



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:40 PM GMT

PDB ID : 1LE5
Title : Crystal structure of a NF-kB heterodimer bound to an IFN γ -kB
Authors : Berkowitz, B.; Huang, D.B.; Chen-Park, F.E.; Sigler, P.B.; Ghosh, G.
Deposited on : 2002-04-09
Resolution : 2.75 Å(reported)

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

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

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

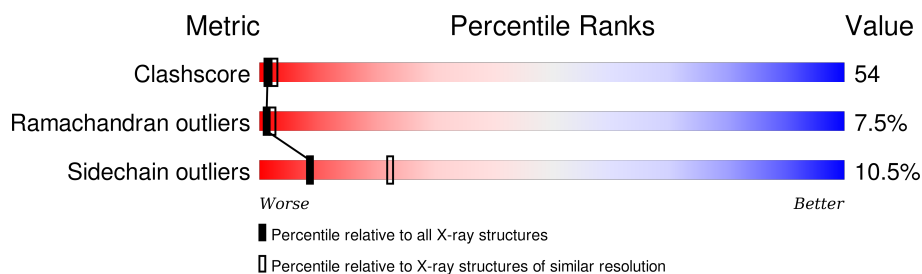
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

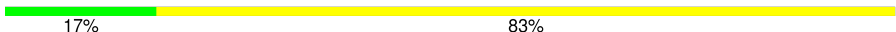






Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)

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

Note EDS was not executed.

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

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Mol	Chain	Length	Quality of chain
4	F	313	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (34%), yellow (52%), and orange (13%). A small red dot is at the end of the bar.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10439 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*AP*AP*TP*TP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			244	118	44	71	11			
1	G	12	Total	C	N	O	P	0	0	0
			244	118	44	71	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			242	117	45	69	11			
2	H	12	Total	C	N	O	P	0	0	0
			242	117	45	69	11			

- Molecule 3 is a protein called Nuclear factor NF-kappa-B p65 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	274	Total	C	N	O	S	0	0	0
			2184	1361	402	409	12			
3	E	274	Total	C	N	O	S	0	0	0
			2184	1361	402	409	12			

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	313	Total 2462	C 1559	N 429	O 461	S 13	0	0	0
4	F	313	Total 2462	C 1559	N 429	O 461	S 13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total 33	O 33	0	0
5	B	32	Total 32	O 32	0	0
5	C	4	Total 4	O 4	0	0
5	D	9	Total 9	O 9	0	0
5	E	32	Total 32	O 32	0	0
5	F	51	Total 51	O 51	0	0
5	G	6	Total 6	O 6	0	0
5	H	8	Total 8	O 8	0	0

3 Residue-property plots

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

Note EDS was not executed.

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

Chain C: 



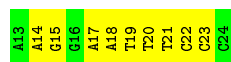
- Molecule 1: 5'-D(*TP*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*T)-3'

Chain G: 



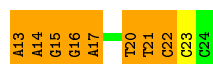
- Molecule 2: 5'-D(*AP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3'

Chain D: 



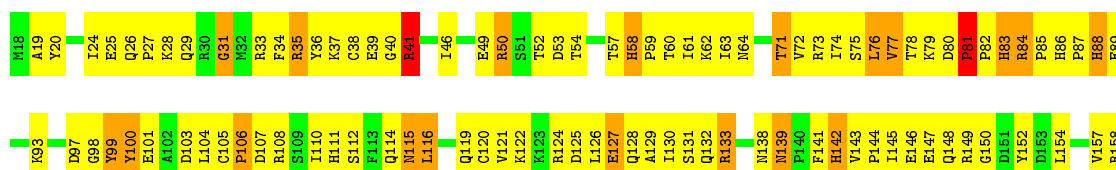
- Molecule 2: 5'-D(*AP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3'

Chain H: 



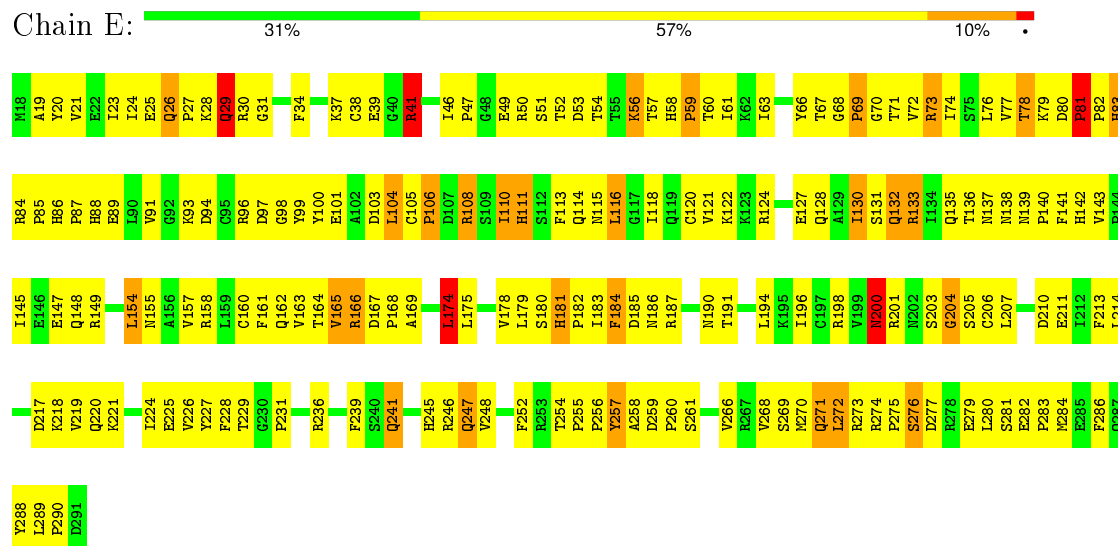
- Molecule 3: Nuclear factor NF-kappa-B p65 subunit

Chain A: 

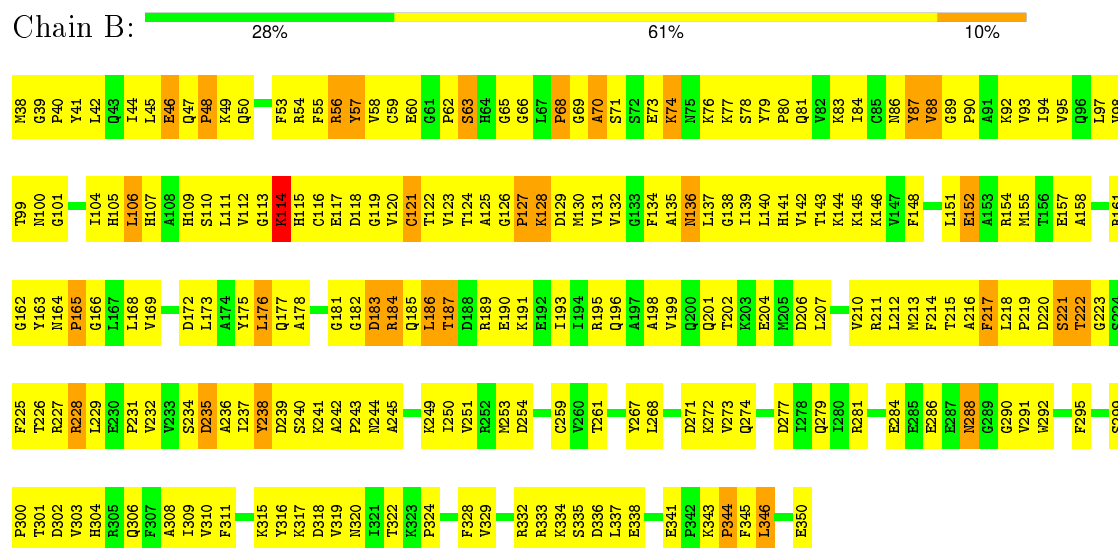




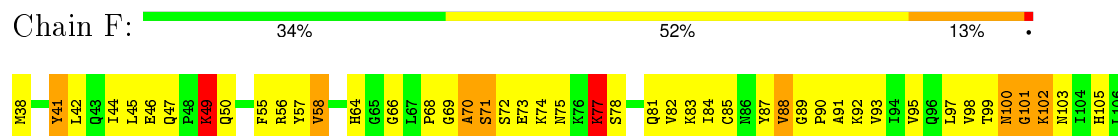
• Molecule 3: Nuclear factor NF-kappa-B p65 subunit



• Molecule 4: Nuclear factor NF-kappa-B p50 subunit



• Molecule 4: Nuclear factor NF-kappa-B p50 subunit



N320	N321	F322	K323	V327	F328	V329	R332	R333	K334	S335	D336	L337	E338	T339	S340	E341	F342	K343	F344	F345	L346	P349	E350																																	
D235	A236	I237	Y238	D239	S240	N244	A245	S246	N247	L248	V249	I250	D254	R255	C259	Y267	L268	D271	K272	V273	Q274	K275	Q279	T280	R281	F282	Y283	E284	E285	E286	E287	N288	G289	G290	V291	F298	S299	P300	V303	H304	R305	Q306	A307	A308	I309	V310	Y316	K317	D318	V319						
H107	A108	H109	S110	L111	V112	G113	K114	H115	C116	E117	D118	G121	T122	V123	T124	A125	G126	P127	M130	V131	V132	G133	F134	A135	M136	L137	G138	T139	L140	H141	V142	T143	K144	K145	K146	V147	F148	E149	T150	L151	E152	A153	R154	M155	T156	E157	I160	R161	G162	Y163	N164	P165	G166	L167	H170	
S171	D172	L173	A174	Y175	L176	Q177	A178	E179	G182	D183	R184	Q185	L186	T187	D188	R189	E190	K191	E192	I193	I194	R195	Q196	A197	A198	V199	Q200	Q201	T202	K203	E204	M205	V209	V210	M213	F214	T215	A216	F217	L218	P219	S221	D220	T222	G223	S224	F225	T226	R227	R228	L229	E230	P231	V232	V233	S234

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.53Å 138.01Å 89.32Å 90.00° 97.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75	Depositor
% Data completeness (in resolution range)	88.0 (20.00-2.75)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.260 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10439	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.32	0/273	0.74	0/420
1	G	0.69	0/273	1.26	3/420 (0.7%)
2	D	0.32	0/271	0.78	0/416
2	H	0.80	0/271	1.31	2/416 (0.5%)
3	A	0.39	0/2236	0.67	0/3031
3	E	0.39	0/2236	0.69	0/3031
4	B	0.35	0/2514	0.60	0/3394
4	F	0.41	0/2514	0.66	0/3394
All	All	0.41	0/10588	0.71	5/14522 (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
1	G	0	5
2	H	0	6
All	All	0	11

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	8	DT	O4'-C4'-C3'	-5.71	102.22	104.50
2	H	17	DA	O4'-C1'-C2'	5.32	110.16	105.90
1	G	7	DA	O4'-C1'-C2'	5.27	110.11	105.90
1	G	5	DA	N9-C1'-C2'	5.21	122.49	112.60
2	H	15	DG	N9-C1'-C2'	5.10	122.29	112.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	11	DC	Sidechain
1	G	4	DG	Sidechain
1	G	5	DA	Sidechain
1	G	6	DA	Sidechain
1	G	7	DA	Sidechain
2	H	13	DA	Sidechain
2	H	14	DA	Sidechain
2	H	16	DG	Sidechain
2	H	20	DT	Sidechain
2	H	21	DT	Sidechain
2	H	22	DC	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	244	0	138	28	0
1	G	244	0	138	33	0
2	D	242	0	137	23	0
2	H	242	0	137	14	0
3	A	2184	0	2146	239	0
3	E	2184	0	2146	245	0
4	B	2462	0	2458	301	0
4	F	2462	0	2458	250	0
5	A	33	0	0	5	0
5	B	32	0	0	4	0
5	C	4	0	0	3	0
5	D	9	0	0	1	0
5	E	32	0	0	7	0
5	F	51	0	0	5	0
5	G	6	0	0	2	0
5	H	8	0	0	1	0
All	All	10439	0	9758	1074	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 54.

All (1074) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:DT:H3'	4:B:65:GLY:HA2	1.30	1.11
4:F:250:ILE:HG23	4:F:268:LEU:HD21	1.29	1.06
4:B:104:ILE:HG22	4:B:211:ARG:HH22	1.23	1.03
3:E:273:ARG:HD2	3:E:280:LEU:HD11	1.41	1.02
4:B:134:PHE:HB3	4:B:137:LEU:HD11	1.42	1.02
3:E:200:ASN:HB2	3:E:213:PHE:H	1.26	0.99
3:A:273:ARG:HE	3:E:81:PRO:HG2	1.26	0.98
3:A:149:ARG:HG2	3:A:150:GLY:H	1.29	0.98
4:F:176:LEU:HD22	4:F:184:ARG:HG3	1.46	0.97
3:E:206:CYS:HA	3:E:288:TYR:HD2	1.28	0.96
3:A:128:GLN:O	3:A:132:GLN:HG3	1.66	0.96
1:G:4:DG:H3'	3:E:246:ARG:NH1	1.80	0.95
3:A:200:ASN:HB2	3:A:213:PHE:H	1.33	0.94
4:F:84:ILE:HB	4:F:130:MET:HB3	1.50	0.93
4:F:332:ARG:HG2	4:F:332:ARG:HH11	1.33	0.93
3:A:165:VAL:HG23	3:A:173:LEU:HB3	1.51	0.92
4:B:195:ARG:HH11	4:B:195:ARG:HA	1.33	0.91
3:E:130:ILE:HD11	3:E:148:GLN:HG2	1.50	0.91
4:B:186:LEU:H	4:B:186:LEU:HD12	1.35	0.91
3:E:74:ILE:HD12	3:E:161:PHE:HD1	1.34	0.90
4:B:84:ILE:HD13	4:B:130:MET:HG2	1.50	0.90
2:D:22:DC:H2''	2:D:23:DC:H5''	1.54	0.90
4:F:88:VAL:HG22	4:F:89:GLY:H	1.34	0.90
3:A:273:ARG:NE	3:E:81:PRO:HG2	1.84	0.90
4:B:111:LEU:HD21	4:B:137:LEU:HB3	1.54	0.89
4:B:244:ASN:HB3	4:B:274:GLN:HE22	1.38	0.89
3:E:174:LEU:H	3:E:174:LEU:HD22	1.36	0.88
4:B:123:VAL:HG11	4:B:132:VAL:HG11	1.56	0.88
3:E:257:TYR:CD2	3:E:258:ALA:N	2.42	0.87
3:E:257:TYR:HD2	3:E:258:ALA:N	1.71	0.87
4:F:156:THR:O	4:F:160:ILE:HG23	1.76	0.86
4:B:215:THR:HG23	4:B:228:ARG:HG3	1.57	0.86
3:E:111:HIS:H	3:E:111:HIS:CD2	1.90	0.85
3:A:201:ARG:HH21	3:A:201:ARG:HG2	1.41	0.85
4:F:46:GLU:HG2	4:F:47:GLN:H	1.40	0.85
3:A:53:ASP:OD1	3:A:54:THR:HG23	1.75	0.85
3:A:35:ARG:HE	3:A:35:ARG:HA	1.39	0.85
1:G:6:DA:H2''	1:G:7:DA:O5'	1.77	0.84
3:A:26:GLN:O	3:A:49:GLU:HB2	1.78	0.83
3:A:63:ILE:HD12	3:A:63:ILE:H	1.43	0.83
4:B:286:GLU:HB2	4:B:290:GLY:HA3	1.57	0.83
4:B:56:ARG:HB3	4:B:56:ARG:NH1	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:155:MET:HE2	4:B:169:VAL:HG22	1.58	0.83
4:B:125:ALA:HB3	4:B:132:VAL:HG22	1.60	0.83
4:F:227:ARG:NE	4:F:227:ARG:HA	1.91	0.83
4:B:329:VAL:HG23	4:B:345:PHE:HB2	1.60	0.83
4:F:107:HIS:HD2	4:F:109:HIS:H	1.26	0.83
2:D:17:DA:H2'	4:B:306:GLN:HE22	1.43	0.83
3:A:114:GLN:O	3:A:115:ASN:HB2	1.78	0.82
3:E:81:PRO:HB2	3:E:82:PRO:HD3	1.60	0.82
4:B:116:CYS:HA	4:B:121:CYS:HA	1.62	0.82
3:E:21:VAL:HG13	3:E:63:ILE:HG22	1.60	0.82
3:E:27:PRO:HD2	3:E:180:SER:HB2	1.62	0.82
4:B:48:PRO:HA	4:B:69:GLY:HA2	1.61	0.81
4:B:45:LEU:HD11	4:B:81:GLN:HB2	1.63	0.81
4:F:123:VAL:HG11	4:F:132:VAL:HG21	1.62	0.81
3:E:258:ALA:O	3:E:260:PRO:HD3	1.80	0.81
2:H:21:DT:H2''	2:H:22:DC:O5'	1.79	0.81
3:A:57:THR:HG22	3:A:58:HIS:H	1.45	0.81
3:A:166:ARG:HH11	3:A:166:ARG:HG3	1.46	0.81
4:B:92:LYS:HB2	4:B:217:PHE:HE1	1.46	0.80
4:F:167:LEU:HD21	4:F:228:ARG:NH2	1.97	0.79
4:F:189:ARG:HD2	4:F:190:GLU:N	1.98	0.79
3:E:76:LEU:HD11	3:E:118:ILE:HD12	1.65	0.79
1:G:4:DG:H3'	3:E:246:ARG:HH12	1.48	0.78
4:F:329:VAL:HG23	4:F:345:PHE:HB2	1.64	0.78
4:B:40:PRO:HB3	4:B:87:TYR:HA	1.64	0.78
3:E:69:PRO:HG2	3:E:166:ARG:NH1	1.98	0.78
3:A:73:ARG:HA	3:A:100:TYR:O	1.84	0.78
3:E:74:ILE:HD12	3:E:161:PHE:CD1	2.18	0.78
2:D:23:DC:H4'	5:D:721:HOH:O	1.84	0.78
4:B:76:LYS:HG3	4:B:77:LYS:H	1.49	0.77
4:F:126:GLY:N	4:F:127:PRO:HD3	2.00	0.77
4:B:261:THR:O	4:B:315:LYS:HG2	1.84	0.77
4:F:88:VAL:HG11	4:F:218:LEU:HD22	1.67	0.77
3:E:79:LYS:HG2	3:E:80:ASP:OD2	1.85	0.77
1:C:9:DT:H2'	3:A:38:CYS:SG	2.24	0.77
3:A:195:LYS:HD2	3:A:217:ASP:OD1	1.84	0.76
4:F:114:LYS:HE2	4:F:134:PHE:HA	1.67	0.76
1:G:5:DA:H2''	1:G:6:DA:O5'	1.86	0.76
4:B:92:LYS:HB2	4:B:217:PHE:CE1	2.20	0.76
3:E:198:ARG:HD2	4:F:310:VAL:HG21	1.67	0.76
1:G:11:DC:O2	2:H:15:DG:N2	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:262:LEU:HD21	3:A:266:VAL:HG23	1.67	0.76
3:A:169:ALA:HB1	3:A:171:ARG:HH21	1.52	0.75
3:A:79:LYS:HA	3:A:158:ARG:CD	2.17	0.75
3:A:93:LYS:HE2	3:A:115:ASN:HB3	1.66	0.75
4:F:105:HIS:HB3	4:F:201:GLN:NE2	2.02	0.75
3:A:84:ARG:H	3:A:84:ARG:HE	1.34	0.75
3:A:108:ARG:HB3	3:A:111:HIS:CE1	2.22	0.74
4:F:250:ILE:HG23	4:F:268:LEU:CD2	2.12	0.74
3:E:204:GLY:HA2	3:E:210:ASP:OD1	1.86	0.74
4:F:115:HIS:HB3	5:F:800:HOH:O	1.87	0.74
3:E:111:HIS:HD2	3:E:111:HIS:H	1.33	0.74
4:F:346:LEU:C	4:F:346:LEU:HD23	2.07	0.74
4:B:79:TYR:HB3	4:B:80:PRO:HD2	1.69	0.73
4:F:116:CYS:HA	4:F:121:CYS:HA	1.68	0.73
1:G:8:DT:H2''	1:G:9:DT:O5'	1.88	0.73
4:F:84:ILE:HB	4:F:130:MET:CB	2.17	0.73
4:F:97:LEU:HD21	4:F:111:LEU:HD21	1.70	0.73
3:E:111:HIS:N	3:E:111:HIS:CD2	2.56	0.73
3:E:58:HIS:HB3	3:E:113:PHE:O	1.87	0.73
4:B:195:ARG:O	4:B:199:VAL:HG23	1.87	0.73
4:B:173:LEU:HD21	4:B:193:ILE:HG21	1.70	0.72
3:A:86:HIS:NE2	3:A:154:LEU:HA	2.04	0.72
4:F:184:ARG:HD2	4:F:184:ARG:H	1.54	0.72
4:B:279:GLN:NE2	4:B:332:ARG:HH21	1.88	0.72
4:F:167:LEU:HD12	4:F:167:LEU:N	2.04	0.72
4:B:254:ASP:HB2	4:B:267:TYR:HB2	1.72	0.72
1:C:8:DT:H2''	1:C:9:DT:H72	1.72	0.72
4:B:329:VAL:CG2	4:B:345:PHE:HB2	2.18	0.72
4:B:104:ILE:HG22	4:B:211:ARG:NH2	2.02	0.72
3:E:72:VAL:O	3:E:101:GLU:HA	1.90	0.72
3:E:80:ASP:HB3	3:E:81:PRO:HD2	1.72	0.71
3:A:236:ARG:HE	3:E:82:PRO:HG2	1.54	0.71
3:E:248:VAL:HG11	4:F:305:ARG:HG3	1.71	0.71
3:A:267:ARG:HD2	3:A:285:GLU:HG3	1.71	0.71
4:F:88:VAL:CG1	4:F:218:LEU:HD22	2.20	0.71
3:E:56:LYS:HD3	3:E:56:LYS:H	1.56	0.71
3:E:108:ARG:NH1	3:E:108:ARG:HB2	2.05	0.71
4:F:72:SER:O	4:F:77:LYS:HG3	1.91	0.71
4:F:189:ARG:HD2	4:F:190:GLU:HB2	1.71	0.71
4:B:111:LEU:HD22	4:B:116:CYS:SG	2.31	0.71
4:F:186:LEU:O	4:F:191:LYS:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:123:VAL:CG1	4:B:132:VAL:HG11	2.21	0.71
3:A:206:CYS:HA	3:A:288:TYR:HD2	1.56	0.70
1:C:3:DG:H1'	1:C:4:DG:C8	2.25	0.70
3:E:241:GLN:HB2	5:E:847:HOH:O	1.90	0.70
4:B:195:ARG:CA	4:B:195:ARG:HH11	2.04	0.70
3:E:271:GLN:NE2	3:E:280:LEU:HD23	2.07	0.69
4:B:88:VAL:HG13	4:B:89:GLY:N	2.07	0.69
4:B:39:GLY:CA	4:B:86:ASN:HD22	2.04	0.69
3:E:282:GLU:HG3	3:E:283:PRO:HD2	1.72	0.69
3:A:166:ARG:NH1	3:A:166:ARG:HG3	2.08	0.69
4:B:55:PHE:HD2	4:B:141:HIS:HE2	1.40	0.69
4:F:41:TYR:CE2	4:F:85:CYS:HB2	2.26	0.69
4:F:42:LEU:HD21	4:F:214:PHE:HB3	1.74	0.69
3:A:76:LEU:HD11	3:A:88:HIS:O	1.91	0.69
3:E:49:GLU:HG3	3:E:50:ARG:HG3	1.73	0.69
2:H:22:DC:H2'	2:H:23:DC:C6	2.27	0.68
4:F:227:ARG:HE	4:F:227:ARG:HA	1.56	0.68
4:F:332:ARG:NH1	4:F:332:ARG:HG2	2.04	0.68
3:E:69:PRO:HG2	3:E:166:ARG:HH11	1.56	0.68
3:A:274:ARG:NH1	3:A:279:GLU:OE1	2.27	0.68
3:A:129:ALA:HA	3:A:132:GLN:OE1	1.94	0.68
1:C:8:DT:H2''	1:C:9:DT:C7	2.22	0.68
3:A:246:ARG:HD3	5:A:734:HOH:O	1.92	0.68
3:A:88:HIS:HB2	3:A:119:GLN:O	1.93	0.68
4:B:215:THR:CG2	4:B:228:ARG:HG3	2.23	0.68
3:A:149:ARG:HG2	3:A:150:GLY:N	2.07	0.68
5:G:705:HOH:O	3:E:246:ARG:HD3	1.94	0.68
4:B:148:PHE:HE1	4:B:199:VAL:HG22	1.58	0.68
3:E:73:ARG:HB3	3:E:162:GLN:HB2	1.76	0.68
4:B:154:ARG:HA	4:B:154:ARG:NE	2.09	0.68
4:F:250:ILE:CG2	4:F:268:LEU:HD21	2.18	0.67
4:F:167:LEU:HD21	4:F:228:ARG:HH21	1.57	0.67
3:E:257:TYR:CE1	3:E:266:VAL:HG11	2.30	0.67
2:D:22:DC:C2'	2:D:23:DC:H5''	2.23	0.67
3:E:108:ARG:HB2	3:E:108:ARG:HH11	1.59	0.67
3:E:190:ASN:HB3	3:E:220:GLN:HE22	1.57	0.67
3:E:182:PRO:HB2	3:E:184:PHE:CE1	2.30	0.67
4:B:218:LEU:HG	4:B:229:LEU:HD21	1.74	0.67
3:A:165:VAL:CG2	3:A:173:LEU:HB3	2.25	0.67
4:F:44:ILE:HG22	4:F:46:GLU:O	1.95	0.67
3:A:79:LYS:HA	3:A:158:ARG:NE	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:72:VAL:HG13	3:E:100:TYR:HE1	1.59	0.67
3:A:88:HIS:CG	3:A:120:CYS:HA	2.30	0.67
4:B:111:LEU:HD23	4:B:112:VAL:H	1.60	0.66
4:F:268:LEU:HD12	4:F:280:ILE:HD12	1.78	0.66
4:B:218:LEU:HD21	4:B:229:LEU:HD11	1.78	0.66
4:F:88:VAL:HG22	4:F:89:GLY:N	2.08	0.66
3:A:24:ILE:HB	3:A:25:GLU:OE2	1.96	0.66
4:F:186:LEU:O	4:F:191:LYS:HE3	1.95	0.66
3:E:122:LYS:NZ	3:E:124:ARG:HH21	1.94	0.66
3:E:70:GLY:HA3	3:E:104:LEU:HD22	1.78	0.66
4:B:114:LYS:HD2	4:B:135:ALA:O	1.96	0.66
3:A:148:GLN:HG2	3:A:152:TYR:OH	1.95	0.66
3:A:72:VAL:O	3:A:101:GLU:HA	1.96	0.66
4:F:84:ILE:CB	4:F:130:MET:HB3	2.24	0.65
4:B:125:ALA:CB	4:B:132:VAL:HG22	2.26	0.65
4:F:107:HIS:NE2	4:F:109:HIS:CD2	2.65	0.65
3:A:262:LEU:HD21	3:A:266:VAL:CG2	2.27	0.65
3:E:84:ARG:HB3	5:E:788:HOH:O	1.96	0.65
3:A:29:GLN:HE22	3:A:181:HIS:HB3	1.61	0.65
4:B:66:GLY:O	4:B:68:PRO:HD3	1.97	0.65
4:F:49:LYS:HE3	4:F:49:LYS:HA	1.77	0.65
4:F:304:HIS:HB3	4:F:308:ALA:HB3	1.79	0.65
4:F:107:HIS:CD2	4:F:109:HIS:H	2.14	0.65
3:E:28:LYS:HG2	3:E:49:GLU:HA	1.79	0.65
4:F:46:GLU:O	4:F:47:GLN:HG2	1.96	0.65
4:B:118:ASP:HB3	4:B:154:ARG:NH2	2.12	0.65
4:B:217:PHE:CD1	4:B:225:PHE:HB3	2.32	0.64
3:E:53:ASP:OD1	3:E:54:THR:HG23	1.97	0.64
4:F:279:GLN:OE1	4:F:332:ARG:NH1	2.30	0.64
3:A:60:THR:HA	3:A:112:SER:HA	1.77	0.64
3:E:31:GLY:CA	3:E:186:ASN:HD22	2.10	0.64
4:B:93:VAL:HG22	4:B:216:ALA:CB	2.27	0.64
4:F:209:VAL:HG22	4:F:238:TYR:HD2	1.62	0.64
3:A:106:PRO:C	3:A:108:ARG:H	2.00	0.64
3:A:165:VAL:O	3:A:166:ARG:HG3	1.98	0.64
4:B:191:LYS:O	4:B:195:ARG:HG2	1.98	0.64
4:B:115:HIS:CE1	4:B:123:VAL:HG23	2.33	0.64
3:E:206:CYS:HA	3:E:288:TYR:CD2	2.21	0.64
3:A:88:HIS:ND1	3:A:120:CYS:HA	2.13	0.64
4:F:97:LEU:HD21	4:F:111:LEU:CD2	2.28	0.64
4:F:45:LEU:HB3	4:F:81:GLN:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:26:GLN:OE1	3:A:181:HIS:N	2.23	0.63
3:E:58:HIS:CG	3:E:114:GLN:HG2	2.34	0.63
2:H:14:DA:H2'	2:H:15:DG:C8	2.33	0.63
4:B:114:LYS:NZ	4:B:136:ASN:HB3	2.13	0.63
3:A:208:GLY:HA2	3:A:254:THR:HG22	1.80	0.63
3:A:219:VAL:O	3:A:247:GLN:HG2	1.99	0.63
4:F:123:VAL:CG1	4:F:132:VAL:HG21	2.27	0.63
4:B:92:LYS:HE3	4:B:124:THR:OG1	1.99	0.63
3:E:190:ASN:HB3	3:E:220:GLN:NE2	2.13	0.63
4:F:50:GLN:HG2	4:F:236:ALA:O	1.98	0.63
4:F:192:GLU:O	4:F:196:GLN:HG3	1.98	0.63
3:E:246:ARG:O	3:E:248:VAL:HG22	1.99	0.63
4:B:56:ARG:HB3	4:B:56:ARG:HH11	1.60	0.63
4:B:73:GLU:O	4:B:74:LYS:HB2	1.99	0.63
4:F:221:SER:O	4:F:222:THR:HB	1.98	0.63
4:B:88:VAL:HG22	4:B:89:GLY:H	1.64	0.62
3:A:166:ARG:HA	3:A:171:ARG:O	2.00	0.62
3:E:51:SER:HB2	3:E:57:THR:OG1	1.99	0.62
3:A:88:HIS:HB3	3:A:121:VAL:N	2.14	0.62
3:E:79:LYS:HA	3:E:158:ARG:HE	1.64	0.62
3:A:79:LYS:NZ	3:A:79:LYS:HB3	2.14	0.62
4:B:94:ILE:HG12	4:B:215:THR:O	1.99	0.62
3:E:279:GLU:O	3:E:280:LEU:HD12	1.98	0.62
3:E:201:ARG:NH2	4:F:255:ARG:NH2	2.47	0.62
4:B:186:LEU:O	4:B:191:LYS:HB3	1.98	0.62
4:F:148:PHE:CD2	4:F:148:PHE:C	2.73	0.62
4:B:55:PHE:HB2	4:B:141:HIS:NE2	2.14	0.62
3:E:201:ARG:NH2	4:F:255:ARG:HH21	1.97	0.62
2:D:21:DT:O4	4:B:54:ARG:NH2	2.32	0.62
4:B:244:ASN:CB	4:B:274:GLN:HE22	2.12	0.62
1:G:10:DC:H2''	1:G:11:DC:C5'	2.30	0.62
4:B:45:LEU:HD12	4:B:46:GLU:HB2	1.82	0.62
4:F:105:HIS:HB3	4:F:201:GLN:HE21	1.63	0.62
4:B:114:LYS:HA	4:B:114:LYS:HE3	1.82	0.62
3:E:155:ASN:HB3	3:E:191:THR:HG21	1.81	0.62
3:A:63:ILE:HD12	3:A:63:ILE:N	2.12	0.62
3:A:206:CYS:HA	3:A:288:TYR:CD2	2.33	0.62
3:A:290:PRO:O	3:A:291:ASP:O	2.18	0.62
4:B:98:VAL:HG23	4:B:211:ARG:HB2	1.82	0.62
4:F:237:ILE:HD12	4:F:237:ILE:N	2.14	0.62
4:F:329:VAL:CG2	4:F:345:PHE:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:178:ALA:O	4:B:226:THR:HG23	1.99	0.61
4:B:244:ASN:HB3	4:B:274:GLN:NE2	2.14	0.61
3:A:24:ILE:HD11	3:A:62:LYS:HB2	1.81	0.61
4:B:279:GLN:HE22	4:B:332:ARG:HH21	1.46	0.61
4:B:93:VAL:HG22	4:B:216:ALA:HB2	1.83	0.61
4:B:129:ASP:HB3	5:B:827:HOH:O	2.00	0.61
4:F:162:GLY:C	4:F:163:TYR:HD1	2.04	0.61
3:E:28:LYS:HG3	3:E:47:PRO:O	2.01	0.61
4:F:42:LEU:HD12	4:F:83:LYS:O	2.00	0.61
4:F:165:PRO:N	4:F:167:LEU:HD13	2.15	0.61
3:A:143:VAL:HG13	3:A:147:GLU:OE1	1.99	0.61
1:G:11:DC:H2'	1:G:12:DT:C6	2.35	0.61
4:F:332:ARG:HD3	4:F:339:THR:HG22	1.83	0.61
4:F:148:PHE:O	4:F:148:PHE:HD2	1.83	0.60
3:A:74:ILE:H	3:A:74:ILE:HD12	1.66	0.60
4:B:143:THR:HG22	4:B:145:LYS:H	1.67	0.60
4:F:254:ASP:HB2	4:F:267:TYR:H	1.65	0.60
4:B:143:THR:HG21	5:B:815:HOH:O	2.01	0.60
3:E:200:ASN:CB	3:E:213:PHE:H	2.08	0.60
3:A:273:ARG:HD2	3:A:280:LEU:HD21	1.82	0.60
4:F:189:ARG:CD	4:F:190:GLU:N	2.64	0.60
1:C:9:DT:OP1	3:A:122:LYS:HD3	2.01	0.60
4:B:164:ASN:ND2	4:B:213:MET:SD	2.75	0.60
4:B:95:VAL:HG12	4:B:214:PHE:HD1	1.66	0.60
4:F:164:ASN:HA	4:F:167:LEU:HD22	1.84	0.60
1:G:6:DA:C2'	1:G:7:DA:O5'	2.50	0.60
3:E:77:VAL:HG12	3:E:85:PRO:HA	1.84	0.60
3:A:46:ILE:HG13	3:A:116:LEU:O	2.00	0.60
4:B:57:TYR:CD2	4:B:57:TYR:N	2.68	0.60
3:A:201:ARG:HG2	3:A:201:ARG:NH2	2.12	0.60
3:A:24:ILE:HD11	3:A:62:LYS:CD	2.32	0.60
4:B:40:PRO:O	4:B:229:LEU:HD22	2.02	0.59
4:B:155:MET:SD	4:B:198:ALA:HB2	2.42	0.59
3:A:93:LYS:CE	3:A:115:ASN:HB3	2.32	0.59
4:F:99:THR:HG23	4:F:105:HIS:O	2.02	0.59
3:A:186:ASN:HD21	3:A:193:GLU:HB2	1.67	0.59
5:H:760:HOH:O	4:F:145:LYS:HD3	2.00	0.59
4:B:106:LEU:HD22	4:B:168:LEU:CG	2.32	0.59
3:E:46:ILE:HG13	3:E:116:LEU:O	2.01	0.59
1:C:1:DT:H3'	4:B:65:GLY:CA	2.18	0.59
4:B:88:VAL:HG13	4:B:89:GLY:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:240:SER:HA	5:F:859:HOH:O	2.02	0.59
4:B:109:HIS:HE1	4:B:207:LEU:O	1.85	0.59
4:B:88:VAL:HG12	4:B:218:LEU:HD22	1.85	0.59
3:E:70:GLY:HA2	3:E:166:ARG:CZ	2.32	0.59
4:F:217:PHE:CE2	4:F:228:ARG:HB3	2.37	0.59
3:A:79:LYS:C	3:A:158:ARG:HE	2.06	0.59
4:F:126:GLY:N	4:F:127:PRO:CD	2.65	0.59
4:B:158:ALA:HA	4:B:163:TYR:CE1	2.38	0.59
3:E:226:VAL:HG23	3:E:239:PHE:CE1	2.37	0.59
1:G:1:DT:H4'	1:G:2:DG:OP1	2.02	0.59
3:E:29:GLN:HA	3:E:29:GLN:HE21	1.68	0.59
4:B:98:VAL:HG22	4:B:211:ARG:O	2.02	0.59
4:F:217:PHE:CD2	4:F:228:ARG:HB3	2.38	0.59
3:E:52:THR:HG22	3:E:53:ASP:N	2.18	0.59
3:E:201:ARG:NH1	3:E:210:ASP:HB3	2.18	0.59
3:A:57:THR:HG22	3:A:58:HIS:N	2.17	0.59
3:A:74:ILE:N	3:A:74:ILE:HD12	2.18	0.59
4:B:84:ILE:HB	4:B:130:MET:SD	2.43	0.58
3:A:24:ILE:HD11	3:A:62:LYS:CB	2.33	0.58
3:A:124:ARG:HG3	3:A:125:ASP:OD2	2.03	0.58
2:D:17:DA:H2''	2:D:18:DA:OP2	2.04	0.58
4:B:76:LYS:CG	4:B:77:LYS:H	2.15	0.58
3:A:108:ARG:HB3	3:A:111:HIS:HE1	1.65	0.58
3:A:163:VAL:O	3:A:174:LEU:HD12	2.03	0.58
4:B:346:LEU:HD13	4:B:346:LEU:C	2.23	0.58
4:B:165:PRO:HG2	4:B:166:GLY:H	1.68	0.58
2:D:14:DA:H2''	2:D:15:DG:O5'	2.04	0.58
1:G:3:DG:H2'	1:G:4:DG:C8	2.38	0.58
3:E:86:HIS:ND1	3:E:87:PRO:HD2	2.18	0.58
4:B:42:LEU:HD23	4:B:84:ILE:HG13	1.84	0.58
3:E:198:ARG:NH2	4:F:310:VAL:HG11	2.19	0.58
3:E:108:ARG:CB	3:E:108:ARG:HH11	2.16	0.58
3:E:46:ILE:HD12	3:E:116:LEU:HD13	1.84	0.58
4:F:66:GLY:O	4:F:68:PRO:HD3	2.04	0.58
1:G:1:DT:H2'	1:G:2:DG:C8	2.39	0.58
4:F:87:TYR:HD2	4:F:88:VAL:O	1.87	0.58
3:E:127:GLU:O	3:E:130:ILE:HG22	2.02	0.58
3:A:262:LEU:HD11	3:A:266:VAL:HG21	1.86	0.58
4:B:83:LYS:C	4:B:84:ILE:HD12	2.23	0.58
2:D:19:DT:H2''	4:B:57:TYR:OH	2.03	0.58
4:B:76:LYS:HG3	4:B:77:LYS:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:277:ASP:OD2	4:B:334:LYS:HB2	2.04	0.58
4:B:219:PRO:HG3	4:B:225:PHE:CE1	2.39	0.58
4:F:45:LEU:HD23	4:F:81:GLN:CB	2.33	0.58
3:A:31:GLY:N	3:A:186:ASN:HD22	2.01	0.58
4:B:228:ARG:HG2	4:B:229:LEU:N	2.19	0.58
3:A:79:LYS:HG2	3:A:79:LYS:O	2.03	0.58
3:E:273:ARG:CD	3:E:280:LEU:HD11	2.25	0.57
4:F:163:TYR:O	4:F:164:ASN:C	2.42	0.57
2:D:21:DT:H2'	4:B:59:CYS:O	2.04	0.57
4:B:333:ARG:HB3	4:B:336:ASP:OD2	2.04	0.57
4:F:254:ASP:HB2	4:F:267:TYR:HB2	1.84	0.57
4:F:88:VAL:HG13	4:F:89:GLY:N	2.19	0.57
3:A:74:ILE:HD13	3:A:100:TYR:CD1	2.39	0.57
3:E:266:VAL:CG1	3:E:288:TYR:HB2	2.33	0.57
2:D:21:DT:H3'	4:B:59:CYS:HG	1.69	0.57
4:B:123:VAL:HG21	4:B:132:VAL:CG1	2.35	0.57
4:B:62:PRO:HD2	5:B:843:HOH:O	2.03	0.57
3:A:86:HIS:CE1	3:A:154:LEU:HA	2.39	0.57
2:H:22:DC:H2'	2:H:23:DC:H6	1.68	0.57
2:D:22:DC:OP2	4:B:59:CYS:SG	2.61	0.57
4:F:343:LYS:HE2	5:F:753:HOH:O	2.04	0.57
3:A:26:GLN:CD	3:A:181:HIS:H	2.06	0.57
3:A:209:GLY:HA2	3:A:253:ARG:CD	2.34	0.57
4:B:38:MET:O	4:B:40:PRO:HD2	2.04	0.57
4:F:46:GLU:OE1	4:F:78:SER:OG	2.20	0.57
3:E:122:LYS:HZ2	3:E:124:ARG:HH21	1.52	0.57
4:F:165:PRO:C	4:F:167:LEU:H	2.07	0.57
2:H:20:DT:H2''	2:H:21:DT:C5'	2.34	0.57
3:A:79:LYS:CA	3:A:158:ARG:HE	2.18	0.57
3:E:131:SER:C	3:E:133:ARG:H	2.09	0.57
3:A:277:ASP:OD1	3:A:279:GLU:HG2	2.05	0.57
3:E:99:TYR:HB3	3:E:138:ASN:HD21	1.70	0.57
4:B:176:LEU:HD21	4:B:184:ARG:HG2	1.87	0.57
1:C:1:DT:H2''	1:C:2:DG:O5'	2.03	0.56
3:E:70:GLY:CA	3:E:104:LEU:HD22	2.35	0.56
3:E:70:GLY:HA2	3:E:166:ARG:NH2	2.19	0.56
3:E:70:GLY:O	3:E:104:LEU:HD13	2.04	0.56
3:E:198:ARG:HH21	4:F:310:VAL:HG11	1.70	0.56
1:G:8:DT:H71	3:E:187:ARG:HD3	1.87	0.56
3:E:184:PHE:CD1	3:E:184:PHE:N	2.74	0.56
3:E:19:ALA:O	3:E:175:LEU:HD22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:175:TYR:CD1	4:F:176:LEU:HG	2.41	0.56
1:C:5:DA:H3'	3:A:247:GLN:HE22	1.70	0.56
3:A:19:ALA:O	3:A:175:LEU:HD22	2.05	0.56
1:G:11:DC:N3	2:H:15:DG:N1	2.40	0.56
4:B:154:ARG:HA	4:B:154:ARG:HE	1.71	0.56
4:B:328:PHE:HE1	4:B:344:PRO:HG3	1.70	0.56
3:A:270:MET:HE2	3:A:286:PHE:HB2	1.87	0.56
3:E:34:PHE:N	3:E:34:PHE:CD2	2.73	0.56
4:F:176:LEU:CD2	4:F:184:ARG:HG3	2.26	0.56
3:A:86:HIS:CD2	3:A:157:VAL:HG12	2.40	0.56
3:E:74:ILE:HG12	3:E:100:TYR:CD1	2.40	0.56
4:F:327:VAL:O	4:F:328:PHE:HD1	1.89	0.56
3:A:229:THR:HG23	3:A:271:GLN:OE1	2.06	0.56
3:A:71:THR:HG23	3:A:164:THR:HB	1.86	0.56
4:B:40:PRO:CG	4:B:218:LEU:HD11	2.36	0.56
3:E:56:LYS:CD	3:E:56:LYS:H	2.19	0.56
4:B:346:LEU:HD13	4:B:346:LEU:O	2.06	0.56
4:B:143:THR:HB	4:B:146:LYS:HD3	1.88	0.56
2:D:17:DA:C2'	4:B:306:GLN:HE22	2.15	0.56
4:B:39:GLY:HA2	4:B:86:ASN:HD22	1.69	0.56
3:E:81:PRO:O	3:E:83:HIS:N	2.39	0.55
3:E:28:LYS:HD3	3:E:47:PRO:CG	2.36	0.55
4:B:58:VAL:HG13	4:B:59:CYS:N	2.20	0.55
1:G:2:DG:H2''	1:G:3:DG:C5'	2.36	0.55
3:A:282:GLU:OE1	3:A:283:PRO:HD2	2.06	0.55
3:E:130:ILE:CG2	3:E:131:SER:N	2.69	0.55
1:C:11:DC:H2'	5:C:763:HOH:O	2.04	0.55
3:A:79:LYS:HA	3:A:158:ARG:HE	1.71	0.55
3:E:24:ILE:HG22	3:E:60:THR:O	2.06	0.55
3:A:79:LYS:HA	3:A:158:ARG:HD2	1.89	0.55
3:E:139:ASN:HD21	3:E:143:VAL:N	2.05	0.55
4:B:187:THR:C	4:B:189:ARG:H	2.11	0.55
4:F:71:SER:O	4:F:77:LYS:HG2	2.07	0.55
3:A:60:THR:HG21	3:A:110:ILE:HG22	1.89	0.55
4:F:273:VAL:O	4:F:306:GLN:HB3	2.07	0.55
4:F:254:ASP:CB	4:F:267:TYR:H	2.19	0.54
4:B:254:ASP:CB	4:B:267:TYR:H	2.21	0.54
4:F:116:CYS:SG	4:F:137:LEU:HD21	2.47	0.54
3:E:66:TYR:CD1	3:E:67:THR:N	2.75	0.54
2:D:19:DT:H4'	2:D:20:DT:OP1	2.06	0.54
4:F:47:GLN:O	4:F:69:GLY:HA2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:167:LEU:CD1	4:F:167:LEU:N	2.69	0.54
3:E:23:ILE:CD1	3:E:161:PHE:HE2	2.20	0.54
4:F:55:PHE:CE2	4:F:239:ASP:HB2	2.43	0.54
4:B:83:LYS:HB2	4:B:131:VAL:HG22	1.89	0.54
3:E:73:ARG:HD2	3:E:99:TYR:CD2	2.42	0.54
3:A:187:ARG:HH11	3:A:187:ARG:HG2	1.71	0.54
1:C:5:DA:H3'	3:A:247:GLN:NE2	2.23	0.54
3:A:35:ARG:NE	3:A:35:ARG:HA	2.17	0.54
2:H:15:DG:H2''	2:H:16:DG:O5'	2.08	0.54
4:B:45:LEU:CD1	4:B:81:GLN:HB2	2.37	0.54
3:A:93:LYS:HB3	3:A:115:ASN:HB3	1.90	0.54
4:B:161:ARG:HB2	4:B:163:TYR:HE1	1.73	0.54
3:E:272:LEU:H	3:E:281:SER:HB3	1.73	0.54
4:B:41:TYR:HA	4:B:229:LEU:HB3	1.87	0.54
4:B:111:LEU:HD23	4:B:112:VAL:N	2.22	0.54
3:A:200:ASN:HD21	4:B:254:ASP:CG	2.11	0.54
1:C:5:DA:H61	4:B:54:ARG:HH22	1.54	0.54
4:B:272:LYS:HD2	4:B:306:GLN:OE1	2.08	0.54
3:E:136:THR:HG23	3:E:138:ASN:HB2	1.90	0.54
2:H:21:DT:C2'	2:H:22:DC:O5'	2.53	0.54
4:B:151:LEU:O	4:B:155:MET:HG3	2.08	0.54
4:B:185:GLN:HA	4:B:185:GLN:HE21	1.72	0.54
4:B:240:SER:C	4:B:242:ALA:H	2.10	0.54
3:A:61:ILE:HD11	3:A:161:PHE:CE2	2.42	0.54
3:A:61:ILE:HG22	3:A:62:LYS:N	2.23	0.54
3:A:146:GLU:HA	3:A:149:ARG:NH1	2.23	0.53
3:E:86:HIS:CD2	3:E:157:VAL:HG12	2.43	0.53
3:A:191:THR:HA	3:A:274:ARG:NH1	2.23	0.53
4:F:117:GLU:O	4:F:118:ASP:HB2	2.09	0.53
3:E:128:GLN:OE1	3:E:128:GLN:O	2.26	0.53
4:B:104:ILE:O	4:B:104:ILE:HG13	2.07	0.53
4:B:114:LYS:HZ2	4:B:136:ASN:HB3	1.74	0.53
3:A:40:GLY:O	3:A:41:ARG:C	2.46	0.53
4:F:341:GLU:HA	4:F:341:GLU:OE1	2.08	0.53
4:F:160:ILE:HG13	4:F:161:ARG:N	2.22	0.53
3:E:91:VAL:O	3:E:116:LEU:HA	2.08	0.53
4:F:157:GLU:OE1	4:F:157:GLU:HA	2.08	0.53
3:A:35:ARG:CA	3:A:35:ARG:HE	2.19	0.53
4:B:329:VAL:HG23	4:B:345:PHE:CB	2.37	0.53
4:B:84:ILE:HD12	4:B:84:ILE:N	2.23	0.53
4:F:45:LEU:HD23	4:F:81:GLN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:209:GLY:HA2	3:A:253:ARG:NE	2.23	0.53
3:E:88:HIS:ND1	3:E:120:CYS:HA	2.24	0.53
4:F:219:PRO:HG3	4:F:225:PHE:CE1	2.44	0.53
1:G:10:DC:H2''	1:G:11:DC:H5'	1.91	0.53
4:F:108:ALA:CB	4:F:142:VAL:HG11	2.38	0.53
3:A:25:GLU:OE2	3:A:60:THR:HB	2.08	0.53
4:B:173:LEU:N	4:B:173:LEU:HD22	2.24	0.53
4:F:203:LYS:HD2	4:F:203:LYS:N	2.24	0.53
2:H:16:DG:H2''	2:H:17:DA:C5'	2.39	0.53
3:A:36:TYR:HB2	3:A:39:GLU:HG2	1.91	0.53
3:A:105:CYS:HB3	3:A:108:ARG:CB	2.38	0.53
4:F:300:PRO:O	4:F:303:VAL:HG23	2.09	0.53
4:F:166:GLY:C	4:F:167:LEU:HD12	2.30	0.52
4:B:148:PHE:HZ	4:B:195:ARG:HH22	1.57	0.52
4:B:286:GLU:HB2	4:B:290:GLY:CA	2.33	0.52
3:A:25:GLU:OE2	3:A:25:GLU:N	2.42	0.52
3:E:27:PRO:HB3	3:E:183:ILE:HD11	1.92	0.52
4:F:209:VAL:HG22	4:F:238:TYR:CD2	2.42	0.52
3:A:190:ASN:HB3	3:A:220:GLN:OE1	2.09	0.52
3:E:210:ASP:O	3:E:254:THR:HG23	2.09	0.52
3:E:78:THR:HG21	5:E:700:HOH:O	2.08	0.52
4:F:165:PRO:HG2	4:F:176:LEU:O	2.09	0.52
1:G:3:DG:N7	4:F:56:ARG:NH2	2.53	0.52
3:E:164:THR:HG22	3:E:164:THR:O	2.09	0.52
4:B:44:ILE:HG22	4:B:46:GLU:O	2.09	0.52
3:A:144:PRO:HG2	3:A:147:GLU:HB2	1.89	0.52
4:B:106:LEU:HD22	4:B:168:LEU:HG	1.90	0.52
4:F:101:GLY:O	4:F:102:LYS:C	2.48	0.52
4:F:165:PRO:O	4:F:167:LEU:N	2.41	0.52
3:A:190:ASN:ND2	3:A:190:ASN:H	2.08	0.52
1:G:10:DC:H2''	1:G:11:DC:O5'	2.09	0.52
1:G:7:DA:H2''	1:G:8:DT:O5'	2.10	0.52
4:B:155:MET:CE	4:B:169:VAL:HG13	2.40	0.52
3:E:257:TYR:HB2	3:E:288:TYR:CD2	2.44	0.52
3:E:96:ARG:O	3:E:98:GLY:N	2.42	0.52
4:F:318:ASP:O	4:F:318:ASP:OD2	2.28	0.52
4:B:53:PHE:CD2	4:B:55:PHE:HD1	2.28	0.52
3:A:255:PRO:HG2	3:A:288:TYR:OH	2.10	0.52
3:A:185:ASP:C	3:A:187:ARG:H	2.13	0.52
4:B:107:HIS:ND1	4:B:210:VAL:HG23	2.25	0.52
4:B:143:THR:HB	4:B:146:LYS:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:218:LEU:HD12	4:B:227:ARG:NH2	2.25	0.52
4:F:72:SER:C	4:F:74:LYS:H	2.12	0.52
3:A:232:GLY:O	3:E:141:PHE:HA	2.10	0.52
3:E:149:ARG:HD2	5:E:741:HOH:O	2.09	0.52
3:E:51:SER:OG	3:E:56:LYS:HA	2.10	0.51
4:B:42:LEU:HD13	4:B:214:PHE:HB3	1.92	0.51
3:A:19:ALA:HB1	3:A:64:ASN:O	2.10	0.51
4:F:115:HIS:HB3	4:F:122:THR:O	2.09	0.51
4:F:175:TYR:HA	4:F:177:GLN:OE1	2.10	0.51
3:E:130:ILE:O	3:E:133:ARG:HB2	2.11	0.51
3:A:25:GLU:HB2	3:A:59:PRO:HA	1.91	0.51
3:E:241:GLN:HA	3:E:241:GLN:HE21	1.75	0.51
3:E:19:ALA:HB3	3:E:175:LEU:HD21	1.92	0.51
3:A:187:ARG:NH1	3:A:187:ARG:HG2	2.24	0.51
4:B:47:GLN:NE2	4:B:235:ASP:OD1	2.44	0.51
4:F:84:ILE:HG13	4:F:130:MET:O	2.11	0.51
4:F:179:GLU:HG2	4:F:184:ARG:NH2	2.26	0.51
4:F:187:THR:C	4:F:189:ARG:H	2.14	0.51
3:A:157:VAL:HG11	5:A:736:HOH:O	2.10	0.51
3:E:106:PRO:C	3:E:108:ARG:H	2.12	0.51
3:E:108:ARG:N	3:E:108:ARG:HH11	2.08	0.51
3:A:190:ASN:HD22	3:A:190:ASN:N	2.08	0.51
4:F:244:ASN:OD1	4:F:244:ASN:C	2.49	0.51
4:B:50:GLN:HG3	4:B:236:ALA:O	2.10	0.51
3:E:201:ARG:NH1	3:E:211:GLU:O	2.43	0.51
3:E:213:PHE:HB3	4:F:267:TYR:HD2	1.76	0.51
4:B:56:ARG:CB	4:B:56:ARG:HH11	2.21	0.51
3:A:24:ILE:HD11	3:A:62:LYS:HD2	1.91	0.51
4:F:95:VAL:HA	4:F:213:MET:O	2.10	0.51
4:F:155:MET:SD	4:F:198:ALA:HB2	2.50	0.51
4:B:84:ILE:HG22	4:B:87:TYR:HB3	1.92	0.51
3:A:146:GLU:HA	3:A:149:ARG:NH2	2.26	0.51
3:A:218:LYS:HA	3:A:247:GLN:O	2.11	0.51
2:D:17:DA:H2'	4:B:306:GLN:NE2	2.21	0.51
4:B:236:ALA:HB3	4:B:238:TYR:CZ	2.46	0.51
3:E:145:ILE:HD12	3:E:145:ILE:N	2.26	0.51
4:F:268:LEU:HD12	4:F:280:ILE:CD1	2.41	0.51
4:F:95:VAL:HG23	4:F:213:MET:O	2.10	0.51
3:A:262:LEU:HD11	3:A:266:VAL:CG2	2.40	0.51
3:A:84:ARG:HB3	3:A:148:GLN:HG3	1.93	0.51
4:B:106:LEU:HD22	4:B:168:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:84:ILE:CB	4:B:130:MET:SD	2.99	0.51
3:E:257:TYR:OH	3:E:266:VAL:HG21	2.11	0.51
3:E:266:VAL:O	3:E:266:VAL:HG13	2.10	0.51
4:B:126:GLY:N	4:B:127:PRO:CD	2.73	0.51
3:E:76:LEU:HD22	3:E:157:VAL:HB	1.93	0.51
4:F:97:LEU:HG	4:F:111:LEU:HG	1.93	0.51
4:F:271:ASP:O	4:F:273:VAL:HG13	2.11	0.51
4:B:291:VAL:HG13	4:B:291:VAL:O	2.11	0.51
3:A:239:PHE:HB3	3:A:252:PHE:CB	2.41	0.51
4:B:254:ASP:HB2	4:B:267:TYR:H	1.75	0.51
3:E:67:THR:HG22	3:E:106:PRO:O	2.10	0.51
4:F:175:TYR:O	4:F:176:LEU:HB2	2.12	0.50
3:A:77:VAL:HG22	3:A:158:ARG:O	2.11	0.50
2:D:21:DT:H3'	4:B:59:CYS:SG	2.52	0.50
4:F:114:LYS:HD2	4:F:135:ALA:O	2.11	0.50
3:A:84:ARG:H	3:A:84:ARG:NE	2.05	0.50
4:F:272:LYS:HA	4:F:306:GLN:O	2.11	0.50
4:F:93:VAL:HA	4:F:216:ALA:HA	1.93	0.50
3:E:41:ARG:HD3	3:E:41:ARG:N	2.27	0.50
4:B:87:TYR:CD1	4:B:130:MET:HB2	2.46	0.50
2:D:21:DT:H73	4:B:60:GLU:HB2	1.93	0.50
4:F:227:ARG:NE	4:F:227:ARG:CA	2.71	0.50
3:A:46:ILE:HD12	3:A:116:LEU:HD22	1.93	0.50
4:F:286:GLU:HB3	4:F:287:GLU:OE2	2.09	0.50
4:B:87:TYR:HB2	4:B:130:MET:SD	2.51	0.50
4:B:152:GLU:OE2	4:B:195:ARG:NH1	2.45	0.50
3:E:31:GLY:HA2	3:E:186:ASN:HD22	1.73	0.50
4:F:148:PHE:HD2	4:F:148:PHE:C	2.14	0.50
4:F:316:TYR:CG	4:F:317:LYS:N	2.79	0.50
4:F:73:GLU:O	4:F:75:ASN:N	2.43	0.50
4:B:222:THR:HG21	5:B:718:HOH:O	2.12	0.50
4:B:42:LEU:HD11	4:B:93:VAL:HG13	1.93	0.50
4:F:95:VAL:CG1	4:F:121:CYS:HB2	2.42	0.50
4:B:299:SER:OG	4:B:300:PRO:HD2	2.12	0.50
4:F:189:ARG:HD2	4:F:190:GLU:CB	2.42	0.50
3:E:27:PRO:O	3:E:181:HIS:NE2	2.44	0.50
3:E:58:HIS:CD2	3:E:114:GLN:HA	2.46	0.50
3:A:267:ARG:HD3	5:A:861:HOH:O	2.12	0.50
4:B:117:GLU:O	4:B:117:GLU:HG3	2.11	0.50
4:B:187:THR:C	4:B:189:ARG:N	2.64	0.50
4:B:237:ILE:O	4:B:238:TYR:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:78:THR:HG22	3:A:79:LYS:N	2.27	0.50
3:E:27:PRO:CB	3:E:183:ILE:HD11	2.42	0.50
3:E:106:PRO:C	3:E:108:ARG:N	2.64	0.50
1:G:4:DG:H3'	3:E:246:ARG:HH11	1.73	0.50
3:A:127:GLU:OE2	3:A:128:GLN:HG3	2.12	0.50
3:E:130:ILE:HG23	3:E:131:SER:N	2.27	0.50
4:F:49:LYS:HG3	4:F:49:LYS:O	2.12	0.50
3:A:203:SER:O	3:A:204:GLY:O	2.30	0.50
4:B:99:THR:HG23	4:B:206:ASP:OD2	2.12	0.50
1:C:5:DA:H2''	1:C:6:DA:H8	1.77	0.49
4:F:329:VAL:HG23	4:F:345:PHE:CB	2.36	0.49
3:A:259:ASP:OD2	3:A:262:LEU:HA	2.12	0.49
3:A:105:CYS:HB3	3:A:108:ARG:HB3	1.92	0.49
4:B:157:GLU:HG3	4:B:163:TYR:OH	2.12	0.49
3:E:167:ASP:O	3:E:169:ALA:N	2.44	0.49
4:B:88:VAL:CG1	4:B:218:LEU:HD13	2.43	0.49
3:E:200:ASN:HB2	3:E:213:PHE:N	2.10	0.49
4:B:118:ASP:HB3	4:B:154:ARG:HH22	1.77	0.49
3:E:271:GLN:HG2	3:E:283:PRO:HA	1.94	0.49
3:A:78:THR:O	3:A:158:ARG:HD2	2.12	0.49
3:E:174:LEU:CD2	3:E:174:LEU:H	2.13	0.49
3:E:255:PRO:HG2	3:E:288:TYR:OH	2.11	0.49
1:C:3:DG:H1'	1:C:4:DG:N7	2.27	0.49
3:E:111:HIS:HD2	3:E:111:HIS:N	2.00	0.49
4:F:108:ALA:HB3	4:F:205:MET:CE	2.43	0.49
3:A:74:ILE:HB	3:A:100:TYR:HB3	1.93	0.49
4:B:112:VAL:HG12	4:B:113:GLY:N	2.27	0.49
1:G:1:DT:H2''	1:G:2:DG:O5'	2.11	0.49
4:B:53:PHE:CE2	4:B:55:PHE:HA	2.47	0.49
4:B:176:LEU:CD2	4:B:184:ARG:HG2	2.42	0.49
4:B:236:ALA:HB3	4:B:238:TYR:CE1	2.47	0.49
4:B:308:ALA:C	4:B:309:ILE:HG13	2.33	0.49
3:E:228:PHE:CD2	3:E:255:PRO:HG3	2.48	0.49
1:G:2:DG:C2'	1:G:3:DG:O5'	2.61	0.49
2:H:20:DT:H2''	2:H:21:DT:H5'	1.93	0.49
4:F:100:ASN:OD1	4:F:101:GLY:N	2.45	0.49
3:E:178:VAL:HG22	3:E:179:LEU:N	2.28	0.49
3:A:89:GLU:HB3	3:A:98:GLY:HA2	1.95	0.49
4:F:237:ILE:CD1	4:F:237:ILE:N	2.75	0.49
1:C:8:DT:C2'	1:C:9:DT:H72	2.39	0.49
4:F:103:ASN:HB3	4:F:105:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:84:ARG:HG2	3:E:143:VAL:HG11	1.95	0.49
3:A:26:GLN:OE1	3:A:27:PRO:HD2	2.13	0.49
4:F:282:PHE:CD2	4:F:329:VAL:HG22	2.48	0.49
3:A:60:THR:CG2	3:A:110:ILE:HG22	2.43	0.49
4:B:83:LYS:HB3	4:B:131:VAL:HG13	1.95	0.49
4:B:215:THR:HG23	4:B:228:ARG:CG	2.38	0.49
4:B:115:HIS:HB3	4:B:122:THR:O	2.13	0.49
4:F:108:ALA:HB3	4:F:142:VAL:HG11	1.94	0.49
3:A:74:ILE:HG13	3:A:161:PHE:CE1	2.48	0.49
4:B:88:VAL:HG22	4:B:89:GLY:N	2.27	0.48
3:E:26:GLN:O	3:E:49:GLU:HB3	2.13	0.48
4:F:287:GLU:O	4:F:288:ASN:C	2.51	0.48
4:F:286:GLU:OE1	4:F:317:LYS:HE2	2.13	0.48
4:B:143:THR:CB	4:B:146:LYS:HD3	2.43	0.48
4:B:228:ARG:HD2	4:B:231:PRO:CG	2.43	0.48
4:B:333:ARG:HG2	4:B:335:SER:OG	2.13	0.48
4:B:284:GLU:O	4:B:291:VAL:HA	2.13	0.48
1:C:1:DT:H2'	1:C:2:DG:C8	2.49	0.48
3:E:201:ARG:HH21	4:F:255:ARG:HH21	1.60	0.48
4:F:187:THR:OG1	4:F:189:ARG:HG3	2.13	0.48
4:B:195:ARG:NH1	4:B:195:ARG:CA	2.74	0.48
4:B:115:HIS:CD2	4:B:115:HIS:N	2.80	0.48
3:A:28:LYS:HD2	3:A:49:GLU:OE2	2.13	0.48
4:B:148:PHE:CE1	4:B:199:VAL:HG22	2.45	0.48
4:B:42:LEU:HD12	4:B:214:PHE:O	2.14	0.48
3:E:282:GLU:CG	3:E:283:PRO:HD2	2.42	0.48
4:B:186:LEU:H	4:B:186:LEU:CD1	2.12	0.48
3:A:74:ILE:H	3:A:74:ILE:CD1	2.27	0.48
3:E:66:TYR:CE1	3:E:68:GLY:N	2.81	0.48
3:A:216:CYS:O	4:B:304:HIS:HE1	1.96	0.48
4:F:321:ILE:HG13	4:F:323:LYS:H	1.79	0.48
4:B:186:LEU:HD12	4:B:186:LEU:N	2.16	0.48
3:E:181:HIS:HB2	3:E:182:PRO:HD2	1.95	0.48
3:A:62:LYS:HG2	3:A:64:ASN:HD21	1.78	0.48
3:A:80:ASP:O	3:A:84:ARG:NH2	2.46	0.48
3:E:132:GLN:O	3:E:136:THR:HG22	2.14	0.48
3:E:37:LYS:O	3:E:39:GLU:N	2.47	0.48
1:G:2:DG:H2''	1:G:3:DG:H5'	1.94	0.48
3:E:71:THR:HG22	3:E:72:VAL:N	2.29	0.48
4:B:57:TYR:CD1	4:B:141:HIS:HB2	2.48	0.48
4:F:90:PRO:HA	4:F:126:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:110:SER:HB3	4:B:119:GLY:CA	2.44	0.48
3:E:274:ARG:NE	3:E:277:ASP:OD1	2.45	0.48
4:F:259:CYS:SG	4:F:350:GLU:HG2	2.54	0.48
4:B:125:ALA:C	4:B:127:PRO:HD2	2.33	0.48
3:E:196:ILE:HG23	3:E:214:LEU:HD21	1.94	0.48
3:A:127:GLU:O	3:A:130:ILE:HG22	2.14	0.48
2:D:22:DC:H2''	2:D:23:DC:C5'	2.36	0.48
3:A:62:LYS:HG2	3:A:64:ASN:ND2	2.28	0.48
4:F:170:HIS:O	4:F:172:ASP:N	2.47	0.48
4:F:187:THR:C	4:F:189:ARG:N	2.66	0.47
3:E:248:VAL:CG1	4:F:305:ARG:HG3	2.43	0.47
4:B:53:PHE:O	4:B:240:SER:HB2	2.14	0.47
4:B:109:HIS:CD2	4:B:142:VAL:HG12	2.49	0.47
4:B:218:LEU:CG	4:B:229:LEU:HD21	2.43	0.47
3:E:63:ILE:O	3:E:63:ILE:HG13	2.13	0.47
4:B:114:LYS:CA	4:B:114:LYS:HE3	2.43	0.47
3:E:218:LYS:HA	3:E:247:GLN:O	2.14	0.47
1:C:6:DA:H5'	5:C:806:HOH:O	2.13	0.47
3:E:59:PRO:O	3:E:113:PHE:HD1	1.97	0.47
4:B:111:LEU:HD23	4:B:138:GLY:O	2.15	0.47
4:F:84:ILE:CG1	4:F:130:MET:HB3	2.44	0.47
4:B:172:ASP:C	4:B:173:LEU:HD22	2.34	0.47
3:A:146:GLU:HA	3:A:149:ARG:CZ	2.44	0.47
3:E:41:ARG:H	3:E:41:ARG:HD3	1.77	0.47
4:F:333:ARG:HD2	4:F:336:ASP:OD1	2.14	0.47
4:B:219:PRO:HG3	4:B:225:PHE:HE1	1.78	0.47
3:A:106:PRO:C	3:A:108:ARG:N	2.68	0.47
4:F:321:ILE:O	4:F:349:PRO:HB3	2.15	0.47
4:B:93:VAL:HA	4:B:216:ALA:HA	1.97	0.47
4:B:41:TYR:O	4:B:84:ILE:HG23	2.15	0.47
3:A:273:ARG:NH1	3:E:81:PRO:HD2	2.30	0.47
3:A:200:ASN:CG	3:A:213:PHE:HB2	2.34	0.47
4:F:70:ALA:O	4:F:71:SER:HB2	2.15	0.47
1:G:6:DA:H2'	1:G:7:DA:C8	2.50	0.47
1:C:9:DT:H2''	1:C:10:DC:OP2	2.15	0.47
4:B:117:GLU:O	4:B:118:ASP:HB2	2.14	0.47
4:F:50:GLN:NE2	4:F:235:ASP:HB3	2.29	0.47
3:E:116:LEU:HD12	3:E:116:LEU:O	2.15	0.47
3:E:194:LEU:HB3	3:E:281:SER:HB2	1.97	0.47
3:A:233:TRP:HA	3:E:141:PHE:O	2.15	0.47
3:A:75:SER:OG	3:A:162:GLN:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:240:SER:OG	3:A:243:ASP:OD2	2.31	0.47
4:F:183:ASP:O	4:F:183:ASP:OD1	2.32	0.47
4:B:57:TYR:HD2	4:B:57:TYR:N	2.12	0.47
3:A:84:ARG:HG2	3:A:148:GLN:HA	1.97	0.47
4:B:216:ALA:O	4:B:229:LEU:HG	2.15	0.47
3:E:227:TYR:CE2	3:E:229:THR:HG22	2.49	0.47
3:E:23:ILE:HB	3:E:26:GLN:HG3	1.97	0.47
2:D:19:DT:H2"	2:D:20:DT:H71	1.96	0.47
4:F:108:ALA:HB3	4:F:205:MET:HE3	1.96	0.47
4:F:116:CYS:SG	4:F:137:LEU:CD2	3.03	0.47
3:A:190:ASN:ND2	3:A:190:ASN:N	2.62	0.47
4:B:95:VAL:HA	4:B:213:MET:O	2.15	0.46
3:A:63:ILE:CD1	3:A:63:ILE:H	2.20	0.46
4:B:69:GLY:O	4:B:71:SER:N	2.48	0.46
4:B:79:TYR:O	4:B:81:GLN:HG2	2.15	0.46
3:A:60:THR:OG1	3:A:112:SER:HB2	2.15	0.46
3:A:261:SER:HA	3:A:291:ASP:OD2	2.15	0.46
3:A:46:ILE:CG1	3:A:116:LEU:HD13	2.45	0.46
4:B:316:TYR:CG	4:B:317:LYS:N	2.83	0.46
3:A:200:ASN:OD1	4:B:254:ASP:OD1	2.33	0.46
4:F:121:CYS:SG	4:F:137:LEU:HD21	2.55	0.46
4:F:55:PHE:CD2	4:F:239:ASP:HB2	2.50	0.46
3:E:140:PRO:HB3	3:E:160:CYS:SG	2.54	0.46
3:A:245:HIS:CE1	4:B:251:VAL:HG21	2.50	0.46
1:C:9:DT:OP2	3:A:36:TYR:HB3	2.14	0.46
3:A:139:ASN:OD1	3:A:142:HIS:HA	2.14	0.46
4:B:318:ASP:C	4:B:320:ASN:H	2.19	0.46
4:F:173:LEU:HB3	4:F:176:LEU:HD12	1.96	0.46
3:A:100:TYR:CD1	3:A:100:TYR:C	2.89	0.46
3:A:191:THR:O	3:A:191:THR:HG23	2.15	0.46
3:A:41:ARG:HD3	3:A:41:ARG:N	2.29	0.46
3:E:160:CYS:HA	3:E:178:VAL:O	2.16	0.46
4:F:247:ASN:HD22	4:F:247:ASN:HA	1.57	0.46
3:A:236:ARG:NE	3:E:82:PRO:HG2	2.26	0.46
4:B:125:ALA:HB3	4:B:132:VAL:CG2	2.40	0.46
3:E:135:GLN:HA	3:E:135:GLN:OE1	2.15	0.46
4:B:93:VAL:HG13	4:B:216:ALA:HB2	1.96	0.46
4:F:77:LYS:HG2	5:F:755:HOH:O	2.15	0.46
4:F:146:LYS:O	4:F:150:THR:HB	2.14	0.46
3:E:227:TYR:CD2	3:E:280:LEU:HD21	2.50	0.46
3:E:78:THR:O	3:E:83:HIS:HD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:81:PRO:HB2	3:E:82:PRO:CD	2.39	0.46
3:A:36:TYR:O	3:A:37:LYS:C	2.54	0.46
3:A:46:ILE:HB	3:A:116:LEU:HD13	1.98	0.46
3:E:196:ILE:HG12	3:E:272:LEU:HD22	1.97	0.46
4:B:311:PHE:C	4:B:311:PHE:CD1	2.88	0.46
3:E:141:PHE:CZ	3:E:179:LEU:HD11	2.51	0.46
4:F:287:GLU:O	4:F:289:GLY:N	2.48	0.46
4:F:172:ASP:C	4:F:174:ALA:H	2.19	0.46
3:E:275:PRO:O	3:E:276:SER:C	2.54	0.46
3:A:160:CYS:SG	3:A:177:PRO:HB2	2.55	0.46
3:E:279:GLU:C	3:E:280:LEU:HD12	2.36	0.46
3:E:203:SER:O	3:E:204:GLY:O	2.34	0.46
3:A:236:ARG:HG2	3:E:147:GLU:OE2	2.16	0.46
3:A:145:ILE:HG23	3:A:146:GLU:CD	2.36	0.46
4:F:161:ARG:HG2	4:F:163:TYR:CE1	2.50	0.46
4:B:195:ARG:NH1	4:B:195:ARG:HA	2.16	0.46
4:B:69:GLY:N	4:B:78:SER:O	2.49	0.46
3:E:105:CYS:HB2	3:E:108:ARG:HB2	1.97	0.46
3:E:155:ASN:CB	3:E:191:THR:HG21	2.46	0.46
3:A:71:THR:HA	3:A:103:ASP:HA	1.97	0.46
4:F:248:LEU:HB2	4:F:340:SER:HB3	1.98	0.46
4:B:93:VAL:HG22	4:B:216:ALA:HB1	1.98	0.45
3:E:86:HIS:CG	3:E:157:VAL:HG12	2.51	0.45
4:F:42:LEU:CD2	4:F:214:PHE:HB3	2.46	0.45
4:B:336:ASP:CG	4:B:338:GLU:HB2	2.37	0.45
4:F:177:GLN:O	4:F:184:ARG:NH2	2.49	0.45
4:B:141:HIS:HE1	4:B:239:ASP:CG	2.20	0.45
4:F:267:TYR:CE1	4:F:310:VAL:HG22	2.51	0.45
4:F:179:GLU:HG2	4:F:184:ARG:HH21	1.81	0.45
4:B:53:PHE:C	4:B:240:SER:HB2	2.37	0.45
3:E:139:ASN:ND2	3:E:142:HIS:HA	2.31	0.45
4:F:222:THR:HG22	4:F:223:GLY:N	2.30	0.45
4:B:162:GLY:HA2	4:B:177:GLN:C	2.36	0.45
3:A:81:PRO:C	3:A:83:HIS:H	2.18	0.45
3:A:200:ASN:HD22	3:A:200:ASN:HA	1.54	0.45
4:F:87:TYR:CD2	4:F:88:VAL:O	2.69	0.45
3:A:165:VAL:O	3:A:172:PRO:HA	2.16	0.45
3:A:26:GLN:HG3	3:A:181:HIS:CD2	2.52	0.45
4:B:176:LEU:HD11	4:B:184:ARG:HB2	1.98	0.45
3:A:33:ARG:HB2	3:A:187:ARG:HD3	1.99	0.45
3:E:72:VAL:HB	3:E:104:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:107:HIS:CE1	4:F:210:VAL:HG12	2.51	0.45
4:B:292:TRP:HZ2	4:B:315:LYS:O	2.00	0.45
3:E:53:ASP:CG	3:E:54:THR:N	2.70	0.45
4:B:185:GLN:HA	4:B:185:GLN:NE2	2.31	0.45
4:B:299:SER:O	4:B:302:ASP:HB2	2.16	0.45
4:B:249:LYS:HG2	4:B:250:ILE:N	2.32	0.45
4:F:189:ARG:C	4:F:189:ARG:CD	2.85	0.45
3:A:61:ILE:CG2	3:A:62:LYS:N	2.80	0.45
1:C:8:DT:H2'	3:A:36:TYR:CZ	2.52	0.45
4:F:346:LEU:HD23	4:F:346:LEU:O	2.16	0.45
3:A:81:PRO:O	3:A:83:HIS:N	2.44	0.45
3:E:93:LYS:HG2	3:E:94:ASP:OD2	2.17	0.45
3:E:72:VAL:CG1	3:E:100:TYR:HE1	2.28	0.45
4:F:107:HIS:HD2	4:F:109:HIS:N	2.04	0.45
4:F:346:LEU:C	4:F:346:LEU:CD2	2.80	0.45
3:A:185:ASP:O	3:A:187:ARG:N	2.50	0.45
4:F:286:GLU:HB3	4:F:287:GLU:H	1.61	0.45
4:B:56:ARG:CZ	4:B:56:ARG:HB3	2.46	0.45
4:F:237:ILE:HG22	4:F:237:ILE:O	2.16	0.45
3:E:257:TYR:HD2	3:E:259:ASP:H	1.64	0.45
1:G:11:DC:H2'	1:G:12:DT:H6	1.82	0.45
3:A:58:HIS:CD2	3:A:114:GLN:NE2	2.85	0.45
3:A:214:LEU:HD21	3:A:216:CYS:HB3	1.99	0.45
4:B:42:LEU:HD13	4:B:214:PHE:CB	2.46	0.45
4:B:88:VAL:CG1	4:B:218:LEU:HD22	2.45	0.45
4:B:73:GLU:O	4:B:74:LYS:CB	2.65	0.45
3:A:185:ASP:C	3:A:187:ARG:N	2.70	0.45
4:F:100:ASN:CG	4:F:101:GLY:H	2.21	0.45
3:A:77:VAL:HA	3:A:86:HIS:H	1.82	0.44
3:A:121:VAL:HG13	3:A:121:VAL:O	2.17	0.44
4:B:98:VAL:HG11	4:B:213:MET:CE	2.47	0.44
4:F:71:SER:HB3	4:F:78:SER:OG	2.17	0.44
4:F:69:GLY:O	4:F:71:SER:N	2.50	0.44
3:E:77:VAL:HA	3:E:86:HIS:H	1.81	0.44
4:B:55:PHE:CB	4:B:141:HIS:NE2	2.81	0.44
3:A:52:THR:HG22	3:A:53:ASP:N	2.32	0.44
4:F:155:MET:O	4:F:194:ILE:HD13	2.18	0.44
3:E:255:PRO:HA	5:E:732:HOH:O	2.17	0.44
3:A:72:VAL:HG12	3:A:163:VAL:HG12	2.00	0.44
4:F:193:ILE:HD13	4:F:193:ILE:HA	1.86	0.44
4:F:343:LYS:HA	4:F:344:PRO:HD3	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:189:ARG:NH1	4:B:189:ARG:O	2.51	0.44
1:C:1:DT:H2'	1:C:2:DG:H8	1.81	0.44
3:E:266:VAL:HG13	3:E:288:TYR:HB2	1.99	0.44
4:F:56:ARG:O	4:F:140:LEU:HA	2.17	0.44
3:A:99:TYR:CD2	3:A:100:TYR:N	2.86	0.44
3:E:30:ARG:HG3	3:E:30:ARG:HH11	1.83	0.44
3:A:183:ILE:HG22	3:A:183:ILE:O	2.18	0.44
4:B:210:VAL:HG22	4:B:211:ARG:N	2.31	0.44
4:B:40:PRO:HG3	4:B:218:LEU:HD11	1.98	0.44
1:G:2:DG:H2''	1:G:3:DG:O5'	2.18	0.44
4:F:193:ILE:HD13	4:F:196:GLN:NE2	2.33	0.44
4:F:275:LYS:HG2	4:F:303:VAL:HB	1.99	0.44
4:B:237:ILE:O	4:B:237:ILE:HG22	2.18	0.44
3:A:273:ARG:CZ	3:E:81:PRO:HG2	2.47	0.44
4:B:58:VAL:HG13	4:B:59:CYS:H	1.83	0.44
2:H:20:DT:H2''	2:H:21:DT:O5'	2.18	0.44
4:B:114:LYS:HZ3	4:B:136:ASN:HB3	1.83	0.44
3:E:141:PHE:N	3:E:141:PHE:CD1	2.86	0.44
3:A:205:SER:C	3:A:207:LEU:H	2.21	0.44
4:B:109:HIS:CD2	4:B:142:VAL:H	2.36	0.44
1:G:2:DG:O6	4:F:64:HIS:CE1	2.71	0.44
1:C:10:DC:P	4:B:144:LYS:HD3	2.58	0.44
4:F:152:GLU:HG3	4:F:198:ALA:HB3	1.99	0.44
3:A:139:ASN:HA	3:A:139:ASN:HD22	1.64	0.44
4:B:271:ASP:O	4:B:273:VAL:HG13	2.18	0.44
4:B:120:VAL:HG13	4:B:120:VAL:O	2.18	0.44
4:F:153:ALA:O	4:F:156:THR:HB	2.18	0.44
3:A:77:VAL:O	3:A:86:HIS:HB2	2.18	0.44
1:G:1:DT:H3'	4:F:64:HIS:C	2.38	0.44
2:D:17:DA:C2	2:D:18:DA:C4	3.06	0.44
3:E:86:HIS:CE1	3:E:87:PRO:HD2	2.53	0.44
4:F:45:LEU:HD23	4:F:81:GLN:HB2	1.99	0.44
3:A:282:GLU:HB2	5:A:873:HOH:O	2.18	0.44
4:F:318:ASP:C	4:F:320:ASN:H	2.21	0.44
4:B:250:ILE:HG21	4:B:253:MET:CE	2.48	0.44
3:E:29:GLN:NE2	3:E:182:PRO:O	2.51	0.43
3:E:136:THR:O	3:E:137:ASN:C	2.56	0.43
3:E:88:HIS:ND1	3:E:121:VAL:HG22	2.33	0.43
5:G:731:HOH:O	3:E:221:LYS:HG2	2.18	0.43
3:E:25:GLU:HG3	3:E:25:GLU:O	2.18	0.43
4:F:46:GLU:HG2	4:F:47:GLN:N	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:56:ARG:O	4:B:140:LEU:HA	2.17	0.43
4:B:106:LEU:HD22	4:B:168:LEU:CD2	2.47	0.43
4:B:328:PHE:CE1	4:B:344:PRO:HG3	2.52	0.43
4:B:250:ILE:HD13	4:B:268:LEU:HD11	1.99	0.43
3:E:164:THR:HG23	3:E:174:LEU:HD13	2.00	0.43
4:F:280:ILE:HG12	4:F:298:PHE:CE1	2.54	0.43
4:B:217:PHE:CD1	4:B:225:PHE:CB	3.01	0.43
4:F:197:ALA:C	4:F:199:VAL:H	2.22	0.43
4:F:88:VAL:HG12	4:F:218:LEU:HD22	1.98	0.43
2:D:20:DT:O2	2:D:21:DT:O4'	2.36	0.43
3:A:198:ARG:HD3	4:B:310:VAL:HG21	2.00	0.43
4:B:143:THR:HB	4:B:146:LYS:HB2	2.00	0.43
3:E:61:ILE:O	3:E:110:ILE:HA	2.18	0.43
3:A:184:PHE:HB3	3:A:191:THR:HG21	2.00	0.43
4:B:189:ARG:CZ	4:B:189:ARG:HB3	2.49	0.43
1:C:3:DG:C2	1:C:4:DG:C6	3.07	0.43
1:G:7:DA:C8	1:G:8:DT:H72	2.53	0.43
3:A:104:LEU:HD22	3:A:111:HIS:CD2	2.54	0.43
4:B:106:LEU:N	4:B:168:LEU:HG	2.34	0.43
4:B:303:VAL:HG22	4:B:309:ILE:HG12	2.01	0.43
4:F:333:ARG:O	4:F:337:LEU:HA	2.18	0.43
4:B:182:GLY:O	4:B:183:ASP:HB2	2.19	0.43
4:B:228:ARG:HD2	4:B:231:PRO:HG3	2.01	0.43
1:C:4:DG:H2''	1:C:5:DA:C8	2.53	0.43
2:D:22:DC:H41	4:B:60:GLU:HG3	1.82	0.43
1:C:11:DC:H6	5:C:763:HOH:O	2.02	0.43
3:A:34:PHE:CE1	3:A:185:ASP:HB2	2.54	0.43
4:F:170:HIS:O	4:F:171:SER:C	2.56	0.43
3:E:257:TYR:CE1	3:E:266:VAL:HG21	2.54	0.43
3:E:104:LEU:N	3:E:104:LEU:CD1	2.81	0.43
4:F:109:HIS:CE1	4:F:142:VAL:H	2.37	0.43
3:E:205:SER:C	3:E:207:LEU:H	2.22	0.43
3:E:224:ILE:HG13	3:E:225:GLU:N	2.34	0.43
3:E:228:PHE:CE1	3:E:270:MET:HB2	2.54	0.43
3:A:87:PRO:O	3:A:129:ALA:HB1	2.18	0.43
4:B:110:SER:HB3	4:B:119:GLY:HA2	2.01	0.43
4:F:88:VAL:CG2	4:F:89:GLY:H	2.11	0.42
3:E:89:GLU:HG3	3:E:133:ARG:HH12	1.84	0.42
4:F:47:GLN:OE1	4:F:234:SER:HB2	2.19	0.42
4:F:46:GLU:CG	4:F:47:GLN:H	2.19	0.42
4:F:125:ALA:C	4:F:127:PRO:HD3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:31:GLY:HA2	3:E:186:ASN:ND2	2.33	0.42
4:F:148:PHE:HB2	4:F:202:THR:HG21	2.01	0.42
3:E:226:VAL:HG21	3:E:252:PHE:CD2	2.54	0.42
4:B:116:CYS:N	4:B:121:CYS:SG	2.92	0.42
1:G:9:DT:H2''	1:G:10:DC:O4'	2.20	0.42
2:H:22:DC:H2'	2:H:23:DC:O4'	2.19	0.42
2:D:18:DA:P	4:B:243:PRO:HG2	2.59	0.42
4:B:76:LYS:CG	4:B:77:LYS:N	2.78	0.42
3:E:73:ARG:HD2	3:E:99:TYR:HD2	1.81	0.42
3:E:52:THR:CG2	3:E:53:ASP:N	2.81	0.42
3:E:52:THR:HG22	3:E:53:ASP:H	1.84	0.42
4:B:259:CYS:SG	4:B:350:GLU:HG2	2.60	0.42
3:A:275:PRO:O	3:A:276:SER:C	2.58	0.42
4:F:154:ARG:C	4:F:156:THR:H	2.23	0.42
4:F:163:TYR:O	4:F:165:PRO:N	2.52	0.42
3:A:79:LYS:HZ2	3:A:79:LYS:HB3	1.84	0.42
3:A:173:LEU:HD13	3:A:173:LEU:C	2.39	0.42
4:B:221:SER:O	4:B:222:THR:HB	2.19	0.42
4:B:84:ILE:HG21	4:B:130:MET:SD	2.59	0.42
4:B:97:LEU:HD12	4:B:109:HIS:C	2.40	0.42
4:F:173:LEU:HD21	4:F:190:GLU:HG3	2.01	0.42
4:B:123:VAL:HG21	4:B:132:VAL:HG11	2.01	0.42
3:E:185:ASP:O	3:E:191:THR:OG1	2.28	0.42
4:B:62:PRO:O	4:B:63:SER:C	2.57	0.42
3:E:219:VAL:O	3:E:247:GLN:HG2	2.19	0.42
4:B:281:ARG:HG3	4:B:295:PHE:CE2	2.54	0.42
3:A:167:ASP:HB2	3:A:168:PRO:CD	2.48	0.42
4:F:175:TYR:CE1	4:F:176:LEU:HG	2.54	0.42
3:E:28:LYS:HE2	3:E:28:LYS:HB3	1.79	0.42
4:B:90:PRO:HA	4:B:126:GLY:O	2.20	0.42
4:B:92:LYS:HG2	4:B:124:THR:HA	2.01	0.42
4:F:202:THR:HG22	4:F:202:THR:O	2.19	0.42
4:B:105:HIS:CB	4:B:201:GLN:HE22	2.32	0.42
3:E:41:ARG:CD	3:E:41:ARG:N	2.82	0.42
4:F:91:ALA:O	4:F:124:THR:O	2.38	0.42
3:A:146:GLU:HA	3:A:149:ARG:HH12	1.84	0.42
3:E:23:ILE:HA	3:E:61:ILE:HA	2.01	0.42
3:A:106:PRO:O	3:A:108:ARG:N	2.52	0.42
3:E:30:ARG:NH2	3:E:277:ASP:OD2	2.53	0.42
4:F:215:THR:OG1	4:F:231:PRO:HB3	2.19	0.42
4:B:181:GLY:HA3	4:B:184:ARG:NE	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:34:PHE:HA	5:E:719:HOH:O	2.18	0.42
4:F:136:ASN:HA	4:F:136:ASN:HD22	1.70	0.42
3:A:86:HIS:HA	3:A:87:PRO:HD2	1.72	0.42
3:E:131:SER:C	3:E:133:ARG:N	2.71	0.42
2:H:13:DA:H2'	2:H:14:DA:C8	2.55	0.42
4:F:57:TYR:O	4:F:58:VAL:C	2.57	0.42
3:A:50:ARG:HE	3:A:50:ARG:HB3	1.49	0.42
3:E:154:LEU:H	3:E:154:LEU:HD22	1.85	0.42
4:B:97:LEU:HB3	4:B:210:VAL:HG21	2.02	0.42
3:E:130:ILE:O	3:E:133:ARG:N	2.46	0.42
4:B:55:PHE:HB2	4:B:141:HIS:CE1	2.54	0.42
3:E:163:VAL:HG12	3:E:164:THR:N	2.34	0.42
1:G:7:DA:H2''	1:G:8:DT:C5'	2.50	0.42
3:A:28:LYS:HA	3:A:28:LYS:HD2	1.92	0.42
3:E:145:ILE:CD1	3:E:145:ILE:N	2.83	0.42
4:F:284:GLU:O	4:F:291:VAL:HG13	2.20	0.42
3:A:168:PRO:HB3	5:A:726:HOH:O	2.19	0.42
4:F:144:LYS:HD2	4:F:144:LYS:HA	1.78	0.42
4:B:97:LEU:HD12	4:B:109:HIS:O	2.20	0.42
4:B:98:VAL:HG11	4:B:213:MET:HE3	2.02	0.42
4:F:254:ASP:O	4:F:255:ARG:NH1	2.50	0.42
4:F:165:PRO:HB2	4:F:166:GLY:H	1.70	0.42
4:F:113:GLY:O	4:F:116:CYS:HB2	2.20	0.42
4:B:187:THR:HG22	4:B:189:ARG:H	1.85	0.42
4:F:77:LYS:HB3	4:F:78:SER:H	1.71	0.41
1:G:8:DT:C7	3:E:187:ARG:HD3	2.49	0.41
3:A:93:LYS:HB3	3:A:93:LYS:HE2	1.81	0.41
3:E:113:PHE:N	3:E:113:PHE:CD1	2.87	0.41
3:A:144:PRO:HG2	3:A:147:GLU:CB	2.50	0.41
3:A:116:LEU:HD12	3:A:116:LEU:N	2.35	0.41
3:A:34:PHE:CD1	3:A:185:ASP:HB2	2.55	0.41
4:B:232:VAL:HG23	4:B:232:VAL:O	2.20	0.41
4:F:184:ARG:N	4:F:184:ARG:HD2	2.29	0.41
1:G:10:DC:C2'	1:G:11:DC:O5'	2.68	0.41
3:A:186:ASN:HA	3:A:192:ALA:HA	2.01	0.41
4:B:105:HIS:HA	4:B:168:LEU:HD12	2.02	0.41
4:B:42:LEU:HD12	4:B:214:PHE:C	2.41	0.41
4:B:41:TYR:HD2	4:B:229:LEU:HB3	1.86	0.41
3:E:29:GLN:HB3	5:E:727:HOH:O	2.19	0.41
4:B:73:GLU:HB2	4:B:76:LYS:O	2.21	0.41
4:B:333:ARG:O	4:B:337:LEU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:187:THR:HB	4:B:190:GLU:HG2	2.02	0.41
4:F:284:GLU:OE1	4:F:316:TYR:OH	2.30	0.41
4:F:232:VAL:HA	5:F:803:HOH:O	2.18	0.41
4:F:175:TYR:HA	4:F:177:GLN:CD	2.41	0.41
1:C:5:DA:O5'	3:A:247:GLN:NE2	2.53	0.41
1:C:8:DT:H2"	1:C:9:DT:H73	2.01	0.41
4:B:181:GLY:HA3	4:B:184:ARG:CD	2.50	0.41
4:F:333:ARG:HG2	4:F:335:SER:OG	2.21	0.41
4:B:250:ILE:HG21	4:B:253:MET:HE1	2.02	0.41
4:B:49:LYS:HG2	4:B:70:ALA:HA	2.01	0.41
4:B:143:THR:C	4:B:145:LYS:H	2.23	0.41
3:E:255:PRO:HA	3:E:256:PRO:HD3	1.96	0.41
3:A:130:ILE:HG22	3:A:131:SER:N	2.35	0.41
3:A:165:VAL:HG22	3:A:173:LEU:O	2.20	0.41
3:E:130:ILE:HD13	3:E:130:ILE:O	2.21	0.41
3:E:70:GLY:N	3:E:166:ARG:NH1	2.68	0.41
3:E:28:LYS:HG2	3:E:49:GLU:CA	2.49	0.41
3:A:105:CYS:HA	3:A:106:PRO:HD3	1.93	0.41
3:A:239:PHE:HB3	3:A:252:PHE:HB3	2.01	0.41
4:F:183:ASP:O	4:F:185:GLN:N	2.54	0.41
3:A:272:LEU:HB2	3:A:281:SER:HB3	2.01	0.41
4:F:160:ILE:C	4:F:160:ILE:HD12	2.41	0.41
4:F:50:GLN:HE21	4:F:236:ALA:H	1.69	0.41
4:B:324:PRO:HB3	4:B:346:LEU:HD21	2.02	0.41
4:B:343:LYS:HA	4:B:344:PRO:HD3	1.82	0.41
3:A:258:ALA:O	3:A:260:PRO:HD3	2.20	0.41
4:F:89:GLY:O	4:F:130:MET:HE2	2.20	0.41
3:E:148:GLN:C	3:E:149:ARG:HG3	2.41	0.41
4:B:175:TYR:O	4:B:176:LEU:CB	2.68	0.41
3:E:214:LEU:C	3:E:214:LEU:HD23	2.41	0.41
4:B:128:LYS:HE3	4:B:128:LYS:HB2	1.92	0.41
3:A:85:PRO:HB2	3:A:133:ARG:HG3	2.02	0.41
4:B:42:LEU:HD21	4:B:216:ALA:HB2	2.02	0.41
3:E:210:ASP:OD2	3:E:210:ASP:N	2.54	0.41
4:F:184:ARG:O	4:F:184:ARG:HG2	2.20	0.41
3:E:165:VAL:O	3:E:166:ARG:HG3	2.20	0.41
3:A:60:THR:HG23	3:A:112:SER:HB2	2.02	0.41
3:A:36:TYR:H	3:A:39:GLU:HG3	1.84	0.41
3:A:46:ILE:HB	3:A:116:LEU:CD1	2.51	0.41
3:A:188:ALA:HA	3:A:189:PRO:HD3	1.94	0.41
4:B:142:VAL:HG22	4:B:143:THR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:78:THR:HG22	3:A:79:LYS:H	1.85	0.41
3:A:86:HIS:CD2	3:A:157:VAL:CG1	3.04	0.41
3:E:245:HIS:O	3:E:246:ARG:C	2.59	0.41
3:E:100:TYR:CD1	3:E:101:GLU:N	2.89	0.41
2:D:19:DT:O3'	4:B:57:TYR:HE1	2.03	0.41
4:B:177:GLN:HG2	4:B:178:ALA:H	1.86	0.41
4:B:189:ARG:NH1	4:B:189:ARG:HB3	2.36	0.41
3:E:217:ASP:O	3:E:218:LYS:C	2.59	0.41
4:B:218:LEU:HD12	4:B:227:ARG:CZ	2.51	0.41
4:B:84:ILE:HB	4:B:130:MET:CG	2.50	0.41
3:E:217:ASP:O	3:E:219:VAL:HG13	2.20	0.41
3:A:198:ARG:CZ	4:B:310:VAL:HG11	2.51	0.41
3:E:200:ASN:HD21	4:F:254:ASP:CG	2.24	0.40
3:E:127:GLU:HG3	3:E:128:GLN:N	2.35	0.40
1:C:4:DG:H2''	1:C:5:DA:H8	1.85	0.40
4:F:113:GLY:O	4:F:114:LYS:C	2.59	0.40
4:F:114:LYS:HE2	4:F:134:PHE:CA	2.45	0.40
3:A:214:LEU:HD23	3:A:214:LEU:C	2.40	0.40
3:E:79:LYS:HA	3:E:158:ARG:NE	2.33	0.40
4:F:332:ARG:CG	4:F:332:ARG:NH1	2.77	0.40
4:F:72:SER:O	4:F:77:LYS:NZ	2.49	0.40
4:F:95:VAL:HG13	4:F:95:VAL:O	2.21	0.40
3:E:19:ALA:HB3	3:E:175:LEU:CD2	2.52	0.40
3:A:229:THR:CG2	3:A:271:GLN:OE1	2.69	0.40
4:F:162:GLY:O	4:F:163:TYR:HD1	2.04	0.40
3:A:29:GLN:NE2	3:A:181:HIS:HB3	2.33	0.40
4:F:49:LYS:CA	4:F:49:LYS:HE3	2.48	0.40
4:F:112:VAL:HG22	4:F:138:GLY:C	2.41	0.40
4:F:229:LEU:O	4:F:230:GLU:C	2.59	0.40
4:F:151:LEU:HD12	4:F:151:LEU:C	2.42	0.40
4:B:212:LEU:HD23	4:B:212:LEU:HA	1.97	0.40
3:A:141:PHE:HE1	3:A:179:LEU:HD21	1.86	0.40
3:E:72:VAL:HB	3:E:104:LEU:CD1	2.51	0.40
4:B:54:ARG:HA	4:B:240:SER:CB	2.52	0.40
4:F:44:ILE:HA	4:F:82:VAL:HG23	2.02	0.40
3:A:28:LYS:O	3:A:29:GLN:C	2.60	0.40
4:B:56:ARG:O	4:B:139:ILE:O	2.38	0.40
3:E:178:VAL:CG2	3:E:179:LEU:N	2.85	0.40
4:B:304:HIS:HB3	4:B:308:ALA:HB3	2.04	0.40
3:E:289:LEU:HB3	3:E:290:PRO:HD2	2.03	0.40
3:A:194:LEU:HD12	3:A:280:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:225:GLU:HG3	3:A:273:ARG:HB3	2.03	0.40
4:B:148:PHE:HB2	4:B:202:THR:HG21	2.03	0.40
3:E:184:PHE:HD1	3:E:184:PHE:N	2.19	0.40
4:B:165:PRO:HG2	4:B:166:GLY:N	2.34	0.40
3:A:81:PRO:HB2	3:A:82:PRO:CD	2.51	0.40
4:B:288:ASN:C	4:B:288:ASN:HD22	2.25	0.40
3:E:268:VAL:HG22	3:E:286:PHE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	272/274 (99%)	204 (75%)	49 (18%)	19 (7%)	1	3
3	E	272/274 (99%)	201 (74%)	50 (18%)	21 (8%)	1	2
4	B	311/313 (99%)	236 (76%)	54 (17%)	21 (7%)	1	3
4	F	311/313 (99%)	240 (77%)	44 (14%)	27 (9%)	1	1
All	All	1166/1174 (99%)	881 (76%)	197 (17%)	88 (8%)	1	2

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	81	PRO
3	A	83	HIS
3	A	115	ASN
3	A	204	GLY
4	B	101	GLY
4	B	127	PRO
4	B	165	PRO
4	B	183	ASP

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Mol	Chain	Res	Type
4	B	187	THR
4	B	238	TYR
3	E	81	PRO
3	E	97	ASP
4	F	70	ALA
4	F	102	LYS
4	F	127	PRO
4	F	238	TYR
4	F	288	ASN
4	B	63	SER
4	B	68	PRO
4	B	100	ASN
4	B	114	LYS
4	B	245	ALA
3	E	38	CYS
3	E	83	HIS
3	E	165	VAL
3	E	204	GLY
3	E	247	GLN
4	F	49	LYS
4	F	71	SER
4	F	77	LYS
4	F	101	GLY
4	F	114	LYS
4	F	165	PRO
4	F	171	SER
4	F	183	ASP
4	F	184	ARG
4	F	187	THR
4	F	221	SER
3	A	41	ARG
3	A	97	ASP
3	A	99	TYR
3	A	126	LEU
3	A	142	HIS
3	A	186	ASN
3	A	191	THR
3	A	261	SER
4	B	70	ALA
4	B	221	SER
4	B	223	GLY
3	E	106	PRO

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Mol	Chain	Res	Type
3	E	174	LEU
3	E	261	SER
4	F	100	ASN
4	F	175	TYR
4	F	222	THR
4	F	223	GLY
3	A	106	PRO
3	A	107	ASP
3	A	185	ASP
4	B	241	LYS
3	E	168	PRO
4	F	173	LEU
4	B	74	LYS
4	B	88	VAL
4	B	222	THR
3	E	59	PRO
3	E	115	ASN
3	E	132	GLN
3	E	200	ASN
3	E	276	SER
4	F	88	VAL
4	F	164	ASN
4	F	182	GLY
3	A	31	GLY
4	B	48	PRO
3	E	29	GLN
3	E	41	ARG
3	E	69	PRO
3	A	165	VAL
4	B	319	VAL
3	E	110	ILE
4	F	319	VAL
3	A	231	PRO
4	B	344	PRO
3	E	231	PRO
3	A	77	VAL
4	F	344	PRO
4	F	166	GLY

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	243/243 (100%)	218 (90%)	25 (10%)	9	23
3	E	243/243 (100%)	215 (88%)	28 (12%)	7	19
4	B	269/269 (100%)	244 (91%)	25 (9%)	11	29
4	F	269/269 (100%)	239 (89%)	30 (11%)	7	20
All	All	1024/1024 (100%)	916 (90%)	108 (10%)	8	22

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	20	TYR
3	A	35	ARG
3	A	41	ARG
3	A	50	ARG
3	A	58	HIS
3	A	71	THR
3	A	76	LEU
3	A	81	PRO
3	A	84	ARG
3	A	88	HIS
3	A	100	TYR
3	A	116	LEU
3	A	127	GLU
3	A	133	ARG
3	A	138	ASN
3	A	139	ASN
3	A	167	ASP
3	A	190	ASN
3	A	200	ASN
3	A	201	ARG
3	A	210	ASP
3	A	254	THR
3	A	263	GLN
3	A	272	LEU

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Mol	Chain	Res	Type
3	A	277	ASP
4	B	46	GLU
4	B	56	ARG
4	B	57	TYR
4	B	87	TYR
4	B	106	LEU
4	B	114	LYS
4	B	121	CYS
4	B	128	LYS
4	B	136	ASN
4	B	152	GLU
4	B	176	LEU
4	B	184	ARG
4	B	186	LEU
4	B	196	GLN
4	B	204	GLU
4	B	217	PHE
4	B	220	ASP
4	B	228	ARG
4	B	234	SER
4	B	235	ASP
4	B	288	ASN
4	B	301	THR
4	B	322	THR
4	B	341	GLU
4	B	346	LEU
3	E	20	TYR
3	E	26	GLN
3	E	29	GLN
3	E	41	ARG
3	E	56	LYS
3	E	73	ARG
3	E	78	THR
3	E	81	PRO
3	E	103	ASP
3	E	104	LEU
3	E	108	ARG
3	E	111	HIS
3	E	116	LEU
3	E	130	ILE
3	E	133	ARG
3	E	154	LEU

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Mol	Chain	Res	Type
3	E	166	ARG
3	E	174	LEU
3	E	181	HIS
3	E	184	PHE
3	E	200	ASN
3	E	236	ARG
3	E	241	GLN
3	E	257	TYR
3	E	269	SER
3	E	271	GLN
3	E	272	LEU
3	E	284	MET
4	F	38	MET
4	F	41	TYR
4	F	49	LYS
4	F	58	VAL
4	F	77	LYS
4	F	92	LYS
4	F	98	VAL
4	F	121	CYS
4	F	130	MET
4	F	148	PHE
4	F	152	GLU
4	F	160	ILE
4	F	161	ARG
4	F	167	LEU
4	F	172	ASP
4	F	184	ARG
4	F	188	ASP
4	F	189	ARG
4	F	190	GLU
4	F	195	ARG
4	F	220	ASP
4	F	227	ARG
4	F	230	GLU
4	F	246	SER
4	F	247	ASN
4	F	268	LEU
4	F	279	GLN
4	F	280	ILE
4	F	285	GLU
4	F	287	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	29	GLN
3	A	83	HIS
3	A	111	HIS
3	A	114	GLN
3	A	138	ASN
3	A	162	GLN
3	A	181	HIS
3	A	186	ASN
3	A	190	ASN
3	A	200	ASN
3	A	247	GLN
3	A	287	GLN
4	B	43	GLN
4	B	47	GLN
4	B	86	ASN
4	B	109	HIS
4	B	136	ASN
4	B	177	GLN
4	B	185	GLN
4	B	196	GLN
4	B	200	GLN
4	B	201	GLN
4	B	274	GLN
4	B	279	GLN
4	B	288	ASN
4	B	306	GLN
4	B	330	GLN
3	E	26	GLN
3	E	29	GLN
3	E	111	HIS
3	E	119	GLN
3	E	128	GLN
3	E	138	ASN
3	E	139	ASN
3	E	162	GLN
3	E	186	ASN
3	E	200	ASN
3	E	220	GLN
3	E	241	GLN
3	E	263	GLN
3	E	271	GLN

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Mol	Chain	Res	Type
3	E	287	GLN
4	F	50	GLN
4	F	103	ASN
4	F	105	HIS
4	F	136	ASN
4	F	141	HIS
4	F	164	ASN
4	F	170	HIS
4	F	247	ASN
4	F	320	ASN
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 carbohydrates 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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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