Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 11:15 AM EDT

PDB ID	:	1LE5
Title	:	Crystal structure of a NF-kB heterodimer bound to an IFNb-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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

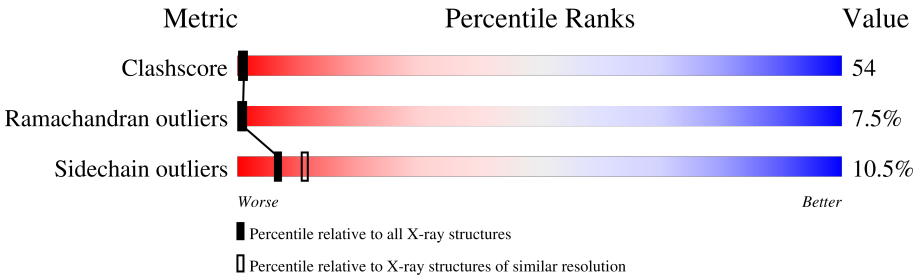
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	12	17% 83%
1	G	12	50% 33% 17%
2	D	12	25% 75%
2	H	12	25% 8% 67%
3	A	274	31% 57% 12%
3	E	274	31% 57% 10%
4	B	313	28% 61% 10%
4	F	313	34% 52% 13%

2 Entry composition (i)

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 methionine	UNP P25799
F	38	MET	-	initiating methionine	UNP P25799

- Molecule 5 is water.

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

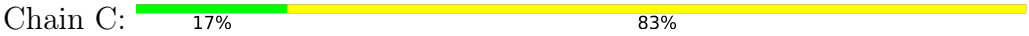
3 Residue-property plots (i)

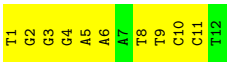
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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*AP*AP*TP*TP*CP*CP*T)-3'

Chain C:



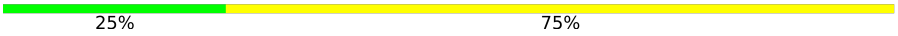


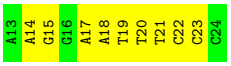
• Molecule 1: 5'-D(*TP*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*T)-3'

Chain G:

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

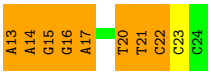
Chain D:





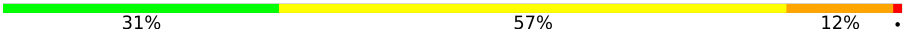
• Molecule 2: 5'-D(*AP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3'

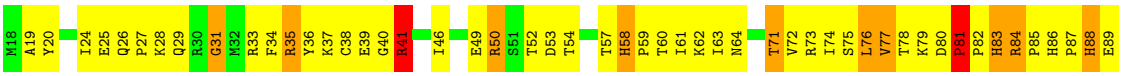
Chain H:

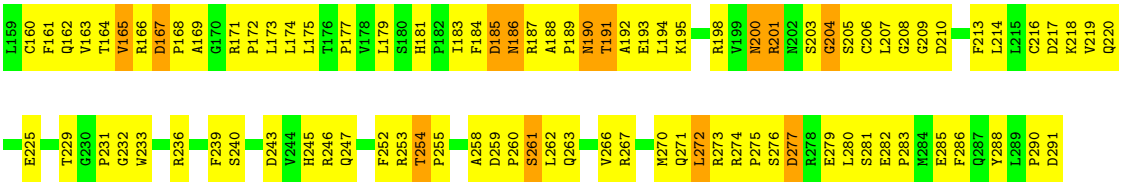


• Molecule 3: Nuclear factor NF-kappa-B p65 subunit

Chain A:

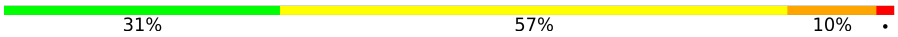


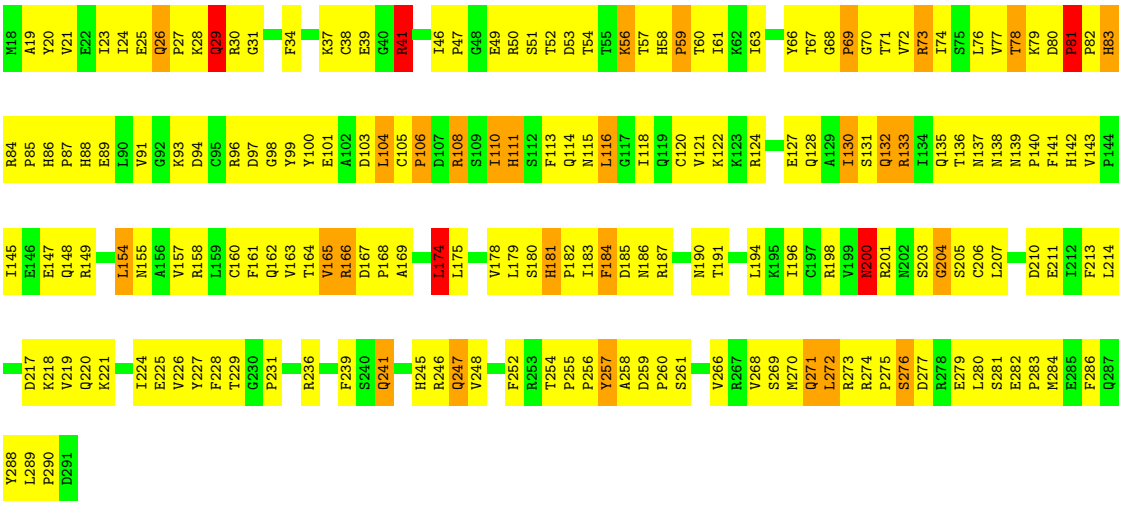




• Molecule 3: Nuclear factor NF-kappa-B p65 subunit

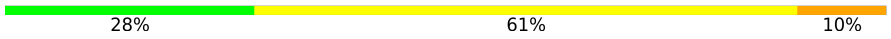
Chain E:

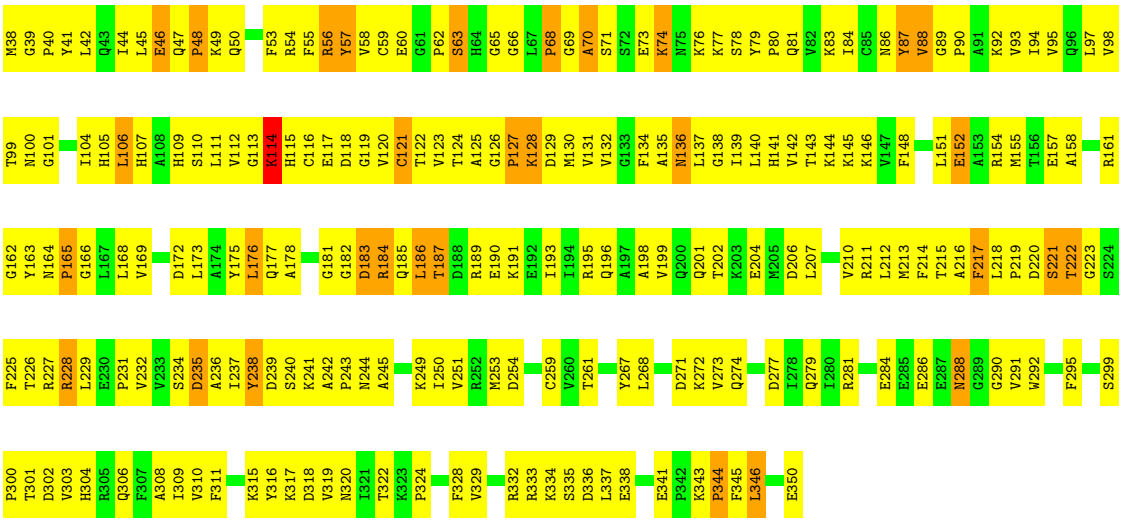




• Molecule 4: Nuclear factor NF-kappa-B p50 subunit

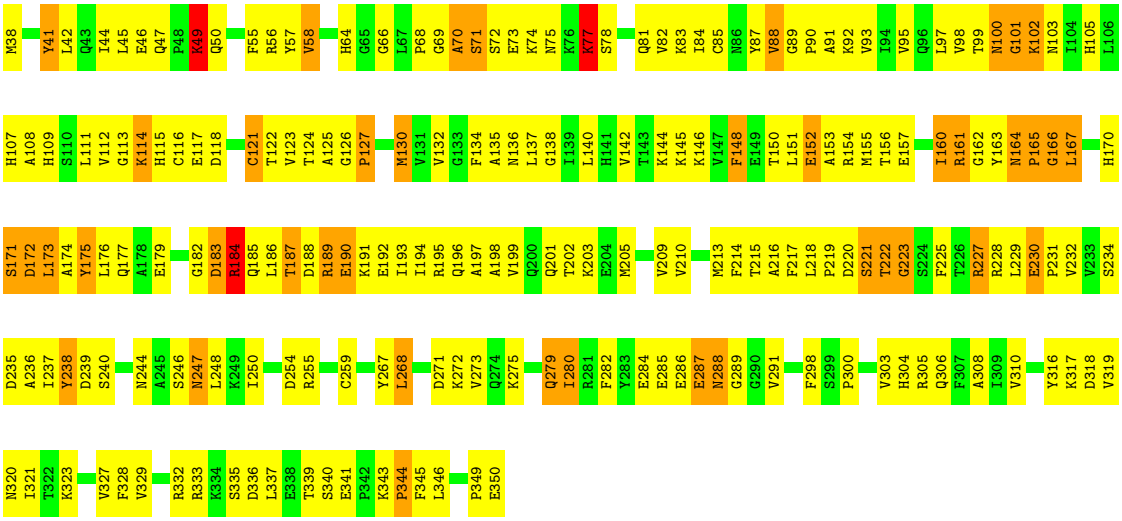
Chain B:





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

Chain F:


M38 Y41 L42 Q43 I44 L45 E46 Q47 P48 K49 Q50 F55 R56 Y57 V58 H64 G65 G66 L67 P68 G69 A70 S71 S72 E73 K74 N75 K76 K77 S78 Q81 V82 K83 I84 C85 N86 Y87 V88 G89 P90 A91 K92 V93 I94 V95 Q96 L97 V98 T99 N100 G101 K102 N103 I104 H105 L106
H107 A108 H109 S110 L111 V112 G113 K114 H115 C116 E117 D118 C121 T122 V123 T124 A125 G126 P127 M130 V131 V132 G133 F134 A135 N136 L137 G138 I139 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 D220 S221 T222 G223 S224 F225 T226 R227 R228 L229 E230 P231 V232 V233 S234
D235 A236 I237 Y238 D239 S240 N244 A245 S246 N247 L248 K249 I250 D254 R255 C259 Y267 L268 D271 K272 V273 Q274 K275 Q279 I280 R281 F282 Y283 E284 E285 E286 E287 N288 G289 G290 V291 F298 S299 P300 V303 H304 R305 Q306 F307 A308 I309 V310 Y316 K317 D318 V319
N320 I321 T322 K323 V327 F328 V329 R332 R333 K334 S335 D336 L337 E338 T339 S340 E341 P342 K343 P344 F345 L346 P349 E350

4 Data and refinement statistics (i)

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	137.53Å 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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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:HD12	4:B:186:LEU:H	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:HG2	3:A:201:ARG:HH21	1.41	0.85
4:F:46:GLU:HG2	4:F:47:GLN:H	1.40	0.85
3:A:35:ARG:HE	3:A:35:ARG:HA	1.39	0.85
3:A:53:ASP:OD1	3:A:54:THR:HG23	1.75	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:56:ARG:NH1	4:B:56:ARG:HB3	1.94	0.83
4:B:155:MET:HE2	4:B:169:VAL:HG22	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:286:GLU:HB2	4:B:290:GLY:HA3	1.57	0.83
4:B:125:ALA:HB3	4:B:132:VAL:HG22	1.60	0.83
4:F:227:ARG:HA	4:F:227:ARG:NE	1.91	0.83
4:B:329:VAL:HG23	4:B:345:PHE:HB2	1.60	0.83
2:D:17:DA:H2'	4:B:306:GLN:HE22	1.43	0.83
4:F:107:HIS:HD2	4:F:109:HIS:H	1.26	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
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:E:258:ALA:O	3:E:260:PRO:HD3	1.80	0.81
3:A:166:ARG:HG3	3:A:166:ARG:HH11	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
2:D:23:DC:H4'	5:D:721:HOH:O	1.84	0.78
3:E:74:ILE:HD12	3:E:161:PHE:CD1	2.18	0.78
4:B:76:LYS:HG3	4:B:77:LYS:H	1.49	0.77
4:B:261:THR:O	4:B:315:LYS:HG2	1.84	0.77
4:F:126:GLY:N	4:F:127:PRO:HD3	2.00	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
3:A:84:ARG:H	3:A:84:ARG:HE	1.34	0.75
4:F:105:HIS:HB3	4:F:201:GLN:NE2	2.02	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:H	3:E:111:HIS:HD2	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:58:HIS:HB3	3:E:113:PHE:O	1.87	0.73
3:E:111:HIS:CD2	3:E:111:HIS:N	2.56	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:H	4:F:184:ARG:HD2	1.54	0.72
4:B:279:GLN:NE2	4:B:332:ARG:HH21	1.88	0.72
1:C:8:DT:H2"	1:C:9:DT:H72	1.72	0.72
4:B:254:ASP:HB2	4:B:267:TYR:HB2	1.72	0.72
4:F:167:LEU:HD12	4:F:167:LEU:N	2.04	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
3:E:56:LYS:H	3:E:56:LYS:HD3	1.56	0.71
3:E:108:ARG:NH1	3:E:108:ARG:HB2	2.05	0.71
4:F:88:VAL:CG1	4:F:218:LEU:HD22	2.20	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:HH11	4:B:195:ARG:CA	2.04	0.70
3:E:271:GLN:NE2	3:E:280:LEU:HD23	2.07	0.69
4:B:39:GLY:CA	4:B:86:ASN:HD22	2.04	0.69
4:B:88:VAL:HG13	4:B:89:GLY:N	2.07	0.69
3:A:166:ARG:HG3	3:A:166:ARG:NH1	2.08	0.69
4:B:55:PHE:HD2	4:B:141:HIS:HE2	1.40	0.69
3:E:282:GLU:HG3	3:E:283:PRO:HD2	1.72	0.69
4:F:41:TYR:CE2	4:F:85:CYS:HB2	2.26	0.69
3:A:76:LEU:HD11	3:A:88:HIS:O	1.91	0.69
4:F:42:LEU:HD21	4:F:214:PHE:HB3	1.74	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:HA	4:F:227:ARG:HE	1.56	0.68
3:A:274:ARG:NH1	3:A:279:GLU:OE1	2.27	0.68
3:E:69:PRO:HG2	3:E:166:ARG:HH11	1.56	0.68
4:F:332:ARG:HG2	4:F:332:ARG:NH1	2.04	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
3:A:149:ARG:HG2	3:A:150:GLY:N	2.07	0.68
4:B:215:THR:CG2	4:B:228:ARG:HG3	2.23	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
4:B:154:ARG:NE	4:B:154:ARG:HA	2.09	0.68
3:E:73:ARG:HB3	3:E:162:GLN:HB2	1.76	0.68
4:F:250:ILE:CG2	4:F:268:LEU:HD21	2.18	0.67
2:D:22:DC:C2'	2:D:23:DC:H5"	2.23	0.67
3:E:257:TYR:CE1	3:E:266:VAL:HG11	2.30	0.67
4:F:167:LEU:HD21	4:F:228:ARG:HH21	1.57	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
3:A:165:VAL:CG2	3:A:173:LEU:HB3	2.25	0.67
4:B:218:LEU:HG	4:B:229:LEU:HD21	1.74	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:A:88:HIS:CG	3:A:120:CYS:HA	2.30	0.67
3:E:72:VAL:HG13	3:E:100:TYR:HE1	1.59	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
3:A:24:ILE:HB	3:A:25:GLU:OE2	1.96	0.66
3:E:122:LYS:NZ	3:E:124:ARG:HH21	1.94	0.66
4:F:88:VAL:HG22	4:F:89:GLY:N	2.08	0.66
4:F:186:LEU:O	4:F:191:LYS:HE3	1.95	0.66
4:B:114:LYS:HD2	4:B:135:ALA:O	1.96	0.66
3:E:70:GLY:HA3	3:E:104:LEU:HD22	1.78	0.66
3:A:72:VAL:O	3:A:101:GLU:HA	1.96	0.66
3:A:148:GLN:HG2	3:A:152:TYR:OH	1.95	0.66
4:B:125:ALA:CB	4:B:132:VAL:HG22	2.26	0.65
4:F:84:ILE:CB	4:F:130:MET:HB3	2.24	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
4:B:118:ASP:HB3	4:B:154:ARG:NH2	2.12	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: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
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:F:279:GLN:OE1	4:F:332:ARG:NH1	2.30	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:115:HIS:CE1	4:B:123:VAL:HG23	2.33	0.64
4:B:191:LYS:O	4:B:195:ARG:HG2	1.98	0.64
3:A:88:HIS:ND1	3:A:120:CYS:HA	2.13	0.64
3:E:206:CYS:HA	3:E:288:TYR:CD2	2.21	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
3:A:208:GLY:HA2	3:A:254:THR:HG22	1.80	0.63
4:B:114:LYS:NZ	4:B:136:ASN:HB3	2.13	0.63
3:A:219:VAL:O	3:A:247:GLN:HG2	1.99	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:123:VAL:CG1	4:F:132:VAL:HG21	2.27	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
3:A:88:HIS:HB3	3:A:121:VAL:N	2.14	0.62
3:A:166:ARG:HA	3:A:171:ARG:O	2.00	0.62
4:B:88:VAL:HG22	4:B:89:GLY:H	1.64	0.62
3:E:51:SER:HB2	3:E:57:THR:OG1	1.99	0.62
3:E:79:LYS:HA	3:E:158:ARG:HE	1.64	0.62
3:A:79:LYS:HB3	3:A:79:LYS:NZ	2.14	0.62
4:B:94:ILE:HG12	4:B:215:THR:O	1.99	0.62
4:B:186:LEU:O	4:B:191:LYS:HB3	1.98	0.62
3:E:201:ARG:NH2	4:F:255:ARG:NH2	2.47	0.62
3:E:279:GLU:O	3:E:280:LEU:HD12	1.98	0.62
4:F:148:PHE:C	4:F:148:PHE:CD2	2.73	0.62
4:B:55:PHE:HB2	4:B:141:HIS:NE2	2.14	0.62
2:D:21:DT:O4	4:B:54:ARG:NH2	2.32	0.62
1:G:10:DC:H2"	1:G:11:DC:C5'	2.30	0.62
4:B:244:ASN:CB	4:B:274:GLN:HE22	2.12	0.62
3:E:201:ARG:NH2	4:F:255:ARG:HH21	1.97	0.62
4:B:45:LEU:HD12	4:B:46:GLU:HB2	1.82	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
4:F:105:HIS:HB3	4:F:201:GLN:HE21	1.63	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:N	4:F:237:ILE:HD12	2.14	0.62
4:B:178:ALA:O	4:B:226:THR:HG23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:329:VAL:CG2	4:F:345:PHE:HB2	2.30	0.61
3:A:24:ILE:HD11	3:A:62:LYS:HB2	1.81	0.61
4:B:244:ASN:HB3	4:B:274:GLN:NE2	2.14	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
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:162:GLY:C	4:F:163:TYR:HD1	2.04	0.61
3:A:143:VAL:HG13	3:A:147:GLU:OE1	1.99	0.61
4:F:165:PRO:N	4:F:167:LEU:HD13	2.15	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:HD2	4:F:148:PHE:O	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
1:G:6:DA:C2'	1:G:7:DA:O5'	2.50	0.60
3:A:46:ILE:HG13	3:A:116:LEU:O	2.00	0.60
4:B:95:VAL:HG12	4:B:214:PHE:HD1	1.66	0.60
4:B:164:ASN:ND2	4:B:213:MET:SD	2.75	0.60
3:E:77:VAL:HG12	3:E:85:PRO:HA	1.84	0.60
4:F:164:ASN:HA	4:F:167:LEU:HD22	1.84	0.60
3:A:24:ILE:HD11	3:A:62:LYS:CD	2.32	0.60
3:A:201:ARG:HG2	3:A:201:ARG:NH2	2.12	0.60
4:B:57:TYR:N	4:B:57:TYR:CD2	2.68	0.60
4:B:40:PRO:O	4:B:229:LEU:HD22	2.02	0.59
3:A:93:LYS:CE	3:A:115:ASN:HB3	2.32	0.59
4:B:155:MET:SD	4:B:198:ALA:HB2	2.42	0.59
4:F:99:THR:HG23	4:F:105:HIS:O	2.02	0.59
5:H:760:HOH:O	4:F:145:LYS:HD3	2.00	0.59
3:A:186:ASN:HD21	3:A:193:GLU:HB2	1.67	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:88:VAL:HG12	4:B:218:LEU:HD22	1.85	0.59
4:B:109:HIS:HE1	4:B:207:LEU:O	1.85	0.59
3:E:70:GLY:HA2	3:E:166:ARG:CZ	2.32	0.59
3:A:79:LYS:C	3:A:158:ARG:HE	2.06	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
4:F:126:GLY:N	4:F:127:PRO:CD	2.65	0.59
4:F:217:PHE:CE2	4:F:228:ARG:HB3	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
3:E:52:THR:HG22	3:E:53:ASP:N	2.18	0.59
4:F:217:PHE:CD2	4:F:228:ARG:HB3	2.38	0.59
3:A:57:THR:HG22	3:A:58:HIS:N	2.17	0.59
3:A:74:ILE:HD12	3:A:74:ILE:N	2.18	0.59
3:E:201:ARG:NH1	3:E:210:ASP:HB3	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:14:DA:H2"	2:D:15:DG:O5'	2.04	0.58
2:D:17:DA:H2"	2:D:18:DA:OP2	2.04	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:76:LYS:CG	4:B:77:LYS:H	2.15	0.58
4:B:165:PRO:HG2	4:B:166:GLY:H	1.68	0.58
4:B:346:LEU:HD13	4:B:346:LEU:C	2.23	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:46:ILE:HD12	3:E:116:LEU:HD13	1.84	0.58
3:E:108:ARG:HH11	3:E:108:ARG:CB	2.16	0.58
3:E:198:ARG:NH2	4:F:310:VAL:HG11	2.19	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
3:E:127:GLU:O	3:E:130:ILE:HG22	2.02	0.58
4:F:87:TYR:HD2	4:F:88:VAL:O	1.87	0.58
3:A:262:LEU:HD11	3:A:266:VAL:HG21	1.86	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
4:B:83:LYS:C	4:B:84:ILE:HD12	2.23	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
3:A:31:GLY:N	3:A:186:ASN:HD22	2.01	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:79:LYS:O	3:A:79:LYS:HG2	2.03	0.58
4:B:228:ARG:HG2	4:B:229:LEU:N	2.19	0.58
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
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
3:A:74:ILE:HD13	3:A:100:TYR:CD1	2.39	0.57
4:F:88:VAL:HG13	4:F:89:GLY:N	2.19	0.57
4:F:254:ASP:HB2	4:F:267:TYR:HB2	1.84	0.57
2:D:21:DT:H3'	4:B:59:CYS:HG	1.69	0.57
4:B:62:PRO:HD2	5:B:843:HOH:O	2.03	0.57
4:B:123:VAL:HG21	4:B:132:VAL:CG1	2.35	0.57
3:E:266:VAL:CG1	3:E:288:TYR:HB2	2.33	0.57
2:H:22:DC:H2'	2:H:23:DC:H6	1.68	0.57
3:A:86:HIS:CE1	3:A:154:LEU:HA	2.39	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
3:E:122:LYS:HZ2	3:E:124:ARG:HH21	1.52	0.57
4:F:46:GLU:OE1	4:F:78:SER:OG	2.20	0.57
2:H:20:DT:H2"	2:H:21:DT:C5'	2.34	0.57
4:F:165:PRO:C	4:F:167:LEU:H	2.07	0.57
3:A:79:LYS:CA	3:A:158:ARG:HE	2.18	0.57
3:A:277:ASP:OD1	3:A:279:GLU:HG2	2.05	0.57
4:B:176:LEU:HD21	4:B:184:ARG:HG2	1.87	0.57
3:E:99:TYR:HB3	3:E:138:ASN:HD21	1.70	0.57
3:E:131:SER:C	3:E:133:ARG:H	2.09	0.57
1:C:1:DT:H2"	1:C:2:DG:O5'	2.03	0.56
3:E:70:GLY:HA2	3:E:166:ARG:NH2	2.19	0.56
3:E:70:GLY:CA	3:E:104:LEU:HD22	2.35	0.56
3:E:70:GLY:O	3:E:104:LEU:HD13	2.04	0.56
1:G:8:DT:H71	3:E:187:ARG:HD3	1.87	0.56
3:E:198:ARG:HH21	4:F:310:VAL:HG11	1.70	0.56
3:E:19:ALA:O	3:E:175:LEU:HD22	2.05	0.56
3:E:184:PHE:CD1	3:E:184:PHE:N	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:F:175:TYR:CD1	4:F:176:LEU:HG	2.41	0.56
1:G:11:DC:N3	2:H:15:DG:N1	2.40	0.56
3:A:270:MET:HE2	3:A:286:PHE:HB2	1.87	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:E:34:PHE:N	3:E:34:PHE:CD2	2.73	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:176:LEU:CD2	4:F:184:ARG:HG3	2.26	0.56
4:F:327:VAL:O	4:F:328:PHE:HD1	1.89	0.56
3:A:71:THR:HG23	3:A:164:THR:HB	1.86	0.56
3:A:229:THR:HG23	3:A:271:GLN:OE1	2.06	0.56
4:B:40:PRO:CG	4:B:218:LEU:HD11	2.36	0.56
4:B:346:LEU:HD13	4:B:346:LEU:O	2.06	0.56
3:E:56:LYS:H	3:E:56:LYS:CD	2.19	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
4:B:143:THR:HB	4:B:146:LYS:HD3	1.88	0.56
4:B:58:VAL:HG13	4:B:59:CYS:N	2.20	0.55
3:E:28:LYS:HD3	3:E:47:PRO:CG	2.36	0.55
3:E:81:PRO:O	3:E:83:HIS:N	2.39	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
1:C:11:DC:H2'	5:C:763:HOH:O	2.04	0.55
3:E:130:ILE:CG2	3:E:131:SER:N	2.69	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
4:B:187:THR:C	4:B:189:ARG:H	2.11	0.55
3:E:139:ASN:HD21	3:E:143:VAL:N	2.05	0.55
3:A:60:THR:HG21	3:A:110:ILE:HG22	1.89	0.55
4:F:71:SER:O	4:F:77:LYS:HG2	2.07	0.55
4:F:273:VAL:O	4:F:306:GLN:HB3	2.07	0.55
4:B:254:ASP:CB	4:B:267:TYR:H	2.21	0.54
3:E:66:TYR:CD1	3:E:67:THR:N	2.75	0.54
4:F:116:CYS:SG	4:F:137:LEU:HD21	2.47	0.54
4:F:254:ASP:CB	4:F:267:TYR:H	2.19	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)
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:F:167:LEU:N	4:F:167:LEU:CD1	2.69	0.54
3:A:187:ARG:HG2	3:A:187:ARG:HH11	1.71	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
1:C:5:DA:H3'	3:A:247:GLN:NE2	2.23	0.54
2:H:15:DG:H2"	2:H:16:DG:O5'	2.08	0.54
3:A:35:ARG:HA	3:A:35:ARG:NE	2.17	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
1:C:5:DA:H61	4:B:54:ARG:HH22	1.54	0.54
3:A:200:ASN:HD21	4:B:254:ASP:CG	2.11	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
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:HE21	4:B:185:GLN:HA	1.72	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
4:B:240:SER:C	4:B:242:ALA:H	2.10	0.54
3:A:146:GLU:HA	3:A:149:ARG:NH1	2.23	0.53
3:A:191:THR:HA	3:A:274:ARG:NH1	2.23	0.53
3:E:86:HIS:CD2	3:E:157:VAL:HG12	2.43	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
3:A:40:GLY:O	3:A:41:ARG:C	2.46	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
4:F:341:GLU:HA	4:F:341:GLU:OE1	2.08	0.53
3:E:91:VAL:O	3:E:116:LEU:HA	2.08	0.53
4:F:157:GLU:HA	4:F:157:GLU:OE1	2.08	0.53
4:F:160:ILE:HG13	4:F:161:ARG:N	2.22	0.53
3:A:35:ARG:HE	3:A:35:ARG:CA	2.19	0.53
4:B:329:VAL:HG23	4:B:345:PHE:CB	2.37	0.53
3:A:209:GLY:HA2	3:A:253:ARG:NE	2.23	0.53
4:B:84:ILE:HD12	4:B:84:ILE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:88:HIS:ND1	3:E:120:CYS:HA	2.24	0.53
4:F:45:LEU:HD23	4:F:81:GLN:HB3	1.91	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
3:A:25:GLU:OE2	3:A:60:THR:HB	2.08	0.53
4:F:108:ALA:CB	4:F:142:VAL:HG11	2.38	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
3:A:25:GLU:OE2	3:A:25:GLU:N	2.42	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
4:F:166:GLY:C	4:F:167:LEU:HD12	2.30	0.52
3:A:190:ASN:HB3	3:A:220:GLN:OE1	2.09	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
1:G:3:DG:N7	4:F:56:ARG:NH2	2.53	0.52
3:A:144:PRO:HG2	3:A:147:GLU:HB2	1.89	0.52
4:B:44:ILE:HG22	4:B:46:GLU:O	2.09	0.52
4:B:106:LEU:HD22	4:B:168:LEU:HG	1.90	0.52
3:E:78:THR:HG21	5:E:700:HOH:O	2.08	0.52
3:E:164:THR:HG22	3:E:164:THR:O	2.09	0.52
3:E:210:ASP:O	3:E:254:THR:HG23	2.09	0.52
4:F:101:GLY:O	4:F:102:LYS:C	2.48	0.52
4:F:165:PRO:HG2	4:F:176:LEU:O	2.09	0.52
3:A:190:ASN:H	3:A:190:ASN:ND2	2.08	0.52
4:F:165:PRO:O	4:F:167:LEU:N	2.41	0.52
1:G:7:DA:H2"	1:G:8:DT:O5'	2.10	0.52
1:G:10:DC:H2"	1:G:11:DC:O5'	2.09	0.52
4:B:155:MET:CE	4:B:169:VAL:HG13	2.40	0.52
3:E:96:ARG:O	3:E:98:GLY:N	2.42	0.52
3:E:257:TYR:HB2	3:E:288:TYR:CD2	2.44	0.52
4:F:318:ASP:O	4:F:318:ASP:OD2	2.28	0.52
3:A:185:ASP:C	3:A:187:ARG:H	2.13	0.52
3:A:255:PRO:HG2	3:A:288:TYR:OH	2.10	0.52
4:B:53:PHE:CD2	4:B:55:PHE:HD1	2.28	0.52
3:A:232:GLY:O	3:E:141:PHE:HA	2.10	0.52
4:B:107:HIS:ND1	4:B:210:VAL:HG23	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:143:THR:HB	4:B:146:LYS:H	1.75	0.52
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: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
3:A:19:ALA:HB1	3:A:64:ASN:O	2.10	0.51
4:B:42:LEU:HD13	4:B:214:PHE:HB3	1.92	0.51
4:F:115:HIS:HB3	4:F:122:THR:O	2.09	0.51
3:A:25:GLU:HB2	3:A:59:PRO:HA	1.91	0.51
3:A:187:ARG:HG2	3:A:187:ARG:NH1	2.24	0.51
4:B:47:GLN:NE2	4:B:235:ASP:OD1	2.44	0.51
3:E:19:ALA:HB3	3:E:175:LEU:HD21	1.92	0.51
3:E:130:ILE:O	3:E:133:ARG:HB2	2.11	0.51
3:E:241:GLN:HE21	3:E:241:GLN:HA	1.75	0.51
4:F:175:TYR:HA	4:F:177:GLN:OE1	2.10	0.51
4:F:84:ILE:HG13	4:F:130:MET:O	2.11	0.51
3:A:157:VAL:HG11	5:A:736:HOH:O	2.10	0.51
3:A:190:ASN:N	3:A:190:ASN:HD22	2.08	0.51
4:B:50:GLN:HG3	4:B:236:ALA:O	2.10	0.51
3:E:106:PRO:C	3:E:108:ARG:H	2.12	0.51
3:E:108:ARG:HH11	3:E:108:ARG:N	2.08	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
4:F:244:ASN:OD1	4:F:244:ASN:C	2.49	0.51
3:A:24:ILE:HD11	3:A:62:LYS:HD2	1.91	0.51
4:B:56:ARG:HH11	4:B:56:ARG:CB	2.21	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: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
2:D:17:DA:H2'	4:B:306:GLN:NE2	2.21	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
4:B:84:ILE:HG22	4:B:87:TYR:HB3	1.92	0.51
4:B:236:ALA:HB3	4:B:238:TYR:CZ	2.46	0.51
3:E:145:ILE:N	3:E:145:ILE:HD12	2.26	0.51
3:A:84:ARG:HB3	3:A:148:GLN:HG3	1.93	0.51
3:A:262:LEU:HD11	3:A:266:VAL:CG2	2.40	0.51
4:B:106:LEU:HD22	4:B:168:LEU:HD23	1.93	0.51
4:F:95:VAL:HG23	4:F:213:MET:O	2.10	0.51
4:F:268:LEU:HD12	4:F:280:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:239:PHE:HB3	3:A:252:PHE:CB	2.41	0.51
4:B:84:ILE:CB	4:B:130:MET:SD	2.99	0.51
4:B:126:GLY:N	4:B:127:PRO:CD	2.73	0.51
4:B:291:VAL:HG13	4:B:291:VAL:O	2.11	0.51
3:E:76:LEU:HD22	3:E:157:VAL:HB	1.93	0.51
3:E:257:TYR:OH	3:E:266:VAL:HG21	2.11	0.51
3:E:266:VAL:HG13	3:E:266:VAL:O	2.10	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: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
2:D:21:DT:H3'	4:B:59:CYS:SG	2.52	0.50
3:A:77:VAL:HG22	3:A:158:ARG:O	2.11	0.50
3:A:84:ARG:H	3:A:84:ARG:NE	2.05	0.50
3:E:41:ARG:HD3	3:E:41:ARG:N	2.27	0.50
4:F:93:VAL:HA	4:F:216:ALA:HA	1.93	0.50
4:F:114:LYS:HD2	4:F:135:ALA:O	2.11	0.50
4:F:175:TYR:O	4:F:176:LEU:HB2	2.12	0.50
4:F:272:LYS:HA	4:F:306:GLN:O	2.11	0.50
2:D:21:DT:H73	4:B:60:GLU:HB2	1.93	0.50
3:A:46:ILE:HD12	3:A:116:LEU:HD22	1.93	0.50
4:B:87:TYR:CD1	4:B:130:MET:HB2	2.46	0.50
4:F:227:ARG:NE	4:F:227:ARG:CA	2.71	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
4:B:222:THR:HG21	5:B:718:HOH:O	2.12	0.50
3:E:31:GLY:HA2	3:E:186:ASN:HD22	1.73	0.50
4:F:73:GLU:O	4:F:75:ASN:N	2.43	0.50
4:F:148:PHE:C	4:F:148:PHE:HD2	2.14	0.50
4:F:316:TYR:CG	4:F:317:LYS:N	2.79	0.50
4:B:42:LEU:HD11	4:B:93:VAL:HG13	1.93	0.50
4:B:299:SER:OG	4:B:300:PRO:HD2	2.12	0.50
4:F:95:VAL:CG1	4:F:121:CYS:HB2	2.42	0.50
3:A:267:ARG:HD3	5:A:861:HOH:O	2.12	0.50
4:B:117:GLU:HG3	4:B:117:GLU:O	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
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
4:F:189:ARG:HD2	4:F:190:GLU:CB	2.42	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: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
3:E:130:ILE:HG23	3:E:131:SER:N	2.27	0.50
4:F:49:LYS:O	4:F:49:LYS:HG3	2.12	0.50
1:C:5:DA:H2"	1:C:6:DA:H8	1.77	0.49
3:A:105:CYS:HB3	3:A:108:ARG:HB3	1.92	0.49
3:A:259:ASP:OD2	3:A:262:LEU:HA	2.12	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:F:329:VAL:HG23	4:F:345:PHE:CB	2.36	0.49
4:B:88:VAL:CG1	4:B:218:LEU:HD13	2.43	0.49
4:B:118:ASP:HB3	4:B:154:ARG:HH22	1.77	0.49
3:E:200:ASN:HB2	3:E:213:PHE:N	2.10	0.49
3:A:78:THR:O	3:A:158:ARG:HD2	2.12	0.49
3:E:174:LEU:H	3:E:174:LEU:CD2	2.13	0.49
3:E:271:GLN:HG2	3:E:283:PRO:HA	1.94	0.49
1:C:3:DG:H1'	1:C:4:DG:N7	2.27	0.49
3:A:74:ILE:HB	3:A:100:TYR:HB3	1.93	0.49
3:E:111:HIS:HD2	3:E:111:HIS:N	2.00	0.49
3:E:255:PRO:HG2	3:E:288:TYR:OH	2.11	0.49
4:F:108:ALA:HB3	4:F:205:MET:CE	2.43	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:112:VAL:HG12	4:B:113:GLY:N	2.27	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
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
3:A:89:GLU:HB3	3:A:98:GLY:HA2	1.95	0.49
3:E:178:VAL:HG22	3:E:179:LEU:N	2.28	0.49
3:E:228:PHE:CD2	3:E:255:PRO:HG3	2.48	0.49
4:F:100:ASN:OD1	4:F:101:GLY:N	2.45	0.49
4:F:237:ILE:N	4:F:237:ILE:CD1	2.75	0.49
1:C:8:DT:C2'	1:C:9:DT:H72	2.39	0.49
3:E:84:ARG:HG2	3:E:143:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:103:ASN:HB3	4:F:105:HIS:CE1	2.48	0.49
3:A:26:GLN:OE1	3:A:27:PRO:HD2	2.13	0.49
3:A:60:THR:CG2	3:A:110:ILE:HG22	2.43	0.49
4:F:282:PHE:CD2	4:F:329:VAL:HG22	2.48	0.49
3:A:74:ILE:HG13	3:A:161:PHE:CE1	2.48	0.49
4:B:83:LYS:HB3	4:B:131:VAL:HG13	1.95	0.49
4:B:115:HIS:HB3	4:B:122:THR:O	2.13	0.49
4:B:215:THR:HG23	4:B:228:ARG:CG	2.38	0.49
4:F:108:ALA:HB3	4:F:142:VAL:HG11	1.94	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:286:GLU:OE1	4:F:317:LYS:HE2	2.13	0.48
4:F:287:GLU:O	4:F:288:ASN:C	2.51	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:284:GLU:O	4:B:291:VAL:HA	2.13	0.48
4:B:333:ARG:HG2	4:B:335:SER:OG	2.13	0.48
1:C:1:DT:H2'	1:C:2:DG:C8	2.49	0.48
3:A:28:LYS:HD2	3:A:49:GLU:OE2	2.13	0.48
4:B:115:HIS:N	4:B:115:HIS:CD2	2.80	0.48
4:B:195:ARG:CA	4:B:195:ARG:NH1	2.74	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:148:PHE:CE1	4:B:199:VAL:HG22	2.45	0.48
3:A:74:ILE:H	3:A:74:ILE:CD1	2.27	0.48
3:A:216:CYS:O	4:B:304:HIS:HE1	1.96	0.48
4:B:42:LEU:HD12	4:B:214:PHE:O	2.14	0.48
4:B:186:LEU:H	4:B:186:LEU:CD1	2.12	0.48
3:E:66:TYR:CE1	3:E:68:GLY:N	2.81	0.48
3:E:282:GLU:CG	3:E:283:PRO:HD2	2.42	0.48
4:F:321:ILE:HG13	4:F:323:LYS:H	1.79	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
4:B:186:LEU:HD12	4:B:186:LEU:N	2.16	0.48
3:E:37:LYS:O	3:E:39:GLU:N	2.47	0.48
3:E:132:GLN:O	3:E:136:THR:HG22	2.14	0.48
3:E:181:HIS:HB2	3:E:182:PRO:HD2	1.95	0.48
1:G:2:DG:H2"	1:G:3:DG:H5'	1.94	0.48
4:B:57:TYR:CD1	4:B:141:HIS:HB2	2.48	0.48
4:B:110:SER:HB3	4:B:119:GLY:CA	2.44	0.48
3:E:71:THR:HG22	3:E:72:VAL:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:274:ARG:NE	3:E:277:ASP:OD1	2.45	0.48
4:F:90:PRO:HA	4:F:126:GLY:O	2.14	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
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
3:A:127:GLU:O	3:A:130:ILE:HG22	2.14	0.48
4:F:170:HIS:O	4:F:172:ASP:N	2.47	0.48
4:B:53:PHE:O	4:B:240:SER:HB2	2.14	0.47
3:E:248:VAL:CG1	4:F:305:ARG:HG3	2.43	0.47
4:F:187:THR:C	4:F:189:ARG:N	2.66	0.47
4:B:109:HIS:CD2	4:B:142:VAL:HG12	2.49	0.47
4:B:114:LYS:HE3	4:B:114:LYS:CA	2.43	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
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:B:172:ASP:C	4:B:173:LEU:HD22	2.34	0.47
4:F:84:ILE:CG1	4:F:130:MET:HB3	2.44	0.47
3:A:146:GLU:HA	3:A:149:ARG:CZ	2.44	0.47
3:E:41:ARG:HD3	3:E:41:ARG:H	1.77	0.47
4:F:333:ARG:HD2	4:F:336:ASP:OD1	2.14	0.47
3:A:106:PRO:C	3:A:108:ARG:N	2.68	0.47
4:B:219:PRO:HG3	4:B:225:PHE:HE1	1.78	0.47
4:F:321:ILE:O	4:F:349:PRO:HB3	2.15	0.47
1:C:9:DT:H2"	1:C:10:DC:OP2	2.15	0.47
1:G:6:DA:H2'	1:G:7:DA:C8	2.50	0.47
3:A:75:SER:OG	3:A:162:GLN:NE2	2.48	0.47
3:A:200:ASN:CG	3:A:213:PHE:HB2	2.34	0.47
3:A:233:TRP:HA	3:E:141:PHE:O	2.15	0.47
3:A:240:SER:OG	3:A:243:ASP:OD2	2.31	0.47
3:A:273:ARG:NH1	3:E:81:PRO:HD2	2.30	0.47
4:B:41:TYR:O	4:B:84:ILE:HG23	2.15	0.47
4:B:93:VAL:HA	4:B:216:ALA:HA	1.97	0.47
4:B:117:GLU:O	4:B:118:ASP:HB2	2.14	0.47
3:E:116:LEU:O	3:E:116:LEU:HD12	2.15	0.47
3:E:194:LEU:HB3	3:E:281:SER:HB2	1.97	0.47
4:F:50:GLN:NE2	4:F:235:ASP:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:70:ALA:O	4:F:71:SER:HB2	2.15	0.47
4:F:183:ASP:OD1	4:F:183:ASP:O	2.32	0.47
3:A:84:ARG:HG2	3:A:148:GLN:HA	1.97	0.47
4:B:57:TYR:N	4:B:57:TYR:HD2	2.12	0.47
4:B:216:ALA:O	4:B:229:LEU:HG	2.15	0.47
3:E:23:ILE:HB	3:E:26:GLN:HG3	1.97	0.47
3:E:227:TYR:CE2	3:E:229:THR:HG22	2.49	0.47
2:D:19:DT:H2"	2:D:20:DT:H71	1.96	0.47
3:A:190:ASN:ND2	3:A:190:ASN:N	2.62	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:46:ILE:CG1	3:A:116:LEU:HD13	2.45	0.46
3:A:60:THR:OG1	3:A:112:SER:HB2	2.15	0.46
3:A:63:ILE:H	3:A:63:ILE:CD1	2.20	0.46
3:A:261:SER:HA	3:A:291:ASP:OD2	2.15	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
4:B:95:VAL:HA	4:B:213:MET:O	2.15	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
3:A:245:HIS:CE1	4:B:251:VAL:HG21	2.50	0.46
3:E:140:PRO:HB3	3:E:160:CYS:SG	2.54	0.46
4:F:55:PHE:CD2	4:F:239:ASP:HB2	2.50	0.46
4:F:121:CYS:SG	4:F:137:LEU:HD21	2.55	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
3:A:41:ARG:HD3	3:A:41:ARG:N	2.29	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
4:F:173:LEU:HB3	4:F:176:LEU:HD12	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:311:PHE:CD1	4:B:311:PHE:C	2.88	0.46
3:E:78:THR:O	3:E:83:HIS:HD2	1.99	0.46
3:E:81:PRO:HB2	3:E:82:PRO:CD	2.39	0.46
3:E:196:ILE:HG12	3:E:272:LEU:HD22	1.97	0.46
3:E:227:TYR:CD2	3:E:280:LEU:HD21	2.50	0.46
3:A:160:CYS:SG	3:A:177:PRO:HB2	2.55	0.46
3:E:141:PHE:CZ	3:E:179:LEU:HD11	2.51	0.46
3:E:275:PRO:O	3:E:276:SER:C	2.54	0.46
4:F:172:ASP:C	4:F:174:ALA:H	2.19	0.46
4:F:287:GLU:O	4:F:289:GLY:N	2.48	0.46
3:A:71:THR:HA	3:A:103:ASP:HA	1.97	0.46
3:A:145:ILE:HG23	3:A:146:GLU:CD	2.36	0.46
3:A:236:ARG:HG2	3:E:147:GLU:OE2	2.16	0.46
4:B:69:GLY:N	4:B:78:SER:O	2.49	0.46
4:B:195:ARG:HA	4:B:195:ARG:NH1	2.16	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:E:203:SER:O	3:E:204:GLY:O	2.34	0.46
3:E:279:GLU:C	3:E:280:LEU:HD12	2.36	0.46
4:F:161:ARG:HG2	4:F:163:TYR:CE1	2.50	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
4:B:336:ASP:CG	4:B:338:GLU:HB2	2.37	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:141:HIS:HE1	4:B:239:ASP:CG	2.20	0.45
4:F:177:GLN:O	4:F:184:ARG:NH2	2.49	0.45
3:A:81:PRO:C	3:A:83:HIS:H	2.18	0.45
4:B:53:PHE:C	4:B:240:SER:HB2	2.37	0.45
4:B:162:GLY:HA2	4:B:177:GLN:C	2.36	0.45
3:E:139:ASN:ND2	3:E:142:HIS:HA	2.31	0.45
4:F:179:GLU:HG2	4:F:184:ARG:HH21	1.81	0.45
4:F:222:THR:HG22	4:F:223:GLY:N	2.30	0.45
4:F:267:TYR:CE1	4:F:310:VAL:HG22	2.51	0.45
3:A:26:GLN:HG3	3:A:181:HIS:CD2	2.52	0.45
3:A:33:ARG:HB2	3:A:187:ARG:HD3	1.99	0.45
3:A:165:VAL:O	3:A:172:PRO:HA	2.16	0.45
3:A:200:ASN:HD22	3:A:200:ASN:HA	1.54	0.45
4:B:176:LEU:HD11	4:B:184:ARG:HB2	1.98	0.45
4:F:87:TYR:CD2	4:F:88:VAL:O	2.69	0.45
4:B:185:GLN:HA	4:B:185:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:249:LYS:HG2	4:B:250:ILE:N	2.32	0.45
4:B:292:TRP:HZ2	4:B:315:LYS:O	2.00	0.45
4:B:299:SER:O	4:B:302:ASP:HB2	2.16	0.45
3:E:53:ASP:CG	3:E:54:THR:N	2.70	0.45
3:E:72:VAL:HB	3:E:104:LEU:HD11	1.97	0.45
4:F:107:HIS:CE1	4:F:210:VAL:HG12	2.51	0.45
1:C:8:DT:H2'	3:A:36:TYR:CZ	2.52	0.45
3:A:61:ILE:CG2	3:A:62:LYS:N	2.80	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
4:F:189:ARG:CD	4:F:189:ARG:C	2.85	0.45
4:F:346:LEU:HD23	4:F:346:LEU:O	2.16	0.45
3:A:185:ASP:O	3:A:187:ARG:N	2.50	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:286:GLU:HB3	4:F:287:GLU:H	1.61	0.45
4:F:346:LEU:C	4:F:346:LEU:CD2	2.80	0.45
4:B:56:ARG:HB3	4:B:56:ARG:CZ	2.46	0.45
4:F:237:ILE:HG22	4:F:237:ILE:O	2.16	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
3:E:257:TYR:HD2	3:E:259:ASP:H	1.64	0.45
3:A:185:ASP:C	3:A:187:ARG:N	2.70	0.45
4:B:42:LEU:HD13	4:B:214:PHE:CB	2.46	0.45
4:B:73:GLU:O	4:B:74:LYS:CB	2.65	0.45
4:B:88:VAL:CG1	4:B:218:LEU:HD22	2.45	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:O	3:A:121:VAL:HG13	2.17	0.44
4:B:98:VAL:HG11	4:B:213:MET:CE	2.47	0.44
3:E:77:VAL:HA	3:E:86:HIS:H	1.81	0.44
4:F:69:GLY:O	4:F:71:SER:N	2.50	0.44
4:F:71:SER:HB3	4:F:78:SER:OG	2.17	0.44
3:A:52:THR:HG22	3:A:53:ASP:N	2.32	0.44
4:B:55:PHE:CB	4:B:141:HIS:NE2	2.81	0.44
4:F:155:MET:O	4:F:194:ILE:HD13	2.18	0.44
3:A:72:VAL:HG12	3:A:163:VAL:HG12	2.00	0.44
4:B:189:ARG:O	4:B:189:ARG:NH1	2.51	0.44
3:E:255:PRO:HA	5:E:732:HOH:O	2.17	0.44
4:F:193:ILE:HD13	4:F:193:ILE:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:343:LYS:HA	4:F:344:PRO:HD3	1.71	0.44
1:C:1:DT:H2'	1:C:2:DG:H8	1.81	0.44
3:A:99:TYR:CD2	3:A:100:TYR:N	2.86	0.44
3:A:183:ILE:O	3:A:183:ILE:HG22	2.18	0.44
3:E:30:ARG:HG3	3:E:30:ARG:HH11	1.83	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
1:G:2:DG:H2"	1:G:3:DG:O5'	2.18	0.44
4:B:40:PRO:HG3	4:B:218:LEU:HD11	1.98	0.44
4:B:210:VAL:HG22	4:B:211:ARG:N	2.31	0.44
4:B:237:ILE:O	4:B:237:ILE:HG22	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
2:H:20:DT:H2"	2:H:21:DT:O5'	2.18	0.44
3:A:205:SER:C	3:A:207:LEU:H	2.21	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
4:B:114:LYS:HZ3	4:B:136:ASN:HB3	1.83	0.44
3:E:141:PHE:CD1	3:E:141:PHE:N	2.86	0.44
1:C:10:DC:P	4:B:144:LYS:HD3	2.58	0.44
1:G:2:DG:O6	4:F:64:HIS:CE1	2.71	0.44
3:A:139:ASN:HD22	3:A:139:ASN:HA	1.64	0.44
4:B:109:HIS:CD2	4:B:142:VAL:H	2.36	0.44
4:B:120:VAL:O	4:B:120:VAL:HG13	2.18	0.44
4:B:271:ASP:O	4:B:273:VAL:HG13	2.18	0.44
4:F:152:GLU:HG3	4:F:198:ALA:HB3	1.99	0.44
2:D:17:DA:C2	2:D:18:DA:C4	3.06	0.44
1:G:1:DT:H3'	4:F:64:HIS:C	2.38	0.44
3:A:77:VAL:O	3:A:86:HIS:HB2	2.18	0.44
3:A:282:GLU:HB2	5:A:873:HOH:O	2.18	0.44
4:B:250:ILE:HG21	4:B:253:MET:CE	2.48	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
4:F:153:ALA:O	4:F:156:THR:HB	2.18	0.44
4:F:318:ASP:C	4:F:320:ASN:H	2.21	0.44
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
3:E:29:GLN:NE2	3:E:182:PRO:O	2.51	0.43
3:E:88:HIS:ND1	3:E:121:VAL:HG22	2.33	0.43
3:E:136:THR:O	3:E:137:ASN:C	2.56	0.43
4:B:56:ARG:O	4:B:140:LEU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:106:LEU:HD22	4:B:168:LEU:CD2	2.47	0.43
4:B:250:ILE:HD13	4:B:268:LEU:HD11	1.99	0.43
4:B:328:PHE:CE1	4:B:344:PRO:HG3	2.52	0.43
4:F:46:GLU:HG2	4:F:47:GLN:N	2.21	0.43
3:E:164:THR:HG23	3:E:174:LEU:HD13	2.00	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:280:ILE:HG12	4:F:298:PHE:CE1	2.54	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:F:88:VAL:HG12	4:F:218:LEU:HD22	1.98	0.43
3:A:184:PHE:HB3	3:A:191:THR:HG21	2.00	0.43
4:B:143:THR:HB	4:B:146:LYS:HB2	2.00	0.43
4:B:189:ARG:HB3	4:B:189:ARG:CZ	2.49	0.43
3:E:61:ILE:O	3:E:110:ILE:HA	2.18	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:182:GLY:O	4:B:183:ASP:HB2	2.19	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
1:C:4:DG:H2"	1:C:5:DA:C8	2.53	0.43
1:C:11:DC:H6	5:C:763:HOH:O	2.02	0.43
2:D:22:DC:H41	4:B:60:GLU:HG3	1.82	0.43
3:A:34:PHE:CE1	3:A:185:ASP:HB2	2.54	0.43
4:B:228:ARG:HD2	4:B:231:PRO:HG3	2.01	0.43
4:F:170:HIS:O	4:F:171:SER:C	2.56	0.43
3:E:104:LEU:N	3:E:104:LEU:CD1	2.81	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:257:TYR:CE1	3:E:266:VAL:HG21	2.54	0.43
4:F:109:HIS:CE1	4:F:142:VAL:H	2.37	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
3:E:228:PHE:CE1	3:E:270:MET:HB2	2.54	0.43
3:E:31:GLY:HA2	3:E:186:ASN:ND2	2.33	0.42
3:E:89:GLU:HG3	3:E:133:ARG:HH12	1.84	0.42
3:E:226:VAL:HG21	3:E:252:PHE:CD2	2.54	0.42
4:F:46:GLU:CG	4:F:47:GLN:H	2.19	0.42
4:F:47:GLN:OE1	4:F:234:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:88:VAL:CG2	4:F:89:GLY:H	2.11	0.42
4:F:125:ALA:C	4:F:127:PRO:HD3	2.39	0.42
4:F:148:PHE:HB2	4:F:202:THR:HG21	2.01	0.42
2:D:18:DA:P	4:B:243:PRO:HG2	2.59	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
3:A:275:PRO:O	3:A:276:SER:C	2.58	0.42
4:B:76:LYS:CG	4:B:77:LYS:N	2.78	0.42
4:B:116:CYS:N	4:B:121:CYS:SG	2.92	0.42
4:B:259:CYS:SG	4:B:350:GLU:HG2	2.60	0.42
3:E:52:THR:HG22	3:E:53:ASP:H	1.84	0.42
3:E:52:THR:CG2	3:E:53:ASP:N	2.81	0.42
3:E:73:ARG:HD2	3:E:99:TYR:HD2	1.81	0.42
3:A:79:LYS:HB3	3:A:79:LYS:HZ2	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: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:167:ASP:HB2	3:A:168:PRO:CD	2.48	0.42
4:B:62:PRO:O	4:B:63:SER:C	2.57	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:B:123:VAL:HG21	4:B:132:VAL:HG11	2.01	0.42
4:B:281:ARG:HG3	4:B:295:PHE:CE2	2.54	0.42
3:E:185:ASP:O	3:E:191:THR:OG1	2.28	0.42
3:E:219:VAL:O	3:E:247:GLN:HG2	2.19	0.42
4:F:173:LEU:HD21	4:F:190:GLU:HG3	2.01	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:B:105:HIS:CB	4:B:201:GLN:HE22	2.32	0.42
3:E:28:LYS:HB3	3:E:28:LYS:HE2	1.79	0.42
3:E:41:ARG:N	3:E:41:ARG:CD	2.82	0.42
4:F:91:ALA:O	4:F:124:THR:O	2.38	0.42
4:F:175:TYR:CE1	4:F:176:LEU:HG	2.54	0.42
4:F:202:THR:O	4:F:202:THR:HG22	2.19	0.42
3:A:106:PRO:O	3:A:108:ARG:N	2.52	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: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:HD22	4:F:136:ASN:HA	1.70	0.42
2:H:13:DA:H2'	2:H:14:DA:C8	2.55	0.42
3:A:50:ARG:HE	3:A:50:ARG:HB3	1.49	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
3:E:154:LEU:H	3:E:154:LEU:HD22	1.85	0.42
4:F:57:TYR:O	4:F:58:VAL:C	2.57	0.42
1:G:7:DA:H2"	1:G:8:DT:C5'	2.50	0.42
3:A:28:LYS:HD2	3:A:28:LYS:HA	1.92	0.42
3:A:168:PRO:HB3	5:A:726:HOH:O	2.19	0.42
4:B:55:PHE:HB2	4:B:141:HIS:CE1	2.54	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
3:E:145:ILE:N	3:E:145:ILE:CD1	2.83	0.42
3:E:163:VAL:HG12	3:E:164:THR:N	2.34	0.42
4:F:144:LYS:HD2	4:F:144:LYS:HA	1.78	0.42
4:F:284:GLU:O	4:F:291:VAL:HG13	2.20	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:B:187:THR:HG22	4:B:189:ARG:H	1.85	0.42
4:F:113:GLY:O	4:F:116:CYS:HB2	2.20	0.42
4:F:165:PRO:HB2	4:F:166:GLY:H	1.70	0.42
4:F:254:ASP:O	4:F:255:ARG:NH1	2.50	0.42
1:G:8:DT:C7	3:E:187:ARG:HD3	2.49	0.41
3:A:34:PHE:CD1	3:A:185:ASP:HB2	2.55	0.41
3:A:93:LYS:HE2	3:A:93:LYS:HB3	1.81	0.41
3:A:116:LEU:N	3:A:116:LEU:HD12	2.35	0.41
3:A:144:PRO:HG2	3:A:147:GLU:CB	2.50	0.41
4:B:232:VAL:O	4:B:232:VAL:HG23	2.20	0.41
3:E:113:PHE:CD1	3:E:113:PHE:N	2.87	0.41
4:F:77:LYS:HB3	4:F:78:SER:H	1.71	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:F:184:ARG:HD2	4:F:184:ARG:N	2.29	0.41
4:B:41:TYR:HD2	4:B:229:LEU:HB3	1.86	0.41
4:B:42:LEU:HD12	4:B:214:PHE:C	2.41	0.41
4:B:73:GLU:HB2	4:B:76:LYS:O	2.21	0.41
4:B:187:THR:HB	4:B:190:GLU:HG2	2.02	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)
3:E:29:GLN:HB3	5:E:727:HOH:O	2.19	0.41
4:F:232:VAL:HA	5:F:803:HOH:O	2.18	0.41
4:F:284:GLU:OE1	4:F:316:TYR:OH	2.30	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:49:LYS:HG2	4:B:70:ALA:HA	2.01	0.41
4:B:181:GLY:HA3	4:B:184:ARG:CD	2.50	0.41
4:B:250:ILE:HG21	4:B:253:MET:HE1	2.02	0.41
4:F:175:TYR:HA	4:F:177:GLN:CD	2.41	0.41
4:F:333:ARG:HG2	4:F:335:SER:OG	2.21	0.41
3:A:105:CYS:HA	3:A:106:PRO:HD3	1.93	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:A:239:PHE:HB3	3:A:252:PHE:HB3	2.01	0.41
3:A:272:LEU:HB2	3:A:281:SER:HB3	2.01	0.41
4:B:143:THR:C	4:B:145:LYS:H	2.23	0.41
3:E:28:LYS:HG2	3:E:49:GLU:CA	2.49	0.41
3:E:70:GLY:N	3:E:166:ARG:NH1	2.68	0.41
3:E:130:ILE:O	3:E:130:ILE:HD13	2.21	0.41
3:E:255:PRO:HA	3:E:256:PRO:HD3	1.96	0.41
4:F:183:ASP:O	4:F:185:GLN:N	2.54	0.41
3:A:258:ALA:O	3:A:260:PRO:HD3	2.20	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
4:F:50:GLN:HE21	4:F:236:ALA:H	1.69	0.41
4:F:160:ILE:C	4:F:160:ILE:HD12	2.41	0.41
3:A:85:PRO:HB2	3:A:133:ARG:HG3	2.02	0.41
4:B:128:LYS:HE3	4:B:128:LYS:HB2	1.92	0.41
4:B:175:TYR:O	4:B:176:LEU:CB	2.68	0.41
3:E:148:GLN:C	3:E:149:ARG:HG3	2.41	0.41
3:E:214:LEU:C	3:E:214:LEU:HD23	2.41	0.41
4:F:89:GLY:O	4:F:130:MET:HE2	2.20	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:60:THR:HG23	3:A:112:SER:HB2	2.02	0.41
3:A:188:ALA:HA	3:A:189:PRO:HD3	1.94	0.41
4:B:42:LEU:HD21	4:B:216:ALA:HB2	2.02	0.41
3:E:165:VAL:O	3:E:166:ARG:HG3	2.20	0.41
3:E:210:ASP:N	3:E:210:ASP:OD2	2.54	0.41
4:F:184:ARG:O	4:F:184:ARG:HG2	2.20	0.41
2:D:19:DT:O3'	4:B:57:TYR:HE1	2.03	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
4:B:142:VAL:HG22	4:B:143:THR:N	2.36	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:100:TYR:CD1	3:E:101:GLU:N	2.89	0.41
3:E:217:ASP:O	3:E:218:LYS:C	2.59	0.41
3:E:245:HIS:O	3:E:246:ARG:C	2.59	0.41
3:A:198:ARG:CZ	4:B:310:VAL:HG11	2.51	0.41
4:B:84:ILE:HB	4:B:130:MET:CG	2.50	0.41
4:B:218:LEU:HD12	4:B:227:ARG:CZ	2.51	0.41
3:E:217:ASP:O	3:E:219:VAL:HG13	2.20	0.41
1:C:4:DG:H2"	1:C:5:DA:H8	1.85	0.40
3:A:214:LEU:C	3:A:214:LEU:HD23	2.40	0.40
3:E:127:GLU:HG3	3:E:128:GLN:N	2.35	0.40
3:E:200:ASN:HD21	4:F:254:ASP:CG	2.24	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:229:THR:CG2	3:A:271:GLN:OE1	2.69	0.40
3:E:19:ALA:HB3	3:E:175:LEU:CD2	2.52	0.40
3:E:79:LYS:HA	3:E:158:ARG:NE	2.33	0.40
4:F:72:SER:O	4:F:77:LYS:NZ	2.49	0.40
4:F:95:VAL:O	4:F:95:VAL:HG13	2.21	0.40
4:F:332:ARG:NH1	4:F:332:ARG:CG	2.77	0.40
3:A:29:GLN:NE2	3:A:181:HIS:HB3	2.33	0.40
3:A:141:PHE:HE1	3:A:179:LEU:HD21	1.86	0.40
4:B:212:LEU:HD23	4:B:212:LEU:HA	1.97	0.40
4:F:49:LYS:HE3	4:F:49:LYS:CA	2.48	0.40
4:F:112:VAL:HG22	4:F:138:GLY:C	2.41	0.40
4:F:151:LEU:C	4:F:151:LEU:HD12	2.42	0.40
4:F:162:GLY:O	4:F:163:TYR:HD1	2.04	0.40
4:F:229:LEU:O	4:F:230:GLU:C	2.59	0.40
3:A:28:LYS:O	3:A:29:GLN:C	2.60	0.40
4:B:54:ARG:HA	4:B:240:SER:CB	2.52	0.40
4:B:56:ARG:O	4:B:139:ILE:O	2.38	0.40
4:B:304:HIS:HB3	4:B:308:ALA:HB3	2.04	0.40
3:E:72:VAL:HB	3:E:104:LEU:CD1	2.51	0.40
3:E:178:VAL:CG2	3:E:179:LEU:N	2.85	0.40
3:E:289:LEU:HB3	3:E:290:PRO:HD2	2.03	0.40
4:F:44:ILE:HA	4:F:82:VAL:HG23	2.02	0.40
3:A:81:PRO:HB2	3:A:82:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:LEU:HD12	3:A:280:LEU:C	2.42	0.40
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
4:B:165:PRO:HG2	4:B:166:GLY:N	2.34	0.40
4:B:288:ASN:C	4:B:288:ASN:HD22	2.25	0.40
3:E:184:PHE:N	3:E:184:PHE:HD1	2.19	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	1
3	E	272/274 (99%)	201 (74%)	50 (18%)	21 (8%)	1	0
4	B	311/313 (99%)	236 (76%)	54 (17%)	21 (7%)	1	1
4	F	311/313 (99%)	240 (77%)	44 (14%)	27 (9%)	1	0
All	All	1166/1174 (99%)	881 (76%)	197 (17%)	88 (8%)	1	0

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	243/243 (100%)	218 (90%)	25 (10%)	7 12
3	E	243/243 (100%)	215 (88%)	28 (12%)	5 9
4	B	269/269 (100%)	244 (91%)	25 (9%)	9 15
4	F	269/269 (100%)	239 (89%)	30 (11%)	6 10
All	All	1024/1024 (100%)	916 (90%)	108 (10%)	7 11

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

Sometimes 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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.