



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2022 – 04:52 PM EST

PDB ID : 1LE9
Title : Crystal structure of a NF-kB heterodimer bound to the Ig/HIV-kB siti
Authors : Benjamin, B.; Huang, D.B.; Chen-Park, F.E.; Sigler, P.B.; Ghosh, G.
Deposited on : 2002-04-09
Resolution : 3.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

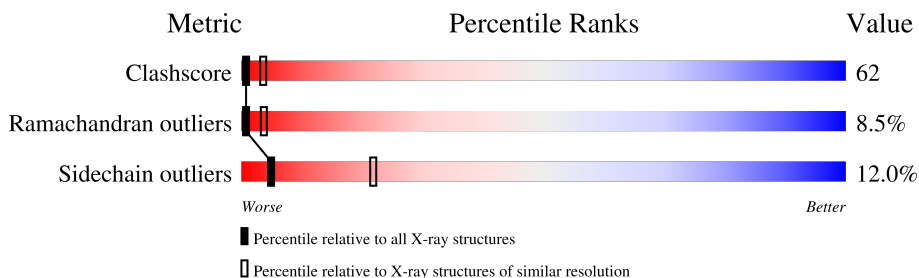
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	12	
1	G	12	
2	D	12	
2	H	12	
3	A	274	
3	E	274	
4	B	313	
4	F	313	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10232 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 DNA chain called 5'-D(*TP*GP*GP*GP*AP*CP*TP*TP*TP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			241	117	39	74	11			
1	G	12	Total	C	N	O	P	0	0	0
			241	117	39	74	11			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*GP*GP*AP*AP*AP*GP*TP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			245	117	51	66	11			
2	H	12	Total	C	N	O	P	0	0	0
			245	117	51	66	11			

- Molecule 3 is a protein called NUCLEAR FACTOR NF-KAPPA-B P65 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			
3	E	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	cloning artifact	UNP Q04207
A	19	ALA	-	cloning artifact	UNP Q04207
E	18	MET	-	cloning artifact	UNP Q04207
E	19	ALA	-	cloning artifact	UNP Q04207

- Molecule 4 is a protein called NUCLEAR FACTOR NF-KAPPA-B P50 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	312	Total	C	N	O	S	0	0	0
			2454	1554	428	460	12			
4	F	312	Total	C	N	O	S	0	0	0
			2454	1554	428	460	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	MET	-	initiating methionine	UNP P25799
F	38	MET	-	initiating methionine	UNP P25799

3 Residue-property plots

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

Note EDS was not executed.

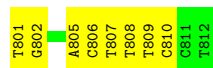
- Molecule 1: 5'-D(*TP*GP*GP*GP*AP*CP*TP*TP*TP*CP*CP*T)-3'

Chain C: 



- Molecule 1: 5'-D(*TP*GP*GP*GP*AP*CP*TP*TP*TP*CP*CP*T)-3'

Chain G: 

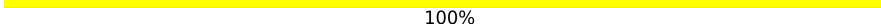


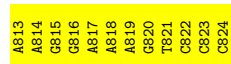
- Molecule 2: 5'-D(*AP*AP*GP*GP*AP*AP*AP*GP*TP*CP*CP*C)-3'

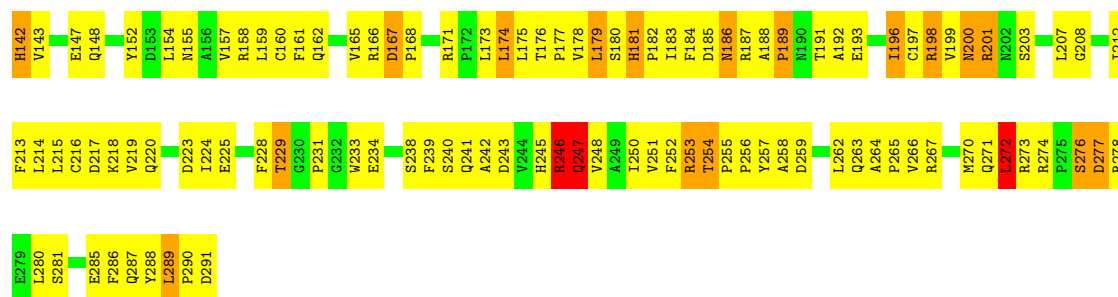
Chain D: 



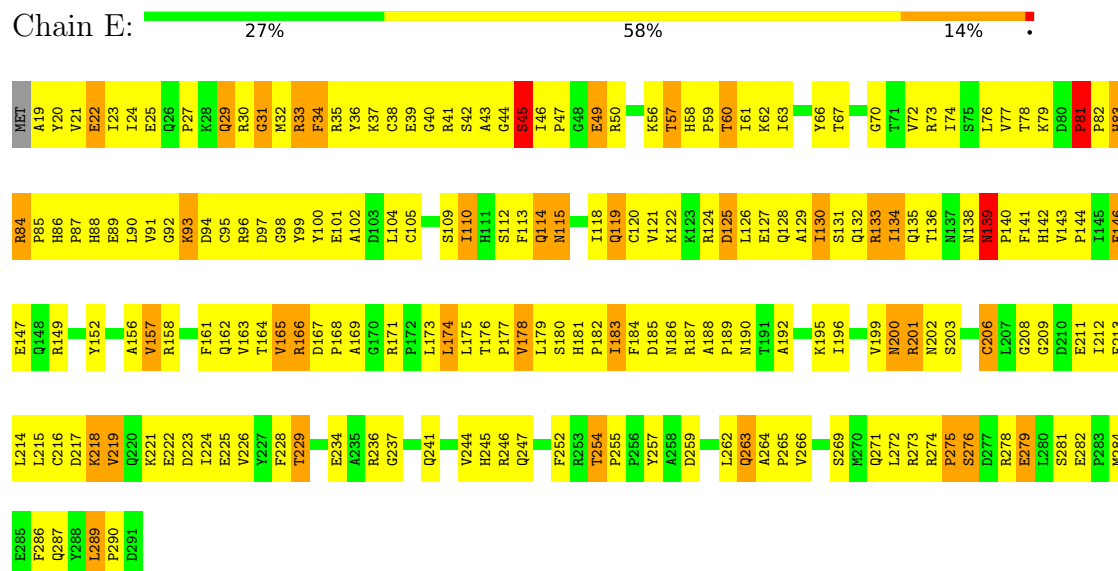
- Molecule 2: 5'-D(*AP*AP*GP*GP*AP*AP*AP*GP*TP*CP*CP*C)-3'

Chain H: 

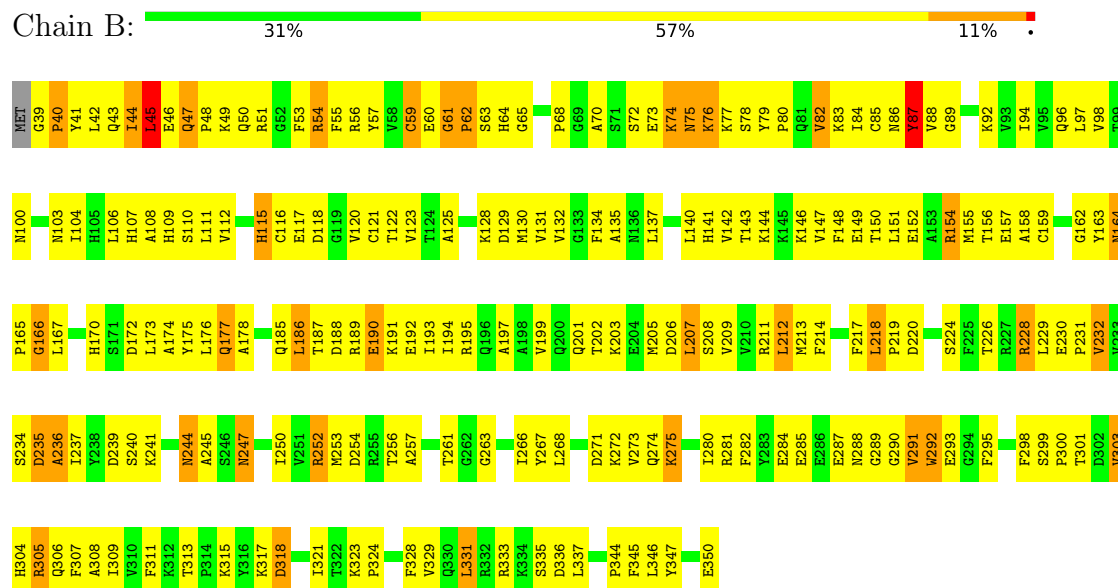




• Molecule 3: NUCLEAR FACTOR NF-KAPPA-B P65 SUBUNIT



• Molecule 4: NUCLEAR FACTOR NF-KAPPA-B P50 SUBUNIT



• Molecule 4: NUCLEAR FACTOR NF-KAPPA-B P50 SUBUNIT

Y316	S234	L167	T104	MET
K317	D235	L168	H105	G39
D318	A236	V169	L106	P40
V319	K237	H170	H107	P41
N320	Y238	S171	A108	L42
I321	D239	D172	H109	Q43
	K240	L173	S110	I44
V327	S241	A174	L111	L45
F328		Y175	V112	E46
V329	S246	L176	G113	Q47
	N247	Q177	K114	P48
R332	L248	A178	H115	K49
R333	K249	E179	C116	Q90
K334	I250			R51
S335	M253	G182	D118	G52
L336	D254	D183		F53
L337		R184	R54	R54
E338	V260	Q185	T122	F55
	G263	L186	V123	R56
F345		T187	T124	Y57
L346	G267	D188	A125	V58
	L268	R189	G126	C59
E350	L269	E190	P127	E60
	D270	K191	K128	G61
	D271	E192		P62
	K272	I193	V131	
	D273	I194	V132	L67
	Q274	R195	G133	P68
	K275	Q196	F134	
	D277		A135	S72
		V199	M136	E73
		Q200	L137	K74
		Q201	G138	N75
		T202	I139	K76
			L140	K77
	F282	M205	H141	S78
	E283	D206	V142	Y79
	D284	L207	T143	P80
	E285		K144	Q81
	E286		K145	V82
	G290	V210	R211	K83
	V291	L212	K146	I84
	E292	M213	V147	C85
	D293	F214	F148	N86
	G294	T215		Y87
	F295	A216	L151	Y88
		F217	A153	V89
		L218	R154	A91
	T301	P219	M155	K92
	D302	D220	T156	V93
	H304	S221	E157	I94
	R305	T222	A158	V95
	Q306	G223	C159	Q96
	F307	S224	T160	L97
	A308	F225	R161	V98
	I309		G162	T99
			Y163	N100
	T313	L229	N164	G101
		E230	P165	T102
			C166	N102

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.84Å 138.00Å 90.04Å 90.00° 97.28° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	85.4 (30.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.249 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10232	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

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	C	0.66	0/268	0.83	0/412
1	G	0.30	0/268	0.71	0/412
2	D	0.69	0/276	0.81	0/424
2	H	0.28	0/276	0.64	0/424
3	A	0.44	0/2228	0.71	1/3021 (0.0%)
3	E	0.44	0/2228	0.69	0/3021
4	B	0.47	0/2506	0.71	0/3384
4	F	0.42	0/2506	0.67	1/3384 (0.0%)
All	All	0.45	0/10556	0.70	2/14482 (0.0%)

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
4	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	272	LEU	CA-CB-CG	6.40	130.03	115.30
4	F	346	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	347	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	C	241	0	139	14	0
1	G	241	0	139	26	0
2	D	245	0	135	5	0
2	H	245	0	135	21	0
3	A	2176	0	2137	328	0
3	E	2176	0	2137	294	0
4	B	2454	0	2449	282	0
4	F	2454	0	2449	327	0
All	All	10232	0	9720	1243	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 62.

All (1243) 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)
4:F:98:VAL:HG12	4:F:168:LEU:HD21	1.19	1.10
2:H:813:DA:H4'	2:H:814:DA:H5'	1.33	1.10
4:F:106:LEU:HD21	4:F:155:MET:HG2	1.38	1.03
4:B:143:THR:HG23	4:B:146:LYS:H	1.24	1.02
4:F:56:ARG:HA	4:F:56:ARG:HH11	1.23	1.00
4:F:164:ASN:HD21	4:F:168:LEU:H	1.03	0.99
3:A:200:ASN:ND2	3:A:201:ARG:H	1.62	0.98
3:E:209:GLY:H	3:E:254:THR:HG22	1.25	0.97
4:F:88:VAL:HG11	4:F:218:LEU:HD22	1.46	0.96
3:A:189:PRO:HG3	3:A:218:LYS:HE3	1.44	0.96
4:F:162:GLY:HA2	4:F:176:LEU:HB2	1.45	0.96
3:E:161:PHE:HB2	3:E:178:VAL:HG12	1.48	0.96
4:F:40:PRO:HB3	4:F:86:ASN:HB2	1.49	0.94
4:F:164:ASN:ND2	4:F:168:LEU:HB2	1.81	0.94
4:F:284:GLU:HB2	4:F:327:VAL:HG23	1.47	0.94
3:A:174:LEU:HD12	3:A:174:LEU:H	1.33	0.94
3:E:72:VAL:HA	3:E:163:VAL:HG12	1.50	0.92
4:B:162:GLY:HA2	4:B:176:LEU:O	1.71	0.91
4:B:72:SER:HB3	4:B:77:LYS:HD2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:91:VAL:HG11	3:E:119:GLN:OE1	1.70	0.90
3:E:165:VAL:HG23	3:E:173:LEU:HB3	1.52	0.90
4:F:105:HIS:HB3	4:F:201:GLN:NE2	1.86	0.90
3:E:87:PRO:HB3	3:E:130:ILE:HG22	1.53	0.89
3:E:201:ARG:HB2	3:E:201:ARG:HH21	1.36	0.89
3:A:80:ASP:HB3	3:A:81:PRO:HD2	1.54	0.88
4:B:47:GLN:HB3	4:B:48:PRO:HD2	1.56	0.88
4:F:303:VAL:HG22	4:F:309:ILE:HG12	1.53	0.88
3:E:215:LEU:HB3	4:F:304:HIS:ND1	1.89	0.88
4:F:56:ARG:HA	4:F:56:ARG:NH1	1.88	0.87
4:F:164:ASN:HD21	4:F:168:LEU:N	1.71	0.87
4:F:67:LEU:HD23	4:F:67:LEU:H	1.39	0.87
3:A:32:MET:O	3:A:186:ASN:HB2	1.75	0.86
4:B:109:HIS:HD2	4:B:142:VAL:H	1.23	0.86
4:B:199:VAL:O	4:B:203:LYS:HD3	1.76	0.86
3:E:21:VAL:HG12	3:E:22:GLU:H	1.40	0.86
4:F:114:LYS:HD3	4:F:114:LYS:H	1.38	0.86
3:E:76:LEU:HD11	3:E:90:LEU:HB2	1.59	0.85
3:A:189:PRO:HB2	3:A:220:GLN:HE21	1.40	0.85
3:A:58:HIS:HB2	3:A:114:GLN:HE21	1.42	0.84
3:E:130:ILE:HA	3:E:133:ARG:HD2	1.57	0.84
4:F:212:LEU:HB2	4:F:234:SER:OG	1.77	0.84
3:A:20:TYR:H	3:A:175:LEU:HG	1.41	0.84
3:A:196:ILE:HD12	3:A:196:ILE:H	1.41	0.84
3:E:74:ILE:HB	3:E:100:TYR:HB3	1.60	0.84
3:E:200:ASN:HD21	3:E:213:PHE:H	1.22	0.83
4:F:97:LEU:HD11	4:F:111:LEU:H	1.40	0.83
1:C:701:DT:H3'	4:B:65:GLY:HA2	1.60	0.83
3:A:28:LYS:HB2	3:A:28:LYS:NZ	1.93	0.82
4:B:47:GLN:HE22	4:B:235:ASP:N	1.78	0.82
3:A:56:LYS:HG2	3:A:57:THR:H	1.42	0.82
4:B:40:PRO:HB3	4:B:86:ASN:HB2	1.59	0.81
4:F:67:LEU:HD21	4:F:137:LEU:HB2	1.60	0.81
4:F:77:LYS:HE2	4:F:77:LYS:H	1.43	0.81
4:F:164:ASN:ND2	4:F:168:LEU:H	1.77	0.81
3:E:19:ALA:HA	3:E:175:LEU:HD22	1.63	0.81
3:A:20:TYR:N	3:A:175:LEU:HG	1.95	0.81
4:F:98:VAL:HG12	4:F:168:LEU:CD2	2.09	0.81
3:E:25:GLU:HB2	3:E:60:THR:H	1.45	0.80
3:E:200:ASN:N	3:E:200:ASN:HD22	1.79	0.80
4:B:42:LEU:HD22	4:B:82:VAL:HG11	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:70:GLY:O	3:A:104:LEU:HG	1.82	0.80
4:B:125:ALA:HA	4:B:132:VAL:HG11	1.64	0.80
3:E:93:LYS:HG3	3:E:115:ASN:O	1.80	0.80
4:F:318:ASP:O	4:F:321:ILE:HG23	1.80	0.80
3:E:77:VAL:O	3:E:157:VAL:HG23	1.82	0.79
4:F:274:GLN:OE1	4:F:333:ARG:HD3	1.82	0.79
3:A:96:ARG:O	3:A:98:GLY:N	2.15	0.79
4:F:96:GLN:HB3	4:F:213:MET:HE2	1.63	0.79
4:F:286:GLU:H	4:F:290:GLY:HA2	1.48	0.79
4:F:42:LEU:HD23	4:F:42:LEU:H	1.49	0.78
4:F:179:GLU:HG2	4:F:184:ARG:HG3	1.65	0.78
4:F:187:THR:HG22	4:F:189:ARG:H	1.46	0.78
4:B:46:GLU:O	4:B:80:PRO:HA	1.82	0.78
1:G:806:DC:H2''	1:G:807:DT:C5'	2.13	0.78
4:F:196:GLN:O	4:F:199:VAL:HG22	1.83	0.78
3:E:128:GLN:O	3:E:132:GLN:HG3	1.82	0.78
3:A:264:ALA:HB1	3:A:265:PRO:HD2	1.66	0.77
4:B:42:LEU:HD22	4:B:82:VAL:CG1	2.13	0.77
4:F:164:ASN:HD21	4:F:168:LEU:HB2	1.47	0.77
4:B:173:LEU:HD23	4:B:175:TYR:H	1.48	0.77
3:E:31:GLY:HA2	3:E:186:ASN:HD21	1.49	0.77
3:E:27:PRO:HB2	3:E:183:ILE:HD11	1.65	0.77
3:E:77:VAL:HG21	3:E:179:LEU:CD2	2.15	0.77
4:B:72:SER:HB3	4:B:77:LYS:CD	2.15	0.77
1:G:809:DT:H1'	1:G:810:DC:H5''	1.66	0.77
3:A:56:LYS:HD3	3:A:56:LYS:H	1.49	0.77
4:B:40:PRO:HB3	4:B:86:ASN:CB	2.15	0.77
4:F:98:VAL:CG1	4:F:168:LEU:HD21	2.09	0.77
3:A:74:ILE:H	3:A:100:TYR:HD1	1.33	0.77
3:A:134:ILE:HG13	3:A:135:GLN:N	2.00	0.76
4:B:176:LEU:O	4:B:176:LEU:HD12	1.86	0.76
3:A:58:HIS:ND1	3:A:114:GLN:HA	2.00	0.76
4:B:96:GLN:OE1	4:B:106:LEU:HD21	1.85	0.76
3:A:134:ILE:HG13	3:A:135:GLN:H	1.51	0.76
3:E:104:LEU:HD23	3:E:104:LEU:H	1.49	0.76
1:G:810:DC:H41	3:E:39:GLU:HG2	1.49	0.76
4:B:47:GLN:HE22	4:B:235:ASP:H	1.33	0.76
3:A:79:LYS:O	3:A:158:ARG:NH1	2.19	0.76
4:B:143:THR:HG23	4:B:146:LYS:N	2.01	0.76
4:B:250:ILE:HG12	4:B:331:LEU:HD22	1.68	0.76
4:F:228:ARG:HD2	4:F:228:ARG:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:184:PHE:HB3	3:A:191:THR:CG2	2.16	0.75
3:E:37:LYS:HD3	3:E:119:GLN:HE22	1.52	0.75
3:E:200:ASN:H	3:E:200:ASN:ND2	1.84	0.75
3:A:46:ILE:HG12	3:A:116:LEU:O	1.87	0.75
3:E:200:ASN:HD22	3:E:200:ASN:H	1.34	0.75
4:F:97:LEU:HD12	4:F:97:LEU:H	1.51	0.75
3:A:28:LYS:HB2	3:A:28:LYS:HZ3	1.50	0.75
3:E:209:GLY:N	3:E:254:THR:HG22	2.00	0.75
3:E:56:LYS:H	3:E:56:LYS:HD3	1.52	0.74
1:G:806:DC:H2''	1:G:807:DT:H5''	1.68	0.74
3:A:175:LEU:HD13	3:A:176:THR:N	2.02	0.74
4:B:165:PRO:HB2	4:B:174:ALA:HA	1.70	0.74
4:F:100:ASN:HA	4:F:211:ARG:CZ	2.18	0.74
3:A:217:ASP:O	3:A:219:VAL:HG13	1.88	0.74
3:E:77:VAL:O	3:E:86:HIS:HB2	1.87	0.74
4:F:147:VAL:O	4:F:151:LEU:HB2	1.88	0.73
4:B:207:LEU:H	4:B:207:LEU:HD22	1.53	0.73
4:B:299:SER:HB3	4:B:300:PRO:HD2	1.69	0.73
3:A:167:ASP:OD1	3:A:168:PRO:HD2	1.87	0.73
4:F:336:ASP:OD1	4:F:338:GLU:HG2	1.87	0.73
3:A:251:VAL:HG11	4:B:252:ARG:NH1	2.02	0.73
3:E:45:SER:O	3:E:47:PRO:HD3	1.88	0.73
3:A:248:VAL:HG22	4:B:304:HIS:NE2	2.04	0.73
4:B:109:HIS:CD2	4:B:142:VAL:H	2.07	0.73
4:B:170:HIS:CE1	4:B:173:LEU:HB2	2.23	0.73
3:E:72:VAL:HG11	3:E:113:PHE:CZ	2.24	0.73
4:F:292:TRP:CZ2	4:F:316:TYR:HA	2.23	0.73
3:A:130:ILE:HD12	3:A:133:ARG:HB2	1.71	0.73
3:E:219:VAL:O	3:E:247:GLN:HB2	1.89	0.73
3:A:27:PRO:HG2	3:A:159:LEU:HD12	1.71	0.72
4:B:186:LEU:HD11	4:B:191:LYS:HD2	1.71	0.72
4:F:199:VAL:HG23	4:F:200:GLN:HE21	1.54	0.72
4:F:219:PRO:HG3	4:F:225:PHE:CE1	2.23	0.72
3:A:20:TYR:H	3:A:175:LEU:CG	2.01	0.72
3:A:93:LYS:HB3	3:A:115:ASN:CB	2.19	0.72
4:F:41:TYR:HD2	4:F:229:LEU:HG	1.53	0.72
3:A:200:ASN:ND2	3:A:201:ARG:N	2.36	0.72
3:A:200:ASN:N	3:A:200:ASN:HD22	1.88	0.72
4:B:217:PHE:HE1	4:B:228:ARG:HG3	1.53	0.72
3:E:73:ARG:HA	3:E:100:TYR:O	1.89	0.72
4:B:212:LEU:HB2	4:B:234:SER:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:173:LEU:HD23	4:B:175:TYR:N	2.04	0.72
4:F:152:GLU:O	4:F:156:THR:HG23	1.90	0.72
1:G:809:DT:H72	3:E:39:GLU:HG3	1.72	0.72
4:F:152:GLU:OE2	4:F:195:ARG:HG3	1.89	0.72
4:F:88:VAL:HG21	4:F:218:LEU:HB3	1.70	0.71
4:F:283:TYR:O	4:F:327:VAL:HG22	1.91	0.71
4:B:40:PRO:HB3	4:B:86:ASN:H	1.53	0.71
4:B:303:VAL:HG13	4:B:309:ILE:CG1	2.20	0.71
3:A:93:LYS:HB3	3:A:115:ASN:HB2	1.71	0.71
4:B:100:ASN:HD22	4:B:211:ARG:HD2	1.56	0.71
4:B:107:HIS:HD2	4:B:109:HIS:H	1.38	0.71
3:A:175:LEU:HD22	3:A:176:THR:H	1.56	0.70
3:A:179:LEU:HD22	3:A:179:LEU:H	1.56	0.70
4:B:112:VAL:HG11	4:B:140:LEU:HD22	1.71	0.70
3:A:26:GLN:HG3	3:A:26:GLN:O	1.91	0.70
3:A:159:LEU:HB2	3:A:180:SER:OG	1.92	0.70
3:A:77:VAL:HG12	3:A:85:PRO:HA	1.72	0.70
3:E:29:GLN:NE2	3:E:30:ARG:HH12	1.89	0.70
3:E:84:ARG:HG3	3:E:152:TYR:CZ	2.27	0.70
4:B:284:GLU:OE1	4:B:317:LYS:HE2	1.92	0.70
3:E:78:THR:HG22	3:E:79:LYS:H	1.56	0.70
3:E:76:LEU:HD22	3:E:88:HIS:O	1.92	0.70
3:A:69:PRO:HB2	3:A:166:ARG:NH2	2.07	0.69
3:A:86:HIS:ND1	3:A:87:PRO:HD2	2.07	0.69
3:A:179:LEU:HD22	3:A:179:LEU:N	2.07	0.69
3:A:199:VAL:HG12	3:A:214:LEU:HA	1.74	0.69
4:F:88:VAL:HG11	4:F:218:LEU:CD2	2.22	0.69
3:A:76:LEU:HD13	3:A:159:LEU:HD23	1.72	0.69
3:E:78:THR:HG21	3:E:84:ARG:HH12	1.58	0.69
1:G:808:DT:H2''	1:G:809:DT:H71	1.74	0.69
2:H:819:DA:H2''	2:H:820:DG:OP2	1.92	0.69
3:A:246:ARG:HG3	3:A:246:ARG:HH11	1.57	0.69
3:A:273:ARG:HD2	3:A:280:LEU:HD21	1.73	0.69
4:F:67:LEU:H	4:F:67:LEU:CD2	2.04	0.69
4:F:67:LEU:HD13	4:F:139:ILE:HD11	1.73	0.69
3:A:189:PRO:HB2	3:A:220:GLN:NE2	2.07	0.69
3:A:72:VAL:HG12	3:A:102:ALA:O	1.93	0.69
3:E:24:ILE:HG13	3:E:25:GLU:OE2	1.91	0.69
4:B:261:THR:O	4:B:315:LYS:HG2	1.92	0.69
3:A:64:ASN:HD22	3:A:65:GLY:N	1.91	0.68
3:A:174:LEU:HD12	3:A:174:LEU:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:47:GLN:NE2	4:B:235:ASP:H	1.90	0.68
4:B:111:LEU:HD23	4:B:121:CYS:SG	2.33	0.68
4:B:271:ASP:O	4:B:273:VAL:HG13	1.93	0.68
4:F:41:TYR:CE1	4:F:230:GLU:HB2	2.27	0.68
3:E:124:ARG:NH1	3:E:124:ARG:HB3	2.08	0.68
3:E:88:HIS:HD2	3:E:121:VAL:HG13	1.58	0.68
4:F:128:LYS:HE2	4:F:128:LYS:O	1.93	0.68
4:B:118:ASP:O	4:B:154:ARG:NH1	2.27	0.68
3:E:92:GLY:H	3:E:95:CYS:HB2	1.59	0.68
1:C:702:DG:H1'	1:C:703:DG:H5'	1.75	0.68
4:B:94:ILE:O	4:B:94:ILE:HD12	1.93	0.68
3:E:82:PRO:HG2	3:E:84:ARG:HH21	1.58	0.68
4:F:100:ASN:HA	4:F:211:ARG:NE	2.09	0.68
3:E:126:LEU:O	3:E:130:ILE:HG23	1.94	0.68
3:A:96:ARG:C	3:A:98:GLY:H	1.98	0.67
4:B:75:ASN:O	4:B:76:LYS:HB2	1.93	0.67
3:A:77:VAL:HG21	3:A:179:LEU:HD12	1.77	0.67
3:A:86:HIS:CE1	3:A:87:PRO:HD2	2.29	0.67
2:H:813:DA:H4'	2:H:814:DA:C5'	2.20	0.67
2:H:823:DC:H2''	2:H:824:DC:C5	2.30	0.67
4:F:84:ILE:HG22	4:F:85:CYS:H	1.59	0.67
4:B:217:PHE:CE1	4:B:228:ARG:HG3	2.29	0.67
3:E:88:HIS:CD2	3:E:120:CYS:HA	2.29	0.67
3:E:200:ASN:ND2	3:E:213:PHE:H	1.91	0.67
4:B:84:ILE:HD12	4:B:130:MET:HE3	1.75	0.67
3:E:35:ARG:HH21	3:E:187:ARG:HH12	1.43	0.67
3:A:223:ASP:OD2	3:A:274:ARG:HG3	1.95	0.66
4:B:88:VAL:HG11	4:B:218:LEU:HG	1.77	0.66
4:F:93:VAL:HG22	4:F:216:ALA:HB2	1.77	0.66
3:A:34:PHE:CD1	3:A:185:ASP:HA	2.31	0.66
4:F:107:HIS:HA	4:F:205:MET:HE1	1.77	0.66
4:F:41:TYR:CD2	4:F:229:LEU:HG	2.31	0.66
3:E:124:ARG:HB3	3:E:124:ARG:HH11	1.61	0.66
3:E:245:HIS:CD2	4:F:269:LEU:HB3	2.31	0.66
3:A:141:PHE:CD1	3:E:234:GLU:HG3	2.31	0.66
4:B:40:PRO:HD3	4:B:86:ASN:HB2	1.77	0.66
4:B:74:LYS:HE3	4:B:75:ASN:HB2	1.77	0.66
4:B:173:LEU:O	4:B:175:TYR:HD1	1.78	0.66
4:B:333:ARG:HD2	4:B:336:ASP:OD2	1.96	0.66
4:F:54:ARG:HG3	4:F:241:LYS:HB2	1.77	0.66
4:F:106:LEU:HD21	4:F:155:MET:CG	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:114:LYS:HD3	4:F:114:LYS:N	2.11	0.66
4:F:84:ILE:HG22	4:F:85:CYS:N	2.11	0.66
4:F:114:LYS:HG2	4:F:115:HIS:H	1.61	0.66
4:F:219:PRO:HA	4:F:224:SER:O	1.96	0.66
4:F:77:LYS:HE2	4:F:77:LYS:N	2.10	0.65
4:B:164:ASN:O	4:B:176:LEU:HD21	1.96	0.65
3:E:60:THR:HA	3:E:112:SER:HA	1.77	0.65
4:B:50:GLN:HG3	4:B:236:ALA:O	1.97	0.65
3:A:58:HIS:CG	3:A:114:GLN:HG3	2.32	0.65
3:E:33:ARG:HH11	3:E:33:ARG:HB2	1.61	0.65
3:E:200:ASN:ND2	3:E:201:ARG:H	1.95	0.65
4:F:159:CYS:SG	4:F:194:ILE:HD11	2.36	0.65
3:A:86:HIS:CD2	3:A:157:VAL:HG12	2.32	0.65
3:A:81:PRO:HG2	3:E:273:ARG:CZ	2.27	0.65
4:B:97:LEU:HG	4:B:111:LEU:HD13	1.78	0.65
4:B:40:PRO:CB	4:B:86:ASN:HB2	2.27	0.65
4:B:304:HIS:HB3	4:B:308:ALA:HB3	1.78	0.65
3:E:186:ASN:HA	3:E:192:ALA:HA	1.77	0.65
4:F:285:GLU:HA	4:F:290:GLY:HA2	1.79	0.65
3:E:25:GLU:HG2	3:E:60:THR:HG23	1.79	0.64
4:F:49:LYS:HA	4:F:49:LYS:HE2	1.77	0.64
3:E:199:VAL:HG22	3:E:284:MET:HE1	1.78	0.64
4:B:170:HIS:CD2	4:B:172:ASP:HB2	2.33	0.64
4:F:207:LEU:N	4:F:207:LEU:HD22	2.13	0.64
4:F:336:ASP:CG	4:F:338:GLU:HG2	2.17	0.64
3:E:41:ARG:HG2	3:E:41:ARG:HH21	1.62	0.64
3:E:91:VAL:HG21	3:E:119:GLN:HG3	1.80	0.64
3:E:203:SER:HB2	3:E:289:LEU:CD2	2.28	0.64
1:C:702:DG:H1'	1:C:703:DG:C5'	2.27	0.64
3:A:52:THR:HG22	3:A:53:ASP:N	2.12	0.64
4:F:190:GLU:O	4:F:193:ILE:HG12	1.97	0.64
4:F:199:VAL:HG23	4:F:200:GLN:NE2	2.13	0.64
3:E:21:VAL:O	3:E:22:GLU:HB2	1.98	0.64
3:A:20:TYR:H	3:A:175:LEU:CD2	2.11	0.63
3:A:81:PRO:HG2	3:E:273:ARG:NH2	2.13	0.63
3:E:78:THR:HG22	3:E:79:LYS:N	2.13	0.63
4:B:60:GLU:HB3	4:B:64:HIS:CE1	2.33	0.63
4:F:98:VAL:HG22	4:F:211:ARG:O	1.98	0.63
4:B:40:PRO:HB3	4:B:86:ASN:N	2.13	0.63
3:E:229:THR:OG1	3:E:269:SER:HB3	1.98	0.63
4:B:55:PHE:CE2	4:B:239:ASP:HB2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:41:TYR:CE2	4:B:85:CYS:HB2	2.33	0.63
3:E:67:THR:HG22	3:E:109:SER:HB3	1.81	0.63
4:F:88:VAL:CG1	4:F:218:LEU:HD22	2.26	0.63
4:F:218:LEU:HD21	4:F:229:LEU:HD21	1.79	0.63
1:G:809:DT:H2''	1:G:810:DC:H5'	1.80	0.63
3:A:33:ARG:HD2	3:A:187:ARG:HG3	1.79	0.63
4:B:303:VAL:HG13	4:B:309:ILE:HG13	1.80	0.63
3:E:165:VAL:CG2	3:E:173:LEU:HB3	2.27	0.63
3:A:184:PHE:HB3	3:A:191:THR:HG22	1.80	0.63
3:E:104:LEU:H	3:E:104:LEU:CD2	2.12	0.63
4:B:109:HIS:HE1	4:B:207:LEU:O	1.82	0.63
4:F:125:ALA:HA	4:F:132:VAL:HG21	1.81	0.62
4:B:250:ILE:CG1	4:B:331:LEU:HD22	2.28	0.62
1:G:808:DT:H2'	3:E:36:TYR:CE2	2.34	0.62
3:A:174:LEU:H	3:A:174:LEU:CD1	2.10	0.62
4:F:50:GLN:HG3	4:F:236:ALA:O	1.99	0.62
3:A:88:HIS:CD2	3:A:120:CYS:HA	2.34	0.62
3:E:201:ARG:HB2	3:E:201:ARG:NH2	2.11	0.62
4:F:92:LYS:NZ	4:F:217:PHE:HB2	2.14	0.62
4:F:156:THR:O	4:F:159:CYS:HB2	1.99	0.62
4:F:166:GLY:HA3	4:F:174:ALA:H	1.65	0.62
3:A:36:TYR:H	3:A:39:GLU:CB	2.12	0.62
3:E:24:ILE:HG21	3:E:62:LYS:HE2	1.80	0.62
3:E:278:ARG:NH2	3:E:278:ARG:HB3	2.14	0.62
4:F:304:HIS:HB3	4:F:308:ALA:HB3	1.82	0.62
4:B:109:HIS:CD2	4:B:141:HIS:HA	2.35	0.62
3:E:24:ILE:CD1	3:E:62:LYS:HB2	2.28	0.62
4:F:97:LEU:HB3	4:F:210:VAL:HG21	1.82	0.62
3:A:64:ASN:HD22	3:A:65:GLY:H	1.46	0.62
3:A:81:PRO:HB2	3:A:82:PRO:CD	2.30	0.62
3:E:144:PRO:O	3:E:147:GLU:N	2.31	0.62
4:B:41:TYR:O	4:B:84:ILE:HA	1.99	0.62
4:B:94:ILE:HD12	4:B:94:ILE:C	2.20	0.62
4:B:207:LEU:HD22	4:B:207:LEU:N	2.14	0.62
3:E:88:HIS:NE2	3:E:120:CYS:HA	2.14	0.62
3:A:90:LEU:HD12	3:A:117:GLY:O	1.99	0.61
4:B:186:LEU:HD12	4:B:187:THR:O	2.00	0.61
4:F:111:LEU:HD12	4:F:111:LEU:O	2.00	0.61
4:F:179:GLU:CG	4:F:184:ARG:HG3	2.29	0.61
1:C:702:DG:H2''	1:C:703:DG:OP2	1.99	0.61
3:E:24:ILE:HG21	3:E:62:LYS:CE	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:54:ARG:HA	4:F:239:ASP:OD2	1.98	0.61
4:B:109:HIS:CD2	4:B:142:VAL:HG12	2.35	0.61
3:A:19:ALA:N	3:A:175:LEU:HB2	2.15	0.61
4:F:109:HIS:HB3	4:F:140:LEU:O	1.99	0.61
4:B:88:VAL:HG21	4:B:218:LEU:CD2	2.31	0.61
3:E:24:ILE:HD13	3:E:62:LYS:HB2	1.82	0.61
3:E:34:PHE:CZ	3:E:185:ASP:HB2	2.36	0.61
3:E:212:ILE:HD11	3:E:286:PHE:CE2	2.36	0.61
4:F:82:VAL:HG22	4:F:83:LYS:N	2.16	0.61
2:H:815:DG:H2''	2:H:816:DG:O5'	2.00	0.61
4:F:76:LYS:HD3	4:F:77:LYS:HE2	1.82	0.61
4:F:165:PRO:C	4:F:174:ALA:HA	2.19	0.61
4:B:143:THR:HG22	4:B:146:LYS:HB2	1.82	0.60
4:B:166:GLY:H	4:B:176:LEU:HD21	1.65	0.60
4:F:55:PHE:HZ	4:F:237:ILE:HG22	1.67	0.60
3:A:77:VAL:CG2	3:A:179:LEU:HD12	2.31	0.60
3:E:20:TYR:O	3:E:63:ILE:HG23	2.01	0.60
3:E:84:ARG:HG3	3:E:152:TYR:OH	2.01	0.60
4:F:55:PHE:HB2	4:F:239:ASP:OD1	2.01	0.60
4:F:163:TYR:O	4:F:164:ASN:HB3	2.01	0.60
4:F:274:GLN:CD	4:F:274:GLN:H	2.05	0.60
3:E:143:VAL:HG12	3:E:147:GLU:HB3	1.84	0.60
1:G:806:DC:H2''	1:G:807:DT:H5'	1.83	0.60
2:H:817:DA:H3'	4:F:306:GLN:NE2	2.16	0.60
3:A:122:LYS:H	3:A:122:LYS:HD2	1.66	0.60
3:E:215:LEU:HD13	4:F:304:HIS:CB	2.31	0.60
4:F:116:CYS:HA	4:F:121:CYS:HA	1.83	0.60
3:A:273:ARG:HB2	3:A:280:LEU:HD13	1.82	0.60
3:E:23:ILE:HD13	3:E:180:SER:OG	2.02	0.60
4:F:115:HIS:ND1	4:F:121:CYS:SG	2.73	0.60
4:B:157:GLU:O	4:B:158:ALA:HB3	2.02	0.60
3:E:96:ARG:O	3:E:97:ASP:HB2	2.02	0.60
3:E:121:VAL:HG23	3:E:122:LYS:O	2.02	0.60
3:E:287:GLN:HE21	3:E:289:LEU:HD11	1.66	0.60
1:G:808:DT:H72	3:E:187:ARG:NE	2.17	0.59
3:E:33:ARG:HH12	3:E:187:ARG:HH11	1.50	0.59
1:C:706:DC:C6	1:C:707:DT:H72	2.37	0.59
2:H:821:DT:H1'	2:H:822:DC:H5'	1.84	0.59
2:H:821:DT:H2''	2:H:822:DC:O5'	2.02	0.59
4:B:39:GLY:N	4:B:40:PRO:HD2	2.17	0.59
3:E:93:LYS:HD2	3:E:93:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:278:ARG:HB3	3:E:278:ARG:HH21	1.66	0.59
3:A:167:ASP:HA	3:A:173:LEU:HD12	1.83	0.59
3:E:41:ARG:HG2	3:E:42:SER:H	1.66	0.59
3:E:72:VAL:CG2	3:E:104:LEU:HB3	2.32	0.59
4:F:97:LEU:HD11	4:F:111:LEU:N	2.15	0.59
3:A:238:SER:HB3	3:A:253:ARG:HD2	1.84	0.59
3:A:200:ASN:ND2	3:A:200:ASN:H	2.01	0.59
4:B:177:GLN:HG2	4:B:178:ALA:H	1.67	0.59
3:A:26:GLN:HG2	3:A:49:GLU:CD	2.23	0.59
3:E:56:LYS:HD3	3:E:56:LYS:N	2.16	0.59
4:F:77:LYS:H	4:F:77:LYS:CE	2.13	0.59
3:A:29:GLN:HG3	3:A:30:ARG:N	2.16	0.59
4:B:187:THR:HG22	4:B:189:ARG:H	1.67	0.59
3:E:25:GLU:CG	3:E:60:THR:HG23	2.32	0.59
4:B:244:ASN:C	4:B:244:ASN:ND2	2.55	0.59
3:A:186:ASN:O	3:A:192:ALA:HB2	2.02	0.59
4:B:82:VAL:CG2	4:B:134:PHE:HE2	2.16	0.59
4:F:55:PHE:CZ	4:F:237:ILE:HG22	2.37	0.59
4:B:84:ILE:HD12	4:B:130:MET:CE	2.32	0.58
4:B:329:VAL:HG23	4:B:345:PHE:HB2	1.85	0.58
3:E:21:VAL:HG12	3:E:61:ILE:HD11	1.85	0.58
3:E:78:THR:HG21	3:E:84:ARG:NH1	2.17	0.58
3:E:199:VAL:HG22	3:E:284:MET:CE	2.32	0.58
3:A:274:ARG:HE	3:A:277:ASP:HB2	1.68	0.58
4:F:143:THR:HG22	4:F:144:LYS:N	2.18	0.58
4:F:195:ARG:O	4:F:199:VAL:HG13	2.03	0.58
3:A:141:PHE:HD1	3:E:234:GLU:HG3	1.68	0.58
4:B:300:PRO:O	4:B:303:VAL:HG23	2.03	0.58
3:E:129:ALA:O	3:E:133:ARG:NE	2.36	0.58
3:A:188:ALA:HB3	3:A:191:THR:HB	1.85	0.58
3:A:141:PHE:CZ	3:A:179:LEU:HD21	2.39	0.58
4:B:116:CYS:HA	4:B:121:CYS:HA	1.85	0.58
4:B:219:PRO:HA	4:B:224:SER:O	2.02	0.58
1:G:808:DT:O2	2:H:819:DA:H2	1.86	0.58
4:B:158:ALA:HA	4:B:163:TYR:HB2	1.84	0.58
3:E:85:PRO:HB2	3:E:133:ARG:HG2	1.86	0.58
4:F:106:LEU:HD11	4:F:151:LEU:HD23	1.85	0.58
4:F:236:ALA:C	4:F:237:ILE:HD12	2.23	0.58
3:A:28:LYS:NZ	3:A:47:PRO:HB2	2.19	0.58
3:A:36:TYR:H	3:A:39:GLU:HB2	1.68	0.58
3:E:41:ARG:HG2	3:E:41:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:96:GLN:HG2	4:F:97:LEU:N	2.17	0.58
4:F:143:THR:HG21	4:F:145:LYS:NZ	2.19	0.58
1:G:806:DC:H5'	3:E:189:PRO:HG3	1.85	0.58
3:A:200:ASN:ND2	3:A:200:ASN:N	2.51	0.58
3:E:23:ILE:HA	3:E:61:ILE:HD12	1.86	0.58
3:E:72:VAL:HG11	3:E:113:PHE:HZ	1.69	0.58
4:F:329:VAL:HG23	4:F:345:PHE:HB2	1.86	0.58
3:A:138:ASN:O	3:A:139:ASN:HB2	2.04	0.57
4:F:327:VAL:HG22	4:F:328:PHE:H	1.69	0.57
3:A:70:GLY:HA2	3:A:166:ARG:HH12	1.68	0.57
4:B:244:ASN:C	4:B:244:ASN:HD22	2.06	0.57
3:A:90:LEU:HG	3:A:116:LEU:HD22	1.85	0.57
4:B:175:TYR:HA	4:B:177:GLN:OE1	2.04	0.57
3:E:203:SER:HB2	3:E:289:LEU:HD21	1.86	0.57
3:A:84:ARG:HD2	3:A:147:GLU:O	2.04	0.57
3:A:229:THR:HG23	3:A:271:GLN:HE21	1.70	0.57
3:E:66:TYR:CZ	3:E:165:VAL:HB	2.40	0.57
3:E:195:LYS:HZ2	3:E:217:ASP:CG	2.07	0.57
3:E:262:LEU:HD12	3:E:263:GLN:H	1.70	0.57
4:F:162:GLY:HA3	4:F:176:LEU:O	2.04	0.57
3:A:257:TYR:CG	3:A:258:ALA:N	2.71	0.57
2:H:819:DA:C8	2:H:820:DG:N7	2.73	0.57
3:E:195:LYS:NZ	3:E:217:ASP:OD1	2.38	0.57
3:E:223:ASP:OD1	3:E:274:ARG:HG3	2.05	0.57
4:B:213:MET:SD	4:B:231:PRO:HB2	2.45	0.57
4:B:164:ASN:O	4:B:176:LEU:HD11	2.05	0.57
4:F:95:VAL:CG1	4:F:134:PHE:HE1	2.18	0.57
4:F:98:VAL:HG13	4:F:213:MET:HB2	1.87	0.57
3:A:246:ARG:HG3	3:A:246:ARG:NH1	2.20	0.56
4:F:92:LYS:HZ1	4:F:217:PHE:HB2	1.68	0.56
3:A:90:LEU:HA	3:A:117:GLY:O	2.04	0.56
2:D:714:DA:H2''	2:D:715:DG:OP2	2.04	0.56
1:G:810:DC:OP1	4:F:144:LYS:HD3	2.04	0.56
3:A:23:ILE:HD11	3:A:161:PHE:HE1	1.70	0.56
3:A:25:GLU:OE2	3:A:49:GLU:HB3	2.05	0.56
3:A:285:GLU:H	3:A:285:GLU:CD	2.07	0.56
4:B:116:CYS:O	4:B:117:GLU:HG3	2.04	0.56
3:E:130:ILE:HD11	3:E:149:ARG:HE	1.71	0.56
4:F:102:LYS:HD2	4:F:103:ASN:N	2.20	0.56
4:F:152:GLU:OE1	4:F:195:ARG:HD2	2.05	0.56
3:A:233:TRP:O	3:A:234:GLU:HG3	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:277:ASP:O	3:A:278:ARG:HB2	2.04	0.56
4:B:87:TYR:CE2	4:B:89:GLY:HA2	2.40	0.56
3:E:186:ASN:O	3:E:192:ALA:HB2	2.06	0.56
3:A:179:LEU:H	3:A:179:LEU:CD2	2.19	0.56
3:E:41:ARG:O	3:E:43:ALA:N	2.32	0.56
4:F:108:ALA:H	4:F:205:MET:HE3	1.71	0.56
4:F:148:PHE:HE2	4:F:199:VAL:HG12	1.71	0.56
4:B:112:VAL:O	4:B:137:LEU:O	2.23	0.56
4:F:68:PRO:HB2	4:F:72:SER:OG	2.04	0.56
4:F:184:ARG:O	4:F:185:GLN:HG2	2.05	0.56
3:A:167:ASP:HA	3:A:173:LEU:CD1	2.36	0.56
4:B:57:TYR:HB2	4:B:59:CYS:SG	2.45	0.56
3:E:215:LEU:HD13	4:F:304:HIS:HB2	1.87	0.56
3:A:196:ILE:HG23	3:A:272:LEU:HD22	1.86	0.56
3:A:274:ARG:NE	3:A:277:ASP:HB2	2.20	0.56
4:B:151:LEU:HD12	4:B:151:LEU:O	2.05	0.56
3:E:34:PHE:CE2	3:E:185:ASP:HB2	2.41	0.56
4:F:43:GLN:C	4:F:82:VAL:HG23	2.26	0.56
4:F:44:ILE:HG12	4:F:44:ILE:O	2.05	0.56
4:F:76:LYS:HD3	4:F:77:LYS:N	2.21	0.56
3:A:80:ASP:CB	3:A:81:PRO:HD2	2.28	0.56
4:F:55:PHE:N	4:F:239:ASP:OD2	2.36	0.56
4:F:72:SER:HA	4:F:76:LYS:O	2.06	0.56
3:A:58:HIS:ND1	3:A:114:GLN:HG3	2.20	0.56
3:E:76:LEU:O	3:E:86:HIS:N	2.38	0.56
3:E:131:SER:O	3:E:134:ILE:HB	2.06	0.56
4:F:55:PHE:H	4:F:239:ASP:CG	2.09	0.56
3:A:73:ARG:HA	3:A:100:TYR:O	2.06	0.55
3:A:93:LYS:HB3	3:A:115:ASN:CG	2.25	0.55
4:B:40:PRO:CD	4:B:86:ASN:HB2	2.36	0.55
4:B:47:GLN:HB3	4:B:48:PRO:CD	2.33	0.55
4:B:83:LYS:HD2	4:B:131:VAL:HB	1.86	0.55
4:B:189:ARG:HG3	4:B:190:GLU:N	2.21	0.55
4:F:148:PHE:CE2	4:F:199:VAL:HG12	2.41	0.55
3:A:122:LYS:HD2	3:A:122:LYS:N	2.21	0.55
4:B:88:VAL:HG12	4:B:88:VAL:O	2.07	0.55
4:B:299:SER:CB	4:B:300:PRO:HD2	2.36	0.55
4:F:94:ILE:HD12	4:F:94:ILE:N	2.21	0.55
4:F:115:HIS:NE2	4:F:123:VAL:HG12	2.22	0.55
3:A:272:LEU:N	3:A:281:SER:OG	2.37	0.55
4:F:55:PHE:CD1	4:F:239:ASP:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:108:ALA:HB3	4:B:142:VAL:HG11	1.88	0.55
3:E:72:VAL:HG12	3:E:72:VAL:O	2.06	0.55
3:E:74:ILE:HD11	3:E:161:PHE:CD1	2.41	0.55
3:E:76:LEU:HD13	3:E:88:HIS:O	2.06	0.55
4:F:164:ASN:HD21	4:F:168:LEU:CB	2.16	0.55
4:F:253:MET:HA	4:F:267:TYR:O	2.06	0.55
3:A:189:PRO:HG3	3:A:218:LYS:CE	2.29	0.55
3:E:33:ARG:HB2	3:E:33:ARG:NH1	2.21	0.55
3:E:200:ASN:HB3	4:F:267:TYR:CE1	2.41	0.55
4:F:207:LEU:HD22	4:F:207:LEU:H	1.72	0.55
3:A:140:PRO:HB2	3:A:160:CYS:SG	2.47	0.55
4:B:147:VAL:HG11	4:B:207:LEU:HD11	1.89	0.55
3:E:224:ILE:HD12	3:E:273:ARG:O	2.07	0.55
3:A:219:VAL:O	3:A:247:GLN:HB2	2.06	0.55
4:B:321:ILE:HG13	4:B:323:LYS:O	2.07	0.55
1:G:805:DA:OP1	3:E:221:LYS:HE3	2.06	0.55
4:F:117:GLU:HA	4:F:117:GLU:OE1	2.06	0.55
4:F:185:GLN:O	4:F:187:THR:N	2.40	0.55
4:B:303:VAL:HG13	4:B:309:ILE:HG12	1.88	0.54
4:F:147:VAL:HG13	4:F:148:PHE:N	2.22	0.54
3:A:19:ALA:O	3:A:20:TYR:HB3	2.06	0.54
3:E:23:ILE:HG12	3:E:61:ILE:CD1	2.37	0.54
3:E:79:LYS:NZ	3:E:79:LYS:HB3	2.22	0.54
3:E:33:ARG:HH12	3:E:187:ARG:NH1	2.06	0.54
3:E:222:GLU:CD	3:E:222:GLU:H	2.11	0.54
4:F:45:LEU:HD22	4:F:83:LYS:HD3	1.89	0.54
4:F:241:LYS:HB3	4:F:241:LYS:NZ	2.21	0.54
3:A:60:THR:HG22	3:A:112:SER:CB	2.37	0.54
4:B:56:ARG:O	4:B:140:LEU:HD12	2.07	0.54
3:E:186:ASN:C	3:E:188:ALA:N	2.59	0.54
4:B:40:PRO:HG3	4:B:86:ASN:O	2.07	0.54
4:B:74:LYS:C	4:B:76:LYS:H	2.10	0.54
4:B:166:GLY:H	4:B:176:LEU:CD2	2.20	0.54
4:B:173:LEU:CD2	4:B:176:LEU:HB3	2.38	0.54
4:B:177:GLN:HB3	4:B:228:ARG:NH1	2.23	0.54
3:E:257:TYR:HD1	3:E:259:ASP:H	1.54	0.54
4:F:102:LYS:HD2	4:F:103:ASN:HB2	1.89	0.54
4:F:112:VAL:HG23	4:F:140:LEU:HB2	1.89	0.54
4:B:192:GLU:OE2	4:B:195:ARG:HD2	2.08	0.54
3:E:70:GLY:HA3	3:E:104:LEU:HD21	1.89	0.54
4:F:43:GLN:H	4:F:82:VAL:HG23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:143:THR:CG2	4:F:145:LYS:HG2	2.37	0.54
4:F:237:ILE:HD12	4:F:237:ILE:N	2.23	0.54
3:A:248:VAL:HG22	4:B:304:HIS:CE1	2.43	0.54
4:B:165:PRO:O	4:B:166:GLY:C	2.45	0.54
4:B:82:VAL:HG21	4:B:134:PHE:HE2	1.73	0.54
4:B:163:TYR:O	4:B:176:LEU:HD11	2.07	0.54
3:E:79:LYS:HB3	3:E:79:LYS:HZ2	1.73	0.54
3:E:140:PRO:HA	3:E:162:GLN:NE2	2.23	0.54
4:F:56:ARG:HH22	4:F:60:GLU:HG3	1.73	0.54
4:F:95:VAL:HG11	4:F:134:PHE:HE1	1.72	0.54
3:A:72:VAL:O	3:A:101:GLU:HA	2.08	0.54
3:A:74:ILE:HG13	3:A:100:TYR:CD1	2.43	0.54
3:A:140:PRO:HB3	3:A:162:GLN:HG2	1.90	0.54
4:B:94:ILE:HG21	4:B:163:TYR:CE2	2.42	0.54
4:B:129:ASP:OD1	4:B:131:VAL:HG12	2.08	0.54
4:B:191:LYS:O	4:B:195:ARG:HG2	2.07	0.53
3:E:229:THR:CG2	3:E:271:GLN:NE2	2.71	0.53
4:F:79:TYR:HD2	4:F:134:PHE:C	2.11	0.53
4:F:286:GLU:H	4:F:290:GLY:CA	2.19	0.53
3:A:200:ASN:HD22	3:A:201:ARG:N	2.05	0.53
4:B:94:ILE:HG21	4:B:163:TYR:CZ	2.44	0.53
3:E:33:ARG:HH12	3:E:187:ARG:HD2	1.72	0.53
4:F:292:TRP:HZ2	4:F:315:LYS:O	1.91	0.53
3:A:26:GLN:HG2	3:A:49:GLU:OE2	2.07	0.53
3:A:77:VAL:HG21	3:A:179:LEU:CD1	2.37	0.53
3:E:72:VAL:HG23	3:E:104:LEU:HB3	1.89	0.53
3:E:143:VAL:CG1	3:E:147:GLU:HB3	2.39	0.53
3:A:41:ARG:C	3:A:43:ALA:N	2.62	0.53
3:A:167:ASP:CB	3:A:168:PRO:HD2	2.38	0.53
4:B:226:THR:O	4:B:228:ARG:HD3	2.08	0.53
3:E:46:ILE:HD11	3:E:118:ILE:CG1	2.39	0.53
3:E:77:VAL:HG21	3:E:179:LEU:HD22	1.89	0.53
4:F:217:PHE:HB3	4:F:225:PHE:HB3	1.89	0.53
1:G:809:DT:H72	3:E:39:GLU:CG	2.39	0.53
3:E:130:ILE:HA	3:E:133:ARG:CD	2.35	0.53
3:E:212:ILE:HD11	3:E:286:PHE:HE2	1.73	0.53
4:F:67:LEU:HD22	4:F:138:GLY:H	1.72	0.53
4:F:147:VAL:HG13	4:F:148:PHE:H	1.74	0.53
4:F:318:ASP:HB3	4:F:320:ASN:OD1	2.09	0.53
4:F:56:ARG:NH2	4:F:60:GLU:HG3	2.24	0.53
4:F:235:ASP:O	4:F:236:ALA:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:32:MET:CE	3:E:46:ILE:HG12	2.39	0.53
4:F:143:THR:HG22	4:F:144:LYS:H	1.73	0.53
4:F:271:ASP:O	4:F:273:VAL:HG13	2.09	0.53
3:A:41:ARG:C	3:A:43:ALA:H	2.11	0.53
3:A:274:ARG:HE	3:A:277:ASP:CB	2.21	0.53
4:F:79:TYR:HB2	4:F:134:PHE:O	2.09	0.53
4:F:212:LEU:HB2	4:F:234:SER:HG	1.74	0.53
3:A:219:VAL:O	3:A:247:GLN:CB	2.57	0.52
4:F:222:THR:HG22	4:F:222:THR:O	2.08	0.52
1:C:710:DC:H2"	1:C:711:DC:OP2	2.09	0.52
3:A:30:ARG:NH1	3:A:30:ARG:HB2	2.25	0.52
3:A:167:ASP:OD2	3:A:173:LEU:HB2	2.09	0.52
3:A:266:VAL:HG13	3:A:288:TYR:HB2	1.91	0.52
3:A:285:GLU:OE2	3:A:285:GLU:N	2.42	0.52
3:E:19:ALA:CA	3:E:175:LEU:HD22	2.37	0.52
4:F:220:ASP:OD1	4:F:224:SER:O	2.27	0.52
4:F:282:PHE:O	4:F:293:GLU:HA	2.08	0.52
3:A:72:VAL:HG13	3:A:100:TYR:HE1	1.74	0.52
4:B:43:GLN:N	4:B:83:LYS:O	2.41	0.52
4:B:282:PHE:HA	4:B:328:PHE:O	2.08	0.52
4:F:59:CYS:O	4:F:60:GLU:OE2	2.28	0.52
4:F:173:LEU:O	4:F:174:ALA:HB3	2.09	0.52
4:F:212:LEU:HD12	4:F:234:SER:OG	2.09	0.52
3:A:225:GLU:OE1	3:A:273:ARG:NH1	2.38	0.52
4:B:186:LEU:HD13	4:B:190:GLU:HB2	1.90	0.52
4:B:272:LYS:HA	4:B:306:GLN:O	2.09	0.52
3:A:132:GLN:O	3:A:136:THR:HG22	2.09	0.52
4:B:107:HIS:CD2	4:B:109:HIS:H	2.23	0.52
3:E:21:VAL:HG12	3:E:22:GLU:N	2.18	0.52
4:F:139:ILE:N	4:F:139:ILE:HD12	2.24	0.52
3:A:219:VAL:HG21	3:A:224:ILE:HD12	1.91	0.52
4:B:185:GLN:O	4:B:187:THR:N	2.42	0.52
3:E:31:GLY:HA2	3:E:186:ASN:ND2	2.22	0.52
4:F:268:LEU:HD23	4:F:268:LEU:C	2.30	0.52
3:A:243:ASP:HB3	3:A:251:VAL:HG13	1.91	0.52
4:B:187:THR:HG22	4:B:188:ASP:N	2.25	0.52
3:E:130:ILE:HD11	3:E:149:ARG:HH21	1.75	0.52
4:F:111:LEU:O	4:F:116:CYS:SG	2.68	0.52
4:F:176:LEU:HD23	4:F:176:LEU:N	2.25	0.52
4:F:329:VAL:CG2	4:F:345:PHE:HB2	2.40	0.52
4:B:281:ARG:NH2	4:B:293:GLU:OE2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:114:GLN:O	3:E:115:ASN:CB	2.58	0.52
3:E:122:LYS:HE3	3:E:125:ASP:OD1	2.10	0.52
3:E:167:ASP:OD1	3:E:171:ARG:HB2	2.10	0.52
4:F:42:LEU:H	4:F:42:LEU:CD2	2.22	0.52
4:F:109:HIS:HE1	4:F:207:LEU:O	1.93	0.52
3:A:197:CYS:O	3:A:198:ARG:HB3	2.08	0.52
3:E:37:LYS:HD3	3:E:119:GLN:NE2	2.21	0.52
4:F:161:ARG:HB3	4:F:163:TYR:CD2	2.45	0.52
4:B:209:VAL:HG23	4:B:237:ILE:O	2.10	0.51
3:E:272:LEU:N	3:E:281:SER:OG	2.40	0.51
3:A:70:GLY:HA3	3:A:104:LEU:HD21	1.92	0.51
3:A:72:VAL:HG13	3:A:100:TYR:CE1	2.46	0.51
3:A:118:ILE:HG22	3:A:118:ILE:O	2.10	0.51
3:A:166:ARG:O	3:A:173:LEU:HB3	2.10	0.51
3:E:114:GLN:O	3:E:115:ASN:HB3	2.09	0.51
3:E:196:ILE:HD11	3:E:271:GLN:HA	1.92	0.51
4:F:79:TYR:N	4:F:79:TYR:CD1	2.78	0.51
4:F:282:PHE:HA	4:F:328:PHE:O	2.10	0.51
4:B:350:GLU:O	4:B:350:GLU:HG2	2.10	0.51
3:E:215:LEU:HB3	4:F:304:HIS:CE1	2.45	0.51
1:C:701:DT:H2''	1:C:702:DG:O5'	2.11	0.51
2:H:814:DA:H2''	2:H:815:DG:O5'	2.10	0.51
4:B:253:MET:HA	4:B:267:TYR:O	2.10	0.51
3:E:241:GLN:O	3:E:244:VAL:HG23	2.09	0.51
4:F:99:THR:HG22	4:F:105:HIS:H	1.74	0.51
4:F:179:GLU:CD	4:F:184:ARG:HG3	2.30	0.51
3:A:257:TYR:HD2	3:A:259:ASP:H	1.51	0.51
3:E:92:GLY:H	3:E:95:CYS:CB	2.23	0.51
3:E:104:LEU:HD23	3:E:104:LEU:N	2.22	0.51
3:E:213:PHE:CE1	4:F:254:ASP:HB3	2.45	0.51
3:A:133:ARG:HD2	3:A:133:ARG:N	2.25	0.51
4:B:110:SER:HB2	4:B:154:ARG:HH21	1.75	0.51
4:B:336:ASP:OD2	4:B:336:ASP:N	2.43	0.51
3:E:21:VAL:O	3:E:22:GLU:CB	2.59	0.51
3:E:24:ILE:HD13	3:E:62:LYS:HE2	1.92	0.51
3:E:89:GLU:HB2	3:E:91:VAL:HG13	1.92	0.51
1:G:810:DC:H41	3:E:39:GLU:CG	2.23	0.51
3:A:219:VAL:CB	3:A:224:ILE:HD12	2.40	0.51
4:B:42:LEU:HD22	4:B:82:VAL:HG12	1.90	0.51
4:B:173:LEU:HD21	4:B:176:LEU:HB3	1.92	0.51
3:E:77:VAL:HG21	3:E:179:LEU:HD21	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:138:ASN:O	3:E:139:ASN:HB2	2.11	0.51
4:F:210:VAL:HG22	4:F:211:ARG:H	1.74	0.51
1:G:801:DT:H3'	1:G:802:DG:H5'	1.92	0.51
3:A:182:PRO:HB2	3:A:184:PHE:CE2	2.46	0.51
4:B:79:TYR:HB3	4:B:134:PHE:O	2.11	0.51
4:F:152:GLU:OE2	4:F:195:ARG:HA	2.09	0.51
4:F:263:GLY:N	4:F:313:THR:O	2.34	0.51
3:E:228:PHE:HZ	3:E:252:PHE:HE1	1.58	0.51
4:F:50:GLN:HA	4:F:237:ILE:HG13	1.93	0.51
4:F:54:ARG:HB2	4:F:240:SER:OG	2.11	0.51
4:F:92:LYS:HZ1	4:F:217:PHE:CB	2.23	0.51
3:A:94:ASP:O	3:A:96:ARG:HG2	2.10	0.51
3:A:238:SER:HB3	3:A:253:ARG:CG	2.41	0.51
3:E:21:VAL:CG1	3:E:61:ILE:HD11	2.40	0.50
4:F:43:GLN:H	4:F:82:VAL:CG2	2.24	0.50
3:A:251:VAL:HG13	3:A:251:VAL:O	2.10	0.50
3:E:25:GLU:CD	3:E:60:THR:HG23	2.31	0.50
3:E:140:PRO:O	3:E:177:PRO:HG2	2.11	0.50
3:A:75:SER:OG	3:A:162:GLN:NE2	2.44	0.50
3:A:214:LEU:CD2	3:A:216:CYS:HB3	2.41	0.50
4:B:129:ASP:OD1	4:B:131:VAL:CG1	2.60	0.50
4:B:163:TYR:C	4:B:176:LEU:HD11	2.32	0.50
4:F:157:GLU:OE2	4:F:158:ALA:N	2.43	0.50
1:C:702:DG:H1'	1:C:703:DG:O5'	2.12	0.50
3:E:30:ARG:HG3	3:E:184:PHE:CD1	2.47	0.50
4:F:107:HIS:HA	4:F:205:MET:CE	2.41	0.50
4:F:161:ARG:HB3	4:F:163:TYR:CE2	2.46	0.50
3:A:267:ARG:HB3	3:A:287:GLN:HG2	1.93	0.50
3:E:90:LEU:N	3:E:98:GLY:O	2.39	0.50
3:A:139:ASN:O	3:A:141:PHE:N	2.44	0.50
3:A:196:ILE:HD12	3:A:196:ILE:N	2.18	0.50
4:B:177:GLN:NE2	4:B:177:GLN:N	2.60	0.50
1:G:806:DC:C2'	1:G:807:DT:H5''	2.41	0.50
3:A:74:ILE:HB	3:A:100:TYR:HB3	1.94	0.50
3:A:246:ARG:HG2	4:B:307:PHE:CD2	2.46	0.50
4:B:46:GLU:OE1	4:B:78:SER:HB2	2.12	0.50
4:B:74:LYS:HG2	4:B:75:ASN:N	2.27	0.50
4:B:109:HIS:CE1	4:B:207:LEU:O	2.62	0.50
4:B:143:THR:O	4:B:147:VAL:HG13	2.12	0.50
4:F:164:ASN:HD21	4:F:168:LEU:CA	2.24	0.50
4:F:316:TYR:CE1	4:F:317:LYS:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:36:TYR:C	3:A:39:GLU:HB2	2.31	0.50
3:E:25:GLU:HB3	3:E:59:PRO:HA	1.94	0.50
4:F:319:VAL:HG12	4:F:319:VAL:O	2.11	0.50
3:A:52:THR:N	3:A:55:THR:O	2.45	0.50
3:A:228:PHE:CE1	3:A:270:MET:HG3	2.46	0.50
3:A:245:HIS:O	3:A:246:ARG:C	2.50	0.50
3:A:32:MET:HG2	3:A:33:ARG:H	1.77	0.49
4:B:94:ILE:HG22	4:B:122:THR:HG23	1.94	0.49
3:E:229:THR:HG23	3:E:271:GLN:NE2	2.26	0.49
3:A:51:SER:HA	3:A:56:LYS:O	2.12	0.49
3:A:52:THR:CG2	3:A:53:ASP:N	2.75	0.49
3:A:92:GLY:HA3	3:A:115:ASN:O	2.12	0.49
3:A:154:LEU:H	3:A:154:LEU:HD12	1.77	0.49
4:B:43:GLN:O	4:B:82:VAL:HA	2.13	0.49
4:B:324:PRO:HB2	4:B:346:LEU:HD11	1.93	0.49
3:E:86:HIS:CD2	3:E:87:PRO:HD2	2.47	0.49
3:E:100:TYR:OH	3:E:102:ALA:HB3	2.11	0.49
3:A:60:THR:HG22	3:A:112:SER:HB3	1.92	0.49
3:A:266:VAL:HG13	3:A:266:VAL:O	2.12	0.49
4:B:244:ASN:HB3	4:B:274:GLN:OE1	2.12	0.49
4:F:83:LYS:HB3	4:F:131:VAL:HG12	1.94	0.49
3:A:200:ASN:HD21	3:A:212:ILE:HG23	1.77	0.49
4:B:50:GLN:OE1	4:B:235:ASP:HB3	2.12	0.49
3:E:37:LYS:O	3:E:39:GLU:N	2.46	0.49
3:E:58:HIS:HB3	3:E:113:PHE:O	2.12	0.49
3:E:134:ILE:C	3:E:136:THR:H	2.16	0.49
1:C:702:DG:N7	4:B:64:HIS:HD2	2.09	0.49
3:A:251:VAL:HG11	4:B:252:ARG:HH12	1.77	0.49
3:A:36:TYR:N	3:A:39:GLU:HB2	2.26	0.49
3:A:56:LYS:CG	3:A:57:THR:H	2.19	0.49
3:A:143:VAL:HG22	3:E:234:GLU:O	2.12	0.49
4:B:73:GLU:O	4:B:75:ASN:N	2.45	0.49
3:E:130:ILE:HD11	3:E:149:ARG:NE	2.28	0.49
4:F:143:THR:HG21	4:F:145:LYS:HZ2	1.77	0.49
4:F:163:TYR:N	4:F:176:LEU:HD12	2.27	0.49
4:F:166:GLY:HA3	4:F:174:ALA:N	2.27	0.49
4:F:211:ARG:HG2	4:F:236:ALA:HA	1.94	0.49
3:A:96:ARG:C	3:A:98:GLY:N	2.65	0.49
4:B:72:SER:HB3	4:B:77:LYS:CE	2.43	0.49
4:F:67:LEU:CD2	4:F:67:LEU:N	2.75	0.49
4:F:95:VAL:HG11	4:F:134:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:109:HIS:CE1	4:F:207:LEU:O	2.66	0.49
3:A:64:ASN:ND2	3:A:65:GLY:N	2.59	0.49
3:A:130:ILE:O	3:A:133:ARG:HB2	2.13	0.49
4:B:197:ALA:O	4:B:201:GLN:HG3	2.13	0.49
4:B:232:VAL:HG22	4:B:232:VAL:O	2.12	0.49
4:F:271:ASP:O	4:F:272:LYS:C	2.52	0.49
3:A:215:LEU:HB3	4:B:304:HIS:CD2	2.48	0.49
4:F:83:LYS:CB	4:F:131:VAL:HG12	2.43	0.49
2:D:713:DA:H8	3:A:43:ALA:HA	1.78	0.48
3:A:22:GLU:O	3:A:22:GLU:HG2	2.13	0.48
3:E:99:TYR:HE2	3:E:101:GLU:HB2	1.78	0.48
4:F:157:GLU:O	4:F:159:CYS:N	2.40	0.48
3:A:219:VAL:HB	3:A:224:ILE:HD12	1.95	0.48
4:B:235:ASP:O	4:B:236:ALA:HB2	2.14	0.48
3:E:165:VAL:O	3:E:166:ARG:HG3	2.12	0.48
3:A:52:THR:HG22	3:A:53:ASP:H	1.79	0.48
3:E:167:ASP:C	3:E:169:ALA:H	2.17	0.48
3:E:174:LEU:HD23	3:E:174:LEU:N	2.28	0.48
3:A:104:LEU:O	3:A:105:CYS:C	2.51	0.48
2:D:718:DA:OP2	4:B:306:GLN:NE2	2.37	0.48
3:A:29:GLN:HG3	3:A:30:ARG:H	1.78	0.48
3:A:36:TYR:CA	3:A:39:GLU:HB2	2.44	0.48
3:A:56:LYS:H	3:A:56:LYS:CD	2.22	0.48
3:E:262:LEU:HD11	3:E:266:VAL:HG23	1.96	0.48
4:F:58:VAL:C	4:F:60:GLU:H	2.15	0.48
4:F:248:LEU:N	4:F:248:LEU:HD12	2.29	0.48
3:A:44:GLY:O	3:A:45:SER:HB2	2.14	0.48
4:B:55:PHE:CD2	4:B:239:ASP:HB2	2.49	0.48
4:B:271:ASP:O	4:B:272:LYS:C	2.50	0.48
3:E:35:ARG:HH21	3:E:187:ARG:NH1	2.10	0.48
3:E:82:PRO:O	3:E:84:ARG:N	2.47	0.48
4:F:317:LYS:HG3	4:F:318:ASP:H	1.77	0.48
3:A:200:ASN:ND2	3:A:213:PHE:H	2.11	0.48
4:B:175:TYR:HA	4:B:177:GLN:HE22	1.78	0.48
4:B:280:ILE:HD11	4:B:309:ILE:HG21	1.96	0.48
4:B:309:ILE:HG22	4:B:311:PHE:HD1	1.79	0.48
3:E:93:LYS:NZ	3:E:115:ASN:O	2.44	0.48
3:E:91:VAL:HG22	3:E:119:GLN:HB2	1.95	0.48
4:F:49:LYS:O	4:F:50:GLN:HB3	2.14	0.48
2:H:816:DG:H2''	2:H:817:DA:O5'	2.13	0.48
3:A:87:PRO:O	3:A:133:ARG:CZ	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:154:LEU:HD12	3:A:154:LEU:N	2.28	0.48
4:B:98:VAL:CG1	4:B:213:MET:HB2	2.44	0.48
4:B:132:VAL:HG23	4:B:132:VAL:O	2.14	0.48
4:B:173:LEU:HD22	4:B:176:LEU:HD23	1.95	0.48
3:E:66:TYR:C	3:E:66:TYR:CD1	2.87	0.48
3:E:272:LEU:HB2	3:E:281:SER:HB3	1.96	0.48
4:F:163:TYR:O	4:F:164:ASN:CB	2.62	0.48
4:F:165:PRO:HA	4:F:176:LEU:HD21	1.96	0.48
3:E:30:ARG:NE	3:E:279:GLU:HG3	2.29	0.48
3:E:132:GLN:HB2	3:E:133:ARG:HH21	1.78	0.48
4:F:49:LYS:HG3	4:F:51:ARG:O	2.13	0.48
3:A:25:GLU:CD	3:A:49:GLU:HB3	2.34	0.47
3:A:184:PHE:N	3:A:184:PHE:CD2	2.81	0.47
4:B:88:VAL:H	4:B:130:MET:HE1	1.78	0.47
3:E:264:ALA:N	3:E:290:PRO:HG3	2.29	0.47
4:F:99:THR:O	4:F:211:ARG:NH2	2.47	0.47
1:C:701:DT:H72	4:B:63:SER:O	2.14	0.47
3:A:45:SER:O	3:A:46:ILE:HD13	2.14	0.47
3:A:56:LYS:HG2	3:A:57:THR:N	2.22	0.47
3:A:155:ASN:HB3	3:A:191:THR:HG21	1.95	0.47
3:A:167:ASP:OD1	3:A:173:LEU:HD12	2.13	0.47
3:A:175:LEU:HD22	3:A:176:THR:N	2.27	0.47
4:B:165:PRO:HA	4:B:176:LEU:HG	1.96	0.47
4:B:206:ASP:OD2	4:B:206:ASP:C	2.53	0.47
3:E:182:PRO:HB2	3:E:184:PHE:CE1	2.49	0.47
3:E:262:LEU:HD11	3:E:266:VAL:CG2	2.44	0.47
4:F:46:GLU:O	4:F:80:PRO:HA	2.14	0.47
4:F:98:VAL:HG23	4:F:211:ARG:HB2	1.96	0.47
3:A:175:LEU:HD13	3:A:175:LEU:C	2.35	0.47
4:B:49:LYS:HE2	4:B:68:PRO:HB2	1.96	0.47
4:B:189:ARG:NH1	4:B:190:GLU:HA	2.30	0.47
4:B:228:ARG:HD3	4:B:228:ARG:N	2.29	0.47
4:F:292:TRP:CD1	4:F:317:LYS:HB3	2.49	0.47
3:A:271:GLN:HG3	3:A:280:LEU:HD12	1.96	0.47
4:B:194:ILE:HG22	4:B:195:ARG:N	2.29	0.47
4:B:329:VAL:CG2	4:B:345:PHE:HB2	2.44	0.47
3:E:130:ILE:HD11	3:E:149:ARG:NH2	2.29	0.47
4:F:188:ASP:OD2	4:F:188:ASP:N	2.48	0.47
3:A:38:CYS:SG	3:A:39:GLU:N	2.87	0.47
3:E:166:ARG:HA	3:E:171:ARG:O	2.14	0.47
4:F:39:GLY:N	4:F:40:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:88:VAL:O	4:F:88:VAL:HG13	2.14	0.47
4:F:92:LYS:HG2	4:F:94:ILE:CD1	2.44	0.47
4:F:123:VAL:HG11	4:F:134:PHE:CE2	2.50	0.47
3:A:45:SER:OG	3:A:46:ILE:N	2.48	0.47
3:A:224:ILE:HD13	3:A:250:ILE:HD11	1.95	0.47
4:B:291:VAL:HG12	4:B:292:TRP:H	1.79	0.47
4:F:77:LYS:HE2	4:F:77:LYS:O	2.14	0.47
4:F:179:GLU:OE1	4:F:184:ARG:HB2	2.14	0.47
3:A:29:GLN:CG	3:A:30:ARG:H	2.28	0.47
3:A:37:LYS:O	3:A:38:CYS:C	2.53	0.47
3:A:71:THR:HG22	3:A:72:VAL:N	2.30	0.47
3:A:208:GLY:HA2	3:A:254:THR:HG22	1.96	0.47
4:B:268:LEU:HD13	4:B:280:ILE:HD12	1.97	0.47
3:E:56:LYS:O	3:E:57:THR:CB	2.61	0.47
4:F:93:VAL:HG22	4:F:216:ALA:CB	2.43	0.47
4:F:100:ASN:ND2	4:F:211:ARG:HD3	2.28	0.47
3:A:86:HIS:CG	3:A:157:VAL:HG12	2.49	0.47
4:B:117:GLU:O	4:B:118:ASP:HB2	2.15	0.47
3:E:174:LEU:HD23	3:E:174:LEU:H	1.80	0.47
3:E:275:PRO:O	3:E:278:ARG:HG2	2.14	0.47
4:F:97:LEU:HD11	4:F:111:LEU:HG	1.97	0.47
4:F:286:GLU:N	4:F:290:GLY:HA2	2.23	0.47
1:G:808:DT:OP2	3:E:36:TYR:OH	2.25	0.47
2:H:815:DG:H4'	2:H:815:DG:OP1	2.14	0.47
3:A:200:ASN:CG	3:A:201:ARG:H	2.16	0.47
3:A:246:ARG:CD	3:A:246:ARG:N	2.78	0.47
3:E:56:LYS:O	3:E:57:THR:HB	2.15	0.47
3:E:66:TYR:CE2	3:E:165:VAL:HB	2.50	0.47
3:E:229:THR:HG23	3:E:271:GLN:HE21	1.80	0.47
4:F:58:VAL:HB	4:F:140:LEU:HD11	1.97	0.47
3:A:58:HIS:HB3	3:A:59:PRO:CD	2.44	0.47
3:A:105:CYS:SG	3:A:108:ARG:NH2	2.88	0.47
3:A:167:ASP:HB3	3:A:168:PRO:HD2	1.97	0.47
4:B:40:PRO:HB3	4:B:86:ASN:CA	2.45	0.47
4:B:44:ILE:O	4:B:46:GLU:N	2.48	0.47
4:B:175:TYR:HA	4:B:177:GLN:NE2	2.30	0.47
4:B:317:LYS:HG3	4:B:318:ASP:H	1.78	0.47
4:F:153:ALA:O	4:F:157:GLU:HB2	2.15	0.47
4:F:220:ASP:N	4:F:224:SER:O	2.48	0.47
3:A:253:ARG:O	3:A:253:ARG:HD3	2.15	0.46
4:B:170:HIS:CD2	4:B:193:ILE:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:81:PRO:C	3:E:83:HIS:H	2.19	0.46
4:F:164:ASN:O	4:F:166:GLY:N	2.48	0.46
3:A:28:LYS:HB2	3:A:28:LYS:HZ2	1.79	0.46
4:B:120:VAL:O	4:B:121:CYS:C	2.52	0.46
4:B:205:MET:HB3	4:B:205:MET:HE2	1.82	0.46
3:E:33:ARG:H	3:E:33:ARG:HG3	1.52	0.46
3:E:45:SER:O	3:E:47:PRO:CD	2.59	0.46
3:E:200:ASN:N	3:E:200:ASN:ND2	2.44	0.46
4:F:195:ARG:HG2	4:F:195:ARG:HH11	1.79	0.46
4:F:268:LEU:HD21	4:F:270:CYS:HB3	1.96	0.46
4:F:305:ARG:HG2	4:F:305:ARG:HH11	1.79	0.46
3:A:158:ARG:HG2	3:A:180:SER:O	2.16	0.46
3:E:72:VAL:HG11	3:E:113:PHE:CE2	2.50	0.46
3:A:180:SER:O	3:A:181:HIS:O	2.33	0.46
4:B:109:HIS:HD2	4:B:142:VAL:HG12	1.77	0.46
4:B:189:ARG:HH11	4:B:189:ARG:C	2.19	0.46
4:B:321:ILE:CG1	4:B:323:LYS:O	2.63	0.46
3:E:109:SER:OG	3:E:110:ILE:N	2.49	0.46
3:E:130:ILE:HG13	3:E:131:SER:N	2.30	0.46
4:F:67:LEU:HD13	4:F:139:ILE:CD1	2.42	0.46
4:F:333:ARG:O	4:F:337:LEU:HA	2.16	0.46
4:F:58:VAL:N	4:F:140:LEU:HD11	2.29	0.46
4:F:105:HIS:C	4:F:168:LEU:HG	2.36	0.46
4:F:170:HIS:NE2	4:F:172:ASP:OD1	2.49	0.46
3:A:108:ARG:HH12	3:A:111:HIS:HA	1.81	0.46
4:B:266:ILE:HG22	4:B:267:TYR:N	2.30	0.46
4:F:295:PHE:O	4:F:314:PRO:HG3	2.16	0.46
1:G:807:DT:H2''	1:G:808:DT:O5'	2.16	0.46
3:A:41:ARG:O	3:A:43:ALA:N	2.49	0.46
3:A:76:LEU:HD21	3:A:118:ILE:HD13	1.97	0.46
3:A:123:LYS:O	3:A:124:ARG:C	2.54	0.46
4:B:156:THR:O	4:B:159:CYS:HB2	2.14	0.46
4:B:291:VAL:HG12	4:B:292:TRP:N	2.31	0.46
3:E:216:CYS:N	4:F:304:HIS:HE1	2.13	0.46
3:E:217:ASP:O	3:E:218:LYS:C	2.53	0.46
3:A:24:ILE:CG2	3:A:60:THR:OG1	2.63	0.46
3:A:224:ILE:HG12	3:A:225:GLU:N	2.31	0.46
3:A:248:VAL:HG21	4:B:305:ARG:HB2	1.98	0.46
3:E:85:PRO:HG3	3:E:139:ASN:HA	1.98	0.46
3:E:88:HIS:CD2	3:E:121:VAL:H	2.33	0.46
3:A:24:ILE:HG21	3:A:110:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:173:LEU:C	4:B:175:TYR:H	2.18	0.46
4:B:202:THR:HG23	4:B:203:LYS:HD2	1.96	0.46
4:F:112:VAL:O	4:F:137:LEU:O	2.33	0.46
4:F:162:GLY:CA	4:F:176:LEU:O	2.64	0.46
2:D:717:DA:OP1	4:B:275:LYS:HE2	2.16	0.46
3:A:179:LEU:N	3:A:179:LEU:CD2	2.76	0.46
3:A:200:ASN:HD21	3:A:213:PHE:H	1.63	0.46
3:A:23:ILE:HD11	3:A:161:PHE:CE1	2.49	0.45
3:A:262:LEU:HG	3:A:263:GLN:N	2.31	0.45
4:B:49:LYS:HA	4:B:70:ALA:HA	1.99	0.45
4:F:82:VAL:CG2	4:F:83:LYS:N	2.79	0.45
3:E:29:GLN:HE21	3:E:30:ARG:HH12	1.59	0.45
4:F:114:LYS:HE3	4:F:115:HIS:CE1	2.52	0.45
4:F:272:LYS:N	4:F:307:PHE:CE1	2.85	0.45
4:F:277:ASP:OD1	4:F:333:ARG:HG3	2.16	0.45
4:F:292:TRP:HZ3	4:F:327:VAL:HG21	1.81	0.45
3:A:214:LEU:HB2	3:A:252:PHE:HE2	1.82	0.45
3:A:219:VAL:CG2	3:A:224:ILE:HD12	2.47	0.45
3:E:59:PRO:O	3:E:113:PHE:N	2.41	0.45
3:E:144:PRO:C	3:E:146:GLU:N	2.68	0.45
3:A:133:ARG:HD2	3:A:133:ARG:H	1.81	0.45
4:B:60:GLU:O	4:B:64:HIS:HE1	2.00	0.45
4:B:144:LYS:O	4:B:147:VAL:HG22	2.16	0.45
3:E:265:PRO:HB3	3:E:287:GLN:CD	2.37	0.45
4:F:45:LEU:HD13	4:F:83:LYS:HE2	1.99	0.45
3:A:238:SER:HB3	3:A:253:ARG:CD	2.47	0.45
3:E:91:VAL:HG23	3:E:91:VAL:O	2.16	0.45
3:E:92:GLY:O	3:E:95:CYS:HB2	2.17	0.45
3:E:201:ARG:HG3	3:E:202:ASN:N	2.31	0.45
4:F:158:ALA:O	4:F:176:LEU:HD12	2.17	0.45
4:F:189:ARG:O	4:F:191:LYS:N	2.49	0.45
1:G:809:DT:H3	2:H:818:DA:H2	1.65	0.45
3:E:27:PRO:CB	3:E:183:ILE:HD11	2.42	0.45
3:E:93:LYS:C	3:E:95:CYS:N	2.69	0.45
3:E:167:ASP:HB2	3:E:168:PRO:CD	2.46	0.45
3:A:24:ILE:HG22	3:A:60:THR:OG1	2.17	0.45
4:B:173:LEU:HD23	4:B:173:LEU:C	2.37	0.45
4:B:256:THR:C	4:B:345:PHE:CD1	2.90	0.45
3:E:164:THR:HG22	3:E:165:VAL:N	2.32	0.45
4:F:88:VAL:CG1	4:F:91:ALA:HB2	2.47	0.45
4:B:57:TYR:CB	4:B:59:CYS:SG	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:229:LEU:O	4:B:230:GLU:C	2.55	0.45
4:F:147:VAL:HG13	4:F:202:THR:OG1	2.17	0.45
3:A:32:MET:HG2	3:A:33:ARG:N	2.32	0.45
3:A:81:PRO:O	3:E:234:GLU:OE1	2.34	0.45
4:B:88:VAL:HG11	4:B:218:LEU:CG	2.45	0.45
3:E:237:GLY:HA2	3:E:255:PRO:HD3	1.98	0.45
4:F:136:ASN:N	4:F:136:ASN:HD22	2.15	0.45
3:A:84:ARG:CZ	3:A:152:TYR:CZ	3.00	0.45
3:A:89:GLU:HG3	3:A:98:GLY:HA2	1.98	0.45
3:A:167:ASP:CG	3:A:173:LEU:HB2	2.37	0.45
3:A:257:TYR:CD2	3:A:258:ALA:N	2.85	0.45
4:B:336:ASP:O	4:B:337:LEU:HB2	2.17	0.45
4:F:92:LYS:HZ3	4:F:94:ILE:CD1	2.30	0.45
3:A:81:PRO:HB2	3:A:82:PRO:HD2	1.99	0.44
3:E:37:LYS:C	3:E:39:GLU:H	2.20	0.44
4:F:305:ARG:HG2	4:F:305:ARG:NH1	2.32	0.44
1:C:712:DT:H4'	1:C:712:DT:OP1	2.17	0.44
3:A:80:ASP:HB3	3:A:81:PRO:CD	2.38	0.44
3:A:84:ARG:NH2	3:A:152:TYR:CD2	2.85	0.44
3:A:223:ASP:OD2	3:A:274:ARG:CG	2.65	0.44
3:A:243:ASP:HB3	3:A:251:VAL:CG1	2.48	0.44
4:B:86:ASN:N	4:B:86:ASN:HD22	2.14	0.44
3:E:89:GLU:HB3	3:E:98:GLY:HA2	1.98	0.44
3:E:186:ASN:C	3:E:188:ALA:H	2.18	0.44
3:E:208:GLY:HA2	3:E:254:THR:CG2	2.46	0.44
4:F:41:TYR:CD2	4:F:41:TYR:N	2.84	0.44
3:A:25:GLU:OE1	3:A:49:GLU:N	2.51	0.44
3:A:36:TYR:O	3:A:39:GLU:HB2	2.18	0.44
4:B:195:ARG:O	4:B:199:VAL:HG23	2.17	0.44
4:B:285:GLU:CD	4:B:285:GLU:O	2.55	0.44
4:F:97:LEU:CD1	4:F:111:LEU:HG	2.48	0.44
3:A:159:LEU:HB2	3:A:180:SER:CB	2.47	0.44
3:A:187:ARG:O	3:A:188:ALA:C	2.55	0.44
4:B:140:LEU:HD12	4:B:140:LEU:HA	1.82	0.44
4:B:214:PHE:HB2	4:B:232:VAL:HG13	1.99	0.44
4:F:153:ALA:HA	4:F:156:THR:OG1	2.17	0.44
4:F:295:PHE:C	4:F:314:PRO:HG3	2.37	0.44
1:G:805:DA:OP2	3:E:246:ARG:NH1	2.51	0.44
3:A:36:TYR:H	3:A:39:GLU:HG3	1.81	0.44
3:A:84:ARG:NH2	3:A:152:TYR:CG	2.86	0.44
3:A:246:ARG:CD	3:A:246:ARG:H	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:247:ASN:HD22	4:B:247:ASN:HA	1.51	0.44
3:E:46:ILE:HD11	3:E:118:ILE:HD11	2.00	0.44
4:F:143:THR:HB	4:F:145:LYS:HG2	2.00	0.44
3:A:125:ASP:HB3	3:A:128:GLN:NE2	2.32	0.44
3:A:139:ASN:OD1	3:A:142:HIS:N	2.50	0.44
3:A:239:PHE:HB3	3:A:252:PHE:HA	1.99	0.44
4:B:292:TRP:CD1	4:B:317:LYS:HB3	2.52	0.44
3:E:156:ALA:HA	3:E:183:ILE:O	2.18	0.44
3:E:206:CYS:SG	3:E:262:LEU:HB3	2.58	0.44
3:E:245:HIS:HD2	4:F:269:LEU:HB3	1.82	0.44
4:B:47:GLN:HB3	4:B:47:GLN:HE21	1.59	0.44
4:B:98:VAL:HG13	4:B:213:MET:HB2	2.00	0.44
3:E:30:ARG:HE	3:E:279:GLU:HG3	1.82	0.44
3:E:93:LYS:HG2	3:E:115:ASN:HB3	2.00	0.44
3:E:245:HIS:ND1	3:E:246:ARG:HG2	2.32	0.44
4:F:84:ILE:CG2	4:F:85:CYS:N	2.79	0.44
4:F:157:GLU:O	4:F:158:ALA:HB3	2.18	0.44
3:A:24:ILE:CG2	3:A:25:GLU:N	2.80	0.44
3:A:108:ARG:CG	3:A:109:SER:N	2.80	0.44
4:B:92:LYS:HG2	4:B:217:PHE:HB2	1.99	0.44
4:B:115:HIS:ND1	4:B:122:THR:O	2.50	0.44
4:B:175:TYR:OH	4:B:190:GLU:OE2	2.35	0.44
3:E:81:PRO:O	3:E:83:HIS:N	2.41	0.44
3:E:183:ILE:O	3:E:183:ILE:HG22	2.17	0.44
4:F:107:HIS:NE2	4:F:206:ASP:O	2.51	0.44
4:F:316:TYR:CZ	4:F:317:LYS:HG2	2.53	0.44
3:A:52:THR:CG2	3:A:53:ASP:H	2.31	0.44
3:A:165:VAL:HG23	3:A:166:ARG:O	2.16	0.44
4:B:108:ALA:CB	4:B:142:VAL:HG11	2.48	0.43
3:A:29:GLN:CG	3:A:30:ARG:N	2.79	0.43
3:A:80:ASP:CB	3:A:81:PRO:CD	2.96	0.43
3:A:134:ILE:O	3:A:136:THR:N	2.51	0.43
3:A:238:SER:O	3:A:253:ARG:HG3	2.18	0.43
4:B:287:GLU:O	4:B:289:GLY:N	2.47	0.43
3:E:90:LEU:O	3:E:95:CYS:HB3	2.18	0.43
4:F:84:ILE:CG2	4:F:85:CYS:H	2.28	0.43
4:F:157:GLU:OE1	4:F:161:ARG:HD2	2.18	0.43
4:F:212:LEU:H	4:F:234:SER:HB2	1.83	0.43
4:F:260:VAL:HG11	4:F:321:ILE:HG12	2.00	0.43
3:A:88:HIS:CG	3:A:120:CYS:HA	2.54	0.43
3:A:89:GLU:OE2	3:A:89:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:100:ASN:HA	4:B:211:ARG:HD2	1.99	0.43
4:B:111:LEU:HD21	4:B:137:LEU:HD13	2.00	0.43
4:B:165:PRO:O	4:B:167:LEU:N	2.51	0.43
4:B:173:LEU:O	4:B:174:ALA:HB3	2.18	0.43
4:B:228:ARG:HD3	4:B:228:ARG:H	1.83	0.43
3:E:133:ARG:H	3:E:133:ARG:HE	1.66	0.43
4:F:57:TYR:HB2	4:F:60:GLU:HG2	1.99	0.43
4:F:163:TYR:HD1	4:F:217:PHE:CE1	2.36	0.43
4:F:219:PRO:HG3	4:F:225:PHE:CZ	2.53	0.43
4:F:274:GLN:H	4:F:274:GLN:NE2	2.16	0.43
3:A:36:TYR:CD1	3:A:39:GLU:HG3	2.53	0.43
3:A:56:LYS:O	3:A:57:THR:HB	2.18	0.43
3:A:62:LYS:HE3	3:A:64:ASN:HB2	2.00	0.43
3:A:76:LEU:HG	3:A:157:VAL:HB	1.99	0.43
4:B:88:VAL:CG1	4:B:218:LEU:HG	2.47	0.43
4:B:147:VAL:O	4:B:151:LEU:HB2	2.18	0.43
4:B:186:LEU:O	4:B:190:GLU:HG3	2.19	0.43
4:F:92:LYS:HG2	4:F:94:ILE:HD11	2.01	0.43
1:C:711:DC:H2''	1:C:712:DT:O5'	2.18	0.43
1:G:807:DT:C2	2:H:820:DG:N2	2.87	0.43
3:A:134:ILE:C	3:A:136:THR:H	2.22	0.43
3:A:159:LEU:O	3:A:180:SER:N	2.48	0.43
3:A:160:CYS:SG	3:A:177:PRO:HB3	2.59	0.43
4:B:207:LEU:H	4:B:207:LEU:CD2	2.27	0.43
4:B:220:ASP:N	4:B:224:SER:O	2.52	0.43
4:B:331:LEU:HD12	4:B:331:LEU:HA	1.92	0.43
3:E:93:LYS:O	3:E:95:CYS:N	2.51	0.43
3:E:186:ASN:O	3:E:188:ALA:N	2.51	0.43
3:A:273:ARG:HB2	3:A:280:LEU:CD1	2.46	0.43
3:E:62:LYS:C	3:E:63:ILE:HD13	2.39	0.43
4:F:57:TYR:CE1	4:F:141:HIS:HB3	2.54	0.43
3:A:85:PRO:HD2	3:A:148:GLN:OE1	2.19	0.43
3:A:93:LYS:CB	3:A:115:ASN:HB2	2.45	0.43
3:A:246:ARG:H	3:A:246:ARG:HD2	1.84	0.43
3:E:82:PRO:O	3:E:84:ARG:NE	2.52	0.43
4:F:131:VAL:HG23	4:F:131:VAL:O	2.18	0.43
3:A:27:PRO:HD2	3:A:180:SER:HB2	1.99	0.43
3:A:58:HIS:CE1	3:A:114:GLN:HA	2.54	0.43
3:A:77:VAL:HA	3:A:86:HIS:H	1.83	0.43
3:A:241:GLN:O	3:A:243:ASP:N	2.51	0.43
4:B:60:GLU:O	4:B:62:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:86:ASN:N	4:B:86:ASN:ND2	2.66	0.43
3:E:78:THR:O	3:E:158:ARG:HD2	2.18	0.43
3:E:127:GLU:OE2	3:E:127:GLU:HA	2.19	0.43
3:E:129:ALA:O	3:E:132:GLN:HB2	2.19	0.43
3:E:199:VAL:HG12	3:E:214:LEU:HA	2.00	0.43
3:A:84:ARG:CD	3:A:147:GLU:O	2.66	0.43
3:A:110:ILE:HG23	3:A:110:ILE:O	2.19	0.43
3:A:134:ILE:C	3:A:136:THR:N	2.73	0.43
3:E:76:LEU:HD11	3:E:90:LEU:N	2.33	0.43
4:F:52:GLY:HA2	4:F:247:ASN:ND2	2.34	0.43
4:F:56:ARG:NH1	4:F:56:ARG:CA	2.72	0.43
4:F:169:VAL:O	4:F:170:HIS:HB2	2.19	0.43
4:F:193:ILE:HG13	4:F:194:ILE:N	2.33	0.43
3:A:76:LEU:CD1	3:A:159:LEU:HD23	2.45	0.43
3:A:81:PRO:CB	3:A:82:PRO:CD	2.97	0.43
4:B:239:ASP:O	4:B:245:ALA:HB3	2.19	0.43
3:E:224:ILE:HD12	3:E:225:GLU:H	1.84	0.43
3:E:246:ARG:HA	3:E:246:ARG:HD2	1.81	0.43
4:F:114:LYS:N	4:F:114:LYS:CD	2.77	0.43
4:F:272:LYS:HA	4:F:306:GLN:O	2.19	0.43
3:A:79:LYS:O	3:A:83:HIS:NE2	2.52	0.42
3:A:224:ILE:CD1	3:A:250:ILE:HD11	2.49	0.42
4:F:111:LEU:O	4:F:111:LEU:CD1	2.67	0.42
4:F:143:THR:HG21	4:F:145:LYS:HG2	2.01	0.42
4:F:317:LYS:HG3	4:F:318:ASP:N	2.34	0.42
3:A:27:PRO:HB3	3:A:183:ILE:HD11	2.01	0.42
3:E:81:PRO:C	3:E:83:HIS:N	2.73	0.42
4:F:187:THR:HG22	4:F:188:ASP:N	2.34	0.42
3:A:48:GLY:HA3	3:A:57:THR:O	2.18	0.42
3:A:76:LEU:HD12	3:A:158:ARG:O	2.19	0.42
4:B:226:THR:O	4:B:226:THR:HG22	2.20	0.42
4:B:288:ASN:OD1	4:B:288:ASN:O	2.37	0.42
3:E:195:LYS:NZ	3:E:217:ASP:CG	2.72	0.42
3:E:229:THR:HG21	3:E:271:GLN:NE2	2.33	0.42
3:A:255:PRO:HA	3:A:256:PRO:HD3	1.84	0.42
4:B:154:ARG:HD2	4:B:154:ARG:N	2.33	0.42
3:E:85:PRO:CG	3:E:139:ASN:HA	2.50	0.42
3:E:131:SER:HA	3:E:134:ILE:HD12	2.00	0.42
2:H:822:DC:H2''	2:H:823:DC:O5'	2.19	0.42
3:E:86:HIS:ND1	3:E:157:VAL:HB	2.35	0.42
4:F:151:LEU:CD1	4:F:202:THR:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:810:DC:N4	3:E:39:GLU:HG2	2.26	0.42
3:A:58:HIS:HB3	3:A:59:PRO:HD2	2.01	0.42
3:A:108:ARG:NH1	3:A:110:ILE:O	2.53	0.42
3:A:196:ILE:H	3:A:196:ILE:CD1	2.14	0.42
4:B:56:ARG:HH11	4:B:60:GLU:HG2	1.84	0.42
4:B:61:GLY:O	4:B:62:PRO:O	2.37	0.42
4:B:148:PHE:CD1	4:B:148:PHE:C	2.92	0.42
3:E:46:ILE:CD1	3:E:118:ILE:HD11	2.49	0.42
3:E:78:THR:CG2	3:E:79:LYS:H	2.29	0.42
4:F:229:LEU:O	4:F:230:GLU:C	2.58	0.42
4:F:333:ARG:HB3	4:F:336:ASP:OD2	2.18	0.42
1:G:809:DT:H2''	1:G:810:DC:OP2	2.20	0.42
2:H:816:DG:C2'	2:H:817:DA:C8	3.02	0.42
4:B:131:VAL:O	4:B:131:VAL:HG13	2.19	0.42
3:E:23:ILE:H	3:E:23:ILE:HG13	1.58	0.42
3:E:76:LEU:HB3	3:E:86:HIS:HB3	2.02	0.42
3:E:124:ARG:NH1	3:E:124:ARG:CB	2.80	0.42
4:F:73:GLU:O	4:F:74:LYS:HB2	2.20	0.42
4:F:246:SER:OG	4:F:247:ASN:N	2.53	0.42
3:A:229:THR:CG2	3:A:271:GLN:HE21	2.33	0.42
4:B:206:ASP:OD2	4:B:208:SER:OG	2.32	0.42
3:E:49:GLU:OE2	3:E:50:ARG:N	2.53	0.42
3:E:134:ILE:O	3:E:136:THR:N	2.53	0.42
3:E:213:PHE:CD1	4:F:254:ASP:HB3	2.55	0.42
4:F:76:LYS:HD3	4:F:77:LYS:H	1.82	0.42
3:A:36:TYR:H	3:A:39:GLU:CG	2.32	0.42
3:A:290:PRO:O	3:A:291:ASP:OXT	2.37	0.42
4:B:87:TYR:CZ	4:B:89:GLY:HA2	2.55	0.42
4:B:147:VAL:CG1	4:B:207:LEU:HD11	2.49	0.42
4:B:155:MET:O	4:B:159:CYS:SG	2.74	0.42
4:B:280:ILE:HG12	4:B:298:PHE:HE2	1.85	0.42
3:E:30:ARG:HE	3:E:279:GLU:CG	2.33	0.42
1:C:705:DA:C2	1:C:706:DC:C2	3.07	0.42
3:A:217:ASP:O	3:A:218:LYS:C	2.58	0.42
4:B:117:GLU:O	4:B:120:VAL:HG22	2.19	0.42
4:B:125:ALA:HA	4:B:132:VAL:CG1	2.41	0.42
4:B:150:THR:O	4:B:154:ARG:HD3	2.20	0.42
4:B:280:ILE:HG12	4:B:298:PHE:CE2	2.55	0.42
3:E:78:THR:CG2	3:E:79:LYS:N	2.82	0.42
3:E:245:HIS:CE1	3:E:246:ARG:HG2	2.55	0.42
4:F:141:HIS:NE2	4:F:207:LEU:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:805:DA:C8	1:G:806:DC:N4	2.88	0.41
3:A:223:ASP:OD2	3:A:276:SER:OG	2.38	0.41
3:A:238:SER:HB3	3:A:253:ARG:HG3	2.02	0.41
4:B:187:THR:CG2	4:B:188:ASP:N	2.83	0.41
3:E:60:THR:HG22	3:E:112:SER:HB3	2.01	0.41
3:E:223:ASP:OD2	3:E:276:SER:HB3	2.20	0.41
4:F:79:TYR:N	4:F:79:TYR:HD1	2.18	0.41
4:F:92:LYS:HZ3	4:F:94:ILE:HD11	1.85	0.41
3:A:28:LYS:HZ3	3:A:47:PRO:HG2	1.85	0.41
4:B:53:PHE:O	4:B:240:SER:N	2.54	0.41
4:B:54:ARG:HG2	4:B:241:LYS:HB2	2.00	0.41
3:E:104:LEU:O	3:E:105:CYS:C	2.57	0.41
4:F:161:ARG:HG2	4:F:161:ARG:HH11	1.85	0.41
3:A:93:LYS:H	3:A:115:ASN:HB2	1.85	0.41
3:A:229:THR:CG2	3:A:271:GLN:NE2	2.83	0.41
3:E:226:VAL:HG11	3:E:252:PHE:CZ	2.56	0.41
4:F:42:LEU:CD1	4:F:214:PHE:HB3	2.51	0.41
4:F:82:VAL:HG22	4:F:83:LYS:H	1.83	0.41
4:F:260:VAL:H	4:F:260:VAL:HG22	1.67	0.41
4:B:50:GLN:O	4:B:51:ARG:HG2	2.19	0.41
4:B:88:VAL:HG21	4:B:218:LEU:HD21	2.02	0.41
4:B:263:GLY:N	4:B:313:THR:O	2.34	0.41
4:B:333:ARG:O	4:B:337:LEU:HA	2.20	0.41
3:E:32:MET:HE1	3:E:46:ILE:HG12	2.01	0.41
4:F:52:GLY:HA2	4:F:247:ASN:HD21	1.84	0.41
4:F:106:LEU:HD11	4:F:151:LEU:CD2	2.49	0.41
4:F:134:PHE:O	4:F:135:ALA:O	2.38	0.41
4:F:250:ILE:HG12	4:F:268:LEU:HD11	2.02	0.41
2:H:817:DA:H3'	4:F:306:GLN:HE22	1.86	0.41
3:A:37:LYS:C	3:A:39:GLU:N	2.73	0.41
4:B:141:HIS:HD2	4:B:142:VAL:O	2.04	0.41
3:E:228:PHE:CZ	3:E:252:PHE:HE1	2.37	0.41
4:F:47:GLN:O	4:F:48:PRO:O	2.38	0.41
4:F:207:LEU:H	4:F:207:LEU:CD2	2.34	0.41
3:A:23:ILE:HG12	3:A:61:ILE:HG22	2.02	0.41
3:A:248:VAL:CG2	4:B:305:ARG:HD2	2.51	0.41
4:B:44:ILE:O	4:B:45:LEU:C	2.59	0.41
4:B:53:PHE:O	4:B:240:SER:HB3	2.21	0.41
3:E:30:ARG:NE	3:E:279:GLU:CG	2.83	0.41
4:F:155:MET:O	4:F:159:CYS:SG	2.76	0.41
4:F:332:ARG:HG3	4:F:332:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:143:THR:OG1	4:B:144:LYS:N	2.53	0.41
3:E:82:PRO:HG2	3:E:84:ARG:NH2	2.31	0.41
4:F:67:LEU:CD2	4:F:138:GLY:H	2.34	0.41
4:F:157:GLU:C	4:F:159:CYS:H	2.20	0.41
4:F:216:ALA:HB3	4:F:229:LEU:CD2	2.51	0.41
4:B:87:TYR:HE2	4:B:128:LYS:H	1.69	0.41
4:B:88:VAL:HG11	4:B:218:LEU:HB3	2.03	0.41
4:B:281:ARG:HD2	4:B:295:PHE:HE1	1.85	0.41
3:E:100:TYR:CZ	3:E:102:ALA:HB3	2.56	0.41
4:F:303:VAL:O	4:F:303:VAL:HG12	2.20	0.41
4:F:332:ARG:HG3	4:F:332:ARG:HH11	1.86	0.41
3:A:33:ARG:CD	3:A:187:ARG:HG3	2.49	0.41
3:A:225:GLU:N	3:A:273:ARG:O	2.49	0.41
3:A:239:PHE:HD2	3:A:240:SER:O	2.04	0.41
3:A:262:LEU:HG	3:A:264:ALA:H	1.85	0.41
3:A:273:ARG:NH1	3:A:273:ARG:HG2	2.36	0.41
4:B:158:ALA:O	4:B:176:LEU:HD13	2.21	0.41
4:B:189:ARG:O	4:B:191:LYS:N	2.53	0.41
4:B:328:PHE:HE1	4:B:344:PRO:HG3	1.86	0.41
3:E:72:VAL:HG21	3:E:104:LEU:HB3	2.03	0.41
3:E:165:VAL:HG23	3:E:166:ARG:N	2.36	0.41
4:F:56:ARG:HH22	4:F:60:GLU:CG	2.34	0.41
4:F:97:LEU:HB3	4:F:210:VAL:CG2	2.49	0.41
4:F:98:VAL:CG1	4:F:213:MET:HB2	2.49	0.41
4:F:151:LEU:HD12	4:F:202:THR:HB	2.02	0.41
4:F:225:PHE:CD2	4:F:225:PHE:N	2.89	0.41
1:C:708:DT:H2'	3:A:36:TYR:CE2	2.56	0.41
2:D:713:DA:H3'	3:A:44:GLY:HA2	2.02	0.41
3:A:40:GLY:O	3:A:43:ALA:HB3	2.21	0.41
3:A:289:LEU:N	3:A:289:LEU:CD1	2.84	0.41
4:B:97:LEU:CG	4:B:111:LEU:HD13	2.48	0.41
4:B:218:LEU:N	4:B:218:LEU:CD1	2.84	0.41
3:E:49:GLU:OE2	3:E:50:ARG:HB2	2.21	0.41
4:F:127:PRO:O	4:F:128:LYS:HB3	2.20	0.41
4:F:237:ILE:N	4:F:237:ILE:CD1	2.84	0.41
4:F:241:LYS:HD2	4:F:241:LYS:O	2.20	0.41
2:H:814:DA:OP2	3:E:44:GLY:HA2	2.21	0.40
2:H:820:DG:H5''	4:F:143:THR:HG23	2.03	0.40
3:A:34:PHE:HB3	3:A:120:CYS:HB3	2.03	0.40
3:A:139:ASN:O	3:A:139:ASN:OD1	2.38	0.40
4:B:173:LEU:O	4:B:175:TYR:CD1	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:176:LEU:N	4:B:177:GLN:NE2	2.69	0.40
3:E:200:ASN:OD1	3:E:213:PHE:HB2	2.21	0.40
3:E:225:GLU:N	3:E:273:ARG:O	2.51	0.40
4:F:117:GLU:O	4:F:118:ASP:CB	2.68	0.40
4:F:346:LEU:HD13	4:F:346:LEU:C	2.41	0.40
2:H:816:DG:N3	2:H:817:DA:O4'	2.54	0.40
3:A:72:VAL:CG1	3:A:100:TYR:HE1	2.35	0.40
3:A:213:PHE:CZ	4:B:252:ARG:HD3	2.55	0.40
4:F:133:GLY:C	4:F:134:PHE:HD2	2.24	0.40
4:F:187:THR:CG2	4:F:188:ASP:N	2.84	0.40
4:F:207:LEU:N	4:F:207:LEU:CD2	2.81	0.40
3:A:30:ARG:HB2	3:A:30:ARG:HH11	1.86	0.40
3:A:86:HIS:ND1	3:A:87:PRO:CD	2.83	0.40
3:A:124:ARG:HD2	3:A:125:ASP:OD1	2.22	0.40
3:A:248:VAL:HG21	4:B:305:ARG:HD2	2.03	0.40
4:B:41:TYR:CD2	4:B:41:TYR:C	2.95	0.40
4:B:186:LEU:CD1	4:B:191:LYS:HD2	2.45	0.40
3:A:60:THR:OG1	3:A:110:ILE:HD11	2.22	0.40
3:A:134:ILE:CG1	3:A:135:GLN:H	2.28	0.40
3:A:167:ASP:CG	3:A:168:PRO:HD2	2.42	0.40
3:A:213:PHE:HZ	4:B:252:ARG:HD3	1.86	0.40
3:A:273:ARG:HD2	3:A:280:LEU:CD2	2.47	0.40
3:A:273:ARG:HG2	3:A:273:ARG:HH11	1.86	0.40
3:A:286:PHE:HE1	3:A:288:TYR:CZ	2.39	0.40
4:B:56:ARG:HD2	4:B:60:GLU:HG2	2.03	0.40
4:B:230:GLU:HA	4:B:231:PRO:HD2	1.96	0.40
4:B:254:ASP:N	4:B:254:ASP:OD2	2.54	0.40
3:E:74:ILE:N	3:E:100:TYR:O	2.49	0.40
4:B:257:ALA:N	4:B:345:PHE:CE1	2.90	0.40
4:B:281:ARG:HD2	4:B:295:PHE:CE1	2.57	0.40
4:B:301:THR:HG22	4:B:301:THR:O	2.21	0.40
3:E:99:TYR:CD2	3:E:100:TYR:N	2.90	0.40
3:E:176:THR:HA	3:E:177:PRO:HD3	1.83	0.40
4:F:53:PHE:CE2	4:F:55:PHE:HA	2.57	0.40
4:F:168:LEU:HD22	4:F:213:MET:SD	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	271/274 (99%)	190 (70%)	55 (20%)	26 (10%)	0	3
3	E	271/274 (99%)	181 (67%)	68 (25%)	22 (8%)	1	4
4	B	310/313 (99%)	227 (73%)	61 (20%)	22 (7%)	1	5
4	F	310/313 (99%)	220 (71%)	61 (20%)	29 (9%)	0	3
All	All	1162/1174 (99%)	818 (70%)	245 (21%)	99 (8%)	1	4

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	SER
3	A	81	PRO
3	A	97	ASP
3	A	115	ASN
3	A	247	GLN
4	B	40	PRO
4	B	45	LEU
4	B	62	PRO
4	B	76	LYS
4	B	135	ALA
4	B	186	LEU
4	B	292	TRP
4	B	335	SER
3	E	22	GLU
3	E	34	PHE
3	E	81	PRO
3	E	83	HIS
3	E	115	ASN
4	F	44	ILE
4	F	48	PRO
4	F	61	GLY
4	F	62	PRO

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Mol	Chain	Res	Type
4	F	72	SER
4	F	87	TYR
4	F	135	ALA
4	F	165	PRO
4	F	177	GLN
4	F	186	LEU
4	F	246	SER
4	F	335	SER
3	A	51	SER
3	A	137	ASN
3	A	142	HIS
3	A	276	SER
4	B	61	GLY
4	B	74	LYS
4	B	87	TYR
4	B	236	ALA
4	B	290	GLY
4	B	291	VAL
3	E	29	GLN
3	E	38	CYS
3	E	45	SER
3	E	135	GLN
3	E	142	HIS
3	E	165	VAL
3	E	276	SER
4	F	45	LEU
4	F	55	PHE
4	F	182	GLY
4	F	183	ASP
4	F	236	ALA
4	F	292	TRP
3	A	49	GLU
3	A	140	PRO
3	A	242	ALA
4	B	164	ASN
4	B	190	GLU
4	B	305	ARG
4	F	68	PRO
4	F	117	GLU
4	F	173	LEU
4	F	190	GLU
4	F	305	ARG

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Mol	Chain	Res	Type
3	A	89	GLU
3	A	90	LEU
3	A	124	ARG
3	A	229	THR
3	A	246	ARG
4	B	235	ASP
3	E	40	GLY
3	E	94	ASP
3	E	139	ASN
3	E	229	THR
4	F	164	ASN
4	F	187	THR
4	F	275	LYS
3	A	57	THR
3	A	181	HIS
4	B	75	ASN
4	B	275	LYS
3	E	57	THR
3	A	110	ILE
3	A	198	ARG
4	F	43	GLN
4	F	59	CYS
3	A	139	ASN
3	A	231	PRO
3	E	31	GLY
3	E	157	VAL
3	A	27	PRO
3	A	31	GLY
4	B	166	GLY
3	E	110	ILE
3	E	134	ILE
3	E	275	PRO
4	F	80	PRO
3	A	189	PRO
4	B	104	ILE

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	
3	A	242/243 (100%)	211 (87%)	31 (13%)	4	19
3	E	242/243 (100%)	209 (86%)	33 (14%)	3	17
4	B	268/269 (100%)	243 (91%)	25 (9%)	9	33
4	F	268/269 (100%)	235 (88%)	33 (12%)	4	21
All	All	1020/1024 (100%)	898 (88%)	122 (12%)	5	22

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	28	LYS
3	A	36	TYR
3	A	53	ASP
3	A	56	LYS
3	A	64	ASN
3	A	75	SER
3	A	81	PRO
3	A	125	ASP
3	A	130	ILE
3	A	133	ARG
3	A	135	GLN
3	A	138	ASN
3	A	167	ASP
3	A	171	ARG
3	A	174	LEU
3	A	178	VAL
3	A	179	LEU
3	A	186	ASN
3	A	193	GLU
3	A	196	ILE
3	A	200	ASN
3	A	201	ARG
3	A	203	SER
3	A	207	LEU
3	A	246	ARG
3	A	247	GLN
3	A	253	ARG
3	A	254	THR
3	A	272	LEU
3	A	277	ASP
3	A	289	LEU

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Mol	Chain	Res	Type
4	B	44	ILE
4	B	45	LEU
4	B	47	GLN
4	B	54	ARG
4	B	59	CYS
4	B	82	VAL
4	B	87	TYR
4	B	103	ASN
4	B	115	HIS
4	B	123	VAL
4	B	149	GLU
4	B	152	GLU
4	B	154	ARG
4	B	177	GLN
4	B	207	LEU
4	B	212	LEU
4	B	218	LEU
4	B	228	ARG
4	B	232	VAL
4	B	244	ASN
4	B	247	ASN
4	B	252	ARG
4	B	303	VAL
4	B	318	ASP
4	B	331	LEU
3	E	33	ARG
3	E	45	SER
3	E	49	GLU
3	E	60	THR
3	E	81	PRO
3	E	84	ARG
3	E	93	LYS
3	E	114	GLN
3	E	119	GLN
3	E	125	ASP
3	E	130	ILE
3	E	133	ARG
3	E	139	ASN
3	E	141	PHE
3	E	146	GLU
3	E	166	ARG
3	E	174	LEU

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Mol	Chain	Res	Type
3	E	178	VAL
3	E	181	HIS
3	E	183	ILE
3	E	190	ASN
3	E	200	ASN
3	E	201	ARG
3	E	206	CYS
3	E	211	GLU
3	E	218	LYS
3	E	219	VAL
3	E	236	ARG
3	E	254	THR
3	E	263	GLN
3	E	279	GLU
3	E	282	GLU
3	E	289	LEU
4	F	46	GLU
4	F	49	LYS
4	F	67	LEU
4	F	77	LYS
4	F	79	TYR
4	F	87	TYR
4	F	97	LEU
4	F	102	LYS
4	F	114	LYS
4	F	115	HIS
4	F	117	GLU
4	F	118	ASP
4	F	121	CYS
4	F	128	LYS
4	F	140	LEU
4	F	151	LEU
4	F	157	GLU
4	F	172	ASP
4	F	176	LEU
4	F	188	ASP
4	F	192	GLU
4	F	201	GLN
4	F	206	ASP
4	F	229	LEU
4	F	230	GLU
4	F	235	ASP

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Mol	Chain	Res	Type
4	F	241	LYS
4	F	260	VAL
4	F	272	LYS
4	F	274	GLN
4	F	301	THR
4	F	305	ARG
4	F	332	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	64	ASN
3	A	88	HIS
3	A	114	GLN
3	A	128	GLN
3	A	137	ASN
3	A	138	ASN
3	A	162	GLN
3	A	181	HIS
3	A	186	ASN
3	A	200	ASN
3	A	220	GLN
3	A	241	GLN
3	A	263	GLN
3	A	271	GLN
4	B	47	GLN
4	B	64	HIS
4	B	86	ASN
4	B	100	ASN
4	B	103	ASN
4	B	105	HIS
4	B	107	HIS
4	B	109	HIS
4	B	136	ASN
4	B	141	HIS
4	B	170	HIS
4	B	177	GLN
4	B	196	GLN
4	B	201	GLN
4	B	244	ASN
4	B	247	ASN
4	B	288	ASN

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Mol	Chain	Res	Type
4	B	320	ASN
3	E	29	GLN
3	E	58	HIS
3	E	88	HIS
3	E	114	GLN
3	E	162	GLN
3	E	200	ASN
3	E	271	GLN
3	E	287	GLN
4	F	47	GLN
4	F	75	ASN
4	F	81	GLN
4	F	96	GLN
4	F	100	ASN
4	F	109	HIS
4	F	136	ASN
4	F	141	HIS
4	F	164	ASN
4	F	185	GLN
4	F	200	GLN
4	F	306	GLN
4	F	330	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.