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PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:07 AM GMT

PDB ID : 2FO1
Title : Crystal Structure of the CSL-Notch-Mastermind ternary complex bound to DNA
Authors : Wilson, J.J.; Kovall, R.A.
Deposited on : 2006-01-12
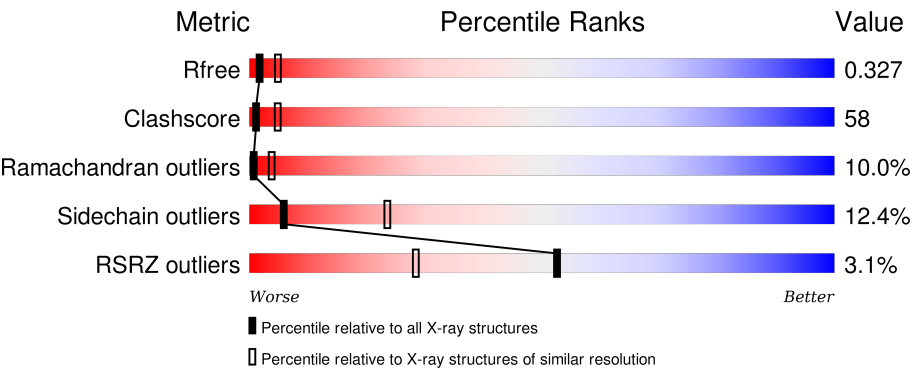Resolution : 3.12 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	Percentile Ranks	Value
Rfree		0.327
Clashscore		58
Ramachandran outliers		10.0%
Sidechain outliers		12.4%
RSRZ outliers		3.1%

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	15	33% / 60% / 7%
2	C	15	33% / 60% / 7%
3	A	477	4% — 34% / 48% / 10% / 8%
4	D	85	21% / 44% / 8% · 26%
5	E	373	2% — 16% / 46% / 16% · 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6939 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*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	15	Total 311	C 149	N 61	O 87	P 14	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total 298	C 145	N 50	O 89	P 14	0	0	0

- Molecule 3 is a protein called Lin-12 and glp-1 phenotype protein 1, isoform b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	439	Total 3497	C 2218	N 608	O 654	S 17	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	GLY	-	CLONING ARTIFACT	GB 22532887
A	188	PRO	-	CLONING ARTIFACT	GB 22532887
A	189	LEU	-	CLONING ARTIFACT	GB 22532887
A	190	GLY	-	CLONING ARTIFACT	GB 22532887
A	191	SER	-	CLONING ARTIFACT	GB 22532887

- Molecule 4 is a protein called Protein lag-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	63	Total 524	C 316	N 102	O 105	S 1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	48	SER	-	CLONING ARTIFACT	UNP Q09260

- Molecule 5 is a protein called Lin-12 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
5	E	297	2309	1420	427	445	3	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	929	GLY	-	CLONING ARTIFACT	UNP P14585
E	930	SER	-	CLONING ARTIFACT	UNP P14585
E	939	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	946	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	949	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1090	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1099	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1114	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1142	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1143	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1146	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1164	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1168	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1220	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1246	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1258	MSE	MET	MODIFIED RESIDUE	UNP P14585

3 Residue-property plots (i)

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.

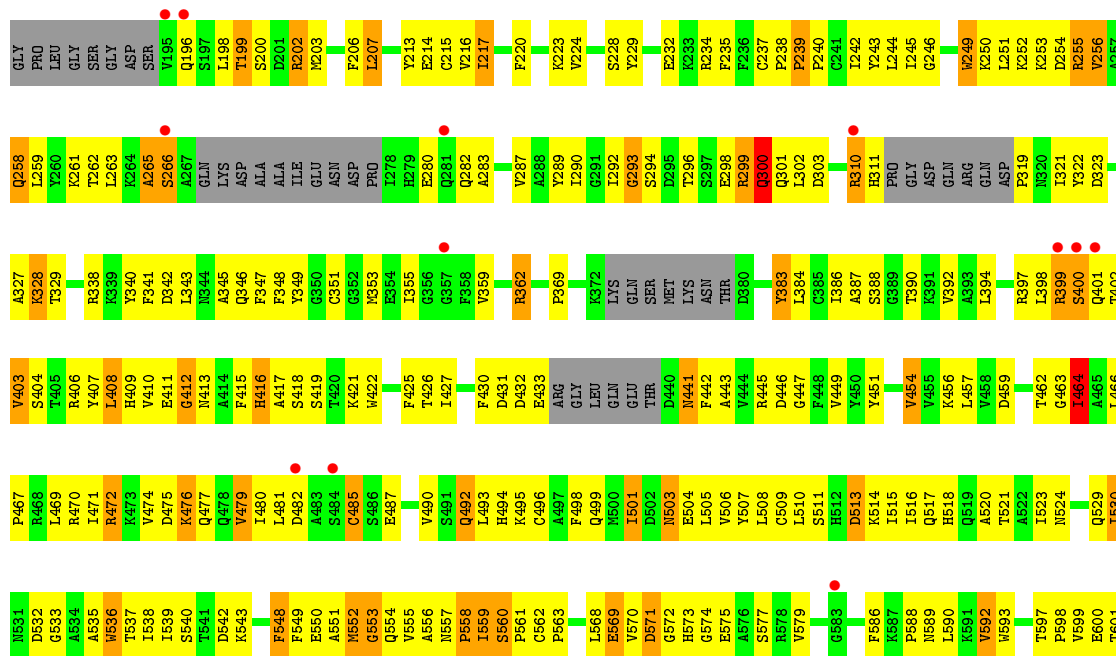- Molecule 1: 5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3'

Chain B:

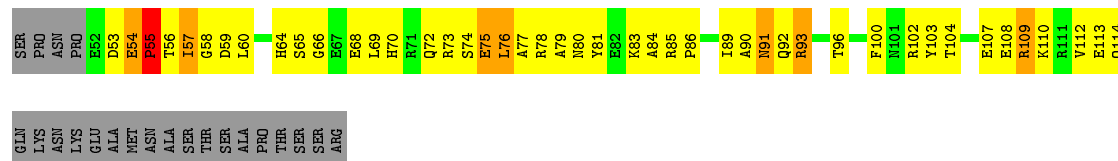- Molecule 2: 5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3'

Chain C:

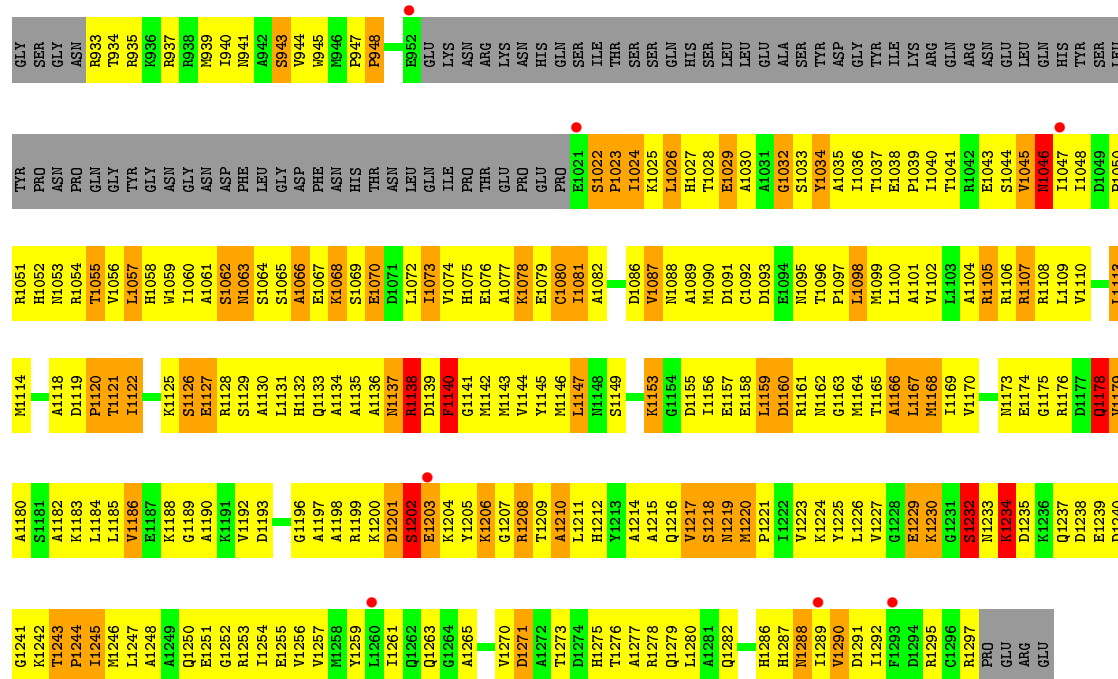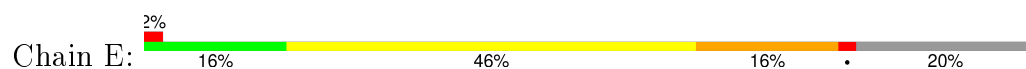- Molecule 3: Lin-12 and glp-1 phenotype protein 1, isoform b

Chain A:

T602 F603 R604 S605 E606 E607 S608 L609 H610 I613 P614 P615 V616 S617 Q618 V619 R620 N621 E622 Q623 T624 W625 W626 M627 F628 T629 N630 R631 T632 T633 G634 D635 V636 E637 V638 P639 I640 S641 L642 V643 R644 D645 G646 G647 V648 E649 Y650 S651 L654 T655 F656 S657 Y658 K659 S660 L661 E662 R663

• Molecule 4: Protein lag-3

Chain D:

21% 44% 8% · 26%

SER PRO ASN PRO E52 D53 E54 P55 T56 I57 G58 D59 L60 H64 S65 G66 E67 E68 L69 H70 R71 Q72 R73 S74 E75 L76 A77 R78 A79 N80 Y81 E82 K83 A84 R85 P86 I89 A90 N91 Q92 R93 T96 F100 N101 R102 Y103 T104 E107 E108 R109 K110 R111 V112 E113 Q114

GLN LYS ASN LYS GLU ALA MET ASN ALA SER THR SER ALA PRO THR SER SER ARG

• Molecule 5: Lin-12 protein

Chain E:

2% 16% 46% 16% · 20%

GLY SER GLY ASN R933 T934 R935 K936 R937 R938 M939 I940 N941 A942 S943 V944 W945 M946 P947 P948 E952 GLU LYS ASN ARG LYS ASN HIS GLN SER ILE THR SER SER GLN HIS SER LEU LEU GLU ALA SER TYR ASP GLY TYR TYR ILE LYS ARG ARG ASN ASN GLU LEU GLN HIS TYR SER LEU

TYR PRO ASN ASN PRO GLN GLY TYR GLY ASN GLY ASN ASP PHE LEU GLY ASP PHE ASN HIS THR ASN LEU GLN ILE PRO THR GLU PRO GLU PRO E1021 S1022 P1023 I1024 K1025 L1026 H1027 T1028 E1029 A1030 A1031 G1032 S1033 Y1034 A1035 I1036 T1037 E1038 P1039 I1040 T1041 R1042 E1043 S1044 V1045 N1046 I1047 I1048 D1049 P1050

R1051 H1052 N1053 R1054 T1055 V1056 L1057 H1058 W1059 I1060 A1061 S1062 N1063 S1064 S1065 E1067 K1068 S1069 E1070 D1071 L1072 I1073 V1074 H1075 E1076 A1077 K1078 E1079 C1080 I1081 A1082 D1086 V1087 N1088 A1089 M1090 D1091 C1092 D1093 E1094 N1095 T1096 P1097 L1098 M1099 L1100 A1101 V1102 L1103 A1104 R1105 R1106 R1107 R1108 L1109 V1110 L1113

M1114 A1118 D1119 P1120 T1121 I1122 K1125 S1126 E1127 R1128 S1129 A1130 L1131 H1132 Q1133 A1134 A1135 A1136 N1137 D1139 F1140 G1141 M1142 M1143 V1144 Y1145 M1146 L1147 N1148 S1149 K1153 G1154 D1155 I1156 E1157 E1158 L1159 D1160 R1161 N1162 G1163 M1164 T1165 A1166 L1167 M1168 I1169 V1170 N1173 E1174 G1175 R1176 D1177 Q1178 V1179

A1180 S1181 A1182 K1183 L1184 L1185 V1186 E1187 K1188 G1189 A1190 K1191 V1192 D1193 G1196 A1197 A1198 R1199 K1200 D1201 S1202 E1203 K1204 Y1205 K1206 G1207 R1208 T1209 A1210 L1211 H1212 Y1213 A1214 A1215 Q1216 V1217 S1218 N1219 M1220 P1221 I1222 V1223 K1224 Y1225 L1226 V1227 G1228 E1229 K1230 G1231 S1232 N1233 K1234 D1235 K1236 Q1237 D1238 E1239 D1240

G1241 K1242 T1243 P1244 I1245 M1246 L1247 A1248 A1249 Q1250 E1251 G1252 R1253 I1254 E1255 V1256 V1257 M1258 Y1259 L1260 I1261 Q1262 G1263 G1264 A1265 V1270 D1271 A1272 T1273 D1274 H1275 T1276 A1277 R1278 Q1279 L1280 A1281 Q1282 H1286 H1287 N1288 I1289 V1290 D1291 I1292 F1293 D1294 R1295 C1296 R1297 PRO GLU ARG GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.09Å 96.78Å 243.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.51 – 3.12	Depositor
	43.51 – 3.12	EDS
% Data completeness	88.6 (43.51-3.12)	Depositor
(in resolution range)	93.0 (43.51-3.12)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.273 , 0.340	Depositor
	0.276 , 0.327	DCC
R_{free} test set	2632 reflections (9.92%)	DCC
Wilson B-factor (Å²)	94.2	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.23 , 72.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Outliers	2 of 52029 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6939	wwPDB-VP
Average B, all atoms (Å²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	B	0.66	0/350	0.80	0/540
2	C	0.64	0/332	0.81	0/509
3	A	0.45	0/3573	0.70	0/4822
4	D	0.37	0/532	0.69	1/714 (0.1%)
5	E	0.42	0/2327	0.76	0/3113
All	All	0.46	0/7114	0.73	1/9698 (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	B	0	2
2	C	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	54	GLU	C-N-CD	-5.81	107.83	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	12	DA	Sidechain
1	B	2	DT	Sidechain
2	C	2	DA	Sidechain
2	C	5	DT	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	B	311	0	171	20	0
2	C	298	0	172	17	0
3	A	3497	0	3441	343	0
4	D	524	0	491	51	0
5	E	2309	0	2301	392	0
All	All	6939	0	6576	785	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 58.

All (785) 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)
5:E:1022:SER:H	5:E:1023:PRO:HD2	1.17	1.08
5:E:1167:LEU:HD12	5:E:1167:LEU:H	1.14	1.07
3:A:283:ALA:HB1	3:A:351:CYS:HB3	1.33	1.07
5:E:935:ARG:NH1	5:E:1158:GLU:HG2	1.69	1.06
2:C:8:DC:H2"	2:C:9:DC:H5'	1.33	1.04
3:A:328:LYS:HD3	3:A:328:LYS:H	1.20	1.04
5:E:1057:LEU:HD12	5:E:1057:LEU:H	1.19	1.03
5:E:1037:THR:HG22	5:E:1038:GLU:H	1.24	1.01
5:E:1063:ASN:ND2	5:E:1106:ARG:HD3	1.74	1.01
5:E:1098:LEU:O	5:E:1098:LEU:HD12	1.58	1.01
3:A:293:GLY:HA3	3:A:338:ARG:HH22	1.25	0.99
3:A:479:VAL:HG12	3:A:481:LEU:HD23	1.39	0.99
5:E:1055:THR:H	5:E:1058:HIS:HD2	1.04	0.98
5:E:1055:THR:H	5:E:1058:HIS:CD2	1.83	0.97
5:E:1246:MSE:HE1	5:E:1271:ASP:HB3	1.43	0.97
3:A:631:ARG:HD2	3:A:631:ARG:H	1.27	0.96
5:E:1129:SER:H	5:E:1132:HIS:HD2	1.12	0.95
5:E:1034:TYR:HD1	5:E:1035:ALA:H	1.11	0.93
5:E:1120:PRO:HG2	5:E:1121:THR:H	1.32	0.93
5:E:1229:GLU:HG3	5:E:1230:LYS:N	1.81	0.93
5:E:1104:ALA:O	5:E:1105:ARG:HG2	1.70	0.92
5:E:1073:ILE:HD11	5:E:1106:ARG:CZ	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:DT:H2"	2:C:8:DC:H5"	1.53	0.91
4:D:54:GLU:HB3	4:D:55:PRO:HD2	1.51	0.91
5:E:1129:SER:H	5:E:1132:HIS:CD2	1.88	0.90
3:A:199:THR:HG23	3:A:202:ARG:HB2	1.51	0.90
3:A:472:ARG:HD3	3:A:499:GLN:OE1	1.72	0.90
3:A:328:LYS:N	3:A:328:LYS:HD3	1.88	0.89
5:E:1063:ASN:HD21	5:E:1106:ARG:HD3	1.37	0.89
5:E:1165:THR:O	5:E:1169:ILE:HG13	1.71	0.88
5:E:1110:VAL:HG21	5:E:1142:MSE:HE1	1.55	0.88
3:A:479:VAL:HG23	3:A:530:ILE:HD12	1.56	0.88
5:E:1119:ASP:OD1	5:E:1121:THR:HB	1.74	0.87
3:A:560:SER:HB3	3:A:561:PRO:HD3	1.56	0.87
3:A:293:GLY:HA3	3:A:338:ARG:NH2	1.90	0.87
5:E:1276:THR:HG22	5:E:1279:GLN:HE21	1.37	0.87
5:E:933:ARG:HH12	5:E:1090:MSE:SE	2.08	0.87
3:A:644:ARG:HB2	3:A:648:VAL:HG12	1.57	0.86
3:A:349:TYR:CE1	3:A:355:ILE:HD11	2.10	0.86
5:E:1156:ILE:HG21	5:E:1190:ALA:HB2	1.56	0.86
3:A:573:HIS:HB2	5:E:1104:ALA:HA	1.58	0.85
5:E:1167:LEU:N	5:E:1167:LEU:HD12	1.91	0.84
3:A:300:GLN:HG2	3:A:329:THR:OG1	1.78	0.84
3:A:388:SER:HB3	5:E:1202:SER:OG	1.76	0.84
3:A:479:VAL:HG12	3:A:479:VAL:O	1.77	0.84
5:E:1205:TYR:O	5:E:1206:LYS:CG	2.26	0.83
5:E:1045:VAL:HG23	5:E:1046:ASN:H	1.43	0.83
5:E:1245:ILE:H	5:E:1245:ILE:HD13	1.44	0.83
5:E:1114:MSE:HE2	5:E:1146:MSE:HG2	1.59	0.82
1:B:1:DT:H2'	1:B:2:DT:H71	1.61	0.82
3:A:644:ARG:HB3	3:A:646:ASP:OD1	1.80	0.81
3:A:292:ILE:C	3:A:294:SER:H	1.84	0.81
3:A:530:ILE:H	3:A:530:ILE:HD13	1.44	0.81
5:E:1114:MSE:HE1	5:E:1146:MSE:HA	1.62	0.81
5:E:1197:ALA:C	5:E:1199:ARG:H	1.83	0.80
3:A:355:ILE:O	3:A:559:ILE:HG12	1.82	0.80
3:A:427:ILE:O	3:A:427:ILE:HG23	1.82	0.79
3:A:283:ALA:CB	3:A:351:CYS:HB3	2.11	0.79
5:E:1074:VAL:O	5:E:1078:LYS:HG3	1.82	0.79
5:E:1129:SER:N	5:E:1132:HIS:HD2	1.80	0.79
3:A:293:GLY:CA	3:A:338:ARG:HH22	1.96	0.79
5:E:1099:MSE:HE1	5:E:1130:ALA:HA	1.63	0.79
5:E:1051:ARG:NH2	5:E:1051:ARG:HB2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1205:TYR:O	5:E:1206:LYS:HG3	1.82	0.79
5:E:1141:GLY:HA2	5:E:1144:VAL:HG12	1.65	0.78
3:A:298:GLU:O	3:A:299:ARG:HB3	1.82	0.78
3:A:251:LEU:CD1	3:A:255:ARG:HD2	2.13	0.78
3:A:631:ARG:CD	3:A:631:ARG:H	1.96	0.77
5:E:1225:TYR:O	5:E:1229:GLU:HB3	1.84	0.77
2:C:7:DT:C2'	2:C:8:DC:H5"	2.15	0.77
5:E:1127:GLU:O	5:E:1160:ASP:HA	1.85	0.77
4:D:65:SER:O	4:D:69:LEU:HD13	1.85	0.77
3:A:199:THR:CG2	3:A:202:ARG:HB2	2.15	0.77
5:E:1056:VAL:O	5:E:1060:ILE:HG12	1.86	0.76
5:E:934:THR:HG22	5:E:935:ARG:N	2.01	0.76
5:E:1037:THR:HG22	5:E:1038:GLU:N	2.00	0.76
5:E:1229:GLU:HG3	5:E:1230:LYS:H	1.47	0.76
3:A:213:TYR:HB3	3:A:549:PHE:CE2	2.20	0.76
3:A:223:LYS:HD2	3:A:383:TYR:HE2	1.51	0.76
5:E:1237:GLN:HB3	5:E:1241:GLY:HA2	1.65	0.76
5:E:1128:ARG:HG2	5:E:1132:HIS:CB	2.15	0.76
5:E:1282:GLN:HG2	5:E:1290:VAL:HG22	1.67	0.75
5:E:1135:ALA:HA	5:E:1143:MSE:HE1	1.65	0.75
3:A:432:ASP:H	3:A:443:ALA:HB3	1.50	0.75
5:E:1217:VAL:HA	5:E:1253:ARG:CG	2.16	0.75
3:A:292:ILE:O	3:A:294:SER:N	2.17	0.75
3:A:579:VAL:HG23	3:A:613:ILE:HD11	1.67	0.75
5:E:934:THR:HG22	5:E:935:ARG:H	1.52	0.75
5:E:1243:THR:HB	5:E:1245:ILE:HG12	1.68	0.75
3:A:447:GLY:H	5:E:1202:SER:HB2	1.51	0.74
3:A:493:LEU:HD21	3:A:539:ILE:HD12	1.70	0.74
3:A:392:VAL:HG12	3:A:540:SER:HA	1.68	0.74
5:E:1051:ARG:HH21	5:E:1051:ARG:HB2	1.50	0.74
3:A:571:ASP:HB3	5:E:1133:GLN:HE22	1.52	0.73
4:D:86:PRO:HA	4:D:89:ILE:HG12	1.70	0.73
3:A:263:LEU:O	3:A:263:LEU:HD23	1.88	0.73
3:A:469:LEU:HB3	3:A:498:PHE:HB3	1.68	0.73
5:E:1141:GLY:HA2	5:E:1144:VAL:CG1	2.19	0.73
3:A:588:PRO:HG3	3:A:603:PHE:CG	2.24	0.73
2:C:8:DC:C2'	2:C:9:DC:H5'	2.15	0.73
5:E:1147:LEU:HG	5:E:1188:LYS:HG3	1.71	0.73
4:D:83:LYS:HD2	4:D:84:ALA:N	2.04	0.72
4:D:69:LEU:O	4:D:72:GLN:HB2	1.89	0.72
3:A:216:VAL:HB	3:A:245:ILE:HB	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1057:LEU:CD1	5:E:1057:LEU:H	1.99	0.72
5:E:1121:THR:HG22	5:E:1122:ILE:N	2.05	0.71
3:A:397:ARG:C	3:A:398:LEU:HD22	2.11	0.71
5:E:1288:ASN:O	5:E:1292:ILE:HG12	1.89	0.71
5:E:1055:THR:O	5:E:1058:HIS:HB2	1.89	0.71
3:A:631:ARG:HD2	3:A:631:ARG:N	2.04	0.71
5:E:1197:ALA:O	5:E:1199:ARG:N	2.23	0.71
4:D:89:ILE:O	4:D:93:ARG:HB2	1.88	0.71
5:E:1057:LEU:N	5:E:1057:LEU:HD12	2.00	0.71
4:D:56:THR:HG23	5:E:1106:ARG:CZ	2.20	0.71
5:E:1218:SER:H	5:E:1253:ARG:HG3	1.55	0.71
3:A:387:ALA:HB3	3:A:390:THR:CG2	2.21	0.71
3:A:569:GLU:HG2	5:E:1128:ARG:NH2	2.06	0.71
5:E:1062:SER:C	5:E:1064:SER:H	1.92	0.71
5:E:1024:ILE:HG22	5:E:1027:HIS:H	1.55	0.70
5:E:1072:LEU:HD12	5:E:1073:ILE:N	2.06	0.70
5:E:1114:MSE:HE3	5:E:1145:TYR:HE2	1.57	0.70
3:A:604:ARG:HH21	3:A:604:ARG:HG2	1.57	0.70
2:C:7:DT:H2"	2:C:8:DC:C5'	2.22	0.70
4:D:54:GLU:CB	4:D:55:PRO:HD2	2.15	0.70
3:A:387:ALA:HB3	3:A:390:THR:HG23	1.74	0.70
5:E:1098:LEU:O	5:E:1101:ALA:HB3	1.91	0.70
5:E:1147:LEU:HB3	5:E:1188:LYS:HE3	1.73	0.70
3:A:293:GLY:CA	3:A:338:ARG:HH12	2.05	0.69
3:A:298:GLU:O	3:A:299:ARG:CB	2.41	0.69
5:E:1100:LEU:HD12	5:E:1100:LEU:H	1.58	0.69
3:A:637:GLU:HA	3:A:656:PHE:O	1.92	0.69
5:E:1200:LYS:HA	5:E:1206:LYS:HD2	1.74	0.69
5:E:1201:ASP:CG	5:E:1202:SER:H	1.96	0.69
5:E:1070:GLU:O	5:E:1073:ILE:HG12	1.91	0.69
5:E:1095:ASN:OD1	5:E:1099:MSE:HG2	1.93	0.69
3:A:293:GLY:HA3	3:A:338:ARG:HH12	1.56	0.69
5:E:1138:ARG:HG3	5:E:1178:GLN:HE22	1.55	0.69
1:B:1:DT:C2'	1:B:2:DT:H71	2.22	0.69
3:A:223:LYS:HB2	3:A:540:SER:O	1.93	0.69
3:A:559:ILE:HA	3:A:644:ARG:HH22	1.56	0.69
3:A:568:LEU:HD23	3:A:568:LEU:C	2.13	0.68
5:E:1257:VAL:O	5:E:1261:ILE:HG12	1.92	0.68
3:A:442:PHE:CE2	3:A:456:LYS:HE2	2.28	0.68
5:E:1045:VAL:HG12	5:E:1056:VAL:HG21	1.74	0.68
5:E:1102:VAL:HG13	5:E:1142:MSE:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:HIS:CE1	5:E:1174:GLU:H	2.11	0.68
3:A:425:PHE:HD2	3:A:459:ASP:HA	1.59	0.68
5:E:1205:TYR:O	5:E:1206:LYS:CB	2.41	0.68
5:E:1128:ARG:HG2	5:E:1132:HIS:HB2	1.76	0.68
3:A:548:PHE:HE1	3:A:559:ILE:HG13	1.59	0.68
3:A:415:PHE:HE1	3:A:464:ILE:HG23	1.58	0.68
1:B:13:DA:H1'	1:B:14:DG:H5"	1.76	0.68
3:A:560:SER:CB	3:A:561:PRO:HD3	2.24	0.68
5:E:1114:MSE:HE3	5:E:1145:TYR:CE2	2.29	0.67
3:A:557:ASN:HD22	3:A:557:ASN:N	1.91	0.67
5:E:1061:ALA:O	5:E:1063:ASN:N	2.27	0.67
5:E:1217:VAL:HA	5:E:1253:ARG:HG3	1.76	0.67
3:A:310:ARG:HD2	3:A:311:HIS:H	1.58	0.67
5:E:1045:VAL:HG23	5:E:1046:ASN:N	2.10	0.67
3:A:474:VAL:HG13	3:A:496:CYS:HA	1.77	0.67
5:E:1156:ILE:CG2	5:E:1190:ALA:HB2	2.24	0.67
5:E:1223:VAL:O	5:E:1227:VAL:HG22	1.94	0.67
5:E:1167:LEU:CD1	5:E:1167:LEU:H	1.96	0.67
5:E:1220:MSE:HA	5:E:1223:VAL:HG22	1.77	0.66
3:A:548:PHE:CE1	3:A:559:ILE:HG13	2.30	0.66
3:A:471:ILE:HG13	3:A:498:PHE:CE1	2.30	0.66
5:E:1098:LEU:C	5:E:1098:LEU:HD12	2.14	0.66
5:E:1120:PRO:CG	5:E:1121:THR:H	2.05	0.66
5:E:1077:ALA:O	5:E:1081:ILE:HG22	1.94	0.66
4:D:91:ASN:HD22	4:D:91:ASN:N	1.94	0.66
3:A:229:TYR:O	3:A:232:GLU:HG2	1.96	0.66
5:E:1297:ARG:HH11	5:E:1297:ARG:HB3	1.61	0.66
3:A:217:ILE:HD13	3:A:217:ILE:C	2.16	0.66
3:A:521:THR:OG1	3:A:529:GLN:HB2	1.95	0.66
5:E:1041:THR:H	5:E:1044:SER:CB	2.09	0.65
4:D:107:GLU:OE1	4:D:110:LYS:HD2	1.94	0.65
3:A:293:GLY:HA3	3:A:338:ARG:NH1	2.11	0.65
3:A:245:ILE:HD12	3:A:245:ILE:N	2.11	0.65
3:A:592:VAL:HG12	3:A:601:THR:OG1	1.96	0.65
5:E:1162:ASN:HB2	5:E:1164:MSE:HE2	1.78	0.65
3:A:431:ASP:HB3	3:A:443:ALA:HB1	1.78	0.65
4:D:76:LEU:HD11	5:E:1253:ARG:HH12	1.62	0.65
5:E:1132:HIS:O	5:E:1136:ALA:N	2.25	0.65
3:A:251:LEU:HD13	3:A:255:ARG:HD2	1.79	0.65
4:D:73:ARG:NH1	5:E:1218:SER:OG	2.30	0.64
3:A:510:LEU:HD23	3:A:533:GLY:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1055:THR:N	5:E:1058:HIS:HD2	1.86	0.64
3:A:447:GLY:N	5:E:1202:SER:HB2	2.12	0.64
5:E:1056:VAL:HG12	5:E:1060:ILE:HD11	1.80	0.64
5:E:1209:THR:O	5:E:1209:THR:HG23	1.97	0.64
3:A:530:ILE:N	3:A:530:ILE:HD13	2.13	0.64
3:A:459:ASP:OD1	3:A:462:THR:HG23	1.97	0.64
5:E:1104:ALA:C	5:E:1105:ARG:HG2	2.17	0.64
5:E:1282:GLN:HG2	5:E:1290:VAL:CG2	2.27	0.64
5:E:1234:LYS:HD3	5:E:1234:LYS:H	1.63	0.64
1:B:6:DG:H4'	3:A:235:PHE:HE2	1.61	0.64
3:A:237:CYS:HA	3:A:238:PRO:C	2.18	0.63
5:E:1157:GLU:O	5:E:1165:THR:HG22	1.97	0.63
3:A:479:VAL:O	3:A:481:LEU:HD23	1.99	0.63
3:A:509:CYS:SG	3:A:510:LEU:N	2.71	0.63
1:B:7:DT:H2"	1:B:8:DG:C8	2.34	0.63
5:E:1143:MSE:O	5:E:1147:LEU:HD22	1.98	0.63
5:E:1197:ALA:C	5:E:1199:ARG:N	2.48	0.63
5:E:1202:SER:O	5:E:1203:GLU:C	2.37	0.63
5:E:1045:VAL:HG11	5:E:1080:CYS:CB	2.28	0.63
3:A:551:ALA:HB3	3:A:647:GLY:O	1.99	0.62
3:A:640:ILE:HD11	3:A:656:PHE:HB2	1.80	0.62
3:A:621:ASN:H	3:A:624:THR:HG1	1.46	0.62
5:E:1241:GLY:O	5:E:1271:ASP:HA	1.99	0.62
3:A:292:ILE:C	3:A:294:SER:N	2.51	0.62
5:E:1217:VAL:HG23	5:E:1251:GLU:HB3	1.81	0.62
4:D:58:GLY:O	4:D:60:LEU:N	2.32	0.62
3:A:244:LEU:HB2	3:A:323:ASP:O	1.99	0.62
5:E:1120:PRO:HG2	5:E:1121:THR:N	2.10	0.62
5:E:1139:ASP:OD2	5:E:1142:MSE:HB2	2.00	0.62
2:C:14:DG:H2'	2:C:15:DT:C7	2.30	0.62
5:E:1243:THR:OG1	5:E:1246:MSE:HG3	1.99	0.62
3:A:408:LEU:HD21	3:A:415:PHE:HD2	1.64	0.62
5:E:1022:SER:N	5:E:1023:PRO:HD2	1.97	0.62
5:E:1245:ILE:HD13	5:E:1245:ILE:N	2.10	0.62
5:E:1040:ILE:N	5:E:1040:ILE:HD12	2.14	0.62
5:E:1091:ASP:OD2	5:E:1095:ASN:N	2.30	0.62
5:E:1270:VAL:HG12	5:E:1276:THR:HB	1.82	0.62
3:A:349:TYR:HE1	3:A:355:ILE:HD11	1.61	0.61
3:A:287:VAL:HB	3:A:348:PHE:CE1	2.35	0.61
5:E:1110:VAL:HG21	5:E:1142:MSE:CE	2.27	0.61
3:A:560:SER:HB3	3:A:561:PRO:CD	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1051:ARG:HH21	5:E:1051:ARG:CB	2.12	0.61
5:E:1078:LYS:HA	5:E:1081:ILE:CG2	2.29	0.61
3:A:289:TYR:CE2	3:A:301:GLN:HB2	2.35	0.61
3:A:513:ASP:O	3:A:514:LYS:HG2	2.01	0.61
3:A:388:SER:HB2	3:A:447:GLY:O	2.00	0.61
5:E:1220:MSE:HE3	5:E:1224:LYS:HG3	1.82	0.61
3:A:259:LEU:O	3:A:263:LEU:HB3	2.01	0.61
3:A:503:ASN:O	3:A:505:LEU:N	2.25	0.61
5:E:1030:ALA:HB1	5:E:1060:ILE:CD1	2.31	0.61
3:A:506:VAL:HA	3:A:518:HIS:O	2.01	0.60
3:A:213:TYR:HB3	3:A:549:PHE:CD2	2.35	0.60
4:D:70:HIS:HE1	5:E:1174:GLU:H	1.48	0.60
5:E:1133:GLN:HA	5:E:1136:ALA:HB3	1.83	0.60
5:E:1229:GLU:O	5:E:1230:LYS:HB2	2.00	0.60
3:A:557:ASN:HB3	3:A:558:PRO:HD2	1.83	0.60
3:A:293:GLY:HA3	3:A:338:ARG:CZ	2.30	0.60
4:D:55:PRO:O	5:E:1108:ARG:HB2	2.01	0.60
3:A:548:PHE:O	3:A:548:PHE:HD2	1.85	0.60
3:A:586:PHE:HB2	3:A:606:GLU:O	2.01	0.60
1:B:3:DA:H1'	1:B:4:DC:H5'	1.83	0.60
3:A:251:LEU:HD11	3:A:255:ARG:HD2	1.82	0.60
3:A:577:SER:HB3	3:A:613:ILE:HD13	1.83	0.60
3:A:477:GLN:HG2	3:A:477:GLN:O	2.00	0.60
5:E:1141:GLY:CA	5:E:1144:VAL:HG12	2.30	0.60
3:A:290:ILE:HD13	3:A:345:ALA:HB2	1.84	0.60
3:A:573:HIS:NE2	5:E:1064:SER:N	2.50	0.60
3:A:402:THR:O	3:A:404:SER:N	2.34	0.60
3:A:255:ARG:HH21	3:A:553:GLY:H	1.48	0.59
5:E:1133:GLN:NE2	5:E:1136:ALA:HB3	2.16	0.59
5:E:944:VAL:HG22	5:E:945:TRP:H	1.67	0.59
5:E:1096:THR:HG23	5:E:1099:MSE:H	1.67	0.59
1:B:1:DT:H2'	1:B:2:DT:C7	2.32	0.59
3:A:637:GLU:HA	3:A:657:SER:HA	1.83	0.59
5:E:1037:THR:CG2	5:E:1038:GLU:H	2.04	0.59
3:A:552:MET:O	3:A:553:GLY:O	2.20	0.59
1:B:6:DG:C8	1:B:7:DT:H72	2.38	0.59
5:E:1027:HIS:CE1	5:E:1048:ILE:HG22	2.37	0.59
3:A:506:VAL:HG11	3:A:517:GLN:HG2	1.84	0.59
4:D:104:THR:O	4:D:108:GLU:N	2.35	0.59
5:E:1102:VAL:HA	5:E:1142:MSE:HE3	1.85	0.59
3:A:633:THR:O	3:A:635:ASP:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1245:ILE:CD1	5:E:1245:ILE:H	2.06	0.58
5:E:1062:SER:C	5:E:1064:SER:N	2.56	0.58
3:A:644:ARG:O	3:A:646:ASP:N	2.31	0.58
5:E:1039:PRO:C	5:E:1040:ILE:HD12	2.24	0.58
5:E:1072:LEU:O	5:E:1076:GLU:N	2.27	0.58
5:E:1133:GLN:HA	5:E:1133:GLN:NE2	2.18	0.58
5:E:1182:ALA:O	5:E:1186:VAL:HG12	2.03	0.58
5:E:1078:LYS:HA	5:E:1081:ILE:HG23	1.86	0.58
5:E:1126:SER:HA	5:E:1161:ARG:HD2	1.85	0.58
3:A:494:HIS:O	3:A:537:THR:HA	2.04	0.58
5:E:944:VAL:HG22	5:E:945:TRP:N	2.18	0.58
4:D:109:ARG:O	4:D:113:GLU:HG2	2.03	0.58
3:A:520:ALA:HB1	3:A:530:ILE:HA	1.85	0.58
3:A:215:CYS:HB3	3:A:548:PHE:HE2	1.68	0.58
3:A:427:ILE:HD13	3:A:449:VAL:HG21	1.86	0.57
3:A:588:PRO:O	4:D:78:ARG:NH1	2.37	0.57
5:E:1086:ASP:O	5:E:1088:ASN:N	2.38	0.57
5:E:1045:VAL:O	5:E:1047:ILE:N	2.38	0.57
5:E:1064:SER:C	5:E:1066:ALA:H	2.07	0.57
3:A:252:LYS:NZ	3:A:554:GLN:HB2	2.19	0.57
5:E:1030:ALA:HB1	5:E:1060:ILE:HD13	1.87	0.57
5:E:1038:GLU:O	5:E:1040:ILE:CD1	2.53	0.57
3:A:479:VAL:HG12	3:A:481:LEU:CD2	2.25	0.57
5:E:1246:MSE:O	5:E:1247:LEU:C	2.43	0.57
5:E:1217:VAL:HA	5:E:1253:ARG:HG2	1.86	0.57
5:E:1022:SER:H	5:E:1023:PRO:CD	2.05	0.57
5:E:1200:LYS:O	5:E:1201:ASP:O	2.22	0.57
5:E:1287:HIS:O	5:E:1288:ASN:C	2.41	0.57
3:A:536:TRP:CD1	3:A:536:TRP:N	2.73	0.57
4:D:66:GLY:C	4:D:68:GLU:N	2.57	0.57
3:A:347:PHE:O	3:A:355:ILE:HB	2.05	0.57
3:A:559:ILE:HA	3:A:644:ARG:NH2	2.19	0.57
3:A:579:VAL:HG23	3:A:613:ILE:CD1	2.34	0.57
5:E:1270:VAL:HB	5:E:1275:HIS:O	2.05	0.56
5:E:935:ARG:CB	5:E:1199:ARG:HH22	2.19	0.56
5:E:1045:VAL:HG11	5:E:1080:CYS:HB2	1.85	0.56
4:D:60:LEU:O	4:D:64:HIS:ND1	2.30	0.56
5:E:1242:LYS:HZ2	5:E:1250:GLN:HE22	1.53	0.56
3:A:252:LYS:HG3	3:A:349:TYR:OH	2.05	0.56
3:A:255:ARG:HH21	3:A:553:GLY:N	2.04	0.56
4:D:83:LYS:O	4:D:86:PRO:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1220:MSE:SE	5:E:1223:VAL:HG21	2.56	0.56
5:E:1167:LEU:O	5:E:1168:MSE:C	2.43	0.56
5:E:1135:ALA:CA	5:E:1143:MSE:HE1	2.35	0.56
3:A:495:LYS:HA	3:A:536:TRP:O	2.05	0.56
3:A:479:VAL:CG1	3:A:479:VAL:O	2.51	0.56
5:E:945:TRP:CZ3	5:E:947:PRO:HB3	2.40	0.56
3:A:203:MET:HG3	3:A:207:LEU:HD12	1.87	0.56
5:E:1109:LEU:O	5:E:1113:LEU:HB2	2.04	0.56
5:E:1066:ALA:O	5:E:1067:GLU:HB3	2.06	0.56
3:A:415:PHE:CE2	3:A:466:LEU:HG	2.40	0.56
5:E:1041:THR:O	5:E:1045:VAL:HG22	2.05	0.56
3:A:441:ASN:HB2	5:E:939:MSE:HE1	1.87	0.56
5:E:1062:SER:O	5:E:1064:SER:N	2.38	0.56
3:A:383:TYR:O	3:A:384:LEU:HD23	2.06	0.56
3:A:408:LEU:HB3	3:A:425:PHE:HE1	1.71	0.56
3:A:615:PRO:O	3:A:618:GLN:HG2	2.05	0.56
5:E:934:THR:CG2	5:E:935:ARG:H	2.17	0.55
5:E:1186:VAL:HG11	5:E:1225:TYR:OH	2.05	0.55
2:C:1:DA:H2"	2:C:2:DA:C8	2.41	0.55
5:E:1109:LEU:HG	5:E:1113:LEU:HD23	1.88	0.55
5:E:1087:VAL:HG22	5:E:1118:ALA:HB2	1.88	0.55
5:E:1129:SER:N	5:E:1132:HIS:CD2	2.63	0.55
3:A:557:ASN:ND2	3:A:557:ASN:N	2.54	0.55
2:C:13:DA:H2"	2:C:14:DG:H8	1.72	0.55
3:A:425:PHE:CD2	3:A:459:ASP:HA	2.40	0.55
5:E:1045:VAL:CG2	5:E:1046:ASN:H	2.09	0.55
3:A:548:PHE:O	3:A:548:PHE:CD2	2.60	0.55
4:D:100:PHE:O	4:D:103:TYR:HB3	2.05	0.55
5:E:1197:ALA:HA	5:E:1200:LYS:HG3	1.87	0.55
5:E:1149:SER:O	5:E:1153:LYS:HD3	2.07	0.55
5:E:1224:LYS:HA	5:E:1259:TYR:HE1	1.71	0.55
3:A:228:SER:OG	3:A:234:ARG:HB2	2.06	0.55
5:E:1242:LYS:NZ	5:E:1250:GLN:HE22	2.04	0.55
3:A:198:LEU:HD12	3:A:199:THR:H	1.72	0.55
4:D:76:LEU:HD13	4:D:77:ALA:N	2.22	0.55
5:E:1217:VAL:O	5:E:1218:SER:O	2.24	0.55
3:A:362:ARG:N	3:A:362:ARG:HD2	2.21	0.55
3:A:548:PHE:HD1	3:A:559:ILE:HG21	1.72	0.55
5:E:1081:ILE:C	5:E:1081:ILE:HD13	2.27	0.55
5:E:1114:MSE:CE	5:E:1146:MSE:HG2	2.32	0.55
5:E:1211:LEU:HD12	5:E:1211:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:261:LYS:HG3	3:A:262:THR:N	2.22	0.55
3:A:220:PHE:HB3	3:A:422:TRP:CZ2	2.42	0.55
3:A:588:PRO:HG3	3:A:603:PHE:CD2	2.42	0.54
4:D:75:GLU:OE1	4:D:75:GLU:HA	2.06	0.54
3:A:415:PHE:CE1	3:A:464:ILE:CG2	2.90	0.54
2:C:8:DC:H5'	2:C:8:DC:H6	1.71	0.54
5:E:1128:ARG:HG2	5:E:1132:HIS:HB3	1.89	0.54
2:C:14:DG:H4'	2:C:14:DG:OP1	2.08	0.54
5:E:1047:ILE:HD12	5:E:1047:ILE:N	2.22	0.54
3:A:259:LEU:O	3:A:263:LEU:CB	2.55	0.54
3:A:586:PHE:HB2	3:A:606:GLU:C	2.28	0.54
3:A:402:THR:HG23	3:A:403:VAL:H	1.72	0.54
3:A:599:VAL:HG12	3:A:600:GLU:N	2.22	0.54
4:D:66:GLY:C	4:D:68:GLU:H	2.09	0.54
5:E:1140:PHE:CD1	5:E:1140:PHE:C	2.81	0.54
1:B:6:DG:N2	3:A:400:SER:HB3	2.22	0.54
4:D:92:GLN:HE21	4:D:96:THR:HB	1.73	0.54
3:A:410:VAL:HG21	3:A:459:ASP:OD1	2.08	0.54
1:B:13:DA:C2'	1:B:14:DG:H5"	2.38	0.54
5:E:1201:ASP:CG	5:E:1202:SER:N	2.61	0.54
3:A:571:ASP:OD1	3:A:571:ASP:N	2.40	0.54
5:E:1133:GLN:HA	5:E:1136:ALA:CB	2.38	0.53
3:A:255:ARG:NH2	3:A:553:GLY:H	2.06	0.53
5:E:1245:ILE:O	5:E:1248:ALA:HB3	2.07	0.53
3:A:287:VAL:HG11	3:A:348:PHE:CZ	2.43	0.53
5:E:935:ARG:CZ	5:E:1158:GLU:HG2	2.37	0.53
5:E:1238:ASP:OD1	5:E:1242:LYS:N	2.37	0.53
3:A:432:ASP:CG	3:A:433:GLU:H	2.11	0.53
3:A:243:TYR:HB3	3:A:245:ILE:HD11	1.89	0.53
3:A:415:PHE:HE1	3:A:464:ILE:CG2	2.21	0.53
5:E:1199:ARG:C	5:E:1201:ASP:N	2.60	0.53
5:E:1096:THR:O	5:E:1100:LEU:HD12	2.08	0.53
5:E:1131:LEU:HD21	5:E:1185:LEU:HD21	1.90	0.53
3:A:572:GLY:N	5:E:1137:ASN:HD22	2.06	0.53
5:E:1200:LYS:HG2	5:E:1206:LYS:HD2	1.90	0.53
5:E:934:THR:CG2	5:E:935:ARG:N	2.69	0.53
5:E:1057:LEU:HA	5:E:1060:ILE:HG12	1.90	0.53
5:E:1126:SER:O	5:E:1127:GLU:C	2.46	0.53
3:A:410:VAL:O	3:A:410:VAL:HG23	2.07	0.53
5:E:1086:ASP:C	5:E:1088:ASN:H	2.11	0.53
3:A:613:ILE:H	3:A:613:ILE:HD12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:77:ALA:HA	4:D:80:ASN:HD22	1.74	0.53
3:A:415:PHE:CE1	3:A:464:ILE:HG23	2.43	0.52
5:E:1203:GLU:HB3	5:E:1205:TYR:CD1	2.44	0.52
5:E:1027:HIS:HE1	5:E:1048:ILE:HG22	1.73	0.52
5:E:1048:ILE:N	5:E:1048:ILE:HD12	2.24	0.52
5:E:1159:LEU:H	5:E:1159:LEU:HD13	1.73	0.52
3:A:199:THR:HG23	3:A:202:ARG:H	1.74	0.52
3:A:442:PHE:CZ	3:A:456:LYS:HG2	2.45	0.52
4:D:91:ASN:HD22	4:D:91:ASN:H	1.57	0.52
2:C:14:DG:H2'	2:C:15:DT:H72	1.90	0.52
5:E:1167:LEU:O	5:E:1170:VAL:N	2.42	0.52
5:E:1196:GLY:O	5:E:1199:ARG:HB2	2.10	0.52
3:A:262:THR:O	3:A:262:THR:HG22	2.08	0.52
3:A:479:VAL:HG11	3:A:507:TYR:OH	2.10	0.52
5:E:1254:ILE:HG22	5:E:1289:ILE:HG12	1.92	0.52
3:A:369:PRO:HG3	3:A:493:LEU:HD12	1.92	0.52
3:A:432:ASP:O	3:A:433:GLU:CB	2.57	0.52
5:E:1046:ASN:HB3	5:E:1047:ILE:HD12	1.90	0.52
5:E:1209:THR:O	5:E:1211:LEU:N	2.43	0.52
3:A:626:TRP:O	3:A:627:MET:HB2	2.10	0.52
5:E:1045:VAL:HG11	5:E:1080:CYS:HB3	1.91	0.51
3:A:249:TRP:HA	3:A:249:TRP:CE3	2.45	0.51
5:E:945:TRP:CH2	5:E:947:PRO:HB3	2.45	0.51
3:A:542:ASP:CG	3:A:543:LYS:H	2.14	0.51
3:A:590:LEU:HA	3:A:643:VAL:O	2.10	0.51
5:E:1038:GLU:O	5:E:1040:ILE:HD12	2.10	0.51
5:E:1131:LEU:HD21	5:E:1185:LEU:CD2	2.40	0.51
5:E:1242:LYS:HG2	5:E:1246:MSE:HE2	1.93	0.51
5:E:1184:LEU:HD13	5:E:1184:LEU:C	2.31	0.51
3:A:509:CYS:O	3:A:515:ILE:HG23	2.11	0.51
5:E:1098:LEU:HD13	5:E:1110:VAL:HG13	1.92	0.51
5:E:1214:ALA:O	5:E:1215:ALA:C	2.49	0.51
4:D:56:THR:HG22	4:D:57:ILE:HD13	1.92	0.51
5:E:1235:ASP:HA	5:E:1243:THR:HG22	1.92	0.51
5:E:1220:MSE:O	5:E:1223:VAL:HG22	2.11	0.51
5:E:1159:LEU:HD23	5:E:1163:GLY:HA2	1.93	0.51
3:A:251:LEU:O	3:A:255:ARG:HG3	2.10	0.51
3:A:427:ILE:CG2	3:A:427:ILE:O	2.54	0.51
3:A:555:VAL:HG11	3:A:646:ASP:OD2	2.10	0.51
3:A:387:ALA:HB3	3:A:390:THR:HG21	1.93	0.51
3:A:220:PHE:HB3	3:A:422:TRP:CH2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:568:LEU:CD2	3:A:568:LEU:C	2.79	0.51
3:A:289:TYR:HB3	3:A:299:ARG:HG2	1.93	0.51
5:E:1297:ARG:NH1	5:E:1297:ARG:HB3	2.24	0.51
3:A:571:ASP:OD2	5:E:1136:ALA:HB1	2.11	0.50
5:E:1178:GLN:O	5:E:1180:ALA:N	2.44	0.50
4:D:104:THR:HA	4:D:107:GLU:HB3	1.92	0.50
3:A:349:TYR:HB2	3:A:353:MET:HB3	1.93	0.50
3:A:644:ARG:C	3:A:646:ASP:H	2.13	0.50
3:A:402:THR:HG23	3:A:403:VAL:N	2.27	0.50
5:E:1159:LEU:N	5:E:1159:LEU:HD13	2.27	0.50
3:A:619:VAL:HG11	3:A:638:VAL:HG11	1.94	0.50
5:E:1141:GLY:O	5:E:1144:VAL:HG12	2.11	0.50
5:E:1252:GLY:HA3	5:E:1286:HIS:CE1	2.46	0.50
1:B:13:DA:H2"	1:B:14:DG:H5"	1.93	0.50
5:E:935:ARG:HB2	5:E:1199:ARG:NH2	2.27	0.50
4:D:66:GLY:O	4:D:68:GLU:N	2.44	0.50
3:A:386:ILE:HD13	3:A:392:VAL:HG11	1.94	0.50
5:E:1276:THR:C	5:E:1280:LEU:HD23	2.32	0.50
3:A:474:VAL:HG21	3:A:535:ALA:HB1	1.93	0.50
3:A:243:TYR:CB	3:A:245:ILE:HD11	2.41	0.50
5:E:1220:MSE:HE1	5:E:1259:TYR:CD1	2.46	0.50
5:E:1276:THR:HG22	5:E:1279:GLN:NE2	2.17	0.50
5:E:1184:LEU:HD13	5:E:1188:LYS:HG2	1.92	0.50
3:A:568:LEU:HB2	3:A:654:LEU:HD23	1.94	0.50
3:A:659:LYS:HD3	5:E:1052:HIS:HD2	1.77	0.50
5:E:1022:SER:O	5:E:1023:PRO:C	2.51	0.49
5:E:1028:THR:HG23	5:E:1029:GLU:N	2.27	0.49
5:E:1099:MSE:C	5:E:1101:ALA:N	2.64	0.49
5:E:1138:ARG:CG	5:E:1178:GLN:HE22	2.23	0.49
2:C:1:DA:H1'	2:C:2:DA:H5'	1.94	0.49
1:B:6:DG:H4'	3:A:235:PHE:CE2	2.45	0.49
3:A:608:SER:O	3:A:609:LEU:HD23	2.12	0.49
5:E:1086:ASP:C	5:E:1088:ASN:N	2.66	0.49
5:E:1072:LEU:HD13	5:E:1076:GLU:OE2	2.12	0.49
5:E:1099:MSE:O	5:E:1101:ALA:N	2.45	0.49
4:D:86:PRO:HA	4:D:89:ILE:CG1	2.39	0.49
5:E:1056:VAL:CG1	5:E:1060:ILE:HD11	2.42	0.49
3:A:560:SER:O	3:A:562:CYS:N	2.46	0.49
5:E:1081:ILE:HD13	5:E:1082:ALA:N	2.27	0.49
3:A:637:GLU:HG3	3:A:637:GLU:O	2.13	0.49
3:A:319:PRO:HG2	3:A:321:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1153:LYS:HA	5:E:1156:ILE:HG12	1.94	0.49
5:E:1252:GLY:HA3	5:E:1286:HIS:ND1	2.28	0.49
5:E:1201:ASP:OD1	5:E:1202:SER:N	2.42	0.49
3:A:245:ILE:HG22	3:A:246:GLY:N	2.27	0.49
3:A:394:LEU:HD11	3:A:457:LEU:HD13	1.94	0.49
3:A:388:SER:CB	5:E:1202:SER:OG	2.56	0.49
3:A:506:VAL:HG13	3:A:518:HIS:H	1.76	0.49
5:E:1110:VAL:CG2	5:E:1142:MSE:HE1	2.36	0.49
5:E:1114:MSE:HA	5:E:1118:ALA:HB3	1.95	0.48
5:E:1233:ASN:C	5:E:1235:ASP:H	2.16	0.48
5:E:1253:ARG:O	5:E:1256:VAL:HG12	2.13	0.48
2:C:1:DA:H1'	2:C:2:DA:C5'	2.43	0.48
3:A:220:PHE:CE2	3:A:543:LYS:HD2	2.48	0.48
3:A:224:VAL:HG11	3:A:492:GLN:HG2	1.94	0.48
5:E:1133:GLN:CA	5:E:1133:GLN:NE2	2.74	0.48
5:E:1220:MSE:HB2	5:E:1221:PRO:HD3	1.94	0.48
3:A:215:CYS:HB2	3:A:548:PHE:O	2.13	0.48
5:E:1064:SER:C	5:E:1066:ALA:N	2.67	0.48
3:A:432:ASP:O	3:A:433:GLU:HB2	2.12	0.48
3:A:462:THR:OG1	3:A:463:GLY:N	2.46	0.48
4:D:76:LEU:C	4:D:76:LEU:HD13	2.33	0.48
4:D:83:LYS:CD	4:D:84:ALA:N	2.75	0.48
3:A:516:ILE:HA	5:E:947:PRO:HB2	1.96	0.48
2:C:14:DG:H2"	2:C:15:DT:O5'	2.12	0.48
5:E:1201:ASP:O	5:E:1202:SER:O	2.31	0.48
5:E:1058:HIS:CE1	5:E:1089:ALA:O	2.66	0.48
3:A:223:LYS:HD2	3:A:383:TYR:CE2	2.40	0.48
5:E:1219:ASN:O	5:E:1220:MSE:C	2.52	0.48
3:A:593:TRP:CE2	3:A:598:PRO:HB3	2.48	0.48
5:E:1099:MSE:HE1	5:E:1130:ALA:CA	2.38	0.48
4:D:91:ASN:ND2	4:D:91:ASN:H	2.12	0.48
5:E:1173:ASN:O	5:E:1178:GLN:HG2	2.14	0.48
3:A:472:ARG:O	3:A:496:CYS:HB2	2.13	0.48
5:E:1253:ARG:HA	5:E:1253:ARG:NE	2.29	0.48
3:A:613:ILE:N	3:A:613:ILE:HD12	2.29	0.48
3:A:604:ARG:HG2	3:A:604:ARG:NH2	2.25	0.48
5:E:935:ARG:HB2	5:E:1199:ARG:HH22	1.79	0.48
3:A:548:PHE:C	3:A:548:PHE:CD2	2.86	0.48
3:A:310:ARG:HG2	3:A:310:ARG:HH11	1.79	0.48
4:D:91:ASN:ND2	4:D:91:ASN:N	2.61	0.48
3:A:242:ILE:N	3:A:242:ILE:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:250:LYS:O	3:A:253:LYS:HB3	2.14	0.48
5:E:1242:LYS:HG2	5:E:1246:MSE:CE	2.44	0.47
3:A:300:GLN:H	3:A:300:GLN:HE21	1.62	0.47
5:E:935:ARG:NH1	5:E:1158:GLU:CG	2.59	0.47
3:A:506:VAL:HG11	3:A:517:GLN:HE21	1.80	0.47
3:A:411:GLU:O	3:A:412:GLY:C	2.50	0.47
5:E:1022:SER:N	5:E:1023:PRO:CD	2.73	0.47
5:E:1167:LEU:CD1	5:E:1167:LEU:N	2.65	0.47
5:E:1040:ILE:N	5:E:1040:ILE:CD1	2.77	0.47
5:E:1087:VAL:CG2	5:E:1118:ALA:HB2	2.44	0.47
3:A:441:ASN:HA	5:E:941:ASN:HA	1.96	0.47
5:E:1182:ALA:C	5:E:1184:LEU:N	2.67	0.47
4:D:64:HIS:C	4:D:66:GLY:N	2.68	0.47
3:A:199:THR:O	3:A:200:SER:C	2.52	0.47
5:E:1252:GLY:HA2	5:E:1289:ILE:HD11	1.96	0.47
4:D:80:ASN:O	4:D:83:LYS:HB3	2.13	0.47
1:B:13:DA:C1'	1:B:14:DG:H5"	2.42	0.47
3:A:508:LEU:HD11	3:A:515:ILE:CG2	2.45	0.47
3:A:418:SER:HB3	3:A:421:LYS:O	2.15	0.47
3:A:451:TYR:CE1	3:A:490:VAL:HG22	2.50	0.47
3:A:550:GLU:HA	3:A:648:VAL:HG23	1.97	0.47
5:E:1045:VAL:HG12	5:E:1056:VAL:CG2	2.41	0.47
5:E:1243:THR:O	5:E:1244:PRO:C	2.53	0.47
5:E:1276:THR:O	5:E:1278:ARG:N	2.48	0.47
5:E:1034:TYR:HD1	5:E:1035:ALA:N	1.94	0.47
1:B:13:DA:H2"	1:B:14:DG:C5'	2.45	0.47
5:E:1093:ASP:HA	5:E:1125:LYS:HD2	1.97	0.47
3:A:254:ASP:C	3:A:256:VAL:H	2.17	0.47
5:E:1196:GLY:O	5:E:1199:ARG:N	2.47	0.47
5:E:1208:ARG:HB3	5:E:1212:HIS:HB2	1.96	0.47
3:A:560:SER:CB	3:A:561:PRO:CD	2.90	0.47
3:A:254:ASP:O	3:A:256:VAL:N	2.47	0.47
5:E:1180:ALA:C	5:E:1182:ALA:N	2.67	0.47
4:D:76:LEU:O	4:D:76:LEU:HD22	2.14	0.47
5:E:1073:ILE:HD11	5:E:1106:ARG:NH2	2.30	0.46
3:A:493:LEU:CD2	3:A:539:ILE:HD12	2.41	0.46
3:A:415:PHE:CZ	3:A:466:LEU:HG	2.50	0.46
5:E:1220:MSE:HE1	5:E:1259:TYR:HD1	1.80	0.46
5:E:1099:MSE:CE	5:E:1130:ALA:HA	2.40	0.46
3:A:555:VAL:HG12	3:A:556:ALA:N	2.31	0.46
5:E:1199:ARG:NH1	5:E:1203:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:569:GLU:CG	5:E:1128:ARG:NH2	2.78	0.46
3:A:510:LEU:HG	3:A:510:LEU:O	2.15	0.46
5:E:1234:LYS:HG3	5:E:1265:ALA:HB2	1.98	0.46
3:A:441:ASN:HB2	5:E:939:MSE:CE	2.46	0.46
3:A:362:ARG:H	3:A:362:ARG:HD2	1.81	0.46
5:E:1097:PRO:HA	5:E:1100:LEU:HD13	1.98	0.46
5:E:1259:TYR:CE2	5:E:1263:GLN:HG3	2.50	0.46
3:A:508:LEU:HD11	3:A:515:ILE:HG21	1.96	0.46
5:E:943:SER:OG	5:E:944:VAL:N	2.46	0.46
3:A:406:ARG:CZ	3:A:419:SER:HB3	2.45	0.46
5:E:1107:ARG:HA	5:E:1142:MSE:HE1	1.96	0.46
5:E:1121:THR:O	5:E:1122:ILE:C	2.53	0.46
3:A:506:VAL:CG1	3:A:517:GLN:HG2	2.46	0.46
3:A:255:ARG:HH21	3:A:553:GLY:HA2	1.80	0.46
3:A:265:ALA:O	3:A:266:SER:HB3	2.15	0.46
3:A:568:LEU:C	3:A:569:GLU:OE1	2.54	0.46
3:A:254:ASP:C	3:A:256:VAL:N	2.69	0.46
3:A:342:ASP:OD1	3:A:342:ASP:N	2.45	0.46
3:A:616:VAL:HG22	3:A:658:TYR:CE1	2.50	0.46
5:E:1029:GLU:O	5:E:1030:ALA:C	2.54	0.46
5:E:1066:ALA:O	5:E:1067:GLU:CB	2.63	0.46
3:A:215:CYS:HB3	3:A:548:PHE:CE2	2.50	0.46
5:E:1193:ASP:OD1	5:E:1232:SER:HA	2.15	0.46
3:A:523:ILE:HG23	3:A:524:ASN:N	2.30	0.46
3:A:568:LEU:HD23	3:A:569:GLU:N	2.30	0.46
5:E:1174:GLU:CG	5:E:1175:GLY:H	2.29	0.46
3:A:290:ILE:CD1	3:A:345:ALA:HB2	2.45	0.46
5:E:1025:LYS:O	5:E:1029:GLU:HG3	2.16	0.46
5:E:1113:LEU:HD13	5:E:1113:LEU:HA	1.73	0.46
3:A:620:ARG:HA	3:A:624:THR:OG1	2.15	0.46
3:A:514:LYS:HA	3:A:514:LYS:HD3	1.76	0.46
3:A:258:GLN:HA	3:A:261:LYS:HE2	1.97	0.46
3:A:563:PRO:HG3	3:A:650:TYR:CD2	2.51	0.46
3:A:447:GLY:HA2	5:E:1201:ASP:OD1	2.16	0.45
5:E:1133:GLN:O	5:E:1137:ASN:OD1	2.34	0.45
5:E:1064:SER:O	5:E:1066:ALA:N	2.40	0.45
3:A:510:LEU:HD23	3:A:510:LEU:H	1.81	0.45
5:E:1056:VAL:C	5:E:1060:ILE:HG12	2.36	0.45
5:E:1087:VAL:CG2	5:E:1113:LEU:HD12	2.46	0.45
5:E:1140:PHE:C	5:E:1140:PHE:HD1	2.17	0.45
3:A:470:ARG:HB3	3:A:499:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:933:ARG:NH1	5:E:1090:MSE:SE	2.88	0.45
1:B:7:DT:H2"	1:B:8:DG:H8	1.80	0.45
3:A:431:ASP:HB3	3:A:443:ALA:CB	2.45	0.45
3:A:542:ASP:CG	3:A:543:LYS:N	2.69	0.45
5:E:1291:ASP:O	5:E:1295:ARG:HB2	2.16	0.45
5:E:1183:LYS:O	5:E:1186:VAL:HG13	2.17	0.45
3:A:255:ARG:HH21	3:A:553:GLY:CA	2.28	0.45
5:E:1218:SER:N	5:E:1253:ARG:HG3	2.27	0.45
5:E:1199:ARG:O	5:E:1201:ASP:N	2.49	0.45
5:E:1289:ILE:O	5:E:1290:VAL:C	2.53	0.45
3:A:280:GLU:C	3:A:282:GLN:H	2.20	0.45
5:E:1063:ASN:C	5:E:1065:SER:H	2.20	0.45
5:E:1273:THR:O	5:E:1275:HIS:HD2	2.00	0.45
3:A:499:GLN:HA	3:A:506:VAL:O	2.17	0.45
5:E:1178:GLN:C	5:E:1180:ALA:H	2.20	0.45
4:D:113:GLU:O	4:D:114:GLN:HG3	2.17	0.45
3:A:593:TRP:NE1	3:A:598:PRO:HB3	2.32	0.45
5:E:1026:LEU:O	5:E:1029:GLU:HB2	2.17	0.45
3:A:588:PRO:HG3	3:A:603:PHE:CD1	2.52	0.45
5:E:1174:GLU:HG2	5:E:1175:GLY:H	1.80	0.45
5:E:1219:ASN:C	5:E:1221:PRO:HD2	2.36	0.45
5:E:1098:LEU:HD11	5:E:1146:MSE:CE	2.47	0.45
5:E:1133:GLN:O	5:E:1134:ALA:C	2.55	0.45
3:A:394:LEU:HD11	3:A:457:LEU:CD1	2.46	0.45
3:A:245:ILE:CD1	3:A:245:ILE:N	2.80	0.45
5:E:1089:ALA:O	5:E:1097:PRO:HD3	2.16	0.45
5:E:1179:VAL:HG22	5:E:1179:VAL:O	2.17	0.45
3:A:430:PHE:HB3	3:A:454:VAL:HB	1.98	0.45
5:E:1026:LEU:C	5:E:1026:LEU:HD12	2.37	0.45
5:E:1073:ILE:HD11	5:E:1106:ARG:NH1	2.31	0.45
5:E:1034:TYR:CD1	5:E:1035:ALA:N	2.75	0.45
3:A:557:ASN:HB3	3:A:558:PRO:CD	2.47	0.45
5:E:1209:THR:N	5:E:1212:HIS:ND1	2.65	0.45
3:A:616:VAL:HG22	3:A:658:TYR:CD1	2.52	0.45
5:E:1234:LYS:H	5:E:1234:LYS:CD	2.25	0.44
5:E:1029:GLU:OE1	5:E:1037:THR:HB	2.17	0.44
5:E:1141:GLY:O	5:E:1142:MSE:C	2.55	0.44
5:E:1244:PRO:O	5:E:1245:ILE:C	2.55	0.44
2:C:12:DC:H2"	2:C:13:DA:C8	2.53	0.44
1:B:8:DG:OP1	3:A:397:ARG:HD3	2.18	0.44
3:A:244:LEU:HD23	3:A:244:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:ILE:HD13	3:A:501:ILE:C	2.38	0.44
1:B:6:DG:H21	3:A:400:SER:HB3	1.82	0.44
3:A:515:ILE:HG22	3:A:516:ILE:N	2.31	0.44
3:A:605:SER:C	3:A:607:GLU:H	2.20	0.44
3:A:244:LEU:O	3:A:322:TYR:HB3	2.18	0.44
3:A:599:VAL:CG1	3:A:600:GLU:N	2.80	0.44
5:E:1233:ASN:C	5:E:1235:ASP:N	2.71	0.44
3:A:644:ARG:C	3:A:646:ASP:N	2.71	0.44
3:A:592:VAL:HA	3:A:641:SER:O	2.18	0.44
5:E:1200:LYS:C	5:E:1201:ASP:O	2.54	0.44
3:A:328:LYS:H	3:A:328:LYS:CD	2.06	0.44
5:E:1025:LYS:HD3	5:E:1038:GLU:OE1	2.17	0.44
4:D:65:SER:O	4:D:68:GLU:HB2	2.17	0.44
5:E:1099:MSE:SE	5:E:1133:GLN:HG3	2.68	0.44
3:A:411:GLU:HG3	3:A:416:HIS:NE2	2.33	0.44
3:A:239:PRO:HA	3:A:240:PRO:HD3	1.88	0.44
5:E:1207:GLY:HA2	5:E:1239:GLU:H	1.83	0.44
3:A:206:PHE:CE2	3:A:649:VAL:HG21	2.53	0.44
3:A:198:LEU:HD12	3:A:199:THR:N	2.33	0.43
4:D:85:ARG:N	4:D:86:PRO:HD2	2.33	0.43
3:A:573:HIS:O	3:A:575:GLU:N	2.51	0.43
3:A:398:LEU:N	3:A:398:LEU:HD22	2.32	0.43
3:A:589:ASN:HD22	4:D:81:TYR:HE2	1.65	0.43
3:A:215:CYS:CB	3:A:548:PHE:HE2	2.31	0.43
3:A:252:LYS:HZ1	3:A:554:GLN:HB2	1.83	0.43
3:A:416:HIS:CG	3:A:417:ALA:N	2.87	0.43
5:E:940:ILE:HG22	5:E:940:ILE:O	2.17	0.43
1:B:6:DG:H2'	1:B:7:DT:C7	2.48	0.43
4:D:76:LEU:O	4:D:79:ALA:HB3	2.19	0.43
3:A:609:LEU:HD12	3:A:642:LEU:HD21	2.00	0.43
5:E:1025:LYS:O	5:E:1028:THR:HG22	2.18	0.43
5:E:1243:THR:O	5:E:1246:MSE:N	2.51	0.43
5:E:1178:GLN:C	5:E:1180:ALA:N	2.71	0.43
1:B:6:DG:H2"	1:B:7:DT:C6	2.54	0.43
3:A:451:TYR:CD1	3:A:490:VAL:HG22	2.54	0.43
5:E:1033:SER:O	5:E:1069:SER:CB	2.66	0.43
5:E:1165:THR:OG1	5:E:1168:MSE:HE3	2.19	0.43
3:A:235:PHE:CD1	3:A:329:THR:HA	2.53	0.43
5:E:1075:HIS:C	5:E:1077:ALA:N	2.71	0.43
3:A:388:SER:HB2	3:A:447:GLY:N	2.33	0.43
5:E:1243:THR:H	5:E:1246:MSE:SE	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1253:ARG:HB2	5:E:1256:VAL:HG12	2.01	0.43
3:A:430:PHE:CD1	3:A:430:PHE:C	2.92	0.43
5:E:1073:ILE:CD1	5:E:1106:ARG:CZ	2.86	0.43
5:E:1217:VAL:HG23	5:E:1251:GLU:CB	2.48	0.43
3:A:603:PHE:CE1	3:A:606:GLU:HA	2.54	0.43
3:A:516:ILE:HG22	5:E:948:PRO:HG2	2.00	0.43
2:C:13:DA:C4	2:C:14:DG:N7	2.87	0.43
3:A:302:LEU:CD2	3:A:327:ALA:HB2	2.49	0.43
5:E:1072:LEU:C	5:E:1072:LEU:HD12	2.39	0.42
5:E:1278:ARG:O	5:E:1279:GLN:C	2.56	0.42
3:A:539:ILE:O	3:A:539:ILE:HG23	2.18	0.42
5:E:1219:ASN:OD1	5:E:1219:ASN:O	2.36	0.42
3:A:530:ILE:N	3:A:530:ILE:CD1	2.81	0.42
3:A:362:ARG:H	3:A:362:ARG:CD	2.32	0.42
5:E:1192:VAL:CG1	5:E:1226:LEU:HD22	2.50	0.42
3:A:196:GLN:HB3	3:A:552:MET:HG3	2.01	0.42
4:D:92:GLN:NE2	4:D:96:THR:HB	2.33	0.42
3:A:341:PHE:CD1	3:A:341:PHE:C	2.92	0.42
3:A:388:SER:OG	3:A:445:ARG:O	2.31	0.42
5:E:1057:LEU:HA	5:E:1060:ILE:CG1	2.49	0.42
5:E:1063:ASN:HD21	5:E:1106:ARG:HH11	1.67	0.42
5:E:1066:ALA:C	5:E:1068:LYS:H	2.22	0.42
3:A:586:PHE:CE2	3:A:642:LEU:HD11	2.54	0.42
4:D:109:ARG:HA	4:D:112:VAL:HG22	2.01	0.42
3:A:215:CYS:CB	3:A:548:PHE:CE2	3.02	0.42
3:A:348:PHE:HA	3:A:355:ILE:HG12	2.02	0.42
3:A:648:VAL:O	3:A:648:VAL:CG1	2.68	0.42
3:A:427:ILE:HG13	3:A:457:LEU:CD2	2.49	0.42
3:A:213:TYR:CB	3:A:549:PHE:CE2	2.99	0.42
3:A:597:THR:HA	3:A:598:PRO:HD2	1.85	0.42
3:A:388:SER:HB2	3:A:447:GLY:H	1.85	0.42
3:A:481:LEU:HD12	3:A:481:LEU:O	2.19	0.42
3:A:251:LEU:HD13	3:A:251:LEU:C	2.40	0.42
3:A:386:ILE:HD12	3:A:538:ILE:HD13	2.00	0.42
5:E:1182:ALA:O	5:E:1183:LYS:C	2.56	0.42
5:E:1188:LYS:HA	5:E:1188:LYS:HD3	1.68	0.42
5:E:1078:LYS:CA	5:E:1081:ILE:HG23	2.49	0.42
3:A:413:ASN:HA	3:A:464:ILE:HD12	2.00	0.42
5:E:1210:ALA:O	5:E:1211:LEU:C	2.58	0.42
3:A:416:HIS:HD1	3:A:417:ALA:H	1.67	0.42
3:A:252:LYS:HD2	3:A:252:LYS:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1043:GLU:O	5:E:1048:ILE:HD13	2.20	0.42
5:E:1034:TYR:O	5:E:1036:ILE:HG13	2.20	0.42
3:A:485:CYS:C	3:A:487:GLU:H	2.23	0.42
5:E:1026:LEU:HD12	5:E:1026:LEU:O	2.20	0.42
5:E:1091:ASP:O	5:E:1092:CYS:C	2.58	0.42
5:E:1237:GLN:HB3	5:E:1241:GLY:CA	2.45	0.42
5:E:1075:HIS:C	5:E:1077:ALA:H	2.24	0.42
5:E:1253:ARG:CB	5:E:1256:VAL:HG12	2.50	0.42
5:E:1167:LEU:HA	5:E:1170:VAL:HB	2.00	0.41
5:E:1059:TRP:O	5:E:1062:SER:HB3	2.19	0.41
3:A:407:TYR:CG	3:A:422:TRP:HB3	2.55	0.41
5:E:1166:ALA:HB1	5:E:1185:LEU:CD1	2.50	0.41
5:E:1126:SER:O	5:E:1128:ARG:N	2.53	0.41
5:E:1182:ALA:O	5:E:1184:LEU:N	2.53	0.41
5:E:1054:ARG:HG2	5:E:1091:ASP:HB3	2.01	0.41
5:E:1135:ALA:N	5:E:1143:MSE:HE2	2.35	0.41
5:E:1078:LYS:CA	5:E:1081:ILE:CG2	2.96	0.41
5:E:935:ARG:HB3	5:E:1199:ARG:HH22	1.84	0.41
5:E:1053:ASN:O	5:E:1091:ASP:HA	2.21	0.41
4:D:53:ASP:OD1	5:E:1108:ARG:NH2	2.53	0.41
3:A:659:LYS:CD	5:E:1052:HIS:HD2	2.33	0.41
3:A:388:SER:HB3	5:E:1202:SER:CB	2.48	0.41
3:A:249:TRP:HB3	3:A:322:TYR:CE1	2.56	0.41
3:A:553:GLY:O	3:A:554:GLN:C	2.58	0.41
5:E:1254:ILE:HG13	5:E:1255:GLU:N	2.36	0.41
3:A:408:LEU:HD22	3:A:425:PHE:CE1	2.55	0.41
3:A:614:PRO:HA	3:A:615:PRO:HD3	1.91	0.41
5:E:1233:ASN:O	5:E:1235:ASP:N	2.54	0.41
3:A:642:LEU:HA	3:A:642:LEU:HD23	1.82	0.41
3:A:217:ILE:HG23	3:A:217:ILE:O	2.21	0.41
5:E:1140:PHE:HD1	5:E:1141:GLY:N	2.19	0.41
3:A:287:VAL:CB	3:A:348:PHE:CE1	3.04	0.41
3:A:559:ILE:O	3:A:561:PRO:N	2.53	0.41
3:A:249:TRP:HB3	3:A:322:TYR:CD1	2.55	0.41
3:A:446:ASP:OD2	5:E:1203:GLU:HG3	2.21	0.41
5:E:1040:ILE:HG22	5:E:1040:ILE:O	2.20	0.41
5:E:1271:ASP:OD2	5:E:1275:HIS:HB2	2.21	0.41
3:A:348:PHE:CD1	3:A:348:PHE:C	2.93	0.41
3:A:348:PHE:HB2	3:A:353:MET:O	2.21	0.41
1:B:6:DG:H2"	1:B:7:DT:H6	1.86	0.41
5:E:1253:ARG:O	5:E:1257:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:442:PHE:CZ	3:A:456:LYS:HE2	2.56	0.41
2:C:1:DA:H1'	2:C:2:DA:O5'	2.21	0.41
5:E:1028:THR:O	5:E:1032:GLY:N	2.38	0.41
3:A:654:LEU:HD12	3:A:654:LEU:HA	1.86	0.41
3:A:255:ARG:NH2	3:A:553:GLY:HA2	2.36	0.41
5:E:1216:GLN:O	5:E:1217:VAL:O	2.39	0.41
5:E:1048:ILE:N	5:E:1048:ILE:CD1	2.83	0.41
3:A:466:LEU:HB3	3:A:467:PRO:HD2	2.03	0.41
3:A:441:ASN:HB3	5:E:941:ASN:HB3	2.02	0.41
5:E:1033:SER:O	5:E:1069:SER:HB3	2.20	0.41
3:A:610:HIS:HE1	5:E:1173:ASN:HD21	1.68	0.40
3:A:475:ASP:O	3:A:476:LYS:C	2.59	0.40
4:D:57:ILE:HB	4:D:58:GLY:H	1.58	0.40
5:E:1061:ALA:HA	5:E:1109:LEU:HD21	2.04	0.40
5:E:1225:TYR:OH	5:E:1229:GLU:OE1	2.37	0.40
3:A:220:PHE:CD2	3:A:220:PHE:N	2.90	0.40
3:A:280:GLU:C	3:A:282:GLN:N	2.74	0.40
3:A:399:ARG:O	3:A:401:GLN:N	2.55	0.40
3:A:343:LEU:O	3:A:359:VAL:HA	2.21	0.40
3:A:340:TYR:CE2	3:A:383:TYR:CE1	3.10	0.40
3:A:409:HIS:ND1	3:A:410:VAL:N	2.69	0.40
4:D:90:ALA:C	4:D:92:GLN:N	2.74	0.40
3:A:602:THR:HG23	4:D:74:SER:HB2	2.02	0.40
3:A:416:HIS:ND1	3:A:417:ALA:N	2.70	0.40
5:E:1238:ASP:C	5:E:1240:ASP:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	429/477 (90%)	324 (76%)	77 (18%)	28 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	61/85 (72%)	44 (72%)	14 (23%)	3 (5%)	3	17
5	E	293/373 (79%)	170 (58%)	76 (26%)	47 (16%)	0	0
All	All	783/935 (84%)	538 (69%)	167 (21%)	78 (10%)	1	4

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	299	ARG
3	A	399	ARG
3	A	400	SER
3	A	403	VAL
3	A	504	GLU
3	A	513	ASP
3	A	553	GLY
3	A	560	SER
3	A	574	GLY
3	A	627	MET
3	A	634	GLY
4	D	55	PRO
4	D	59	ASP
5	E	943	SER
5	E	1023	PRO
5	E	1032	GLY
5	E	1045	VAL
5	E	1046	ASN
5	E	1062	SER
5	E	1066	ALA
5	E	1070	GLU
5	E	1122	ILE
5	E	1198	ALA
5	E	1201	ASP
5	E	1202	SER
5	E	1204	LYS
5	E	1206	LYS
5	E	1217	VAL
5	E	1218	SER
5	E	1219	ASN
5	E	1230	LYS
5	E	1277	ALA
3	A	266	SER
3	A	300	GLN

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type
3	A	303	ASP
3	A	412	GLY
5	E	948	PRO
5	E	1022	SER
5	E	1050	PRO
5	E	1063	ASN
5	E	1087	VAL
5	E	1121	THR
5	E	1138	ARG
5	E	1203	GLU
5	E	1232	SER
5	E	1271	ASP
3	A	265	ALA
3	A	416	HIS
3	A	645	ASP
5	E	1024	ILE
5	E	1078	LYS
5	E	1140	PHE
5	E	1160	ASP
5	E	1166	ALA
5	E	1189	GLY
5	E	1210	ALA
3	A	207	LEU
3	A	214	GLU
3	A	255	ARG
3	A	479	VAL
3	A	532	ASP
5	E	1107	ARG
5	E	1127	GLU
5	E	1179	VAL
5	E	1234	LYS
5	E	1029	GLU
5	E	1068	LYS
5	E	1178	GLN
5	E	1208	ARG
5	E	1220	MSE
3	A	476	LYS
3	A	480	ILE
5	E	1120	PRO
5	E	1290	VAL
3	A	464	ILE
3	A	293	GLY

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Mol	Chain	Res	Type
3	A	558	PRO
4	D	57	ILE

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	385/416 (92%)	341 (89%)	44 (11%)	7	28
4	D	54/73 (74%)	47 (87%)	7 (13%)	5	22
5	E	244/298 (82%)	210 (86%)	34 (14%)	4	19
All	All	683/787 (87%)	598 (88%)	85 (12%)	6	23

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	199	THR
3	A	202	ARG
3	A	217	ILE
3	A	239	PRO
3	A	249	TRP
3	A	256	VAL
3	A	258	GLN
3	A	296	THR
3	A	300	GLN
3	A	310	ARG
3	A	328	LYS
3	A	346	GLN
3	A	362	ARG
3	A	383	TYR
3	A	408	LEU
3	A	426	THR
3	A	441	ASN
3	A	454	VAL
3	A	464	ILE
3	A	472	ARG

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Mol	Chain	Res	Type
3	A	482	ASP
3	A	485	CYS
3	A	492	GLN
3	A	501	ILE
3	A	503	ASN
3	A	511	SER
3	A	530	ILE
3	A	536	TRP
3	A	548	PHE
3	A	552	MET
3	A	559	ILE
3	A	569	GLU
3	A	570	VAL
3	A	571	ASP
3	A	592	VAL
3	A	620	ARG
3	A	623	GLN
3	A	630	ASN
3	A	631	ARG
3	A	644	ARG
3	A	648	VAL
3	A	651	SER
3	A	660	SER
3	A	662	GLU
4	D	55	PRO
4	D	75	GLU
4	D	76	LEU
4	D	91	ASN
4	D	93	ARG
4	D	102	ARG
4	D	109	ARG
5	E	937	ARG
5	E	1026	LEU
5	E	1034	TYR
5	E	1046	ASN
5	E	1055	THR
5	E	1057	LEU
5	E	1073	ILE
5	E	1079	GLU
5	E	1080	CYS
5	E	1081	ILE
5	E	1098	LEU

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Mol	Chain	Res	Type
5	E	1105	ARG
5	E	1113	LEU
5	E	1126	SER
5	E	1137	ASN
5	E	1138	ARG
5	E	1140	PHE
5	E	1147	LEU
5	E	1153	LYS
5	E	1155	ASP
5	E	1159	LEU
5	E	1167	LEU
5	E	1168	MSE
5	E	1176	ARG
5	E	1178	GLN
5	E	1186	VAL
5	E	1202	SER
5	E	1229	GLU
5	E	1232	SER
5	E	1234	LYS
5	E	1243	THR
5	E	1244	PRO
5	E	1245	ILE
5	E	1288	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	221	HIS
3	A	258	GLN
3	A	301	GLN
3	A	320	ASN
3	A	361	GLN
3	A	401	GLN
3	A	478	GLN
3	A	503	ASN
3	A	517	GLN
3	A	519	GLN
3	A	524	ASN
3	A	528	HIS
3	A	557	ASN
3	A	610	HIS
3	A	630	ASN

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Mol	Chain	Res	Type
4	D	70	HIS
4	D	80	ASN
4	D	91	ASN
4	D	92	GLN
4	D	114	GLN
5	E	1027	HIS
5	E	1046	ASN
5	E	1053	ASN
5	E	1058	HIS
5	E	1063	ASN
5	E	1132	HIS
5	E	1133	GLN
5	E	1137	ASN
5	E	1162	ASN
5	E	1172	HIS
5	E	1250	GLN
5	E	1263	GLN
5	E	1275	HIS
5	E	1279	GLN
5	E	1285	ASN

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	15/15 (100%)	-0.31	0	100	100	72, 88, 113, 115	0
2	C	15/15 (100%)	-0.36	0	100	100	66, 85, 113, 113	0
3	A	439/477 (92%)	0.05	18 (4%)	41	19	37, 97, 165, 197	0
4	D	63/85 (74%)	-0.49	0	100	100	68, 123, 174, 200	0
5	E	283/373 (75%)	-0.20	7 (2%)	61	39	52, 94, 165, 202	0
All	All	815/965 (84%)	-0.09	25 (3%)	52	28	37, 98, 166, 202	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	400	SER	8.2
3	A	484	SER	5.4
5	E	1203	GLU	4.3
3	A	626	TRP	3.8
3	A	661	LEU	3.7
3	A	399	ARG	3.6
5	E	1047	ILE	3.5
3	A	583	GLY	3.1
3	A	401	GLN	3.1
5	E	1021	GLU	3.0
3	A	195	VAL	2.9
3	A	662	GLU	2.9
3	A	196	GLN	2.9
5	E	1289	ILE	2.9
3	A	629	THR	2.8
3	A	266	SER	2.8
5	E	1260	LEU	2.6
3	A	663	ARG	2.6
3	A	623	GLN	2.5
5	E	952	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	482	ASP	2.3
5	E	1293	PHE	2.3
3	A	281	GLN	2.2
3	A	357	GLY	2.1
3	A	310	ARG	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.