



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:28 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

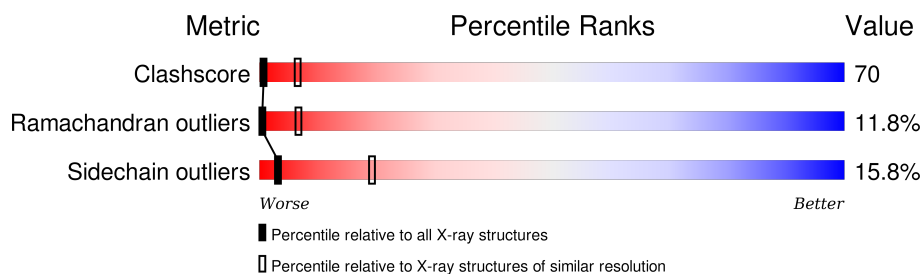
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	328	
1	C	328	
1	E	328	
2	B	175	
2	D	175	
2	F	175	
3	L	213	

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Mol	Chain	Length	Quality of chain
3	U	213	
4	H	221	
4	T	221	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	A	452	X	-	-	-
5	MAN	C	452	X	-	-	-
5	MAN	E	452	X	-	-	-

2 Entry composition

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

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

- Molecule 1 is a protein called 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).

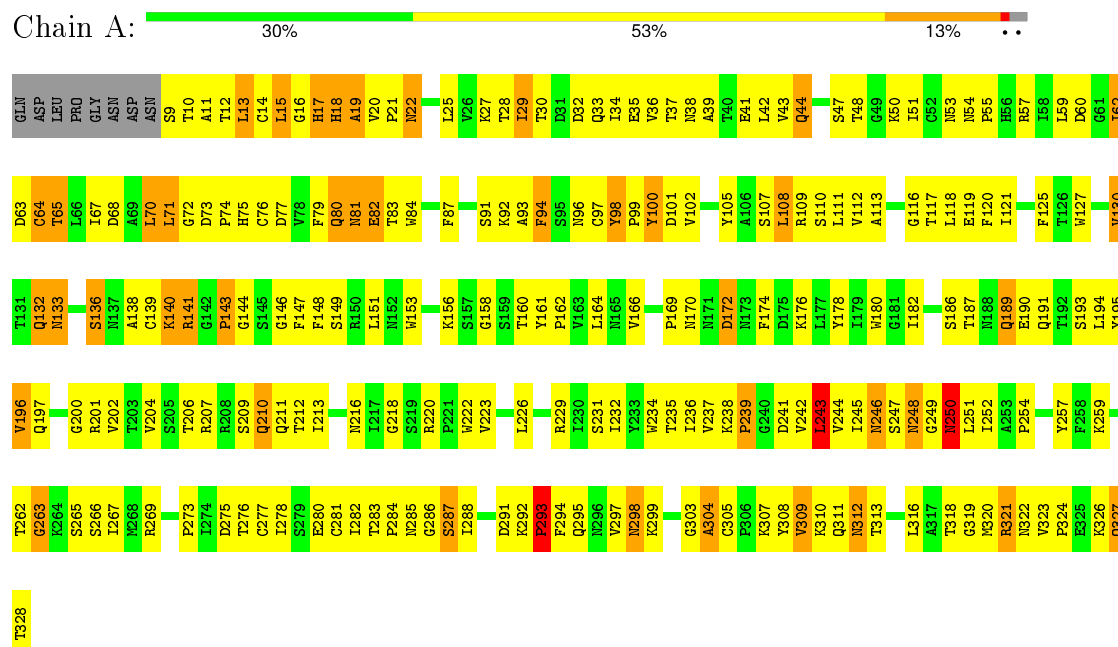
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	C	3	Total	C	N	O	0	0
			39	22	2	15		
5	E	3	Total	C	N	O	0	0
			39	22	2	15		

3 Residue-property plots

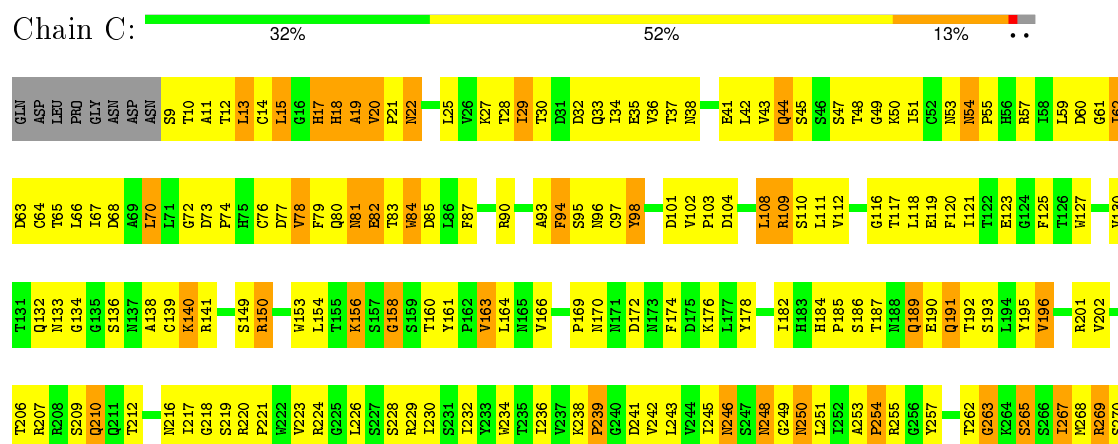
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

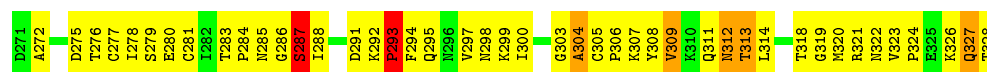
Note EDS was not executed.

• Molecule 1: hemagglutinin HA1



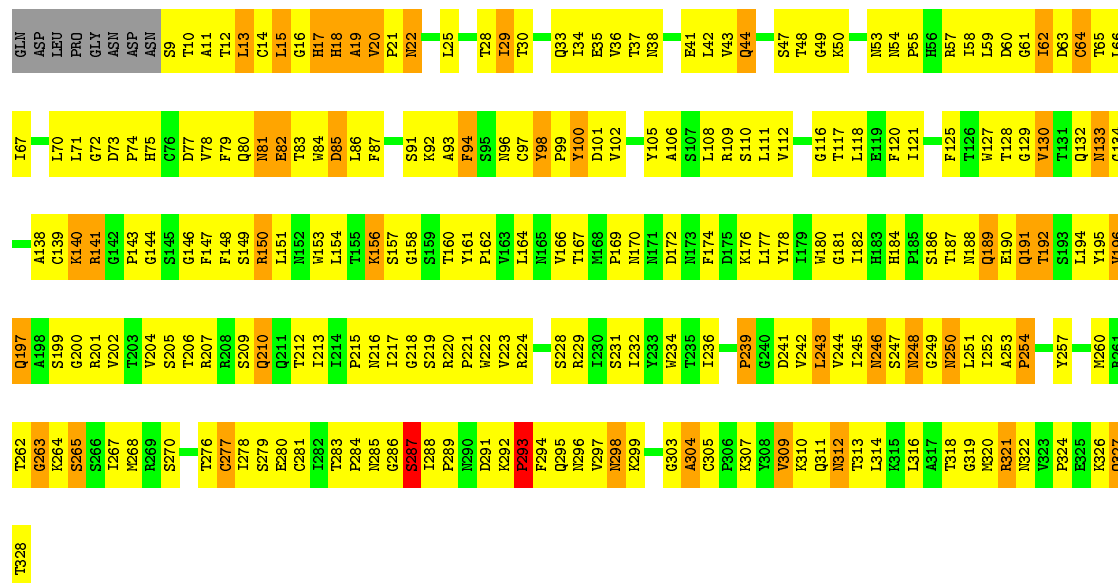
• Molecule 1: hemagglutinin HA1





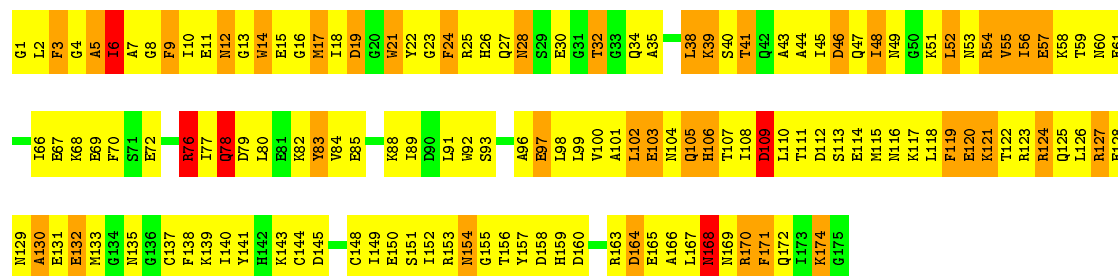
• Molecule 1: hemagglutinin HA1

Chain E: 27% 57% 13% ..



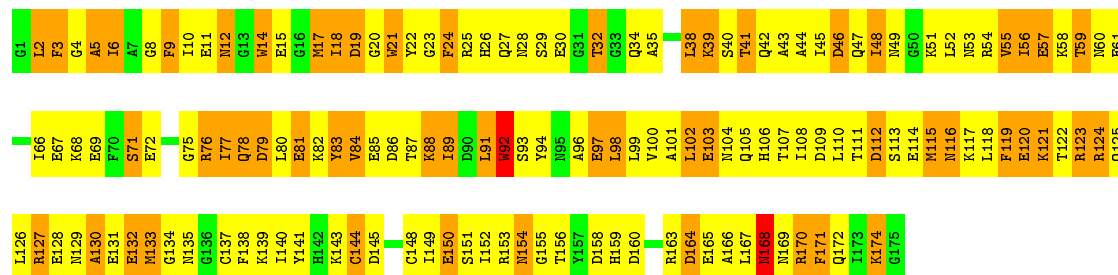
• Molecule 2: hemagglutinin HA2

Chain B: 18% 57% 22% .

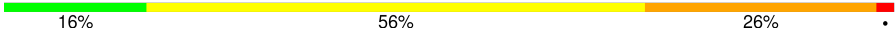


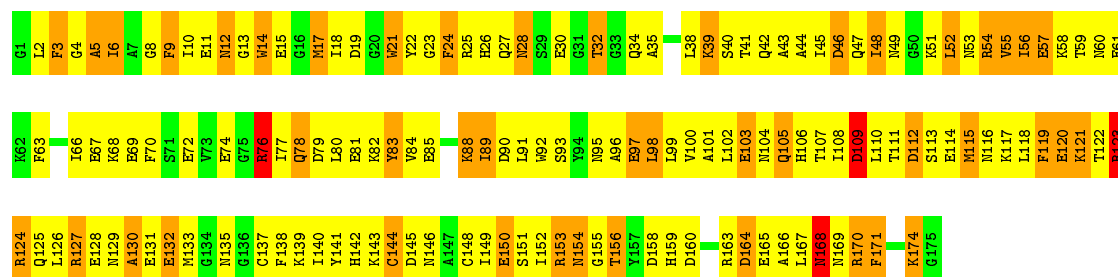
• Molecule 2: hemagglutinin HA2

Chain D: 15% 51% 32% .

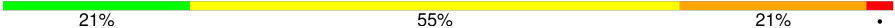


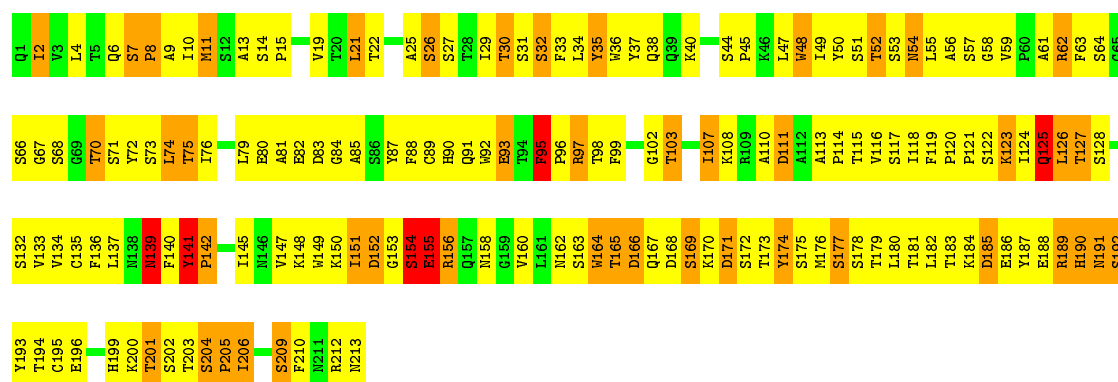
• Molecule 2: hemagglutinin HA2

Chain F:  16% 56% 26%

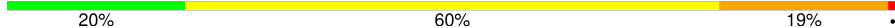


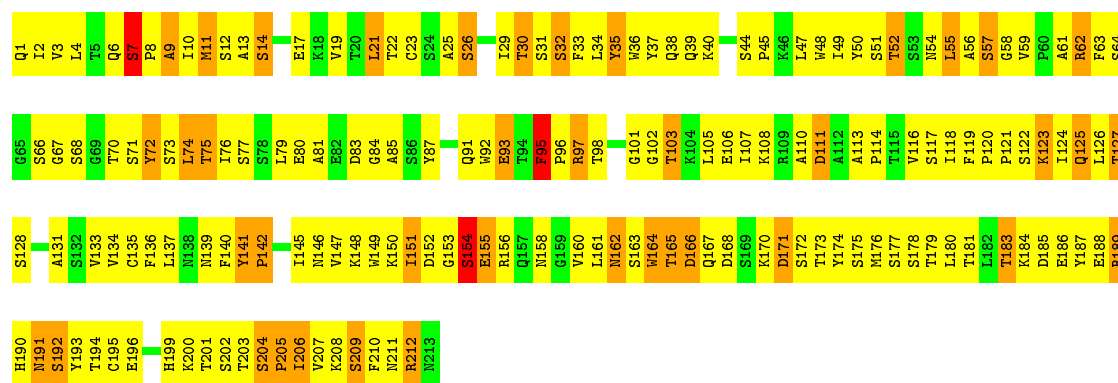
- Molecule 3: influenza virus infectivity neutralizing antibody (light chain)

Chain L:  21% 55% 21%

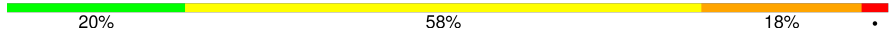


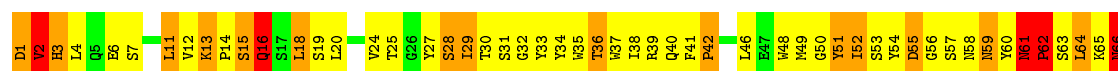
- Molecule 3: influenza virus infectivity neutralizing antibody (light chain)

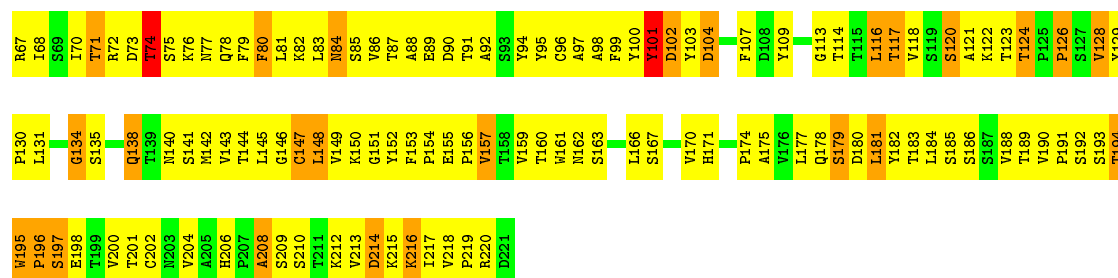
Chain U:  20% 60% 19%



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

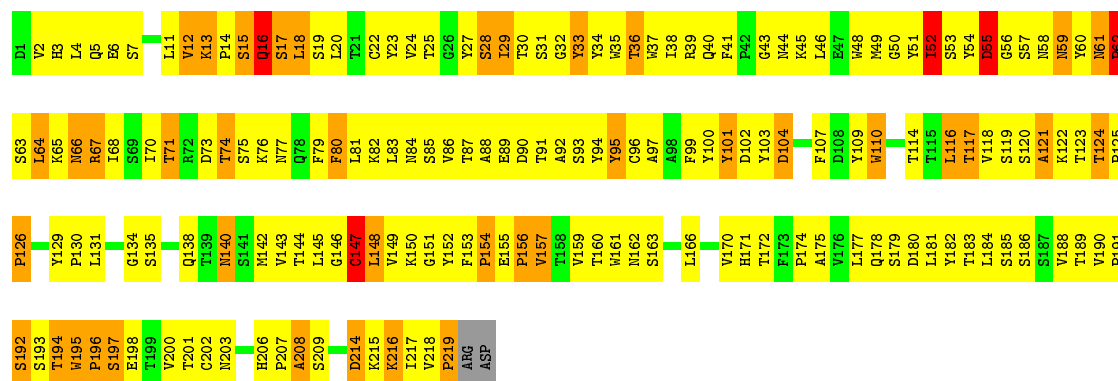
Chain H:  20% 58% 18%





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

Chain T: 19% 59% 18% ..



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, α , β , γ	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 ²)	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 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 70.

All (2549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASN:HD21	1:C:140:LYS:HE2	1.10	1.10
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:9:PHE:C	2:F:9:PHE:CD1	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:28:SER:HA	4:T:77:ASN:ND2	2.30	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/328 (97%)	247 (78%)	43 (14%)	28 (9%)	1	12
1	C	318/328 (97%)	241 (76%)	53 (17%)	24 (8%)	1	15
1	E	318/328 (97%)	250 (79%)	41 (13%)	27 (8%)	1	13
2	B	173/175 (99%)	96 (56%)	44 (25%)	33 (19%)	0	2
2	D	173/175 (99%)	89 (51%)	48 (28%)	36 (21%)	0	1
2	F	173/175 (99%)	89 (51%)	49 (28%)	35 (20%)	0	1
3	L	211/213 (99%)	141 (67%)	46 (22%)	24 (11%)	0	7
3	U	211/213 (99%)	139 (66%)	51 (24%)	21 (10%)	1	9
4	H	219/221 (99%)	158 (72%)	38 (17%)	23 (10%)	1	8
4	T	217/221 (98%)	147 (68%)	47 (22%)	23 (11%)	0	8
All	All	2331/2377 (98%)	1597 (68%)	460 (20%)	274 (12%)	0	7

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	8	38
1	C	282/289 (98%)	249 (88%)	33 (12%)	7	32
1	E	282/289 (98%)	248 (88%)	34 (12%)	6	30
2	B	149/149 (100%)	120 (80%)	29 (20%)	2	10
2	D	149/149 (100%)	116 (78%)	33 (22%)	1	6
2	F	149/149 (100%)	118 (79%)	31 (21%)	1	8
3	L	187/187 (100%)	147 (79%)	40 (21%)	1	7
3	U	187/187 (100%)	152 (81%)	35 (19%)	2	11
4	H	196/196 (100%)	163 (83%)	33 (17%)	2	15
4	T	194/196 (99%)	167 (86%)	27 (14%)	4	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2057/2080 (99%)	1732 (84%)	325 (16%)	3 19

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	14,14,15	0.68	0	15,19,21	1.53	2 (13%)
5	NAG	A	451	5	14,14,15	0.51	0	15,19,21	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	452	5	11,11,12	0.96	1 (9%)	14,15,17	0.97	1 (7%)
5	NAG	C	450	1,5	14,14,15	0.67	0	15,19,21	1.12	2 (13%)
5	NAG	C	451	5	14,14,15	0.73	0	15,19,21	0.94	1 (6%)
5	MAN	C	452	5	11,11,12	1.11	1 (9%)	14,15,17	1.05	1 (7%)
5	NAG	E	450	1,5	14,14,15	0.78	0	15,19,21	1.22	2 (13%)
5	NAG	E	451	5	14,14,15	1.24	1 (7%)	15,19,21	1.20	2 (13%)
5	MAN	E	452	5	11,11,12	0.85	0	14,15,17	1.13	1 (7%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	451	NAG	C1-C2	-3.37	1.47	1.52
5	C	452	MAN	C4-C5	2.04	1.57	1.53
5	A	452	MAN	C4-C5	2.16	1.57	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	450	NAG	C2-N2-C7	-4.25	117.58	123.04
5	A	450	NAG	C4-C3-C2	-3.16	106.31	111.23
5	E	451	NAG	C2-N2-C7	-2.92	119.29	123.04
5	C	451	NAG	C2-N2-C7	-2.91	119.30	123.04
5	A	451	NAG	C2-N2-C7	-2.78	119.46	123.04
5	E	450	NAG	C2-N2-C7	-2.72	119.55	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	450	NAG	C2-N2-C7	-2.61	119.69	123.04
5	E	450	NAG	C4-C3-C2	-2.39	107.51	111.23
5	C	450	NAG	C4-C3-C2	-2.36	107.56	111.23
5	A	452	MAN	C6-C5-C4	2.36	118.84	113.02
5	E	451	NAG	C4-C3-C2	2.52	115.14	111.23
5	E	452	MAN	C6-C5-C4	2.67	119.61	113.02
5	C	452	MAN	C6-C5-C4	2.86	120.06	113.02

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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	451	NAG	3	0
5	C	450	NAG	2	0
5	C	451	NAG	2	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section 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.