



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 06:43 AM JST

PDB ID : 7F4S
Title : Crystal structure of TthMTA1-PteMTA9 complex
Authors : Chen, J.; Liu, L.
Deposited on : 2021-06-21
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

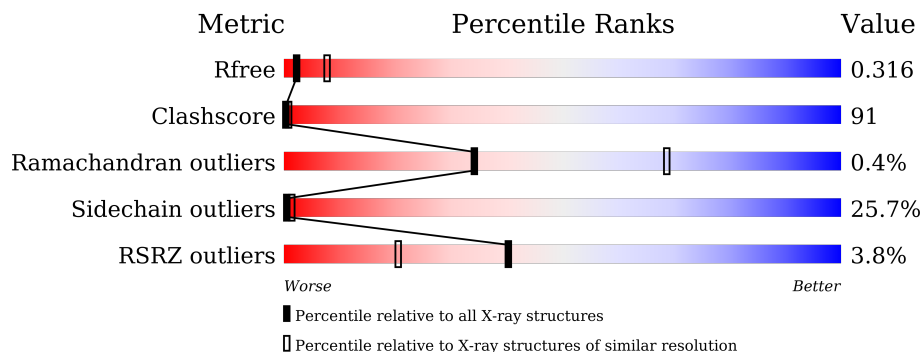
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	202	
1	B	202	
1	C	202	
2	D	237	
2	E	237	
2	F	237	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9145 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 MT-a70 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	178	1422	909	244	261	8	0	0	0
1	B	178	1426	906	249	263	8	0	0	0
1	C	176	1411	898	244	261	8	0	0	0

- Molecule 2 is a protein called MTA9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	215	1632	1041	269	315	7	0	0	0
2	E	213	1608	1034	270	297	7	0	0	0
2	F	192	1434	927	239	262	6	0	0	0

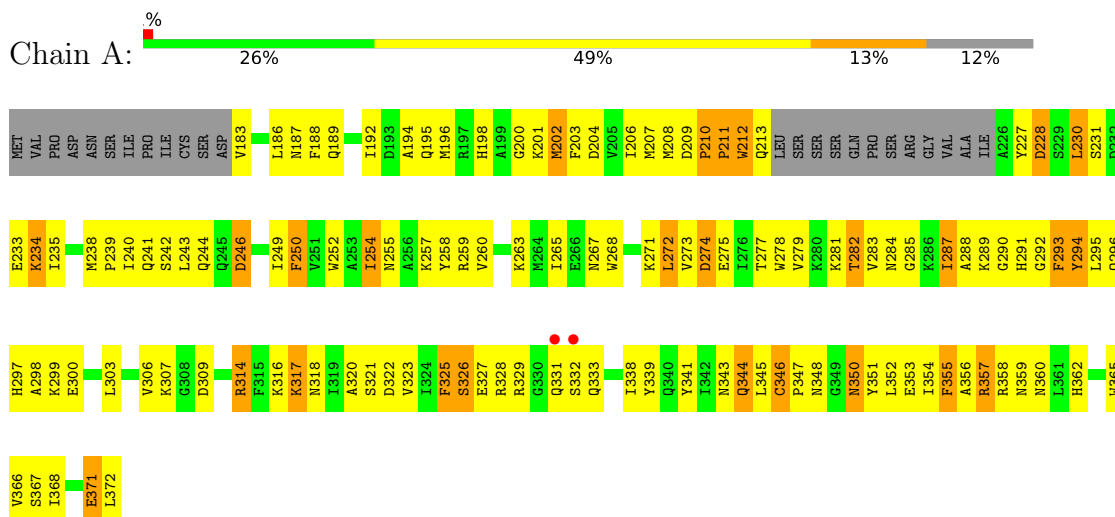
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	28	Total	O	0	0
			28	28		
3	C	24	Total	O	0	0
			24	24		
3	D	43	Total	O	0	0
			43	43		
3	E	43	Total	O	0	0
			43	43		
3	F	42	Total	O	0	0
			42	42		

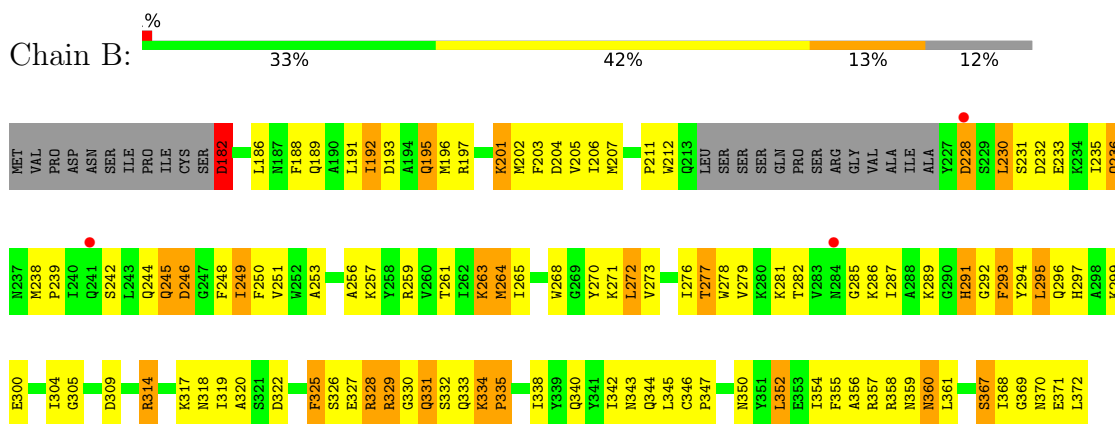
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

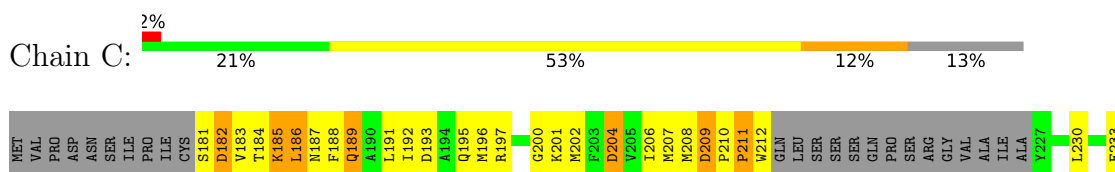
- Molecule 1: MT-a70 family protein



- Molecule 1: MT-a70 family protein



- Molecule 1: MT-a70 family protein

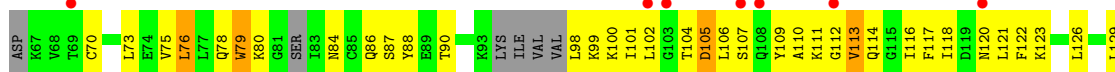




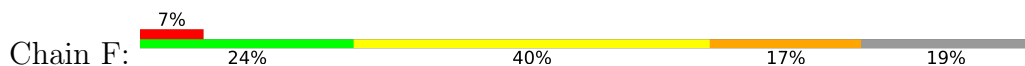
• Molecule 2: MTA9

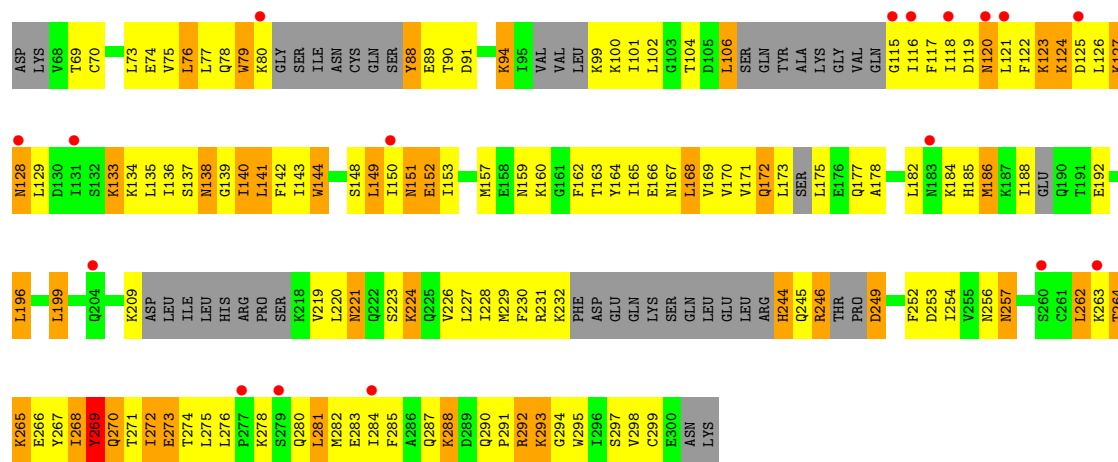


• Molecule 2: MTA9



• Molecule 2: MTA9





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.70Å 75.65Å 142.47Å 90.00° 99.16° 90.00°	Depositor
Resolution (Å)	44.93 – 3.09 44.93 – 3.09	Depositor EDS
% Data completeness (in resolution range)	57.1 (44.93-3.09) 77.2 (44.93-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.304 , 0.316 0.304 , 0.316	Depositor DCC
R_{free} test set	2000 reflections (8.66%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtrriage
Anisotropy	0.081	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 103.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	9145	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	0.57	3/1453 (0.2%)	0.77	7/1962 (0.4%)
1	B	0.57	2/1457 (0.1%)	0.70	4/1967 (0.2%)
1	C	0.62	3/1440 (0.2%)	0.72	5/1943 (0.3%)
2	D	0.55	2/1646 (0.1%)	0.73	4/2223 (0.2%)
2	E	0.48	1/1623 (0.1%)	0.69	3/2186 (0.1%)
2	F	0.45	0/1445	0.70	2/1943 (0.1%)
All	All	0.54	11/9064 (0.1%)	0.72	25/12224 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	F	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	277	PRO	N-CD	5.33	1.55	1.47
1	A	239	PRO	N-CD	5.29	1.55	1.47
1	A	347	PRO	N-CD	5.23	1.55	1.47
2	D	248	PRO	N-CD	5.22	1.55	1.47
2	D	277	PRO	N-CD	5.22	1.55	1.47
1	B	239	PRO	N-CD	5.13	1.55	1.47
1	C	239	PRO	N-CD	5.11	1.55	1.47
1	C	210	PRO	N-CD	5.11	1.55	1.47
1	A	211	PRO	N-CD	5.10	1.54	1.47
1	C	211	PRO	N-CD	5.08	1.54	1.47
1	B	335	PRO	N-CD	5.00	1.54	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	TRP	N-CA-CB	-10.94	90.91	110.60
1	A	211	PRO	N-CA-C	-8.73	89.40	112.10
1	A	212	TRP	N-CA-C	-7.13	91.74	111.00
1	A	211	PRO	CB-CA-C	-6.95	94.62	112.00
2	D	291	PRO	N-CA-CB	6.30	110.86	103.30
2	E	291	PRO	N-CA-CB	6.28	110.83	103.30
1	B	346	CYS	C-N-CD	6.26	141.54	128.40
2	F	276	LEU	C-N-CD	6.10	141.22	128.40
1	C	346	CYS	C-N-CD	6.02	141.04	128.40
1	B	204	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	334	LYS	C-N-CD	5.94	140.88	128.40
1	C	238	MET	C-N-CD	5.79	140.55	128.40
1	A	209	ASP	C-N-CD	5.78	140.54	128.40
2	F	290	GLN	C-N-CD	5.72	140.41	128.40
2	D	276	LEU	C-N-CD	5.70	140.38	128.40
1	A	210	PRO	C-N-CD	5.70	140.37	128.40
1	B	238	MET	C-N-CD	5.70	140.36	128.40
1	C	210	PRO	C-N-CD	5.68	140.32	128.40
1	B	334	LYS	C-N-CD	5.68	140.32	128.40
1	A	346	CYS	C-N-CD	5.62	140.20	128.40
1	C	209	ASP	C-N-CD	5.59	140.14	128.40
2	E	276	LEU	C-N-CD	5.53	140.00	128.40
2	D	247	THR	C-N-CD	5.49	139.93	128.40
2	E	248	PRO	N-CA-CB	5.44	109.83	103.30
2	D	200	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	182	ASP	Peptide
2	F	269	TYR	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1422	0	1371	289	0
1	B	1426	0	1364	262	1
1	C	1411	0	1357	243	2
2	D	1632	0	1554	314	1
2	E	1608	0	1552	272	0
2	F	1434	0	1364	384	1
3	A	32	0	0	2	0
3	B	28	0	0	4	1
3	C	24	0	0	10	0
3	D	43	0	0	9	0
3	E	43	0	0	9	0
3	F	42	0	0	11	0
All	All	9145	0	8562	1591	3

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 91.

All (1591) 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:292:GLY:HA2	1:A:297:HIS:CE1	1.23	1.68
2:D:134:LYS:HE2	2:D:282:MET:SD	1.14	1.67
2:F:118:ILE:CG1	2:F:284:ILE:HD12	1.29	1.60
2:F:144:TRP:HE1	2:F:264:THR:CG2	1.12	1.59
2:E:79:TRP:CZ3	2:E:190:GLN:NE2	1.68	1.57
1:A:292:GLY:CA	1:A:297:HIS:CE1	1.79	1.56
2:F:118:ILE:HG12	2:F:284:ILE:CD1	1.10	1.55
2:E:242:LEU:CB	2:E:277:PRO:HD2	1.36	1.54
2:D:97:VAL:CG2	2:D:109:TYR:CE1	1.90	1.51
2:F:70:CYS:H	2:F:199:LEU:CD2	1.18	1.51
2:D:97:VAL:CG2	2:D:109:TYR:CZ	1.94	1.50
1:B:272:LEU:CB	2:F:151:ASN:ND2	1.72	1.50
1:B:320:ALA:CB	2:F:220:LEU:CD2	1.87	1.49
1:A:287:ILE:CG2	1:B:371:GLU:HB2	1.41	1.47
1:A:289:LYS:NZ	1:B:186:LEU:HD13	1.19	1.46
1:C:321:SER:HB2	2:E:208:VAL:CG2	1.41	1.46
2:E:175:LEU:HD21	2:E:191:THR:CB	1.44	1.46
1:B:320:ALA:CB	2:F:220:LEU:HD22	1.43	1.45
1:B:293:PHE:HE2	2:F:244:HIS:CD2	1.36	1.43
1:C:293:PHE:O	2:E:245:GLN:CB	1.67	1.43
1:C:353:GLU:OE1	1:C:356:ALA:CB	1.64	1.43
1:B:320:ALA:HB3	2:F:220:LEU:CD2	0.99	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:242:LEU:CB	2:E:277:PRO:CD	1.95	1.43
1:B:296:GLN:HE21	2:F:246:ARG:C	1.21	1.42
2:F:74:GLU:O	2:F:78:GLN:CB	1.65	1.41
2:F:118:ILE:CG1	2:F:284:ILE:CD1	1.84	1.41
2:D:97:VAL:HG22	2:D:109:TYR:CE1	1.50	1.40
2:F:116:ILE:CD1	2:F:135:LEU:HD21	1.48	1.40
2:D:68:VAL:CB	2:D:199:LEU:HG	1.50	1.40
2:F:142:PHE:C	2:F:143:ILE:HD12	1.38	1.39
2:F:144:TRP:NE1	2:F:264:THR:HG21	1.30	1.39
2:D:134:LYS:CE	2:D:282:MET:SD	2.11	1.38
1:A:281:LYS:O	1:A:327:GLU:CB	1.71	1.37
1:A:292:GLY:CA	1:A:297:HIS:HE1	1.19	1.36
1:A:358:ARG:N	1:A:372:LEU:HD22	1.42	1.35
1:B:206:ILE:CG1	1:B:244:GLN:NE2	1.90	1.34
2:F:70:CYS:CB	2:F:199:LEU:CD2	2.04	1.34
1:B:206:ILE:HG13	1:B:244:GLN:NE2	1.42	1.34
1:A:356:ALA:O	1:A:372:LEU:CD2	1.74	1.34
2:D:273:GLU:OE2	2:D:292:ARG:NH2	1.59	1.33
2:D:127:LYS:O	2:D:160:LYS:NZ	1.61	1.33
1:B:293:PHE:CE2	2:F:244:HIS:CD2	2.15	1.33
2:D:104:THR:CG2	3:D:418:HOH:O	1.77	1.32
2:F:173:LEU:HD11	2:F:254:ILE:CG2	1.60	1.31
1:C:322:ASP:OD2	2:E:222:GLN:HA	1.21	1.31
2:E:79:TRP:HZ3	2:E:190:GLN:NE2	0.84	1.30
1:A:289:LYS:NZ	1:B:186:LEU:CD1	1.92	1.29
2:F:70:CYS:N	2:F:199:LEU:CD2	1.91	1.29
1:A:316:LYS:CE	1:A:344:GLN:OE1	1.81	1.29
1:B:358:ARG:HG2	1:B:372:LEU:O	1.29	1.29
2:D:68:VAL:CB	2:D:199:LEU:CG	2.10	1.29
1:A:263:LYS:O	1:A:267:ASN:ND2	1.66	1.28
1:A:274:ASP:OD1	2:D:220:LEU:HD12	1.23	1.28
1:B:314:ARG:O	1:B:347:PRO:HD3	1.24	1.28
1:A:357:ARG:CA	1:A:372:LEU:HD23	1.63	1.27
1:A:316:LYS:NZ	1:A:344:GLN:OE1	1.69	1.26
2:D:189:GLU:CB	2:D:192:GLU:OE1	1.83	1.26
1:B:197:ARG:NH2	2:D:231:ARG:HG2	1.50	1.26
1:A:321:SER:OG	1:A:341:TYR:CE1	1.88	1.25
1:A:329:ARG:HH21	1:A:333:GLN:CD	1.36	1.25
1:B:206:ILE:CD1	1:B:244:GLN:HE21	1.50	1.25
1:B:296:GLN:O	2:F:249:ASP:N	1.68	1.24
1:A:356:ALA:C	1:A:372:LEU:HD21	1.58	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:HIS:O	2:E:246:ARG:CB	1.86	1.23
1:A:293:PHE:O	2:D:244:HIS:HB3	1.26	1.23
2:D:146:ASP:OD1	2:D:225:GLN:HG2	1.28	1.23
2:F:173:LEU:CD1	2:F:254:ILE:HB	1.68	1.23
1:B:300:GLU:OE2	1:B:334:LYS:NZ	1.70	1.23
2:D:168:LEU:HG	2:D:249:ASP:O	1.06	1.23
2:E:144:TRP:CZ2	2:E:264:THR:OG1	1.89	1.23
2:F:70:CYS:CB	2:F:199:LEU:HD23	1.63	1.23
1:A:281:LYS:O	1:A:327:GLU:HB3	1.08	1.22
1:B:293:PHE:CE2	2:F:244:HIS:HD2	1.52	1.22
2:F:172:GLN:HG3	2:F:223:SER:O	1.34	1.22
2:E:131:ILE:CG1	2:E:160:LYS:HD3	1.69	1.22
2:F:173:LEU:CG	2:F:254:ILE:HB	1.70	1.21
2:F:171:VAL:HB	2:F:252:PHE:CD1	1.75	1.21
2:D:243:ARG:CG	2:D:246:ARG:HD3	1.70	1.21
2:D:94:LYS:N	2:D:295:TRP:O	1.74	1.20
2:E:165:ILE:HD11	2:E:231:ARG:CB	1.70	1.20
2:F:196:LEU:HD11	3:F:429:HOH:O	1.06	1.20
1:B:272:LEU:HD12	2:F:151:ASN:ND2	1.55	1.20
2:D:137:SER:O	2:D:233:PHE:HB2	1.37	1.20
1:B:272:LEU:CG	2:F:151:ASN:ND2	2.05	1.19
1:A:357:ARG:CA	1:A:372:LEU:CD2	2.20	1.19
2:F:116:ILE:HD11	2:F:135:LEU:CD2	1.73	1.19
1:B:272:LEU:CD1	2:F:151:ASN:ND2	2.04	1.18
1:B:320:ALA:CA	2:F:220:LEU:HD22	1.72	1.18
1:B:272:LEU:HB2	2:F:151:ASN:ND2	1.57	1.18
1:C:321:SER:CB	2:E:208:VAL:CG2	2.21	1.18
1:A:358:ARG:N	1:A:372:LEU:CD2	2.06	1.18
2:F:70:CYS:N	2:F:199:LEU:HD22	1.52	1.18
2:F:118:ILE:CD1	2:F:284:ILE:HD13	1.75	1.17
2:E:116:ILE:HD11	2:E:134:LYS:CD	1.75	1.17
2:F:142:PHE:O	2:F:143:ILE:HD12	1.41	1.17
2:E:90:THR:HG22	3:E:427:HOH:O	1.37	1.17
1:B:358:ARG:CG	1:B:372:LEU:O	1.92	1.16
1:A:323:VAL:CG2	2:D:224:LYS:HE2	1.75	1.16
1:A:356:ALA:O	1:A:372:LEU:HD21	1.01	1.16
2:F:76:LEU:HD12	2:F:77:LEU:H	1.07	1.16
2:E:113:VAL:O	2:E:135:LEU:CD2	1.93	1.15
2:E:265:LYS:HD2	3:E:402:HOH:O	1.01	1.15
1:A:357:ARG:C	1:A:372:LEU:CD2	2.15	1.15
1:A:371:GLU:OE2	3:A:401:HOH:O	1.63	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:269:TYR:OH	2:E:283:GLU:OE1	1.63	1.15
1:C:249:ILE:HG22	1:C:270:TYR:CE1	1.81	1.15
2:D:175:LEU:HD12	2:D:257:ASN:OD1	1.48	1.14
1:A:316:LYS:HE2	1:A:344:GLN:OE1	1.41	1.14
2:D:97:VAL:HG21	2:D:109:TYR:CE1	1.73	1.14
1:B:272:LEU:HB3	2:F:151:ASN:ND2	1.54	1.14
1:C:321:SER:HB2	2:E:208:VAL:HG22	1.17	1.14
1:A:296:GLN:O	2:D:249:ASP:OD1	1.65	1.13
2:D:68:VAL:CB	2:D:199:LEU:CD2	2.26	1.13
1:C:283:VAL:HG21	1:C:327:GLU:OE2	1.46	1.13
1:C:339:TYR:OH	1:C:360:ASN:OD1	1.64	1.13
2:F:172:GLN:CG	2:F:223:SER:O	1.96	1.13
1:B:230:LEU:HB3	1:B:235:ILE:HD11	1.29	1.12
1:B:197:ARG:HH22	2:D:231:ARG:CG	1.61	1.12
2:F:116:ILE:HD11	2:F:135:LEU:HD21	1.16	1.12
2:F:281:LEU:O	2:F:295:TRP:CE3	2.02	1.12
1:A:287:ILE:HG22	1:B:371:GLU:HB2	1.20	1.11
1:C:249:ILE:CG2	1:C:270:TYR:CE1	2.32	1.11
2:E:131:ILE:HD11	2:E:160:LYS:HD2	1.24	1.11
1:B:206:ILE:HG13	1:B:244:GLN:CD	1.69	1.11
2:D:243:ARG:H	2:D:243:ARG:HD3	1.15	1.11
2:F:173:LEU:CD1	2:F:254:ILE:CG2	2.28	1.11
2:F:118:ILE:HA	2:F:284:ILE:HB	1.32	1.11
1:B:296:GLN:NE2	2:F:246:ARG:C	2.04	1.11
1:C:209:ASP:OD1	3:C:401:HOH:O	1.66	1.11
2:D:120:ASN:HB3	2:D:144:TRP:O	1.50	1.11
2:D:168:LEU:CG	2:D:249:ASP:O	1.97	1.10
2:D:253:ASP:CB	2:D:265:LYS:HE3	1.81	1.10
2:F:70:CYS:CB	2:F:199:LEU:HD21	1.74	1.10
1:A:287:ILE:HG21	1:B:371:GLU:HB2	1.23	1.10
1:A:329:ARG:HH21	1:A:333:GLN:NE2	1.48	1.10
2:E:107:SER:HA	2:E:133:LYS:NZ	1.64	1.10
2:F:135:LEU:HD11	2:F:141:LEU:HD21	1.29	1.10
1:A:329:ARG:NH2	1:A:333:GLN:NE2	2.00	1.10
2:F:269:TYR:HA	2:F:272:ILE:HD11	1.30	1.10
1:A:292:GLY:HA3	1:A:297:HIS:CE1	1.76	1.10
2:E:113:VAL:O	2:E:135:LEU:HD23	1.51	1.09
2:E:175:LEU:CD2	2:E:191:THR:CB	2.30	1.09
1:B:206:ILE:HD11	1:B:244:GLN:HE21	1.10	1.09
2:E:131:ILE:HG12	2:E:160:LYS:HD3	1.33	1.09
1:A:323:VAL:HG21	2:D:224:LYS:HE2	1.09	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:THR:HG22	2:D:195:VAL:HG12	1.10	1.09
2:D:241:GLU:O	2:D:274:THR:O	1.70	1.09
1:B:195:GLN:HG3	1:B:203:PHE:CZ	1.88	1.09
2:F:173:LEU:CD1	2:F:254:ILE:CB	2.30	1.09
1:B:203:PHE:HB2	1:B:244:GLN:HE22	1.17	1.08
1:C:321:SER:HB2	2:E:208:VAL:HG21	1.22	1.08
2:D:146:ASP:OD1	2:D:225:GLN:CG	2.01	1.08
1:B:191:LEU:HD22	1:B:368:ILE:HD11	1.29	1.08
2:D:97:VAL:HG23	2:D:109:TYR:CZ	1.71	1.08
2:F:137:SER:O	2:F:232:LYS:HD2	1.54	1.08
1:C:353:GLU:OE1	1:C:356:ALA:HB2	1.34	1.08
1:C:353:GLU:OE1	1:C:356:ALA:HB1	1.41	1.08
2:F:144:TRP:CZ3	2:F:226:VAL:O	2.07	1.08
2:D:97:VAL:HG23	2:D:109:TYR:OH	1.53	1.07
2:F:144:TRP:NE1	2:F:264:THR:CG2	1.95	1.07
1:A:274:ASP:OD1	2:D:220:LEU:CD1	2.01	1.07
1:C:242:SER:O	1:C:245:GLN:NE2	1.88	1.07
1:A:329:ARG:NH2	1:A:333:GLN:CD	2.07	1.07
2:D:243:ARG:HG3	2:D:246:ARG:HD3	1.34	1.06
2:F:168:LEU:HB3	3:F:414:HOH:O	1.55	1.06
2:F:144:TRP:HE1	2:F:264:THR:HG23	1.12	1.06
2:F:168:LEU:CB	3:F:414:HOH:O	2.03	1.06
2:F:281:LEU:HB2	2:F:295:TRP:CE3	1.91	1.06
2:E:165:ILE:HD11	2:E:231:ARG:HB2	1.31	1.06
2:F:144:TRP:HZ3	2:F:226:VAL:C	1.56	1.06
1:A:211:PRO:HG2	1:A:211:PRO:O	1.55	1.06
1:B:191:LEU:CD2	1:B:368:ILE:HD11	1.84	1.06
2:D:243:ARG:NH1	3:D:401:HOH:O	1.89	1.06
2:D:223:SER:O	2:D:224:LYS:NZ	1.88	1.05
2:E:116:ILE:CD1	2:E:134:LYS:CD	2.32	1.05
2:E:116:ILE:CD1	2:E:134:LYS:HD2	1.86	1.05
1:A:287:ILE:CG2	1:B:371:GLU:CB	2.34	1.05
2:F:163:THR:O	2:F:230:PHE:HD2	1.39	1.05
2:F:116:ILE:HG21	2:F:284:ILE:HD11	1.36	1.05
1:B:327:GLU:OE2	1:B:328:ARG:NH1	1.88	1.05
2:D:162:PHE:CE1	2:D:232:LYS:HB2	1.90	1.05
2:F:118:ILE:HG12	2:F:284:ILE:HD13	1.24	1.05
2:D:69:THR:HG22	2:D:195:VAL:CG1	1.84	1.05
2:F:173:LEU:HD11	2:F:254:ILE:HG21	1.35	1.04
1:A:354:ILE:HG22	1:A:355:PHE:HD2	1.20	1.04
1:A:354:ILE:HG22	1:A:355:PHE:CD2	1.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD22	1:A:235:ILE:HG13	1.34	1.04
2:F:118:ILE:HG13	2:F:284:ILE:HD12	1.31	1.04
2:F:173:LEU:HG	2:F:254:ILE:HB	1.32	1.04
2:F:135:LEU:CD1	2:F:141:LEU:HD21	1.86	1.03
1:B:206:ILE:CG1	1:B:244:GLN:HE21	1.58	1.03
2:F:88:TYR:OH	2:F:293:LYS:N	1.91	1.03
1:B:206:ILE:HD12	1:B:244:GLN:HG2	1.35	1.02
1:B:358:ARG:CD	1:B:372:LEU:O	2.07	1.02
2:D:109:TYR:HE2	2:D:296:ILE:CG2	1.70	1.02
1:A:322:ASP:OD1	2:D:220:LEU:HD13	1.56	1.02
2:E:222:GLN:OE1	2:E:224:LYS:NZ	1.92	1.02
2:F:144:TRP:CE3	2:F:226:VAL:O	2.12	1.02
1:A:290:GLY:HA3	1:B:372:LEU:HD12	1.39	1.02
1:B:256:ALA:CB	3:B:416:HOH:O	2.06	1.02
2:D:149:LEU:HD11	2:D:152:GLU:HB2	1.36	1.02
2:F:122:PHE:HB3	2:F:126:LEU:HG	1.39	1.02
2:E:242:LEU:CB	2:E:277:PRO:HD3	1.86	1.01
1:B:320:ALA:C	2:F:220:LEU:HD22	1.80	1.01
1:A:198:HIS:CD2	1:C:294:TYR:OH	2.13	1.01
1:A:202:MET:HG3	1:A:243:LEU:O	1.60	1.01
1:B:320:ALA:CB	2:F:220:LEU:HD21	1.64	1.01
2:E:116:ILE:HD11	2:E:134:LYS:HD2	1.40	1.01
2:D:120:ASN:HD21	2:D:123:LYS:HA	1.24	1.01
2:D:120:ASN:ND2	2:D:120:ASN:O	1.93	1.00
2:D:253:ASP:HB3	2:D:265:LYS:HE3	1.40	1.00
2:F:127:LYS:O	2:F:159:ASN:ND2	1.94	1.00
2:F:76:LEU:HD12	2:F:77:LEU:N	1.76	1.00
2:E:106:LEU:HD13	2:E:134:LYS:HE2	1.41	1.00
1:B:354:ILE:HG22	1:B:355:PHE:CD2	1.95	1.00
2:F:265:LYS:NZ	3:F:401:HOH:O	1.93	1.00
1:B:293:PHE:HE2	2:F:244:HIS:CG	1.80	0.99
2:D:109:TYR:HE2	2:D:296:ILE:HG21	1.24	0.99
1:A:357:ARG:HA	1:A:372:LEU:HD23	1.01	0.99
2:D:253:ASP:OD2	2:D:265:LYS:HE2	1.61	0.99
1:B:206:ILE:CD1	1:B:244:GLN:HG2	1.93	0.99
2:F:281:LEU:HB3	2:F:295:TRP:CH2	1.98	0.99
1:C:322:ASP:CG	2:E:222:GLN:HA	1.82	0.99
2:E:165:ILE:HD11	2:E:231:ARG:HB3	1.45	0.99
1:A:194:ALA:O	1:A:198:HIS:ND1	1.96	0.99
1:A:186:LEU:HD22	1:A:187:ASN:H	1.24	0.98
1:A:265:ILE:HD11	1:A:272:LEU:HD22	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:PHE:O	2:E:245:GLN:HB3	0.82	0.98
2:D:182:LEU:HD22	2:D:183:ASN:H	1.23	0.98
2:F:281:LEU:O	2:F:295:TRP:CZ3	2.16	0.98
1:A:198:HIS:CD2	1:C:294:TYR:HH	1.80	0.98
2:F:118:ILE:CD1	2:F:284:ILE:CD1	2.38	0.98
1:A:289:LYS:HZ1	1:B:186:LEU:HD13	1.28	0.98
2:F:70:CYS:CA	2:F:199:LEU:CD2	2.41	0.98
1:A:357:ARG:HA	1:A:372:LEU:CD2	1.87	0.98
1:C:325:PHE:CD1	2:E:204:GLN:HG3	1.97	0.98
1:C:353:GLU:CD	1:C:356:ALA:HB2	1.83	0.98
2:D:253:ASP:OD2	2:D:265:LYS:CE	2.11	0.98
2:D:68:VAL:CB	2:D:199:LEU:HD21	1.93	0.97
2:F:173:LEU:HD12	2:F:254:ILE:HB	1.43	0.97
2:F:73:LEU:O	2:F:76:LEU:CD1	2.12	0.97
2:F:136:ILE:HD12	2:F:137:SER:H	1.29	0.97
2:D:104:THR:HG21	3:D:418:HOH:O	1.49	0.97
2:F:142:PHE:C	2:F:143:ILE:CD1	2.32	0.97
1:B:314:ARG:O	1:B:347:PRO:CD	2.12	0.97
2:F:281:LEU:CB	2:F:295:TRP:CZ3	2.46	0.97
1:A:289:LYS:HZ1	1:B:186:LEU:CG	1.76	0.97
2:D:176:GLU:OE1	2:D:176:GLU:N	1.96	0.97
1:B:328:ARG:HB2	1:B:331:GLN:NE2	1.79	0.97
2:F:136:ILE:HG23	2:F:139:GLY:N	1.80	0.97
1:A:356:ALA:O	1:A:372:LEU:CG	2.13	0.96
1:C:202:MET:CE	1:C:243:LEU:O	2.13	0.96
1:A:322:ASP:OD2	2:D:222:GLN:HA	1.65	0.96
2:F:120:ASN:OD1	2:F:285:PHE:CE2	2.18	0.96
1:C:273:VAL:HG23	1:C:306:VAL:HG12	1.48	0.96
1:C:322:ASP:OD2	2:E:222:GLN:CA	2.13	0.96
2:D:97:VAL:HG21	2:D:109:TYR:CZ	1.83	0.96
1:B:281:LYS:O	1:B:327:GLU:HG3	1.67	0.95
1:C:257:LYS:HB3	1:C:260:VAL:HG21	1.48	0.95
2:F:196:LEU:HD21	3:F:429:HOH:O	1.66	0.95
1:A:289:LYS:HE3	1:B:182:ASP:N	1.79	0.95
1:A:320:ALA:HB3	2:D:220:LEU:CD2	1.96	0.95
1:A:346:CYS:O	1:A:351:TYR:OH	1.83	0.95
1:A:274:ASP:OD2	2:D:218:LYS:HD3	1.65	0.95
1:C:316:LYS:HZ1	1:C:347:PRO:HG2	1.28	0.95
2:F:144:TRP:CZ3	2:F:226:VAL:C	2.39	0.95
1:C:314:ARG:O	1:C:347:PRO:HD3	1.63	0.95
2:F:163:THR:O	2:F:230:PHE:CD2	2.19	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:208:VAL:HG13	2:E:209:LYS:CB	1.95	0.94
2:E:284:ILE:HG22	2:E:285:PHE:HD2	1.31	0.94
2:F:74:GLU:O	2:F:78:GLN:CA	2.15	0.94
2:F:70:CYS:N	2:F:199:LEU:HD21	1.80	0.94
1:B:246:ASP:OD1	1:B:309:ASP:N	1.99	0.94
2:F:118:ILE:HG23	2:F:284:ILE:HG21	1.49	0.94
1:C:293:PHE:C	2:E:245:GLN:HB3	1.87	0.94
2:D:137:SER:O	2:D:233:PHE:CB	2.15	0.94
1:B:203:PHE:HB2	1:B:244:GLN:NE2	1.82	0.94
1:B:357:ARG:HH21	1:B:360:ASN:HD21	1.12	0.94
2:F:171:VAL:HB	2:F:252:PHE:HD1	1.31	0.94
2:E:106:LEU:CD1	2:E:134:LYS:HE2	1.97	0.94
2:E:121:LEU:O	2:E:121:LEU:HD12	1.67	0.94
2:E:131:ILE:HD11	2:E:160:LYS:CD	1.96	0.94
2:E:101:ILE:HA	2:E:104:THR:HG21	1.49	0.93
2:E:284:ILE:HG22	2:E:285:PHE:CD2	2.02	0.93
1:B:286:LYS:CB	1:B:325:PHE:HZ	1.80	0.93
1:A:287:ILE:HG22	1:B:371:GLU:CB	1.97	0.93
2:F:281:LEU:HB3	2:F:295:TRP:CZ3	2.04	0.93
1:B:327:GLU:HG2	1:B:328:ARG:H	1.30	0.93
2:D:204:GLN:O	2:D:208:VAL:HG23	1.68	0.93
2:E:245:GLN:H	2:E:245:GLN:HE21	1.17	0.93
2:E:129:LEU:O	2:E:160:LYS:NZ	2.01	0.93
2:E:196:LEU:HD23	2:E:196:LEU:H	1.32	0.93
2:F:173:LEU:HD11	2:F:254:ILE:HG22	1.49	0.93
2:F:116:ILE:CD1	2:F:135:LEU:CD2	2.34	0.93
1:B:286:LYS:CB	1:B:325:PHE:CZ	2.51	0.93
2:F:70:CYS:CA	2:F:199:LEU:HD21	1.99	0.93
1:A:288:ALA:HB1	1:A:298:ALA:HA	1.49	0.93
2:D:75:VAL:HG21	2:D:252:PHE:H	1.34	0.92
2:D:146:ASP:CG	2:D:225:GLN:HE21	1.73	0.92
1:C:322:ASP:OD1	2:E:222:GLN:CB	2.17	0.92
2:D:138:ASN:O	2:D:138:ASN:ND2	2.03	0.92
2:E:116:ILE:HD11	2:E:134:LYS:HD3	1.46	0.92
2:E:283:GLU:HG2	2:E:286:ALA:HB2	1.47	0.92
2:D:243:ARG:HG2	2:D:246:ARG:HD3	1.47	0.92
2:F:118:ILE:HG12	2:F:284:ILE:CG1	1.98	0.92
2:F:175:LEU:CB	2:F:254:ILE:HG21	1.99	0.92
1:B:206:ILE:CD1	1:B:244:GLN:NE2	2.25	0.92
2:E:107:SER:HA	2:E:133:LYS:HZ3	1.29	0.92
1:A:281:LYS:O	1:A:327:GLU:HB2	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:O	1:B:261:THR:OG1	1.86	0.92
1:C:320:ALA:O	2:E:220:LEU:HB3	1.68	0.92
2:F:116:ILE:CG2	2:F:284:ILE:HD11	1.99	0.91
1:A:265:ILE:HD11	1:A:272:LEU:CD2	1.99	0.91
1:A:274:ASP:OD2	2:D:218:LYS:CD	2.18	0.91
2:F:118:ILE:CG1	2:F:284:ILE:HD13	1.73	0.91
2:F:173:LEU:HD12	2:F:254:ILE:CB	1.98	0.91
1:A:289:LYS:HZ2	1:B:186:LEU:CD1	1.63	0.91
2:E:144:TRP:CE2	2:E:264:THR:OG1	2.20	0.91
1:A:292:GLY:HA3	1:A:295:LEU:O	1.71	0.91
2:F:73:LEU:O	2:F:76:LEU:HD11	1.69	0.91
2:E:177:GLN:HE22	2:E:206:VAL:HA	1.34	0.91
1:B:326:SER:OG	1:B:335:PRO:HG3	1.71	0.91
1:A:230:LEU:HD22	1:A:235:ILE:CG1	2.01	0.90
1:B:340:GLN:O	1:B:343:ASN:OD1	1.89	0.90
1:C:321:SER:CB	2:E:208:VAL:HG21	1.91	0.90
2:E:137:SER:HG	2:E:233:PHE:HD1	1.03	0.90
2:F:173:LEU:HG	2:F:254:ILE:CB	1.99	0.90
1:A:213:GLN:HG3	1:A:230:LEU:O	1.72	0.90
2:D:147:LYS:CA	2:D:222:GLN:OE1	2.19	0.90
2:E:114:GLN:HG2	2:E:278:LYS:HD2	1.50	0.90
2:D:120:ASN:OD1	2:D:126:LEU:HD11	1.71	0.90
2:F:135:LEU:HD12	2:F:162:PHE:HE2	1.36	0.90
1:A:254:ILE:HG13	1:A:257:LYS:HB2	1.53	0.90
2:E:162:PHE:HB3	2:E:230:PHE:HB3	1.54	0.90
2:D:109:TYR:CE2	2:D:296:ILE:HG21	2.07	0.90
2:E:106:LEU:CD1	2:E:134:LYS:CE	2.50	0.90
2:F:74:GLU:O	2:F:78:GLN:N	2.05	0.90
2:E:174:SER:OG	2:E:177:GLN:HB2	1.72	0.90
2:F:167:ASN:C	2:F:168:LEU:HD13	1.91	0.90
2:E:100:LYS:HA	2:E:300:GLU:HG3	1.52	0.89
2:F:172:GLN:HG3	2:F:223:SER:C	1.93	0.89
1:C:246:ASP:OD1	1:C:309:ASP:N	2.04	0.89
2:F:173:LEU:N	2:F:253:ASP:O	2.04	0.89
2:D:147:LYS:HA	2:D:222:GLN:OE1	1.73	0.89
2:E:116:ILE:CD1	2:E:134:LYS:HD3	1.99	0.89
1:C:182:ASP:OD1	1:C:370:ASN:OD1	1.89	0.89
1:A:316:LYS:HE2	1:A:344:GLN:CD	1.92	0.89
1:C:249:ILE:HG21	1:C:270:TYR:CE1	2.06	0.89
2:F:143:ILE:O	2:F:227:LEU:HG	1.72	0.89
1:B:244:GLN:HB2	1:B:270:TYR:OH	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLY:HA3	1:B:372:LEU:HD21	1.55	0.88
1:A:278:TRP:NE1	1:A:326:SER:O	2.06	0.88
2:F:76:LEU:CD1	2:F:77:LEU:N	2.35	0.88
1:B:314:ARG:HH11	1:B:314:ARG:HG2	1.36	0.88
1:A:288:ALA:CB	1:A:298:ALA:HA	2.03	0.88
2:F:142:PHE:O	2:F:143:ILE:CD1	2.20	0.88
2:E:121:LEU:HB3	2:E:144:TRP:O	1.74	0.88
1:B:203:PHE:CB	1:B:244:GLN:HE22	1.87	0.88
2:D:97:VAL:HG22	2:D:109:TYR:HE1	1.16	0.88
2:D:177:GLN:HG3	2:D:209:LYS:CB	2.03	0.88
2:E:131:ILE:CG1	2:E:160:LYS:CD	2.52	0.88
1:A:211:PRO:O	1:A:211:PRO:CG	2.18	0.88
2:E:231:ARG:HH21	2:E:231:ARG:HG3	1.37	0.87
2:F:118:ILE:HG23	2:F:284:ILE:CG2	2.04	0.87
2:D:175:LEU:CD1	2:D:257:ASN:OD1	2.22	0.87
2:E:100:LYS:O	2:E:104:THR:HB	1.74	0.87
2:E:101:ILE:HA	2:E:104:THR:CG2	2.04	0.87
1:B:206:ILE:HD12	1:B:244:GLN:CG	2.05	0.87
2:F:76:LEU:CD1	2:F:77:LEU:H	1.86	0.87
2:D:149:LEU:HD11	2:D:152:GLU:CB	2.04	0.87
2:D:256:ASN:ND2	3:D:402:HOH:O	2.00	0.87
1:C:322:ASP:OD1	2:E:222:GLN:CG	2.21	0.87
2:D:127:LYS:C	2:D:160:LYS:HZ2	1.78	0.87
2:E:144:TRP:HZ2	2:E:264:THR:OG1	1.54	0.87
2:D:120:ASN:ND2	2:D:123:LYS:HA	1.90	0.86
1:A:297:HIS:NE2	2:D:166:GLU:OE2	2.08	0.86
1:B:328:ARG:O	1:B:331:GLN:HG2	1.75	0.86
2:D:109:TYR:CE2	2:D:296:ILE:CG2	2.59	0.86
2:F:281:LEU:O	2:F:295:TRP:HE3	1.57	0.86
2:D:261:CYS:O	2:D:262:LEU:HD23	1.75	0.86
1:B:294:TYR:CE2	2:F:165:ILE:HG12	2.10	0.86
1:C:293:PHE:CE2	1:C:294:TYR:HE2	1.93	0.86
2:E:166:GLU:O	2:E:229:MET:HB3	1.76	0.86
2:F:117:PHE:O	2:F:284:ILE:CG1	2.24	0.86
2:F:168:LEU:HD23	2:F:227:LEU:HD22	1.55	0.86
1:C:280:LYS:O	1:C:288:ALA:HB2	1.75	0.86
2:F:262:LEU:HD23	2:F:262:LEU:H	1.40	0.86
1:C:278:TRP:CE2	1:C:335:PRO:HD3	2.11	0.85
2:F:116:ILE:CG1	2:F:135:LEU:HD21	2.06	0.85
1:B:189:GLN:NE2	1:B:192:ILE:HD11	1.92	0.85
1:C:322:ASP:OD1	2:E:222:GLN:HG3	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:VAL:CG2	2:D:252:PHE:H	1.89	0.85
1:B:285:GLY:HA2	2:F:69:THR:CB	2.07	0.85
1:A:356:ALA:HB3	1:A:367:SER:OG	1.77	0.85
1:A:263:LYS:HG2	1:A:267:ASN:HD21	1.39	0.85
1:A:293:PHE:O	2:D:244:HIS:CB	2.21	0.85
1:B:358:ARG:HD2	1:B:372:LEU:O	1.73	0.85
2:F:173:LEU:CD1	2:F:254:ILE:HG21	2.01	0.85
1:C:322:ASP:OD2	2:E:221:ASN:O	1.95	0.84
2:F:70:CYS:H	2:F:199:LEU:HD22	0.68	0.84
2:F:283:GLU:O	2:F:298:VAL:HG23	1.76	0.84
1:B:338:ILE:O	1:B:342:ILE:HG13	1.75	0.84
1:C:283:VAL:HG13	3:C:421:HOH:O	1.76	0.84
2:E:269:TYR:CD1	2:E:292:ARG:HD2	2.13	0.84
1:A:186:LEU:HD22	1:A:187:ASN:N	1.92	0.84
1:A:246:ASP:OD1	1:A:309:ASP:N	2.11	0.84
1:C:293:PHE:O	2:E:245:GLN:CG	2.25	0.84
2:D:162:PHE:HE1	2:D:232:LYS:HB2	1.38	0.84
1:A:211:PRO:CB	1:A:228:ASP:HB3	2.08	0.84
2:E:209:LYS:CB	2:E:221:ASN:CB	2.55	0.84
1:B:206:ILE:HD11	1:B:244:GLN:NE2	1.90	0.83
1:A:263:LYS:C	1:A:267:ASN:HD22	1.80	0.83
2:E:283:GLU:CG	2:E:286:ALA:HB2	2.08	0.83
2:F:162:PHE:CE1	2:F:232:LYS:HG3	2.13	0.83
2:D:144:TRP:HZ2	2:D:268:ILE:CD1	1.91	0.83
1:A:289:LYS:NZ	1:B:186:LEU:HD22	1.92	0.83
2:F:116:ILE:HD12	2:F:135:LEU:HD21	1.56	0.83
2:D:179:LEU:HD21	2:D:191:THR:HG22	1.60	0.83
1:A:290:GLY:HA3	1:B:372:LEU:CD1	2.09	0.83
1:B:295:LEU:N	2:F:166:GLU:OE2	2.11	0.83
2:F:148:SER:O	2:F:149:LEU:HD23	1.79	0.83
2:E:101:ILE:O	2:E:104:THR:HG22	1.79	0.83
2:F:196:LEU:HD12	2:F:196:LEU:O	1.78	0.82
2:F:159:ASN:OD1	2:F:160:LYS:HG2	1.79	0.82
1:A:186:LEU:HG	1:A:368:ILE:HD11	1.59	0.82
1:B:272:LEU:HD12	2:F:151:ASN:CG	2.00	0.82
1:A:288:ALA:HB3	1:A:298:ALA:CB	2.09	0.82
2:D:179:LEU:CD2	2:D:191:THR:HB	2.09	0.82
2:D:146:ASP:CG	2:D:225:GLN:HG2	1.99	0.82
2:F:171:VAL:CB	2:F:252:PHE:CD1	2.58	0.82
1:A:213:GLN:CG	1:A:230:LEU:O	2.28	0.82
1:A:233:GLU:OE2	3:A:402:HOH:O	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:TYR:O	2:E:246:ARG:N	2.13	0.81
2:E:131:ILE:CD1	2:E:160:LYS:CD	2.58	0.81
2:F:117:PHE:O	2:F:284:ILE:HG13	1.80	0.81
2:E:131:ILE:CD1	2:E:160:LYS:HD2	2.07	0.81
2:F:116:ILE:CG2	2:F:284:ILE:CD1	2.58	0.81
1:B:206:ILE:CD1	1:B:244:GLN:CG	2.56	0.81
1:C:280:LYS:HB2	1:C:288:ALA:HB2	1.61	0.81
2:F:125:ASP:O	2:F:128:ASN:ND2	2.13	0.81
2:D:179:LEU:HD21	2:D:191:THR:CG2	2.11	0.81
2:E:131:ILE:HG13	2:E:160:LYS:HD3	1.63	0.81
2:F:101:ILE:HA	2:F:104:THR:HB	1.59	0.81
1:A:289:LYS:NZ	1:B:186:LEU:CD2	2.43	0.80
1:B:292:GLY:O	1:B:297:HIS:CD2	2.34	0.80
1:C:322:ASP:OD1	2:E:222:GLN:HB2	1.79	0.80
2:E:79:TRP:CE3	2:E:190:GLN:NE2	2.47	0.80
2:F:170:VAL:O	2:F:224:LYS:HB3	1.82	0.80
2:E:114:GLN:HG2	2:E:278:LYS:CD	2.11	0.80
2:F:165:ILE:O	2:F:166:GLU:HG2	1.80	0.80
1:B:357:ARG:HH21	1:B:360:ASN:ND2	1.80	0.80
2:F:168:LEU:CD2	2:F:227:LEU:HD22	2.11	0.80
2:D:124:LYS:O	2:D:126:LEU:CD2	2.30	0.80
2:D:149:LEU:CD1	2:D:152:GLU:HB2	2.11	0.80
1:A:322:ASP:OD1	2:D:220:LEU:CD1	2.29	0.80
1:C:182:ASP:OD1	1:C:370:ASN:CG	2.20	0.80
2:F:122:PHE:H	2:F:126:LEU:CD1	1.94	0.80
1:A:289:LYS:HZ1	1:B:186:LEU:CD1	1.75	0.80
1:B:281:LYS:HB2	1:B:286:LYS:HA	1.64	0.80
2:D:168:LEU:HG	2:D:249:ASP:C	2.03	0.80
2:E:79:TRP:HZ3	2:E:190:GLN:CD	1.83	0.80
2:E:129:LEU:O	2:E:160:LYS:CE	2.30	0.80
1:C:249:ILE:HG21	1:C:270:TYR:CZ	2.17	0.79
1:B:293:PHE:O	2:F:245:GLN:N	2.14	0.79
1:B:360:ASN:O	1:B:361:LEU:HD23	1.82	0.79
1:B:299:LYS:NZ	3:B:401:HOH:O	2.15	0.79
2:E:174:SER:CB	2:E:177:GLN:HB2	2.12	0.79
2:D:127:LYS:C	2:D:160:LYS:NZ	2.33	0.79
2:E:129:LEU:O	2:E:160:LYS:HE2	1.82	0.79
2:F:101:ILE:HA	2:F:104:THR:CB	2.12	0.79
1:B:195:GLN:CG	1:B:203:PHE:CZ	2.65	0.79
1:B:319:ILE:O	1:B:344:GLN:NE2	2.14	0.79
1:C:186:LEU:HD23	1:C:187:ASN:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:HIS:HA	2:F:249:ASP:OD1	1.82	0.79
1:C:316:LYS:NZ	1:C:347:PRO:HG2	1.97	0.79
2:E:175:LEU:HG	2:E:254:ILE:HG21	1.63	0.79
2:E:266:GLU:O	2:E:269:TYR:HB2	1.83	0.79
1:C:343:ASN:O	1:C:346:CYS:O	2.01	0.78
1:B:326:SER:OG	1:B:335:PRO:CG	2.30	0.78
1:C:316:LYS:NZ	1:C:347:PRO:CG	2.45	0.78
2:F:118:ILE:CA	2:F:284:ILE:HB	2.12	0.78
1:A:230:LEU:CD2	1:A:235:ILE:HG13	2.13	0.78
1:A:289:LYS:HD3	1:A:291:HIS:CB	2.12	0.78
2:F:141:LEU:HB2	2:F:230:PHE:HB2	1.64	0.78
2:D:99:LYS:O	2:D:300:GLU:HA	1.83	0.78
1:C:354:ILE:HG22	1:C:355:PHE:CD2	2.18	0.78
2:F:101:ILE:CD1	2:F:106:LEU:HD21	2.12	0.78
1:A:211:PRO:CB	1:A:228:ASP:CB	2.62	0.78
1:B:244:GLN:CB	1:B:270:TYR:OH	2.32	0.78
2:F:135:LEU:HD11	2:F:141:LEU:CD2	2.14	0.78
1:A:358:ARG:CA	1:A:372:LEU:HD22	2.12	0.78
2:F:88:TYR:HH	2:F:293:LYS:N	1.81	0.78
1:C:278:TRP:CZ3	1:C:300:GLU:OE2	2.36	0.78
2:D:121:LEU:HD11	2:D:144:TRP:CE3	2.18	0.77
1:C:316:LYS:HZ2	1:C:347:PRO:HG3	1.47	0.77
1:A:230:LEU:HB3	1:A:235:ILE:HD11	1.65	0.77
1:A:289:LYS:NZ	1:B:186:LEU:CG	2.41	0.77
2:D:253:ASP:CG	2:D:265:LYS:HE3	2.04	0.77
1:C:182:ASP:CB	1:C:185:LYS:HB2	2.14	0.77
1:C:273:VAL:CG2	1:C:306:VAL:CG1	2.62	0.77
1:C:202:MET:HE3	1:C:243:LEU:O	1.85	0.77
1:A:258:TYR:OH	1:A:275:GLU:OE1	2.03	0.77
2:E:165:ILE:CD1	2:E:231:ARG:HB2	2.12	0.77
1:C:249:ILE:HG22	1:C:270:TYR:HE1	1.48	0.77
1:C:291:HIS:O	2:E:246:ARG:CA	2.32	0.77
1:C:321:SER:CB	2:E:208:VAL:HG22	1.98	0.76
1:A:186:LEU:HD13	1:A:187:ASN:N	2.00	0.76
1:A:289:LYS:HZ1	1:B:186:LEU:CD2	1.96	0.76
1:A:357:ARG:C	1:A:372:LEU:HD21	2.06	0.76
1:B:230:LEU:CB	1:B:235:ILE:HD11	2.14	0.76
1:C:293:PHE:CD2	1:C:294:TYR:CE2	2.74	0.76
1:C:296:GLN:CD	2:E:247:THR:O	2.24	0.76
1:C:323:VAL:O	2:E:204:GLN:NE2	2.18	0.76
1:C:278:TRP:HZ3	1:C:300:GLU:OE2	1.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:168:LEU:HD21	2:F:229:MET:CE	2.16	0.76
2:E:133:LYS:HG3	2:E:134:LYS:N	2.01	0.76
2:E:245:GLN:HE21	2:E:245:GLN:N	1.82	0.76
2:D:165:ILE:O	2:D:166:GLU:HG2	1.86	0.75
2:D:179:LEU:HD23	2:D:191:THR:HB	1.68	0.75
2:D:273:GLU:CD	2:D:292:ARG:NH2	2.38	0.75
2:F:159:ASN:OD1	2:F:160:LYS:N	2.19	0.75
1:A:353:GLU:HB2	1:A:365:TRP:CE3	2.21	0.75
2:E:131:ILE:HG12	2:E:160:LYS:CD	2.12	0.75
2:D:144:TRP:HZ2	2:D:268:ILE:HD11	1.49	0.75
2:D:223:SER:C	2:D:224:LYS:HG2	2.07	0.75
2:F:262:LEU:HD23	2:F:262:LEU:N	2.01	0.75
1:B:188:PHE:O	1:B:192:ILE:HG23	1.87	0.75
1:C:257:LYS:HB3	1:C:260:VAL:CG2	2.17	0.75
2:D:253:ASP:CB	2:D:265:LYS:CE	2.62	0.75
2:E:177:GLN:NE2	2:E:206:VAL:HA	2.01	0.75
1:A:186:LEU:HD12	1:A:188:PHE:CE2	2.21	0.75
1:B:207:MET:CE	1:B:342:ILE:HD11	2.16	0.75
1:C:280:LYS:O	1:C:288:ALA:CB	2.34	0.75
2:D:135:LEU:CD2	2:D:139:GLY:HA3	2.17	0.75
2:F:283:GLU:O	2:F:298:VAL:CG2	2.34	0.75
2:F:173:LEU:HG	2:F:254:ILE:N	2.02	0.75
1:A:288:ALA:CB	1:A:298:ALA:CB	2.65	0.75
1:B:256:ALA:HB3	3:B:416:HOH:O	1.77	0.75
1:B:326:SER:OG	1:B:335:PRO:CB	2.35	0.74
1:C:182:ASP:O	1:C:186:LEU:N	2.18	0.74
1:B:207:MET:HE1	1:B:342:ILE:HD11	1.69	0.74
2:D:171:VAL:HG22	2:D:224:LYS:HE3	1.68	0.74
2:F:269:TYR:HA	2:F:272:ILE:CD1	2.16	0.74
1:A:211:PRO:HB3	1:A:228:ASP:CB	2.16	0.74
2:D:296:ILE:HD12	2:D:296:ILE:N	2.02	0.74
2:F:116:ILE:HD11	2:F:135:LEU:HD23	1.67	0.74
1:C:273:VAL:HG23	1:C:306:VAL:CG1	2.16	0.74
1:C:296:GLN:HG3	2:E:247:THR:N	2.03	0.74
2:F:73:LEU:O	2:F:76:LEU:HD12	1.86	0.74
1:A:282:THR:HG23	1:A:284:ASN:O	1.88	0.74
2:D:165:ILE:O	2:D:165:ILE:HD12	1.87	0.74
2:D:243:ARG:HD3	2:D:243:ARG:N	2.00	0.74
2:F:77:LEU:CB	2:F:252:PHE:O	2.36	0.74
1:A:352:LEU:HD12	1:A:366:VAL:O	1.87	0.74
1:B:291:HIS:ND1	1:B:292:GLY:N	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:125:ASP:HA	2:F:128:ASN:ND2	2.03	0.74
1:A:314:ARG:NH1	1:A:348:ASN:O	2.20	0.74
1:C:280:LYS:O	1:C:288:ALA:N	2.20	0.74
1:A:292:GLY:N	1:A:297:HIS:CE1	2.54	0.74
2:E:87:SER:OG	3:E:401:HOH:O	2.04	0.74
2:D:104:THR:HG23	3:D:418:HOH:O	1.59	0.73
2:F:284:ILE:O	2:F:284:ILE:HG22	1.87	0.73
1:A:188:PHE:CD1	1:A:243:LEU:HD11	2.23	0.73
1:B:357:ARG:NH2	1:B:360:ASN:HD21	1.86	0.73
1:C:280:LYS:HB2	1:C:288:ALA:CB	2.18	0.73
2:D:121:LEU:CD1	2:D:144:TRP:CE3	2.71	0.73
2:E:163:THR:OG1	2:E:231:ARG:O	2.05	0.73
1:B:326:SER:OG	1:B:335:PRO:HB3	1.88	0.73
2:F:249:ASP:N	2:F:249:ASP:OD1	2.20	0.73
1:A:291:HIS:O	1:A:297:HIS:CE1	2.42	0.73
1:A:357:ARG:N	1:A:372:LEU:HD21	2.04	0.73
1:B:354:ILE:HG22	1:B:355:PHE:CE2	2.24	0.73
2:F:144:TRP:CD1	2:F:264:THR:HG21	2.21	0.73
1:A:252:TRP:CE3	1:A:300:GLU:HG2	2.24	0.73
1:A:288:ALA:HB3	1:A:298:ALA:HB2	1.70	0.73
1:B:320:ALA:HB3	2:F:220:LEU:HD21	0.74	0.73
2:D:97:VAL:HG21	2:D:109:TYR:CD1	2.23	0.73
2:E:231:ARG:HG3	2:E:231:ARG:NH2	2.02	0.73
2:D:204:GLN:O	2:D:208:VAL:CG2	2.37	0.73
2:F:118:ILE:HG12	2:F:284:ILE:HD12	0.81	0.73
2:F:292:ARG:HB2	2:F:295:TRP:HB2	1.71	0.73
1:C:278:TRP:CZ2	1:C:335:PRO:HD3	2.24	0.73
2:F:168:LEU:HD22	2:F:168:LEU:N	2.03	0.72
1:B:191:LEU:CD2	1:B:368:ILE:CD1	2.67	0.72
1:B:314:ARG:HG2	1:B:314:ARG:NH1	1.99	0.72
2:F:136:ILE:HG13	2:F:138:ASN:H	1.54	0.72
2:E:196:LEU:HD23	2:E:196:LEU:N	2.03	0.72
2:F:133:LYS:N	2:F:133:LYS:HD2	2.04	0.72
1:C:265:ILE:HD11	1:C:272:LEU:HD11	1.70	0.72
1:C:292:GLY:HA2	1:C:297:HIS:CE1	2.25	0.72
2:D:247:THR:HG22	3:D:407:HOH:O	1.89	0.72
2:E:135:LEU:HD12	2:E:162:PHE:HZ	1.54	0.72
2:F:122:PHE:H	2:F:126:LEU:HD12	1.54	0.72
2:D:149:LEU:HD11	2:D:152:GLU:CG	2.20	0.72
2:F:273:GLU:OE2	2:F:274:THR:N	2.23	0.72
1:A:211:PRO:HB2	1:A:228:ASP:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:GLU:CD	1:C:356:ALA:CB	2.48	0.72
2:E:286:ALA:O	2:E:299:CYS:SG	2.48	0.72
2:F:118:ILE:HD11	2:F:284:ILE:HD13	1.69	0.72
2:F:291:PRO:HG3	2:F:297:SER:OG	1.88	0.72
2:D:249:ASP:OD1	2:D:249:ASP:N	2.22	0.71
2:F:125:ASP:HA	2:F:128:ASN:HD21	1.55	0.71
2:F:269:TYR:CA	2:F:272:ILE:HD11	2.15	0.71
1:A:201:LYS:NZ	1:A:204:ASP:OD2	2.22	0.71
1:A:231:SER:HB3	1:A:234:LYS:HD2	1.72	0.71
2:D:100:LYS:HE3	2:D:300:GLU:OE1	1.90	0.71
2:E:269:TYR:O	2:E:273:GLU:HG3	1.90	0.71
1:A:263:LYS:C	1:A:267:ASN:ND2	2.42	0.71
2:D:120:ASN:H	2:D:144:TRP:HB2	1.55	0.71
2:E:86:GLN:O	2:E:291:PRO:CB	2.38	0.71
2:F:136:ILE:HG23	2:F:139:GLY:CA	2.19	0.71
2:F:144:TRP:HE3	2:F:226:VAL:O	1.72	0.71
2:F:159:ASN:OD1	2:F:160:LYS:NZ	2.22	0.71
1:A:289:LYS:HZ2	1:B:186:LEU:HD13	0.73	0.71
2:E:101:ILE:N	2:E:101:ILE:HD12	2.06	0.71
2:E:113:VAL:O	2:E:135:LEU:HD21	1.87	0.71
1:A:287:ILE:HG21	1:B:371:GLU:CB	2.11	0.71
1:A:353:GLU:HB2	1:A:365:TRP:CZ3	2.25	0.71
2:F:136:ILE:HD12	2:F:137:SER:N	2.04	0.71
2:F:142:PHE:CZ	2:F:272:ILE:HG21	2.26	0.71
2:F:171:VAL:HG21	2:F:252:PHE:CE1	2.25	0.71
1:A:194:ALA:C	1:A:198:HIS:HD1	1.94	0.70
2:F:281:LEU:CB	2:F:295:TRP:CE3	2.66	0.70
1:C:246:ASP:OD1	1:C:308:GLY:HA3	1.91	0.70
2:D:124:LYS:O	2:D:126:LEU:HD21	1.91	0.70
1:B:251:VAL:CG1	1:B:265:ILE:HD11	2.21	0.70
1:C:191:LEU:HD23	1:C:191:LEU:O	1.92	0.70
2:D:253:ASP:OD2	2:D:265:LYS:HE3	1.92	0.70
2:D:136:ILE:HG22	2:D:137:SER:N	2.06	0.70
2:F:127:LYS:HE2	2:F:159:ASN:HB3	1.73	0.70
2:E:100:LYS:HD2	2:E:100:LYS:N	2.06	0.70
2:E:105:ASP:OD2	2:E:107:SER:OG	2.09	0.70
1:A:186:LEU:HD12	1:A:188:PHE:CD2	2.26	0.70
1:A:192:ILE:HD11	1:A:242:SER:OG	1.92	0.70
1:B:293:PHE:CZ	2:F:244:HIS:CD2	2.77	0.70
2:D:98:LEU:HA	2:D:299:CYS:O	1.92	0.70
1:A:213:GLN:CG	1:A:230:LEU:C	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:MET:SD	1:B:202:MET:HG3	2.32	0.70
1:B:197:ARG:HH22	2:D:231:ARG:HG2	0.68	0.70
2:F:117:PHE:HA	2:F:142:PHE:HB2	1.74	0.70
2:F:135:LEU:CD1	2:F:162:PHE:HE2	2.05	0.70
2:F:175:LEU:CA	2:F:254:ILE:HG21	2.22	0.70
2:F:182:LEU:HD23	2:F:182:LEU:O	1.92	0.70
1:B:279:VAL:HG23	1:B:325:PHE:CD2	2.27	0.70
1:B:281:LYS:CB	1:B:286:LYS:HA	2.21	0.70
1:B:296:GLN:O	2:F:249:ASP:OD1	2.10	0.70
2:F:168:LEU:HD23	2:F:227:LEU:HB3	1.73	0.69
2:E:106:LEU:HD13	2:E:134:LYS:CE	2.15	0.69
1:A:288:ALA:CB	1:A:298:ALA:CA	2.71	0.69
1:B:233:GLU:HA	1:B:236:GLN:OE1	1.91	0.69
2:F:74:GLU:C	2:F:78:GLN:CB	2.59	0.69
1:A:263:LYS:HG2	1:A:267:ASN:ND2	2.08	0.69
1:B:191:LEU:HD22	1:B:368:ILE:CD1	2.17	0.69
1:A:211:PRO:HB2	1:A:228:ASP:CB	2.22	0.69
1:A:357:ARG:CA	1:A:372:LEU:HD21	2.09	0.69
2:E:265:LYS:CD	3:E:402:HOH:O	1.82	0.69
2:F:284:ILE:CG2	2:F:284:ILE:O	2.40	0.69
1:A:230:LEU:HD22	1:A:235:ILE:CD1	2.22	0.69
1:A:289:LYS:HZ1	1:B:186:LEU:HD22	1.56	0.69
1:C:293:PHE:CD2	1:C:294:TYR:HE2	2.10	0.69
2:D:242:LEU:HD13	2:D:277:PRO:HG3	1.74	0.69
2:D:243:ARG:H	2:D:243:ARG:CD	1.97	0.69
2:F:136:ILE:CD1	2:F:137:SER:H	2.05	0.69
2:F:118:ILE:HD11	2:F:284:ILE:CD1	2.20	0.69
1:A:358:ARG:H	1:A:372:LEU:HD22	1.54	0.69
1:C:299:LYS:HE2	3:C:407:HOH:O	1.92	0.69
2:F:196:LEU:CD1	3:F:429:HOH:O	1.82	0.69
1:C:196:MET:O	1:C:200:GLY:N	2.23	0.68
2:F:142:PHE:HZ	2:F:272:ILE:HG21	1.58	0.68
1:B:329:ARG:HD3	1:B:329:ARG:C	2.13	0.68
1:C:296:GLN:CG	2:E:247:THR:O	2.41	0.68
2:D:169:VAL:HG23	2:D:171:VAL:HG23	1.76	0.68
2:F:168:LEU:HB2	3:F:414:HOH:O	1.76	0.68
1:A:213:GLN:HG2	1:A:230:LEU:C	2.14	0.68
1:A:259:ARG:HD2	1:A:259:ARG:O	1.93	0.68
1:B:294:TYR:HB2	2:F:166:GLU:OE2	1.93	0.68
1:C:283:VAL:CG1	3:C:421:HOH:O	2.38	0.68
1:C:337:GLU:O	1:C:340:GLN:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:117:PHE:O	2:F:284:ILE:CB	2.41	0.68
2:E:245:GLN:H	2:E:245:GLN:NE2	1.88	0.68
2:E:270:GLN:O	2:E:274:THR:HG23	1.92	0.68
2:F:122:PHE:CB	2:F:126:LEU:HG	2.19	0.68
2:E:201:PHE:HA	2:E:205:LYS:HD3	1.76	0.68
1:A:275:GLU:HG3	1:A:303:LEU:HD13	1.75	0.68
1:B:203:PHE:O	1:B:244:GLN:OE1	2.11	0.68
1:C:313:GLY:O	1:C:316:LYS:HE3	1.93	0.68
1:C:349:GLY:O	1:C:351:TYR:CE1	2.46	0.68
2:D:143:ILE:HD12	2:D:157:MET:HE2	1.76	0.68
2:E:118:ILE:HG22	2:E:120:ASN:H	1.59	0.68
1:B:281:LYS:O	1:B:327:GLU:CG	2.42	0.68
2:F:173:LEU:HG	2:F:253:ASP:C	2.15	0.67
1:C:363:ASP:OD1	3:C:402:HOH:O	2.10	0.67
2:D:136:ILE:HG22	2:D:137:SER:H	1.59	0.67
2:F:116:ILE:CG1	2:F:135:LEU:CD2	2.70	0.67
1:B:282:THR:HG23	1:B:287:ILE:O	1.93	0.67
1:C:361:LEU:CD2	1:C:367:SER:OG	2.42	0.67
2:F:118:ILE:O	2:F:143:ILE:HA	1.94	0.67
2:D:146:ASP:CG	2:D:225:GLN:NE2	2.48	0.67
2:E:116:ILE:HD13	2:E:134:LYS:CD	2.21	0.67
2:F:115:GLY:HA2	2:F:140:ILE:HG13	1.74	0.67
2:F:167:ASN:OD1	2:F:226:VAL:CG1	2.43	0.67
2:F:281:LEU:C	2:F:295:TRP:CZ3	2.67	0.67
1:B:206:ILE:HG12	1:B:244:GLN:NE2	2.03	0.67
2:E:262:LEU:HD23	2:E:262:LEU:C	2.15	0.67
2:F:168:LEU:HD22	2:F:168:LEU:H	1.60	0.67
2:F:175:LEU:CB	2:F:254:ILE:CG2	2.72	0.67
1:C:188:PHE:HB3	1:C:243:LEU:HD11	1.77	0.67
1:C:196:MET:HG3	1:C:197:ARG:HD3	1.76	0.67
2:D:89:GLU:HG2	2:D:90:THR:N	2.09	0.67
2:E:135:LEU:HD12	2:E:162:PHE:CZ	2.28	0.67
2:F:135:LEU:CD1	2:F:141:LEU:CD2	2.69	0.67
1:B:320:ALA:CA	2:F:220:LEU:CD2	2.52	0.67
2:E:107:SER:HA	2:E:133:LYS:CE	2.24	0.67
1:C:296:GLN:HG3	2:E:247:THR:C	2.16	0.66
1:B:228:ASP:OD2	1:B:228:ASP:N	2.24	0.66
1:A:252:TRP:HE3	1:A:300:GLU:HG2	1.60	0.66
2:D:125:ASP:C	2:D:126:LEU:HD23	2.15	0.66
2:E:131:ILE:CD1	2:E:160:LYS:HD3	2.24	0.66
2:F:125:ASP:C	2:F:128:ASN:HD22	1.99	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:ASP:N	2:D:66:ASP:OD1	2.27	0.66
2:F:101:ILE:HD12	2:F:106:LEU:HD21	1.77	0.66
2:E:100:LYS:HA	2:E:300:GLU:CG	2.26	0.66
1:A:203:PHE:O	1:A:244:GLN:HB2	1.95	0.66
2:F:162:PHE:HE1	2:F:232:LYS:HG3	1.61	0.66
2:D:228:ILE:HG22	2:D:230:PHE:CE1	2.30	0.66
1:A:186:LEU:HD13	1:A:186:LEU:C	2.15	0.65
1:C:316:LYS:NZ	1:C:347:PRO:HG3	2.10	0.65
2:F:117:PHE:O	2:F:284:ILE:HB	1.96	0.65
1:C:191:LEU:HD23	1:C:191:LEU:C	2.16	0.65
2:E:177:GLN:NE2	2:E:206:VAL:C	2.50	0.65
1:C:273:VAL:CG2	1:C:306:VAL:HG11	2.26	0.65
2:D:179:LEU:HD12	2:D:185:HIS:O	1.96	0.65
1:B:292:GLY:HA2	2:F:245:GLN:CB	2.26	0.65
1:B:293:PHE:CZ	2:F:244:HIS:HD2	2.09	0.65
1:C:182:ASP:HB2	1:C:185:LYS:HB2	1.78	0.65
1:B:358:ARG:HD2	1:B:372:LEU:C	2.17	0.65
2:D:162:PHE:HB3	2:D:230:PHE:HB3	1.78	0.65
2:D:182:LEU:HD22	2:D:183:ASN:N	2.05	0.65
2:D:284:ILE:HA	2:D:298:VAL:CG2	2.27	0.65
2:E:99:LYS:O	2:E:101:ILE:HD12	1.96	0.65
2:E:121:LEU:HD13	2:E:149:LEU:HD13	1.78	0.65
1:A:368:ILE:HA	1:C:291:HIS:CB	2.27	0.65
1:B:281:LYS:HA	1:B:287:ILE:H	1.62	0.65
1:C:193:ASP:O	1:C:197:ARG:HG2	1.96	0.65
2:E:106:LEU:C	2:E:133:LYS:HE2	2.17	0.65
2:E:247:THR:HG23	2:E:248:PRO:N	2.11	0.65
1:A:211:PRO:HA	1:A:227:TYR:CE1	2.32	0.65
1:C:188:PHE:HD1	1:C:243:LEU:HD11	1.61	0.65
1:C:204:ASP:HB3	1:C:315:PHE:CE2	2.31	0.65
2:F:134:LYS:O	2:F:135:LEU:HD23	1.96	0.65
1:B:370:ASN:O	1:B:371:GLU:HG2	1.97	0.65
1:C:291:HIS:O	2:E:246:ARG:HA	1.97	0.65
2:D:140:ILE:HD11	2:D:142:PHE:CZ	2.31	0.65
2:F:196:LEU:HD12	2:F:196:LEU:C	2.16	0.65
1:A:329:ARG:HH21	1:A:333:GLN:CG	2.10	0.64
2:D:195:VAL:O	2:D:199:LEU:HB2	1.96	0.64
2:D:167:ASN:O	2:D:249:ASP:HB3	1.97	0.64
2:D:243:ARG:HG2	2:D:246:ARG:CD	2.23	0.64
2:F:281:LEU:HB2	2:F:295:TRP:CD2	2.32	0.64
2:E:174:SER:HB3	2:E:177:GLN:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:ILE:HG13	2:F:135:LEU:CD2	2.27	0.64
1:B:201:LYS:HB2	1:B:201:LYS:HZ2	1.61	0.64
1:C:276:ILE:HG23	1:C:322:ASP:O	1.97	0.64
1:C:353:GLU:CG	1:C:356:ALA:HB2	2.27	0.64
2:F:101:ILE:O	2:F:104:THR:N	2.30	0.64
1:A:367:SER:O	1:C:291:HIS:CB	2.45	0.64
2:D:179:LEU:HD11	2:D:187:LYS:C	2.17	0.64
1:A:320:ALA:HB3	2:D:220:LEU:HD21	1.77	0.64
2:E:107:SER:HA	2:E:133:LYS:HZ1	1.60	0.64
2:F:168:LEU:HD13	2:F:168:LEU:N	2.11	0.64
1:C:188:PHE:CD1	1:C:243:LEU:HD11	2.33	0.64
2:F:171:VAL:HB	2:F:252:PHE:CE1	2.33	0.64
2:F:173:LEU:HG	2:F:254:ILE:CA	2.27	0.64
1:A:188:PHE:CE1	1:A:243:LEU:HD11	2.32	0.64
2:E:175:LEU:O	2:E:179:LEU:N	2.30	0.64
1:A:195:GLN:HG3	1:A:203:PHE:CZ	2.33	0.64
1:C:322:ASP:CG	2:E:222:GLN:CA	2.63	0.63
1:B:206:ILE:CG1	1:B:244:GLN:CD	2.51	0.63
1:C:211:PRO:O	1:C:212:TRP:HB2	1.98	0.63
2:D:144:TRP:CZ2	2:D:268:ILE:CD1	2.79	0.63
2:F:159:ASN:HD21	2:F:160:LYS:HZ1	1.46	0.63
1:B:326:SER:CB	1:B:335:PRO:HB3	2.29	0.63
1:C:257:LYS:CB	1:C:260:VAL:HG21	2.27	0.63
1:C:283:VAL:CG2	1:C:327:GLU:OE2	2.37	0.63
2:F:100:LYS:O	2:F:104:THR:OG1	2.13	0.63
1:A:292:GLY:N	1:A:297:HIS:HE1	1.93	0.63
1:C:182:ASP:HB3	1:C:185:LYS:HB2	1.81	0.63
1:C:206:ILE:HA	1:C:352:LEU:O	1.98	0.63
1:C:283:VAL:HG21	1:C:327:GLU:CD	2.19	0.63
2:F:116:ILE:HG21	2:F:284:ILE:CD1	2.20	0.63
1:B:326:SER:CB	1:B:335:PRO:CB	2.77	0.63
1:C:354:ILE:HG22	1:C:355:PHE:CE2	2.33	0.63
1:A:208:MET:HE2	1:A:210:PRO:HG3	1.80	0.63
2:D:88:TYR:OH	2:D:293:LYS:CB	2.46	0.63
1:A:318:ASN:OD1	2:D:219:VAL:HA	1.98	0.63
1:B:242:SER:O	1:B:245:GLN:NE2	2.31	0.63
1:C:296:GLN:HG3	2:E:247:THR:CA	2.28	0.63
2:E:255:VAL:HG22	2:E:256:ASN:N	2.12	0.63
1:C:212:TRP:CE3	1:C:235:ILE:HD12	2.34	0.63
2:F:143:ILE:HD12	2:F:143:ILE:N	2.07	0.63
1:C:359:ASN:ND2	1:C:360:ASN:HD22	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:101:ILE:HA	2:F:104:THR:OG1	1.98	0.62
1:B:251:VAL:HG11	1:B:265:ILE:HD11	1.80	0.62
2:D:147:LYS:HB3	2:D:222:GLN:OE1	1.99	0.62
1:A:356:ALA:O	1:A:372:LEU:CD1	2.46	0.62
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.13	0.62
1:B:329:ARG:NH1	1:B:333:GLN:OE1	2.32	0.62
2:D:158:GLU:HG3	2:D:159:ASN:N	2.15	0.62
2:E:243:ARG:HH21	2:E:274:THR:HA	1.63	0.62
2:F:173:LEU:CG	2:F:254:ILE:CB	2.54	0.62
1:A:316:LYS:HD3	1:A:344:GLN:O	2.00	0.62
2:D:75:VAL:HG21	2:D:252:PHE:N	2.12	0.62
2:D:208:VAL:HG12	2:D:208:VAL:O	2.00	0.62
2:E:114:GLN:CG	2:E:278:LYS:HD2	2.27	0.62
2:F:168:LEU:HD23	2:F:227:LEU:CD2	2.29	0.62
2:F:171:VAL:HG21	2:F:252:PHE:HE1	1.63	0.62
1:B:328:ARG:HB2	1:B:331:GLN:HE21	1.65	0.61
2:D:143:ILE:HD12	2:D:157:MET:CE	2.30	0.61
2:D:146:ASP:O	2:D:225:GLN:HA	2.00	0.61
2:E:140:ILE:HD11	2:E:276:LEU:HD11	1.82	0.61
2:E:177:GLN:NE2	2:E:206:VAL:O	2.33	0.61
2:F:256:ASN:OD1	2:F:257:ASN:OD1	2.18	0.61
1:A:289:LYS:HZ1	1:B:186:LEU:CB	2.12	0.61
2:D:242:LEU:CD2	2:D:242:LEU:H	2.13	0.61
1:A:339:TYR:OH	1:A:360:ASN:ND2	2.33	0.61
1:A:282:THR:OG1	1:A:283:VAL:N	2.34	0.61
1:A:356:ALA:O	1:A:372:LEU:HD11	2.00	0.61
1:C:212:TRP:HZ2	1:C:261:THR:HG23	1.65	0.61
1:C:183:VAL:HB	1:C:188:PHE:HZ	1.64	0.61
2:D:111:LYS:CB	2:D:112:GLY:HA2	2.30	0.61
2:F:171:VAL:CB	2:F:252:PHE:HD1	2.05	0.61
2:F:269:TYR:O	2:F:272:ILE:HG13	2.00	0.61
1:A:186:LEU:HD13	1:A:187:ASN:C	2.21	0.61
1:B:329:ARG:HD3	1:B:330:GLY:N	2.15	0.61
1:B:371:GLU:O	1:B:371:GLU:HG3	2.00	0.61
1:A:323:VAL:CG2	2:D:224:LYS:CE	2.67	0.61
1:C:329:ARG:HD3	3:C:406:HOH:O	2.01	0.61
2:D:179:LEU:HD21	2:D:191:THR:CB	2.31	0.61
2:D:183:ASN:O	3:D:403:HOH:O	2.15	0.61
1:C:265:ILE:HG13	1:C:266:GLU:N	2.14	0.61
2:D:99:LYS:O	2:D:300:GLU:HB3	2.00	0.61
2:E:262:LEU:HD23	2:E:262:LEU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:271:THR:O	2:F:271:THR:HG22	2.00	0.61
1:A:289:LYS:HZ3	1:B:186:LEU:CD2	2.13	0.61
2:D:138:ASN:HA	2:D:233:PHE:HB3	1.83	0.61
2:D:68:VAL:CB	2:D:199:LEU:CD1	2.79	0.60
2:F:144:TRP:NE1	2:F:264:THR:HG23	1.91	0.60
1:B:264:MET:SD	1:B:268:TRP:CH2	2.93	0.60
2:D:175:LEU:CD2	2:D:179:LEU:HG	2.31	0.60
2:E:287:GLN:O	2:E:290:GLN:N	2.34	0.60
2:D:127:LYS:C	2:D:127:LYS:HD3	2.21	0.60
2:F:143:ILE:HG22	2:F:144:TRP:N	2.17	0.60
2:F:171:VAL:CB	2:F:252:PHE:CE1	2.84	0.60
2:F:178:ALA:O	2:F:182:LEU:HB2	2.01	0.60
1:C:299:LYS:CE	3:C:407:HOH:O	2.48	0.60
2:D:232:LYS:HD2	2:D:232:LYS:O	2.01	0.60
2:E:262:LEU:O	2:E:263:LYS:HD2	2.00	0.60
2:F:118:ILE:CG2	2:F:284:ILE:HG21	2.29	0.60
1:A:202:MET:HG3	1:A:244:GLN:HA	1.83	0.60
2:F:144:TRP:HZ3	2:F:226:VAL:CA	2.14	0.60
1:A:354:ILE:HG22	1:A:355:PHE:CE2	2.37	0.60
1:A:213:GLN:HG3	1:A:230:LEU:C	2.21	0.60
1:A:274:ASP:OD1	2:D:220:LEU:CG	2.49	0.60
1:A:357:ARG:C	1:A:372:LEU:HD22	1.99	0.60
1:C:206:ILE:HD13	1:C:244:GLN:OE1	2.01	0.60
2:D:121:LEU:CD1	2:D:144:TRP:HE3	2.14	0.60
2:D:298:VAL:HG23	2:D:298:VAL:O	2.01	0.60
2:E:167:ASN:O	2:E:167:ASN:ND2	2.35	0.60
2:F:178:ALA:O	2:F:182:LEU:N	2.28	0.60
1:A:294:TYR:CE1	2:D:165:ILE:HG12	2.37	0.60
2:E:274:THR:HG21	3:E:409:HOH:O	2.02	0.60
1:A:211:PRO:HG3	1:A:230:LEU:HD13	1.84	0.59
2:D:147:LYS:CB	2:D:222:GLN:OE1	2.49	0.59
1:C:331:GLN:HA	1:C:332:SER:C	2.20	0.59
1:A:202:MET:CG	1:A:243:LEU:O	2.43	0.59
1:C:350:ASN:N	1:C:350:ASN:OD1	2.32	0.59
2:D:284:ILE:HG23	2:D:298:VAL:CG2	2.32	0.59
2:E:129:LEU:C	2:E:160:LYS:HZ3	2.06	0.59
1:B:322:ASP:OD2	2:F:221:ASN:O	2.21	0.59
2:F:196:LEU:CG	3:F:429:HOH:O	2.29	0.59
1:A:357:ARG:O	1:A:359:ASN:N	2.29	0.59
1:A:358:ARG:H	1:A:372:LEU:CD2	2.08	0.59
2:E:121:LEU:CD1	2:E:149:LEU:HD13	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:VAL:HG23	1:A:183:VAL:O	2.01	0.59
1:A:195:GLN:OE1	1:A:201:LYS:O	2.21	0.59
2:D:162:PHE:CD1	2:D:232:LYS:HB2	2.36	0.59
2:E:76:LEU:O	2:E:76:LEU:HD22	2.02	0.59
2:E:107:SER:N	2:E:133:LYS:HE2	2.18	0.59
2:F:157:MET:O	2:F:160:LYS:O	2.21	0.59
2:F:159:ASN:CG	2:F:160:LYS:HZ2	2.05	0.59
1:C:297:HIS:CD2	2:E:166:GLU:OE1	2.56	0.59
2:D:124:LYS:O	2:D:126:LEU:HD23	2.02	0.59
2:F:79:TRP:HD1	2:F:80:LYS:N	2.01	0.59
2:F:163:THR:HG22	2:F:164:TYR:N	2.17	0.59
2:F:171:VAL:CG2	2:F:252:PHE:CE1	2.86	0.59
1:A:321:SER:OG	1:A:341:TYR:HE1	1.76	0.59
2:E:177:GLN:HE22	2:E:206:VAL:CA	2.12	0.59
2:F:118:ILE:HG12	2:F:284:ILE:CB	2.33	0.59
2:F:135:LEU:CD1	2:F:162:PHE:CE2	2.86	0.59
1:A:186:LEU:CD1	1:A:188:PHE:CD2	2.85	0.58
1:A:292:GLY:HA2	1:A:297:HIS:HE1	0.48	0.58
1:B:293:PHE:CE2	2:F:244:HIS:CG	2.72	0.58
2:E:117:PHE:HD2	2:E:272:ILE:HD11	1.68	0.58
2:F:162:PHE:CE1	2:F:232:LYS:CG	2.87	0.58
1:B:292:GLY:O	1:B:297:HIS:NE2	2.36	0.58
1:C:293:PHE:CE2	1:C:294:TYR:CE2	2.82	0.58
2:D:97:VAL:CG2	2:D:109:TYR:OH	2.25	0.58
2:F:123:LYS:HE3	2:F:123:LYS:H	1.69	0.58
2:D:147:LYS:C	2:D:222:GLN:OE1	2.41	0.58
1:A:321:SER:OG	1:A:341:TYR:CZ	2.32	0.58
2:E:101:ILE:HD12	2:E:101:ILE:H	1.67	0.58
1:A:281:LYS:C	1:A:327:GLU:HB3	2.11	0.58
1:B:191:LEU:HD23	1:B:368:ILE:HD11	1.81	0.58
1:B:212:TRP:CD2	1:B:257:LYS:HG3	2.38	0.58
1:C:296:GLN:OE1	2:E:247:THR:O	2.21	0.58
2:D:246:ARG:HB3	3:D:407:HOH:O	2.03	0.58
2:D:281:LEU:O	2:D:296:ILE:CD1	2.52	0.58
2:E:175:LEU:HD23	2:E:178:ALA:HB3	1.86	0.58
2:E:112:GLY:HA2	2:E:134:LYS:O	2.04	0.58
2:F:125:ASP:CA	2:F:128:ASN:ND2	2.66	0.58
1:C:253:ALA:HB2	1:C:261:THR:HG21	1.86	0.58
2:D:182:LEU:CD2	2:D:183:ASN:H	2.08	0.58
2:E:90:THR:CG2	3:E:427:HOH:O	2.14	0.58
2:F:172:GLN:HG2	2:F:223:SER:O	1.98	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:HIS:CD2	2:E:231:ARG:CD	2.86	0.57
1:C:282:THR:O	1:C:283:VAL:HB	2.01	0.57
2:E:84:ASN:CB	3:E:417:HOH:O	2.51	0.57
2:F:116:ILE:HG22	2:F:284:ILE:CD1	2.33	0.57
2:F:167:ASN:O	2:F:168:LEU:HD13	2.03	0.57
1:B:281:LYS:HA	1:B:287:ILE:N	2.19	0.57
2:D:95:ILE:HG22	2:D:96:VAL:N	2.19	0.57
2:E:253:ASP:OD1	3:E:402:HOH:O	2.17	0.57
2:F:76:LEU:HD13	2:F:77:LEU:N	2.19	0.57
1:B:354:ILE:CG2	1:B:355:PHE:CE2	2.88	0.57
1:C:336:GLU:O	1:C:338:ILE:N	2.38	0.57
2:E:174:SER:O	2:E:177:GLN:HB3	2.03	0.57
2:D:179:LEU:CD1	2:D:185:HIS:O	2.52	0.57
2:D:280:GLN:HA	2:D:280:GLN:OE1	2.03	0.57
2:E:75:VAL:HG12	2:E:75:VAL:O	2.05	0.57
2:E:174:SER:HB3	2:E:177:GLN:CB	2.34	0.57
1:A:281:LYS:HG3	1:A:285:GLY:O	2.04	0.57
1:A:211:PRO:CG	1:A:230:LEU:HB2	2.35	0.57
1:B:206:ILE:HG13	1:B:244:GLN:CG	2.33	0.57
2:E:283:GLU:HG2	2:E:286:ALA:CB	2.29	0.57
2:F:88:TYR:HH	2:F:293:LYS:H	1.36	0.57
1:C:265:ILE:HD11	1:C:272:LEU:CD1	2.35	0.57
1:C:296:GLN:HG3	2:E:247:THR:O	2.04	0.57
1:C:299:LYS:HD3	2:E:250:VAL:CG1	2.34	0.57
2:D:281:LEU:O	2:D:296:ILE:HD13	2.05	0.57
2:E:211:LEU:CB	2:E:221:ASN:HA	2.35	0.57
1:A:291:HIS:C	1:A:297:HIS:CE1	2.78	0.56
1:C:293:PHE:O	2:E:245:GLN:HG2	2.02	0.56
1:C:296:GLN:HG3	2:E:246:ARG:C	2.26	0.56
2:D:286:ALA:O	2:D:299:CYS:HB3	2.05	0.56
2:D:102:LEU:O	2:D:102:LEU:HD22	2.06	0.56
2:E:116:ILE:HB	2:E:141:LEU:HD12	1.87	0.56
2:E:269:TYR:CD1	2:E:292:ARG:CD	2.85	0.56
2:F:122:PHE:CD1	2:F:123:LYS:N	2.74	0.56
2:F:159:ASN:HD21	2:F:160:LYS:NZ	2.02	0.56
1:A:250:PHE:CD1	1:A:250:PHE:N	2.73	0.56
1:A:281:LYS:H	1:A:327:GLU:HA	1.70	0.56
1:A:317:LYS:HD2	1:A:317:LYS:N	2.20	0.56
1:C:314:ARG:O	1:C:347:PRO:CD	2.46	0.56
1:C:338:ILE:O	1:C:341:TYR:HB2	2.06	0.56
2:D:94:LYS:O	2:D:95:ILE:HG13	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:ILE:CD1	2:D:157:MET:HE2	2.35	0.56
2:E:100:LYS:HD2	2:E:100:LYS:H	1.70	0.56
2:F:144:TRP:HZ3	2:F:226:VAL:O	1.58	0.56
1:A:368:ILE:HG23	1:A:368:ILE:O	2.05	0.56
2:F:167:ASN:OD1	2:F:226:VAL:HG13	2.04	0.56
1:C:204:ASP:HB3	1:C:315:PHE:HE2	1.70	0.56
1:C:330:GLY:O	1:C:333:GLN:HB2	2.05	0.56
2:E:168:LEU:HD11	2:E:250:VAL:HA	1.88	0.56
1:A:355:PHE:CD2	1:A:355:PHE:N	2.73	0.56
2:E:116:ILE:HD13	2:E:134:LYS:HD3	1.81	0.56
1:B:195:GLN:HE22	1:B:350:ASN:ND2	2.04	0.56
2:D:241:GLU:CB	2:D:243:ARG:CZ	2.84	0.56
2:D:242:LEU:N	2:D:242:LEU:HD22	2.21	0.56
2:E:78:GLN:O	2:E:265:LYS:NZ	2.36	0.56
2:E:144:TRP:NE1	2:E:264:THR:OG1	2.37	0.56
2:E:177:GLN:NE2	2:E:206:VAL:CA	2.69	0.56
2:E:253:ASP:HB3	2:E:265:LYS:HE3	1.87	0.56
2:E:76:LEU:HD22	2:E:76:LEU:C	2.27	0.56
2:E:286:ALA:O	2:E:299:CYS:HB2	2.06	0.56
2:F:116:ILE:HD11	2:F:282:MET:HE1	1.87	0.56
2:F:283:GLU:O	2:F:298:VAL:CB	2.54	0.56
1:B:261:THR:O	1:B:265:ILE:HG13	2.05	0.56
1:B:328:ARG:NH1	1:B:328:ARG:HG3	2.20	0.56
2:D:270:GLN:O	2:D:274:THR:HG23	2.06	0.56
1:C:183:VAL:O	1:C:188:PHE:HE2	1.88	0.55
1:B:327:GLU:HG2	1:B:328:ARG:N	2.09	0.55
1:A:186:LEU:HG	1:A:368:ILE:CD1	2.34	0.55
1:A:289:LYS:HG3	1:B:182:ASP:N	2.21	0.55
1:C:257:LYS:CA	1:C:260:VAL:CG2	2.84	0.55
1:C:357:ARG:HB2	1:C:359:ASN:OD1	2.06	0.55
2:D:143:ILE:HG22	2:D:144:TRP:N	2.22	0.55
1:B:206:ILE:CG1	1:B:244:GLN:CG	2.84	0.55
2:F:291:PRO:HB3	2:F:297:SER:HB2	1.88	0.55
2:D:126:LEU:HD23	2:D:126:LEU:N	2.20	0.55
1:A:355:PHE:HD2	1:A:355:PHE:N	2.05	0.55
1:C:315:PHE:CE2	1:C:346:CYS:SG	2.99	0.55
2:F:140:ILE:HG22	2:F:231:ARG:CB	2.36	0.55
2:F:151:ASN:OD1	2:F:151:ASN:N	2.40	0.55
2:F:151:ASN:O	2:F:152:GLU:OE1	2.25	0.55
1:B:232:ASP:HB3	1:B:236:GLN:HE22	1.71	0.55
1:B:264:MET:SD	1:B:268:TRP:CZ2	3.00	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:181:GLU:O	2:D:181:GLU:HG3	2.05	0.55
1:C:280:LYS:C	1:C:288:ALA:HB2	2.28	0.55
2:D:119:ASP:O	2:D:124:LYS:HE2	2.06	0.55
2:D:210:ASP:CB	2:D:223:SER:OG	2.55	0.55
1:A:211:PRO:HB3	1:A:228:ASP:HB3	1.79	0.55
1:B:195:GLN:HE22	1:B:350:ASN:HD22	1.54	0.55
2:E:106:LEU:HD12	2:E:134:LYS:CE	2.34	0.55
1:A:289:LYS:HZ3	1:B:186:LEU:CD1	2.11	0.55
1:C:250:PHE:CE2	1:C:304:ILE:HD13	2.42	0.55
2:D:167:ASN:HD21	2:D:226:VAL:CG1	2.20	0.55
2:F:135:LEU:HD12	2:F:162:PHE:CE2	2.28	0.55
2:F:136:ILE:CG2	2:F:139:GLY:CA	2.85	0.55
1:A:292:GLY:CA	1:A:295:LEU:O	2.51	0.54
2:D:179:LEU:HD11	2:D:186:MET:O	2.06	0.54
2:D:134:LYS:CD	2:D:282:MET:SD	2.92	0.54
2:D:187:LYS:O	2:D:191:THR:HG22	2.07	0.54
1:A:211:PRO:CB	1:A:228:ASP:HB2	2.37	0.54
1:C:318:ASN:N	2:E:219:VAL:O	2.40	0.54
2:D:97:VAL:HG21	2:D:109:TYR:CE2	2.39	0.54
2:F:137:SER:O	2:F:232:LYS:CD	2.44	0.54
2:F:244:HIS:N	2:F:275:LEU:CB	2.71	0.54
1:B:327:GLU:CG	1:B:328:ARG:H	2.10	0.54
1:C:212:TRP:CE3	1:C:212:TRP:HA	2.42	0.54
1:A:230:LEU:CD2	1:A:235:ILE:CD1	2.86	0.54
2:D:149:LEU:HD11	2:D:152:GLU:HG3	1.89	0.54
2:F:118:ILE:HD13	2:F:284:ILE:HD13	1.80	0.54
1:B:278:TRP:CZ2	1:B:335:PRO:HD3	2.42	0.54
1:C:272:LEU:N	1:C:272:LEU:HD22	2.21	0.54
2:D:68:VAL:C	2:D:69:THR:HG23	2.28	0.54
2:D:127:LYS:O	2:D:127:LYS:HD3	2.08	0.54
2:E:110:ALA:HB1	2:E:111:LYS:HG2	1.89	0.54
2:F:94:LYS:NZ	2:F:94:LYS:HB3	2.22	0.54
1:A:323:VAL:HG23	2:D:224:LYS:HE2	1.80	0.54
2:D:126:LEU:O	2:D:129:LEU:HB2	2.07	0.54
2:E:117:PHE:HD2	2:E:272:ILE:CD1	2.20	0.54
2:E:253:ASP:CB	2:E:265:LYS:HE3	2.38	0.54
2:F:116:ILE:HG13	2:F:135:LEU:HD21	1.85	0.54
2:F:125:ASP:C	2:F:128:ASN:ND2	2.59	0.54
1:A:201:LYS:HE3	1:A:350:ASN:OD1	2.08	0.54
1:A:211:PRO:HD3	1:A:355:PHE:CD1	2.43	0.54
1:A:320:ALA:HB3	2:D:220:LEU:HD22	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:141:LEU:HD13	2:E:162:PHE:CE2	2.43	0.54
2:F:136:ILE:HG23	2:F:139:GLY:H	1.70	0.54
2:E:174:SER:O	2:E:178:ALA:N	2.40	0.54
1:A:322:ASP:OD1	2:D:220:LEU:HB3	2.08	0.54
1:B:253:ALA:HB2	1:B:261:THR:HG21	1.90	0.54
2:D:284:ILE:HA	2:D:298:VAL:HG22	1.90	0.54
1:A:288:ALA:CB	1:A:298:ALA:HB1	2.38	0.53
1:A:294:TYR:N	1:A:294:TYR:CD2	2.73	0.53
2:E:226:VAL:HG12	2:E:227:LEU:N	2.23	0.53
1:B:249:ILE:HG22	1:B:305:GLY:O	2.09	0.53
1:B:282:THR:H	1:B:287:ILE:H	1.57	0.53
1:C:286:LYS:HA	2:E:70:CYS:SG	2.48	0.53
1:C:297:HIS:NE2	2:E:166:GLU:OE1	2.41	0.53
1:C:321:SER:OG	2:E:208:VAL:CG2	2.56	0.53
1:C:363:ASP:O	1:C:364:ASN:HB2	2.08	0.53
2:D:247:THR:HG21	2:D:271:THR:HG23	1.91	0.53
2:D:282:MET:CE	2:D:298:VAL:HG11	2.38	0.53
2:F:283:GLU:O	2:F:298:VAL:HB	2.07	0.53
1:C:204:ASP:OD1	1:C:204:ASP:N	2.37	0.53
2:F:281:LEU:O	2:F:295:TRP:HZ3	1.86	0.53
1:B:278:TRP:O	1:B:299:LYS:HA	2.07	0.53
1:C:331:GLN:HA	1:C:333:GLN:N	2.23	0.53
2:E:98:LEU:N	2:E:109:TYR:HH	2.05	0.53
2:E:222:GLN:CD	2:E:224:LYS:NZ	2.62	0.53
2:F:75:VAL:O	2:F:78:GLN:O	2.27	0.53
2:F:168:LEU:CD2	2:F:227:LEU:CD2	2.84	0.53
1:C:238:MET:O	1:C:238:MET:HG3	2.08	0.53
1:C:249:ILE:CG2	1:C:270:TYR:CD1	2.90	0.53
1:C:249:ILE:CG2	1:C:270:TYR:CZ	2.80	0.53
2:F:153:ILE:HD11	2:F:228:ILE:HG13	1.91	0.53
2:F:281:LEU:CB	2:F:295:TRP:CH2	2.80	0.53
1:B:191:LEU:O	1:B:195:GLN:HB2	2.08	0.53
1:C:183:VAL:O	1:C:188:PHE:CE2	2.61	0.53
2:F:101:ILE:CD1	2:F:106:LEU:CD2	2.86	0.53
1:A:198:HIS:HD2	2:E:231:ARG:NE	2.07	0.53
2:D:143:ILE:CD1	2:D:157:MET:CE	2.87	0.53
1:A:265:ILE:HD11	1:A:272:LEU:HD21	1.88	0.52
1:B:232:ASP:OD1	1:B:257:LYS:NZ	2.32	0.52
1:B:248:PHE:HD1	1:B:304:ILE:HG23	1.73	0.52
1:C:320:ALA:O	2:E:220:LEU:CB	2.50	0.52
2:E:173:LEU:O	2:E:254:ILE:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:88:TYR:HD1	2:F:88:TYR:O	1.92	0.52
2:F:122:PHE:O	2:F:126:LEU:HB2	2.09	0.52
1:A:211:PRO:HD3	1:A:355:PHE:CE1	2.43	0.52
1:B:201:LYS:NZ	1:B:201:LYS:CB	2.73	0.52
2:D:233:PHE:CG	2:D:234:ASP:N	2.78	0.52
2:E:101:ILE:N	2:E:101:ILE:CD1	2.73	0.52
1:A:317:LYS:N	1:A:317:LYS:CD	2.73	0.52
1:B:281:LYS:HB3	1:B:286:LYS:CB	2.40	0.52
1:C:361:LEU:HD23	1:C:367:SER:OG	2.08	0.52
2:E:121:LEU:HD12	2:E:121:LEU:C	2.30	0.52
2:E:168:LEU:CD1	2:E:250:VAL:HA	2.39	0.52
1:A:231:SER:CB	1:A:234:LYS:NZ	2.73	0.52
2:D:175:LEU:O	2:D:175:LEU:HD22	2.09	0.52
2:D:242:LEU:CD2	2:D:242:LEU:N	2.73	0.52
2:F:142:PHE:CA	2:F:143:ILE:HD12	2.34	0.52
2:F:267:TYR:N	2:F:267:TYR:CD2	2.74	0.52
1:A:213:GLN:HG3	1:A:231:SER:HA	1.92	0.52
2:D:179:LEU:HD21	2:D:191:THR:HB	1.86	0.52
2:E:101:ILE:H	2:E:101:ILE:CD1	2.23	0.52
2:F:221:ASN:OD1	2:F:221:ASN:N	2.42	0.52
1:A:329:ARG:HH22	1:A:333:GLN:NE2	2.01	0.52
1:C:204:ASP:OD2	1:C:349:GLY:HA3	2.10	0.52
2:E:100:LYS:N	2:E:100:LYS:CD	2.73	0.52
1:A:183:VAL:HG22	1:A:238:MET:HE3	1.92	0.51
1:B:357:ARG:HB2	1:B:360:ASN:OD1	2.09	0.51
1:A:188:PHE:HD1	1:A:243:LEU:HD11	1.72	0.51
2:D:91:ASP:HB2	2:D:291:PRO:O	2.11	0.51
2:D:99:LYS:O	2:D:300:GLU:CB	2.58	0.51
2:D:233:PHE:CD1	2:D:234:ASP:N	2.75	0.51
2:D:253:ASP:CG	2:D:265:LYS:CE	2.68	0.51
1:B:207:MET:CE	1:B:342:ILE:CD1	2.86	0.51
1:B:231:SER:O	1:B:235:ILE:HG12	2.10	0.51
1:B:360:ASN:C	1:B:361:LEU:HD23	2.30	0.51
2:D:140:ILE:HD11	2:D:142:PHE:HZ	1.72	0.51
2:D:171:VAL:HG22	2:D:224:LYS:CE	2.40	0.51
2:F:141:LEU:HG	2:F:162:PHE:CD2	2.46	0.51
2:F:143:ILE:CG2	2:F:144:TRP:N	2.73	0.51
1:A:207:MET:HA	1:A:250:PHE:O	2.11	0.51
1:A:211:PRO:O	1:A:211:PRO:CD	2.49	0.51
1:A:356:ALA:O	1:A:372:LEU:HG	2.06	0.51
1:B:232:ASP:HB3	1:B:236:GLN:NE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ARG:HA	1:C:262:ILE:HG13	1.92	0.51
1:B:294:TYR:HB2	2:F:166:GLU:HG3	1.92	0.51
1:C:299:LYS:HD3	2:E:250:VAL:HG11	1.92	0.51
2:D:99:LYS:O	2:D:300:GLU:CA	2.56	0.51
2:D:228:ILE:CG2	2:D:230:PHE:CE1	2.93	0.51
2:D:283:GLU:HG2	2:D:286:ALA:HB2	1.91	0.51
1:A:273:VAL:HG13	1:A:274:ASP:N	2.26	0.51
1:B:326:SER:HG	1:B:335:PRO:HG3	1.75	0.51
2:D:88:TYR:OH	2:D:293:LYS:HB3	2.11	0.51
2:D:223:SER:O	2:D:224:LYS:HG2	2.10	0.51
2:D:286:ALA:O	2:D:299:CYS:CB	2.59	0.51
2:F:134:LYS:HD3	2:F:134:LYS:C	2.31	0.51
1:A:198:HIS:CD2	2:E:231:ARG:HD3	2.45	0.51
1:A:240:ILE:HD12	1:A:240:ILE:N	2.25	0.51
1:A:299:LYS:HG2	2:D:249:ASP:OD2	2.10	0.51
1:C:293:PHE:CD2	1:C:294:TYR:CD2	2.98	0.51
2:D:284:ILE:HG23	2:D:298:VAL:HG23	1.93	0.51
1:C:272:LEU:N	1:C:272:LEU:CD2	2.73	0.51
2:D:136:ILE:CG2	2:D:137:SER:N	2.73	0.51
2:D:253:ASP:HB2	2:D:265:LYS:NZ	2.26	0.51
1:A:238:MET:HB2	1:A:240:ILE:CD1	2.40	0.51
1:A:274:ASP:OD2	2:D:218:LYS:HD2	2.08	0.51
1:A:289:LYS:HG2	1:A:290:GLY:N	2.26	0.51
1:C:296:GLN:N	2:E:248:PRO:O	2.44	0.51
1:C:316:LYS:HZ2	1:C:347:PRO:CG	2.11	0.51
2:D:146:ASP:OD1	2:D:225:GLN:HG3	2.06	0.51
2:E:253:ASP:HB2	2:E:265:LYS:CE	2.41	0.51
1:A:195:GLN:HE22	1:A:350:ASN:HD22	1.59	0.51
2:F:88:TYR:OH	2:F:292:ARG:CA	2.59	0.51
1:B:328:ARG:HH11	1:B:328:ARG:HG3	1.75	0.50
2:D:280:GLN:O	2:D:281:LEU:HD23	2.11	0.50
1:A:254:ILE:CG1	1:A:257:LYS:HB2	2.36	0.50
1:A:350:ASN:OD1	1:A:350:ASN:N	2.41	0.50
1:A:357:ARG:C	1:A:359:ASN:H	2.11	0.50
1:B:293:PHE:C	1:B:293:PHE:CD2	2.85	0.50
2:D:187:LYS:O	2:D:191:THR:CG2	2.60	0.50
2:D:241:GLU:CB	2:D:243:ARG:NE	2.74	0.50
2:F:163:THR:CG2	2:F:164:TYR:N	2.74	0.50
1:A:192:ILE:CD1	1:A:242:SER:OG	2.57	0.50
1:B:189:GLN:HE22	1:B:192:ILE:HD11	1.71	0.50
1:C:296:GLN:CG	2:E:246:ARG:C	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:286:ALA:O	2:E:299:CYS:CB	2.60	0.50
1:A:206:ILE:HA	1:A:352:LEU:O	2.12	0.50
1:B:248:PHE:CE1	1:B:304:ILE:CG2	2.95	0.50
1:C:211:PRO:HG2	1:C:230:LEU:HB2	1.92	0.50
2:D:255:VAL:HG23	3:D:404:HOH:O	2.11	0.50
2:E:134:LYS:HZ3	2:E:284:ILE:HD11	1.76	0.50
2:F:269:TYR:H	2:F:269:TYR:HD2	1.58	0.50
1:A:358:ARG:N	1:A:372:LEU:HD23	2.09	0.50
1:B:279:VAL:HG23	1:B:325:PHE:HD2	1.76	0.50
1:C:250:PHE:CE2	1:C:304:ILE:CD1	2.95	0.50
2:D:136:ILE:CG2	2:D:137:SER:H	2.23	0.50
2:E:154:LEU:HD23	2:E:230:PHE:CE2	2.47	0.50
1:B:195:GLN:NE2	1:B:350:ASN:ND2	2.60	0.50
1:C:257:LYS:CB	1:C:260:VAL:CG2	2.86	0.50
2:F:244:HIS:N	2:F:244:HIS:ND1	2.60	0.50
1:B:248:PHE:CD1	1:B:304:ILE:HG23	2.47	0.50
2:D:95:ILE:CG2	2:D:96:VAL:N	2.75	0.50
2:F:101:ILE:CA	2:F:104:THR:HB	2.38	0.50
1:C:315:PHE:CD2	1:C:346:CYS:SG	3.02	0.49
2:F:101:ILE:O	2:F:104:THR:HB	2.12	0.49
2:F:100:LYS:C	2:F:104:THR:OG1	2.50	0.49
1:B:246:ASP:OD1	1:B:309:ASP:O	2.30	0.49
2:D:159:ASN:O	2:D:159:ASN:ND2	2.45	0.49
2:F:118:ILE:HA	2:F:284:ILE:CB	2.22	0.49
2:F:297:SER:OG	2:F:299:CYS:SG	2.70	0.49
1:A:255:ASN:O	2:D:164:TYR:HE1	1.94	0.49
2:D:173:LEU:O	2:D:254:ILE:HA	2.11	0.49
2:F:79:TRP:CD1	2:F:80:LYS:N	2.80	0.49
1:A:198:HIS:HD2	2:E:231:ARG:CD	2.24	0.49
1:C:233:GLU:O	1:C:236:GLN:HB3	2.12	0.49
2:D:155:GLU:HA	2:D:158:GLU:HG2	1.94	0.49
1:C:250:PHE:HE2	1:C:304:ILE:CD1	2.25	0.49
1:A:289:LYS:CG	1:B:369:GLY:O	2.61	0.49
1:B:207:MET:HE3	1:B:342:ILE:CD1	2.43	0.49
1:C:299:LYS:CD	2:E:250:VAL:CG1	2.91	0.49
1:C:325:PHE:HB2	3:C:405:HOH:O	2.12	0.49
2:F:170:VAL:O	2:F:224:LYS:CB	2.59	0.49
1:A:208:MET:CE	1:A:210:PRO:HG3	2.43	0.49
1:B:256:ALA:HB1	3:B:416:HOH:O	1.95	0.49
1:C:211:PRO:CG	1:C:230:LEU:HB2	2.42	0.49
1:C:354:ILE:CG2	1:C:355:PHE:CE2	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:TYR:OH	2:D:293:LYS:N	2.42	0.49
2:E:117:PHE:CD1	2:E:117:PHE:C	2.86	0.49
1:B:328:ARG:NH1	1:B:328:ARG:CG	2.73	0.49
1:C:340:GLN:O	1:C:344:GLN:HG3	2.13	0.49
2:D:71:ASP:OD1	2:D:71:ASP:N	2.45	0.49
2:F:164:TYR:CD1	2:F:164:TYR:C	2.86	0.49
1:A:353:GLU:HB2	1:A:365:TRP:HE3	1.71	0.48
1:B:206:ILE:CD1	1:B:244:GLN:CD	2.79	0.48
1:C:212:TRP:HA	1:C:212:TRP:HE3	1.77	0.48
2:D:175:LEU:HD22	2:D:179:LEU:HG	1.94	0.48
1:A:258:TYR:OH	1:A:275:GLU:CD	2.51	0.48
1:C:353:GLU:HG2	1:C:356:ALA:HB2	1.95	0.48
2:D:179:LEU:CD2	2:D:191:THR:CG2	2.89	0.48
2:E:219:VAL:HG13	2:E:220:LEU:HG	1.95	0.48
2:E:244:HIS:ND1	2:E:244:HIS:N	2.60	0.48
1:A:252:TRP:CZ3	1:A:300:GLU:HG2	2.48	0.48
2:D:242:LEU:CD1	2:D:277:PRO:HG3	2.43	0.48
2:F:122:PHE:HA	2:F:123:LYS:HE3	1.94	0.48
2:F:138:ASN:N	2:F:138:ASN:ND2	2.60	0.48
2:F:159:ASN:ND2	2:F:160:LYS:NZ	2.60	0.48
1:A:271:LYS:O	1:A:306:VAL:HG12	2.13	0.48
1:B:293:PHE:CE2	2:F:244:HIS:CB	2.95	0.48
1:C:207:MET:HA	1:C:250:PHE:O	2.13	0.48
2:F:269:TYR:CD2	2:F:269:TYR:N	2.76	0.48
1:B:314:ARG:H	1:B:314:ARG:HD3	1.77	0.48
1:B:345:LEU:C	1:B:345:LEU:HD13	2.34	0.48
2:F:121:LEU:CD1	2:F:153:ILE:CG2	2.92	0.48
2:F:281:LEU:HD12	2:F:294:GLY:O	2.13	0.48
1:C:352:LEU:HD12	1:C:366:VAL:HB	1.95	0.48
1:C:359:ASN:ND2	1:C:360:ASN:ND2	2.61	0.48
2:D:144:TRP:CZ2	2:D:268:ILE:HD11	2.39	0.48
2:E:107:SER:CA	2:E:133:LYS:NZ	2.57	0.48
2:F:116:ILE:HG13	2:F:135:LEU:HD22	1.94	0.48
1:A:289:LYS:CE	1:B:182:ASP:N	2.67	0.48
1:A:317:LYS:HD2	1:A:317:LYS:H	1.78	0.48
2:D:146:ASP:O	2:D:224:LYS:O	2.32	0.48
2:D:244:HIS:ND1	2:D:244:HIS:N	2.60	0.48
1:A:227:TYR:O	1:A:228:ASP:HB2	2.12	0.48
2:E:165:ILE:HG22	2:E:166:GLU:HG2	1.96	0.48
2:F:196:LEU:CD2	3:F:429:HOH:O	2.24	0.48
1:A:282:THR:HG21	1:A:287:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:PHE:HA	3:C:405:HOH:O	2.13	0.48
1:B:197:ARG:NH2	2:D:231:ARG:CG	2.42	0.48
2:F:122:PHE:N	2:F:126:LEU:CD1	2.73	0.48
2:F:268:ILE:H	2:F:268:ILE:HG12	1.53	0.48
1:C:249:ILE:HG22	1:C:270:TYR:CD1	2.43	0.47
1:C:280:LYS:CB	1:C:288:ALA:HB2	2.39	0.47
2:E:232:LYS:O	2:E:233:PHE:CB	2.61	0.47
2:D:90:THR:HG22	2:D:91:ASP:N	2.29	0.47
1:C:317:LYS:HD3	2:E:213:LEU:CB	2.44	0.47
2:D:121:LEU:HG	2:D:146:ASP:HB2	1.96	0.47
2:D:223:SER:C	2:D:224:LYS:HZ2	1.98	0.47
1:A:203:PHE:CD1	1:A:352:LEU:HB2	2.49	0.47
2:F:116:ILE:HG22	2:F:284:ILE:HD12	1.97	0.47
2:F:177:GLN:NE2	2:F:209:LYS:CB	2.78	0.47
2:D:168:LEU:CD2	2:D:249:ASP:O	2.58	0.47
2:D:243:ARG:O	2:D:246:ARG:HB2	2.14	0.47
2:E:254:ILE:HG22	2:E:255:VAL:H	1.78	0.47
1:A:292:GLY:CA	1:A:297:HIS:ND1	2.61	0.47
1:C:315:PHE:HD2	1:C:346:CYS:HG	1.56	0.47
2:D:121:LEU:HD11	2:D:144:TRP:HE3	1.70	0.47
2:D:296:ILE:N	2:D:296:ILE:CD1	2.73	0.47
2:E:142:PHE:CZ	2:E:272:ILE:HG12	2.49	0.47
2:F:79:TRP:HD1	2:F:80:LYS:H	1.60	0.47
2:F:298:VAL:C	2:F:299:CYS:SG	2.93	0.47
1:A:271:LYS:HB3	1:A:271:LYS:HE3	1.62	0.47
1:C:212:TRP:CE3	1:C:235:ILE:CD1	2.98	0.47
2:D:189:GLU:CB	2:D:192:GLU:HB2	2.44	0.47
2:F:69:THR:N	2:F:199:LEU:HD22	2.30	0.47
2:D:181:GLU:HA	2:D:182:LEU:C	2.35	0.47
2:E:106:LEU:HD12	2:E:134:LYS:HE3	1.96	0.47
2:F:137:SER:OG	2:F:138:ASN:ND2	2.48	0.47
1:A:186:LEU:HD13	1:A:187:ASN:CA	2.43	0.47
1:B:249:ILE:HG12	1:B:250:PHE:N	2.29	0.47
1:C:293:PHE:HD2	1:C:294:TYR:CE2	2.32	0.47
1:A:231:SER:CB	1:A:234:LYS:HZ2	2.28	0.47
1:B:201:LYS:HZ2	1:B:201:LYS:CB	2.25	0.47
2:E:255:VAL:CG2	2:E:256:ASN:N	2.77	0.46
1:C:202:MET:HE1	1:C:243:LEU:O	2.12	0.46
2:D:242:LEU:H	2:D:242:LEU:HD22	1.80	0.46
2:F:168:LEU:HD21	2:F:227:LEU:HD22	1.95	0.46
2:F:291:PRO:HB3	2:F:297:SER:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLN:NE2	1:B:192:ILE:CD1	2.73	0.46
1:C:183:VAL:HG23	1:C:184:THR:N	2.28	0.46
1:C:353:GLU:OE1	1:C:356:ALA:CA	2.52	0.46
1:C:363:ASP:O	1:C:365:TRP:HD1	1.97	0.46
2:D:179:LEU:CD1	2:D:186:MET:O	2.64	0.46
2:D:293:LYS:HG2	2:D:294:GLY:N	2.29	0.46
2:F:171:VAL:CG1	2:F:252:PHE:HD1	2.29	0.46
2:F:281:LEU:C	2:F:295:TRP:HZ3	2.17	0.46
1:A:322:ASP:OD1	2:D:220:LEU:CB	2.63	0.46
1:C:277:THR:HG23	2:E:224:LYS:HE2	1.98	0.46
2:D:171:VAL:HG13	2:D:224:LYS:HE3	1.97	0.46
2:D:179:LEU:CD2	2:D:191:THR:CB	2.83	0.46
2:F:136:ILE:CD1	2:F:137:SER:N	2.73	0.46
2:F:288:LYS:HB2	2:F:288:LYS:HE2	1.70	0.46
1:A:211:PRO:HG3	1:A:230:LEU:HB2	1.98	0.46
1:A:231:SER:HB3	1:A:234:LYS:NZ	2.31	0.46
1:B:192:ILE:HG13	1:B:193:ASP:N	2.31	0.46
1:B:314:ARG:HH11	1:B:314:ARG:CG	2.14	0.46
2:D:261:CYS:C	2:D:262:LEU:HD23	2.35	0.46
2:E:100:LYS:H	2:E:100:LYS:CD	2.29	0.46
2:F:265:LYS:HD3	2:F:265:LYS:HA	1.76	0.46
2:D:69:THR:HA	2:D:195:VAL:HG11	1.97	0.46
2:D:169:VAL:HG23	2:D:169:VAL:O	2.16	0.46
2:D:284:ILE:HG23	2:D:298:VAL:HG21	1.97	0.46
2:F:171:VAL:CG1	2:F:252:PHE:CD1	2.99	0.46
1:B:296:GLN:NE2	2:F:246:ARG:O	2.35	0.46
1:C:321:SER:O	1:C:341:TYR:HE1	1.98	0.46
2:D:135:LEU:HD22	2:D:139:GLY:HA3	1.96	0.46
2:E:123:LYS:HD2	2:E:152:GLU:CB	2.45	0.46
2:F:122:PHE:CD1	2:F:122:PHE:C	2.89	0.46
2:F:129:LEU:HA	2:F:129:LEU:HD23	1.77	0.46
1:A:186:LEU:CD2	1:A:187:ASN:N	2.73	0.46
1:B:286:LYS:CB	1:B:325:PHE:CE2	2.99	0.46
2:F:116:ILE:CD1	2:F:282:MET:CE	2.93	0.46
2:F:165:ILE:C	2:F:166:GLU:HG2	2.37	0.46
2:F:192:GLU:CB	3:F:409:HOH:O	2.64	0.46
2:F:227:LEU:CD1	2:F:268:ILE:HG21	2.46	0.46
1:C:183:VAL:HB	1:C:188:PHE:CZ	2.48	0.45
1:C:315:PHE:HE2	1:C:346:CYS:SG	2.39	0.45
1:A:196:MET:O	1:A:200:GLY:N	2.48	0.45
1:A:277:THR:O	1:A:323:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLN:HA	1:B:192:ILE:HG12	1.98	0.45
1:B:343:ASN:OD1	1:B:343:ASN:N	2.49	0.45
2:F:117:PHE:O	2:F:284:ILE:CD1	2.64	0.45
1:C:242:SER:HA	1:C:245:GLN:HE22	1.80	0.45
1:C:277:THR:CG2	2:E:224:LYS:HE2	2.46	0.45
1:C:336:GLU:O	1:C:337:GLU:C	2.52	0.45
2:E:175:LEU:HA	2:E:178:ALA:HB3	1.99	0.45
1:A:288:ALA:O	1:B:371:GLU:HA	2.16	0.45
1:B:317:LYS:O	2:F:219:VAL:O	2.35	0.45
1:C:239:PRO:O	1:C:243:LEU:HD13	2.16	0.45
1:C:357:ARG:HD2	3:C:409:HOH:O	2.16	0.45
2:E:135:LEU:HD23	2:E:135:LEU:HA	1.84	0.45
2:E:206:VAL:O	2:E:206:VAL:HG12	2.16	0.45
2:F:173:LEU:HG	2:F:253:ASP:O	2.16	0.45
2:F:262:LEU:N	2:F:262:LEU:CD2	2.73	0.45
1:A:188:PHE:HD1	1:A:243:LEU:HD21	1.82	0.45
1:A:289:LYS:HG3	1:B:369:GLY:O	2.17	0.45
1:A:329:ARG:HE	1:A:333:GLN:HG2	1.82	0.45
1:B:230:LEU:HG	1:B:235:ILE:HD13	1.98	0.45
2:D:146:ASP:OD1	2:D:146:ASP:O	2.35	0.45
2:E:114:GLN:O	2:E:139:GLY:CA	2.64	0.45
1:A:273:VAL:CG1	1:A:274:ASP:N	2.80	0.45
1:B:327:GLU:OE2	1:B:328:ARG:HG3	2.17	0.45
1:C:330:GLY:C	1:C:333:GLN:HB2	2.37	0.45
2:D:284:ILE:HA	2:D:298:VAL:HG23	1.97	0.45
1:A:260:VAL:O	1:A:263:LYS:HB3	2.17	0.45
1:B:278:TRP:HE1	1:B:326:SER:HG	1.62	0.45
1:C:248:PHE:CD2	1:C:345:LEU:HD21	2.52	0.45
2:D:97:VAL:HB	2:D:298:VAL:HA	1.99	0.45
1:B:248:PHE:CD1	1:B:304:ILE:CG2	3.00	0.45
1:C:317:LYS:O	1:C:318:ASN:CB	2.64	0.45
2:D:122:PHE:O	2:D:122:PHE:HD1	2.00	0.45
2:E:76:LEU:C	2:E:76:LEU:CD2	2.85	0.45
2:F:88:TYR:O	2:F:88:TYR:CD1	2.70	0.45
2:F:266:GLU:O	2:F:270:GLN:NE2	2.50	0.45
1:A:289:LYS:HZ1	1:B:186:LEU:HB2	1.81	0.45
1:A:297:HIS:CD2	2:D:166:GLU:OE2	2.69	0.45
1:B:276:ILE:HG22	1:B:276:ILE:O	2.17	0.45
1:C:201:LYS:HB2	1:C:201:LYS:HE2	1.84	0.45
1:C:206:ILE:CG1	1:C:249:ILE:HG13	2.47	0.45
1:C:265:ILE:HD11	1:C:272:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:174:SER:OG	2:D:176:GLU:OE1	2.33	0.45
1:A:329:ARG:NH2	1:A:333:GLN:OE1	2.47	0.44
1:B:264:MET:HG3	1:B:265:ILE:N	2.32	0.44
1:C:322:ASP:OD2	1:C:322:ASP:N	2.50	0.44
1:A:287:ILE:CG2	1:B:371:GLU:CA	2.93	0.44
1:B:279:VAL:CG2	1:B:325:PHE:CD2	2.99	0.44
2:D:88:TYR:CE1	2:D:90:THR:O	2.70	0.44
2:D:143:ILE:HG22	2:D:144:TRP:H	1.81	0.44
1:A:210:PRO:O	1:A:212:TRP:CD1	2.71	0.44
2:D:246:ARG:HD2	2:D:246:ARG:HA	1.57	0.44
2:F:173:LEU:HD12	2:F:254:ILE:CG1	2.48	0.44
2:F:262:LEU:O	2:F:263:LYS:C	2.53	0.44
1:A:325:PHE:O	1:A:325:PHE:CD1	2.71	0.44
1:C:202:MET:HE2	1:C:243:LEU:O	2.11	0.44
1:C:248:PHE:HD1	1:C:305:GLY:O	1.99	0.44
1:C:350:ASN:O	1:C:351:TYR:CD1	2.70	0.44
2:E:268:ILE:O	2:E:272:ILE:HG13	2.18	0.44
1:B:211:PRO:HB2	1:B:228:ASP:O	2.18	0.44
1:B:230:LEU:HG	1:B:235:ILE:CD1	2.47	0.44
1:C:181:SER:OG	1:C:182:ASP:N	2.50	0.44
1:C:350:ASN:O	1:C:351:TYR:HD1	2.01	0.44
2:D:120:ASN:ND2	2:D:123:LYS:CA	2.73	0.44
2:E:253:ASP:CG	3:E:402:HOH:O	2.56	0.44
1:A:211:PRO:CD	1:A:355:PHE:CE1	3.00	0.44
1:A:289:LYS:CD	1:A:291:HIS:CB	2.89	0.44
1:B:295:LEU:CD1	1:B:296:GLN:H	2.31	0.44
1:A:331:GLN:HA	1:A:332:SER:HA	1.62	0.44
1:A:353:GLU:HB2	1:A:365:TRP:HZ3	1.79	0.44
1:B:331:GLN:HA	1:B:332:SER:HA	1.71	0.44
2:E:196:LEU:H	2:E:196:LEU:CD2	2.02	0.44
2:F:151:ASN:C	2:F:152:GLU:OE1	2.56	0.44
2:F:219:VAL:O	2:F:220:LEU:HD23	2.18	0.44
1:B:295:LEU:HG	2:F:168:LEU:HD12	1.99	0.44
2:D:100:LYS:HD2	2:D:100:LYS:HA	1.73	0.44
2:F:118:ILE:HG23	2:F:284:ILE:HG22	1.94	0.44
2:F:256:ASN:C	2:F:257:ASN:OD1	2.55	0.44
1:A:192:ILE:HG23	1:A:202:MET:HE1	2.00	0.44
1:B:203:PHE:CZ	1:B:352:LEU:HD13	2.53	0.44
2:E:146:ASP:HB3	2:E:147:LYS:H	1.66	0.44
2:E:253:ASP:CB	2:E:265:LYS:CE	2.96	0.44
2:F:128:ASN:ND2	2:F:128:ASN:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:ILE:CG1	2:F:137:SER:N	2.80	0.44
2:E:262:LEU:C	2:E:262:LEU:CD2	2.85	0.43
1:A:277:THR:CG2	1:A:299:LYS:HE2	2.48	0.43
1:C:204:ASP:HB3	1:C:315:PHE:CZ	2.53	0.43
1:C:322:ASP:OD1	2:E:222:GLN:CA	2.67	0.43
2:E:134:LYS:NZ	2:E:284:ILE:HD11	2.33	0.43
2:E:174:SER:O	2:E:177:GLN:CB	2.66	0.43
2:F:123:LYS:HE3	2:F:123:LYS:N	2.33	0.43
1:A:211:PRO:CD	1:A:355:PHE:HE1	2.32	0.43
1:B:295:LEU:HD12	2:F:249:ASP:HA	1.99	0.43
1:C:258:TYR:O	1:C:261:THR:OG1	2.30	0.43
2:D:165:ILE:C	2:D:166:GLU:HG2	2.38	0.43
1:A:183:VAL:HG22	1:A:238:MET:CE	2.48	0.43
1:A:210:PRO:HB3	1:A:235:ILE:HG21	2.00	0.43
2:E:105:ASP:OD2	2:E:107:SER:CB	2.66	0.43
2:F:141:LEU:O	2:F:142:PHE:CD1	2.70	0.43
1:A:354:ILE:O	1:A:355:PHE:HB2	2.18	0.43
1:B:259:ARG:HA	1:B:259:ARG:HD2	1.80	0.43
1:C:350:ASN:C	1:C:351:TYR:CD1	2.92	0.43
2:D:113:VAL:O	2:D:113:VAL:HG23	2.19	0.43
2:D:124:LYS:H	2:D:124:LYS:CD	2.31	0.43
2:D:127:LYS:C	2:D:127:LYS:CD	2.85	0.43
2:F:140:ILE:C	2:F:141:LEU:HD23	2.39	0.43
2:F:274:THR:O	2:F:275:LEU:CB	2.65	0.43
1:A:211:PRO:HB2	1:A:228:ASP:HB2	1.94	0.43
1:A:240:ILE:N	1:A:240:ILE:CD1	2.81	0.43
1:A:249:ILE:C	1:A:250:PHE:CD1	2.92	0.43
2:D:124:LYS:H	2:D:124:LYS:HD2	1.83	0.43
2:D:282:MET:HE3	2:D:298:VAL:HG11	1.99	0.43
2:F:167:ASN:OD1	2:F:227:LEU:O	2.36	0.43
2:D:88:TYR:OH	2:D:293:LYS:HB2	2.18	0.43
2:E:152:GLU:O	2:E:156:THR:OG1	2.27	0.43
2:E:243:ARG:NH2	2:E:274:THR:HA	2.31	0.43
2:E:254:ILE:HG22	2:E:255:VAL:N	2.33	0.43
2:F:116:ILE:CD1	2:F:282:MET:HE2	2.48	0.43
2:F:184:LYS:HA	2:F:185:HIS:HA	1.76	0.43
2:F:227:LEU:HD23	2:F:228:ILE:N	2.34	0.43
1:A:289:LYS:HZ3	1:B:186:LEU:HD22	1.72	0.43
1:B:273:VAL:HG22	1:B:273:VAL:O	2.18	0.43
1:C:299:LYS:CD	2:E:250:VAL:HG11	2.48	0.43
2:D:146:ASP:HA	2:D:225:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:LEU:HB2	2:D:254:ILE:HG22	2.00	0.43
2:E:242:LEU:CB	2:E:277:PRO:CG	2.87	0.43
2:F:123:LYS:H	2:F:123:LYS:CE	2.30	0.43
1:B:197:ARG:O	1:B:197:ARG:HG2	2.19	0.43
1:B:261:THR:HA	1:B:264:MET:HG2	2.00	0.43
2:D:91:ASP:OD1	2:D:91:ASP:O	2.36	0.43
2:D:277:PRO:HD2	2:D:278:LYS:NZ	2.33	0.43
2:F:88:TYR:OH	2:F:292:ARG:HA	2.19	0.43
1:B:277:THR:HG21	2:F:169:VAL:HG21	2.01	0.43
2:E:218:LYS:HA	2:E:218:LYS:HD3	1.86	0.43
1:A:241:GLN:HG2	1:A:268:TRP:O	2.19	0.42
1:A:250:PHE:N	1:A:250:PHE:HD1	2.14	0.42
1:A:263:LYS:CG	1:A:267:ASN:HD21	2.21	0.42
1:A:289:LYS:HD3	1:A:291:HIS:H	1.84	0.42
1:B:322:ASP:CB	2:F:224:LYS:HE3	2.49	0.42
1:C:189:GLN:HA	1:C:192:ILE:HD12	2.00	0.42
1:C:333:GLN:HG2	1:C:359:ASN:HD22	1.83	0.42
1:A:211:PRO:HG2	1:A:235:ILE:HD11	2.01	0.42
1:A:299:LYS:HE2	1:A:299:LYS:HB2	1.68	0.42
2:E:269:TYR:HD1	2:E:292:ARG:CD	2.31	0.42
1:C:271:LYS:O	1:C:306:VAL:HG12	2.20	0.42
2:E:144:TRP:CZ2	2:E:268:ILE:HG13	2.54	0.42
1:B:293:PHE:O	2:F:245:GLN:CA	2.67	0.42
1:B:356:ALA:HB2	1:B:367:SER:OG	2.20	0.42
2:E:154:LEU:HD23	2:E:230:PHE:HE2	1.84	0.42
1:C:191:LEU:C	1:C:191:LEU:CD2	2.87	0.42
2:D:159:ASN:ND2	2:D:159:ASN:C	2.73	0.42
1:B:193:ASP:O	1:B:197:ARG:HB3	2.19	0.42
1:C:183:VAL:CG2	1:C:184:THR:N	2.82	0.42
1:C:325:PHE:CE1	2:E:204:GLN:HG3	2.50	0.42
1:C:325:PHE:HD1	2:E:204:GLN:HG3	1.73	0.42
2:E:140:ILE:CD1	2:E:276:LEU:HD11	2.49	0.42
2:F:226:VAL:CG1	2:F:227:LEU:N	2.83	0.42
1:A:186:LEU:CD1	1:A:187:ASN:C	2.85	0.42
1:B:289:LYS:O	1:B:297:HIS:O	2.38	0.42
1:B:293:PHE:C	1:B:293:PHE:HD2	2.22	0.42
1:C:324:ILE:HG22	1:C:326:SER:H	1.85	0.42
1:C:343:ASN:O	1:C:346:CYS:C	2.56	0.42
2:D:127:LYS:CA	2:D:160:LYS:NZ	2.81	0.42
2:D:203:GLN:O	2:D:206:VAL:N	2.37	0.42
2:D:284:ILE:O	2:D:285:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:76:LEU:HD23	2:E:80:LYS:HD2	2.01	0.42
1:C:183:VAL:HG21	1:C:355:PHE:CE1	2.55	0.42
2:D:109:TYR:HE2	2:D:296:ILE:HG23	1.71	0.42
2:E:99:LYS:O	2:E:101:ILE:CD1	2.66	0.42
2:F:99:LYS:HD2	2:F:106:LEU:HB3	2.02	0.42
2:F:162:PHE:HB3	2:F:230:PHE:HB3	2.02	0.42
2:F:266:GLU:O	2:F:269:TYR:HD2	2.02	0.42
2:F:293:LYS:O	2:F:293:LYS:HG3	2.20	0.42
1:B:259:ARG:NH2	1:B:263:LYS:HG2	2.35	0.42
2:F:124:LYS:O	2:F:127:LYS:HB2	2.20	0.42
1:B:205:VAL:CG1	1:B:250:PHE:CE1	3.02	0.42
1:B:291:HIS:ND1	1:B:291:HIS:C	2.73	0.42
1:B:293:PHE:CD2	2:F:244:HIS:HB2	2.54	0.42
2:D:122:PHE:HB3	2:D:124:LYS:HG3	2.02	0.42
2:D:144:TRP:NE1	2:D:227:LEU:HD13	2.34	0.42
2:E:222:GLN:CD	2:E:224:LYS:HZ2	2.12	0.42
1:B:276:ILE:CG1	1:B:304:ILE:HD11	2.50	0.41
1:B:282:THR:HG23	1:B:287:ILE:C	2.41	0.41
1:C:317:LYS:HA	2:E:219:VAL:HG23	2.02	0.41
1:A:211:PRO:HG2	1:A:230:LEU:HB2	2.01	0.41
1:A:230:LEU:HD22	1:A:235:ILE:HD11	1.99	0.41
1:A:288:ALA:HB2	1:A:298:ALA:HB1	2.00	0.41
2:D:94:LYS:C	2:D:95:ILE:HG13	2.40	0.41
2:E:110:ALA:HA	2:E:111:LYS:HA	1.69	0.41
1:A:186:LEU:CD1	1:A:187:ASN:N	2.79	0.41
2:D:138:ASN:ND2	2:D:138:ASN:C	2.73	0.41
2:D:251:LEU:HD23	2:D:251:LEU:HA	1.89	0.41
2:F:122:PHE:H	2:F:126:LEU:HD11	1.80	0.41
1:A:338:ILE:O	1:A:341:TYR:HB2	2.20	0.41
2:F:185:HIS:HA	2:F:186:MET:HA	1.86	0.41
1:B:206:ILE:HD11	1:B:244:GLN:HG2	1.92	0.41
1:B:235:ILE:HG12	1:B:235:ILE:H	1.64	0.41
1:B:326:SER:HB2	1:B:335:PRO:HB3	1.99	0.41
1:C:322:ASP:CG	2:E:222:GLN:CB	2.85	0.41
2:F:283:GLU:HB3	2:F:297:SER:HA	2.02	0.41
1:B:201:LYS:HB2	1:B:201:LYS:NZ	2.26	0.41
1:B:340:GLN:C	1:B:343:ASN:OD1	2.55	0.41
1:C:294:TYR:HA	2:E:245:GLN:HA	2.02	0.41
1:C:312:ASN:OD1	1:C:312:ASN:N	2.53	0.41
1:C:337:GLU:O	1:C:341:TYR:HD2	2.04	0.41
2:D:173:LEU:O	2:D:255:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:154:LEU:HD21	2:E:164:TYR:CD2	2.55	0.41
2:E:283:GLU:HG3	2:E:284:ILE:N	2.35	0.41
2:F:226:VAL:HG12	2:F:227:LEU:N	2.35	0.41
1:B:292:GLY:O	1:B:297:HIS:HD2	1.95	0.41
1:C:193:ASP:O	1:C:197:ARG:CG	2.65	0.41
1:C:257:LYS:HA	1:C:260:VAL:CG2	2.50	0.41
1:C:327:GLU:CG	1:C:328:ARG:N	2.84	0.41
2:D:75:VAL:HG22	2:D:251:LEU:HD22	2.03	0.41
2:D:243:ARG:HE	2:D:246:ARG:HG2	1.86	0.41
2:D:269:TYR:CD1	2:D:292:ARG:HD3	2.55	0.41
1:A:206:ILE:O	1:A:249:ILE:HG13	2.20	0.41
1:B:338:ILE:O	1:B:342:ILE:CG1	2.59	0.41
2:D:73:LEU:O	2:D:76:LEU:O	2.39	0.41
2:E:101:ILE:CG2	2:E:129:LEU:HD11	2.51	0.41
2:E:167:ASN:ND2	2:E:167:ASN:C	2.73	0.41
2:F:196:LEU:HG	3:F:413:HOH:O	2.20	0.41
1:B:232:ASP:CG	1:B:257:LYS:HZ2	2.21	0.41
1:C:336:GLU:C	1:C:338:ILE:N	2.74	0.41
2:D:76:LEU:HD23	2:D:76:LEU:HA	1.88	0.41
2:D:144:TRP:CD1	2:D:227:LEU:HD12	2.56	0.41
2:D:284:ILE:HG12	2:D:298:VAL:HG21	2.02	0.41
2:E:196:LEU:N	2:E:196:LEU:CD2	2.73	0.41
2:F:117:PHE:O	2:F:284:ILE:HD12	2.21	0.41
2:F:168:LEU:HD21	2:F:229:MET:HE1	1.99	0.41
2:F:281:LEU:CA	2:F:295:TRP:CZ3	3.03	0.41
1:A:238:MET:HE3	1:A:355:PHE:HZ	1.86	0.41
1:C:246:ASP:OD1	1:C:308:GLY:CA	2.66	0.41
1:C:330:GLY:O	1:C:332:SER:O	2.39	0.41
2:D:147:LYS:O	2:D:222:GLN:OE1	2.39	0.41
2:F:168:LEU:CD2	2:F:168:LEU:N	2.73	0.41
1:A:235:ILE:O	1:A:238:MET:SD	2.79	0.40
2:D:75:VAL:HG22	2:D:252:PHE:H	1.78	0.40
1:B:338:ILE:HD12	1:B:338:ILE:HA	1.80	0.40
1:A:202:MET:HG3	1:A:243:LEU:C	2.37	0.40
1:A:282:THR:CG2	1:A:287:ILE:HB	2.51	0.40
1:C:277:THR:OG1	1:C:323:VAL:HG12	2.22	0.40
2:D:95:ILE:HB	2:D:296:ILE:HG23	2.03	0.40
2:D:277:PRO:HD2	2:D:278:LYS:HZ3	1.86	0.40
2:E:129:LEU:HD23	2:E:129:LEU:HA	1.76	0.40
2:E:261:CYS:O	2:E:261:CYS:SG	2.78	0.40
2:F:94:LYS:NZ	2:F:94:LYS:CB	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HD12	2:D:166:GLU:HB3	2.03	0.40
1:C:321:SER:OG	2:E:208:VAL:HG23	2.22	0.40
2:D:167:ASN:HD22	2:D:167:ASN:HA	1.74	0.40
2:F:101:ILE:C	2:F:104:THR:H	2.24	0.40
2:F:143:ILE:CD1	2:F:143:ILE:N	2.73	0.40
1:B:207:MET:HA	1:B:250:PHE:O	2.22	0.40
1:B:293:PHE:O	1:B:293:PHE:HD2	2.04	0.40
2:D:144:TRP:HE1	2:D:227:LEU:HD13	1.86	0.40
2:D:146:ASP:CA	2:D:225:GLN:HG2	2.51	0.40
2:E:231:ARG:NH2	2:E:231:ARG:CG	2.73	0.40
2:F:136:ILE:O	2:F:232:LYS:HE3	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:HIS:O	2:F:246:ARG:NH2[1_545]	1.87	0.33
2:D:102:LEU:CD1	3:B:422:HOH:O[2_646]	2.07	0.13
1:B:291:HIS:O	1:C:367:SER:O[1_565]	2.13	0.07

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	174/202 (86%)	163 (94%)	11 (6%)	0	100	100
1	B	174/202 (86%)	168 (97%)	6 (3%)	0	100	100
1	C	170/202 (84%)	162 (95%)	8 (5%)	0	100	100
2	D	203/237 (86%)	187 (92%)	15 (7%)	1 (0%)	29	64
2	E	201/237 (85%)	189 (94%)	9 (4%)	3 (2%)	10	39
2	F	174/237 (73%)	166 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1096/1317 (83%)	1035 (94%)	57 (5%)	4 (0%)	34 69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	247	THR
2	E	290	GLN
2	E	291	PRO
2	D	290	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	148/178 (83%)	119 (80%)	29 (20%)	1 6
1	B	149/178 (84%)	121 (81%)	28 (19%)	1 6
1	C	149/178 (84%)	119 (80%)	30 (20%)	1 5
2	D	169/225 (75%)	122 (72%)	47 (28%)	0 1
2	E	162/225 (72%)	111 (68%)	51 (32%)	0 0
2	F	140/225 (62%)	89 (64%)	51 (36%)	0 0
All	All	917/1209 (76%)	681 (74%)	236 (26%)	0 1

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	202	MET
1	A	228	ASP
1	A	230	LEU
1	A	234	LYS
1	A	246	ASP
1	A	250	PHE
1	A	254	ILE

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Mol	Chain	Res	Type
1	A	272	LEU
1	A	274	ASP
1	A	279	VAL
1	A	282	THR
1	A	287	ILE
1	A	293	PHE
1	A	294	TYR
1	A	307	LYS
1	A	314	ARG
1	A	317	LYS
1	A	325	PHE
1	A	326	SER
1	A	328	ARG
1	A	343	ASN
1	A	344	GLN
1	A	345	LEU
1	A	350	ASN
1	A	355	PHE
1	A	357	ARG
1	A	362	HIS
1	A	371	GLU
1	B	182	ASP
1	B	192	ILE
1	B	195	GLN
1	B	201	LYS
1	B	228	ASP
1	B	230	LEU
1	B	236	GLN
1	B	245	GLN
1	B	246	ASP
1	B	249	ILE
1	B	263	LYS
1	B	264	MET
1	B	271	LYS
1	B	272	LEU
1	B	277	THR
1	B	291	HIS
1	B	293	PHE
1	B	295	LEU
1	B	314	ARG
1	B	318	ASN
1	B	325	PHE

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Mol	Chain	Res	Type
1	B	328	ARG
1	B	329	ARG
1	B	331	GLN
1	B	352	LEU
1	B	359	ASN
1	B	360	ASN
1	B	367	SER
1	C	182	ASP
1	C	185	LYS
1	C	186	LEU
1	C	189	GLN
1	C	195	GLN
1	C	204	ASP
1	C	208	MET
1	C	241	GLN
1	C	246	ASP
1	C	249	ILE
1	C	259	ARG
1	C	261	THR
1	C	274	ASP
1	C	280	LYS
1	C	299	LYS
1	C	301	SER
1	C	311	ASP
1	C	312	ASN
1	C	316	LYS
1	C	317	LYS
1	C	322	ASP
1	C	326	SER
1	C	328	ARG
1	C	333	GLN
1	C	345	LEU
1	C	346	CYS
1	C	350	ASN
1	C	362	HIS
1	C	368	ILE
1	C	372	LEU
2	D	66	ASP
2	D	71	ASP
2	D	73	LEU
2	D	89	GLU
2	D	100	LYS

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Mol	Chain	Res	Type
2	D	102	LEU
2	D	104	THR
2	D	107	SER
2	D	108	GLN
2	D	120	ASN
2	D	122	PHE
2	D	124	LYS
2	D	127	LYS
2	D	129	LEU
2	D	131	ILE
2	D	135	LEU
2	D	137	SER
2	D	138	ASN
2	D	140	ILE
2	D	148	SER
2	D	150	ILE
2	D	157	MET
2	D	158	GLU
2	D	159	ASN
2	D	167	ASN
2	D	175	LEU
2	D	181	GLU
2	D	182	LEU
2	D	186	MET
2	D	191	THR
2	D	192	GLU
2	D	199	LEU
2	D	224	LYS
2	D	231	ARG
2	D	234	ASP
2	D	242	LEU
2	D	243	ARG
2	D	244	HIS
2	D	246	ARG
2	D	249	ASP
2	D	256	ASN
2	D	264	THR
2	D	279	SER
2	D	292	ARG
2	D	293	LYS
2	D	297	SER
2	D	300	GLU

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Mol	Chain	Res	Type
2	E	73	LEU
2	E	76	LEU
2	E	79	TRP
2	E	88	TYR
2	E	102	LEU
2	E	105	ASP
2	E	113	VAL
2	E	122	PHE
2	E	126	LEU
2	E	131	ILE
2	E	133	LYS
2	E	138	ASN
2	E	146	ASP
2	E	148	SER
2	E	149	LEU
2	E	166	GLU
2	E	167	ASN
2	E	175	LEU
2	E	177	GLN
2	E	181	GLU
2	E	183	ASN
2	E	196	LEU
2	E	197	ASP
2	E	199	LEU
2	E	205	LYS
2	E	212	ILE
2	E	220	LEU
2	E	224	LYS
2	E	227	LEU
2	E	228	ILE
2	E	243	ARG
2	E	244	HIS
2	E	245	GLN
2	E	247	THR
2	E	251	LEU
2	E	253	ASP
2	E	256	ASN
2	E	262	LEU
2	E	264	THR
2	E	265	LYS
2	E	266	GLU
2	E	270	GLN

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Mol	Chain	Res	Type
2	E	279	SER
2	E	283	GLU
2	E	287	GLN
2	E	288	LYS
2	E	289	ASP
2	E	292	ARG
2	E	293	LYS
2	E	297	SER
2	E	300	GLU
2	F	76	LEU
2	F	79	TRP
2	F	88	TYR
2	F	89	GLU
2	F	90	THR
2	F	91	ASP
2	F	94	LYS
2	F	102	LEU
2	F	106	LEU
2	F	119	ASP
2	F	120	ASN
2	F	123	LYS
2	F	124	LYS
2	F	127	LYS
2	F	128	ASN
2	F	133	LYS
2	F	138	ASN
2	F	140	ILE
2	F	141	LEU
2	F	144	TRP
2	F	149	LEU
2	F	150	ILE
2	F	151	ASN
2	F	152	GLU
2	F	168	LEU
2	F	172	GLN
2	F	186	MET
2	F	188	ILE
2	F	196	LEU
2	F	199	LEU
2	F	221	ASN
2	F	224	LYS
2	F	244	HIS

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Mol	Chain	Res	Type
2	F	246	ARG
2	F	249	ASP
2	F	257	ASN
2	F	262	LEU
2	F	264	THR
2	F	265	LYS
2	F	268	ILE
2	F	269	TYR
2	F	270	GLN
2	F	272	ILE
2	F	273	GLU
2	F	278	LYS
2	F	280	GLN
2	F	281	LEU
2	F	287	GLN
2	F	288	LYS
2	F	292	ARG
2	F	293	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	267	ASN
1	A	333	GLN
1	A	360	ASN
1	B	189	GLN
1	B	244	GLN
1	B	267	ASN
1	B	296	GLN
1	B	297	HIS
1	B	312	ASN
1	B	331	GLN
1	B	350	ASN
1	C	189	GLN
1	C	241	GLN
1	C	245	GLN
1	C	318	ASN
1	C	333	GLN
1	C	359	ASN
2	D	159	ASN
2	D	167	ASN

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Mol	Chain	Res	Type
2	D	225	GLN
2	D	290	GLN
2	E	114	GLN
2	E	177	GLN
2	E	183	ASN
2	E	204	GLN
2	E	245	GLN
2	E	287	GLN
2	F	128	ASN
2	F	138	ASN
2	F	244	HIS
2	F	270	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	178/202 (88%)	-0.34	2 (1%) 80 64	37, 57, 85, 115	0
1	B	178/202 (88%)	-0.34	3 (1%) 70 49	36, 57, 81, 101	0
1	C	176/202 (87%)	-0.11	4 (2%) 60 39	43, 68, 95, 111	0
2	D	215/237 (90%)	-0.30	5 (2%) 60 39	31, 54, 81, 111	0
2	E	213/237 (89%)	0.00	13 (6%) 21 9	45, 73, 99, 125	0
2	F	192/237 (81%)	0.37	17 (8%) 9 3	53, 83, 104, 120	0
All	All	1152/1317 (87%)	-0.12	44 (3%) 40 20	31, 65, 97, 125	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	284	ILE	6.1
2	F	116	ILE	5.1
2	E	69	THR	5.1
2	F	115	GLY	5.0
1	C	308	GLY	4.3
2	E	107	SER	3.8
1	A	331	GLN	3.7
2	F	128	ASN	3.6
2	D	258	GLY	3.5
2	E	262	LEU	3.3
2	E	261	CYS	3.3
1	C	359	ASN	3.2
2	F	120	ASN	3.1
2	F	204	GLN	2.8
2	F	118	ILE	2.8
1	B	241	GLN	2.8
2	E	259	LYS	2.8
2	E	112	GLY	2.7
2	E	102	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	332	SER	2.6
1	C	309	ASP	2.5
2	D	302	LYS	2.5
1	B	284	ASN	2.4
2	F	80	LYS	2.4
2	F	150	ILE	2.4
2	E	260	SER	2.3
2	E	120	ASN	2.3
2	E	264	THR	2.3
2	D	260	SER	2.3
2	D	103	GLY	2.2
2	F	277	PRO	2.2
2	F	263	LYS	2.2
2	F	279	SER	2.2
2	F	183	ASN	2.2
1	C	360	ASN	2.2
2	E	108	GLN	2.1
2	F	131	ILE	2.1
2	D	261	CYS	2.1
1	B	228	ASP	2.1
2	F	260	SER	2.1
2	E	134	LYS	2.0
2	E	103	GLY	2.0
2	F	125	ASP	2.0
2	F	121	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.