



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:40 AM GMT

PDB ID : 1KEN  
Title : INFLUENZA VIRUS HEMAGGLUTININ COMPLEXED WITH AN AN-  
TIBODY THAT PREVENTS THE HEMAGGLUTININ LOW PH FUSO-  
GENIC TRANSITION  
Authors : Barbey-Martin, C.; Gigant, B.; Bizebard, T.; Calder, L.J.; Wharto, S.A.;  
Skehel, J.J.; Knossow, M.  
Deposited on : 2001-11-16  
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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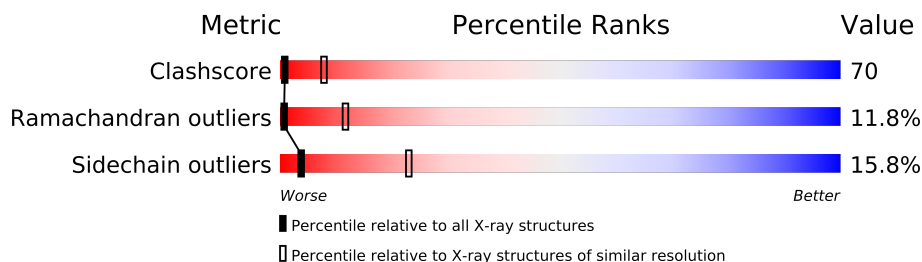
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	328	
1	C	328	
1	E	328	
2	B	175	
2	D	175	
2	F	175	
3	L	213	
3	U	213	
4	H	221	
4	T	221	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18492 atoms, of which 0 are hydrogen and 0 are deuterium.

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 hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2472	1547	434	478	13			
1	C	320	Total	C	N	O	S	0	0	0
			2472	1547	434	478	13			
1	E	320	Total	C	N	O	S	0	0	0
			2472	1547	434	478	13			

- Molecule 2 is a protein called hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	D	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	F	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			

- Molecule 3 is a protein called influenza virus infectivity neutralizing antibody (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1638	1028	272	332	6			
3	U	213	Total	C	N	O	S	0	0	0
			1638	1028	272	332	6			

- Molecule 4 is a protein called influenza virus infectivity neutralizing antibody (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	221	Total	C	N	O	S	0	0	0
			1720	1102	272	340	6			
4	T	219	Total	C	N	O	S	0	0	0
			1700	1092	267	335	6			

- Molecule 5 is a polymer of unknown type called SUGAR (NAG-NAG-MAN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	C	3	Total	C	N	O	0	0
			39	22	2	15		
5	E	3	Total	C	N	O	0	0
			39	22	2	15		

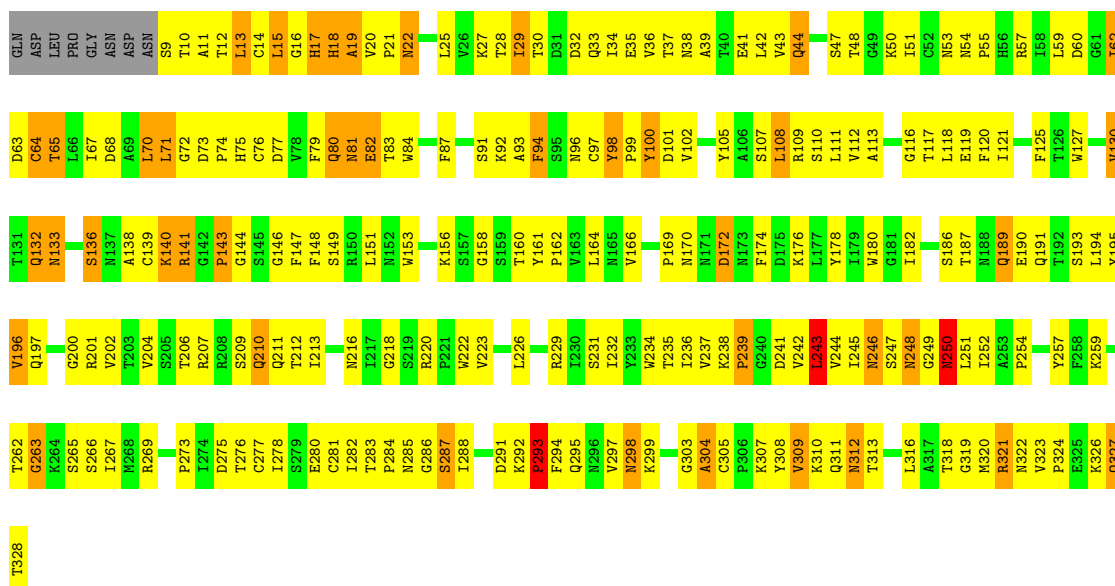
### 3 Residue-property plots

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

Note EDS was not executed.

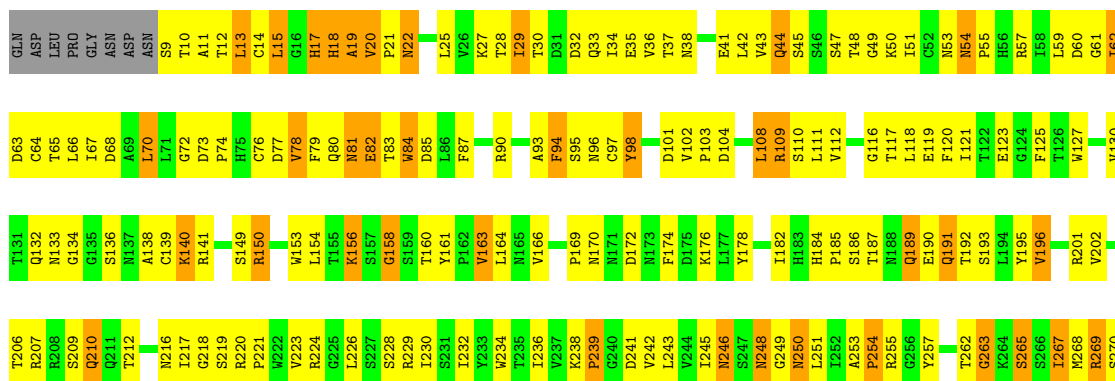
#### • Molecule 1: hemagglutinin HA1

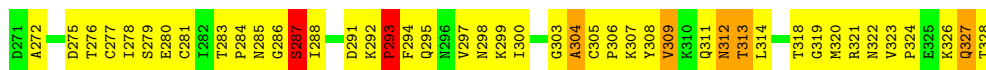
Chain A: 



#### • Molecule 1: hemagglutinin HA1

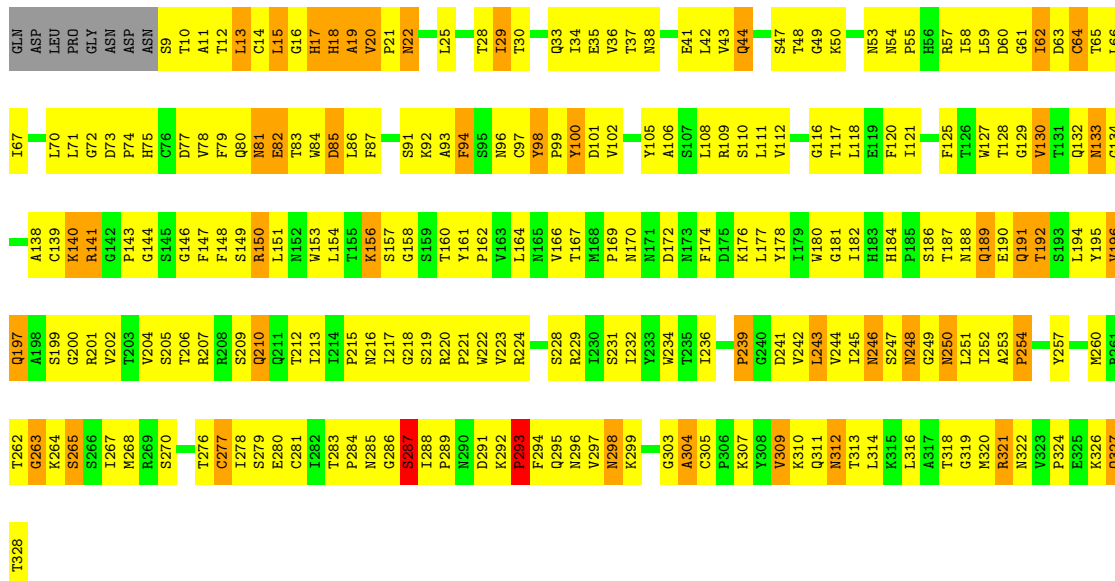
Chain C: 

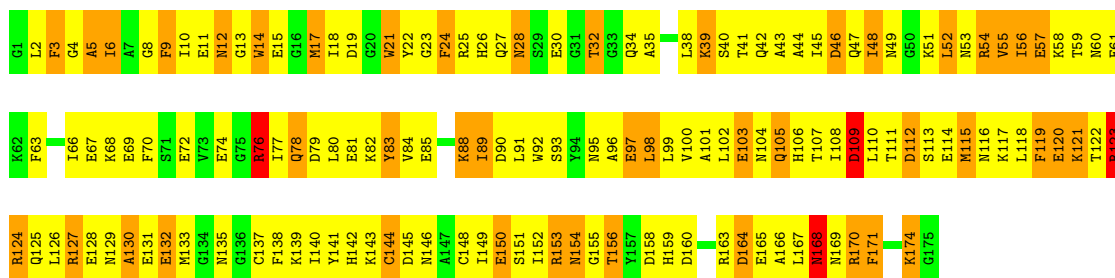




• Molecule 1: hemagglutinin HA1

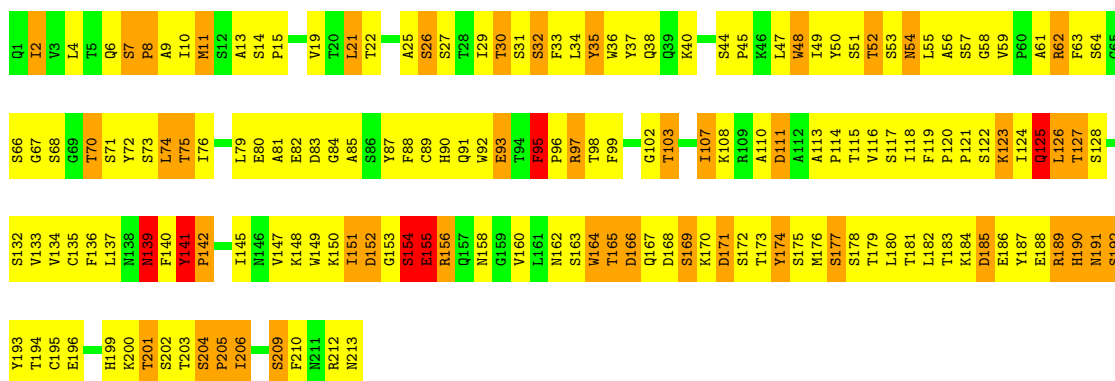
Chain E:





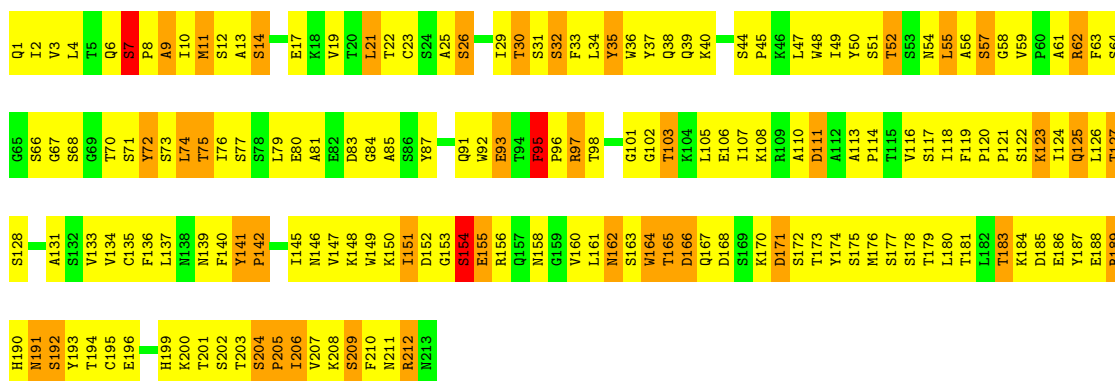
• Molecule 3: influenza virus infectivity neutralizing antibody (light chain)

Chain L:



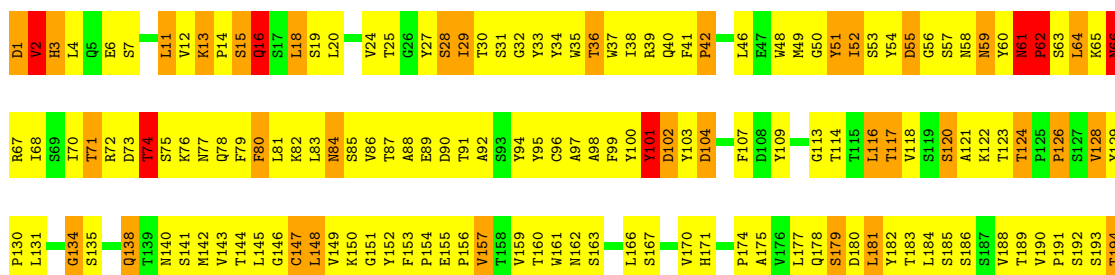
• Molecule 3: influenza virus infectivity neutralizing antibody (light chain)

Chain U:



• Molecule 4: influenza virus infectivity neutralizing antibody (heavy chain)

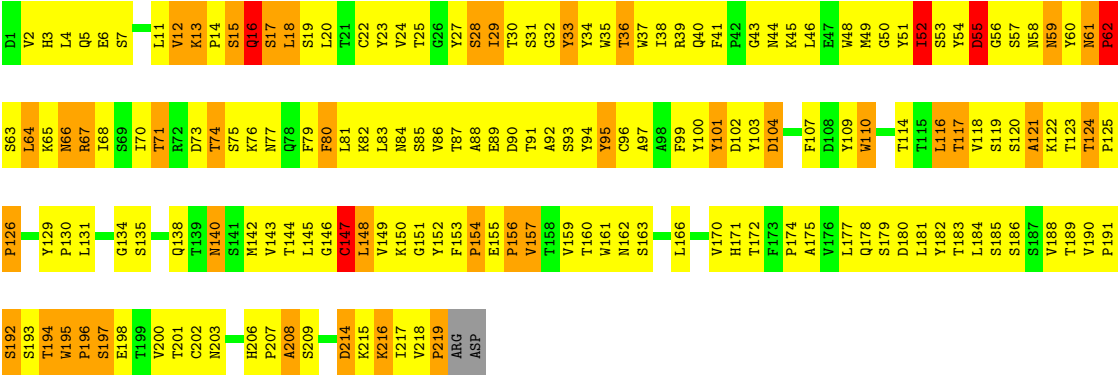
Chain H:





● Molecule 4: influenza virus infectivity neutralizing antibody (heavy chain)

Chain T:





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.04Å 315.59Å 97.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.50	Depositor
% Data completeness (in resolution range)	91.8 (25.00-3.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.255 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18492	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0/2528	0.91	3/3443 (0.1%)
1	C	0.77	1/2528 (0.0%)	0.96	2/3443 (0.1%)
1	E	0.71	0/2528	0.93	2/3443 (0.1%)
2	B	0.74	0/1445	0.86	0/1939
2	D	0.77	1/1445 (0.1%)	0.89	3/1939 (0.2%)
2	F	0.73	0/1445	0.84	0/1939
3	L	0.82	2/1679 (0.1%)	1.05	7/2281 (0.3%)
3	U	0.76	0/1679	0.97	3/2281 (0.1%)
4	H	0.85	2/1774 (0.1%)	1.00	2/2431 (0.1%)
4	T	0.78	1/1754 (0.1%)	1.00	2/2406 (0.1%)
All	All	0.76	7/18805 (0.0%)	0.95	24/25545 (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
3	L	0	1
3	U	0	1
4	H	0	1
4	T	0	2
5	A	1	0
5	C	1	0
5	E	1	0
All	All	3	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	ASP	CB-CG	7.47	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	155	GLU	CB-CG	7.10	1.65	1.52
3	L	155	GLU	CG-CD	6.60	1.61	1.51
4	H	61	ASN	CB-CG	5.86	1.64	1.51
2	D	92	TRP	CB-CG	-5.42	1.40	1.50
1	C	163	VAL	CA-CB	-5.18	1.43	1.54
4	T	110	TRP	CB-CG	-5.18	1.41	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	64	LEU	CA-CB-CG	-10.84	90.37	115.30
3	L	111	ASP	N-CA-C	-9.85	84.40	111.00
4	H	64	LEU	CA-CB-CG	-7.90	97.13	115.30
3	U	111	ASP	N-CA-C	-7.69	90.24	111.00
2	D	79	ASP	CB-CG-OD2	7.20	124.78	118.30
3	L	7	SER	N-CA-C	7.16	130.34	111.00
3	L	152	ASP	CB-CG-OD1	-6.92	112.07	118.30
3	L	156	ARG	NE-CZ-NH2	-6.74	116.93	120.30
3	L	152	ASP	CB-CG-OD2	6.56	124.20	118.30
3	U	95	PHE	N-CA-C	6.35	128.15	111.00
1	C	108	LEU	CA-CB-CG	-5.93	101.66	115.30
1	A	64	CYS	CA-CB-SG	-5.92	103.34	114.00
1	A	243	LEU	CA-CB-CG	5.88	128.82	115.30
4	H	181	LEU	CA-CB-CG	5.87	128.81	115.30
1	E	66	LEU	CA-CB-CG	-5.82	101.91	115.30
4	T	219	PRO	N-CA-C	5.76	127.07	112.10
1	C	109	ARG	NE-CZ-NH1	-5.38	117.61	120.30
3	L	95	PHE	N-CA-C	5.37	125.50	111.00
3	U	7	SER	N-CA-C	5.31	125.33	111.00
1	A	108	LEU	CA-CB-CG	-5.29	103.14	115.30
3	L	115	THR	N-CA-C	-5.14	97.12	111.00
2	D	2	LEU	N-CA-C	-5.10	97.24	111.00
1	E	64	CYS	CA-CB-SG	-5.04	104.93	114.00
2	D	59	THR	N-CA-C	5.01	124.52	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	452	MAN	C1
5	C	452	MAN	C1
5	E	452	MAN	C1

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	101	TYR	Sidechain
3	L	141	TYR	Sidechain
4	T	33	TYR	Sidechain
4	T	95	TYR	Sidechain
3	U	72	TYR	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2472	0	2424	336	0
1	C	2472	0	2424	328	0
1	E	2472	0	2424	334	0
2	B	1421	0	1346	259	0
2	D	1421	0	1346	273	0
2	F	1421	0	1346	276	0
3	L	1638	0	1578	232	0
3	U	1638	0	1578	260	0
4	H	1720	0	1639	264	0
4	T	1700	0	1622	276	0
5	A	39	0	34	3	0
5	C	39	0	34	4	0
5	E	39	0	34	0	0
All	All	18492	0	17829	2549	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 70.

All (2549) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:PRO:HA	1:A:141:ARG:HH12	1.11	1.16
3:U:199:HIS:HB3	3:U:201:THR:HG22	1.28	1.11
3:U:134:VAL:HG22	3:U:179:THR:HG23	1.30	1.11
1:C:77:ASP:O	1:C:80:GLN:HG2	1.47	1.10
1:C:96:ASN:HD21	1:C:140:LYS:HE2	1.10	1.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:321:ARG:HG2	1:E:322:ASN:H	1.14	1.10
1:E:28:THR:HG22	2:F:104:ASN:HB3	1.23	1.09
2:B:25:ARG:HG2	2:B:34:GLN:HG2	1.31	1.09
2:D:3:PHE:HD2	2:D:113:SER:HA	1.14	1.09
2:B:3:PHE:HD2	2:B:113:SER:HA	1.10	1.08
1:A:54:ASN:HB3	1:A:278:ILE:HD13	1.35	1.08
4:T:18:LEU:HD12	4:T:19:SER:N	1.68	1.08
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.12	1.08
1:E:14:CYS:HB2	2:F:25:ARG:HB2	1.32	1.06
1:A:28:THR:HG22	2:B:104:ASN:HB3	1.37	1.06
3:U:137:LEU:HD23	3:U:145:ILE:HD13	1.38	1.05
1:E:29:ILE:HD11	2:F:102:LEU:HD23	1.31	1.05
4:T:2:VAL:HB	4:T:109:TYR:CE2	1.93	1.04
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.41	1.03
1:A:186:SER:HA	1:A:218:GLY:O	1.56	1.03
2:F:25:ARG:HG2	2:F:34:GLN:HG2	1.40	1.03
2:B:167:LEU:O	2:B:170:ARG:HB2	1.60	1.02
2:F:3:PHE:HD2	2:F:113:SER:HA	1.23	1.02
3:L:199:HIS:HB3	3:L:201:THR:HG22	1.42	1.02
1:C:14:CYS:HB2	2:D:25:ARG:HB2	1.40	1.02
4:T:2:VAL:HB	4:T:109:TYR:HE2	1.19	1.01
1:C:29:ILE:HD11	2:D:102:LEU:HD23	1.41	1.01
3:L:67:GLY:HA3	3:L:72:TYR:CD2	1.94	1.01
1:E:96:ASN:HD21	1:E:140:LYS:HE2	1.21	1.01
2:B:130:ALA:HB1	2:B:139:LYS:O	1.61	1.01
2:D:28:ASN:HD22	2:D:145:ASP:HA	1.19	1.01
2:F:28:ASN:HD22	2:F:145:ASP:HA	1.19	1.00
2:D:25:ARG:HG2	2:D:34:GLN:HG2	1.39	1.00
2:B:3:PHE:CD2	2:B:113:SER:HA	1.96	1.00
3:L:201:THR:HG23	3:L:202:SER:H	1.23	1.00
1:C:286:GLY:O	1:C:287:SER:HB2	1.62	1.00
3:L:199:HIS:CD2	3:L:200:LYS:H	1.80	0.99
3:L:151:ILE:HG22	3:L:152:ASP:N	1.76	0.99
1:A:216:ASN:HB3	1:C:212:THR:HG21	1.43	0.99
4:T:126:PRO:HB3	4:T:152:TYR:HB3	1.45	0.99
3:L:121:PRO:HB2	3:L:126:LEU:HD21	1.45	0.98
3:U:164:TRP:H	3:U:164:TRP:HE3	1.00	0.98
1:A:281:CYS:HB2	1:A:304:ALA:O	1.62	0.97
4:H:18:LEU:HD12	4:H:19:SER:N	1.77	0.97
1:A:22:ASN:H	1:A:22:ASN:HD22	1.10	0.97
1:A:18:HIS:HA	2:B:14:TRP:HB2	1.44	0.97
2:D:132:GLU:HA	2:D:138:PHE:HA	1.47	0.97

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:22:ASN:HD22	1:C:22:ASN:H	1.09	0.97
2:F:167:LEU:O	2:F:170:ARG:HB2	1.66	0.96
2:F:145:ASP:H	2:F:148:CYS:HB3	1.31	0.95
1:A:14:CYS:HB2	2:B:25:ARG:HB2	1.47	0.94
4:T:218:VAL:HG12	4:T:219:PRO:HD2	1.46	0.94
1:A:74:PRO:HA	1:A:141:ARG:NH1	1.82	0.94
3:U:14:SER:HA	3:U:108:LYS:HB2	1.49	0.94
1:A:77:ASP:O	1:A:80:GLN:HG2	1.67	0.94
1:C:18:HIS:HA	2:D:14:TRP:HB2	1.50	0.94
2:F:127:ARG:HH11	2:F:127:ARG:HB3	1.33	0.94
2:B:132:GLU:HA	2:B:138:PHE:HA	1.49	0.94
1:A:111:LEU:HD12	1:A:112:VAL:N	1.82	0.94
1:C:170:ASN:HB2	1:C:176:LYS:HE2	1.50	0.94
2:F:121:LYS:HZ1	2:F:122:THR:CG2	1.80	0.94
3:L:141:TYR:HB3	3:L:142:PRO:HD3	1.49	0.94
3:L:164:TRP:HE3	3:L:164:TRP:H	0.97	0.93
1:C:28:THR:HG22	2:D:104:ASN:HB3	1.48	0.93
1:C:13:LEU:HD11	2:D:24:PHE:HB3	1.48	0.93
4:H:63:SER:O	4:H:64:LEU:HG	1.68	0.93
3:L:201:THR:HG23	3:L:202:SER:N	1.83	0.93
1:A:54:ASN:HD22	1:A:55:PRO:HA	1.31	0.93
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.51	0.93
1:E:108:LEU:O	1:E:112:VAL:HG23	1.69	0.93
3:L:95:PHE:CZ	4:H:60:TYR:HB3	2.04	0.93
3:U:199:HIS:CD2	3:U:200:LYS:H	1.85	0.92
2:B:145:ASP:H	2:B:148:CYS:HB3	1.33	0.92
2:F:55:VAL:HG12	2:F:56:ILE:N	1.82	0.92
1:A:170:ASN:HB2	1:A:176:LYS:HE2	1.51	0.92
2:D:3:PHE:CD2	2:D:113:SER:HA	2.03	0.92
4:H:126:PRO:HB3	4:H:152:TYR:HB3	1.48	0.92
1:A:321:ARG:HG2	1:A:322:ASN:H	1.33	0.92
1:A:172:ASP:HB3	1:A:174:PHE:CE2	2.05	0.91
3:U:137:LEU:HD23	3:U:145:ILE:CD1	2.01	0.91
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.05	0.91
4:H:52:ILE:HG23	4:H:52:ILE:O	1.67	0.91
4:H:191:PRO:HB2	4:H:194:THR:HB	1.53	0.91
1:A:9:SER:O	2:B:143:LYS:HE3	1.71	0.91
2:F:126:LEU:O	2:F:126:LEU:HD12	1.71	0.91
1:C:283:THR:HG22	1:C:287:SER:H	1.35	0.91
2:F:125:GLN:HE22	2:F:155:GLY:HA2	1.34	0.91
1:E:13:LEU:HD11	2:F:24:PHE:HB3	1.54	0.90
2:D:167:LEU:O	2:D:170:ARG:HB2	1.72	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:283:THR:HG23	1:A:286:GLY:N	1.86	0.90
1:A:283:THR:HG23	1:A:286:GLY:H	1.35	0.90
1:E:72:GLY:HA3	1:E:149:SER:OG	1.70	0.90
1:C:186:SER:HA	1:C:218:GLY:O	1.72	0.90
4:H:195:TRP:HB3	4:H:196:PRO:HD3	1.53	0.89
4:T:24:VAL:HG13	4:T:77:ASN:OD1	1.72	0.89
1:A:74:PRO:HG3	1:A:139:CYS:SG	2.11	0.89
1:E:18:HIS:HA	2:F:14:TRP:HB2	1.54	0.89
2:D:127:ARG:HH11	2:D:127:ARG:HB3	1.36	0.89
2:F:17:MET:HE1	2:F:19:ASP:H	1.37	0.89
1:A:84:TRP:CZ2	1:A:116:GLY:HA2	2.07	0.89
4:T:18:LEU:HD12	4:T:19:SER:H	1.31	0.88
2:B:127:ARG:HH11	2:B:127:ARG:HB3	1.37	0.88
2:F:127:ARG:NH1	2:F:127:ARG:HB3	1.89	0.88
2:D:48:ILE:HD11	2:D:107:THR:HG23	1.54	0.88
1:C:96:ASN:ND2	1:C:140:LYS:HE2	1.88	0.88
2:F:3:PHE:CD2	2:F:113:SER:HA	2.08	0.87
3:L:151:ILE:O	3:L:192:SER:HB2	1.72	0.87
2:F:121:LYS:HZ1	2:F:122:THR:HG22	1.37	0.87
1:C:172:ASP:HB3	1:C:174:PHE:CE2	2.09	0.87
1:E:74:PRO:HD3	1:E:97:CYS:HB2	1.56	0.87
3:L:134:VAL:HG22	3:L:179:THR:HG23	1.57	0.87
1:A:17:HIS:HD2	2:B:6:ILE:HG23	1.40	0.87
4:H:63:SER:C	4:H:64:LEU:HG	1.95	0.87
3:U:121:PRO:HB2	3:U:126:LEU:HD21	1.55	0.87
4:H:34:TYR:CD2	4:H:53:SER:HB3	2.09	0.87
3:U:97:ARG:HB2	4:T:48:TRP:CD2	2.10	0.87
4:H:1:ASP:O	4:H:2:VAL:HG22	1.73	0.86
3:L:201:THR:CG2	3:L:202:SER:H	1.88	0.86
4:H:142:MET:HA	4:H:192:SER:HA	1.58	0.86
2:B:127:ARG:NH1	2:B:127:ARG:HB3	1.89	0.86
4:H:32:GLY:O	4:H:33:TYR:HB2	1.75	0.86
2:B:28:ASN:HD22	2:B:145:ASP:CA	1.88	0.86
4:H:18:LEU:HD12	4:H:19:SER:H	1.38	0.86
2:D:165:GLU:HA	2:D:168:ASN:HD21	1.39	0.86
3:L:48:TRP:O	3:L:49:ILE:HG13	1.75	0.86
3:L:151:ILE:HG22	3:L:152:ASP:H	1.37	0.86
1:E:321:ARG:HG2	1:E:322:ASN:N	1.90	0.85
2:F:165:GLU:HA	2:F:168:ASN:HD21	1.37	0.85
4:H:56:GLY:O	4:H:58:ASN:N	2.09	0.85
1:E:307:LYS:HE2	2:F:60:ASN:ND2	1.90	0.85
4:H:131:LEU:HB2	4:H:146:GLY:HA3	1.59	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:132:GLU:HA	2:F:138:PHE:HA	1.56	0.85
4:H:151:GLY:C	4:H:181:LEU:HD12	1.97	0.85
4:T:206:HIS:CE1	4:T:208:ALA:HB3	2.11	0.85
3:L:40:LYS:HD3	3:L:85:ALA:HB2	1.59	0.85
3:U:47:LEU:HD12	3:U:48:TRP:H	1.40	0.85
1:C:108:LEU:HD13	1:C:234:TRP:CE3	2.12	0.85
1:C:283:THR:HG23	1:C:286:GLY:N	1.92	0.84
3:L:97:ARG:HB2	4:H:48:TRP:CD2	2.11	0.84
1:C:64:CYS:HB2	1:C:79:PHE:CE1	2.11	0.84
2:D:100:VAL:HG23	2:D:101:ALA:H	1.42	0.84
1:A:28:THR:HB	2:B:105:GLN:HB2	1.58	0.84
1:A:176:LYS:HD2	1:A:257:TYR:CD2	2.13	0.84
2:F:28:ASN:HD22	2:F:145:ASP:CA	1.91	0.84
1:A:309:VAL:HG12	2:B:93:SER:HA	1.60	0.84
1:A:74:PRO:HD3	1:A:97:CYS:HB2	1.59	0.83
3:U:201:THR:HG23	3:U:202:SER:H	1.43	0.83
1:C:283:THR:HG23	1:C:286:GLY:H	1.38	0.83
1:E:17:HIS:HD2	2:F:6:ILE:HG23	1.43	0.83
1:E:77:ASP:O	1:E:80:GLN:HG2	1.78	0.83
1:A:11:ALA:O	2:B:140:ILE:HB	1.78	0.83
1:A:207:ARG:HG2	1:E:223:VAL:HG22	1.60	0.83
1:C:98:TYR:H	1:C:139:CYS:HB2	1.44	0.83
2:F:165:GLU:HA	2:F:168:ASN:ND2	1.93	0.83
1:A:13:LEU:HD11	2:B:24:PHE:HB3	1.58	0.83
4:T:142:MET:HA	4:T:192:SER:HA	1.59	0.83
1:C:81:ASN:ND2	1:C:120:PHE:H	1.76	0.83
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.59	0.83
3:L:9:ALA:N	3:L:103:THR:HG23	1.92	0.83
1:C:81:ASN:HD21	1:C:120:PHE:H	1.27	0.83
1:C:74:PRO:HD3	1:C:97:CYS:HB2	1.61	0.82
4:T:190:VAL:HG21	4:T:195:TRP:HB2	1.60	0.82
1:E:98:TYR:H	1:E:139:CYS:HB2	1.44	0.82
2:D:80:LEU:HD21	2:F:80:LEU:HD21	1.60	0.82
1:E:170:ASN:ND2	1:E:239:PRO:HA	1.94	0.82
2:D:28:ASN:HD22	2:D:145:ASP:CA	1.92	0.82
1:E:73:ASP:OD1	1:E:74:PRO:HD2	1.79	0.82
1:C:84:TRP:CZ2	1:C:116:GLY:HA2	2.14	0.82
1:E:74:PRO:HA	1:E:141:ARG:HH12	1.44	0.82
2:D:125:GLN:HE22	2:D:155:GLY:HA2	1.43	0.82
2:B:100:VAL:HG23	2:B:101:ALA:H	1.42	0.82
3:U:194:THR:HA	3:U:209:SER:HB2	1.59	0.82
3:L:164:TRP:N	3:L:164:TRP:CE3	2.47	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22:ASN:HD22	1:A:22:ASN:N	1.76	0.81
4:T:63:SER:O	4:T:64:LEU:HG	1.80	0.81
2:D:171:PHE:HD2	2:F:167:LEU:HB3	1.43	0.81
4:H:162:ASN:ND2	4:H:201:THR:H	1.78	0.81
2:D:131:GLU:O	2:D:139:LYS:HB3	1.78	0.81
1:A:54:ASN:ND2	1:A:55:PRO:HA	1.94	0.81
3:L:9:ALA:H	3:L:103:THR:HG23	1.43	0.81
3:L:148:LYS:HD2	3:L:155:GLU:O	1.81	0.81
4:T:28:SER:O	4:T:30:THR:N	2.13	0.81
4:T:53:SER:OG	4:T:55:ASP:HB2	1.80	0.81
3:L:164:TRP:N	3:L:164:TRP:HE3	1.78	0.81
1:E:108:LEU:HD13	1:E:234:TRP:CE3	2.16	0.81
3:U:151:ILE:HG12	3:U:193:TYR:CD2	2.15	0.81
4:H:122:LYS:HD3	4:H:123:THR:O	1.80	0.81
1:C:307:LYS:HE2	2:D:60:ASN:ND2	1.96	0.81
4:T:65:LYS:O	4:T:67:ARG:N	2.14	0.81
2:F:130:ALA:HB1	2:F:139:LYS:O	1.80	0.80
2:F:166:ALA:N	2:F:168:ASN:HD21	1.80	0.80
3:U:95:PHE:CE2	4:T:60:TYR:HB3	2.16	0.80
4:H:29:ILE:HG22	4:H:35:TRP:CE2	2.17	0.80
4:T:61:ASN:HB3	4:T:62:PRO:HD2	1.62	0.80
2:B:145:ASP:O	2:B:149:ILE:HG12	1.80	0.80
1:C:22:ASN:N	1:C:22:ASN:HD22	1.79	0.80
4:T:131:LEU:HB2	4:T:146:GLY:HA3	1.64	0.80
1:A:220:ARG:HH21	1:C:210:GLN:NE2	1.79	0.80
4:H:188:VAL:HG22	4:H:189:THR:N	1.97	0.80
4:T:86:VAL:HG23	4:T:90:ASP:HB2	1.63	0.80
1:A:237:VAL:HG12	1:A:241:ASP:HB3	1.64	0.80
3:U:141:TYR:HB3	3:U:142:PRO:HD3	1.62	0.80
1:C:42:LEU:O	1:C:293:PRO:HD2	1.80	0.79
4:T:81:LEU:HD12	4:T:82:LYS:H	1.46	0.79
4:T:218:VAL:CG1	4:T:219:PRO:HD2	2.11	0.79
3:U:118:ILE:HD13	3:U:195:CYS:HB2	1.63	0.79
2:F:121:LYS:HZ3	2:F:121:LYS:HB3	1.45	0.79
3:L:95:PHE:HZ	4:H:60:TYR:HB3	1.46	0.79
1:A:72:GLY:HA3	1:A:149:SER:OG	1.82	0.79
3:U:164:TRP:N	3:U:164:TRP:CE3	2.49	0.79
3:U:29:ILE:HD11	3:U:34:LEU:HB2	1.63	0.79
1:A:98:TYR:H	1:A:139:CYS:HB2	1.48	0.79
4:T:52:ILE:O	4:T:52:ILE:HG23	1.82	0.79
3:L:19:VAL:HG21	3:L:79:LEU:HD23	1.64	0.79
4:T:151:GLY:C	4:T:181:LEU:HD12	2.03	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:T:2:VAL:CG2	4:T:27:TYR:HB2	2.12	0.79
1:A:22:ASN:ND2	1:A:22:ASN:H	1.76	0.79
1:E:9:SER:O	2:F:143:LYS:HE3	1.82	0.79
1:C:22:ASN:H	1:C:22:ASN:ND2	1.77	0.79
4:H:24:VAL:HG13	4:H:77:ASN:OD1	1.83	0.79
1:A:96:ASN:HD21	1:A:140:LYS:HE2	1.48	0.79
2:F:110:LEU:HD13	2:F:110:LEU:O	1.82	0.79
1:E:11:ALA:O	2:F:140:ILE:HB	1.83	0.79
4:T:64:LEU:HD23	4:T:66:ASN:HD21	1.48	0.79
4:T:33:TYR:HD2	4:T:99:PHE:O	1.65	0.78
2:D:145:ASP:H	2:D:148:CYS:HB3	1.47	0.78
1:C:182:ILE:O	1:C:230:ILE:HG23	1.83	0.78
1:E:283:THR:HG23	1:E:286:GLY:N	1.96	0.78
3:U:14:SER:OG	3:U:108:LYS:HD2	1.84	0.78
2:B:167:LEU:HB3	2:F:171:PHE:HD2	1.46	0.78
3:L:48:TRP:CE2	3:L:59:VAL:HG13	2.19	0.78
2:B:121:LYS:HZ1	2:B:122:THR:HG22	1.49	0.78
1:E:186:SER:HA	1:E:218:GLY:O	1.84	0.78
4:T:195:TRP:HB3	4:T:196:PRO:HD3	1.64	0.78
4:H:28:SER:O	4:H:30:THR:N	2.17	0.78
3:U:151:ILE:HG12	3:U:193:TYR:CE2	2.19	0.78
1:A:147:PHE:CE2	1:A:153:TRP:HB2	2.18	0.78
3:U:116:VAL:HG12	3:U:117:SER:N	1.99	0.78
2:B:125:GLN:HE22	2:B:155:GLY:HA2	1.49	0.78
1:C:320:MET:HA	2:D:111:THR:HG21	1.65	0.78
2:D:6:ILE:HG13	2:D:112:ASP:HA	1.66	0.78
3:U:201:THR:HG23	3:U:202:SER:N	1.98	0.77
2:D:165:GLU:HA	2:D:168:ASN:ND2	1.98	0.77
1:C:320:MET:CA	2:D:111:THR:HG21	2.14	0.77
2:F:28:ASN:HB2	2:F:144:CYS:O	1.82	0.77
4:T:142:MET:SD	4:T:191:PRO:HA	2.24	0.77
2:B:55:VAL:HG12	2:B:56:ILE:N	2.00	0.77
4:H:37:TRP:CZ3	4:H:96:CYS:HB3	2.18	0.77
1:E:96:ASN:ND2	1:E:140:LYS:HE2	1.98	0.77
2:F:121:LYS:NZ	2:F:122:THR:CG2	2.47	0.77
3:L:194:THR:HA	3:L:209:SER:HB2	1.64	0.77
3:U:113:ALA:HB2	3:U:201:THR:OG1	1.83	0.77
3:U:67:GLY:HA3	3:U:72:TYR:CD2	2.20	0.77
2:B:28:ASN:ND2	2:B:145:ASP:HA	1.96	0.77
2:F:6:ILE:HG13	2:F:112:ASP:HA	1.66	0.77
4:H:97:ALA:HB1	4:H:109:TYR:O	1.85	0.77
1:C:321:ARG:HG2	1:C:322:ASN:H	1.49	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:28:THR:HB	2:F:105:GLN:HB2	1.66	0.77
1:C:283:THR:CG2	1:C:286:GLY:H	1.97	0.77
2:F:129:ASN:ND2	2:F:159:HIS:HA	1.99	0.76
1:A:12:THR:HG23	2:B:138:PHE:O	1.86	0.76
3:U:164:TRP:N	3:U:164:TRP:HE3	1.81	0.76
3:U:14:SER:CA	3:U:108:LYS:HB2	2.14	0.76
1:E:170:ASN:HB2	1:E:176:LYS:HE2	1.66	0.76
3:L:137:LEU:HD23	3:L:145:ILE:HD13	1.67	0.76
3:U:107:ILE:H	3:U:167:GLN:HE22	1.31	0.76
1:C:73:ASP:OD1	1:C:74:PRO:HD2	1.85	0.76
2:B:167:LEU:HD12	2:B:172:GLN:OE1	1.85	0.76
2:D:127:ARG:NH1	2:D:127:ARG:HB3	1.99	0.76
3:U:184:LYS:O	3:U:188:GLU:HG3	1.85	0.76
1:A:312:ASN:H	1:A:312:ASN:HD22	1.33	0.76
1:C:201:ARG:HG2	1:C:201:ARG:HH11	1.51	0.76
1:C:29:ILE:HD13	2:D:101:ALA:HB1	1.67	0.76
1:C:9:SER:O	2:D:143:LYS:HE3	1.85	0.76
2:D:149:ILE:C	2:D:151:SER:H	1.86	0.76
1:C:87:PHE:HB3	1:C:267:ILE:HG13	1.67	0.76
4:H:28:SER:C	4:H:30:THR:H	1.88	0.76
2:F:100:VAL:HG23	2:F:101:ALA:H	1.49	0.76
4:H:37:TRP:HB3	4:H:49:MET:HE3	1.68	0.76
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.20	0.76
1:A:47:SER:HB2	1:A:288:ILE:HG22	1.67	0.76
1:E:28:THR:CG2	2:F:104:ASN:HB3	2.11	0.76
2:D:28:ASN:ND2	2:D:145:ASP:HA	1.99	0.76
1:C:36:VAL:HG23	1:C:320:MET:O	1.86	0.76
2:D:130:ALA:HB1	2:D:139:LYS:O	1.85	0.76
1:E:141:ARG:HH11	1:E:141:ARG:HG3	1.50	0.76
1:A:172:ASP:HB3	1:A:174:PHE:HE2	1.49	0.76
3:U:48:TRP:CE2	3:U:59:VAL:HG13	2.21	0.76
3:U:122:SER:O	3:U:126:LEU:HG	1.87	0.75
2:F:121:LYS:NZ	2:F:122:THR:HG22	2.01	0.75
2:F:170:ARG:HB3	2:F:171:PHE:HD1	1.52	0.75
1:A:81:ASN:ND2	1:A:120:PHE:H	1.85	0.75
4:H:121:ALA:HB3	4:H:153:PHE:CE2	2.22	0.75
4:H:32:GLY:HA2	4:H:54:TYR:CD2	2.22	0.75
1:E:64:CYS:HB2	1:E:79:PHE:CE1	2.22	0.75
4:H:88:ALA:O	4:H:91:THR:HG22	1.85	0.75
3:L:141:TYR:HB3	3:L:142:PRO:CD	2.16	0.75
2:B:80:LEU:HD21	2:F:80:LEU:HD21	1.68	0.75
1:A:160:THR:HA	1:A:196:VAL:HG21	1.68	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:170:VAL:HG12	4:H:188:VAL:HA	1.68	0.74
1:C:80:GLN:O	1:C:82:GLU:N	2.21	0.74
1:C:74:PRO:CD	1:C:97:CYS:HB2	2.18	0.74
4:T:63:SER:C	4:T:64:LEU:HG	2.05	0.74
1:A:54:ASN:HB3	1:A:278:ILE:CD1	2.16	0.74
1:E:74:PRO:CD	1:E:97:CYS:HB2	2.15	0.74
2:D:28:ASN:HB2	2:D:144:CYS:O	1.88	0.74
1:A:25:LEU:HA	1:A:34:ILE:O	1.85	0.74
3:L:201:THR:CG2	3:L:202:SER:N	2.49	0.74
3:L:29:ILE:CD1	3:L:34:LEU:HB2	2.18	0.74
3:L:141:TYR:CB	3:L:142:PRO:HD3	2.17	0.74
3:U:148:LYS:HD2	3:U:155:GLU:O	1.87	0.74
1:C:246:ASN:C	1:C:246:ASN:HD22	1.90	0.74
2:D:121:LYS:HZ1	2:D:122:THR:HG22	1.51	0.74
3:U:125:GLN:HA	3:U:125:GLN:HE21	1.52	0.74
4:T:34:TYR:CD2	4:T:53:SER:HB3	2.22	0.74
1:C:313:THR:O	1:C:314:LEU:HD23	1.88	0.74
1:C:11:ALA:O	2:D:140:ILE:HB	1.87	0.74
4:T:191:PRO:HB2	4:T:194:THR:HB	1.67	0.74
3:U:29:ILE:HD11	3:U:34:LEU:HD12	1.70	0.74
1:A:47:SER:HB2	1:A:288:ILE:CG2	2.18	0.74
1:E:286:GLY:O	1:E:287:SER:HB2	1.87	0.74
2:D:149:ILE:O	2:D:151:SER:N	2.19	0.74
1:E:67:ILE:O	1:E:70:LEU:HB3	1.88	0.74
4:H:194:THR:O	4:H:194:THR:HG22	1.88	0.74
3:U:122:SER:HB3	3:U:125:GLN:HB3	1.68	0.74
1:C:10:THR:HG21	2:D:141:TYR:O	1.86	0.74
4:H:190:VAL:HG21	4:H:195:TRP:HB2	1.69	0.74
3:U:29:ILE:HD11	3:U:34:LEU:CD1	2.18	0.74
1:E:81:ASN:ND2	1:E:120:PHE:H	1.86	0.74
1:A:62:ILE:HG22	1:A:63:ASP:H	1.51	0.74
2:D:166:ALA:N	2:D:168:ASN:HD21	1.86	0.74
3:L:47:LEU:HD12	3:L:48:TRP:H	1.53	0.74
3:U:95:PHE:CZ	4:T:60:TYR:HB3	2.23	0.73
1:A:164:LEU:O	1:A:246:ASN:HA	1.87	0.73
1:A:73:ASP:OD1	1:A:74:PRO:HD2	1.88	0.73
3:U:14:SER:CB	3:U:108:LYS:HD2	2.19	0.73
1:E:29:ILE:HD13	2:F:101:ALA:HB1	1.68	0.73
1:A:293:PRO:O	1:A:294:PHE:HD2	1.71	0.73
2:F:149:ILE:O	2:F:151:SER:N	2.22	0.73
3:L:38:GLN:HG3	3:L:87:TYR:HE1	1.54	0.73
1:E:84:TRP:CE2	1:E:116:GLY:HA2	2.22	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:309:VAL:HG12	2:D:93:SER:HA	1.71	0.73
4:H:29:ILE:HG12	4:H:77:ASN:ND2	2.04	0.73
4:H:73:ASP:O	4:H:75:SER:N	2.22	0.73
2:B:117:LYS:HE3	2:F:4:GLY:HA2	1.69	0.73
2:B:28:ASN:HB2	2:B:144:CYS:O	1.87	0.73
2:B:17:MET:HE1	2:B:19:ASP:H	1.54	0.73
2:F:115:MET:O	2:F:117:LYS:N	2.22	0.73
1:E:17:HIS:ND1	1:E:18:HIS:N	2.37	0.73
2:F:165:GLU:CA	2:F:168:ASN:HD21	2.01	0.73
2:B:47:GLN:OE1	2:B:110:LEU:HD21	1.89	0.72
1:E:47:SER:HB2	1:E:288:ILE:CG2	2.19	0.72
2:D:154:ASN:HB3	2:D:156:THR:OG1	1.87	0.72
3:L:150:LYS:O	3:L:151:ILE:HB	1.88	0.72
3:U:118:ILE:HG21	3:U:209:SER:HA	1.71	0.72
1:A:311:GLN:HE22	2:B:93:SER:HB3	1.53	0.72
3:L:36:TRP:HB2	3:L:49:ILE:HD12	1.70	0.72
1:C:17:HIS:HD2	2:D:6:ILE:HG23	1.54	0.72
3:U:141:TYR:HB3	3:U:142:PRO:CD	2.18	0.72
4:T:29:ILE:HG22	4:T:35:TRP:CE2	2.24	0.72
4:T:170:VAL:HG12	4:T:188:VAL:HA	1.69	0.72
4:H:37:TRP:HB3	4:H:49:MET:CE	2.20	0.72
3:L:13:ALA:O	3:L:108:LYS:HG3	1.90	0.72
1:E:22:ASN:H	1:E:22:ASN:HD22	1.36	0.72
2:D:131:GLU:HB2	2:F:127:ARG:HH21	1.52	0.72
2:D:28:ASN:HD21	2:D:30:GLU:HB2	1.55	0.72
4:H:100:TYR:O	4:H:101:TYR:HB3	1.90	0.72
1:A:81:ASN:HD21	1:A:120:PHE:H	1.34	0.72
3:L:51:SER:HB2	3:L:54:ASN:OD1	1.89	0.72
2:D:170:ARG:HB3	2:D:171:PHE:HD1	1.53	0.72
1:C:283:THR:CG2	1:C:286:GLY:N	2.53	0.72
4:T:177:LEU:HB2	4:T:182:TYR:CE1	2.24	0.72
4:T:48:TRP:CZ2	4:T:50:GLY:HA2	2.25	0.72
3:U:51:SER:HB2	3:U:54:ASN:OD1	1.90	0.72
1:A:210:GLN:NE2	1:E:220:ARG:HH21	1.86	0.72
1:E:294:PHE:CE1	2:F:96:ALA:HB1	2.24	0.72
3:U:47:LEU:HD12	3:U:48:TRP:N	2.04	0.72
4:H:86:VAL:HG23	4:H:90:ASP:HB2	1.72	0.72
2:D:171:PHE:CD2	2:F:167:LEU:HB3	2.24	0.72
1:C:87:PHE:O	1:C:267:ILE:HA	1.90	0.72
3:U:183:THR:OG1	3:U:186:GLU:HB2	1.90	0.72
2:F:115:MET:C	2:F:117:LYS:H	1.93	0.71
2:F:89:ILE:HD12	2:F:89:ILE:H	1.53	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:T:206:HIS:HD2	4:T:209:SER:OG	1.72	0.71
1:E:160:THR:HA	1:E:196:VAL:HG21	1.73	0.71
2:D:106:HIS:ND1	2:D:106:HIS:O	2.24	0.71
1:E:202:VAL:O	1:E:212:THR:HG23	1.91	0.71
3:L:151:ILE:HG12	3:L:193:TYR:CE2	2.26	0.71
4:T:180:ASP:O	4:T:181:LEU:HD22	1.90	0.71
3:L:125:GLN:HE21	3:L:125:GLN:HA	1.56	0.71
2:B:166:ALA:N	2:B:168:ASN:HD21	1.87	0.71
3:L:126:LEU:O	3:L:128:SER:N	2.24	0.71
1:C:170:ASN:ND2	1:C:239:PRO:HA	2.05	0.71
4:H:54:TYR:O	4:H:56:GLY:N	2.24	0.71
3:U:141:TYR:CB	3:U:142:PRO:HD3	2.21	0.71
2:B:2:LEU:HB2	2:B:109:ASP:OD1	1.91	0.71
2:D:141:TYR:CZ	2:D:170:ARG:HG2	2.26	0.71
3:U:29:ILE:CD1	3:U:34:LEU:HB2	2.20	0.71
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.72	0.71
2:F:10:ILE:O	2:F:12:ASN:N	2.23	0.71
1:C:50:LYS:O	1:C:286:GLY:O	2.09	0.71
1:E:172:ASP:HB3	1:E:174:PHE:CE2	2.26	0.71
4:T:131:LEU:HG	4:T:147:CYS:H	1.55	0.70
1:E:10:THR:HG21	2:F:141:TYR:C	2.12	0.70
4:H:29:ILE:H	4:H:77:ASN:HD21	1.37	0.70
1:A:172:ASP:CB	1:A:174:PHE:CE2	2.74	0.70
3:U:211:ASN:O	3:U:212:ARG:HG2	1.89	0.70
2:B:166:ALA:H	2:B:168:ASN:HD21	1.38	0.70
2:F:111:THR:C	2:F:113:SER:H	1.93	0.70
2:D:84:VAL:HG12	2:D:85:GLU:N	2.06	0.70
2:D:141:TYR:CE2	2:D:170:ARG:HG2	2.26	0.70
1:E:191:GLN:O	1:E:194:LEU:N	2.24	0.70
1:E:295:GLN:OE1	1:E:297:VAL:HB	1.89	0.70
3:U:66:SER:OG	3:U:67:GLY:N	2.25	0.70
1:E:321:ARG:CG	1:E:322:ASN:H	1.96	0.70
1:A:321:ARG:HG2	1:A:322:ASN:N	2.04	0.70
3:U:14:SER:OG	3:U:17:GLU:OE2	2.09	0.70
2:D:4:GLY:HA2	2:F:117:LYS:HE3	1.74	0.70
3:L:151:ILE:HG12	3:L:193:TYR:CD2	2.27	0.70
4:T:161:TRP:CE2	4:T:188:VAL:HB	2.27	0.70
1:C:304:ALA:H	2:D:61:GLU:HG3	1.56	0.70
3:L:212:ARG:NH2	4:H:138:GLN:H	1.89	0.70
2:F:149:ILE:C	2:F:151:SER:H	1.93	0.70
3:L:199:HIS:HD2	3:L:200:LYS:H	1.37	0.70
3:L:21:LEU:HD21	3:L:87:TYR:CD2	2.27	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:PRO:CD	1:A:97:CYS:HB2	2.21	0.69
3:U:201:THR:CG2	3:U:202:SER:H	2.05	0.69
2:F:108:ILE:C	2:F:110:LEU:H	1.94	0.69
4:H:52:ILE:CG2	4:H:52:ILE:O	2.40	0.69
4:H:29:ILE:H	4:H:77:ASN:ND2	1.89	0.69
1:A:33:GLN:O	1:A:34:ILE:HG13	1.91	0.69
4:H:33:TYR:HD2	4:H:99:PHE:O	1.74	0.69
3:L:97:ARG:HB2	4:H:48:TRP:CG	2.27	0.69
1:A:170:ASN:CB	1:A:176:LYS:HE2	2.22	0.69
1:C:25:LEU:HD22	1:C:33:GLN:OE1	1.90	0.69
1:C:35:GLU:O	1:C:322:ASN:HB3	1.93	0.69
4:H:126:PRO:HB3	4:H:152:TYR:CB	2.19	0.69
4:H:142:MET:SD	4:H:191:PRO:HA	2.32	0.69
4:T:53:SER:H	4:T:58:ASN:HD21	1.40	0.69
4:H:121:ALA:HB3	4:H:153:PHE:CZ	2.27	0.69
1:A:206:THR:OG1	1:A:209:SER:HB3	1.93	0.69
1:E:217:ILE:HD12	1:E:217:ILE:N	2.08	0.69
2:F:129:ASN:HD21	2:F:159:HIS:HA	1.58	0.69
4:T:188:VAL:HG22	4:T:189:THR:N	2.07	0.69
4:T:13:LYS:O	4:T:16:GLN:HG3	1.93	0.69
3:L:167:GLN:HE21	3:L:172:SER:HB3	1.58	0.69
2:D:166:ALA:H	2:D:168:ASN:HD21	1.40	0.69
2:F:96:ALA:O	2:F:98:LEU:N	2.25	0.69
3:L:95:PHE:CE2	4:H:60:TYR:HB3	2.27	0.69
1:E:59:LEU:HD21	1:E:82:GLU:HG3	1.75	0.69
3:U:8:PRO:HG2	3:U:11:MET:HE3	1.74	0.69
1:A:10:THR:HG22	2:B:143:LYS:HD2	1.75	0.69
1:C:28:THR:HB	2:D:105:GLN:HB2	1.74	0.69
1:C:47:SER:HB2	1:C:288:ILE:CG2	2.23	0.69
4:T:102:ASP:O	4:T:103:TYR:HB2	1.93	0.69
3:U:193:TYR:O	3:U:209:SER:OG	2.10	0.69
3:L:118:ILE:HD13	3:L:195:CYS:HB2	1.74	0.69
2:F:48:ILE:HD11	2:F:107:THR:HG23	1.73	0.68
3:L:151:ILE:CG2	3:L:152:ASP:N	2.50	0.68
3:L:48:TRP:C	3:L:49:ILE:HG13	2.13	0.68
2:D:80:LEU:HD21	2:F:80:LEU:CD2	2.22	0.68
3:U:106:GLU:HA	3:U:167:GLN:OE1	1.93	0.68
1:C:54:ASN:HD22	1:C:55:PRO:HA	1.56	0.68
4:T:28:SER:C	4:T:30:THR:H	1.95	0.68
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.75	0.68
1:E:206:THR:HB	1:E:241:ASP:OD1	1.93	0.68
1:A:29:ILE:HD13	2:B:101:ALA:HB1	1.76	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:PHE:CE1	2:B:96:ALA:HB1	2.28	0.68
4:T:29:ILE:H	4:T:77:ASN:ND2	1.92	0.68
1:A:216:ASN:HB3	1:C:212:THR:CG2	2.21	0.68
4:T:195:TRP:O	4:T:196:PRO:C	2.31	0.68
4:T:195:TRP:HZ2	4:T:217:ILE:HG22	1.57	0.68
3:U:48:TRP:O	3:U:49:ILE:HG13	1.91	0.68
3:U:141:TYR:CG	3:U:142:PRO:HD3	2.29	0.68
2:B:100:VAL:O	2:B:104:ASN:HB2	1.94	0.68
1:E:12:THR:HB	2:F:27:GLN:HB3	1.73	0.68
1:C:18:HIS:O	1:C:19:ALA:HB2	1.93	0.68
1:C:12:THR:HB	2:D:27:GLN:HB3	1.75	0.68
4:H:58:ASN:O	4:H:60:TYR:N	2.22	0.68
4:H:131:LEU:HB2	4:H:146:GLY:CA	2.23	0.68
2:B:131:GLU:O	2:B:139:LYS:HB3	1.92	0.68
4:H:58:ASN:HB2	4:H:60:TYR:CE2	2.29	0.68
3:U:48:TRP:C	3:U:49:ILE:HG13	2.13	0.68
1:E:191:GLN:OE1	1:E:195:TYR:HD1	1.77	0.68
1:A:298:ASN:HD22	1:A:299:LYS:N	1.92	0.68
1:C:295:GLN:OE1	1:C:297:VAL:HB	1.93	0.68
1:C:29:ILE:HD11	2:D:102:LEU:CD2	2.21	0.68
2:B:124:ARG:HH21	2:F:132:GLU:HB3	1.59	0.68
4:H:195:TRP:HH2	4:H:219:PRO:HA	1.58	0.68
4:T:184:LEU:HD12	4:T:185:SER:N	2.07	0.68
1:C:176:LYS:HE3	1:C:178:TYR:OH	1.94	0.68
3:L:167:GLN:NE2	3:L:172:SER:HB3	2.09	0.68
1:A:189:GLN:O	1:A:193:SER:OG	2.09	0.68
4:H:86:VAL:HG23	4:H:90:ASP:CB	2.25	0.67
2:B:108:ILE:C	2:B:110:LEU:H	1.96	0.67
1:A:252:ILE:HG22	1:A:252:ILE:O	1.92	0.67
2:B:78:GLN:O	2:B:79:ASP:C	2.32	0.67
2:B:171:PHE:HZ	2:F:171:PHE:CE2	2.13	0.67
1:C:61:GLY:O	1:C:79:PHE:CZ	2.48	0.67
2:F:166:ALA:H	2:F:168:ASN:HD21	1.40	0.67
1:E:311:GLN:HE22	2:F:93:SER:HB3	1.59	0.67
3:L:199:HIS:CD2	3:L:200:LYS:N	2.59	0.67
4:H:13:LYS:HG3	4:H:120:SER:HA	1.76	0.67
1:C:98:TYR:HE2	1:C:229:ARG:HA	1.59	0.67
3:U:13:ALA:O	3:U:108:LYS:N	2.28	0.67
4:H:56:GLY:C	4:H:58:ASN:H	1.98	0.67
4:T:51:TYR:HD1	4:T:52:ILE:N	1.92	0.67
1:C:10:THR:HG22	2:D:143:LYS:HD2	1.77	0.67
1:C:36:VAL:HG22	1:C:37:THR:N	2.10	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:ASN:CB	1:A:278:ILE:HD13	2.19	0.67
3:U:35:TYR:HD2	3:U:50:TYR:HA	1.60	0.67
2:B:23:GLY:HA3	2:B:35:ALA:O	1.93	0.67
2:D:23:GLY:HA3	2:D:35:ALA:O	1.95	0.67
1:E:37:THR:HG23	1:E:320:MET:O	1.95	0.67
4:H:61:ASN:HB3	4:H:62:PRO:HD2	1.77	0.67
1:A:319:GLY:HA2	2:B:21:TRP:HH2	1.60	0.67
1:E:91:SER:C	1:E:93:ALA:H	1.97	0.67
3:U:126:LEU:C	3:U:128:SER:H	1.96	0.67
2:D:115:MET:O	2:D:117:LYS:N	2.27	0.67
2:D:126:LEU:O	2:D:126:LEU:HD12	1.95	0.67
1:C:12:THR:HG23	2:D:138:PHE:O	1.96	0.67
1:A:41:GLU:HG3	1:A:43:VAL:H	1.61	0.66
2:B:3:PHE:HB2	2:B:112:ASP:O	1.94	0.66
4:T:86:VAL:HG23	4:T:90:ASP:CB	2.25	0.66
3:U:32:SER:O	3:U:33:PHE:CD1	2.48	0.66
1:E:10:THR:HG21	2:F:141:TYR:O	1.95	0.66
4:T:162:ASN:ND2	4:T:201:THR:H	1.93	0.66
1:A:77:ASP:O	1:A:80:GLN:CG	2.43	0.66
1:E:319:GLY:HA2	2:F:21:TRP:HH2	1.59	0.66
3:U:168:ASP:OD1	3:U:171:ASP:HB2	1.96	0.66
1:E:294:PHE:HB3	1:E:309:VAL:HG21	1.77	0.66
1:E:121:ILE:HG13	1:E:257:TYR:CZ	2.30	0.66
3:L:30:THR:O	3:L:32:SER:N	2.28	0.66
1:A:310:LYS:HG3	2:B:93:SER:OG	1.94	0.66
1:C:47:SER:HB2	1:C:288:ILE:HG22	1.78	0.66
2:D:127:ARG:HG3	2:D:159:HIS:CG	2.31	0.66
3:U:119:PHE:CD2	4:T:131:LEU:HB3	2.30	0.66
1:A:303:GLY:O	1:A:305:CYS:SG	2.53	0.66
1:E:102:VAL:HG22	1:E:232:ILE:CB	2.23	0.66
2:D:28:ASN:ND2	2:D:30:GLU:HB2	2.11	0.66
3:U:147:VAL:HA	3:U:196:GLU:O	1.96	0.66
3:U:151:ILE:O	3:U:192:SER:HB2	1.96	0.66
3:U:212:ARG:HA	3:U:212:ARG:HE	1.61	0.66
4:H:188:VAL:CG2	4:H:189:THR:N	2.58	0.66
3:L:116:VAL:HG12	3:L:117:SER:N	2.10	0.66
1:E:125:PHE:HB2	1:E:127:TRP:NE1	2.10	0.66
3:U:8:PRO:O	3:U:10:ILE:N	2.27	0.66
1:C:90:ARG:NH1	1:C:270:SER:O	2.29	0.66
1:C:77:ASP:O	1:C:80:GLN:CG	2.36	0.66
1:E:140:LYS:HD2	1:E:140:LYS:O	1.96	0.66
4:H:162:ASN:HD21	4:H:201:THR:H	1.41	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:68:LYS:HE2	2:D:85:GLU:CD	2.16	0.66
2:B:25:ARG:CG	2:B:34:GLN:HG2	2.20	0.66
4:H:51:TYR:HD1	4:H:52:ILE:N	1.94	0.66
4:T:61:ASN:HB3	4:T:62:PRO:CD	2.26	0.66
3:U:175:SER:HG	4:T:171:HIS:CE1	2.14	0.66
1:A:36:VAL:HG23	1:A:320:MET:O	1.96	0.66
2:B:170:ARG:HB3	2:B:171:PHE:HD1	1.59	0.66
1:C:283:THR:HG22	1:C:287:SER:N	2.10	0.66
4:T:14:PRO:O	4:T:15:SER:CB	2.43	0.66
4:H:65:LYS:O	4:H:67:ARG:N	2.28	0.66
2:B:6:ILE:HG13	2:B:112:ASP:HA	1.77	0.66
2:B:51:LYS:O	2:B:54:ARG:HB2	1.96	0.66
2:B:149:ILE:C	2:B:151:SER:H	2.00	0.66
4:T:13:LYS:HG3	4:T:120:SER:HA	1.78	0.66
1:A:140:LYS:N	1:A:140:LYS:HD2	2.10	0.66
2:F:28:ASN:ND2	2:F:145:ASP:HA	2.02	0.65
1:E:141:ARG:HG3	1:E:141:ARG:NH1	2.08	0.65
3:U:141:TYR:CB	3:U:142:PRO:CD	2.73	0.65
2:B:121:LYS:HZ1	2:B:122:THR:CG2	2.09	0.65
4:H:11:LEU:O	4:H:12:VAL:HG13	1.96	0.65
4:T:150:LYS:CB	4:T:183:THR:HG23	2.27	0.65
1:E:47:SER:HB2	1:E:288:ILE:HG22	1.78	0.65
3:L:38:GLN:HG3	3:L:87:TYR:CE1	2.30	0.65
1:C:318:THR:O	2:D:48:ILE:HG12	1.96	0.65
3:U:19:VAL:HG21	3:U:79:LEU:HD23	1.78	0.65
1:A:18:HIS:O	1:A:19:ALA:HB2	1.96	0.65
2:F:126:LEU:HA	2:F:159:HIS:HB3	1.77	0.65
4:H:18:LEU:HD22	4:H:116:LEU:CD1	2.27	0.65
4:T:131:LEU:HB2	4:T:146:GLY:CA	2.26	0.65
4:H:195:TRP:CH2	4:H:219:PRO:HA	2.31	0.65
3:U:163:SER:HB2	4:T:174:PRO:HD2	1.77	0.65
3:L:32:SER:HA	3:L:51:SER:HA	1.79	0.65
2:D:108:ILE:C	2:D:110:LEU:H	1.99	0.65
2:D:48:ILE:HD11	2:D:107:THR:CG2	2.27	0.65
4:T:6:GLU:OE1	4:T:95:TYR:HA	1.96	0.65
2:B:121:LYS:HZ3	2:B:122:THR:N	1.94	0.65
2:F:44:ALA:HB2	2:F:114:GLU:HG3	1.77	0.65
1:A:17:HIS:ND1	1:A:18:HIS:N	2.44	0.65
2:B:39:LYS:O	2:B:43:ALA:HB2	1.97	0.65
4:H:54:TYR:C	4:H:56:GLY:H	2.00	0.65
4:H:195:TRP:CZ2	4:H:219:PRO:HG3	2.31	0.65
2:B:141:TYR:CE2	2:B:170:ARG:HG2	2.32	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:118:ILE:HD11	3:U:149:TRP:CH2	2.32	0.65
3:L:91:GLN:HE21	3:L:93:GLU:HB3	1.62	0.65
1:A:59:LEU:HD12	1:A:60:ASP:N	2.12	0.65
3:U:199:HIS:HD2	3:U:200:LYS:H	1.38	0.65
1:C:41:GLU:HG3	1:C:43:VAL:H	1.61	0.65
4:T:148:LEU:HD23	4:T:148:LEU:O	1.97	0.65
3:U:125:GLN:CA	3:U:125:GLN:HE21	2.07	0.65
3:U:151:ILE:HG22	3:U:152:ASP:N	2.12	0.65
4:H:13:LYS:HB2	4:H:16:GLN:OE1	1.97	0.65
1:C:74:PRO:HG3	1:C:139:CYS:SG	2.37	0.64
1:E:294:PHE:HB3	1:E:309:VAL:CG2	2.27	0.64
4:T:100:TYR:O	4:T:101:TYR:HB3	1.96	0.64
1:C:111:LEU:HD12	1:C:112:VAL:N	2.11	0.64
1:A:293:PRO:O	1:A:294:PHE:CD2	2.51	0.64
1:A:9:SER:C	2:B:143:LYS:HE3	2.18	0.64
1:C:169:PRO:CA	1:C:242:VAL:HG23	2.27	0.64
1:E:54:ASN:HB3	1:E:278:ILE:HD13	1.79	0.64
4:H:80:PHE:N	4:H:80:PHE:CD2	2.65	0.64
3:U:116:VAL:HG12	3:U:117:SER:H	1.61	0.64
1:A:294:PHE:CE1	2:B:96:ALA:CB	2.80	0.64
4:T:206:HIS:NE2	4:T:208:ALA:HB3	2.13	0.64
3:L:8:PRO:HG2	3:L:11:MET:CE	2.28	0.64
3:U:151:ILE:HA	3:U:192:SER:O	1.98	0.64
1:E:187:THR:C	1:E:189:GLN:H	2.00	0.64
1:A:74:PRO:CG	1:A:139:CYS:SG	2.84	0.64
1:C:18:HIS:HA	2:D:14:TRP:CB	2.24	0.64
3:L:29:ILE:HD12	3:L:34:LEU:HB2	1.79	0.64
4:H:53:SER:OG	4:H:55:ASP:HB2	1.97	0.64
4:T:51:TYR:CD1	4:T:52:ILE:N	2.66	0.64
3:U:29:ILE:CD1	3:U:34:LEU:HD12	2.27	0.64
3:U:199:HIS:CD2	3:U:200:LYS:N	2.63	0.64
3:U:212:ARG:HG2	4:T:138:GLN:HE22	1.63	0.64
2:B:100:VAL:HG23	2:B:101:ALA:N	2.12	0.64
4:T:91:THR:OG1	4:T:117:THR:HA	1.97	0.64
1:A:216:ASN:ND2	1:C:212:THR:HB	2.12	0.64
4:T:67:ARG:HB3	4:T:84:ASN:HB2	1.80	0.64
4:T:2:VAL:HG21	4:T:27:TYR:HB2	1.78	0.64
4:T:177:LEU:HD12	4:T:181:LEU:O	1.98	0.64
3:L:141:TYR:CB	3:L:142:PRO:CD	2.75	0.64
4:T:56:GLY:C	4:T:58:ASN:H	2.01	0.64
3:U:149:TRP:O	3:U:154:SER:HB3	1.98	0.64
2:B:168:ASN:O	2:B:170:ARG:N	2.31	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:126:LEU:HA	2:D:159:HIS:HB3	1.80	0.64
2:D:165:GLU:CA	2:D:168:ASN:HD21	2.09	0.64
1:E:83:THR:O	1:E:84:TRP:HB3	1.97	0.64
1:E:13:LEU:O	2:F:138:PHE:N	2.29	0.63
5:C:451:NAG:H5	4:H:54:TYR:OH	1.97	0.63
1:C:61:GLY:O	1:C:79:PHE:HZ	1.81	0.63
2:D:39:LYS:O	2:D:43:ALA:HB2	1.98	0.63
3:U:133:VAL:HB	3:U:180:LEU:HB3	1.79	0.63
4:H:87:THR:O	4:H:118:VAL:HG11	1.97	0.63
1:A:318:THR:O	2:B:48:ILE:HG21	1.98	0.63
1:E:303:GLY:O	1:E:305:CYS:SG	2.56	0.63
1:C:117:THR:HG23	1:C:117:THR:O	1.98	0.63
1:A:29:ILE:CD1	2:B:102:LEU:HD23	2.26	0.63
2:B:165:GLU:HA	2:B:168:ASN:HD21	1.62	0.63
4:T:155:GLU:OE2	4:T:156:PRO:HA	1.97	0.63
1:A:141:ARG:O	1:A:143:PRO:HD2	1.99	0.63
2:B:111:THR:C	2:B:113:SER:H	2.01	0.63
2:B:126:LEU:HA	2:B:159:HIS:HB3	1.79	0.63
1:C:13:LEU:O	2:D:138:PHE:N	2.30	0.63
4:T:58:ASN:O	4:T:59:ASN:HB2	1.98	0.63
5:A:451:NAG:H61	1:E:222:TRP:CZ2	2.34	0.63
2:B:47:GLN:OE1	2:B:110:LEU:HD11	1.98	0.63
2:D:21:TRP:HB2	2:D:41:THR:HG23	1.80	0.63
2:F:128:GLU:HA	2:F:170:ARG:NH2	2.13	0.63
1:A:80:GLN:O	1:A:82:GLU:N	2.31	0.63
3:U:96:PRO:O	3:U:98:THR:HG23	1.98	0.63
3:L:19:VAL:CG2	3:L:79:LEU:HD23	2.29	0.63
4:H:87:THR:CG2	4:H:89:GLU:HB2	2.28	0.63
4:H:149:VAL:HB	4:H:184:LEU:HG	1.81	0.63
4:T:194:THR:HG22	4:T:194:THR:O	1.98	0.63
3:U:14:SER:HB3	3:U:108:LYS:HD2	1.80	0.63
1:A:119:GLU:OE2	1:A:259:LYS:HD2	1.98	0.63
4:H:13:LYS:O	4:H:16:GLN:HG3	1.99	0.63
1:A:13:LEU:O	2:B:138:PHE:N	2.26	0.63
4:H:18:LEU:CD2	4:H:116:LEU:HD13	2.29	0.63
3:U:9:ALA:H	3:U:103:THR:HG23	1.63	0.63
3:U:134:VAL:HG13	3:U:179:THR:OG1	1.99	0.63
2:D:170:ARG:HB3	2:D:171:PHE:CD1	2.34	0.63
4:T:120:SER:O	4:T:121:ALA:O	2.15	0.63
3:L:163:SER:HB2	4:H:174:PRO:HD2	1.81	0.63
2:D:129:ASN:O	2:D:130:ALA:HB2	1.98	0.63
1:A:108:LEU:HD13	1:A:234:TRP:CE3	2.33	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:184:HIS:O	1:C:228:SER:HB2	1.98	0.63
3:U:4:LEU:N	3:U:4:LEU:HD12	2.14	0.63
1:C:19:ALA:O	1:C:20:VAL:HG13	1.99	0.62
4:H:37:TRP:CB	4:H:49:MET:HE3	2.28	0.62
3:U:8:PRO:HG2	3:U:11:MET:CE	2.29	0.62
3:L:2:ILE:O	3:L:2:ILE:HG12	1.97	0.62
1:A:321:ARG:CG	1:A:322:ASN:H	2.10	0.62
1:C:30:THR:HG23	2:D:105:GLN:HE22	1.64	0.62
3:U:9:ALA:N	3:U:103:THR:HG23	2.14	0.62
1:E:62:ILE:HG22	1:E:63:ASP:H	1.64	0.62
3:L:125:GLN:HE21	3:L:125:GLN:CA	2.11	0.62
3:L:141:TYR:O	3:L:142:PRO:C	2.37	0.62
1:C:25:LEU:HD13	1:C:33:GLN:OE1	2.00	0.62
1:C:160:THR:HA	1:C:196:VAL:HG21	1.80	0.62
1:E:25:LEU:HD13	1:E:33:GLN:OE1	1.98	0.62
4:T:97:ALA:HB1	4:T:109:TYR:O	1.99	0.62
3:L:122:SER:HB3	3:L:125:GLN:HB3	1.82	0.62
3:L:126:LEU:C	3:L:128:SER:H	2.02	0.62
4:T:195:TRP:CZ2	4:T:217:ILE:HG22	2.34	0.62
4:H:131:LEU:HG	4:H:147:CYS:H	1.64	0.62
3:U:118:ILE:CD1	3:U:195:CYS:HB2	2.29	0.62
1:E:319:GLY:HA2	2:F:21:TRP:CH2	2.35	0.62
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.64	0.62
4:H:18:LEU:HD22	4:H:116:LEU:HD13	1.81	0.62
3:U:38:GLN:HG3	3:U:87:TYR:HE1	1.65	0.62
3:U:153:GLY:O	3:U:154:SER:HB2	1.99	0.62
1:E:187:THR:O	1:E:190:GLU:N	2.25	0.62
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.35	0.62
1:E:17:HIS:HB2	1:E:320:MET:SD	2.38	0.62
2:F:96:ALA:C	2:F:98:LEU:H	2.02	0.62
3:L:56:ALA:O	3:L:58:GLY:N	2.32	0.62
3:L:8:PRO:O	3:L:10:ILE:N	2.28	0.62
4:H:67:ARG:HB3	4:H:84:ASN:HB2	1.80	0.62
1:E:191:GLN:OE1	1:E:250:ASN:ND2	2.32	0.62
3:L:133:VAL:HB	3:L:180:LEU:HB3	1.80	0.62
2:D:44:ALA:HB2	2:D:114:GLU:HG3	1.81	0.62
1:A:29:ILE:HG23	2:D:103:GLU:OE1	1.99	0.62
2:D:54:ARG:NH1	2:D:103:GLU:OE2	2.32	0.62
3:U:126:LEU:O	3:U:128:SER:N	2.33	0.62
1:C:223:VAL:HG22	1:E:207:ARG:HG2	1.81	0.62
2:F:150:GLU:O	2:F:150:GLU:HG3	1.99	0.62
1:A:91:SER:O	1:A:93:ALA:N	2.33	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:201:THR:CG2	3:U:202:SER:N	2.63	0.62
2:D:115:MET:C	2:D:117:LYS:H	2.02	0.62
2:D:127:ARG:HG3	2:D:159:HIS:CD2	2.34	0.62
4:T:18:LEU:HD22	4:T:116:LEU:HD13	1.81	0.62
1:A:108:LEU:O	1:A:108:LEU:HG	1.97	0.62
3:U:80:GLU:O	3:U:81:ALA:C	2.38	0.62
3:U:118:ILE:HD13	3:U:195:CYS:CB	2.30	0.62
1:E:246:ASN:HD22	1:E:246:ASN:C	2.03	0.62
2:F:10:ILE:HG22	2:F:10:ILE:O	1.99	0.62
1:A:91:SER:C	1:A:93:ALA:H	2.01	0.62
2:B:3:PHE:CB	2:B:112:ASP:O	2.48	0.62
1:C:298:ASN:HD22	1:C:299:LYS:N	1.97	0.62
1:E:283:THR:HG23	1:E:286:GLY:H	1.62	0.62
4:T:29:ILE:H	4:T:77:ASN:HD21	1.44	0.62
1:E:176:LYS:HE3	1:E:178:TYR:OH	2.00	0.62
3:L:118:ILE:HD13	3:L:195:CYS:CB	2.30	0.62
3:U:7:SER:CB	3:U:8:PRO:HD3	2.30	0.62
1:C:191:GLN:OE1	1:C:195:TYR:HD1	1.83	0.62
1:E:94:PHE:CD1	1:E:94:PHE:C	2.72	0.62
1:A:10:THR:HG23	2:B:143:LYS:HZ2	1.64	0.62
2:B:108:ILE:O	2:B:110:LEU:N	2.33	0.62
1:C:318:THR:O	2:D:48:ILE:HG21	2.00	0.62
1:E:283:THR:HG22	1:E:287:SER:H	1.65	0.62
1:C:176:LYS:HD2	1:C:257:TYR:CD2	2.35	0.62
4:H:142:MET:CA	4:H:192:SER:HA	2.29	0.62
3:U:141:TYR:CD2	3:U:142:PRO:HD3	2.35	0.62
1:A:138:ALA:O	1:A:140:LYS:NZ	2.33	0.62
3:U:21:LEU:HD13	3:U:21:LEU:N	2.15	0.61
1:E:82:GLU:OE2	1:E:82:GLU:HA	2.00	0.61
3:U:187:TYR:C	3:U:189:ARG:H	2.04	0.61
2:D:38:LEU:C	2:D:40:SER:H	2.04	0.61
1:C:83:THR:O	1:C:84:TRP:HB3	1.99	0.61
1:A:29:ILE:HD11	2:B:102:LEU:CD2	2.28	0.61
4:H:206:HIS:HD2	4:H:209:SER:OG	1.83	0.61
2:B:139:LYS:C	2:B:140:ILE:HD12	2.20	0.61
2:F:121:LYS:NZ	2:F:122:THR:N	2.48	0.61
1:C:221:PRO:HG2	1:E:206:THR:HA	1.81	0.61
2:D:42:GLN:O	2:D:46:ASP:N	2.33	0.61
2:D:141:TYR:OH	2:D:170:ARG:HG2	1.99	0.61
1:E:35:GLU:O	1:E:322:ASN:HB3	2.00	0.61
4:H:29:ILE:HG22	4:H:35:TRP:CZ2	2.35	0.61
3:U:6:GLN:OE1	3:U:87:TYR:O	2.18	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:ARG:HG2	1:E:223:VAL:CG2	2.30	0.61
3:L:118:ILE:HG21	3:L:209:SER:HA	1.81	0.61
2:D:105:GLN:O	2:D:108:ILE:HB	2.00	0.61
1:A:12:THR:HB	2:B:27:GLN:HB3	1.83	0.61
3:U:21:LEU:N	3:U:21:LEU:CD1	2.63	0.61
1:C:25:LEU:HA	1:C:34:ILE:O	2.00	0.61
2:B:130:ALA:CB	2:B:139:LYS:O	2.45	0.61
4:H:58:ASN:O	4:H:59:ASN:HB2	2.00	0.61
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.36	0.61
3:U:91:GLN:HE21	3:U:93:GLU:N	1.99	0.61
2:B:66:ILE:O	2:B:66:ILE:HG13	2.00	0.61
4:H:38:ILE:O	4:H:95:TYR:HB2	2.00	0.61
4:H:49:MET:O	4:H:62:PRO:HD3	2.00	0.61
3:U:2:ILE:HG22	3:U:4:LEU:CD1	2.30	0.61
2:F:43:ALA:O	2:F:46:ASP:HB2	2.01	0.61
1:E:150:ARG:O	1:E:151:LEU:HD23	2.01	0.61
1:C:59:LEU:HD12	1:C:60:ASP:N	2.16	0.61
3:L:62:ARG:O	3:L:76:ILE:HA	2.00	0.61
1:C:64:CYS:HB2	1:C:79:PHE:HE1	1.63	0.61
4:H:122:LYS:HD3	4:H:124:THR:HG23	1.82	0.61
3:U:162:ASN:HA	3:U:177:SER:O	1.99	0.61
1:C:51:ILE:HD11	1:C:272:ALA:HB3	1.82	0.61
3:L:171:ASP:HB3	3:L:173:THR:HG23	1.81	0.61
3:U:136:PHE:O	3:U:137:LEU:HD12	2.01	0.61
1:C:10:THR:HG21	2:D:141:TYR:C	2.20	0.61
4:T:3:HIS:O	4:T:24:VAL:HA	2.01	0.61
4:H:33:TYR:CE2	4:H:100:TYR:HB2	2.35	0.61
1:C:209:SER:O	1:C:210:GLN:HB2	2.01	0.61
1:E:81:ASN:HD21	1:E:120:PHE:H	1.49	0.61
1:A:202:VAL:HG22	1:A:247:SER:HB2	1.83	0.61
3:L:25:ALA:O	3:L:26:SER:C	2.40	0.61
1:A:18:HIS:HA	2:B:14:TRP:CB	2.27	0.61
1:A:294:PHE:HB3	1:A:309:VAL:CG2	2.30	0.61
2:F:108:ILE:C	2:F:110:LEU:N	2.52	0.61
2:B:149:ILE:O	2:B:151:SER:N	2.30	0.61
1:E:73:ASP:OD1	1:E:75:HIS:CD2	2.54	0.61
1:A:27:LYS:HG3	1:A:32:ASP:HA	1.83	0.61
1:C:187:THR:O	1:C:190:GLU:N	2.34	0.61
1:A:295:GLN:OE1	1:A:297:VAL:HB	2.01	0.61
4:H:40:GLN:HB3	4:H:46:LEU:HD23	1.83	0.61
4:T:38:ILE:O	4:T:95:TYR:HB2	2.01	0.60
1:A:96:ASN:ND2	1:A:140:LYS:HE2	2.13	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:221:PRO:HG2	1:E:206:THR:CA	2.31	0.60
3:L:189:ARG:HB3	3:L:190:HIS:CE1	2.35	0.60
1:E:109:ARG:HG2	1:E:109:ARG:HH11	1.66	0.60
4:H:27:TYR:HE1	4:H:31:SER:O	1.84	0.60
1:E:184:HIS:O	1:E:228:SER:HB2	2.01	0.60
1:C:97:CYS:O	1:C:98:TYR:C	2.37	0.60
1:E:43:VAL:HA	1:E:294:PHE:O	2.00	0.60
1:C:283:THR:C	1:C:285:ASN:N	2.53	0.60
1:A:36:VAL:HG22	1:A:37:THR:N	2.16	0.60
3:U:97:ARG:HB2	4:T:48:TRP:CG	2.37	0.60
1:E:80:GLN:O	1:E:82:GLU:N	2.34	0.60
1:E:294:PHE:CE1	2:F:96:ALA:CB	2.84	0.60
5:C:450:NAG:H83	4:H:100:TYR:CE1	2.37	0.60
2:F:57:GLU:O	2:F:58:LYS:HG2	2.00	0.60
4:T:32:GLY:O	4:T:33:TYR:HB2	2.01	0.60
4:T:87:THR:O	4:T:118:VAL:HG11	2.02	0.60
1:A:298:ASN:HD22	1:A:299:LYS:H	1.50	0.60
3:U:3:VAL:O	3:U:3:VAL:HG12	2.01	0.60
2:B:171:PHE:CD1	2:B:171:PHE:N	2.70	0.60
4:H:28:SER:C	4:H:30:THR:N	2.55	0.60
1:C:193:SER:HA	3:U:57:SER:HB2	1.83	0.60
3:L:191:ASN:HD22	3:L:191:ASN:N	2.00	0.60
3:L:29:ILE:HD11	3:L:34:LEU:HB2	1.83	0.60
3:U:6:GLN:NE2	3:U:101:GLY:O	2.35	0.60
3:U:107:ILE:H	3:U:167:GLN:NE2	1.97	0.60
1:A:148:PHE:HB2	1:A:151:LEU:HB2	1.83	0.60
2:B:44:ALA:HB2	2:B:114:GLU:HG3	1.84	0.60
1:C:18:HIS:CA	2:D:14:TRP:HB2	2.29	0.60
2:D:21:TRP:CE2	2:D:45:ILE:HD11	2.36	0.60
1:E:283:THR:CG2	1:E:286:GLY:N	2.65	0.60
4:H:51:TYR:CD1	4:H:52:ILE:N	2.69	0.60
3:U:52:THR:HG23	3:U:72:TYR:CE2	2.36	0.60
1:C:201:ARG:NH1	1:C:201:ARG:HG2	2.16	0.60
4:H:87:THR:HG21	4:H:89:GLU:HB2	1.82	0.60
1:E:71:LEU:HD11	1:E:100:TYR:CE1	2.36	0.60
4:T:130:PRO:HD3	4:T:215:LYS:HG2	1.84	0.60
3:U:36:TRP:CD2	3:U:74:LEU:HD23	2.37	0.60
1:A:247:SER:CB	1:A:251:LEU:HB2	2.32	0.60
2:F:23:GLY:HA3	2:F:35:ALA:O	2.01	0.60
1:C:41:GLU:HG3	1:C:42:LEU:N	2.17	0.60
3:U:14:SER:HB3	3:U:108:LYS:CB	2.32	0.60
4:T:86:VAL:CG2	4:T:87:THR:N	2.64	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:108:LEU:O	1:C:112:VAL:HG23	2.01	0.60
1:E:9:SER:C	2:F:143:LYS:HE3	2.21	0.59
2:F:100:VAL:HG23	2:F:101:ALA:N	2.17	0.59
3:U:61:ALA:O	3:U:63:PHE:N	2.36	0.59
4:H:67:ARG:CB	4:H:84:ASN:HB2	2.31	0.59
1:C:293:PRO:O	1:C:294:PHE:CD2	2.55	0.59
4:T:24:VAL:HG11	4:T:29:ILE:HG23	1.84	0.59
1:E:97:CYS:O	1:E:98:TYR:C	2.41	0.59
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.02	0.59
1:C:220:ARG:HH21	1:E:210:GLN:NE2	2.00	0.59
2:B:68:LYS:HE2	2:B:85:GLU:CD	2.23	0.59
3:U:165:THR:HG23	3:U:175:SER:O	2.03	0.59
2:B:141:TYR:HB3	2:B:165:GLU:HB3	1.83	0.59
2:D:121:LYS:NZ	2:D:122:THR:HG22	2.17	0.59
3:U:37:TYR:OH	4:T:99:PHE:HE2	1.83	0.59
3:L:137:LEU:HD23	3:L:145:ILE:CD1	2.32	0.59
3:L:212:ARG:HG2	3:L:213:ASN:H	1.65	0.59
1:E:187:THR:C	1:E:189:GLN:N	2.55	0.59
1:C:123:GLU:O	1:C:255:ARG:O	2.21	0.59
4:T:80:PHE:CD2	4:T:80:PHE:N	2.69	0.59
1:C:319:GLY:HA2	2:D:21:TRP:HH2	1.67	0.59
1:C:294:PHE:CE1	2:D:96:ALA:HB1	2.37	0.59
2:D:25:ARG:HG2	2:D:34:GLN:CG	2.25	0.59
4:H:6:GLU:OE1	4:H:95:TYR:HA	2.03	0.59
3:L:147:VAL:HA	3:L:196:GLU:O	2.03	0.59
1:A:312:ASN:H	1:A:312:ASN:ND2	1.99	0.59
1:C:68:ASP:OD2	1:C:95:SER:HB3	2.02	0.59
1:E:169:PRO:CA	1:E:242:VAL:HG23	2.32	0.59
4:H:102:ASP:O	4:H:103:TYR:HB2	2.02	0.59
1:A:139:CYS:O	1:A:146:GLY:C	2.41	0.59
1:A:291:ASP:OD2	1:A:292:LYS:N	2.35	0.59
1:C:17:HIS:HA	2:D:22:TYR:CD2	2.38	0.59
2:F:85:GLU:O	2:F:89:ILE:HD13	2.02	0.59
2:D:151:SER:O	2:D:156:THR:N	2.33	0.59
2:B:129:ASN:HD21	2:B:159:HIS:HA	1.68	0.59
2:F:170:ARG:HB3	2:F:171:PHE:CD1	2.34	0.59
1:C:206:THR:OG1	1:C:209:SER:HB3	2.03	0.59
1:C:185:PRO:HB3	1:C:190:GLU:HG2	1.85	0.59
1:C:324:PRO:HB3	1:C:328:THR:HB	1.85	0.59
1:E:262:THR:O	1:E:263:GLY:O	2.21	0.59
2:B:141:TYR:CZ	2:B:170:ARG:HG2	2.37	0.59
2:D:98:LEU:O	2:D:99:LEU:C	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:2:LEU:HB2	2:F:109:ASP:OD1	2.02	0.59
3:L:187:TYR:C	3:L:189:ARG:H	2.05	0.59
1:A:17:HIS:HE1	2:B:13:GLY:HA2	1.67	0.59
2:F:166:ALA:N	2:F:168:ASN:ND2	2.50	0.59
2:F:48:ILE:HG22	2:F:49:ASN:N	2.17	0.59
1:E:74:PRO:HD2	1:E:96:ASN:O	2.02	0.59
3:U:167:GLN:HG2	3:U:172:SER:HA	1.85	0.59
1:A:28:THR:O	1:A:30:THR:N	2.36	0.59
1:A:10:THR:HG23	2:B:143:LYS:NZ	2.18	0.59
2:D:96:ALA:O	2:D:98:LEU:N	2.35	0.59
1:E:309:VAL:CG1	2:F:93:SER:HA	2.33	0.59
4:T:146:GLY:O	4:T:147:CYS:HB3	2.01	0.59
2:F:121:LYS:NZ	2:F:122:THR:HG23	2.18	0.59
1:C:62:ILE:HG22	1:C:63:ASP:H	1.67	0.59
2:D:2:LEU:HB2	2:D:109:ASP:OD1	2.01	0.59
2:D:71:SER:HB2	2:D:72:GLU:OE2	2.03	0.59
4:H:39:ARG:NH1	4:H:94:TYR:OH	2.35	0.59
2:B:165:GLU:HA	2:B:168:ASN:ND2	2.18	0.59
1:A:108:LEU:O	1:A:112:VAL:HG23	2.02	0.59
1:E:281:CYS:HB2	1:E:304:ALA:O	2.03	0.59
1:A:166:VAL:HG22	1:A:245:ILE:HB	1.84	0.59
2:D:100:VAL:HG23	2:D:101:ALA:N	2.14	0.58
2:D:111:THR:C	2:D:113:SER:H	2.05	0.58
2:F:100:VAL:O	2:F:104:ASN:HB2	2.02	0.58
4:T:142:MET:CA	4:T:192:SER:HA	2.33	0.58
2:D:25:ARG:HE	2:D:34:GLN:CD	2.07	0.58
2:B:26:HIS:ND1	2:B:26:HIS:O	2.36	0.58
4:T:75:SER:OG	4:T:76:LYS:N	2.35	0.58
2:D:47:GLN:OE1	2:D:110:LEU:HD11	2.03	0.58
3:L:118:ILE:HD12	3:L:135:CYS:HB2	1.85	0.58
1:A:25:LEU:HD23	1:A:34:ILE:N	2.18	0.58
1:C:169:PRO:HA	1:C:242:VAL:HG23	1.85	0.58
1:A:262:THR:O	1:A:263:GLY:O	2.21	0.58
1:C:217:ILE:N	1:C:217:ILE:HD12	2.18	0.58
1:E:29:ILE:CD1	2:F:102:LEU:HD23	2.21	0.58
2:F:108:ILE:O	2:F:110:LEU:N	2.36	0.58
4:H:195:TRP:HB3	4:H:196:PRO:CD	2.30	0.58
3:L:21:LEU:HD21	3:L:87:TYR:HD2	1.66	0.58
1:E:91:SER:O	1:E:93:ALA:N	2.37	0.58
1:C:251:LEU:HD21	1:C:253:ALA:HB2	1.85	0.58
2:D:6:ILE:CG1	2:D:112:ASP:HA	2.32	0.58
3:U:125:GLN:HB2	4:T:129:TYR:CD2	2.37	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:6:GLN:NE2	3:U:102:GLY:HA2	2.19	0.58
4:H:13:LYS:N	4:H:16:GLN:OE1	2.30	0.58
2:B:171:PHE:HD2	2:D:167:LEU:HB3	1.69	0.58
1:C:17:HIS:HB2	1:C:320:MET:SD	2.43	0.58
2:D:27:GLN:HG3	2:D:27:GLN:O	2.03	0.58
4:H:146:GLY:O	4:H:147:CYS:CB	2.50	0.58
3:L:7:SER:CB	3:L:8:PRO:HD3	2.33	0.58
4:H:188:VAL:CG2	4:H:189:THR:H	2.16	0.58
2:D:168:ASN:O	2:D:170:ARG:N	2.36	0.58
1:E:310:LYS:HG3	2:F:93:SER:OG	2.03	0.58
4:H:29:ILE:HG22	4:H:35:TRP:CD2	2.39	0.58
4:T:49:MET:O	4:T:62:PRO:HD3	2.03	0.58
2:D:167:LEU:HD12	2:D:172:GLN:OE1	2.03	0.58
2:D:6:ILE:CD1	2:D:112:ASP:HA	2.34	0.58
3:U:92:TRP:O	3:U:97:ARG:NH2	2.37	0.58
3:U:119:PHE:O	3:U:133:VAL:HG13	2.03	0.58
1:A:206:THR:HA	1:E:221:PRO:HG2	1.85	0.58
3:U:7:SER:HB2	3:U:8:PRO:HD3	1.86	0.58
1:E:17:HIS:HA	2:F:22:TYR:CD2	2.38	0.58
1:E:309:VAL:HG12	2:F:93:SER:HA	1.85	0.58
2:D:151:SER:HA	2:D:156:THR:O	2.04	0.58
4:T:162:ASN:HD21	4:T:201:THR:H	1.50	0.58
4:T:188:VAL:HG22	4:T:189:THR:H	1.67	0.58
1:C:166:VAL:CG2	1:C:245:ILE:HB	2.34	0.58
4:T:149:VAL:HB	4:T:184:LEU:HG	1.84	0.58
2:F:38:LEU:O	2:F:40:SER:N	2.37	0.58
1:A:53:ASN:OD1	1:A:276:THR:HA	2.04	0.58
1:C:248:ASN:HD22	1:C:248:ASN:C	2.07	0.58
1:E:252:ILE:HG22	1:E:252:ILE:O	2.04	0.58
1:A:37:THR:HG23	1:A:321:ARG:O	2.04	0.57
2:B:126:LEU:HD12	2:B:126:LEU:O	2.04	0.57
2:B:168:ASN:C	2:B:170:ARG:H	2.06	0.57
1:C:108:LEU:HA	1:C:111:LEU:HD21	1.85	0.57
3:L:8:PRO:HG2	3:L:11:MET:HE3	1.86	0.57
1:A:324:PRO:HB3	1:A:328:THR:HB	1.85	0.57
3:U:199:HIS:HB3	3:U:201:THR:CG2	2.18	0.57
1:A:17:HIS:CD2	2:B:6:ILE:HG23	2.29	0.57
1:C:268:MET:SD	1:C:284:PRO:HG3	2.44	0.57
4:T:150:LYS:HB2	4:T:183:THR:HG23	1.85	0.57
1:E:94:PHE:HD1	1:E:94:PHE:C	2.06	0.57
1:A:44:GLN:HB3	1:A:295:GLN:CB	2.32	0.57
4:T:160:THR:OG1	4:T:203:ASN:HB2	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:ARG:HG3	1:A:269:ARG:HH11	1.69	0.57
3:U:116:VAL:CG1	3:U:117:SER:N	2.67	0.57
2:B:3:PHE:HE2	2:B:113:SER:HG	1.50	0.57
1:E:41:GLU:HG3	1:E:43:VAL:H	1.68	0.57
4:H:122:LYS:CD	4:H:124:THR:HG23	2.35	0.57
1:E:33:GLN:O	1:E:34:ILE:HG13	2.05	0.57
1:A:94:PHE:C	1:A:94:PHE:CD1	2.78	0.57
1:E:18:HIS:O	1:E:19:ALA:HB2	2.04	0.57
1:E:41:GLU:HG3	1:E:42:LEU:N	2.18	0.57
2:F:141:TYR:CE2	2:F:170:ARG:HG2	2.40	0.57
2:F:152:ILE:C	2:F:154:ASN:H	2.06	0.57
4:H:91:THR:OG1	4:H:117:THR:HA	2.04	0.57
1:E:148:PHE:HB2	1:E:151:LEU:HB2	1.86	0.57
1:C:186:SER:CA	1:C:218:GLY:O	2.50	0.57
1:E:121:ILE:HG13	1:E:257:TYR:CE1	2.39	0.57
2:D:96:ALA:C	2:D:98:LEU:H	2.07	0.57
2:F:166:ALA:H	2:F:168:ASN:ND2	2.01	0.57
4:T:17:SER:HA	4:T:84:ASN:O	2.04	0.57
3:U:21:LEU:HD21	3:U:87:TYR:CD2	2.40	0.57
1:A:140:LYS:H	1:A:140:LYS:CD	2.15	0.57
1:E:291:ASP:OD2	1:E:292:LYS:N	2.38	0.57
2:F:89:ILE:HD12	2:F:89:ILE:N	2.19	0.57
1:A:283:THR:CG2	1:A:286:GLY:N	2.65	0.57
1:C:172:ASP:CB	1:C:174:PHE:CE2	2.87	0.57
2:D:106:HIS:O	2:D:106:HIS:CG	2.58	0.57
2:D:66:ILE:HG13	2:D:66:ILE:O	2.02	0.57
3:L:174:TYR:N	3:L:174:TYR:CD2	2.73	0.57
3:U:3:VAL:H	3:U:26:SER:CB	2.18	0.57
1:C:220:ARG:HE	1:E:210:GLN:HG3	1.69	0.57
3:U:40:LYS:HD3	3:U:85:ALA:HB2	1.84	0.57
2:F:47:GLN:OE1	2:F:110:LEU:HD11	2.05	0.57
2:F:89:ILE:CD1	2:F:89:ILE:H	2.17	0.57
2:B:27:GLN:HG3	2:B:27:GLN:O	2.05	0.57
1:A:191:GLN:OE1	1:A:195:TYR:HD1	1.86	0.57
4:H:87:THR:OG1	4:H:88:ALA:N	2.37	0.57
3:U:3:VAL:HB	3:U:26:SER:HB2	1.86	0.57
2:D:26:HIS:O	2:D:32:THR:HG22	2.04	0.57
1:A:64:CYS:HB2	1:A:79:PHE:CE1	2.40	0.57
2:F:141:TYR:CZ	2:F:170:ARG:HG2	2.39	0.57
4:T:146:GLY:O	4:T:147:CYS:CB	2.52	0.57
1:A:283:THR:HG22	1:A:287:SER:H	1.69	0.57
1:E:25:LEU:HD22	1:E:33:GLN:OE1	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:120:GLU:OE1	2:D:120:GLU:HA	2.04	0.57
1:C:74:PRO:HD3	1:C:97:CYS:CB	2.34	0.56
1:C:36:VAL:HG22	1:C:37:THR:H	1.70	0.56
4:T:131:LEU:HG	4:T:147:CYS:N	2.19	0.56
1:E:187:THR:O	1:E:189:GLN:N	2.38	0.56
2:B:48:ILE:HD11	2:B:107:THR:HG23	1.86	0.56
2:D:122:THR:O	2:D:126:LEU:HG	2.04	0.56
1:E:13:LEU:O	2:F:138:PHE:HB2	2.05	0.56
1:E:17:HIS:CG	1:E:18:HIS:H	2.23	0.56
4:T:27:TYR:CE1	4:T:31:SER:HB2	2.40	0.56
4:T:14:PRO:O	4:T:15:SER:HB3	2.05	0.56
4:H:91:THR:HB	4:H:118:VAL:H	1.70	0.56
2:D:3:PHE:CB	2:D:112:ASP:O	2.53	0.56
1:E:44:GLN:HB3	1:E:295:GLN:CB	2.35	0.56
2:F:102:LEU:O	2:F:103:GLU:C	2.43	0.56
4:T:2:VAL:CB	4:T:109:TYR:HE2	2.06	0.56
4:T:86:VAL:HG22	4:T:87:THR:N	2.19	0.56
2:B:80:LEU:HD21	2:D:80:LEU:HD21	1.87	0.56
1:C:164:LEU:O	1:C:246:ASN:HA	2.05	0.56
1:A:246:ASN:HD22	1:A:246:ASN:C	2.09	0.56
1:A:38:ASN:HD22	1:A:318:THR:CG2	2.17	0.56
1:E:209:SER:O	1:E:210:GLN:CB	2.53	0.56
3:U:191:ASN:HD22	3:U:191:ASN:H	1.52	0.56
1:C:37:THR:HG23	1:C:321:ARG:O	2.05	0.56
4:H:162:ASN:HD21	4:H:201:THR:N	2.02	0.56
4:H:37:TRP:CH2	4:H:96:CYS:HB3	2.40	0.56
1:E:91:SER:C	1:E:93:ALA:N	2.58	0.56
1:E:304:ALA:H	2:F:61:GLU:HG3	1.70	0.56
3:L:176:MET:HG2	3:L:177:SER:H	1.70	0.56
3:U:134:VAL:HG22	3:U:179:THR:CG2	2.20	0.56
4:T:3:HIS:HB3	4:T:25:THR:OG1	2.04	0.56
3:U:14:SER:OG	3:U:108:LYS:CD	2.53	0.56
3:L:184:LYS:O	3:L:188:GLU:HG3	2.05	0.56
1:A:200:GLY:HA3	1:A:250:ASN:OD1	2.05	0.56
1:C:295:GLN:HG3	1:C:306:PRO:O	2.05	0.56
1:A:82:GLU:HA	1:A:82:GLU:OE2	2.06	0.56
5:C:450:NAG:H83	4:H:100:TYR:HE1	1.69	0.56
3:L:147:VAL:HG21	3:L:178:SER:OG	2.05	0.56
2:B:21:TRP:HB2	2:B:41:THR:HG23	1.87	0.56
4:T:159:VAL:HG22	4:T:160:THR:N	2.20	0.56
1:A:182:ILE:HG22	1:A:231:SER:HB2	1.87	0.56
2:D:102:LEU:O	2:D:104:ASN:N	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:108:LEU:HD13	1:E:234:TRP:CD2	2.40	0.56
3:L:199:HIS:HB3	3:L:201:THR:CG2	2.27	0.56
1:C:286:GLY:O	1:C:287:SER:CB	2.44	0.56
3:U:95:PHE:HE2	4:T:60:TYR:HB3	1.68	0.56
1:A:242:VAL:CG1	1:E:221:PRO:HB3	2.35	0.56
3:L:165:THR:OG1	3:L:166:ASP:N	2.37	0.56
1:A:319:GLY:HA2	2:B:21:TRP:CH2	2.40	0.56
1:C:53:ASN:OD1	1:C:276:THR:HA	2.06	0.56
1:A:293:PRO:C	1:A:294:PHE:CD2	2.79	0.56
2:B:108:ILE:C	2:B:110:LEU:N	2.59	0.56
2:F:27:GLN:O	2:F:27:GLN:HG3	2.06	0.56
1:E:140:LYS:HD2	1:E:140:LYS:N	2.21	0.56
2:D:150:GLU:O	2:D:156:THR:OG1	2.24	0.56
1:A:176:LYS:HD2	1:A:257:TYR:CE2	2.40	0.56
4:T:87:THR:OG1	4:T:88:ALA:N	2.36	0.56
1:A:87:PHE:HB3	1:A:267:ILE:HG13	1.88	0.56
2:D:118:LEU:O	2:D:122:THR:HG23	2.06	0.56
4:T:162:ASN:HD21	4:T:200:VAL:HA	1.71	0.56
4:H:32:GLY:H	4:H:54:TYR:HB3	1.71	0.56
2:B:68:LYS:HE2	2:B:85:GLU:OE2	2.06	0.56
1:C:138:ALA:O	1:C:140:LYS:NZ	2.39	0.56
2:D:166:ALA:N	2:D:168:ASN:ND2	2.54	0.56
1:C:254:PRO:O	1:C:254:PRO:HG2	2.06	0.56
1:C:74:PRO:HA	1:C:141:ARG:HH12	1.70	0.55
4:T:201:THR:HG21	4:T:214:ASP:HB2	1.88	0.55
4:H:33:TYR:HE2	4:H:100:TYR:HB2	1.71	0.55
3:U:50:TYR:O	3:U:51:SER:C	2.44	0.55
1:E:153:TRP:O	1:E:154:LEU:HD23	2.06	0.55
1:A:74:PRO:HD3	1:A:97:CYS:CB	2.31	0.55
2:B:105:GLN:O	2:B:108:ILE:HB	2.06	0.55
1:E:293:PRO:O	1:E:294:PHE:HD2	1.89	0.55
2:F:98:LEU:C	2:F:100:VAL:N	2.55	0.55
1:A:14:CYS:O	2:B:25:ARG:N	2.38	0.55
4:T:87:THR:CG2	4:T:89:GLU:HB2	2.37	0.55
3:U:32:SER:HA	3:U:51:SER:HA	1.88	0.55
3:L:21:LEU:HB2	3:L:74:LEU:HB2	1.87	0.55
1:E:82:GLU:CA	1:E:82:GLU:OE2	2.54	0.55
2:B:121:LYS:HB3	2:B:121:LYS:HZ3	1.70	0.55
1:A:91:SER:C	1:A:93:ALA:N	2.59	0.55
3:L:4:LEU:HD23	3:L:89:CYS:SG	2.47	0.55
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.41	0.55
2:D:57:GLU:O	2:D:58:LYS:HG2	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:19:ALA:C	1:C:20:VAL:HG22	2.26	0.55
4:H:162:ASN:HD21	4:H:200:VAL:HA	1.71	0.55
2:F:118:LEU:O	2:F:121:LYS:HB3	2.07	0.55
4:H:35:TRP:HB3	4:H:79:PHE:CZ	2.41	0.55
1:A:283:THR:CG2	1:A:286:GLY:H	2.13	0.55
3:U:149:TRP:HE1	3:U:178:SER:HB3	1.71	0.55
1:C:326:LYS:O	1:C:327:GLN:HB2	2.05	0.55
1:E:87:PHE:HB3	1:E:267:ILE:HG13	1.88	0.55
1:C:82:GLU:OE2	1:C:83:THR:N	2.37	0.55
2:B:115:MET:O	2:B:117:LYS:N	2.36	0.55
1:E:74:PRO:HA	1:E:141:ARG:NH1	2.19	0.55
4:H:51:TYR:CE1	4:H:60:TYR:HB2	2.42	0.55
3:U:147:VAL:HG21	3:U:178:SER:OG	2.07	0.55
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.88	0.55
2:B:10:ILE:O	2:B:12:ASN:N	2.39	0.55
3:U:116:VAL:HG13	3:U:136:PHE:O	2.07	0.55
4:T:65:LYS:C	4:T:67:ARG:N	2.60	0.55
3:U:80:GLU:O	3:U:83:ASP:N	2.39	0.55
4:H:15:SER:O	4:H:16:GLN:O	2.24	0.55
1:E:84:TRP:CZ2	1:E:116:GLY:HA2	2.42	0.55
3:U:171:ASP:HB3	3:U:173:THR:OG1	2.06	0.55
3:U:113:ALA:HB2	3:U:201:THR:CB	2.37	0.55
4:T:190:VAL:HB	4:T:191:PRO:CD	2.36	0.55
2:F:119:PHE:O	2:F:123:ARG:HB2	2.06	0.55
4:H:142:MET:HA	4:H:192:SER:CA	2.35	0.55
4:H:177:LEU:HD12	4:H:181:LEU:O	2.07	0.55
3:L:139:ASN:HA	3:L:174:TYR:O	2.06	0.55
2:B:170:ARG:HB3	2:B:171:PHE:CD1	2.41	0.55
1:E:138:ALA:O	1:E:140:LYS:NZ	2.40	0.55
3:U:19:VAL:O	3:U:75:THR:HA	2.07	0.55
2:B:121:LYS:NZ	2:B:122:THR:N	2.55	0.55
3:L:118:ILE:HD11	3:L:149:TRP:CH2	2.42	0.55
3:U:183:THR:OG1	3:U:186:GLU:CB	2.55	0.55
1:C:36:VAL:CG2	1:C:320:MET:O	2.54	0.55
1:E:286:GLY:O	1:E:287:SER:CB	2.54	0.55
1:E:13:LEU:CD1	2:F:24:PHE:HB3	2.34	0.55
4:T:190:VAL:HB	4:T:191:PRO:HD2	1.89	0.55
4:T:6:GLU:OE1	4:T:96:CYS:N	2.38	0.55
1:C:304:ALA:N	2:D:61:GLU:HG3	2.22	0.55
2:B:115:MET:C	2:B:117:LYS:H	2.08	0.55
2:D:128:GLU:HA	2:D:170:ARG:NH2	2.22	0.55
1:E:17:HIS:HE1	2:F:13:GLY:HA2	1.72	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:29:ILE:HB	2:F:105:GLN:NE2	2.22	0.55
4:H:24:VAL:HG11	4:H:29:ILE:HG23	1.88	0.55
4:T:58:ASN:O	4:T:60:TYR:N	2.37	0.55
3:L:175:SER:OG	4:H:171:HIS:CE1	2.60	0.55
1:A:187:THR:OG1	1:A:189:GLN:HG2	2.06	0.55
1:A:295:GLN:HE22	1:A:308:TYR:HD1	1.54	0.55
4:H:27:TYR:CE1	4:H:31:SER:O	2.59	0.55
4:T:20:LEU:HD11	4:T:94:TYR:CB	2.37	0.55
1:A:174:PHE:N	1:A:174:PHE:CD2	2.75	0.55
4:T:11:LEU:O	4:T:12:VAL:HG13	2.07	0.55
1:E:186:SER:CA	1:E:218:GLY:O	2.54	0.55
2:D:38:LEU:O	2:D:40:SER:N	2.39	0.55
2:B:126:LEU:CD2	2:B:152:ILE:HD11	2.37	0.54
4:H:195:TRP:O	4:H:197:SER:N	2.40	0.54
1:E:64:CYS:HB2	1:E:79:PHE:HE1	1.72	0.54
2:F:131:GLU:O	2:F:139:LYS:HB3	2.07	0.54
2:D:166:ALA:H	2:D:168:ASN:ND2	2.04	0.54
2:F:47:GLN:OE1	2:F:110:LEU:HD21	2.07	0.54
3:L:19:VAL:HG21	3:L:79:LEU:CD2	2.35	0.54
4:H:15:SER:N	4:H:86:VAL:O	2.40	0.54
1:E:22:ASN:H	1:E:22:ASN:ND2	2.03	0.54
1:E:106:ALA:O	1:E:109:ARG:HB3	2.06	0.54
1:C:94:PHE:C	1:C:94:PHE:CD1	2.79	0.54
1:A:42:LEU:O	1:A:293:PRO:HD2	2.08	0.54
1:C:17:HIS:HA	2:D:22:TYR:HD2	1.72	0.54
1:E:292:LYS:HB3	1:E:293:PRO:HD2	1.89	0.54
4:H:201:THR:HG23	4:H:216:LYS:N	2.22	0.54
4:T:144:THR:O	4:T:145:LEU:HD23	2.07	0.54
1:C:121:ILE:HG13	1:C:257:TYR:CE1	2.42	0.54
1:A:27:LYS:NZ	2:B:97:GLU:OE1	2.40	0.54
1:E:42:LEU:O	1:E:293:PRO:HD2	2.07	0.54
4:T:58:ASN:HB2	4:T:60:TYR:CE2	2.43	0.54
3:U:79:LEU:HD13	3:U:80:GLU:N	2.23	0.54
3:L:47:LEU:HD12	3:L:48:TRP:N	2.21	0.54
4:H:150:LYS:CB	4:H:183:THR:HG23	2.37	0.54
4:H:150:LYS:HB2	4:H:183:THR:HG23	1.90	0.54
2:D:76:ARG:HD2	2:F:81:GLU:OE2	2.06	0.54
2:B:100:VAL:O	2:B:101:ALA:C	2.46	0.54
1:C:320:MET:CB	2:D:111:THR:HG21	2.37	0.54
1:E:293:PRO:C	1:E:294:PHE:CD2	2.81	0.54
4:T:41:PHE:HD1	4:T:92:ALA:HB2	1.72	0.54
1:A:10:THR:HG21	2:B:141:TYR:C	2.27	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:44:GLN:N	1:E:294:PHE:O	2.37	0.54
4:H:56:GLY:O	4:H:58:ASN:OD1	2.26	0.54
4:H:217:ILE:O	4:H:219:PRO:HD3	2.08	0.54
1:A:169:PRO:CA	1:A:242:VAL:HG23	2.38	0.54
3:L:191:ASN:HD22	3:L:191:ASN:H	1.55	0.54
1:C:43:VAL:O	1:C:43:VAL:HG12	2.06	0.54
4:T:61:ASN:CB	4:T:62:PRO:HD2	2.37	0.54
1:E:307:LYS:HE2	2:F:60:ASN:HD22	1.71	0.54
3:U:150:LYS:O	3:U:151:ILE:HB	2.08	0.54
1:A:17:HIS:HA	2:B:22:TYR:CD2	2.43	0.54
1:C:44:GLN:HB3	1:C:295:GLN:CB	2.37	0.54
1:E:313:THR:O	1:E:314:LEU:HD23	2.07	0.54
2:F:98:LEU:O	2:F:99:LEU:C	2.45	0.54
4:T:145:LEU:HB2	4:T:188:VAL:CG1	2.38	0.54
1:A:83:THR:O	1:A:84:TRP:HB3	2.08	0.54
1:A:206:THR:HB	1:A:241:ASP:OD1	2.08	0.54
3:L:149:TRP:HE1	3:L:178:SER:HB3	1.73	0.54
1:A:109:ARG:NH2	1:A:267:ILE:HD13	2.22	0.54
1:E:102:VAL:HB	1:E:105:TYR:HD2	1.73	0.54
1:E:74:PRO:HG3	1:E:139:CYS:SG	2.48	0.54
3:U:151:ILE:HA	3:U:193:TYR:HA	1.90	0.54
3:U:91:GLN:NE2	3:U:93:GLU:N	2.56	0.54
3:L:173:THR:C	3:L:174:TYR:CD2	2.81	0.54
1:A:17:HIS:HD2	2:B:6:ILE:CG2	2.15	0.53
4:T:29:ILE:HG22	4:T:35:TRP:CZ2	2.43	0.53
1:E:140:LYS:H	1:E:140:LYS:CD	2.20	0.53
3:L:118:ILE:CD1	3:L:195:CYS:HB2	2.37	0.53
3:L:81:ALA:O	3:L:107:ILE:HD11	2.07	0.53
2:B:83:TYR:CD2	2:D:66:ILE:HG23	2.43	0.53
2:D:10:ILE:O	2:D:10:ILE:HG22	2.09	0.53
4:T:73:ASP:O	4:T:75:SER:N	2.41	0.53
2:B:129:ASN:ND2	2:B:159:HIS:HA	2.24	0.53
3:U:32:SER:C	3:U:33:PHE:HD1	2.12	0.53
3:L:116:VAL:HG13	3:L:136:PHE:O	2.08	0.53
1:E:109:ARG:NH1	1:E:109:ARG:HG2	2.23	0.53
4:H:195:TRP:O	4:H:196:PRO:C	2.47	0.53
3:U:141:TYR:O	3:U:142:PRO:C	2.46	0.53
3:U:52:THR:CG2	3:U:72:TYR:HE2	2.21	0.53
1:A:38:ASN:HD22	1:A:318:THR:HB	1.74	0.53
3:U:123:LYS:HD2	3:U:123:LYS:H	1.72	0.53
1:A:294:PHE:HB3	1:A:309:VAL:HG21	1.90	0.53
2:F:165:GLU:C	2:F:168:ASN:HD21	2.12	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:66:SER:OG	3:L:67:GLY:N	2.42	0.53
3:U:14:SER:CB	3:U:108:LYS:HB2	2.39	0.53
4:T:87:THR:HG21	4:T:89:GLU:HB2	1.91	0.53
1:A:38:ASN:ND2	1:A:318:THR:HB	2.23	0.53
3:L:52:THR:HG23	3:L:72:TYR:CE2	2.44	0.53
3:L:123:LYS:HB3	3:L:123:LYS:NZ	2.24	0.53
4:T:195:TRP:HB3	4:T:196:PRO:CD	2.37	0.53
4:H:11:LEU:HB2	4:H:117:THR:O	2.08	0.53
1:A:187:THR:HB	1:A:189:GLN:OE1	2.09	0.53
1:C:67:ILE:O	1:C:70:LEU:HB3	2.08	0.53
1:A:117:THR:O	1:A:117:THR:HG23	2.09	0.53
2:B:168:ASN:C	2:B:170:ARG:N	2.62	0.53
2:D:129:ASN:ND2	2:D:159:HIS:HA	2.23	0.53
1:E:44:GLN:OE1	1:E:289:PRO:HG2	2.08	0.53
3:L:67:GLY:HA2	3:L:72:TYR:HA	1.90	0.53
3:U:38:GLN:HG3	3:U:87:TYR:CE1	2.41	0.53
3:L:56:ALA:O	3:L:59:VAL:HG23	2.09	0.53
3:U:167:GLN:CG	3:U:172:SER:HA	2.38	0.53
5:A:451:NAG:H2	1:E:222:TRP:CD1	2.43	0.53
1:A:17:HIS:CG	1:A:18:HIS:H	2.26	0.53
2:D:152:ILE:C	2:D:154:ASN:H	2.12	0.53
4:H:35:TRP:CD1	4:H:35:TRP:N	2.77	0.53
2:F:21:TRP:CE2	2:F:45:ILE:HD11	2.43	0.53
2:F:39:LYS:O	2:F:43:ALA:HB2	2.08	0.53
3:L:113:ALA:HB1	3:L:114:PRO:HD2	1.91	0.53
2:D:17:MET:HE1	2:D:19:ASP:H	1.74	0.53
1:C:293:PRO:O	1:C:294:PHE:HD2	1.89	0.53
2:D:108:ILE:C	2:D:110:LEU:N	2.62	0.53
2:D:168:ASN:C	2:D:170:ARG:H	2.11	0.53
4:T:194:THR:HG23	4:T:198:GLU:OE2	2.09	0.53
3:L:141:TYR:O	3:L:142:PRO:O	2.27	0.53
4:T:125:PRO:HG3	4:T:209:SER:HB2	1.89	0.53
1:C:291:ASP:OD2	1:C:292:LYS:N	2.42	0.53
1:A:223:VAL:HG22	1:C:207:ARG:HG2	1.90	0.53
3:U:149:TRP:CD1	3:U:160:VAL:HG11	2.44	0.53
1:E:25:LEU:HA	1:E:34:ILE:O	2.09	0.53
2:D:76:ARG:O	2:D:77:ILE:C	2.47	0.53
1:C:298:ASN:ND2	1:C:299:LYS:N	2.56	0.53
3:U:126:LEU:C	3:U:128:SER:N	2.61	0.53
3:U:19:VAL:CG2	3:U:79:LEU:HD23	2.38	0.53
1:A:250:ASN:N	1:A:250:ASN:OD1	2.41	0.53
1:E:36:VAL:HG22	1:E:37:THR:N	2.25	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:T:62:PRO:HG2	4:T:64:LEU:H	1.75	0.52
4:H:179:SER:O	4:H:180:ASP:HB2	2.08	0.52
1:C:303:GLY:O	1:C:305:CYS:SG	2.68	0.52
3:U:8:PRO:C	3:U:10:ILE:H	2.12	0.52
2:B:48:ILE:HG22	2:B:49:ASN:N	2.24	0.52
2:F:145:ASP:N	2:F:148:CYS:HB3	2.13	0.52
2:F:3:PHE:HB2	2:F:112:ASP:OD2	2.09	0.52
4:T:24:VAL:O	4:T:25:THR:HG23	2.08	0.52
4:T:201:THR:HG23	4:T:216:LYS:N	2.23	0.52
3:L:61:ALA:O	3:L:63:PHE:N	2.43	0.52
1:A:220:ARG:HE	1:C:210:GLN:HE21	1.57	0.52
2:B:121:LYS:NZ	2:B:122:THR:CG2	2.73	0.52
3:L:167:GLN:CG	3:L:172:SER:HA	2.40	0.52
3:U:39:GLN:HB2	3:U:45:PRO:HA	1.92	0.52
1:A:320:MET:HA	2:B:111:THR:HG21	1.91	0.52
2:D:127:ARG:H	2:D:159:HIS:HB2	1.74	0.52
3:L:95:PHE:HA	3:L:97:ARG:NH1	2.24	0.52
4:T:6:GLU:O	4:T:7:SER:HB2	2.09	0.52
3:L:8:PRO:C	3:L:10:ILE:H	2.10	0.52
1:A:312:ASN:HD22	1:A:312:ASN:N	1.96	0.52
1:C:166:VAL:HG22	1:C:245:ILE:HB	1.92	0.52
2:F:5:ALA:HB1	2:F:115:MET:HG2	1.91	0.52
1:A:87:PHE:O	1:A:267:ILE:HA	2.09	0.52
1:C:59:LEU:HD12	1:C:59:LEU:C	2.28	0.52
1:E:169:PRO:HA	1:E:242:VAL:HA	1.91	0.52
3:L:156:ARG:O	3:L:158:ASN:OD1	2.27	0.52
1:A:17:HIS:N	2:B:115:MET:HE1	2.25	0.52
2:D:98:LEU:C	2:D:100:VAL:N	2.58	0.52
3:L:95:PHE:HZ	4:H:60:TYR:CB	2.20	0.52
1:E:202:VAL:HG22	1:E:247:SER:OG	2.09	0.52
1:E:177:LEU:CD1	1:E:236:ILE:HG22	2.40	0.52
1:C:74:PRO:HD2	1:C:96:ASN:O	2.10	0.52
2:F:145:ASP:O	2:F:149:ILE:N	2.40	0.52
4:H:131:LEU:HG	4:H:147:CYS:N	2.24	0.52
3:L:116:VAL:HG12	3:L:117:SER:H	1.73	0.52
1:A:94:PHE:C	1:A:94:PHE:HD1	2.13	0.52
1:C:299:LYS:HA	1:C:308:TYR:CD1	2.44	0.52
1:E:17:HIS:CD2	2:F:6:ILE:HG23	2.34	0.52
2:F:154:ASN:HB3	2:F:156:THR:OG1	2.09	0.52
1:A:102:VAL:HB	1:A:105:TYR:HD2	1.74	0.52
1:A:38:ASN:HD22	1:A:318:THR:CB	2.23	0.52
1:A:307:LYS:HE2	2:B:60:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:6:ILE:O	2:B:8:GLY:N	2.43	0.52
2:D:121:LYS:HZ1	2:D:122:THR:CG2	2.20	0.52
2:D:121:LYS:HB3	2:D:121:LYS:HZ3	1.75	0.52
2:F:17:MET:SD	2:F:17:MET:C	2.88	0.52
4:H:155:GLU:OE2	4:H:156:PRO:HA	2.09	0.52
1:E:201:ARG:HG2	1:E:201:ARG:HH11	1.75	0.52
1:C:303:GLY:O	1:C:304:ALA:C	2.47	0.52
4:H:184:LEU:HD12	4:H:185:SER:N	2.24	0.52
2:D:78:GLN:O	2:D:79:ASP:C	2.46	0.52
2:B:110:LEU:HD13	2:B:110:LEU:O	2.10	0.52
2:B:3:PHE:HB2	2:B:112:ASP:OD2	2.10	0.52
1:A:42:LEU:HD22	2:B:55:VAL:HG11	1.91	0.52
1:C:294:PHE:HB3	1:C:309:VAL:CG2	2.40	0.52
2:F:111:THR:C	2:F:113:SER:N	2.62	0.52
2:F:139:LYS:C	2:F:140:ILE:HD12	2.29	0.52
3:L:52:THR:O	3:L:52:THR:HG22	2.10	0.52
3:L:141:TYR:CG	3:L:142:PRO:HD3	2.44	0.52
4:T:56:GLY:O	4:T:58:ASN:OD1	2.27	0.52
3:U:30:THR:O	3:U:32:SER:N	2.40	0.52
4:H:1:ASP:C	4:H:2:VAL:HG22	2.30	0.52
1:C:248:ASN:ND2	1:C:248:ASN:C	2.63	0.52
3:U:116:VAL:CG1	3:U:117:SER:H	2.22	0.52
1:A:316:LEU:HD12	2:B:104:ASN:OD1	2.09	0.52
1:C:319:GLY:HA2	2:D:21:TRP:CH2	2.44	0.52
2:F:51:LYS:O	2:F:54:ARG:HB2	2.10	0.52
4:T:33:TYR:CD2	4:T:99:PHE:O	2.55	0.52
2:F:38:LEU:C	2:F:40:SER:H	2.13	0.52
5:A:451:NAG:H2	1:E:222:TRP:CG	2.44	0.52
1:C:250:ASN:N	1:C:250:ASN:OD1	2.42	0.52
3:U:91:GLN:HE21	3:U:93:GLU:HB3	1.74	0.52
2:B:6:ILE:C	2:B:8:GLY:H	2.11	0.52
2:D:100:VAL:O	2:D:104:ASN:HB2	2.09	0.52
1:E:298:ASN:HD22	1:E:299:LYS:N	2.07	0.52
3:L:32:SER:O	3:L:33:PHE:CD1	2.62	0.52
1:E:127:TRP:CE3	1:E:164:LEU:HD23	2.45	0.52
4:H:206:HIS:CE1	4:H:208:ALA:HB3	2.44	0.52
3:U:91:GLN:HE21	3:U:93:GLU:CB	2.23	0.52
1:A:238:LYS:HE2	2:F:72:GLU:HG3	1.92	0.52
2:B:152:ILE:C	2:B:154:ASN:H	2.13	0.51
4:T:18:LEU:O	4:T:82:LYS:O	2.28	0.51
4:H:162:ASN:O	4:H:163:SER:HB2	2.10	0.51
4:T:195:TRP:O	4:T:197:SER:N	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:209:SER:OG	1:A:210:GLN:N	2.42	0.51
1:A:138:ALA:C	1:A:140:LYS:NZ	2.64	0.51
1:E:249:GLY:C	1:E:250:ASN:OD1	2.49	0.51
1:A:187:THR:C	1:A:189:GLN:H	2.12	0.51
1:E:62:ILE:HG22	1:E:63:ASP:N	2.25	0.51
1:A:320:MET:CA	2:B:111:THR:HG21	2.41	0.51
2:B:4:GLY:O	2:B:8:GLY:HA3	2.09	0.51
2:D:129:ASN:HD21	2:D:159:HIS:HA	1.75	0.51
2:F:171:PHE:HD1	2:F:171:PHE:H	1.55	0.51
4:H:34:TYR:O	4:H:36:THR:HG22	2.09	0.51
4:T:32:GLY:H	4:T:54:TYR:HB3	1.74	0.51
4:T:65:LYS:O	4:T:66:ASN:C	2.49	0.51
3:U:52:THR:HG23	3:U:72:TYR:HE2	1.73	0.51
4:H:67:ARG:HD2	4:H:83:LEU:O	2.09	0.51
1:A:187:THR:C	1:A:189:GLN:N	2.62	0.51
3:L:96:PRO:O	3:L:98:THR:HG23	2.10	0.51
2:F:42:GLN:O	2:F:46:ASP:N	2.43	0.51
2:B:102:LEU:O	2:B:103:GLU:C	2.49	0.51
2:B:3:PHE:CZ	2:F:2:LEU:O	2.63	0.51
2:D:6:ILE:C	2:D:8:GLY:N	2.63	0.51
2:B:91:LEU:HD21	2:D:92:TRP:NE1	2.25	0.51
4:T:207:PRO:O	4:T:208:ALA:C	2.48	0.51
4:H:65:LYS:C	4:H:67:ARG:N	2.63	0.51
1:A:109:ARG:NH1	1:A:109:ARG:HG2	2.25	0.51
1:A:211:GLN:NE2	1:A:235:THR:OG1	2.44	0.51
4:T:56:GLY:O	4:T:58:ASN:N	2.43	0.51
3:L:21:LEU:CD2	3:L:87:TYR:CD2	2.93	0.51
3:L:167:GLN:HG3	3:L:172:SER:HA	1.91	0.51
1:C:163:VAL:HG22	1:C:248:ASN:HB3	1.91	0.51
2:B:9:PHE:C	2:B:9:PHE:CD1	2.84	0.51
1:A:326:LYS:O	1:A:327:GLN:HB2	2.09	0.51
1:A:97:CYS:O	1:A:98:TYR:C	2.49	0.51
2:B:108:ILE:HG22	2:B:109:ASP:N	2.26	0.51
2:B:129:ASN:O	2:B:130:ALA:HB2	2.11	0.51
2:B:57:GLU:O	2:B:58:LYS:HG2	2.11	0.51
1:E:12:THR:HG23	2:F:138:PHE:O	2.10	0.51
4:H:61:ASN:HB3	4:H:62:PRO:CD	2.41	0.51
4:H:194:THR:HG23	4:H:198:GLU:OE2	2.10	0.51
1:E:172:ASP:CB	1:E:174:PHE:CE2	2.94	0.51
1:A:169:PRO:HA	1:A:242:VAL:HG23	1.93	0.51
2:F:9:PHE:HD1	2:F:10:ILE:N	2.09	0.51
1:A:143:PRO:HG2	1:A:144:GLY:H	1.75	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:67:GLU:O	2:F:68:LYS:HG3	2.11	0.51
4:H:128:VAL:HG11	4:H:204:VAL:HG21	1.92	0.51
3:L:36:TRP:CD2	3:L:74:LEU:HD23	2.45	0.51
3:U:168:ASP:CG	3:U:171:ASP:HB2	2.31	0.51
1:E:303:GLY:O	1:E:304:ALA:C	2.48	0.51
1:E:248:ASN:HD22	1:E:248:ASN:C	2.13	0.51
2:B:6:ILE:C	2:B:8:GLY:N	2.62	0.51
4:T:20:LEU:CD1	4:T:94:TYR:HB3	2.40	0.51
2:B:88:LYS:O	2:B:89:ILE:C	2.47	0.51
1:A:125:PHE:HB2	1:A:127:TRP:NE1	2.26	0.51
1:E:294:PHE:HE1	2:F:96:ALA:HB1	1.71	0.51
4:T:18:LEU:C	4:T:18:LEU:HD12	2.29	0.51
3:L:29:ILE:HD11	3:L:34:LEU:HD13	1.92	0.51
4:H:54:TYR:C	4:H:56:GLY:N	2.64	0.51
4:T:33:TYR:CE2	4:T:100:TYR:HB2	2.46	0.51
4:T:64:LEU:O	4:T:66:ASN:OD1	2.28	0.51
1:C:209:SER:O	1:C:210:GLN:CB	2.59	0.51
3:U:141:TYR:CG	3:U:142:PRO:CD	2.93	0.51
1:E:217:ILE:HG22	1:E:218:GLY:N	2.26	0.51
2:B:151:SER:O	2:B:156:THR:N	2.44	0.51
3:L:119:PHE:CD2	4:H:131:LEU:HB3	2.45	0.51
1:E:186:SER:O	1:E:218:GLY:O	2.29	0.51
2:F:52:LEU:O	2:F:53:ASN:C	2.45	0.51
1:C:140:LYS:HD2	1:C:140:LYS:N	2.26	0.51
2:D:102:LEU:O	2:D:103:GLU:C	2.49	0.51
1:E:288:ILE:HG21	1:E:297:VAL:HG21	1.91	0.51
4:H:161:TRP:CZ3	4:H:202:CYS:HB3	2.45	0.51
1:C:108:LEU:HG	1:C:108:LEU:O	2.10	0.51
1:C:320:MET:HB3	2:D:111:THR:HG21	1.93	0.50
4:T:161:TRP:HB3	4:T:166:LEU:HB2	1.93	0.50
1:A:121:ILE:HG13	1:A:257:TYR:CZ	2.46	0.50
4:H:195:TRP:CB	4:H:196:PRO:HD3	2.34	0.50
3:L:153:GLY:O	3:L:154:SER:HB2	2.10	0.50
3:U:174:TYR:CD2	3:U:174:TYR:N	2.79	0.50
1:A:294:PHE:HE1	2:B:96:ALA:HB1	1.72	0.50
2:D:121:LYS:HZ3	2:D:122:THR:N	2.09	0.50
1:E:316:LEU:HD12	2:F:104:ASN:OD1	2.11	0.50
1:C:29:ILE:O	2:F:51:LYS:HA	2.11	0.50
4:T:4:LEU:HD12	4:T:110:TRP:O	2.12	0.50
1:C:283:THR:O	1:C:285:ASN:N	2.44	0.50
4:H:201:THR:HG23	4:H:215:LYS:C	2.31	0.50
4:H:58:ASN:O	4:H:59:ASN:CB	2.58	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:127:TRP:CZ3	1:C:164:LEU:HD23	2.46	0.50
1:C:166:VAL:HG23	1:C:166:VAL:O	2.12	0.50
1:E:54:ASN:HB2	1:E:277:CYS:O	2.10	0.50
1:A:38:ASN:HD22	1:A:318:THR:HG21	1.76	0.50
2:F:26:HIS:O	2:F:32:THR:HA	2.11	0.50
2:B:3:PHE:CD2	2:B:113:SER:CA	2.85	0.50
1:C:15:LEU:HD23	1:C:15:LEU:N	2.26	0.50
1:C:294:PHE:HB3	1:C:309:VAL:HG21	1.92	0.50
1:E:10:THR:HG22	2:F:143:LYS:HD2	1.94	0.50
1:E:43:VAL:O	1:E:43:VAL:HG12	2.10	0.50
4:T:29:ILE:HG22	4:T:35:TRP:CD2	2.45	0.50
4:T:35:TRP:CD1	4:T:35:TRP:N	2.80	0.50
3:L:125:GLN:HB2	4:H:129:TYR:CD2	2.45	0.50
4:H:177:LEU:HB2	4:H:182:TYR:CE1	2.46	0.50
4:H:14:PRO:O	4:H:15:SER:CB	2.59	0.50
3:L:107:ILE:N	3:L:167:GLN:OE1	2.40	0.50
1:A:187:THR:O	1:A:190:GLU:N	2.44	0.50
2:F:163:ARG:O	2:F:164:ASP:C	2.50	0.50
2:D:91:LEU:O	2:D:92:TRP:C	2.46	0.50
1:E:285:ASN:HD22	1:E:298:ASN:HB2	1.75	0.50
1:C:13:LEU:O	2:D:138:PHE:HB2	2.10	0.50
1:E:72:GLY:CA	1:E:149:SER:OG	2.52	0.50
1:E:201:ARG:O	1:E:247:SER:HA	2.12	0.50
2:B:79:ASP:O	2:B:82:LYS:HB2	2.10	0.50
2:F:40:SER:OG	2:F:114:GLU:HB3	2.12	0.50
3:L:183:THR:OG1	3:L:186:GLU:HB2	2.11	0.50
1:A:191:GLN:HE22	1:A:250:ASN:HD21	1.58	0.50
2:D:76:ARG:O	2:D:78:GLN:N	2.44	0.50
3:L:44:SER:O	3:L:45:PRO:C	2.50	0.50
1:C:66:LEU:HD11	1:C:118:LEU:HD21	1.93	0.50
2:B:127:ARG:HG3	2:B:159:HIS:CG	2.47	0.50
2:B:25:ARG:HE	2:B:34:GLN:CD	2.15	0.50
1:C:283:THR:O	1:C:283:THR:HG23	2.12	0.50
3:L:8:PRO:HB2	3:L:103:THR:CG2	2.41	0.50
3:L:209:SER:OG	3:L:210:PHE:CD1	2.64	0.50
2:D:56:ILE:HG12	2:D:57:GLU:HG3	1.93	0.50
1:C:94:PHE:C	1:C:94:PHE:HD1	2.15	0.50
3:U:113:ALA:HB1	3:U:114:PRO:HD2	1.94	0.50
1:C:43:VAL:O	1:C:45:SER:N	2.45	0.50
2:F:127:ARG:HH11	2:F:127:ARG:CB	2.16	0.50
4:T:28:SER:O	4:T:31:SER:N	2.39	0.50
3:U:74:LEU:O	3:U:75:THR:HB	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:21:TRP:CD2	2:D:45:ILE:HD11	2.45	0.50
1:E:19:ALA:O	1:E:20:VAL:HG13	2.12	0.50
1:C:283:THR:O	1:C:284:PRO:C	2.49	0.50
4:H:128:VAL:CG1	4:H:204:VAL:HG21	2.41	0.50
4:T:12:VAL:O	4:T:118:VAL:HA	2.12	0.50
1:A:64:CYS:SG	1:A:75:HIS:CE1	3.04	0.50
1:C:312:ASN:O	1:C:313:THR:HB	2.12	0.50
4:T:3:HIS:ND1	4:T:4:LEU:N	2.60	0.50
3:L:141:TYR:CD2	3:L:142:PRO:HD3	2.46	0.50
4:H:145:LEU:HB2	4:H:188:VAL:CG1	2.42	0.50
1:A:140:LYS:H	1:A:140:LYS:HD2	1.70	0.50
1:A:140:LYS:HD2	1:A:140:LYS:O	2.11	0.50
1:C:251:LEU:CD2	1:C:253:ALA:HB2	2.41	0.50
2:B:128:GLU:HA	2:B:170:ARG:NH2	2.26	0.50
1:C:9:SER:C	2:D:143:LYS:HE3	2.32	0.50
1:E:320:MET:O	1:E:321:ARG:O	2.30	0.50
1:E:41:GLU:OE2	1:E:314:LEU:N	2.41	0.50
2:F:102:LEU:O	2:F:104:ASN:N	2.45	0.50
3:L:126:LEU:C	3:L:128:SER:N	2.65	0.50
4:H:190:VAL:CG2	4:H:195:TRP:HB2	2.42	0.50
4:T:37:TRP:CZ3	4:T:96:CYS:HB3	2.47	0.50
3:L:8:PRO:HG2	3:L:11:MET:HE2	1.94	0.50
3:U:186:GLU:HG3	3:U:189:ARG:CZ	2.42	0.50
2:D:18:ILE:C	2:D:20:GLY:H	2.15	0.50
2:B:166:ALA:H	2:B:168:ASN:ND2	2.09	0.49
1:E:17:HIS:HA	2:F:22:TYR:HD2	1.77	0.49
4:T:195:TRP:O	4:T:198:GLU:N	2.45	0.49
2:F:17:MET:CE	2:F:19:ASP:H	2.15	0.49
4:T:61:ASN:CB	4:T:62:PRO:CD	2.90	0.49
1:A:212:THR:CG2	1:E:216:ASN:HB3	2.37	0.49
3:L:118:ILE:CD1	3:L:135:CYS:HB2	2.42	0.49
1:A:62:ILE:HG22	1:A:63:ASP:N	2.22	0.49
2:F:6:ILE:CG1	2:F:112:ASP:HA	2.38	0.49
4:T:4:LEU:HA	4:T:23:TYR:O	2.12	0.49
3:L:29:ILE:HD11	3:L:34:LEU:CD1	2.42	0.49
1:E:169:PRO:HA	1:E:242:VAL:HG23	1.94	0.49
3:U:191:ASN:HD22	3:U:191:ASN:N	2.09	0.49
1:E:147:PHE:CE2	1:E:153:TRP:HB2	2.47	0.49
4:H:114:THR:HG23	4:H:114:THR:O	2.12	0.49
4:H:129:TYR:HB2	4:H:148:LEU:CD2	2.42	0.49
4:H:3:HIS:O	4:H:24:VAL:HA	2.11	0.49
4:H:159:VAL:HG11	4:H:186:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:217:ILE:CD1	1:E:217:ILE:N	2.75	0.49
2:F:115:MET:C	2:F:117:LYS:N	2.61	0.49
3:U:4:LEU:N	3:U:4:LEU:CD1	2.75	0.49
1:E:138:ALA:HB1	1:E:224:ARG:HG2	1.93	0.49
3:L:125:GLN:HB2	4:H:129:TYR:CG	2.48	0.49
1:C:161:TYR:N	1:C:196:VAL:HG21	2.28	0.49
4:H:20:LEU:HB2	4:H:81:LEU:HB3	1.95	0.49
3:U:137:LEU:CD2	3:U:145:ILE:HD13	2.26	0.49
1:C:226:LEU:HD21	4:T:104:ASP:CB	2.42	0.49
2:D:110:LEU:HD13	2:D:110:LEU:O	2.12	0.49
2:F:24:PHE:CE1	2:F:153:ARG:HG3	2.48	0.49
3:L:127:THR:HG22	3:L:127:THR:O	2.12	0.49
4:T:161:TRP:CB	4:T:166:LEU:HB2	2.42	0.49
3:U:14:SER:HB3	3:U:108:LYS:HB2	1.94	0.49
2:F:125:GLN:OE1	2:F:152:ILE:HG23	2.13	0.49
2:D:68:LYS:HE2	2:D:85:GLU:OE2	2.12	0.49
3:U:151:ILE:CA	3:U:192:SER:O	2.60	0.49
4:H:65:LYS:O	4:H:66:ASN:C	2.50	0.49
1:E:153:TRP:C	1:E:154:LEU:HD23	2.33	0.49
2:D:52:LEU:O	2:D:53:ASN:C	2.51	0.49
2:B:51:LYS:NZ	2:B:106:HIS:ND1	2.58	0.49
2:B:140:ILE:HD12	2:B:140:ILE:N	2.27	0.49
1:C:312:ASN:ND2	1:C:313:THR:HG22	2.28	0.49
1:E:29:ILE:HD11	2:F:102:LEU:CD2	2.23	0.49
2:D:149:ILE:C	2:D:151:SER:N	2.57	0.49
4:T:6:GLU:O	4:T:7:SER:CB	2.61	0.49
3:U:205:PRO:O	3:U:206:ILE:C	2.50	0.49
1:C:136:SER:OG	4:T:104:ASP:OD1	2.23	0.49
1:A:39:ALA:HA	1:A:316:LEU:O	2.13	0.49
1:C:10:THR:CG2	2:D:141:TYR:O	2.60	0.49
3:L:151:ILE:HA	3:L:192:SER:O	2.12	0.49
3:U:96:PRO:HA	4:T:48:TRP:CZ3	2.47	0.49
3:L:58:GLY:O	3:L:59:VAL:C	2.50	0.49
2:B:9:PHE:C	2:B:9:PHE:HD1	2.16	0.49
3:U:134:VAL:HA	3:U:179:THR:HA	1.94	0.49
1:C:80:GLN:O	1:C:81:ASN:C	2.51	0.49
1:C:82:GLU:OE2	1:C:82:GLU:CA	2.59	0.49
1:C:74:PRO:CG	1:C:139:CYS:SG	3.00	0.49
2:D:88:LYS:O	2:D:89:ILE:C	2.51	0.49
1:E:37:THR:HG23	1:E:321:ARG:O	2.12	0.49
1:C:283:THR:HG23	1:C:285:ASN:CA	2.42	0.49
3:L:124:ILE:O	3:L:127:THR:N	2.46	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:ILE:HG13	1:A:257:TYR:CE1	2.47	0.49
1:A:50:LYS:O	1:A:286:GLY:O	2.31	0.49
2:B:48:ILE:HD11	2:B:107:THR:CG2	2.43	0.49
3:L:168:ASP:CG	3:L:169:SER:N	2.66	0.49
1:A:19:ALA:HB1	1:A:322:ASN:OD1	2.12	0.49
2:D:24:PHE:CE1	2:D:153:ARG:HG3	2.48	0.49
3:L:29:ILE:HA	3:L:93:GLU:OE1	2.13	0.49
1:A:59:LEU:HD12	1:A:59:LEU:C	2.32	0.49
4:H:190:VAL:HB	4:H:191:PRO:CD	2.42	0.49
1:A:139:CYS:SG	1:A:147:PHE:O	2.70	0.49
2:B:117:LYS:HE3	2:F:4:GLY:CA	2.42	0.49
1:C:321:ARG:HG2	1:C:322:ASN:N	2.24	0.49
2:D:127:ARG:HD2	2:D:159:HIS:CE1	2.48	0.49
1:E:10:THR:HG22	2:F:142:HIS:C	2.34	0.49
2:D:150:GLU:HG3	2:D:150:GLU:O	2.12	0.49
4:T:180:ASP:C	4:T:181:LEU:HD22	2.32	0.49
4:T:188:VAL:CG2	4:T:189:THR:N	2.74	0.49
1:A:82:GLU:OE2	1:A:82:GLU:CA	2.61	0.49
2:D:67:GLU:O	2:D:68:LYS:HG3	2.13	0.49
2:D:106:HIS:ND1	2:D:106:HIS:C	2.65	0.49
1:C:221:PRO:HG2	1:E:206:THR:C	2.34	0.49
2:F:70:PHE:HD1	2:F:82:LYS:HE3	1.77	0.49
2:F:55:VAL:HG12	2:F:56:ILE:H	1.71	0.48
3:U:33:PHE:CZ	4:T:101:TYR:HE1	2.31	0.48
3:U:74:LEU:O	3:U:75:THR:CB	2.60	0.48
3:L:63:PHE:HE1	3:L:76:ILE:HD11	1.78	0.48
3:L:137:LEU:O	3:L:140:PHE:HE1	1.96	0.48
1:A:307:LYS:HD3	2:B:92:TRP:CZ2	2.48	0.48
1:C:43:VAL:HA	1:C:294:PHE:O	2.13	0.48
1:C:36:VAL:CG2	1:C:37:THR:N	2.77	0.48
2:D:168:ASN:C	2:D:170:ARG:N	2.67	0.48
1:E:12:THR:HB	2:F:27:GLN:CB	2.40	0.48
1:E:14:CYS:HA	2:F:137:CYS:HA	1.95	0.48
2:F:171:PHE:N	2:F:171:PHE:CD1	2.73	0.48
3:L:124:ILE:O	3:L:126:LEU:N	2.46	0.48
1:E:170:ASN:OD1	1:E:176:LYS:HD3	2.12	0.48
1:C:209:SER:OG	1:C:210:GLN:N	2.41	0.48
2:B:76:ARG:O	2:B:77:ILE:C	2.49	0.48
2:B:38:LEU:O	2:B:40:SER:N	2.47	0.48
1:E:283:THR:HG22	1:E:287:SER:N	2.28	0.48
2:F:107:THR:O	2:F:110:LEU:HB3	2.13	0.48
2:F:149:ILE:C	2:F:151:SER:N	2.64	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:97:ARG:CB	4:H:48:TRP:CG	2.96	0.48
1:C:61:GLY:O	1:C:62:ILE:HB	2.14	0.48
3:L:116:VAL:HG13	3:L:137:LEU:HD12	1.95	0.48
1:E:130:VAL:HG13	1:E:162:PRO:HD2	1.95	0.48
4:H:27:TYR:CE1	4:H:31:SER:HB2	2.48	0.48
4:T:159:VAL:CG2	4:T:160:THR:N	2.76	0.48
3:L:162:ASN:HA	3:L:177:SER:O	2.14	0.48
3:U:131:ALA:O	3:U:181:THR:HA	2.13	0.48
1:C:17:HIS:ND1	1:C:18:HIS:N	2.60	0.48
1:C:54:ASN:ND2	1:C:55:PRO:HA	2.23	0.48
4:H:149:VAL:O	4:H:183:THR:HA	2.13	0.48
3:L:183:THR:O	3:L:184:LYS:C	2.49	0.48
3:U:137:LEU:O	3:U:175:SER:HA	2.14	0.48
1:C:76:CYS:O	1:C:77:ASP:C	2.52	0.48
1:A:18:HIS:CA	2:B:14:TRP:HB2	2.31	0.48
2:B:167:LEU:HB3	2:F:171:PHE:CD2	2.37	0.48
2:B:170:ARG:NH1	2:D:127:ARG:HH22	2.10	0.48
2:B:56:ILE:HG12	2:B:57:GLU:HG3	1.94	0.48
1:C:320:MET:HB3	2:D:111:THR:CG2	2.44	0.48
2:F:108:ILE:HG22	2:F:109:ASP:N	2.27	0.48
2:B:124:ARG:NH2	2:F:132:GLU:HB3	2.26	0.48
3:L:122:SER:O	3:L:126:LEU:HG	2.14	0.48
2:F:121:LYS:HZ1	2:F:122:THR:CA	2.27	0.48
2:F:122:THR:O	2:F:124:ARG:N	2.33	0.48
1:A:283:THR:C	1:A:285:ASN:N	2.63	0.48
2:D:80:LEU:O	2:D:81:GLU:C	2.51	0.48
3:L:81:ALA:O	3:L:107:ILE:CD1	2.61	0.48
2:B:21:TRP:CE2	2:B:45:ILE:HD11	2.49	0.48
2:D:91:LEU:O	2:D:93:SER:N	2.46	0.48
2:B:149:ILE:C	2:B:151:SER:N	2.65	0.48
1:E:108:LEU:HG	1:E:108:LEU:O	2.13	0.48
1:C:176:LYS:HD2	1:C:257:TYR:CG	2.49	0.48
3:U:141:TYR:CG	3:U:142:PRO:N	2.81	0.48
4:T:184:LEU:HD12	4:T:185:SER:CA	2.42	0.48
3:U:2:ILE:HG22	3:U:4:LEU:HD12	1.96	0.48
2:D:10:ILE:O	2:D:12:ASN:N	2.44	0.48
1:A:275:ASP:CG	1:A:276:THR:N	2.67	0.48
1:C:72:GLY:HA3	1:C:149:SER:OG	2.13	0.48
1:C:236:ILE:O	1:C:236:ILE:HG13	2.13	0.48
4:T:2:VAL:HB	4:T:109:TYR:CD2	2.47	0.48
1:A:121:ILE:CG1	1:A:257:TYR:CE1	2.96	0.48
1:E:22:ASN:N	1:E:22:ASN:HD22	2.01	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:9:PHE:C	2:F:9:PHE:CD1	2.87	0.48
1:A:17:HIS:CG	1:A:18:HIS:N	2.80	0.48
2:D:89:ILE:HD12	2:D:89:ILE:H	1.79	0.48
1:E:283:THR:C	1:E:285:ASN:N	2.66	0.48
4:T:161:TRP:CD1	4:T:170:VAL:HG11	2.47	0.48
1:C:186:SER:O	1:C:218:GLY:O	2.31	0.48
4:H:146:GLY:O	4:H:161:TRP:HH2	1.97	0.48
3:L:149:TRP:O	3:L:154:SER:HB3	2.14	0.48
1:C:191:GLN:OE1	1:C:250:ASN:ND2	2.45	0.48
1:A:10:THR:CG2	2:B:143:LYS:HD2	2.41	0.48
2:B:4:GLY:O	2:B:5:ALA:O	2.31	0.48
2:D:3:PHE:HB3	2:D:112:ASP:O	2.14	0.48
3:L:121:PRO:HB2	3:L:126:LEU:CD2	2.32	0.48
4:T:201:THR:OG1	4:T:216:LYS:HA	2.13	0.48
1:A:111:LEU:C	1:A:111:LEU:HD12	2.33	0.48
4:H:177:LEU:HD12	4:H:178:GLN:H	1.79	0.48
1:E:164:LEU:O	1:E:246:ASN:HA	2.14	0.48
1:E:54:ASN:HD22	1:E:55:PRO:HA	1.79	0.48
2:D:43:ALA:O	2:D:46:ASP:HB2	2.13	0.48
1:C:275:ASP:CG	1:C:276:THR:N	2.67	0.48
2:F:26:HIS:O	2:F:26:HIS:ND1	2.47	0.48
1:C:309:VAL:CG1	2:D:93:SER:HA	2.40	0.48
1:E:18:HIS:HA	2:F:14:TRP:CB	2.36	0.48
2:F:88:LYS:O	2:F:89:ILE:C	2.52	0.48
1:A:13:LEU:CD1	2:B:24:PHE:HB3	2.38	0.48
3:L:91:GLN:HE21	3:L:93:GLU:CB	2.27	0.48
1:C:202:VAL:O	1:C:212:THR:HG23	2.13	0.48
1:A:176:LYS:HE3	1:A:178:TYR:OH	2.14	0.48
1:E:182:ILE:HG22	1:E:231:SER:HB2	1.95	0.48
2:B:96:ALA:C	2:B:98:LEU:H	2.17	0.47
1:E:318:THR:O	2:F:48:ILE:HG21	2.13	0.47
1:E:36:VAL:HG23	1:E:320:MET:O	2.14	0.47
2:B:28:ASN:CB	2:B:144:CYS:O	2.58	0.47
4:T:201:THR:HG22	4:T:202:CYS:O	2.14	0.47
3:U:32:SER:C	3:U:33:PHE:CD1	2.88	0.47
3:L:63:PHE:CE1	3:L:76:ILE:HD11	2.48	0.47
2:B:82:LYS:O	2:B:84:VAL:N	2.47	0.47
3:U:207:VAL:O	3:U:208:LYS:HG2	2.14	0.47
1:E:318:THR:O	1:E:318:THR:HG22	2.13	0.47
1:E:98:TYR:HE2	1:E:229:ARG:HA	1.78	0.47
4:T:188:VAL:CG2	4:T:189:THR:H	2.27	0.47
3:U:97:ARG:N	4:T:48:TRP:CE3	2.82	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:19:VAL:O	3:L:75:THR:HA	2.14	0.47
1:C:108:LEU:CD1	1:C:234:TRP:CE3	2.92	0.47
4:H:188:VAL:HG22	4:H:189:THR:H	1.69	0.47
4:H:87:THR:HG23	4:H:90:ASP:H	1.78	0.47
3:L:107:ILE:HG22	3:L:108:LYS:H	1.79	0.47
3:U:186:GLU:O	3:U:189:ARG:HB2	2.14	0.47
1:C:55:PRO:HG3	1:C:280:GLU:CD	2.34	0.47
1:E:242:VAL:HG22	1:E:243:LEU:N	2.29	0.47
1:E:48:THR:HG23	1:E:49:GLY:N	2.29	0.47
4:T:5:GLN:HA	4:T:5:GLN:OE1	2.14	0.47
2:D:94:TYR:CE2	2:F:95:ASN:HB3	2.48	0.47
1:A:73:ASP:OD1	1:A:75:HIS:CD2	2.68	0.47
1:A:36:VAL:CG2	1:A:320:MET:O	2.62	0.47
1:C:38:ASN:HD22	1:C:318:THR:HB	1.79	0.47
2:F:140:ILE:N	2:F:140:ILE:HD12	2.28	0.47
1:A:13:LEU:O	2:B:138:PHE:HB2	2.15	0.47
1:A:283:THR:HG22	1:A:287:SER:N	2.29	0.47
3:U:150:LYS:HB2	3:U:194:THR:OG1	2.13	0.47
1:C:109:ARG:HH11	1:C:109:ARG:HG2	1.79	0.47
1:C:33:GLN:O	1:C:34:ILE:HG13	2.13	0.47
1:C:249:GLY:C	1:C:250:ASN:OD1	2.52	0.47
2:D:38:LEU:C	2:D:40:SER:N	2.66	0.47
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.50	0.47
1:C:81:ASN:ND2	1:C:119:GLU:HA	2.29	0.47
1:C:44:GLN:N	1:C:294:PHE:O	2.45	0.47
4:T:91:THR:HB	4:T:118:VAL:H	1.80	0.47
4:T:86:VAL:HG22	4:T:87:THR:O	2.13	0.47
1:C:220:ARG:HH21	1:E:210:GLN:HE21	1.63	0.47
2:D:3:PHE:HB2	2:D:112:ASP:O	2.13	0.47
2:D:129:ASN:O	2:D:130:ALA:CB	2.62	0.47
1:E:50:LYS:O	1:E:286:GLY:O	2.32	0.47
2:B:145:ASP:N	2:B:148:CYS:HB3	2.16	0.47
4:T:56:GLY:C	4:T:58:ASN:N	2.67	0.47
4:T:54:TYR:C	4:T:56:GLY:H	2.17	0.47
1:A:266:SER:OG	1:A:267:ILE:N	2.47	0.47
1:E:209:SER:OG	1:E:210:GLN:N	2.45	0.47
2:D:57:GLU:O	2:D:58:LYS:CG	2.62	0.47
2:F:26:HIS:O	2:F:32:THR:HG22	2.14	0.47
4:H:41:PHE:HD1	4:H:92:ALA:HB2	1.80	0.47
1:E:324:PRO:HB3	1:E:328:THR:HB	1.96	0.47
4:T:22:CYS:HB3	4:T:79:PHE:CE1	2.49	0.47
4:T:28:SER:HA	4:T:77:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:164:TRP:CG	3:U:176:MET:HG3	2.49	0.47
4:T:146:GLY:O	4:T:161:TRP:HH2	1.96	0.47
3:L:95:PHE:HD1	3:L:97:ARG:HH12	1.63	0.47
4:H:126:PRO:CB	4:H:152:TYR:HB3	2.34	0.47
4:T:88:ALA:O	4:T:91:THR:HG22	2.14	0.47
3:L:35:TYR:HD2	3:L:50:TYR:HA	1.78	0.47
2:D:67:GLU:C	2:D:68:LYS:HG3	2.35	0.47
3:U:141:TYR:O	3:U:142:PRO:O	2.32	0.47
3:U:173:THR:C	3:U:174:TYR:CD2	2.88	0.47
2:F:39:LYS:O	2:F:39:LYS:HG2	2.15	0.47
1:E:182:ILE:HD11	1:E:215:PRO:HD3	1.95	0.47
2:F:120:GLU:HA	2:F:120:GLU:OE1	2.14	0.47
2:B:103:GLU:OE1	1:E:29:ILE:HG23	2.14	0.47
1:C:312:ASN:N	1:C:312:ASN:HD22	2.11	0.47
2:B:125:GLN:OE1	2:B:152:ILE:HG23	2.15	0.47
1:C:35:GLU:HG2	1:C:322:ASN:HD22	1.79	0.47
2:F:141:TYR:OH	2:F:170:ARG:HG2	2.15	0.47
2:F:85:GLU:HG3	2:F:89:ILE:HD13	1.96	0.47
2:D:28:ASN:CB	2:D:144:CYS:O	2.59	0.47
3:U:125:GLN:HB2	4:T:129:TYR:CG	2.49	0.47
3:L:35:TYR:CD1	3:L:35:TYR:N	2.81	0.47
3:L:74:LEU:O	3:L:75:THR:CB	2.63	0.47
3:L:74:LEU:O	3:L:75:THR:HB	2.15	0.47
1:E:176:LYS:HD2	1:E:257:TYR:CD2	2.49	0.47
1:A:32:ASP:O	1:A:33:GLN:NE2	2.46	0.47
3:U:11:MET:O	3:U:105:LEU:HA	2.14	0.47
1:C:54:ASN:HB3	1:C:278:ILE:HD13	1.95	0.47
2:F:38:LEU:C	2:F:40:SER:N	2.68	0.47
1:E:54:ASN:CB	1:E:278:ILE:HD13	2.44	0.47
1:C:117:THR:O	1:C:117:THR:CG2	2.62	0.47
2:B:117:LYS:CE	2:F:4:GLY:HA2	2.42	0.47
2:F:67:GLU:C	2:F:68:LYS:HG3	2.35	0.47
2:F:96:ALA:C	2:F:98:LEU:N	2.68	0.47
1:C:13:LEU:HD13	1:C:14:CYS:N	2.30	0.47
4:T:126:PRO:HB3	4:T:152:TYR:CB	2.32	0.47
3:L:123:LYS:CD	3:L:124:ILE:HG13	2.45	0.47
1:C:246:ASN:C	1:C:246:ASN:ND2	2.63	0.47
1:E:251:LEU:HD21	1:E:253:ALA:HB2	1.97	0.47
4:H:20:LEU:HD23	4:H:20:LEU:HA	1.63	0.47
1:E:270:SER:HB2	1:E:284:PRO:HA	1.97	0.47
1:A:35:GLU:O	1:A:322:ASN:HB3	2.14	0.47
1:C:15:LEU:HD11	2:D:119:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:295:GLN:OE1	1:C:297:VAL:N	2.46	0.47
2:F:55:VAL:CG1	2:F:56:ILE:N	2.55	0.47
1:C:174:PHE:N	1:C:174:PHE:CD2	2.83	0.47
2:B:21:TRP:CD2	2:B:45:ILE:HD11	2.50	0.47
1:A:41:GLU:HG3	1:A:42:LEU:N	2.29	0.47
2:B:2:LEU:O	2:D:3:PHE:CZ	2.68	0.47
1:C:294:PHE:CE1	2:D:96:ALA:CB	2.97	0.47
2:D:121:LYS:NZ	2:D:122:THR:CG2	2.76	0.47
2:D:130:ALA:CB	2:D:139:LYS:O	2.59	0.47
1:E:14:CYS:O	2:F:25:ARG:N	2.48	0.47
2:F:129:ASN:O	2:F:130:ALA:HB2	2.14	0.47
1:E:141:ARG:HH11	1:E:141:ARG:CG	2.21	0.47
4:T:123:THR:HA	4:T:154:PRO:HD3	1.96	0.47
4:T:54:TYR:O	4:T:56:GLY:N	2.48	0.47
4:T:40:GLN:HB3	4:T:46:LEU:HD23	1.97	0.47
2:D:48:ILE:HG22	2:D:49:ASN:N	2.30	0.46
1:C:121:ILE:HG13	1:C:257:TYR:CZ	2.50	0.46
4:H:177:LEU:HD12	4:H:178:GLN:N	2.30	0.46
2:B:67:GLU:O	2:B:68:LYS:HG3	2.15	0.46
1:C:323:VAL:HA	1:C:324:PRO:HD3	1.79	0.46
1:A:29:ILE:CG2	2:D:103:GLU:OE1	2.62	0.46
2:D:119:PHE:O	2:D:123:ARG:HB2	2.15	0.46
1:E:283:THR:HG23	1:E:285:ASN:C	2.35	0.46
2:F:145:ASP:O	2:F:149:ILE:HG12	2.14	0.46
2:B:30:GLU:OE2	2:B:145:ASP:HB2	2.15	0.46
4:T:2:VAL:HG13	4:T:24:VAL:HG23	1.97	0.46
4:T:177:LEU:HD12	4:T:178:GLN:N	2.31	0.46
3:U:133:VAL:N	3:U:180:LEU:O	2.32	0.46
3:L:63:PHE:CE1	3:L:76:ILE:CD1	2.98	0.46
3:U:118:ILE:HD11	3:U:149:TRP:CZ3	2.51	0.46
1:E:247:SER:CB	1:E:251:LEU:HB2	2.46	0.46
2:D:9:PHE:CD1	2:D:9:PHE:C	2.89	0.46
1:E:87:PHE:O	1:E:267:ILE:HA	2.15	0.46
2:B:166:ALA:N	2:B:168:ASN:ND2	2.59	0.46
2:B:165:GLU:CA	2:B:168:ASN:HD21	2.29	0.46
1:E:283:THR:O	1:E:283:THR:HG23	2.14	0.46
2:F:106:HIS:O	2:F:106:HIS:CG	2.68	0.46
2:F:132:GLU:HG3	2:F:137:CYS:O	2.16	0.46
2:F:6:ILE:C	2:F:8:GLY:H	2.18	0.46
1:E:70:LEU:HD22	1:E:112:VAL:HG21	1.97	0.46
2:F:121:LYS:HZ1	2:F:122:THR:N	2.12	0.46
1:E:132:GLN:O	1:E:133:ASN:C	2.53	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:48:ILE:CD1	2:D:107:THR:HG23	2.36	0.46
4:T:28:SER:C	4:T:30:THR:N	2.64	0.46
1:C:283:THR:C	1:C:285:ASN:H	2.17	0.46
3:L:124:ILE:O	3:L:125:GLN:C	2.54	0.46
4:H:201:THR:HG21	4:H:214:ASP:HB2	1.97	0.46
4:T:62:PRO:HG2	4:T:63:SER:N	2.29	0.46
3:L:79:LEU:HD13	3:L:80:GLU:N	2.30	0.46
4:H:84:ASN:HB3	4:H:85:SER:H	1.42	0.46
1:A:25:LEU:HD23	1:A:34:ILE:C	2.36	0.46
1:A:118:LEU:N	1:A:118:LEU:HD23	2.30	0.46
1:C:85:ASP:HA	1:C:265:SER:HB3	1.96	0.46
1:E:312:ASN:H	1:E:312:ASN:ND2	2.14	0.46
3:U:175:SER:OG	4:T:171:HIS:ND1	2.49	0.46
2:D:171:PHE:H	2:D:171:PHE:HD1	1.56	0.46
1:C:121:ILE:CG1	1:C:257:TYR:CE1	2.98	0.46
1:A:222:TRP:CG	5:C:451:NAG:H2	2.50	0.46
4:T:67:ARG:CB	4:T:84:ASN:HB2	2.45	0.46
2:D:80:LEU:O	2:D:82:LYS:N	2.49	0.46
4:H:87:THR:HG23	4:H:89:GLU:HB2	1.97	0.46
1:E:195:TYR:O	1:E:196:VAL:HB	2.15	0.46
3:L:25:ALA:O	3:L:27:SER:O	2.34	0.46
1:E:248:ASN:ND2	1:E:248:ASN:C	2.69	0.46
1:E:268:MET:SD	1:E:284:PRO:HG3	2.56	0.46
1:E:53:ASN:OD1	1:E:276:THR:HA	2.16	0.46
1:E:167:THR:HG23	1:E:167:THR:O	2.13	0.46
2:D:89:ILE:CD1	2:D:89:ILE:H	2.28	0.46
2:D:89:ILE:N	2:D:89:ILE:HD12	2.30	0.46
1:E:29:ILE:HG12	2:F:101:ALA:O	2.15	0.46
3:L:34:LEU:HD22	3:L:72:TYR:CD2	2.50	0.46
4:T:142:MET:HA	4:T:192:SER:CA	2.37	0.46
4:T:143:VAL:O	4:T:189:THR:HG23	2.16	0.46
1:E:15:LEU:HD11	2:F:119:PHE:HB2	1.97	0.46
4:H:107:PHE:HE1	4:H:109:TYR:HE1	1.63	0.46
1:A:237:VAL:CG1	1:A:241:ASP:HB3	2.41	0.46
3:U:66:SER:HB3	3:U:73:SER:OG	2.15	0.46
1:E:217:ILE:HD12	1:E:217:ILE:H	1.79	0.46
1:E:48:THR:HG23	1:E:49:GLY:H	1.81	0.46
1:E:312:ASN:HD22	1:E:312:ASN:N	2.13	0.46
1:C:98:TYR:CZ	1:C:226:LEU:HD13	2.50	0.46
1:A:17:HIS:CE1	2:B:13:GLY:HA2	2.48	0.46
2:B:5:ALA:O	2:B:8:GLY:N	2.47	0.46
2:F:168:ASN:O	2:F:170:ARG:N	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:145:ASP:O	2:D:149:ILE:HG12	2.16	0.46
4:H:128:VAL:O	4:H:215:LYS:HE3	2.16	0.46
4:H:216:LYS:HE2	4:T:194:THR:OG1	2.15	0.46
1:A:84:TRP:HZ2	1:A:113:ALA:HA	1.80	0.46
4:T:33:TYR:HE2	4:T:100:TYR:HB2	1.80	0.46
3:U:25:ALA:O	3:U:26:SER:C	2.54	0.46
1:A:191:GLN:OE1	1:A:250:ASN:ND2	2.48	0.46
2:D:76:ARG:O	2:D:79:ASP:N	2.48	0.46
2:B:16:GLY:O	2:B:18:ILE:HG23	2.16	0.46
2:B:51:LYS:HA	1:E:29:ILE:O	2.15	0.46
1:C:15:LEU:HD23	1:C:15:LEU:H	1.80	0.46
2:D:6:ILE:N	2:D:112:ASP:OD1	2.49	0.46
1:C:170:ASN:CB	1:C:176:LYS:HE2	2.33	0.46
4:T:33:TYR:HD2	4:T:99:PHE:C	2.19	0.46
4:T:51:TYR:CE1	4:T:60:TYR:HB2	2.51	0.46
3:U:38:GLN:NE2	3:U:48:TRP:CZ2	2.84	0.46
1:A:209:SER:O	1:A:210:GLN:CB	2.64	0.46
1:A:206:THR:CA	1:E:221:PRO:HG2	2.46	0.46
1:A:201:ARG:HH12	1:A:246:ASN:ND2	2.12	0.46
3:U:11:MET:O	3:U:105:LEU:HD12	2.16	0.46
3:L:187:TYR:C	3:L:189:ARG:N	2.68	0.46
1:E:209:SER:O	1:E:210:GLN:HB2	2.15	0.46
1:A:139:CYS:O	1:A:146:GLY:O	2.34	0.46
2:B:43:ALA:O	2:B:46:ASP:HB2	2.15	0.46
2:D:127:ARG:HG3	2:D:159:HIS:CE1	2.51	0.46
2:F:105:GLN:O	2:F:108:ILE:HB	2.16	0.46
2:F:4:GLY:O	2:F:8:GLY:HA3	2.16	0.46
1:A:55:PRO:HG3	1:A:280:GLU:OE1	2.15	0.46
4:T:70:ILE:CG2	4:T:71:THR:N	2.79	0.46
4:T:140:ASN:HD22	4:T:140:ASN:HA	1.64	0.46
1:C:136:SER:CB	4:T:104:ASP:OD1	2.64	0.46
2:B:40:SER:HA	2:B:43:ALA:HB3	1.97	0.46
1:C:44:GLN:HG3	1:C:44:GLN:O	2.16	0.46
4:T:162:ASN:HD21	4:T:201:THR:N	2.14	0.46
4:T:15:SER:N	4:T:86:VAL:O	2.49	0.46
3:U:32:SER:O	3:U:33:PHE:HD1	1.98	0.46
4:H:144:THR:O	4:H:145:LEU:HD23	2.16	0.46
3:U:12:SER:HA	3:U:106:GLU:O	2.17	0.46
4:H:41:PHE:HB3	4:H:42:PRO:HD2	1.97	0.46
1:E:85:ASP:O	1:E:265:SER:HA	2.16	0.46
2:D:14:TRP:CH2	2:D:23:GLY:O	2.69	0.45
2:F:127:ARG:HG3	2:F:159:HIS:CG	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:24:PHE:O	2:F:34:GLN:HA	2.16	0.45
4:T:155:GLU:HG2	4:T:182:TYR:CE2	2.51	0.45
1:A:174:PHE:CE1	1:A:259:LYS:HG3	2.51	0.45
3:L:48:TRP:CZ2	3:L:59:VAL:HG13	2.51	0.45
4:H:67:ARG:NH1	4:H:90:ASP:OD1	2.47	0.45
1:A:298:ASN:ND2	1:A:299:LYS:N	2.61	0.45
3:L:185:ASP:O	3:L:188:GLU:N	2.49	0.45
1:A:98:TYR:CD2	1:A:99:PRO:HD2	2.51	0.45
2:F:168:ASN:C	2:F:170:ARG:H	2.19	0.45
2:B:28:ASN:HD21	2:B:30:GLU:HB2	1.81	0.45
4:T:201:THR:HG22	4:T:202:CYS:N	2.31	0.45
4:H:58:ASN:HB2	4:H:60:TYR:CD2	2.51	0.45
1:A:170:ASN:ND2	1:A:239:PRO:HA	2.32	0.45
2:F:9:PHE:HD1	2:F:9:PHE:C	2.19	0.45
4:H:175:ALA:HB2	4:H:184:LEU:HB3	1.98	0.45
3:U:3:VAL:H	3:U:26:SER:HB3	1.82	0.45
1:C:300:ILE:HD11	2:D:69:GLU:HG3	1.98	0.45
1:C:82:GLU:OE2	1:C:82:GLU:HA	2.16	0.45
4:T:193:SER:O	4:T:196:PRO:HD2	2.16	0.45
4:H:76:LYS:O	4:H:77:ASN:C	2.52	0.45
1:A:178:TYR:CE1	1:A:243:LEU:HG	2.51	0.45
2:B:89:ILE:H	2:B:89:ILE:HD12	1.81	0.45
1:C:81:ASN:HD22	1:C:119:GLU:HA	1.80	0.45
1:C:18:HIS:O	1:C:19:ALA:CB	2.60	0.45
2:D:83:TYR:CG	2:F:66:ILE:HG23	2.51	0.45
1:E:67:ILE:HG13	1:E:105:TYR:CE2	2.52	0.45
1:C:283:THR:HG23	1:C:285:ASN:N	2.32	0.45
4:T:177:LEU:HD12	4:T:178:GLN:H	1.81	0.45
4:H:59:ASN:OD1	4:H:61:ASN:OD1	2.34	0.45
4:H:141:SER:O	4:H:192:SER:HA	2.15	0.45
1:A:283:THR:O	1:A:284:PRO:C	2.54	0.45
4:H:151:GLY:CA	4:H:181:LEU:HD12	2.45	0.45
1:E:170:ASN:ND2	1:E:239:PRO:CA	2.75	0.45
1:E:191:GLN:O	1:E:192:THR:C	2.53	0.45
1:E:196:VAL:O	1:E:197:GLN:C	2.54	0.45
3:L:132:SER:HA	3:L:180:LEU:O	2.17	0.45
3:U:136:PHE:C	3:U:137:LEU:HD12	2.37	0.45
1:E:10:THR:HB	1:E:11:ALA:H	1.57	0.45
4:T:2:VAL:HG21	4:T:27:TYR:CB	2.46	0.45
4:H:56:GLY:C	4:H:58:ASN:N	2.64	0.45
2:D:85:GLU:O	2:D:86:ASP:C	2.55	0.45
1:C:195:TYR:O	1:C:196:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:GLN:HB3	1:A:295:GLN:HA	1.97	0.45
3:L:168:ASP:CG	3:L:169:SER:H	2.20	0.45
1:A:17:HIS:HB2	1:A:320:MET:SD	2.57	0.45
2:D:5:ALA:HB1	2:D:115:MET:HG2	1.98	0.45
1:C:14:CYS:O	2:D:25:ARG:N	2.49	0.45
1:C:283:THR:O	1:C:283:THR:CG2	2.64	0.45
3:L:90:HIS:ND1	3:L:98:THR:O	2.49	0.45
2:D:167:LEU:HD23	2:D:167:LEU:N	2.32	0.45
2:D:6:ILE:C	2:D:8:GLY:H	2.18	0.45
1:E:13:LEU:HD13	1:E:14:CYS:N	2.32	0.45
3:U:14:SER:CB	3:U:108:LYS:CD	2.94	0.45
1:C:176:LYS:HD2	1:C:257:TYR:CE2	2.51	0.45
4:H:64:LEU:HA	4:H:64:LEU:HD23	1.82	0.45
4:T:37:TRP:HB3	4:T:49:MET:HE3	1.99	0.45
3:U:95:PHE:CD1	3:U:97:ARG:NH1	2.85	0.45
3:L:21:LEU:CD1	3:L:21:LEU:N	2.79	0.45
1:E:164:LEU:N	1:E:164:LEU:HD12	2.31	0.45
3:U:7:SER:CB	3:U:8:PRO:CD	2.94	0.45
1:E:204:VAL:HA	1:E:244:VAL:O	2.17	0.45
2:F:130:ALA:CB	2:F:139:LYS:O	2.60	0.45
2:B:24:PHE:O	2:B:34:GLN:HA	2.16	0.45
1:E:73:ASP:OD1	1:E:75:HIS:HD2	2.00	0.45
3:L:55:LEU:HB3	3:L:59:VAL:HB	1.99	0.45
3:L:74:LEU:HB3	3:L:75:THR:H	1.58	0.45
3:L:119:PHE:HA	3:L:120:PRO:HD3	1.71	0.45
1:C:108:LEU:HD12	1:C:111:LEU:HD21	1.98	0.45
1:E:117:THR:C	1:E:118:LEU:HD23	2.37	0.45
2:B:38:LEU:C	2:B:40:SER:H	2.19	0.45
4:H:216:LYS:H	4:H:216:LYS:HD2	1.81	0.45
4:H:37:TRP:CE3	4:H:96:CYS:HB3	2.50	0.45
4:H:53:SER:H	4:H:58:ASN:HD21	1.65	0.45
1:A:176:LYS:HD2	1:A:257:TYR:CG	2.52	0.45
3:U:55:LEU:HD21	3:U:63:PHE:O	2.17	0.45
1:A:191:GLN:OE1	1:A:195:TYR:CD1	2.68	0.45
4:T:71:THR:O	4:T:79:PHE:HB2	2.16	0.45
1:C:150:ARG:N	1:C:150:ARG:CD	2.79	0.45
4:H:76:LYS:HD2	4:H:76:LYS:HA	1.76	0.45
4:H:190:VAL:HB	4:H:191:PRO:HD2	1.99	0.45
3:L:36:TRP:CZ2	3:L:73:SER:O	2.70	0.45
4:H:146:GLY:O	4:H:147:CYS:HB2	2.15	0.45
3:L:120:PRO:HG2	4:H:220:ARG:NH2	2.32	0.45
2:B:118:LEU:O	2:B:122:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:61:GLY:O	1:E:79:PHE:CZ	2.70	0.45
3:U:2:ILE:HG22	3:U:4:LEU:HD11	1.98	0.45
1:C:248:ASN:HD22	1:C:248:ASN:H	1.65	0.45
1:A:191:GLN:NE2	1:A:250:ASN:HD21	2.15	0.45
2:B:77:ILE:HD13	2:B:77:ILE:HA	1.52	0.45
2:F:78:GLN:O	2:F:79:ASP:C	2.54	0.45
1:A:197:GLN:CD	1:A:197:GLN:H	2.19	0.45
4:T:20:LEU:CD1	4:T:94:TYR:CB	2.96	0.44
3:U:14:SER:HB3	3:U:108:LYS:CD	2.45	0.44
3:L:141:TYR:CG	3:L:142:PRO:N	2.83	0.44
4:H:76:LYS:CE	4:H:76:LYS:HA	2.46	0.44
3:L:92:TRP:O	3:L:97:ARG:NH2	2.50	0.44
4:T:52:ILE:O	4:T:52:ILE:CG2	2.54	0.44
1:E:200:GLY:HA3	1:E:250:ASN:OD1	2.17	0.44
1:C:184:HIS:CE1	1:C:216:ASN:ND2	2.85	0.44
4:T:172:THR:HA	4:T:186:SER:HA	1.99	0.44
2:B:98:LEU:O	2:B:99:LEU:C	2.55	0.44
1:C:298:ASN:HD22	1:C:299:LYS:H	1.61	0.44
1:C:43:VAL:HG23	1:C:314:LEU:HB2	1.99	0.44
4:H:35:TRP:CE3	4:H:98:ALA:HB2	2.52	0.44
4:H:6:GLU:OE1	4:H:96:CYS:N	2.41	0.44
3:L:32:SER:C	3:L:33:PHE:CD1	2.90	0.44
3:U:127:THR:HG22	3:U:127:THR:O	2.18	0.44
3:L:182:LEU:HA	3:L:182:LEU:HD23	1.77	0.44
3:U:114:PRO:HD3	3:U:140:PHE:CB	2.48	0.44
1:A:10:THR:HG21	2:B:141:TYR:O	2.17	0.44
1:A:36:VAL:HG22	1:A:37:THR:H	1.80	0.44
1:C:28:THR:HG22	2:D:105:GLN:N	2.32	0.44
2:D:159:HIS:C	2:D:159:HIS:ND1	2.70	0.44
1:E:42:LEU:O	1:E:294:PHE:HB2	2.17	0.44
2:D:83:TYR:OH	2:F:85:GLU:OE1	2.24	0.44
4:T:39:ARG:HB2	4:T:93:SER:O	2.18	0.44
2:F:122:THR:C	2:F:124:ARG:N	2.71	0.44
3:L:38:GLN:CG	3:L:87:TYR:HE1	2.27	0.44
3:L:116:VAL:CG1	3:L:117:SER:N	2.80	0.44
3:U:2:ILE:HA	3:U:2:ILE:HD13	1.67	0.44
2:B:85:GLU:OE1	2:F:83:TYR:OH	2.27	0.44
1:C:96:ASN:O	1:C:97:CYS:HB2	2.17	0.44
2:F:48:ILE:HD11	2:F:107:THR:CG2	2.43	0.44
4:T:195:TRP:CB	4:T:196:PRO:CD	2.96	0.44
2:F:122:THR:C	2:F:124:ARG:H	2.18	0.44
2:F:152:ILE:C	2:F:154:ASN:N	2.71	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:134:GLY:HA3	4:H:220:ARG:HE	1.82	0.44
1:C:111:LEU:HD12	1:C:111:LEU:C	2.37	0.44
1:E:16:GLY:HA2	2:F:115:MET:HE3	2.00	0.44
1:E:16:GLY:HA2	2:F:115:MET:SD	2.58	0.44
4:T:149:VAL:O	4:T:184:LEU:N	2.45	0.44
4:H:7:SER:O	4:H:20:LEU:HD22	2.17	0.44
1:A:292:LYS:HB3	1:A:293:PRO:HD2	1.99	0.44
2:B:111:THR:C	2:B:113:SER:N	2.70	0.44
2:D:130:ALA:HB2	2:D:140:ILE:HA	1.99	0.44
1:E:10:THR:CG2	2:F:141:TYR:O	2.62	0.44
2:F:66:ILE:HG13	2:F:66:ILE:O	2.12	0.44
4:T:152:TYR:CE2	4:T:157:VAL:HG22	2.52	0.44
4:T:34:TYR:O	4:T:36:THR:HG22	2.18	0.44
4:T:58:ASN:O	4:T:59:ASN:CB	2.60	0.44
3:L:6:GLN:HE22	3:L:88:PHE:HA	1.83	0.44
2:D:82:LYS:O	2:D:84:VAL:N	2.51	0.44
2:B:121:LYS:NZ	2:B:122:THR:HG22	2.24	0.44
3:U:166:ASP:O	3:U:167:GLN:C	2.55	0.44
4:H:86:VAL:HG22	4:H:87:THR:O	2.18	0.44
1:C:191:GLN:O	1:C:192:THR:C	2.55	0.44
2:B:9:PHE:HD1	2:B:10:ILE:N	2.16	0.44
3:L:82:GLU:C	3:L:84:GLY:H	2.21	0.44
1:A:71:LEU:CD1	1:A:100:TYR:CE1	3.00	0.44
1:A:17:HIS:HA	2:B:22:TYR:HD2	1.81	0.44
2:D:103:GLU:O	2:D:107:THR:OG1	2.20	0.44
2:D:91:LEU:HD13	2:F:91:LEU:HD13	1.99	0.44
2:F:146:ASN:O	2:F:149:ILE:HB	2.18	0.44
2:F:28:ASN:HD21	2:F:30:GLU:HB2	1.83	0.44
1:C:14:CYS:HA	2:D:137:CYS:HA	1.99	0.44
3:U:49:ILE:HA	3:U:54:ASN:O	2.17	0.44
1:E:121:ILE:HG13	1:E:257:TYR:OH	2.17	0.44
1:E:121:ILE:CG1	1:E:257:TYR:CE1	3.01	0.44
4:H:13:LYS:O	4:H:14:PRO:C	2.55	0.44
2:B:17:MET:HE3	2:B:19:ASP:HB2	1.98	0.44
3:U:187:TYR:C	3:U:189:ARG:N	2.69	0.44
2:D:9:PHE:C	2:D:9:PHE:HD1	2.21	0.44
3:L:186:GLU:HG3	3:L:189:ARG:CZ	2.48	0.44
4:H:20:LEU:HD11	4:H:94:TYR:CB	2.47	0.44
3:L:4:LEU:HD12	3:L:4:LEU:N	2.32	0.44
1:A:136:SER:HB2	4:H:104:ASP:OD1	2.18	0.44
1:A:147:PHE:CG	1:A:148:PHE:N	2.85	0.44
1:A:311:GLN:CD	1:A:311:GLN:H	2.21	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:283:THR:HG23	1:E:285:ASN:CA	2.48	0.44
2:B:3:PHE:HZ	2:F:2:LEU:O	2.00	0.44
2:F:84:VAL:HG12	2:F:85:GLU:N	2.32	0.44
4:T:97:ALA:CB	4:T:109:TYR:O	2.65	0.44
4:H:72:ARG:O	4:H:72:ARG:HG3	2.18	0.44
1:A:127:TRP:CZ3	1:A:166:VAL:HG11	2.53	0.44
2:D:55:VAL:HG12	2:D:56:ILE:N	2.33	0.44
1:A:226:LEU:HD21	4:H:104:ASP:HB2	1.98	0.44
1:A:65:THR:HG23	1:A:68:ASP:OD2	2.18	0.44
1:A:18:HIS:CE1	1:A:320:MET:SD	3.11	0.44
2:D:127:ARG:C	2:D:129:ASN:H	2.21	0.44
2:D:3:PHE:CD2	2:D:113:SER:CA	2.90	0.44
2:D:6:ILE:HG13	2:D:112:ASP:OD1	2.18	0.44
1:E:283:THR:HG23	1:E:285:ASN:N	2.33	0.44
2:F:168:ASN:C	2:F:170:ARG:N	2.71	0.44
4:T:51:TYR:HE1	4:T:58:ASN:HD22	1.65	0.44
4:T:59:ASN:OD1	4:T:61:ASN:OD1	2.35	0.44
4:T:206:HIS:CD2	4:T:209:SER:OG	2.60	0.44
3:L:194:THR:HG22	3:L:209:SER:CB	2.48	0.44
2:D:4:GLY:CA	2:F:117:LYS:HE3	2.46	0.44
1:A:248:ASN:HD22	1:A:248:ASN:C	2.20	0.44
1:A:74:PRO:HD3	1:A:97:CYS:SG	2.58	0.44
1:E:13:LEU:HB3	2:F:138:PHE:HB2	1.99	0.44
2:F:89:ILE:O	2:F:90:ASP:C	2.56	0.44
1:E:138:ALA:C	1:E:140:LYS:NZ	2.71	0.44
4:H:100:TYR:O	4:H:101:TYR:CB	2.58	0.44
4:H:51:TYR:C	4:H:59:ASN:O	2.56	0.44
3:L:95:PHE:CD1	3:L:97:ARG:NH1	2.86	0.44
3:U:122:SER:HB3	3:U:125:GLN:CB	2.43	0.44
3:U:122:SER:OG	3:U:124:ILE:HG13	2.17	0.44
4:H:130:PRO:C	4:H:131:LEU:HD23	2.38	0.44
2:F:9:PHE:CE1	2:F:10:ILE:HG13	2.52	0.44
2:F:74:GLU:HB2	2:F:78:GLN:HB2	2.00	0.44
3:L:204:SER:HA	3:L:205:PRO:HD2	1.65	0.44
2:D:98:LEU:O	2:D:100:VAL:N	2.51	0.43
2:B:132:GLU:HG3	2:B:137:CYS:O	2.18	0.43
2:B:28:ASN:ND2	2:B:30:GLU:HB2	2.33	0.43
4:H:54:TYR:HA	4:H:72:ARG:HH22	1.81	0.43
3:U:35:TYR:CD2	3:U:50:TYR:HA	2.46	0.43
3:U:95:PHE:HD1	3:U:97:ARG:HH12	1.66	0.43
3:U:194:THR:HG22	3:U:209:SER:CB	2.47	0.43
4:T:184:LEU:C	4:T:184:LEU:HD12	2.38	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:9:PHE:HD1	2:D:10:ILE:N	2.15	0.43
1:C:187:THR:C	1:C:189:GLN:N	2.72	0.43
1:C:326:LYS:O	1:C:327:GLN:CB	2.66	0.43
4:T:40:GLN:HA	4:T:45:LYS:O	2.18	0.43
4:T:114:THR:HG23	4:T:114:THR:O	2.18	0.43
3:U:56:ALA:O	3:U:58:GLY:N	2.45	0.43
1:A:18:HIS:O	1:A:19:ALA:CB	2.63	0.43
1:C:311:GLN:HE22	2:D:93:SER:HB3	1.82	0.43
2:B:171:PHE:CZ	2:F:171:PHE:CE2	3.00	0.43
1:E:12:THR:CB	2:F:27:GLN:HB3	2.45	0.43
2:F:6:ILE:CD1	2:F:112:ASP:HA	2.49	0.43
1:C:13:LEU:CD1	2:D:24:PHE:HB3	2.34	0.43
2:F:56:ILE:O	2:F:58:LYS:HG3	2.17	0.43
3:U:74:LEU:HB3	3:U:75:THR:H	1.52	0.43
4:H:155:GLU:HG2	4:H:182:TYR:CE2	2.53	0.43
1:A:209:SER:O	1:A:210:GLN:HB2	2.18	0.43
1:C:182:ILE:O	1:C:230:ILE:CG2	2.60	0.43
3:L:165:THR:HG23	3:L:175:SER:O	2.18	0.43
1:A:38:ASN:ND2	1:A:318:THR:CB	2.81	0.43
1:C:223:VAL:HG12	1:C:223:VAL:O	2.17	0.43
1:E:205:SER:HB3	1:E:210:GLN:HA	1.99	0.43
2:B:153:ARG:HG2	2:B:153:ARG:O	2.18	0.43
1:A:229:ARG:HE	1:A:229:ARG:HB3	1.61	0.43
1:C:288:ILE:HG21	1:C:297:VAL:HG21	1.99	0.43
2:F:51:LYS:NZ	2:F:106:HIS:ND1	2.64	0.43
1:A:286:GLY:O	1:A:287:SER:CB	2.65	0.43
3:U:96:PRO:HA	4:T:48:TRP:HZ3	1.84	0.43
4:T:53:SER:H	4:T:58:ASN:ND2	2.10	0.43
4:H:86:VAL:CG2	4:H:90:ASP:HB2	2.45	0.43
1:A:25:LEU:HD22	1:A:33:GLN:OE1	2.18	0.43
4:H:206:HIS:CD2	4:H:209:SER:OG	2.66	0.43
3:U:44:SER:O	3:U:45:PRO:C	2.57	0.43
3:L:82:GLU:O	3:L:84:GLY:N	2.52	0.43
3:U:125:GLN:CA	3:U:125:GLN:NE2	2.79	0.43
3:L:36:TRP:CE3	3:L:74:LEU:HD23	2.53	0.43
1:C:160:THR:C	1:C:196:VAL:HG21	2.38	0.43
1:A:323:VAL:HA	1:A:324:PRO:HD3	1.88	0.43
1:E:134:GLY:HA3	1:E:153:TRP:HB3	2.00	0.43
1:C:140:LYS:HD2	1:C:140:LYS:O	2.18	0.43
2:B:127:ARG:H	2:B:159:HIS:HB2	1.84	0.43
2:B:165:GLU:HA	2:B:165:GLU:OE1	2.18	0.43
2:D:121:LYS:NZ	2:D:122:THR:N	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:102:LEU:CD1	2:F:102:LEU:HD11	2.48	0.43
2:F:3:PHE:CB	2:F:112:ASP:OD2	2.66	0.43
2:F:14:TRP:CH2	2:F:25:ARG:HG3	2.53	0.43
2:F:6:ILE:C	2:F:8:GLY:N	2.71	0.43
1:E:108:LEU:HA	1:E:108:LEU:HD12	1.70	0.43
3:U:119:PHE:HA	3:U:120:PRO:HD3	1.82	0.43
4:T:32:GLY:HA2	4:T:54:TYR:CD2	2.53	0.43
3:U:55:LEU:HG	3:U:55:LEU:H	1.65	0.43
1:C:108:LEU:HD13	1:C:234:TRP:CD2	2.52	0.43
1:E:246:ASN:C	1:E:246:ASN:ND2	2.70	0.43
1:A:130:VAL:HG13	1:A:162:PRO:HD2	2.00	0.43
2:B:44:ALA:O	2:B:47:GLN:N	2.52	0.43
2:D:165:GLU:C	2:D:168:ASN:HD21	2.22	0.43
3:U:212:ARG:NE	3:U:212:ARG:HA	2.32	0.43
3:L:171:ASP:HB3	3:L:173:THR:CG2	2.47	0.43
2:F:76:ARG:O	2:F:77:ILE:C	2.55	0.43
1:C:262:THR:O	1:C:263:GLY:O	2.36	0.43
1:A:42:LEU:HD22	2:B:55:VAL:CG1	2.49	0.43
1:C:27:LYS:HG3	1:C:32:ASP:HA	2.00	0.43
1:E:37:THR:OG1	1:E:38:ASN:N	2.51	0.43
1:E:140:LYS:N	1:E:140:LYS:CD	2.79	0.43
3:L:75:THR:HG22	3:L:76:ILE:N	2.34	0.43
1:C:109:ARG:CZ	1:C:269:ARG:NH2	2.82	0.43
1:E:127:TRP:HE3	1:E:164:LEU:HD23	1.84	0.43
1:E:254:PRO:HG2	1:E:254:PRO:O	2.19	0.43
3:U:91:GLN:HE21	3:U:93:GLU:H	1.64	0.43
3:L:191:ASN:ND2	3:L:191:ASN:N	2.65	0.43
4:H:20:LEU:CD1	4:H:94:TYR:HB3	2.49	0.43
1:A:143:PRO:HG2	1:A:144:GLY:N	2.34	0.43
1:C:298:ASN:C	1:C:298:ASN:ND2	2.71	0.43
2:D:117:LYS:HB3	2:D:117:LYS:HE2	1.88	0.43
4:H:76:LYS:HE3	4:H:76:LYS:HA	2.01	0.43
4:T:64:LEU:HB2	4:T:68:ILE:CD1	2.48	0.43
4:T:84:ASN:HB3	4:T:85:SER:H	1.43	0.43
1:E:307:LYS:HD3	2:F:92:TRP:CZ2	2.53	0.43
4:H:161:TRP:HB3	4:H:166:LEU:HB2	2.01	0.43
1:A:210:GLN:HE21	1:E:220:ARG:HE	1.65	0.43
1:E:253:ALA:HB1	1:E:254:PRO:HD2	2.00	0.43
2:F:21:TRP:CD2	2:F:45:ILE:HD11	2.54	0.43
3:L:25:ALA:O	3:L:27:SER:N	2.52	0.43
3:U:207:VAL:HG22	3:U:208:LYS:N	2.33	0.43
1:A:153:TRP:CD1	1:A:153:TRP:C	2.91	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:GLY:HA2	2:B:115:MET:HE3	2.01	0.43
1:C:27:LYS:HE2	2:F:54:ARG:HD2	2.00	0.43
2:D:100:VAL:O	2:D:101:ALA:C	2.57	0.43
2:F:104:ASN:O	2:F:107:THR:N	2.50	0.43
4:T:20:LEU:HB2	4:T:81:LEU:HB3	2.00	0.43
4:T:194:THR:HG23	4:T:198:GLU:CD	2.39	0.43
4:T:216:LYS:H	4:T:216:LYS:HD2	1.82	0.43
4:H:6:GLU:CD	4:H:113:GLY:HA2	2.39	0.43
1:C:127:TRP:CH2	1:C:166:VAL:HG21	2.53	0.43
2:B:26:HIS:CE1	2:B:32:THR:C	2.92	0.43
1:A:117:THR:C	1:A:118:LEU:HD23	2.39	0.43
1:E:264:LYS:HD2	2:F:63:PHE:CE2	2.54	0.43
1:A:98:TYR:HE2	1:A:229:ARG:HA	1.83	0.43
3:U:137:LEU:O	3:U:140:PHE:CE1	2.72	0.43
2:B:3:PHE:HA	2:B:3:PHE:HD1	1.67	0.43
1:A:309:VAL:CG1	2:B:93:SER:HA	2.38	0.43
2:D:119:PHE:C	2:D:121:LYS:H	2.22	0.43
2:B:171:PHE:CD2	2:D:167:LEU:HB3	2.50	0.43
1:E:11:ALA:HB2	2:F:28:ASN:HA	2.01	0.43
4:T:14:PRO:O	4:T:15:SER:OG	2.37	0.43
3:L:137:LEU:O	3:L:175:SER:HA	2.19	0.43
4:H:41:PHE:HB3	4:H:42:PRO:CD	2.49	0.43
3:U:1:GLN:HG2	3:U:1:GLN:O	2.19	0.43
3:L:70:THR:OG1	3:L:70:THR:O	2.36	0.43
1:C:74:PRO:HA	1:C:141:ARG:NH1	2.34	0.42
1:A:42:LEU:HD11	1:A:316:LEU:HB2	2.01	0.42
2:B:91:LEU:O	2:B:92:TRP:C	2.56	0.42
1:C:28:THR:HG21	2:D:105:GLN:HA	2.00	0.42
2:D:167:LEU:HG	2:D:168:ASN:N	2.34	0.42
4:T:81:LEU:HD12	4:T:82:LYS:N	2.23	0.42
1:E:15:LEU:HD23	1:E:15:LEU:N	2.33	0.42
4:H:37:TRP:O	4:H:49:MET:HB2	2.20	0.42
4:H:70:ILE:CG2	4:H:71:THR:N	2.81	0.42
2:B:17:MET:C	2:B:17:MET:SD	2.98	0.42
1:A:204:VAL:HA	1:A:244:VAL:O	2.19	0.42
1:A:67:ILE:HA	1:A:67:ILE:HD13	1.89	0.42
1:A:248:ASN:ND2	1:A:248:ASN:C	2.73	0.42
2:B:163:ARG:O	2:B:164:ASP:C	2.57	0.42
2:B:72:GLU:HG3	1:C:238:LYS:HE2	2.01	0.42
2:D:171:PHE:N	2:D:171:PHE:CD1	2.77	0.42
1:C:29:ILE:HG23	2:F:103:GLU:OE1	2.19	0.42
1:A:54:ASN:O	1:A:278:ILE:HA	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:21:LEU:HD22	3:U:74:LEU:HG	2.00	0.42
1:C:206:THR:HB	1:C:241:ASP:OD1	2.19	0.42
4:T:174:PRO:O	4:T:175:ALA:C	2.57	0.42
1:E:132:GLN:HA	1:E:154:LEU:CD2	2.49	0.42
2:D:58:LYS:HE2	2:D:58:LYS:HB3	1.86	0.42
1:A:18:HIS:CG	1:A:19:ALA:N	2.86	0.42
2:B:3:PHE:HE2	2:B:113:SER:OG	2.00	0.42
1:C:47:SER:OG	1:C:48:THR:N	2.53	0.42
2:F:25:ARG:HE	2:F:34:GLN:CD	2.22	0.42
4:H:218:VAL:HG13	4:H:218:VAL:O	2.19	0.42
4:T:13:LYS:HA	4:T:14:PRO:HD3	1.81	0.42
4:H:180:ASP:O	4:H:181:LEU:HD22	2.20	0.42
2:D:86:ASP:O	2:D:87:THR:C	2.56	0.42
3:U:34:LEU:HD22	3:U:72:TYR:CD2	2.55	0.42
1:C:54:ASN:CB	1:C:278:ILE:HD13	2.49	0.42
4:T:150:LYS:HG3	4:T:183:THR:OG1	2.19	0.42
1:E:304:ALA:N	2:F:61:GLU:HG3	2.34	0.42
2:D:140:ILE:N	2:D:140:ILE:HD12	2.35	0.42
1:E:13:LEU:C	1:E:13:LEU:HD13	2.40	0.42
1:E:283:THR:HG21	1:E:297:VAL:HG11	2.01	0.42
1:E:111:LEU:HD12	1:E:112:VAL:N	2.33	0.42
4:H:195:TRP:CB	4:H:196:PRO:CD	2.90	0.42
4:H:161:TRP:CB	4:H:166:LEU:HB2	2.49	0.42
1:E:187:THR:HB	1:E:189:GLN:CD	2.40	0.42
1:C:189:GLN:HB3	1:C:189:GLN:HE21	1.57	0.42
1:C:217:ILE:HD12	1:C:217:ILE:H	1.85	0.42
1:E:58:ILE:CD1	1:E:86:LEU:HB3	2.49	0.42
1:A:291:ASP:OD2	1:A:292:LYS:HG2	2.19	0.42
2:B:102:LEU:O	2:B:104:ASN:N	2.52	0.42
1:E:28:THR:HA	2:F:101:ALA:HA	2.01	0.42
2:B:151:SER:HB2	2:B:157:TYR:HB2	2.02	0.42
4:T:217:ILE:O	4:T:218:VAL:HG22	2.20	0.42
1:C:111:LEU:HG	1:C:111:LEU:H	1.73	0.42
3:U:194:THR:HG22	3:U:209:SER:HB2	2.02	0.42
3:U:209:SER:OG	3:U:210:PHE:CD1	2.71	0.42
3:U:34:LEU:HD13	3:U:72:TYR:CD1	2.54	0.42
4:T:150:LYS:CA	4:T:183:THR:HG23	2.49	0.42
4:T:122:LYS:HG3	4:T:124:THR:HG23	2.01	0.42
1:C:36:VAL:CG2	1:C:37:THR:H	2.31	0.42
2:D:132:GLU:HG3	2:D:137:CYS:O	2.19	0.42
4:T:119:SER:HB3	4:T:153:PHE:HZ	1.84	0.42
3:U:14:SER:CB	3:U:108:LYS:CB	2.96	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:212:THR:HG22	1:A:213:ILE:N	2.33	0.42
2:B:80:LEU:CD2	2:F:80:LEU:HD21	2.44	0.42
1:C:109:ARG:NH2	1:C:267:ILE:HD13	2.35	0.42
1:C:127:TRP:CE3	1:C:164:LEU:HD23	2.54	0.42
3:L:32:SER:C	3:L:33:PHE:HD1	2.23	0.42
1:C:281:CYS:HB2	1:C:304:ALA:O	2.20	0.42
3:U:40:LYS:NZ	3:U:84:GLY:O	2.35	0.42
3:U:175:SER:OG	4:T:171:HIS:CE1	2.71	0.42
1:A:29:ILE:CG1	2:B:102:LEU:HD23	2.49	0.42
1:C:17:HIS:CG	1:C:18:HIS:H	2.36	0.42
2:F:3:PHE:CB	2:F:112:ASP:O	2.67	0.42
1:E:98:TYR:CD2	1:E:99:PRO:HD2	2.55	0.42
4:T:152:TYR:CE1	4:T:182:TYR:HB3	2.55	0.42
3:L:97:ARG:HB2	4:H:48:TRP:CE2	2.52	0.42
1:E:172:ASP:O	1:E:239:PRO:HB3	2.20	0.42
1:C:37:THR:OG1	1:C:319:GLY:HA3	2.19	0.42
2:D:21:TRP:CE3	2:D:45:ILE:HG13	2.55	0.42
1:E:283:THR:O	1:E:283:THR:CG2	2.68	0.42
1:E:28:THR:O	1:E:30:THR:N	2.52	0.42
4:H:18:LEU:O	4:H:82:LYS:O	2.37	0.42
1:A:22:ASN:ND2	1:A:22:ASN:N	2.46	0.42
2:F:121:LYS:HB3	2:F:121:LYS:NZ	2.24	0.42
4:H:73:ASP:OD1	4:H:75:SER:OG	2.38	0.42
4:T:37:TRP:O	4:T:49:MET:HB2	2.20	0.42
3:L:51:SER:O	3:L:53:SER:N	2.53	0.42
2:F:42:GLN:O	2:F:46:ASP:HB2	2.19	0.42
1:A:191:GLN:O	1:A:194:LEU:N	2.53	0.42
1:E:177:LEU:HB2	1:E:260:MET:SD	2.60	0.42
1:C:309:VAL:HG12	2:D:93:SER:CA	2.44	0.42
2:D:51:LYS:O	2:D:54:ARG:HB2	2.19	0.42
1:E:318:THR:O	1:E:318:THR:CG2	2.68	0.42
2:B:127:ARG:HH21	2:F:131:GLU:HB2	1.85	0.42
4:T:153:PHE:CG	4:T:154:PRO:HA	2.54	0.42
1:A:176:LYS:O	1:A:236:ILE:HA	2.19	0.42
3:U:35:TYR:HB3	3:U:49:ILE:O	2.20	0.42
3:L:8:PRO:HB3	3:L:11:MET:HB3	2.01	0.42
4:H:167:SER:O	4:H:170:VAL:HG22	2.20	0.42
3:U:29:ILE:O	3:U:29:ILE:HG13	2.20	0.42
1:A:47:SER:CB	1:A:288:ILE:HG22	2.45	0.42
4:H:67:ARG:O	4:H:68:ILE:C	2.57	0.42
1:A:25:LEU:HD13	1:A:33:GLN:OE1	2.20	0.42
1:E:187:THR:HB	1:E:189:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:2:ILE:HG23	3:L:98:THR:HG21	2.02	0.42
3:U:3:VAL:N	3:U:26:SER:HB2	2.34	0.42
1:A:166:VAL:CG2	1:A:245:ILE:HB	2.47	0.42
4:T:73:ASP:O	4:T:76:LYS:N	2.53	0.42
1:A:182:ILE:O	1:A:182:ILE:CG2	2.68	0.42
1:A:70:LEU:O	1:A:71:LEU:C	2.58	0.42
3:U:156:ARG:O	3:U:158:ASN:OD1	2.38	0.42
1:C:226:LEU:HD21	4:T:104:ASP:HB2	2.02	0.42
2:B:40:SER:OG	2:B:114:GLU:HB3	2.20	0.42
1:A:29:ILE:O	2:D:51:LYS:HA	2.19	0.42
2:F:141:TYR:HB3	2:F:165:GLU:HB3	2.02	0.42
2:F:68:LYS:HE2	2:F:85:GLU:OE2	2.20	0.42
1:A:80:GLN:HE21	1:A:80:GLN:HB3	1.63	0.42
3:U:55:LEU:HB3	3:U:59:VAL:HB	2.02	0.42
3:U:160:VAL:O	3:U:161:LEU:HD23	2.19	0.42
3:L:149:TRP:CD1	3:L:160:VAL:HG11	2.55	0.42
1:A:308:TYR:CD2	2:B:89:ILE:HG13	2.54	0.42
3:L:190:HIS:ND1	3:L:190:HIS:N	2.67	0.42
2:B:68:LYS:HE2	2:B:85:GLU:OE1	2.19	0.42
2:B:54:ARG:NH1	2:B:103:GLU:OE2	2.53	0.41
2:F:110:LEU:HD13	2:F:110:LEU:C	2.37	0.41
2:F:165:GLU:OE1	2:F:168:ASN:ND2	2.53	0.41
4:T:18:LEU:CD2	4:T:116:LEU:HD13	2.48	0.41
4:T:29:ILE:HG12	4:T:77:ASN:ND2	2.34	0.41
4:H:218:VAL:O	4:H:219:PRO:C	2.56	0.41
4:H:180:ASP:C	4:H:181:LEU:HD22	2.40	0.41
2:D:68:LYS:HE2	2:D:85:GLU:OE1	2.20	0.41
1:E:130:VAL:HG21	1:E:164:LEU:HD21	2.02	0.41
1:E:280:GLU:HB3	1:E:304:ALA:HB3	2.02	0.41
1:E:71:LEU:CD1	1:E:100:TYR:CE1	3.03	0.41
4:H:41:PHE:O	4:H:42:PRO:C	2.58	0.41
1:E:180:TRP:CE2	1:E:204:VAL:HG21	2.55	0.41
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.85	0.41
2:B:4:GLY:O	2:B:5:ALA:C	2.59	0.41
2:D:6:ILE:O	2:D:8:GLY:N	2.54	0.41
1:C:13:LEU:C	1:C:13:LEU:HD13	2.41	0.41
4:H:107:PHE:CE1	4:H:109:TYR:HE1	2.38	0.41
4:H:193:SER:O	4:H:196:PRO:HD2	2.20	0.41
1:A:50:LYS:HG2	1:A:273:PRO:HG2	2.03	0.41
3:L:6:GLN:NE2	3:L:102:GLY:HA2	2.35	0.41
1:E:176:LYS:CE	1:E:178:TYR:OH	2.68	0.41
4:H:67:ARG:NH1	4:H:85:SER:O	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:196:VAL:O	1:E:197:GLN:O	2.38	0.41
3:L:4:LEU:CD1	3:L:4:LEU:N	2.84	0.41
1:C:67:ILE:HA	1:C:67:ILE:HD13	1.92	0.41
3:U:137:LEU:O	3:U:140:PHE:HE1	2.03	0.41
1:C:140:LYS:CD	1:C:140:LYS:H	2.34	0.41
2:B:126:LEU:HD23	2:B:152:ILE:HD11	2.02	0.41
2:F:167:LEU:HG	2:F:168:ASN:N	2.36	0.41
2:F:68:LYS:HE2	2:F:85:GLU:CD	2.41	0.41
2:D:132:GLU:O	2:D:134:GLY:N	2.53	0.41
3:L:123:LYS:HG2	3:L:124:ILE:N	2.35	0.41
3:L:125:GLN:NE2	4:H:129:TYR:CE2	2.88	0.41
1:A:111:LEU:HD12	1:A:112:VAL:CA	2.48	0.41
4:H:51:TYR:O	4:H:70:ILE:HD12	2.20	0.41
4:H:159:VAL:HG22	4:H:160:THR:N	2.34	0.41
3:U:3:VAL:O	3:U:25:ALA:HA	2.20	0.41
3:U:204:SER:HA	3:U:205:PRO:HD2	1.57	0.41
4:T:43:GLY:O	4:T:44:ASN:HB2	2.20	0.41
1:A:294:PHE:CE1	2:B:96:ALA:HB2	2.54	0.41
1:C:18:HIS:CG	1:C:19:ALA:N	2.88	0.41
2:F:142:HIS:N	2:F:142:HIS:ND1	2.68	0.41
4:T:107:PHE:CE1	4:T:109:TYR:HE1	2.39	0.41
1:A:304:ALA:H	2:B:61:GLU:HG3	1.85	0.41
4:T:130:PRO:HB2	4:T:217:ILE:HD13	2.02	0.41
4:H:34:TYR:CE2	4:H:53:SER:HB3	2.53	0.41
1:A:51:ILE:CG2	1:A:282:ILE:HD13	2.50	0.41
3:U:118:ILE:HD12	3:U:135:CYS:HB2	2.01	0.41
4:H:86:VAL:HG22	4:H:87:THR:N	2.34	0.41
1:E:181:GLY:C	1:E:252:ILE:HB	2.41	0.41
1:E:143:PRO:HG2	1:E:144:GLY:H	1.85	0.41
1:C:141:ARG:HG3	1:C:141:ARG:HH11	1.86	0.41
2:B:171:PHE:HD1	2:B:171:PHE:H	1.57	0.41
2:B:5:ALA:HB1	2:B:115:MET:HG2	2.02	0.41
1:C:44:GLN:HB3	1:C:295:GLN:HB3	2.01	0.41
1:C:48:THR:HG23	1:C:49:GLY:H	1.83	0.41
2:D:111:THR:C	2:D:113:SER:N	2.72	0.41
2:D:131:GLU:HB3	2:F:127:ARG:HE	1.85	0.41
1:E:298:ASN:HD22	1:E:299:LYS:H	1.68	0.41
1:E:139:CYS:O	1:E:146:GLY:C	2.58	0.41
3:L:151:ILE:HA	3:L:193:TYR:HA	2.02	0.41
3:L:141:TYR:CG	3:L:142:PRO:CD	3.03	0.41
4:H:4:LEU:CD1	4:H:97:ALA:HA	2.51	0.41
3:L:37:TYR:OH	4:H:99:PHE:HE2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:164:LEU:HB2	1:E:247:SER:O	2.21	0.41
1:C:223:VAL:O	1:C:224:ARG:HB3	2.20	0.41
1:E:326:LYS:O	1:E:327:GLN:HB2	2.20	0.41
1:C:103:PRO:O	1:C:104:ASP:C	2.59	0.41
1:A:15:LEU:C	2:B:14:TRP:CZ2	2.94	0.41
1:C:313:THR:O	1:C:313:THR:HG23	2.19	0.41
2:D:108:ILE:O	2:D:110:LEU:N	2.53	0.41
2:D:167:LEU:HA	2:D:171:PHE:CE1	2.56	0.41
2:F:100:VAL:O	2:F:101:ALA:C	2.59	0.41
2:F:121:LYS:HZ3	2:F:122:THR:N	2.18	0.41
4:H:33:TYR:CD2	4:H:99:PHE:O	2.65	0.41
1:A:51:ILE:HA	1:A:287:SER:HG	1.85	0.41
4:H:160:THR:O	4:H:202:CYS:HA	2.21	0.41
1:C:78:VAL:HG13	1:C:79:PHE:N	2.36	0.41
4:T:150:LYS:HG3	4:T:183:THR:CG2	2.50	0.41
1:C:191:GLN:OE1	1:C:195:TYR:CD1	2.69	0.41
1:A:269:ARG:HG3	1:A:269:ARG:NH1	2.34	0.41
2:B:69:GLU:O	2:B:70:PHE:CD2	2.73	0.41
3:U:76:ILE:O	3:U:77:SER:C	2.57	0.41
2:B:5:ALA:O	2:B:6:ILE:C	2.58	0.41
2:B:96:ALA:O	2:B:98:LEU:N	2.50	0.41
1:C:308:TYR:CD2	2:D:89:ILE:HG13	2.56	0.41
2:F:28:ASN:ND2	2:F:146:ASN:N	2.68	0.41
4:T:130:PRO:C	4:T:131:LEU:HD23	2.41	0.41
1:A:76:CYS:O	1:A:77:ASP:C	2.56	0.41
4:T:51:TYR:HE1	4:T:58:ASN:ND2	2.18	0.41
1:E:59:LEU:HD12	1:E:60:ASP:N	2.36	0.41
3:U:29:ILE:HD12	3:U:34:LEU:HB2	2.01	0.41
1:E:151:LEU:HD23	1:E:151:LEU:HA	1.87	0.41
3:U:3:VAL:CB	3:U:26:SER:HB2	2.50	0.41
1:C:254:PRO:CG	1:C:254:PRO:O	2.68	0.41
1:A:71:LEU:HD11	1:A:100:TYR:CE1	2.56	0.41
3:L:205:PRO:O	3:L:206:ILE:C	2.59	0.41
1:A:309:VAL:HG12	2:B:93:SER:CA	2.39	0.41
2:B:115:MET:C	2:B:117:LYS:N	2.74	0.41
2:B:1:GLY:HA2	2:B:112:ASP:CG	2.41	0.41
1:C:15:LEU:C	2:D:14:TRP:CZ2	2.94	0.41
2:D:100:VAL:CG2	2:D:101:ALA:H	2.22	0.41
2:D:115:MET:C	2:D:117:LYS:N	2.71	0.41
2:F:127:ARG:NH1	2:F:128:GLU:HG2	2.36	0.41
1:A:13:LEU:HD13	1:A:14:CYS:N	2.36	0.41
1:E:74:PRO:HD3	1:E:97:CYS:CB	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:T:193:SER:OG	4:T:194:THR:N	2.54	0.41
4:T:129:TYR:HB2	4:T:148:LEU:CD2	2.51	0.41
4:T:87:THR:HG23	4:T:90:ASP:H	1.85	0.41
4:T:83:LEU:HD21	4:T:90:ASP:OD1	2.21	0.41
1:C:63:ASP:O	1:C:93:ALA:HB1	2.21	0.41
1:A:102:VAL:HG22	1:A:232:ILE:CB	2.46	0.41
1:C:140:LYS:CD	1:C:140:LYS:N	2.84	0.41
4:T:154:PRO:O	4:T:155:GLU:C	2.58	0.41
4:T:195:TRP:CG	4:T:196:PRO:N	2.88	0.41
4:H:73:ASP:N	4:H:78:GLN:O	2.50	0.41
1:A:172:ASP:HB3	1:A:174:PHE:CD2	2.53	0.41
4:H:84:ASN:HD22	4:H:84:ASN:HA	1.66	0.41
3:L:167:GLN:HG3	3:L:172:SER:CA	2.51	0.41
1:E:161:TYR:CE2	1:E:249:GLY:HA2	2.56	0.41
1:E:247:SER:OG	1:E:251:LEU:HB2	2.21	0.41
2:D:39:LYS:HG2	2:D:39:LYS:O	2.20	0.41
3:L:139:ASN:CA	3:L:174:TYR:O	2.69	0.41
1:A:247:SER:OG	1:A:249:GLY:O	2.39	0.41
4:T:159:VAL:HG11	4:T:172:THR:OG1	2.20	0.41
2:D:26:HIS:O	2:D:32:THR:HA	2.21	0.41
2:F:69:GLU:O	2:F:70:PHE:CD2	2.74	0.41
1:A:67:ILE:O	1:A:70:LEU:HB3	2.20	0.41
2:F:77:ILE:HD13	2:F:77:ILE:HA	1.80	0.41
1:E:129:GLY:O	1:E:157:SER:HB3	2.21	0.41
2:B:120:GLU:HA	2:B:120:GLU:OE1	2.21	0.41
1:C:154:LEU:N	1:C:154:LEU:HD23	2.36	0.41
2:B:24:PHE:N	2:B:24:PHE:CD1	2.89	0.41
4:T:195:TRP:O	4:T:198:GLU:O	2.39	0.41
4:T:201:THR:HG23	4:T:215:LYS:C	2.42	0.41
4:H:48:TRP:CZ2	4:H:50:GLY:HA2	2.56	0.41
4:T:53:SER:C	4:T:55:ASP:N	2.73	0.41
4:T:64:LEU:HA	4:T:64:LEU:HD23	1.74	0.41
3:U:61:ALA:O	3:U:62:ARG:C	2.58	0.41
2:D:56:ILE:O	2:D:58:LYS:HG3	2.21	0.41
1:E:177:LEU:HD12	1:E:236:ILE:HG22	2.02	0.41
2:D:115:MET:HB3	2:D:116:ASN:H	1.65	0.40
4:H:148:LEU:HD23	4:H:148:LEU:O	2.22	0.40
4:T:190:VAL:CG2	4:T:195:TRP:HB2	2.41	0.40
1:A:59:LEU:HD21	1:A:82:GLU:HG3	2.03	0.40
4:H:72:ARG:HD3	4:H:74:THR:HG22	2.02	0.40
1:C:158:GLY:O	3:U:59:VAL:O	2.39	0.40
3:U:52:THR:CG2	3:U:72:TYR:CE2	3.00	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:137:LEU:HD21	3:L:147:VAL:CG1	2.50	0.40
1:E:212:THR:O	1:E:213:ILE:HD13	2.20	0.40
1:E:312:ASN:N	1:E:312:ASN:ND2	2.68	0.40
1:E:166:VAL:HG22	1:E:245:ILE:HB	2.02	0.40
2:B:2:LEU:O	2:D:3:PHE:HZ	2.04	0.40
1:C:28:THR:CG2	2:D:105:GLN:N	2.84	0.40
2:D:5:ALA:O	2:D:8:GLY:N	2.54	0.40
4:T:162:ASN:O	4:T:163:SER:HB2	2.21	0.40
1:A:107:SER:O	1:A:111:LEU:HG	2.20	0.40
4:H:3:HIS:CG	4:H:4:LEU:N	2.88	0.40
1:A:51:ILE:HA	1:A:287:SER:OG	2.21	0.40
4:T:67:ARG:NH1	4:T:90:ASP:OD1	2.49	0.40
3:L:7:SER:HB2	3:L:8:PRO:HD3	2.04	0.40
3:U:107:ILE:HG13	3:U:167:GLN:NE2	2.37	0.40
1:A:25:LEU:HD23	1:A:34:ILE:H	1.85	0.40
1:E:125:PHE:HB2	1:E:127:TRP:HE1	1.80	0.40
3:U:8:PRO:HB2	3:U:11:MET:HG2	2.03	0.40
1:C:160:THR:CA	1:C:196:VAL:HG21	2.49	0.40
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.57	0.40
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.56	0.40
3:U:145:ILE:HG12	3:U:146:ASN:N	2.36	0.40
2:B:106:HIS:CG	2:B:106:HIS:O	2.72	0.40
1:C:293:PRO:C	1:C:294:PHE:CD2	2.95	0.40
2:D:165:GLU:OE1	2:D:168:ASN:ND2	2.55	0.40
1:A:13:LEU:HB3	2:B:138:PHE:HB2	2.03	0.40
4:T:39:ARG:NH1	4:T:94:TYR:OH	2.53	0.40
4:H:73:ASP:O	4:H:74:THR:C	2.60	0.40
4:H:73:ASP:O	4:H:76:LYS:N	2.51	0.40
3:L:35:TYR:HB3	3:L:49:ILE:O	2.22	0.40
1:A:187:THR:HB	1:A:189:GLN:CD	2.41	0.40
4:T:150:LYS:HA	4:T:183:THR:HG23	2.02	0.40
1:A:326:LYS:O	1:A:327:GLN:CB	2.70	0.40
2:D:163:ARG:O	2:D:164:ASP:C	2.59	0.40
3:U:113:ALA:HB2	3:U:201:THR:HG21	2.02	0.40
1:A:15:LEU:HD11	2:B:119:PHE:HB2	2.03	0.40
2:B:52:LEU:O	2:B:55:VAL:N	2.55	0.40
2:B:52:LEU:O	2:B:53:ASN:C	2.59	0.40
1:C:306:PRO:O	1:C:307:LYS:C	2.60	0.40
2:D:107:THR:O	2:D:110:LEU:HB3	2.21	0.40
2:D:159:HIS:C	2:D:159:HIS:HD1	2.25	0.40
1:E:13:LEU:HD13	1:E:14:CYS:O	2.22	0.40
1:E:296:ASN:ND2	1:E:309:VAL:O	2.55	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:170:ARG:CB	2:F:171:PHE:CD1	3.02	0.40
2:F:88:LYS:O	2:F:91:LEU:N	2.54	0.40
2:F:122:THR:OG1	2:F:123:ARG:N	2.53	0.40
3:U:125:GLN:NE2	4:T:129:TYR:CE2	2.88	0.40
3:L:6:GLN:OE1	3:L:87:TYR:O	2.39	0.40
3:L:8:PRO:C	3:L:10:ILE:N	2.72	0.40
2:B:80:LEU:HD21	2:D:80:LEU:CD2	2.51	0.40
4:H:14:PRO:O	4:H:15:SER:OG	2.33	0.40
3:L:180:LEU:HD12	3:L:181:THR:N	2.36	0.40
1:A:132:GLN:HB3	1:A:133:ASN:H	1.65	0.40
1:C:308:TYR:CD2	1:C:309:VAL:N	2.89	0.40
2:F:98:LEU:HD23	2:F:102:LEU:HG	2.03	0.40
4:H:97:ALA:CB	4:H:109:TYR:O	2.63	0.40
4:H:152:TYR:CZ	4:H:157:VAL:HG22	2.57	0.40
4:H:217:ILE:HD12	4:H:217:ILE:HG23	1.86	0.40
3:L:149:TRP:HE1	3:L:178:SER:CB	2.34	0.40
1:C:125:PHE:HB2	1:C:127:TRP:NE1	2.37	0.40
1:A:246:ASN:C	1:A:246:ASN:ND2	2.75	0.40
3:L:212:ARG:NH2	4:H:138:GLN:N	2.63	0.40
2:B:82:LYS:O	2:B:83:TYR:C	2.59	0.40
1:E:94:PHE:HD1	1:E:94:PHE:O	2.03	0.40
1:A:308:TYR:HD2	2:B:89:ILE:HG13	1.86	0.40
1:C:232:ILE:HG23	1:C:232:ILE:HD12	1.71	0.40
4:H:212:LYS:O	4:H:213:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/328 (97%)	247 (78%)	43 (14%)	28 (9%)	1	19
1	C	318/328 (97%)	241 (76%)	53 (17%)	24 (8%)	2	24
1	E	318/328 (97%)	250 (79%)	41 (13%)	27 (8%)	1	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	173/175 (99%)	96 (56%)	44 (25%)	33 (19%)	0	3
2	D	173/175 (99%)	89 (51%)	48 (28%)	36 (21%)	0	2
2	F	173/175 (99%)	89 (51%)	49 (28%)	35 (20%)	0	2
3	L	211/213 (99%)	141 (67%)	46 (22%)	24 (11%)	1	12
3	U	211/213 (99%)	139 (66%)	51 (24%)	21 (10%)	1	15
4	H	219/221 (99%)	158 (72%)	38 (17%)	23 (10%)	1	14
4	T	217/221 (98%)	147 (68%)	47 (22%)	23 (11%)	1	14
All	All	2331/2377 (98%)	1597 (68%)	460 (20%)	274 (12%)	1	12

All (274) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	81	ASN
1	A	210	GLN
1	A	263	GLY
1	A	287	SER
1	A	304	ALA
2	B	5	ALA
2	B	11	GLU
2	B	55	VAL
2	B	56	ILE
2	B	59	THR
2	B	116	ASN
2	B	154	ASN
2	B	168	ASN
2	B	170	ARG
1	C	44	GLN
1	C	70	LEU
1	C	81	ASN
1	C	156	LYS
1	C	210	GLN
1	C	263	GLY
1	C	287	SER
2	D	5	ALA
2	D	11	GLU
2	D	15	GLU
2	D	55	VAL
2	D	59	THR
2	D	97	GLU

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Mol	Chain	Res	Type
2	D	116	ASN
2	D	127	ARG
2	D	150	GLU
2	D	164	ASP
2	D	168	ASN
2	D	170	ARG
1	E	44	GLN
1	E	81	ASN
1	E	156	LYS
1	E	210	GLN
1	E	263	GLY
1	E	287	SER
1	E	321	ARG
2	F	5	ALA
2	F	11	GLU
2	F	14	TRP
2	F	15	GLU
2	F	55	VAL
2	F	56	ILE
2	F	59	THR
2	F	97	GLU
2	F	116	ASN
2	F	127	ARG
2	F	150	GLU
2	F	168	ASN
2	F	170	ARG
2	F	174	LYS
3	L	26	SER
3	L	31	SER
3	L	32	SER
3	L	57	SER
3	L	93	GLU
3	L	127	THR
3	L	141	TYR
3	L	142	PRO
3	L	206	ILE
3	L	209	SER
4	H	2	VAL
4	H	16	GLN
4	H	29	ILE
4	H	52	ILE
4	H	55	ASP

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Mol	Chain	Res	Type
4	H	57	SER
4	H	66	ASN
4	H	74	THR
4	H	135	SER
4	H	147	CYS
4	H	194	THR
4	H	195	TRP
3	U	31	SER
3	U	57	SER
3	U	62	ARG
3	U	93	GLU
3	U	111	ASP
3	U	127	THR
3	U	139	ASN
3	U	141	TYR
3	U	142	PRO
4	T	29	ILE
4	T	52	ILE
4	T	66	ASN
4	T	74	THR
4	T	121	ALA
4	T	135	SER
4	T	147	CYS
4	T	195	TRP
1	A	19	ALA
1	A	44	GLN
1	A	70	LEU
1	A	92	LYS
1	A	133	ASN
1	A	321	ARG
2	B	7	ALA
2	B	14	TRP
2	B	15	GLU
2	B	28	ASN
2	B	39	LYS
2	B	57	GLU
2	B	83	TYR
2	B	97	GLU
2	B	109	ASP
2	B	127	ARG
2	B	150	GLU
2	B	164	ASP

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Mol	Chain	Res	Type
2	B	169	ASN
2	B	174	LYS
1	C	19	ALA
1	C	62	ILE
1	C	132	GLN
1	C	133	ASN
1	C	277	CYS
1	C	304	ALA
1	C	327	GLN
2	D	14	TRP
2	D	39	LYS
2	D	56	ILE
2	D	57	GLU
2	D	75	GLY
2	D	77	ILE
2	D	83	TYR
2	D	102	LEU
2	D	103	GLU
2	D	115	MET
2	D	130	ALA
2	D	132	GLU
2	D	133	MET
2	D	154	ASN
2	D	169	ASN
2	D	174	LYS
1	E	29	ILE
1	E	92	LYS
1	E	133	ASN
1	E	191	GLN
1	E	197	GLN
1	E	279	SER
2	F	39	LYS
2	F	57	GLU
2	F	83	TYR
2	F	89	ILE
2	F	132	GLU
2	F	154	ASN
2	F	164	ASP
2	F	169	ASN
3	L	62	ARG
3	L	75	THR
3	L	111	ASP

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Mol	Chain	Res	Type
3	L	139	ASN
3	L	151	ILE
3	L	205	PRO
4	H	15	SER
4	H	62	PRO
4	H	134	GLY
3	U	110	ALA
3	U	151	ILE
3	U	154	SER
3	U	205	PRO
3	U	206	ILE
3	U	209	SER
4	T	15	SER
4	T	16	GLN
4	T	55	ASP
4	T	57	SER
4	T	61	ASN
4	T	62	PRO
4	T	194	THR
1	A	21	PRO
1	A	172	ASP
1	A	327	GLN
2	B	78	GLN
2	B	102	LEU
2	B	132	GLU
1	C	18	HIS
1	C	29	ILE
1	C	279	SER
1	C	293	PRO
1	C	313	THR
2	D	92	TRP
2	D	124	ARG
1	E	19	ALA
1	E	110	SER
1	E	192	THR
1	E	196	VAL
1	E	277	CYS
1	E	304	ALA
2	F	88	LYS
2	F	103	GLU
2	F	109	ASP
2	F	133	MET

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Mol	Chain	Res	Type
3	L	83	ASP
3	L	154	SER
3	L	169	SER
3	L	201	THR
4	H	102	ASP
4	H	208	ALA
4	H	210	SER
3	U	9	ALA
3	U	26	SER
3	U	75	THR
4	T	134	GLY
4	T	192	SER
4	T	197	SER
1	A	18	HIS
1	A	62	ILE
1	A	80	GLN
1	A	132	GLN
1	A	158	GLY
1	A	196	VAL
1	A	250	ASN
1	A	277	CYS
1	A	313	THR
2	B	103	GLU
2	B	124	ARG
2	B	133	MET
1	C	21	PRO
1	C	158	GLY
2	D	19	ASP
2	D	81	GLU
2	D	88	LYS
2	D	112	ASP
1	E	18	HIS
1	E	21	PRO
1	E	62	ILE
1	E	327	GLN
2	F	28	ASN
2	F	54	ARG
2	F	112	ASP
2	F	124	ARG
2	F	130	ALA
3	L	52	THR
4	H	3	HIS

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Mol	Chain	Res	Type
4	H	197	SER
3	U	52	THR
4	T	208	ALA
1	A	71	LEU
1	A	98	TYR
1	A	293	PRO
2	B	6	ILE
2	B	19	ASP
2	B	76	ARG
2	B	130	ALA
1	C	84	TRP
1	C	196	VAL
1	E	98	TYR
1	E	188	ASN
1	E	293	PRO
2	F	115	MET
2	F	123	ARG
2	F	153	ARG
3	L	125	GLN
4	H	101	TYR
4	H	196	PRO
4	T	179	SER
1	A	143	PRO
2	D	89	ILE
2	D	91	LEU
1	E	158	GLY
2	F	76	ARG
3	L	110	ALA
3	U	32	SER
4	T	101	TYR
3	U	7	SER
4	T	196	PRO
1	C	98	TYR
4	H	61	ASN
3	L	15	PRO
4	T	156	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/289 (98%)	252 (89%)	30 (11%)	10	45
1	C	282/289 (98%)	249 (88%)	33 (12%)	8	38
1	E	282/289 (98%)	248 (88%)	34 (12%)	7	36
2	B	149/149 (100%)	120 (80%)	29 (20%)	2	12
2	D	149/149 (100%)	116 (78%)	33 (22%)	1	8
2	F	149/149 (100%)	118 (79%)	31 (21%)	2	10
3	L	187/187 (100%)	147 (79%)	40 (21%)	1	9
3	U	187/187 (100%)	152 (81%)	35 (19%)	2	13
4	H	196/196 (100%)	163 (83%)	33 (17%)	3	19
4	T	194/196 (99%)	167 (86%)	27 (14%)	5	29
All	All	2057/2080 (99%)	1732 (84%)	325 (16%)	4	23

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	15	LEU
1	A	17	HIS
1	A	20	VAL
1	A	22	ASN
1	A	48	THR
1	A	57	ARG
1	A	65	THR
1	A	82	GLU
1	A	94	PHE
1	A	100	TYR
1	A	101	ASP
1	A	110	SER
1	A	130	VAL
1	A	136	SER
1	A	140	LYS
1	A	141	ARG
1	A	156	LYS
1	A	189	GLN
1	A	239	PRO
1	A	243	LEU
1	A	246	ASN
1	A	248	ASN
1	A	250	ASN

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Mol	Chain	Res	Type
1	A	254	PRO
1	A	265	SER
1	A	293	PRO
1	A	298	ASN
1	A	309	VAL
1	A	312	ASN
2	B	3	PHE
2	B	6	ILE
2	B	9	PHE
2	B	12	ASN
2	B	17	MET
2	B	21	TRP
2	B	24	PHE
2	B	32	THR
2	B	38	LEU
2	B	41	THR
2	B	46	ASP
2	B	48	ILE
2	B	52	LEU
2	B	54	ARG
2	B	76	ARG
2	B	78	GLN
2	B	105	GLN
2	B	106	HIS
2	B	109	ASP
2	B	119	PHE
2	B	120	GLU
2	B	121	LYS
2	B	123	ARG
2	B	135	ASN
2	B	158	ASP
2	B	160	ASP
2	B	168	ASN
2	B	171	PHE
2	B	174	LYS
1	C	13	LEU
1	C	15	LEU
1	C	17	HIS
1	C	20	VAL
1	C	22	ASN
1	C	54	ASN
1	C	57	ARG

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Mol	Chain	Res	Type
1	C	65	THR
1	C	78	VAL
1	C	82	GLU
1	C	94	PHE
1	C	101	ASP
1	C	110	SER
1	C	130	VAL
1	C	140	LYS
1	C	150	ARG
1	C	156	LYS
1	C	189	GLN
1	C	191	GLN
1	C	219	SER
1	C	239	PRO
1	C	243	LEU
1	C	246	ASN
1	C	248	ASN
1	C	250	ASN
1	C	254	PRO
1	C	265	SER
1	C	267	ILE
1	C	269	ARG
1	C	287	SER
1	C	293	PRO
1	C	309	VAL
1	C	312	ASN
2	D	3	PHE
2	D	6	ILE
2	D	9	PHE
2	D	12	ASN
2	D	17	MET
2	D	18	ILE
2	D	21	TRP
2	D	24	PHE
2	D	29	SER
2	D	32	THR
2	D	38	LEU
2	D	41	THR
2	D	46	ASP
2	D	48	ILE
2	D	71	SER
2	D	76	ARG

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Mol	Chain	Res	Type
2	D	78	GLN
2	D	84	VAL
2	D	97	GLU
2	D	98	LEU
2	D	119	PHE
2	D	120	GLU
2	D	121	LYS
2	D	123	ARG
2	D	124	ARG
2	D	133	MET
2	D	135	ASN
2	D	144	CYS
2	D	158	ASP
2	D	160	ASP
2	D	168	ASN
2	D	171	PHE
2	D	174	LYS
1	E	13	LEU
1	E	15	LEU
1	E	17	HIS
1	E	20	VAL
1	E	22	ASN
1	E	57	ARG
1	E	65	THR
1	E	78	VAL
1	E	82	GLU
1	E	85	ASP
1	E	94	PHE
1	E	100	TYR
1	E	101	ASP
1	E	128	THR
1	E	130	VAL
1	E	140	LYS
1	E	141	ARG
1	E	150	ARG
1	E	156	LYS
1	E	189	GLN
1	E	199	SER
1	E	219	SER
1	E	239	PRO
1	E	243	LEU
1	E	246	ASN

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Mol	Chain	Res	Type
1	E	248	ASN
1	E	250	ASN
1	E	254	PRO
1	E	265	SER
1	E	287	SER
1	E	293	PRO
1	E	298	ASN
1	E	309	VAL
1	E	312	ASN
2	F	3	PHE
2	F	6	ILE
2	F	9	PHE
2	F	12	ASN
2	F	17	MET
2	F	18	ILE
2	F	21	TRP
2	F	24	PHE
2	F	32	THR
2	F	41	THR
2	F	46	ASP
2	F	48	ILE
2	F	52	LEU
2	F	76	ARG
2	F	78	GLN
2	F	97	GLU
2	F	98	LEU
2	F	105	GLN
2	F	109	ASP
2	F	119	PHE
2	F	120	GLU
2	F	121	LYS
2	F	123	ARG
2	F	135	ASN
2	F	144	CYS
2	F	156	THR
2	F	158	ASP
2	F	160	ASP
2	F	168	ASN
2	F	171	PHE
2	F	174	LYS
3	L	2	ILE
3	L	8	PRO

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Mol	Chain	Res	Type
3	L	11	MET
3	L	14	SER
3	L	21	LEU
3	L	22	THR
3	L	30	THR
3	L	35	TYR
3	L	48	TRP
3	L	54	ASN
3	L	64	SER
3	L	68	SER
3	L	70	THR
3	L	71	SER
3	L	74	LEU
3	L	95	PHE
3	L	97	ARG
3	L	99	PHE
3	L	103	THR
3	L	107	ILE
3	L	123	LYS
3	L	125	GLN
3	L	126	LEU
3	L	139	ASN
3	L	154	SER
3	L	155	GLU
3	L	164	TRP
3	L	165	THR
3	L	166	ASP
3	L	170	LYS
3	L	171	ASP
3	L	174	TYR
3	L	177	SER
3	L	185	ASP
3	L	189	ARG
3	L	190	HIS
3	L	191	ASN
3	L	192	SER
3	L	203	THR
3	L	204	SER
4	H	2	VAL
4	H	11	LEU
4	H	13	LYS
4	H	16	GLN

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Mol	Chain	Res	Type
4	H	18	LEU
4	H	25	THR
4	H	28	SER
4	H	36	THR
4	H	42	PRO
4	H	51	TYR
4	H	59	ASN
4	H	62	PRO
4	H	66	ASN
4	H	71	THR
4	H	74	THR
4	H	80	PHE
4	H	84	ASN
4	H	104	ASP
4	H	116	LEU
4	H	117	THR
4	H	120	SER
4	H	124	THR
4	H	126	PRO
4	H	128	VAL
4	H	138	GLN
4	H	140	ASN
4	H	143	VAL
4	H	148	LEU
4	H	154	PRO
4	H	157	VAL
4	H	179	SER
4	H	214	ASP
4	H	216	LYS
3	U	11	MET
3	U	14	SER
3	U	21	LEU
3	U	22	THR
3	U	23	CYS
3	U	30	THR
3	U	35	TYR
3	U	55	LEU
3	U	64	SER
3	U	68	SER
3	U	70	THR
3	U	71	SER
3	U	74	LEU

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Mol	Chain	Res	Type
3	U	95	PHE
3	U	97	ARG
3	U	103	THR
3	U	123	LYS
3	U	125	GLN
3	U	154	SER
3	U	155	GLU
3	U	162	ASN
3	U	164	TRP
3	U	165	THR
3	U	166	ASP
3	U	170	LYS
3	U	171	ASP
3	U	183	THR
3	U	185	ASP
3	U	189	ARG
3	U	190	HIS
3	U	191	ASN
3	U	192	SER
3	U	203	THR
3	U	204	SER
3	U	212	ARG
4	T	12	VAL
4	T	13	LYS
4	T	16	GLN
4	T	17	SER
4	T	18	LEU
4	T	28	SER
4	T	36	THR
4	T	52	ILE
4	T	55	ASP
4	T	59	ASN
4	T	62	PRO
4	T	67	ARG
4	T	71	THR
4	T	74	THR
4	T	80	PHE
4	T	104	ASP
4	T	116	LEU
4	T	117	THR
4	T	124	THR
4	T	126	PRO

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Mol	Chain	Res	Type
4	T	140	ASN
4	T	147	CYS
4	T	148	LEU
4	T	154	PRO
4	T	157	VAL
4	T	214	ASP
4	T	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	22	ASN
1	A	38	ASN
1	A	54	ASN
1	A	80	GLN
1	A	81	ASN
1	A	96	ASN
1	A	188	ASN
1	A	189	GLN
1	A	191	GLN
1	A	210	GLN
1	A	211	GLN
1	A	216	ASN
1	A	246	ASN
1	A	248	ASN
1	A	250	ASN
1	A	296	ASN
1	A	298	ASN
1	A	312	ASN
2	B	28	ASN
2	B	49	ASN
2	B	60	ASN
2	B	78	GLN
2	B	125	GLN
2	B	154	ASN
2	B	168	ASN
1	C	17	HIS
1	C	22	ASN
1	C	38	ASN
1	C	54	ASN
1	C	81	ASN

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Mol	Chain	Res	Type
1	C	96	ASN
1	C	170	ASN
1	C	188	ASN
1	C	189	GLN
1	C	210	GLN
1	C	211	GLN
1	C	216	ASN
1	C	246	ASN
1	C	248	ASN
1	C	285	ASN
1	C	296	ASN
1	C	298	ASN
1	C	311	GLN
1	C	312	ASN
1	C	322	ASN
2	D	28	ASN
2	D	49	ASN
2	D	60	ASN
2	D	78	GLN
2	D	125	GLN
2	D	154	ASN
2	D	168	ASN
1	E	22	ASN
1	E	38	ASN
1	E	54	ASN
1	E	75	HIS
1	E	80	GLN
1	E	81	ASN
1	E	96	ASN
1	E	188	ASN
1	E	189	GLN
1	E	210	GLN
1	E	248	ASN
1	E	285	ASN
1	E	296	ASN
1	E	298	ASN
1	E	312	ASN
2	F	28	ASN
2	F	49	ASN
2	F	60	ASN
2	F	78	GLN
2	F	105	GLN

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Mol	Chain	Res	Type
2	F	125	GLN
2	F	168	ASN
3	L	6	GLN
3	L	39	GLN
3	L	91	GLN
3	L	191	ASN
3	L	199	HIS
4	H	40	GLN
4	H	61	ASN
4	H	77	ASN
4	H	78	GLN
4	H	84	ASN
4	H	140	ASN
4	H	162	ASN
4	H	206	HIS
3	U	1	GLN
3	U	6	GLN
3	U	38	GLN
3	U	91	GLN
3	U	191	ASN
3	U	199	HIS
4	T	58	ASN
4	T	61	ASN
4	T	77	ASN
4	T	78	GLN
4	T	84	ASN
4	T	140	ASN
4	T	162	ASN
4	T	206	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

9 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	450	1,5	12,14,15	0.76	0	15,19,21	1.26	2 (13%)
5	NAG	A	451	5	12,14,15	0.58	0	15,19,21	0.85	1 (6%)
5	MAN	A	452	5	10,11,12	0.95	1 (10%)	11,15,17	1.02	1 (9%)
5	NAG	C	450	1,5	12,14,15	0.64	0	15,19,21	0.86	1 (6%)
5	NAG	C	451	5	12,14,15	0.73	0	15,19,21	0.86	1 (6%)
5	MAN	C	452	5	10,11,12	1.05	0	11,15,17	1.16	1 (9%)
5	NAG	E	450	1,5	12,14,15	0.69	0	15,19,21	1.09	1 (6%)
5	NAG	E	451	5	12,14,15	0.96	0	15,19,21	1.03	1 (6%)
5	MAN	E	452	5	10,11,12	0.85	0	11,15,17	1.19	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	451	5	-	0/6/23/26	0/1/1/1
5	MAN	A	452	5	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	C	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	451	5	-	0/6/23/26	0/1/1/1
5	MAN	C	452	5	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	E	450	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	451	5	-	0/6/23/26	0/1/1/1
5	MAN	E	452	5	1/1/4/5	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	452	MAN	C4-C5	2.11	1.57	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	450	NAG	C2-N2-C7	-3.28	117.58	123.09
5	C	452	MAN	C6-C5-C4	2.92	120.06	113.00
5	E	452	MAN	C6-C5-C4	2.74	119.61	113.00
5	A	452	MAN	C6-C5-C4	2.42	118.84	113.00
5	E	451	NAG	C2-N2-C7	-2.26	119.29	123.09
5	C	451	NAG	C2-N2-C7	-2.26	119.30	123.09
5	A	451	NAG	C2-N2-C7	-2.16	119.46	123.09
5	E	450	NAG	C2-N2-C7	-2.11	119.55	123.09
5	A	450	NAG	C4-C3-C2	-2.04	106.31	111.32
5	C	450	NAG	C2-N2-C7	-2.02	119.69	123.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	452	MAN	C1
5	A	452	MAN	C1
5	C	452	MAN	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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