ASN:HA	2.11	0.51
2:B:326:ILE:O	2:B:341:ILE:HA	2.10	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: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:E:540:LYS:NZ	2:F:276:VAL:HG21	2.26	0.51
1:G:326:ILE:CG2	1:G:342:TYR:CE1	2.94	0.51
1:G:451:LYS:O	1:G:471:ASN:HA	2.11	0.51
1:A:363:ASN:ND2	1:A:365:VAL:HB	2.26	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
2:D:329:ILE:HA	2:D:338:THR:O	2.10	0.50
1:E:391:LEU:HD12	1:E:414:TRP:CZ3	2.46	0.50
1:E:402:TRP:O	1:E:402:TRP:HE3	1.93	0.50
1:E:542:ILE:O	1:E:545:ASN:HB3	2.11	0.50
1:G:361:HIS:NE2	1:G:518:VAL:HG21	2.26	0.50
1:A:414:TRP:CE3	1:A:415:GLU:N	2.78	0.50
2:B:54:ASN:ND2	2:B:56:TYR:HB2	2.25	0.50
1:C:361:HIS:CD2	1:C:505:ILE:CG2	2.93	0.50
1:C:363:ASN:ND2	1:C:365:VAL:HB	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:402:TRP:O	1:G:402:TRP:HE3	1.93	0.50
2:H:72:ARG:NH1	2:H:409:THR:HA	2.26	0.50
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.46	0.50
1:A:240:THR:HG22	1:A:315:HIS:CB	2.42	0.50
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.46	0.50
1:C:417:VAL:CG1	1:G:346:PHE:HE2	2.12	0.50
1:E:160:PHE:CZ	1:E:164:MET:HG2	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:244:ILE:HB	1:G:310:LEU:HD22	1.94	0.50
1:G:249:LYS:HG2	1:G:250:ASP:H	1.75	0.50
2:H:97:PRO:HB3	2:H:179:VAL:HG11	1.93	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:A:419:THR:CG2	1:A:420:PRO:HD2	2.41	0.50
1:A:542:ILE:O	1:A:545:ASN:HB3	2.11	0.50
1:C:417:VAL:HG22	1:G:346:PHE:CG	2.47	0.50
1:C:419:THR:CG2	1:C:420:PRO:HD2	2.41	0.50
1:C:468:PRO:HG2	1:C:468:PRO:O	2.12	0.50
1:E:540:LYS:NZ	2:F:261:VAL:O	2.45	0.50
1:G:324:ASP:O	1:G:343:GLN:HG2	2.09	0.50
1:A:345:PRO:HG3	1:E:326:ILE:HD13	1.94	0.50
1:A:361:HIS:NE2	1:A:518:VAL:HG21	2.26	0.50
2:B:27:THR:C	2:B:29:GLU:H	2.15	0.50
1:C:361:HIS:NE2	1:C:518:VAL:HG21	2.26	0.50
1:E:244:ILE:HB	1:E:310:LEU:HD22	1.94	0.50
1:E:451:LYS:O	1:E:471:ASN:HA	2.11	0.50
2:F:10:VAL:HG21	2:F:153:TRP:HH2	1.76	0.50
1:G:318:TYR:N	1:G:318:TYR:HD1	2.10	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
1:A:328:GLU:HG2	1:A:330:GLN:HE21	1.77	0.50
1:A:540:LYS:NZ	2:B:276:VAL:HG21	2.26	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
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:206:ARG:NH2	1:A:218:ASP:HA	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:PHE:CZ	2:D:402:TRP:HZ2	2.30	0.50
1:G:540:LYS:NZ	2:H:276:VAL:HG21	2.26	0.50
2:H:194:GLU:HG2	2:H:195:ILE:N	2.26	0.50
2:B:156:SER:N	2:B:157:PRO:HD2	2.27	0.50
1:C:194:GLU:O	1:C:196:GLY:N	2.45	0.50
1:C:342:TYR:CZ	1:G:345:PRO:CG	2.92	0.50
1:C:540:LYS:NZ	2:D:261:VAL:O	2.45	0.50
1:E:90:VAL:HG12	1:E:90:VAL:O	2.12	0.50
1:E:363:ASN:ND2	1:E:365:VAL:HB	2.27	0.50
1:E:399:GLU:O	1:E:399:GLU:HG2	2.12	0.50
2:F:246:LEU:HB2	2:F:307:ARG:HH12	1.75	0.50
1:G:468:PRO:O	1:G:468:PRO:HG2	2.12	0.50
2:H:61:PHE:CZ	2:H:402:TRP:HZ2	2.30	0.50
1:A:540:LYS:NZ	2:B:261:VAL:O	2.45	0.50
1:C:328:GLU:HG2	1:C:330:GLN:HE21	1.76	0.50
2:D:194:GLU:HG2	2:D:195:ILE:N	2.26	0.50
1:E:12:LEU:HD11	1:E:127:TYR:CE1	2.46	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:G:12:LEU:HD11	1:G:127:TYR:CE1	2.46	0.50
1:G:399:GLU:O	1:G:399:GLU:HG2	2.12	0.50
1:G:540:LYS:NZ	2:H:261:VAL:O	2.45	0.50
2:B:61:PHE:CZ	2:B:402:TRP:HZ2	2.30	0.49
2:B:72:ARG:NH1	2:B:409:THR:HA	2.26	0.49
1:C:244:ILE:HB	1:C:310:LEU:HD22	1.94	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
1:G:194:GLU:O	1:G:196:GLY:N	2.45	0.49
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
2:H:27:THR:C	2:H:29:GLU:H	2.15	0.49
1:C:90:VAL:HG12	1:C:90:VAL:O	2.12	0.49
2:D:27:THR:C	2:D:29:GLU:H	2.15	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: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:G:447:ASN:HB3	1:G:450:THR:OG1	2.12	0.49
1:A:90:VAL:O	1:A:91:GLN:NE2	2.45	0.49
1:A:468:PRO:HG2	1:A:468:PRO:O	2.12	0.49
2:B:54:ASN:HD22	2:B:56:TYR:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:GLU:HG2	2:B:195:ILE:N	2.26	0.49
1:C:132:ILE:HD11	1:C:144:TYR:HE2	1.77	0.49
1:C:169:GLU:HB3	1:C:170:PRO:HD3	1.95	0.49
1:C:345:PRO:HG3	1:G:326:ILE:HD13	1.34	0.49
1:G:183:TYR:CD2	1:G:230:MET:HG2	2.47	0.49
1:G:240:THR:HG22	1:G:315:HIS:CB	2.42	0.49
1:C:229:TRP:O	1:C:230:MET:HB2	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
1:E:326:ILE:CG2	1:E:342:TYR:CE1	2.94	0.49
2:F:97:PRO:HB3	2:F:179:VAL:HG11	1.93	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
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:90:VAL:HG12	2:F:141:GLY:N	2.25	0.49
1:E:318:TYR:N	1:E:318:TYR:HD1	2.10	0.49
1:E:468:PRO:O	1:E:468:PRO:HG2	2.12	0.49
2:F:27:THR:C	2:F:29:GLU:H	2.15	0.49
2:F:61:PHE:CZ	2:F:402:TRP:HZ2	2.30	0.49
2:B:142:ILE:HG22	2:B:144:TYR:CE1	2.48	0.49
1:C:90:VAL:HG12	2:D:141:GLY:N	2.24	0.49
1:C:318:TYR:N	1:C:318:TYR:HD1	2.10	0.49
2:D:72:ARG:NH1	2:D:409:THR:HA	2.26	0.49
1:E:132:ILE:HD11	1:E:144:TYR:HE2	1.77	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
2:F:27:THR:C	2:F:29:GLU:N	2.66	0.49
2:F:54:ASN:HD22	2:F:56:TYR:H	1.60	0.49
1:G:164:MET:HE2	1:G:187:LEU:HD21	1.95	0.49
2:H:72:ARG:NH1	2:H:409:THR:HG22	2.25	0.49
1:G:473:THR:OG1	1:G:476:LYS:HG2	2.13	0.49
2:H:156:SER:N	2:H:157:PRO:HD2	2.27	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:A:394:GLN:HG2	1:A:416:PHE:CE2	2.47	0.49
1:C:346:PHE:HZ	1:G:328:GLU:OE1	1.96	0.49
2:D:24:TRP:CZ3	2:D:61:PHE:CG	3.00	0.49
2:D:108:VAL:HG12	2:D:188:TYR:CD2	2.48	0.49
1:E:183:TYR:CD2	1:E:230:MET:HG2	2.47	0.49
1:E:328:GLU:HG2	1:E:330:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:540:LYS:HZ3	2:F:261:VAL:HG13	1.76	0.49
1:G:169:GLU:HB3	1:G:170:PRO:HD3	1.95	0.49
2:H:27:THR:C	2:H:29:GLU:N	2.66	0.49
1:A:46:LYS:HD2	1:A:116:PHE:HB3	1.94	0.49
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.95	0.49
1:A:191:SER:OG	1:A:198:HIS:CD2	2.66	0.49
1:A:318:TYR:N	1:A:318:TYR:HD1	2.10	0.49
2:D:27:THR:C	2:D:29:GLU:N	2.66	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:E:447:ASN:HB3	1:E:450:THR:OG1	2.12	0.49
2:F:207:GLN:O	2:F:210:LEU:N	2.46	0.49
1:G:344:GLU:HB2	1:G:347:LYS:HB2	1.94	0.49
2:H:108:VAL:HG12	2:H:188:TYR:CD2	2.48	0.49
1:A:229:TRP:O	1:A:230:MET:HB2	2.12	0.49
1:C:46:LYS:HD2	1:C:116:PHE:HB3	1.94	0.49
1:E:229:TRP:O	1:E:230:MET:HB2	2.12	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
2:H:207:GLN:O	2:H:210:LEU:N	2.46	0.49
1:A:342:TYR:C	1:A:342:TYR:CD1	2.87	0.48
2:B:108:VAL:HG12	2:B:188:TYR:CD2	2.48	0.48
1:C:183:TYR:CD2	1:C:230:MET:HG2	2.47	0.48
2:D:142:ILE:HG22	2:D:144:TYR:CE1	2.48	0.48
1:E:473:THR:OG1	1:E:476:LYS:HG2	2.13	0.48
2:H:395:LYS:HG3	2:H:416:PHE:HE2	1.78	0.48
1:A:337:TRP:N	1:A:337:TRP:CD1	2.81	0.48
1:A:344:GLU:HB2	1:A:347:LYS:HB2	1.94	0.48
1:C:416:PHE:HD1	1:C:417:VAL:H	1.61	0.48
1:G:90:VAL:O	1:G:91:GLN:NE2	2.45	0.48
1:G:191:SER:OG	1:G:198:HIS:CD2	2.66	0.48
1:G:326:ILE:CB	1:G:342:TYR:CE1	2.92	0.48
1:A:88:TRP:CZ2	2:B:57:ASN:CB	2.96	0.48
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.12	0.48
2:B:97:PRO:HD3	2:B:181:TYR:CD1	2.49	0.48
1:C:10:VAL:HA	1:C:85:GLN:OE1	2.13	0.48
1:C:344:GLU:HB2	1:C:347:LYS:HB2	1.94	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
2:F:103:LYS:HZ2	2:F:179:VAL:HG23	1.74	0.48
2:F:108:VAL:HG12	2:F:188:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:ILE:HG22	2:F:144:TYR:CE1	2.48	0.48
1:G:452:LEU:HD23	1:G:471:ASN:H	1.78	0.48
1:A:98:ALA:O	1:A:383:TRP:CZ3	2.66	0.48
1:A:356:ARG:HH21	1:A:358:ARG:NH1	2.11	0.48
1:A:452:LEU:HD23	1:A:471:ASN:H	1.78	0.48
2:B:153:TRP:CE3	2:B:156:SER:N	2.82	0.48
2:B:241:VAL:HG12	2:B:242:GLN:N	2.28	0.48
1:C:191:SER:OG	1:C:198:HIS:CD2	2.66	0.48
1:C:447:ASN:HB3	1:C:450:THR:OG1	2.12	0.48
2:D:97:PRO:HD3	2:D:181:TYR:CD1	2.49	0.48
2:D:153:TRP:CE3	2:D:156:SER:N	2.82	0.48
2:D:241:VAL:HG12	2:D:242:GLN:N	2.28	0.48
1:E:96:HIS:CG	1:E:97:PRO:HD2	2.49	0.48
1:E:342:TYR:CD1	1:E:342:TYR:C	2.87	0.48
1:E:356:ARG:HH21	1:E:358:ARG:NH1	2.11	0.48
1:G:98:ALA:O	1:G:383:TRP:CZ3	2.66	0.48
1:G:342:TYR:CD1	1:G:342:TYR:C	2.87	0.48
1:G:416:PHE:HD1	1:G:417:VAL:H	1.61	0.48
1:G:511:ASP:O	1:G:512:LYS:HD3	2.14	0.48
1:A:10:VAL:HA	1:A:85:GLN:OE1	2.13	0.48
1:A:183:TYR:CD2	1:A:230:MET:HG2	2.47	0.48
2:B:27:THR:C	2:B:29:GLU:N	2.66	0.48
2:D:24:TRP:CH2	2:D:61:PHE:CE1	2.88	0.48
1:E:98:ALA:O	1:E:383:TRP:CZ3	2.66	0.48
1:E:164:MET:HE2	1:E:187:LEU:HD21	1.96	0.48
1:G:419:THR:CG2	1:G:420:PRO:HD2	2.42	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:76:ASP:OD1	1:A:78:ARG:HG3	2.14	0.48
1:C:342:TYR:CD1	1:C:342:TYR:C	2.87	0.48
1:C:399:GLU:HG2	1:C:399:GLU:O	2.12	0.48
1:C:452:LEU:HD23	1:C:471:ASN:H	1.78	0.48
1:E:46:LYS:HD2	1:E:116:PHE:HB3	1.94	0.48
1:E:510:PRO:O	1:E:522:ILE:HD13	2.14	0.48
2:F:268:SER:HA	2:F:274:ILE:CG2	2.43	0.48
1:G:510:PRO:O	1:G:522:ILE:HD13	2.14	0.48
1:A:90:VAL:HG12	2:B:141:GLY:N	2.24	0.48
2:D:268:SER:HA	2:D:274:ILE:CG2	2.43	0.48
1:E:88:TRP:CZ2	2:F:57:ASN:CB	2.96	0.48
1:E:108:VAL:HG22	1:E:188:TYR:HA	1.96	0.48
2:F:153:TRP:CE3	2:F:156:SER:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:VAL:HA	1:G: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:A:473:THR:OG1	1:A:476:LYS:HG2	2.13	0.48
2:D:207:GLN:O	2:D:210:LEU:N	2.46	0.48
2:D:395:LYS:HG3	2:D:416:PHE:HE2	1.78	0.48
1:E:10:VAL:HA	1:E:85:GLN:OE1	2.13	0.48
1:E:90:VAL:O	1:E:91:GLN:NE2	2.45	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:G:46:LYS:HD2	1:G:116:PHE:HB3	1.94	0.48
1:A:455:ALA:HB2	1:A:469:LEU:HD11	1.96	0.48
2:B:207:GLN:O	2:B:210:LEU:N	2.46	0.48
1:C:88:TRP:CZ2	2:D:57:ASN:CB	2.96	0.48
1:C:98:ALA:O	1:C:383:TRP:CZ3	2.66	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:76:ASP:OD1	1:E:78:ARG:HG3	2.14	0.48
1:E:511:ASP:O	1:E:512:LYS:HD3	2.14	0.48
1:E:540:LYS:HZ3	2:F:261:VAL:HG12	1.77	0.48
2:F:241:VAL:HG12	2:F:242:GLN:N	2.28	0.48
1:G:76:ASP:OD1	1:G:78:ARG:HG3	2.14	0.48
1:G:455:ALA:HB2	1:G:469:LEU:HD11	1.96	0.48
2:H:54:ASN:HD22	2:H:56:TYR:H	1.60	0.48
1:A:108:VAL:HG22	1:A:188:TYR:HA	1.96	0.48
2:B:52:PRO:HD2	2:B:53:GLU:OE1	2.14	0.48
2:D:52:PRO:HD2	2:D:53:GLU:OE1	2.14	0.48
1:G:132:ILE:HB	1:G:142:ILE:HG12	1.96	0.48
1:G:164:MET:HG3	1:G:182:GLN:NE2	2.29	0.48
2:H:241:VAL:HG12	2:H:242:GLN:N	2.28	0.48
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.49	0.47
1:C:76:ASP:OD1	1:C:78:ARG:HG3	2.14	0.47
1:C:108:VAL:HG22	1:C:188:TYR:HA	1.96	0.47
1:C:356:ARG:HH21	1:C:358:ARG:NH1	2.11	0.47
1:E:169:GLU:HB3	1:E:170:PRO:HD3	1.95	0.47
2:F:158:ALA:O	2:F:161:GLN:HB2	2.15	0.47
1:G:108:VAL:HG22	1:G:188:TYR:HA	1.96	0.47
1:G:337:TRP:N	1:G:337:TRP:CD1	2.81	0.47
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.96	0.47
1:A:399:GLU:HG2	1:A:399:GLU:O	2.12	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:G:336:GLN:HG2	1:G:355:ALA:HB2	1.97	0.47
1:A:46:LYS:HG3	1:A:116:PHE:CD2	2.50	0.47
2:B:268:SER:HA	2:B:274:ILE:CG2	2.43	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
2:F:24:TRP:HZ3	2:F:61:PHE:HB3	1.76	0.47
2:F:97:PRO:HD3	2:F:181:TYR:CD1	2.49	0.47
1:A:354:TYR:CZ	1:A:356:ARG:HD3	2.49	0.47
1:A:511:ASP:O	1:A:512:LYS:HD3	2.14	0.47
1:C:46:LYS:HG3	1:C:116:PHE:CD2	2.50	0.47
1:C:132:ILE:HB	1:C:142:ILE:HG12	1.96	0.47
1:C:390:LYS:HB3	1:C:417:VAL:HG21	1.96	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: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
1:G:88:TRP:CZ2	2:H:57:ASN:CB	2.96	0.47
1:G:354:TYR:CZ	1:G:356:ARG:HD3	2.49	0.47
2:H:158:ALA:O	2:H:161:GLN:HB2	2.14	0.47
2:H:336:GLN:HG2	2:H:355:ALA:CB	2.44	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
1:A:304:ALA:HA	1:A:307:ARG:HD2	1.96	0.47
1:A:510:PRO:O	1:A:522:ILE:HD13	2.14	0.47
2:B:24:TRP:CH2	2:B:61:PHE:CE1	2.88	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:C:455:ALA:HB2	1:C:469:LEU:HD11	1.96	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
2:F:41:MET:HE1	2:F:73:LYS:HD2	1.95	0.47
2:H:97:PRO:HD3	2:H:181:TYR:CD1	2.48	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:A:342:TYR:HB3	1:A:348:ASN:CB	2.44	0.47
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.96	0.47
1:C:23:GLN:HG2	1:C:59:PRO:HA	1.97	0.47
1:C:228:LEU:HD21	1:C:233:GLU:HG2	1.96	0.47
1:C:354:TYR:CZ	1:C:356:ARG:HD3	2.49	0.47
2:F:56:TYR:O	2:F:143:ARG:NH2	2.48	0.47
2:F:64:LYS:HB2	2:F:71:TRP:CZ3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:GLN:HG2	1:G:59:PRO:HA	1.97	0.47
1:G:46:LYS:HG3	1:G:116:PHE:CD2	2.50	0.47
2:H:24:TRP:HZ3	2:H:61:PHE:HB3	1.76	0.47
2:H:56:TYR:O	2:H:143:ARG:NH2	2.48	0.47
2:H:64:LYS:HB2	2:H:71:TRP:CZ3	2.50	0.47
2:H:268:SER:HA	2:H:274:ILE:CG2	2.43	0.47
1:A:6:GLU:CD	1:A:6:GLU:N	2.66	0.47
1:A:336:GLN:HG2	1:A:355:ALA:HB2	1.97	0.47
1:A:345:PRO:HG3	1:E:326:ILE:CD1	2.44	0.47
1:A:540:LYS:HZ3	2:B:261:VAL:HG13	1.78	0.47
2:B:336:GLN:HG2	2:B:355:ALA:CB	2.44	0.47
1:C:326:ILE:HB	1:C:342:TYR:CD1	2.50	0.47
1:C:417:VAL:CG2	1:G:346:PHE:CD2	2.98	0.47
1:C:442:VAL:HG12	1:C:443:ASP:N	2.30	0.47
2:D:56:TYR:O	2:D:143:ARG:NH2	2.48	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:228:LEU:HD21	1:E:233:GLU:HG2	1.96	0.47
1:E:337:TRP:CD1	1:E:337:TRP:N	2.81	0.47
1:E:442:VAL:HG12	1:E:443:ASP:N	2.30	0.47
1:G:102:LYS:CG	1:G:318:TYR:HB2	2.45	0.47
1:G:318:TYR:N	1:G:318:TYR:CD1	2.82	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
2:H:52:PRO:HD2	2:H:53:GLU:OE1	2.14	0.47
1:A:442:VAL:HG12	1:A:443:ASP:N	2.30	0.47
2:B:158:ALA:O	2:B:161:GLN:HB2	2.15	0.47
2:D:64:LYS:HB2	2:D:71:TRP:CZ3	2.50	0.47
1:E:20:LYS:HG2	1:E:56:TYR:HA	1.96	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:G:228:LEU:HD21	1:G:233:GLU:HG2	1.96	0.47
1:C:6:GLU:CD	1:C:6:GLU:N	2.66	0.47
1:C:20:LYS:HG2	1:C:56:TYR:HA	1.96	0.47
1:C:121:ASP:O	1:C:125:ARG:HG3	2.15	0.47
1:C:191:SER:OG	1:C:198:HIS:HD2	1.98	0.47
1:C:318:TYR:N	1:C:318:TYR:CD1	2.82	0.47
1:C:342:TYR:HB3	1:C:348:ASN:CB	2.44	0.47
1:C:391:LEU:HA	1:C:392:PRO:HD3	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:PHE:HD1	1:E:417:VAL:H	1.61	0.47
2:F:24:TRP:HZ3	2:F:61:PHE:CB	2.28	0.47
2:H:276:VAL:HG12	2:H:279:LEU:HD12	1.97	0.47
1:A:33:ALA:O	1:A:36:GLU:HB3	2.15	0.47
1:A:102:LYS:CG	1:A:318:TYR:HB2	2.45	0.47
1:A:326:ILE:HB	1:A:342:TYR:CD1	2.50	0.47
2:B:64:LYS:HB2	2:B:71:TRP:CZ3	2.50	0.47
1:C:336:GLN:HG2	1:C:355:ALA:HB2	1.97	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
1:E:537:PRO:HB2	1:E:540:LYS:HD2	1.97	0.47
2:F:52:PRO:HD2	2:F:53:GLU:OE1	2.14	0.47
2:F:108:VAL:HA	2:F:187:LEU:O	2.15	0.47
1:G:96:HIS:CG	1:G:97:PRO:HD2	2.49	0.47
1:A:191:SER:OG	1:A:198:HIS:HD2	1.98	0.46
2:B:55:PRO:HG2	2:B:56:TYR:CD2	2.51	0.46
2:B:56:TYR:O	2:B:143:ARG:NH2	2.48	0.46
1:C:510:PRO:O	1:C:522:ILE:HD13	2.14	0.46
2:D:108:VAL:HA	2:D:187:LEU:O	2.15	0.46
1:E:437:ALA:HB1	1:E:493:VAL:HA	1.97	0.46
2:F:135:ILE:H	2:F:135:ILE:HG12	1.38	0.46
2:F:345:PRO:O	2:F:346:PHE:HB2	2.15	0.46
1:G:33:ALA:O	1:G:36:GLU:HB3	2.15	0.46
1:G:442:VAL:HG12	1:G:443:ASP:N	2.30	0.46
2:H:55:PRO:HG2	2:H:56:TYR:CD2	2.51	0.46
1:A:121:ASP:O	1:A:125:ARG:HG3	2.15	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:C:346:PHE:CB	1:G:390:LYS:HZ1	1.98	0.46
2:D:55:PRO:HG2	2:D:56:TYR:CD2	2.51	0.46
2:F:64:LYS:HB2	2:F:71:TRP:CE3	2.50	0.46
1:G:121:ASP:O	1:G:125:ARG:HG3	2.15	0.46
1:G:240:THR:HG22	1:G:315:HIS:HB3	1.97	0.46
1:G:248:GLU:CG	1:G:307:ARG:HH21	2.28	0.46
1:A:503:LEU:O	1:A:507:GLN:HG2	2.16	0.46
1:C:33:ALA:O	1:C:36:GLU:HB3	2.15	0.46
1:C:337:TRP:N	1:C:337:TRP:CD1	2.81	0.46
1:C:503:LEU:O	1:C:507:GLN:HG2	2.16	0.46
1:E:33:ALA:O	1:E:36:GLU:HB3	2.15	0.46
1:E:248:GLU:CG	1:E:307:ARG:HH21	2.28	0.46
1:E:326:ILE:HB	1:E:342:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:TYR:HB3	1:G:348:ASN:CB	2.44	0.46
2:H:108:VAL:HA	2:H:187:LEU:O	2.15	0.46
1:A:102:LYS:HG3	1:A:318:TYR:HB2	1.97	0.46
1:A:398:TRP:CZ3	1:A:411:ILE:HD11	2.51	0.46
2:B:276:VAL:HG12	2:B:279:LEU:HD12	1.98	0.46
2:F:259:LYS:HE3	2:F:263:LYS:NZ	2.30	0.46
2:F:330:GLN:HG3	2:F:419:THR:HG21	1.96	0.46
1:G:191:SER:OG	1:G:198:HIS:HD2	1.99	0.46
2:H:64:LYS:HB2	2:H:71:TRP:CE3	2.50	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:E:115:TYR:CE2	1:E:156:SER:HB3	2.51	0.46
1:E:516:GLU:O	1:E:520:GLN:HG2	2.15	0.46
1:G:229:TRP:CZ3	1:G:230:MET:HE1	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:A:118:VAL:C	1:A:148:VAL:HG13	2.36	0.46
1:E:6:GLU:CD	1:E:6:GLU:N	2.66	0.46
1:E:59:PRO:HG2	1:E:76:ASP:HB3	1.98	0.46
1:E:240:THR:HG22	1:E:315:HIS:HB3	1.97	0.46
1:E:451:LYS:O	1:E:452:LEU:HD23	2.15	0.46
1:E:540:LYS:NZ	2:F:261:VAL:HG12	2.31	0.46
2:F:55:PRO:HG2	2:F:56:TYR:CD2	2.51	0.46
2:H:345:PRO:O	2:H:346:PHE:HB2	2.15	0.46
2:B:259:LYS:HE3	2:B:263:LYS:NZ	2.30	0.46
2:B:345:PRO:O	2:B:346:PHE:HB2	2.15	0.46
1:C:91:GLN:HE21	1:C:91:GLN:CA	2.21	0.46
1:C:102:LYS:CG	1:C:318:TYR:HB2	2.45	0.46
1:C:451:LYS:O	1:C:452:LEU:HD23	2.15	0.46
2:D:276:VAL:HG12	2:D:279:LEU:HD12	1.98	0.46
1:E:121:ASP:O	1:E:125:ARG:HG3	2.15	0.46
2:F:276:VAL:HG12	2:F:279:LEU:HD12	1.98	0.46
1:G:59:PRO:HG2	1:G:76:ASP:HB3	1.98	0.46
1:G:342:TYR:C	1:G:342:TYR:HD1	2.19	0.46
2:H:259:LYS:HE3	2:H:263:LYS:NZ	2.30	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
1:A:540:LYS:NZ	2:B:261:VAL:HG12	2.31	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:TYR:C	1:C:342:TYR:HD1	2.19	0.46
2:D:259:LYS:HE3	2:D:263:LYS:NZ	2.30	0.46
1:E:342:TYR:C	1:E:342:TYR:HD1	2.19	0.46
1:G:46:LYS:HG3	1:G:116:PHE:HD2	1.81	0.46
1:G:398:TRP:CZ3	1:G:411:ILE:HD11	2.51	0.46
2:H:10:VAL:HG11	2:H:153:TRP:HH2	1.81	0.46
2:H:135:ILE:C	2:H:137:ASN:H	2.20	0.46
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.98	0.46
1:A:91:GLN:HE21	1:A:91:GLN:CA	2.22	0.46
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.51	0.46
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.64	0.46
1:A:241:VAL:HB	1:A:314:VAL:HG22	1.98	0.46
1:A:342:TYR:C	1:A:342:TYR:HD1	2.19	0.46
2:B:297:GLU:HA	2:B:300:GLU:HB3	1.98	0.46
2:B:365:VAL:HG12	2:B:405:TYR:HE2	1.80	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:C:175:ASN:ND2	1:C:201:LYS:NZ	2.64	0.46
1:C:417:VAL:HG22	1:G:346:PHE:CD2	2.51	0.46
2:D:72:ARG:HH22	2:D:409:THR:HB	1.81	0.46
2:D:297:GLU:HA	2:D:300:GLU:HB3	1.98	0.46
1:E:46:LYS:HG3	1:E:116:PHE:CD2	2.50	0.46
1:E:102:LYS:HG3	1:E:318:TYR:HB2	1.97	0.46
1:E:398:TRP:CZ3	1:E:411:ILE:HD11	2.51	0.46
1:G:102:LYS:HG3	1:G:318:TYR:HB2	1.97	0.46
1:G:540:LYS:NZ	2:H:261:VAL:HG12	2.31	0.46
1:A:116:PHE:C	1:A:148:VAL:HG11	2.37	0.46
1:C:102:LYS:HG3	1:C:318:TYR:HB2	1.97	0.46
1:C:398:TRP:CZ3	1:C:411:ILE:HD11	2.51	0.46
1:C:537:PRO:HB2	1:C:540:LYS:HD2	1.97	0.46
1:E:175:ASN:ND2	1:E:201:LYS:NZ	2.64	0.46
1:E:229:TRP:CZ3	1:E:230:MET:HE1	2.51	0.46
2:F:103:LYS:HZ1	2:F:179:VAL:HG23	1.80	0.46
2:F:135:ILE:C	2:F:137:ASN:H	2.19	0.46
2:F:390:LYS:HA	2:F:415:GLU:O	2.17	0.46
1:G:20:LYS:HG2	1:G:56:TYR:HA	1.96	0.46
1:G:118:VAL:C	1:G:148:VAL:HG13	2.36	0.46
1:G:125:ARG:O	1:G:126:LYS:C	2.55	0.46
2:B:24:TRP:HZ3	2:B:61:PHE:CB	2.28	0.45
2:B:135:ILE:C	2:B:137:ASN:H	2.19	0.45
2:B:330:GLN:HG3	2:B:419:THR:HG21	1.96	0.45

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:ILE:CB	1:G:342:TYR:HE1	2.28	0.45
1:G:361:HIS:CD2	1:G:505:ILE:HG23	2.52	0.45
1:G:445:ALA:O	1:G:453:GLY:HA3	2.16	0.45
1:G:537:PRO:HB2	1:G:540:LYS:HD2	1.97	0.45
2:H:24:TRP:HZ3	2:H:61:PHE:CB	2.28	0.45
1:A:361:HIS:CD2	1:A:505:ILE:HG23	2.52	0.45
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.51	0.45
1:C:53:GLU:H	1:C:53:GLU:CD	2.20	0.45
1:C:115:TYR:O	1:C:117:SER:N	2.50	0.45
2:D:390:LYS:HA	2:D:415:GLU:O	2.16	0.45
1:E:445:ALA:O	1:E:453:GLY:HA3	2.16	0.45
1:E:503:LEU:O	1:E:507:GLN:HG2	2.16	0.45
2:F:10:VAL:HG11	2:F:153:TRP:HH2	1.81	0.45
2:F:116:PHE:CZ	2:F:151:GLN:HG2	2.52	0.45
2:F:255:ASN:HA	2:F:258:GLN:HB2	1.98	0.45
1:G:53:GLU:CD	1:G:53:GLU:H	2.20	0.45
2:H:116:PHE:CZ	2:H:151:GLN:HG2	2.52	0.45
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.99	0.45
1:A:46:LYS:HG3	1:A:116:PHE:HD2	1.81	0.45
1:A:329:ILE:HA	1:A:338:THR:O	2.17	0.45
2:B:195:ILE:O	2:B:199:ARG:HG3	2.17	0.45
2:D:135:ILE:C	2:D:137:ASN:H	2.20	0.45
1:G:95:PRO:HG2	1:G:230:MET:CE	2.47	0.45
1:G:116:PHE:C	1:G:148:VAL:HG11	2.37	0.45
1:G:503:LEU:O	1:G:507:GLN:HG2	2.16	0.45
1:G:546:GLU:O	1:G:549:ASP:HB3	2.17	0.45
2:H:195:ILE:O	2:H:199:ARG:HG3	2.17	0.45
1:A:85:GLN:O	1:A:85:GLN:CG	2.55	0.45
1:A:148:VAL:HG12	1:A:149:LEU:N	2.31	0.45
2:D:195:ILE:O	2:D:199:ARG:HG3	2.17	0.45
1:E:191:SER:OG	1:E:198:HIS:HD2	1.98	0.45
1:G:241:VAL:HB	1:G:314:VAL:HG22	1.98	0.45
1:G:327:ALA:HA	1:G:340:GLN:O	2.17	0.45
2:H:135:ILE:H	2:H:135:ILE:HG12	1.38	0.45
2:H:171:PHE:CZ	2:H:205:LEU:HB2	2.51	0.45
2:H:259:LYS:HE3	2:H:263:LYS:HZ1	1.81	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
2:B:120:LEU:O	2:B:125:ARG:CZ	2.65	0.45
1:C:248:GLU:CG	1:C:307:ARG:HH21	2.28	0.45
1:C:516:GLU:O	1:C:520:GLN:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:ASN:OD1	1:E:130:PHE:HA	2.17	0.45
1:E:95:PRO:HG2	1:E:230:MET:CE	2.47	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: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
2:H:390:LYS:HA	2:H:415:GLU:O	2.16	0.45
2:H:390:LYS:HG2	2:H:415:GLU:OE1	2.17	0.45
1:A:53:GLU:CD	1:A:53:GLU:H	2.20	0.45
1:A:248:GLU:CG	1:A:307:ARG:HH21	2.28	0.45
2:B:207:GLN:O	2:B:208:HIS:C	2.56	0.45
1:C:78:ARG:NH1	1:C:287:LYS:O	2.39	0.45
1:C:95:PRO:HG2	1:C:230:MET:CE	2.47	0.45
1:C:125:ARG:O	1:C:126:LYS:C	2.55	0.45
1:C:410:TRP:HZ3	2:D:401:TRP:CZ2	2.35	0.45
2:D:108:VAL:HG11	2:D:188:TYR:CE2	2.52	0.45
2:D:365:VAL:HG12	2:D:405:TYR:HE2	1.80	0.45
2:D:376:THR:HG22	2:D:389:PHE:HE1	1.80	0.45
2:F:72:ARG:HH22	2:F:409:THR:HB	1.81	0.45
2:F:241:VAL:O	2:F:243:PRO:HD3	2.17	0.45
1:G:57:ASN:OD1	1:G:130:PHE:HA	2.17	0.45
2:H:72:ARG:HH22	2:H:409:THR:HB	1.81	0.45
1:A:115:TYR:O	1:A:117:SER:N	2.50	0.45
2:B:104:LYS:HZ1	2:B:194:GLU:HA	1.82	0.45
1:C:46:LYS:HG3	1:C:116:PHE:HD2	1.81	0.45
1:C:326:ILE:CB	1:C:342:TYR:HE1	2.28	0.45
1:C:440:PHE:CE2	1:C:457:TYR:CE2	3.05	0.45
2:D:78:ARG:O	2:D:82:LYS:HG3	2.17	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: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
2:F:195:ILE:O	2:F:199:ARG:HG3	2.17	0.45
1:G:34:LEU:HD21	1:G:62:ALA:HB2	1.99	0.45
1:G:167:ILE:O	1:G:208:HIS:CE1	2.66	0.45
1:G:329:ILE:HA	1:G:338:THR:O	2.17	0.45
1:A:440:PHE:CE2	1:A:457:TYR:CE2	3.05	0.44
1:A:546:GLU:O	1:A:549:ASP:HB3	2.17	0.44
2:B:108:VAL:HG11	2:B:188:TYR:CE2	2.52	0.44
1:C:10:VAL:HG11	1:C:153:TRP:CZ2	2.52	0.44
2:D:193:LEU:CD1	2:D:201:LYS:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:VAL:HG11	1:E:153:TRP:CZ2	2.52	0.44
2:F:78:ARG:O	2:F:82:LYS:HG3	2.17	0.44
2:F:120:LEU:O	2:F:125:ARG:CZ	2.65	0.44
1:G:410:TRP:HZ3	2:H:401:TRP:CZ2	2.35	0.44
2:H:241:VAL:O	2:H:243:PRO:HD3	2.17	0.44
1:A:57:ASN:OD1	1:A:130:PHE:HA	2.17	0.44
1:A:78:ARG:NH1	1:A:287:LYS:O	2.39	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:A:379:SER:HB3	1:A:383:TRP:HD1	1.82	0.44
1:A:439:THR:HG22	1:A:441:TYR:HE1	1.82	0.44
2:B:162:SER:O	2:B:166:LYS:HG2	2.17	0.44
2:B:193:LEU:CD1	2:B:201:LYS:HG3	2.47	0.44
2:B:390:LYS:HG2	2:B:415:GLU:OE1	2.17	0.44
1:C:379:SER:HB3	1:C:383:TRP:HD1	1.83	0.44
2:D:255:ASN:HA	2:D:258:GLN:HB2	1.99	0.44
1:E:329:ILE:HA	1:E:338:THR:O	2.17	0.44
2:F:171:PHE:HA	2:F:174:GLN:HB3	1.98	0.44
2:F:292:VAL:HG12	2:F:293:ILE:N	2.33	0.44
1:G:160:PHE:CZ	1:G:164:MET:CG	3.01	0.44
2:H:297:GLU:HA	2:H:300:GLU:HB3	1.98	0.44
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.52	0.44
1:C:540:LYS:NZ	2:D:261:VAL:HG12	2.31	0.44
1:C:546:GLU:O	1:C:549:ASP:HB3	2.17	0.44
1:E:546:GLU:O	1:E:549:ASP:HB3	2.17	0.44
2:F:100:LEU:HD23	2:F:100:LEU:HA	1.81	0.44
2:F:390:LYS:HG2	2:F:415:GLU:OE1	2.17	0.44
1:A:327:ALA:HA	1:A:340:GLN:O	2.17	0.44
2:B:78:ARG:O	2:B:82:LYS:HG3	2.17	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:E:327:ALA:HA	1:E:340:GLN:O	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
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:C:327:ALA:HA	1:C:340:GLN:O	2.17	0.44
1:C:451:LYS:O	1:C:471:ASN:N	2.51	0.44
1:E:53:GLU:H	1:E:53:GLU:CD	2.20	0.44
1:E:116:PHE:C	1:E:148:VAL:HG11	2.37	0.44
1:E:160:PHE:CZ	1:E:164:MET:CG	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:VAL:HB	1:E:314:VAL:HG22	1.98	0.44
1:E:410:TRP:HZ3	2:F:401:TRP:CZ2	2.35	0.44
1:E:441:TYR:O	1:E:548:VAL:HG21	2.18	0.44
1:G:412:PRO:HG2	1:G:413:GLU:H	1.83	0.44
1:G:451:LYS:O	1:G:471:ASN:N	2.51	0.44
2:H:78:ARG:O	2:H:82:LYS:HG3	2.17	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:B:292:VAL:HG12	2:B:293:ILE:N	2.33	0.44
1:C:229:TRP:CH2	1:C:230:MET:CE	3.01	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
2:D:162:SER:O	2:D:166:LYS:HG2	2.17	0.44
2:D:292:VAL:HG12	2:D:293:ILE:N	2.33	0.44
2:D:390:LYS:HG2	2:D:415:GLU:OE1	2.17	0.44
2:F:395:LYS:HG3	2:F:416:PHE:HE2	1.78	0.44
2:H:292:VAL:HG12	2:H:293:ILE:N	2.33	0.44
2:H:354:TYR:CE1	2:H:374:LYS:HD3	2.53	0.44
1:A:326:ILE:CB	1:A:342:TYR:HE1	2.28	0.44
2:B:255:ASN:HA	2:B:258:GLN:HB2	1.99	0.44
1:C:160:PHE:CZ	1:C:164:MET:CG	3.00	0.44
1:C:417:VAL:HG21	1:G:346:PHE:CG	2.53	0.44
2:D:47:ILE:HG22	2:D:48:SER:N	2.30	0.44
1:E:540:LYS:C	1:E:542:ILE:H	2.20	0.44
1:G:95:PRO:HG2	1:G:230:MET:HE1	2.00	0.44
1:G:229:TRP:CH2	1:G:230:MET:CE	3.01	0.44
1:G:379:SER:HB3	1:G:383:TRP:HD1	1.83	0.44
2:H:120:LEU:O	2:H:125:ARG:CZ	2.65	0.44
2:H:162:SER:O	2:H:166:LYS:HG2	2.17	0.44
2:H:319:TYR:O	2:H:321:PRO:HD3	2.18	0.44
2:B:249:LYS:HB2	2:B:252:TRP:CZ2	2.52	0.44
2:B:354:TYR:CE1	2:B:374:LYS:HD3	2.53	0.44
2:D:24:TRP:CZ3	2:D:61:PHE:CB	3.00	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:24:TRP:CZ3	2:F:61:PHE:CB	3.01	0.44
2:F:365:VAL:HG12	2:F:405:TYR:HE2	1.81	0.44
2:F:376:THR:HG22	2:F:389:PHE:HE1	1.80	0.44
2:F:420:PRO:HB2	2:F:421:PRO:CD	2.42	0.44
1:G:1:PRO:HG2	1:G:1:PRO:O	2.18	0.44
1:G:10:VAL:HG11	1:G:153:TRP:CZ2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:VAL:HG11	2:H:188:TYR:CE2	2.52	0.44
2:H:255:ASN:HA	2:H:258:GLN:HB2	1.99	0.44
1:A:441:TYR:O	1:A:548:VAL:HG21	2.18	0.44
2:B:241:VAL:O	2:B:243:PRO:HD3	2.17	0.44
2:B:286:THR:HG22	2:B:286:THR:O	2.18	0.44
1:C:439:THR:HG22	1:C:441:TYR:HE1	1.82	0.44
2:D:286:THR:HG22	2:D:286:THR:O	2.18	0.44
1:E:88:TRP:CH2	2:F:57:ASN:CB	3.01	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:451:LYS:O	1:E:471:ASN:N	2.51	0.44
2:F:38:CYS:SG	2:F:132:ILE:HD11	2.58	0.44
2:B:376:THR:HG22	2:B:389:PHE:HE1	1.80	0.43
1:C:336:GLN:C	1:C:337:TRP:CD1	2.92	0.43
1:C:363:ASN:OD1	1:C:365:VAL:N	2.50	0.43
1:E:412:PRO:HG2	1:E:413:GLU:H	1.83	0.43
1:E:543:GLY:C	1:E:545:ASN:H	2.22	0.43
1:G:336:GLN:C	1:G:337:TRP:CD1	2.92	0.43
1:G:440:PHE:CE2	1:G:457:TYR:CE2	3.05	0.43
1:G:441:TYR:O	1:G:548:VAL:HG21	2.18	0.43
1:C:441:TYR:O	1:C:548:VAL:HG21	2.18	0.43
1:E:336:GLN:HG2	1:E:355:ALA:CB	2.48	0.43
2:F:286:THR:O	2:F:286:THR:HG22	2.18	0.43
1:G:132:ILE:HD11	1:G:144:TYR:CE2	2.54	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
2:H:286:THR:O	2:H:286:THR:HG22	2.18	0.43
1:A:536:VAL:HB	1:A:542:ILE:HD13	2.01	0.43
2:B:28:GLU:HG2	2:B:32:LYS:HZ2	1.84	0.43
1:C:167:ILE:O	1:C:208:HIS:CE1	2.66	0.43
2:D:100:LEU:HA	2:D:100:LEU:HD23	1.81	0.43
2:D:319:TYR:O	2:D:321:PRO:HD3	2.18	0.43
1:E:368:LEU:HD11	1:E:391:LEU:HD22	2.00	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:F:354:TYR:CE1	2:F:374:LYS:HD3	2.53	0.43
1:G:148:VAL:HG12	1:G:149:LEU:N	2.31	0.43
1:G:540:LYS:HZ3	2:H:276:VAL:HG21	1.83	0.43
2:B:324:ASP:O	2:B:343:GLN:HG2	2.19	0.43
2:D:28:GLU:HG2	2:D:32:LYS:HZ3	1.83	0.43
2:D:395:LYS:HE2	2:D:399:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:LEU:HD21	1:E:62:ALA:HB2	1.99	0.43
1:E:229:TRP:CH2	1:E:230:MET:CE	3.01	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
1:G:540:LYS:HB2	1:G:542:ILE:HG13	2.00	0.43
2:H:38:CYS:SG	2:H:132:ILE:HD11	2.58	0.43
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.43
1:C:320:ASP:HA	1:C:321:PRO:HD2	1.85	0.43
2:D:241:VAL:O	2:D:243:PRO:HD3	2.17	0.43
2:D:274:ILE:HG13	2:D:306:ASN:CG	2.39	0.43
1:E:95:PRO:HG2	1:E:230:MET:HE1	2.00	0.43
1:E:336:GLN:C	1:E:337:TRP:CD1	2.92	0.43
2:F:207:GLN:O	2:F:208:HIS:C	2.55	0.43
2:F:312:GLU:HA	2:F:313:PRO:HD3	1.72	0.43
1:G:88:TRP:CH2	2:H:57:ASN:CB	3.01	0.43
1:G:540:LYS:C	1:G:542:ILE:H	2.20	0.43
2:H:320:ASP:HA	2:H:321:PRO:HD3	1.84	0.43
2:H:324:ASP:O	2:H:343:GLN:HG2	2.19	0.43
1:A:12:LEU:HD23	1:A:124:PHE:HE2	1.83	0.43
1:A:88:TRP:CH2	2:B:57:ASN:CB	3.01	0.43
1:A:336:GLN:C	1:A:337:TRP:CD1	2.92	0.43
1:A:412:PRO:HG2	1:A:413:GLU:H	1.83	0.43
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.58	0.43
1:C:188:TYR:HB2	1:C:229:TRP:CD1	2.54	0.43
1:C:540:LYS:C	1:C:542:ILE:H	2.20	0.43
2:F:324:ASP:O	2:F:343:GLN:HG2	2.19	0.43
2:F:395:LYS:HE2	2:F:399:GLU:OE1	2.18	0.43
1:G:84:THR:CG2	1:G:154:LYS:HE2	2.49	0.43
2:H:91:GLN:CD	2:H:94:ILE:HG23	2.39	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:A:467:VAL:HG12	1:A:468:PRO:O	2.18	0.43
1:A:476:LYS:O	1:A:480:GLN:HG2	2.19	0.43
2:B:274:ILE:HG13	2:B:306:ASN:CG	2.39	0.43
2:B:395:LYS:HE2	2:B:399:GLU:OE1	2.18	0.43
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.52	0.43
1:C:412:PRO:HG2	1:C:413:GLU:H	1.83	0.43
1:E:14:PRO:HG2	1:E:14:PRO:O	2.18	0.43
1:E:391:LEU:HA	1:E:392:PRO:HD3	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:395:LYS:HE2	2:H:399:GLU:OE1	2.18	0.43
2:H:420:PRO:HB2	2:H:421:PRO:CD	2.42	0.43
1:A:14:PRO:O	1:A:14:PRO:HG2	2.18	0.43
1:A:50:ILE:HD13	1:A:145:GLN:HB2	2.01	0.43
1:A:84:THR:CG2	1:A:154:LYS:HE2	2.49	0.43
1:A:356:ARG:HH21	1:A:358:ARG:CZ	2.32	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
2:B:91:GLN:CD	2:B:94:ILE:HG23	2.39	0.43
1:C:12:LEU:HD23	1:C:124:PHE:HE2	1.83	0.43
1:C:132:ILE:HD11	1:C:144:TYR:CE2	2.54	0.43
2:D:108:VAL:CG1	2:D:188:TYR:CE2	3.02	0.43
2:D:324:ASP:O	2:D:343:GLN:HG2	2.19	0.43
2:D:354:TYR:CE1	2:D:374:LYS:HD3	2.53	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:F:319:TYR:O	2:F:321:PRO:HD3	2.18	0.43
1:G:476:LYS:O	1:G:480:GLN:HG2	2.19	0.43
2:H:108:VAL:CG1	2:H:188:TYR:CE2	3.02	0.43
2:B:61:PHE:CZ	2:B:411:ILE:HD11	2.54	0.43
2:B:160:PHE:O	2:B:160:PHE:CD1	2.72	0.43
1:C:50:ILE:HD13	1:C:145:GLN:HB2	2.01	0.43
1:C:368:LEU:HD11	1:C:391:LEU:HD22	2.00	0.43
1:C:467:VAL:HG12	1:C:468:PRO:O	2.18	0.43
1:C:536:VAL:HB	1:C:542:ILE:HD13	2.01	0.43
1:G:238:LYS:HE3	1:G:315:HIS:CG	2.54	0.43
1:G:536:VAL:HB	1:G:542:ILE:HD13	2.01	0.43
1:A:132:ILE:HD11	1:A:144:TYR:CE2	2.54	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
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.58	0.43
2:D:72:ARG:HH12	2:D:409:THR:CG2	2.29	0.43
1:E:1:PRO:HG2	1:E:1:PRO:O	2.18	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
1:G:336:GLN:HG2	1:G:355:ALA:CB	2.48	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
1:A:175:ASN:HB3	1:A:178:ILE:HD12	2.00	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:THR:CG2	1:C:154:LYS:HE2	2.49	0.42
1:C:476:LYS:O	1:C:480:GLN:HG2	2.19	0.42
2:D:61:PHE:CZ	2:D:411:ILE:HD11	2.54	0.42
2:D:160:PHE:CD1	2:D:160:PHE:O	2.72	0.42
1:E:238:LYS:HE3	1:E:315:HIS:CG	2.54	0.42
1:G:356:ARG:HH21	1:G:358:ARG:CZ	2.32	0.42
2:H:274:ILE:HG13	2:H:306:ASN:CG	2.39	0.42
1:A:90:VAL:CG1	2:B:141:GLY:H	2.29	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
1:E:175:ASN:CB	1:E:178:ILE:HD12	2.49	0.42
1:E:363:ASN:OD1	1:E:365:VAL:N	2.50	0.42
2:F:61:PHE:CZ	2:F:411:ILE:HD11	2.54	0.42
1:G:12:LEU:HD23	1:G:124:PHE:HE2	1.83	0.42
1:G:104:LYS:N	1:G:192:ASP:OD1	2.52	0.42
1:G:175:ASN:HB3	1:G:178:ILE:HD12	2.00	0.42
1:A:368:LEU:HD11	1:A:391:LEU:HD22	2.00	0.42
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.85	0.42
2:B:47:ILE:HG22	2:B:48:SER:N	2.30	0.42
1:C:90:VAL:CG1	2:D:141:GLY:H	2.29	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:D:207:GLN:O	2:D:208:HIS:C	2.55	0.42
2:F:204:GLU:O	2:F:208:HIS:CD2	2.72	0.42
2:F:316:GLY:O	2:F:318:TYR:CD1	2.66	0.42
1:G:467:VAL:HG12	1:G:468:PRO:O	2.18	0.42
2:B:262:GLY:O	2:B:265:ASN:HB3	2.20	0.42
1:C:345:PRO:HB3	1:G:342:TYR:CE1	2.54	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:G:363:ASN:OD1	1:G:365:VAL:N	2.50	0.42
2:H:249:LYS:HB2	2:H:252:TRP:CZ2	2.52	0.42
1:A:23:GLN:NE2	1:A:131:THR:H	2.18	0.42
1:A:175:ASN:CB	1:A:178:ILE:HD12	2.49	0.42
1:A:346:PHE:HE1	1:E:342:TYR:OH	2.02	0.42
2:B:41:MET:HE1	2:B:73:LYS:HD2	2.01	0.42
2:B:108:VAL:CG1	2:B:188:TYR:CE2	3.02	0.42
2:B:204:GLU:O	2:B:208:HIS:CD2	2.72	0.42
1:C:14:PRO:HG2	1:C:14:PRO:O	2.18	0.42
1:C:44:GLU:HB2	1:C:46:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLN:HG2	1:C:355:ALA:CB	2.48	0.42
1:E:483:TYR:O	1:E:486:LEU:HB2	2.20	0.42
2:F:47:ILE:HG21	2:F:47:ILE:HD13	1.82	0.42
1:G:50:ILE:HD13	1:G:145:GLN:HB2	2.01	0.42
1:G:368:LEU:HD11	1:G:391:LEU:HD22	2.00	0.42
1:G:432:GLU:HB3	1:G:433:PRO:HD2	2.01	0.42
2:H:204:GLU:O	2:H:208:HIS:CD2	2.72	0.42
2:H:246:LEU:HD13	2:H:260:LEU:HD11	2.02	0.42
1:C:1:PRO:O	1:C:1:PRO:HG2	2.18	0.42
1:C:23:GLN:NE2	1:C:131:THR:H	2.18	0.42
1:C:175:ASN:HB3	1:C:178:ILE:HD12	2.00	0.42
2:D:204:GLU:O	2:D:208:HIS:CD2	2.72	0.42
2:D:262:GLY:O	2:D:265:ASN:HB3	2.20	0.42
1:E:164:MET:HE1	1:E:187:LEU:HD11	2.01	0.42
1:E:175:ASN:HB3	1:E:178:ILE:HD12	2.00	0.42
2:F:160:PHE:CD1	2:F:160:PHE:O	2.72	0.42
2:F:278:GLN:OE1	2:F:278:GLN:HA	2.20	0.42
1:G:23:GLN:NE2	1:G:131:THR:H	2.18	0.42
1:G:363:ASN:HB3	1:G:366:LYS:HB2	2.02	0.42
1:C:96:HIS:ND1	1:C:98:ALA:HB3	2.35	0.42
1:C:175:ASN:CB	1:C:178:ILE:HD12	2.49	0.42
1:C:238:LYS:HE3	1:C:315:HIS:CG	2.54	0.42
2:D:91:GLN:CD	2:D:94:ILE:HG23	2.39	0.42
1:E:23:GLN:NE2	1:E:131:THR:H	2.18	0.42
1:E:432:GLU:HB3	1:E:433:PRO:HD2	2.01	0.42
1:E:476:LYS:O	1:E:480:GLN:HG2	2.19	0.42
2:F:5:ILE:HG22	2:F:6:GLU:H	1.85	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:F:380:ILE:O	2:F:384:GLY:HA2	2.20	0.42
1:G:175:ASN:CB	1:G:178:ILE:HD12	2.50	0.42
1:G:232:TYR:CD1	1:G:241:VAL:HG22	2.53	0.42
2:H:61:PHE:CZ	2:H:411:ILE:HD11	2.54	0.42
2:H:72:ARG:HH12	2:H:409:THR:CG2	2.29	0.42
2:H:380:ILE:O	2:H:384:GLY:HA2	2.20	0.42
1:A:104:LYS:N	1:A:192:ASP:OD1	2.52	0.42
1:A:483:TYR:O	1:A:486:LEU:HB2	2.20	0.42
1:C:54:ASN:HA	1:C:55:PRO:HD3	1.77	0.42
1:C:104:LYS:N	1:C:192:ASP:OD1	2.52	0.42
1:C:483:TYR:O	1:C:486:LEU:HB2	2.20	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
2:F:123:ASP:HA	2:F:126:LYS:HZ1	1.83	0.42
2:F:271:TYR:CD1	2:F:271:TYR:N	2.88	0.42
1:G:164:MET:HE1	1:G:187:LEU:HD11	2.02	0.42
2:H:47:ILE:HG22	2:H:48:SER:N	2.30	0.42
1:A:1:PRO:O	1:A:1:PRO:HG2	2.18	0.42
1:A:96:HIS:ND1	1:A:98:ALA:HB3	2.35	0.42
1:A:432:GLU:HB3	1:A:433:PRO:HD2	2.01	0.42
1:A:540:LYS:HZ3	2:B:261:VAL:HG12	1.85	0.42
2:B:278:GLN:HA	2:B:278:GLN:OE1	2.20	0.42
2:B:420:PRO:HB2	2:B:421:PRO:CD	2.43	0.42
1:C:88:TRP:CH2	2:D:57:ASN:CB	3.01	0.42
1:C:225:PRO:N	1:C:226:PRO:HD2	2.35	0.42
1:C:363:ASN:HB3	1:C:366:LYS:HB2	2.02	0.42
1:C:421:PRO:HG2	1:C:421:PRO:O	2.20	0.42
2:D:393:ILE:HG12	2:D:394:GLN:N	2.35	0.42
1:E:132:ILE:N	1:E:142:ILE:O	2.52	0.42
1:E:356:ARG:HH21	1:E:358:ARG:CZ	2.32	0.42
1:E:439:THR:HG22	1:E:441:TYR:HE1	1.82	0.42
2:F:28:GLU:O	2:F:32:LYS:HG3	2.20	0.42
1:G:53:GLU:CD	1:G:53:GLU:N	2.73	0.42
1:G:331:LYS:O	1:G:331:LYS:HG2	2.20	0.42
2:H:262:GLY:O	2:H:265:ASN:HB3	2.20	0.42
1:A:44:GLU:HB2	1:A:46:LYS:HG2	2.02	0.42
1:A:312:GLU:HA	1:A:313:PRO:HD2	1.89	0.42
1:C:96:HIS:CD2	1:C:97:PRO:HD2	2.55	0.42
1:C:342:TYR:CZ	1:G:345:PRO:HB3	2.54	0.42
1:E:18:GLY:HA3	1:E:127:TYR:HD1	1.85	0.42
1:E:50:ILE:HD13	1:E:145:GLN:HB2	2.01	0.42
1:G:96:HIS:ND1	1:G:98:ALA:HB3	2.35	0.42
1:G:116:PHE:N	1:G:116:PHE:CD1	2.88	0.42
1:G:483:TYR:O	1:G:486:LEU:HB2	2.20	0.42
2:H:109:LEU:O	2:H:186:ASP:HA	2.20	0.42
2:H:160:PHE:O	2:H:160:PHE:CD1	2.72	0.42
2:H:271:TYR:CD1	2:H:271:TYR:N	2.88	0.42
2:H:278:GLN:OE1	2:H:278:GLN:HA	2.20	0.42
1:A:427:TYR:CD1	1:A:427:TYR:N	2.88	0.41
2:B:24:TRP:HZ3	2:B:61:PHE:CG	2.38	0.41
2:B:395:LYS:O	2:B:399:GLU:N	2.48	0.41
1:C:232:TYR:CD1	1:C:241:VAL:HG22	2.53	0.41
2:D:28:GLU:O	2:D:32:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:LEU:HB3	2:D:125:ARG:NH1	2.34	0.41
1:G:8:VAL:HA	1:G:9:PRO:HD2	1.78	0.41
1:G:38:CYS:HB3	1:G:144:TYR:CE2	2.55	0.41
1:G:96:HIS:CD2	1:G:97:PRO:HD2	2.55	0.41
1:G:201:LYS:HD3	1:G:201:LYS:HA	1.85	0.41
1:G:439:THR:CG2	1:G:441:TYR:HE1	2.33	0.41
2:H:78:ARG:HD3	2:H:411:ILE:O	2.20	0.41
2:H:365:VAL:HG12	2:H:405:TYR:HE2	1.81	0.41
2:H:393:ILE:HG12	2:H:394:GLN:N	2.35	0.41
1:A:249:LYS:CG	1:A:250:ASP:N	2.83	0.41
2:B:28:GLU:O	2:B:32:LYS:HG3	2.20	0.41
2:B:120:LEU:HB3	2:B:125:ARG:NH1	2.34	0.41
2:B:380:ILE:O	2:B:384:GLY:HA2	2.20	0.41
1:C:38:CYS:HB3	1:C:144:TYR:CE2	2.55	0.41
1:C:427:TYR:N	1:C:427:TYR:CD1	2.88	0.41
1:E:77:PHE:CE2	1:E:150:PRO:HB3	2.55	0.41
1:E:96:HIS:ND1	1:E:98:ALA:HB3	2.35	0.41
1:E:427:TYR:N	1:E:427:TYR:CD1	2.88	0.41
1:E:439:THR:CG2	1:E:441:TYR:HE1	2.33	0.41
2:F:18:GLY:HA3	2:F:127:TYR:CD1	2.56	0.41
2:F:78:ARG:HD3	2:F:411:ILE:O	2.19	0.41
2:F:246:LEU:HD13	2:F:260:LEU:HD11	2.02	0.41
1:G:18:GLY:HA3	1:G:127:TYR:HD1	1.85	0.41
1:G:77:PHE:CE2	1:G:150:PRO:HB3	2.55	0.41
1:G:116:PHE:N	1:G:116:PHE:HD1	2.18	0.41
1:G:320:ASP:HA	1:G:321:PRO:HD2	1.85	0.41
1:G:439:THR:HG22	1:G:441:TYR:HE1	1.82	0.41
2:H:336:GLN:HG2	2:H:355:ALA:HB1	2.02	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
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.55	0.41
1:A:363:ASN:HB3	1:A:366:LYS:HB2	2.02	0.41
2:B:100:LEU:HD23	2:B:100:LEU:HA	1.81	0.41
1:C:53:GLU:CD	1:C:53:GLU:N	2.73	0.41
1:C:77:PHE:CE2	1:C:150:PRO:HB3	2.55	0.41
1:C:116:PHE:HD1	1:C:116:PHE:N	2.18	0.41
1:C:432:GLU:HB3	1:C:433:PRO:HD2	2.01	0.41
2:D:24:TRP:HZ3	2:D:61:PHE:CG	2.38	0.41
2:D:246:LEU:HD13	2:D:260:LEU:HD11	2.02	0.41
1:E:116:PHE:N	1:E:116:PHE:HD1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:GLY:HA3	1:E:466:VAL:HA	2.02	0.41
1:G:409:THR:O	1:G:410:TRP:HB2	2.21	0.41
1:G:427:TYR:N	1:G:427:TYR:CD1	2.88	0.41
2:H:10:VAL:HA	2:H:85:GLN:OE1	2.20	0.41
1:A:238:LYS:HE3	1:A:315:HIS:CG	2.54	0.41
2:B:109:LEU:O	2:B:186:ASP:HA	2.20	0.41
2:B:136:ASN:O	2:B:137:ASN:HB2	2.21	0.41
1:C:10:VAL:HG11	1:C:153:TRP:HZ2	1.86	0.41
1:C:331:LYS:O	1:C:331:LYS:HG2	2.20	0.41
2:D:278:GLN:OE1	2:D:278:GLN:HA	2.20	0.41
1:E:12:LEU:HD23	1:E:124:PHE:HE2	1.83	0.41
1:E:78:ARG:NH1	1:E:287:LYS:O	2.39	0.41
1:E:116:PHE:N	1:E:116:PHE:CD1	2.88	0.41
1:E:249:LYS:CG	1:E:250:ASP:N	2.83	0.41
2:F:136:ASN:O	2:F:137:ASN:HB2	2.21	0.41
2:F:393:ILE:HG12	2:F:394:GLN:N	2.35	0.41
1:G:53:GLU:N	1:G:53:GLU:OE2	2.54	0.41
1:G:344:GLU:HA	1:G:345:PRO:HD2	1.81	0.41
1:G:421:PRO:O	1:G:421:PRO:HG2	2.20	0.41
2:B:391:LEU:HD12	2:B:416:PHE:HE1	1.86	0.41
1:C:53:GLU:N	1:C:53:GLU:OE2	2.54	0.41
1:C:349:LEU:HA	1:C:349:LEU:HD23	1.84	0.41
2:D:136:ASN:O	2:D:137:ASN:HB2	2.21	0.41
2:D:395:LYS:O	2:D:399:GLU:N	2.48	0.41
1:E:53:GLU:CD	1:E:53:GLU:N	2.73	0.41
1:E:225:PRO:N	1:E:226:PRO:HD2	2.35	0.41
2:F:10:VAL:HA	2:F:85:GLN:OE1	2.20	0.41
2:F:109:LEU:O	2:F:186:ASP:HA	2.20	0.41
2:F:153:TRP:CE3	2:F:155:GLY:CA	3.03	0.41
2:F:193:LEU:HD12	2:F:201:LYS:HG3	2.03	0.41
1:G:44:GLU:HB2	1:G:46:LYS:HG2	2.02	0.41
1:G:225:PRO:N	1:G:226:PRO:HD2	2.35	0.41
1:G:408:ALA:HB2	2:H:337:TRP:HH2	1.85	0.41
1:A:18:GLY:HA3	1:A:127:TYR:HD1	1.85	0.41
1:A:456:GLY:HA3	1:A:466:VAL:HA	2.02	0.41
2:B:61:PHE:CD2	2:B:403:THR:HG22	2.56	0.41
2:B:108:VAL:CG1	2:B:188:TYR:CD2	3.04	0.41
2:B:246:LEU:HD13	2:B:260:LEU:HD11	2.02	0.41
2:B:393:ILE:HG12	2:B:394:GLN:N	2.35	0.41
1:C:409:THR:O	1:C:410:TRP:HB2	2.21	0.41
2:D:61:PHE:CD2	2:D:403:THR:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:LYS:HB3	2:D:191:SER:O	2.21	0.41
2:D:156:SER:HB2	2:D:157:PRO:CD	2.51	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
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:E:472:THR:HB	1:E:476:LYS:HB2	2.03	0.41
2:F:24:TRP:HZ3	2:F:61:PHE:CG	2.38	0.41
2:F:104:LYS:O	2:F:235:HIS:CD2	2.74	0.41
1:G:418:ASN:C	1:G:418:ASN:ND2	2.74	0.41
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.55	0.41
1:A:116:PHE:HD1	1:A:116:PHE:N	2.18	0.41
1:A:225:PRO:N	1:A:226:PRO:HD2	2.35	0.41
1:A:439:THR:CG2	1:A:441:TYR:HE1	2.33	0.41
2:B:58:THR:HG21	2:B:77:PHE:CD1	2.56	0.41
2:B:94:ILE:H	2:B:94:ILE:HG13	1.54	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:116:PHE:N	1:C:116:PHE:CD1	2.88	0.41
1:C:118:VAL:HA	1:C:119:PRO:HD2	1.71	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
2:D:18:GLY:HA3	2:D:127:TYR:CD1	2.56	0.41
1:E:44:GLU:HB2	1:E:46:LYS:HG2	2.02	0.41
1:E:53:GLU:N	1:E:53:GLU:OE2	2.54	0.41
1:E:440:PHE:HD2	1:E:457:TYR:CD2	2.39	0.41
2:F:202:ILE:O	2:F:206:ARG:N	2.54	0.41
1:G:90:VAL:CG1	2:H:141:GLY:H	2.29	0.41
1:G:391:LEU:HA	1:G:392:PRO:HD3	1.73	0.41
1:G:440:PHE:HD2	1:G:457:TYR:CD2	2.39	0.41
2:H:61:PHE:CD2	2:H:403:THR:HG22	2.56	0.41
2:H:108:VAL:CG1	2:H:188:TYR:CD2	3.04	0.41
2:H:175:ASN:O	2:H:177:ASP:N	2.54	0.41
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.86	0.41
1:A:53:GLU:CD	1:A:53:GLU:N	2.73	0.41
1:A:53:GLU:N	1:A:53:GLU:OE2	2.54	0.41
1:A:54:ASN:O	1:A:143:ARG:NH1	2.54	0.41
1:A:57:ASN:HB2	1:A:143:ARG:HH21	1.86	0.41
1:A:77:PHE:CE2	1:A:150:PRO:HB3	2.55	0.41
1:A:116:PHE:N	1:A:116:PHE:CD1	2.88	0.41
1:A:132:ILE:CD1	1:A:144:TYR:HE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.85	0.41
1:A:331:LYS:O	1:A:331:LYS:HG2	2.20	0.41
1:A:388:LYS:HA	1:A:413:GLU:HB2	2.03	0.41
1:A:418:ASN:C	1:A:418:ASN:ND2	2.74	0.41
1:A:463:ARG:HG3	1:A:463:ARG:NH1	2.35	0.41
1:A:484:LEU:O	1:A:487:GLN:N	2.54	0.41
2:B:11:LYS:N	2:B:85:GLN:OE1	2.49	0.41
2:B:103:LYS:HB3	2:B:191:SER:O	2.21	0.41
2:B:153:TRP:CE3	2:B:155:GLY:CA	3.03	0.41
2:B:175:ASN:O	2:B:177:ASP:N	2.54	0.41
2:B:193:LEU:HD12	2:B:201:LYS:HG3	2.03	0.41
1:C:116:PHE:HA	1:C:148:VAL:HG11	2.03	0.41
1:C:417:VAL:HG21	1:G:346:PHE:CD1	2.56	0.41
1:C:420:PRO:CG	1:C:421:PRO:HD2	2.35	0.41
1:C:463:ARG:HG3	1:C:463:ARG:NH1	2.35	0.41
1:C:484:LEU:O	1:C:487:GLN:N	2.54	0.41
2:D:58:THR:HG21	2:D:77:PHE:CD1	2.56	0.41
2:D:63:ILE:HG12	2:D:64:LYS:H	1.86	0.41
2:D:271:TYR:CD1	2:D:271:TYR:N	2.88	0.41
2:D:391:LEU:HD12	2:D:416:PHE:HE1	1.86	0.41
1:E:96:HIS:CD2	1:E:97:PRO:HD2	2.55	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:E:421:PRO:O	1:E:421:PRO:HG2	2.20	0.41
1:E:484:LEU:O	1:E:487:GLN:N	2.54	0.41
2:F:252:TRP:CH2	2:F:260:LEU:HD22	2.56	0.41
2:F:336:GLN:HG2	2:F:355:ALA:HB1	2.02	0.41
1:G:132:ILE:CD1	1:G:144:TYR:HE2	2.33	0.41
1:G:317:VAL:CG2	1:G:347:LYS:HB3	2.41	0.41
1:G:472:THR:HB	1:G:476:LYS:HB2	2.03	0.41
2:H:18:GLY:HA3	2:H:127:TYR:CD1	2.56	0.41
2:H:24:TRP:HZ3	2:H:61:PHE:CG	2.38	0.41
2:H:74:LEU:HD12	2:H:74:LEU:HA	1.83	0.41
2:H:100:LEU:HA	2:H:100:LEU:HD23	1.81	0.41
2:H:104:LYS:O	2:H:235:HIS:CD2	2.74	0.41
2:H:136:ASN:O	2:H:137:ASN:HB2	2.21	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:H:193:LEU:HD12	2:H:201:LYS:HG3	2.03	0.41
2:H:252:TRP:CH2	2:H:260:LEU:HD22	2.56	0.41
2:H:391:LEU:HD12	2:H:416:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:THR:O	1:A:410:TRP:HB2	2.21	0.41
2:B:10:VAL:HA	2:B:85:GLN:OE1	2.20	0.41
2:B:37:ILE:HG13	2:B:37:ILE:H	1.69	0.41
2:B:271:TYR:CD1	2:B:271:TYR:N	2.88	0.41
2:B:336:GLN:HG2	2:B:355:ALA:HB1	2.02	0.41
1:C:8:VAL:HA	1:C:9:PRO:HD2	1.78	0.41
1:C:54:ASN:O	1:C:143:ARG:NH1	2.54	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:D:175:ASN:O	2:D:177:ASP:N	2.54	0.41
2:D:420:PRO:HB2	2:D:421:PRO:CD	2.43	0.41
1:E:116:PHE:HA	1:E:148:VAL:HG11	2.03	0.41
1:E:331:LYS:O	1:E:331:LYS:HG2	2.20	0.41
1:E:363:ASN:HB3	1:E:366:LYS:HB2	2.02	0.41
2:F:156:SER:HB2	2:F:157:PRO:CD	2.51	0.41
2:F:175:ASN:O	2:F:177:ASP:N	2.54	0.41
1:G:116:PHE:HA	1:G:148:VAL:HG11	2.03	0.41
2:H:34:LEU:HD23	2:H:34:LEU:HA	1.92	0.41
2:H:52:PRO:HG2	2:H:53:GLU:N	2.36	0.41
2:H:274:ILE:HG13	2:H:306:ASN:OD1	2.21	0.41
1:A:116:PHE:HA	1:A:148:VAL:HG11	2.03	0.40
1:A:164:MET:HE1	1:A:187:LEU:HD11	2.02	0.40
2:B:104:LYS:O	2:B:235:HIS:CD2	2.74	0.40
1:C:18:GLY:HA3	1:C:127:TYR:HD1	1.85	0.40
1:C:418:ASN:C	1:C:418:ASN:ND2	2.74	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
2:D:153:TRP:CE3	2:D:155:GLY:CA	3.03	0.40
2:D:274:ILE:HG13	2:D:306:ASN:OD1	2.21	0.40
1:E:229:TRP:CE2	1:E:230:MET:HE3	2.56	0.40
2:F:61:PHE:CD2	2:F:403:THR:HG22	2.56	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
1:G:377:THR:O	1:G:380:ILE:N	2.54	0.40
1:G:536:VAL:HA	1:G:537:PRO:HD3	1.77	0.40
1:A:132:ILE:N	1:A:142:ILE:O	2.52	0.40
1:C:252:TRP:HA	1:C:252:TRP:CE3	2.56	0.40
1:C:331:LYS:O	1:C:333:GLY:N	2.54	0.40
1:C:402:TRP:CE3	1:C:402:TRP:O	2.74	0.40
2:D:419:THR:HA	2:D:420:PRO:HD2	1.96	0.40
1:E:232:TYR:CD1	1:E:241:VAL:HG22	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:ILE:HG12	2:F:64:LYS:H	1.86	0.40
1:G:229:TRP:CE2	1:G:230:MET:HE3	2.56	0.40
1:G:349:LEU:HA	1:G:349:LEU:HD23	1.84	0.40
2:H:28:GLU:O	2:H:32:LYS:HG3	2.20	0.40
2:H:47:ILE:HG21	2:H:47:ILE:HD13	1.82	0.40
1:A:232:TYR:CD1	1:A:241:VAL:HG22	2.53	0.40
1:A:246:LEU:O	1:A:307:ARG:NH1	2.54	0.40
1:A:252:TRP:HA	1:A:252:TRP:CE3	2.56	0.40
1:A:402:TRP:CE3	1:A:402:TRP:O	2.74	0.40
1:A:440:PHE:HD2	1:A:457:TYR:CD2	2.39	0.40
2:D:104:LYS:O	2:D:235:HIS:CD2	2.74	0.40
2:D:109:LEU:O	2:D:186:ASP:HA	2.20	0.40
1:E:252:TRP:HA	1:E:252:TRP:CE3	2.56	0.40
1:E:326:ILE:CG2	1:E:342:TYR:HE1	2.35	0.40
1:E:344:GLU:HA	1:E:345:PRO:HD2	1.82	0.40
1:E:377:THR:O	1:E:380:ILE:N	2.55	0.40
2:F:72:ARG:HH12	2:F:409:THR:CA	2.35	0.40
2:F:274:ILE:HG13	2:F:306:ASN:OD1	2.21	0.40
1:G:452:LEU:HD22	1:G:470:THR:HA	2.04	0.40
1:G:456:GLY:HA3	1:G:466:VAL:HA	2.02	0.40
1:A:472:THR:HB	1:A:476:LYS:HB2	2.03	0.40
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.04	0.40
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.56	0.40
1:C:30:LYS:HB3	1:C:62:ALA:HB3	2.04	0.40
1:C:132:ILE:CD1	1:C:144:TYR:HE2	2.33	0.40
1:C:239:TRP:N	1:C:318:TYR:HE1	2.20	0.40
1:C:246:LEU:O	1:C:307:ARG:NH1	2.54	0.40
1:C:388:LYS:HA	1:C:413:GLU:HB2	2.03	0.40
1:C:472:THR:HB	1:C:476:LYS:HB2	2.03	0.40
2:D:7:THR:HG22	2:D:119:PRO:HG2	2.04	0.40
2:D:10:VAL:HA	2:D:85:GLN:OE1	2.20	0.40
2:D:193:LEU:HD12	2:D:201:LYS:HG3	2.03	0.40
2:D:252:TRP:CH2	2:D:260:LEU:HD22	2.56	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
1:E:243:PRO:HD3	1:E:313:PRO:HB3	2.04	0.40
1:E:246:LEU:O	1:E:307:ARG:NH1	2.54	0.40
1:E:312:GLU:HA	1:E:313:PRO:HD2	1.90	0.40
1:E:452:LEU:HD22	1:E:470:THR:HA	2.04	0.40
2:F:28:GLU:HG3	2:F:135:ILE:HD13	2.02	0.40
2:F:52:PRO:HG2	2:F:53:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:58:THR:HG21	2:F:77:PHE:CD1	2.56	0.40
2:F:103:LYS:HB3	2:F:191:SER:O	2.21	0.40
2:F:108:VAL:CG1	2:F:188:TYR:CD2	3.04	0.40
2:F:391:LEU:HD12	2:F:416:PHE:HE1	1.86	0.40
1:G:10:VAL:HG11	1:G:153:TRP:HZ2	1.86	0.40
1:G:239:TRP:N	1:G:318:TYR:HE1	2.20	0.40
1:G:244:ILE:HD12	1:G:267:ALA:CB	2.40	0.40
2:H:7:THR:HG22	2:H:119:PRO:HG2	2.03	0.40
2:B:252:TRP:CH2	2:B:260:LEU:HD22	2.56	0.40
2:B:316:GLY:O	2:B:318:TYR:CD1	2.65	0.40
1:C:201:LYS:HD3	1:C:201:LYS:HA	1.85	0.40
1:C:442:VAL:HG12	1:C:481:ALA:CB	2.46	0.40
2:D:41:MET:HE1	2:D:73:LYS:HD2	2.02	0.40
1:E:104:LYS:N	1:E:192:ASP:OD1	2.52	0.40
2:F:330:GLN:HB2	2:F:338:THR:OG1	2.22	0.40
1:G:377:THR:OG1	1:G:378:GLU:N	2.55	0.40
1:G:484:LEU:O	1:G:487:GLN:N	2.54	0.40
2:H:103:LYS:HB3	2:H:191:SER:O	2.21	0.40
2:H:395:LYS:HG2	2:H:399:GLU:OE1	2.21	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
1:C:53:GLU:O	2:H:88:TRP:CE2[3_445]	2.04	0.16
2:D:208:HIS:O	1:E:211:ARG:NE[2_657]	2.04	0.16
2:B:200:THR:CB	1:C:211:ARG:NE[2_657]	2.09	0.11
1:C:54:ASN:C	2:H:88:TRP:NE1[3_445]	2.14	0.06
2:D:211:ARG:O	1:E:207:GLN:OE1[2_657]	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 [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	4	26
1	C	530/560 (95%)	438 (83%)	75 (14%)	17 (3%)	4	26
1	E	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	4	26
1	G	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	4	26
2	B	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	4	26
2	D	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	4	26
2	F	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	4	26
2	H	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3676/4000 (92%)	3035 (83%)	525 (14%)	116 (3%)	4	26

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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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 [i](#)

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%)	27	63
1	C	431/500 (86%)	411 (95%)	20 (5%)	27	63
1	E	431/500 (86%)	410 (95%)	21 (5%)	25	61
1	G	431/500 (86%)	411 (95%)	20 (5%)	27	63
2	B	343/400 (86%)	323 (94%)	20 (6%)	20	55
2	D	343/400 (86%)	323 (94%)	20 (6%)	20	55
2	F	343/400 (86%)	323 (94%)	20 (6%)	20	55
2	H	343/400 (86%)	323 (94%)	20 (6%)	20	55
All	All	3096/3600 (86%)	2935 (95%)	161 (5%)	23	59

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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

Sometimes 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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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 [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.