



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2017 – 10:34 PM EDT

PDB ID : 5U1T  
Title : Crystal structure of the *Saccharomyces cerevisiae* separase-securin complex at 2.6 angstrom resolution  
Authors : Luo, S.; Tong, L.  
Deposited on : unknown  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

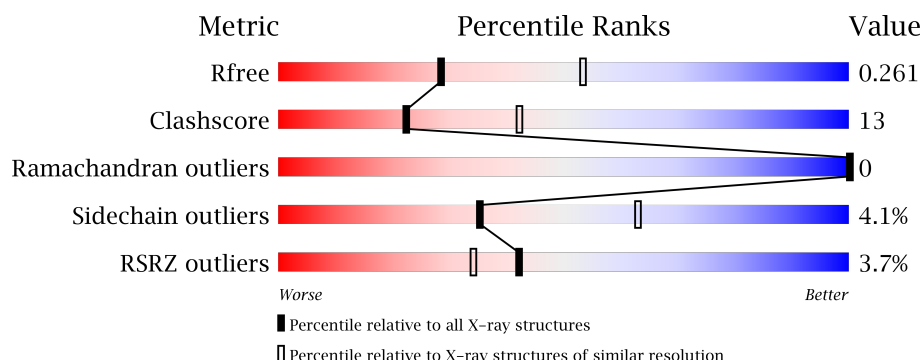
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1596	
2	B	117	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12633 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Separin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1486	Total	C	N	O	S	0	0	0
			12078	7811	1979	2220	68			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	expression tag	UNP Q03018
A	36	HIS	-	expression tag	UNP Q03018
A	37	HIS	-	expression tag	UNP Q03018
A	38	HIS	-	expression tag	UNP Q03018
A	39	HIS	-	expression tag	UNP Q03018
A	40	HIS	-	expression tag	UNP Q03018
A	41	HIS	-	expression tag	UNP Q03018
A	42	SER	-	expression tag	UNP Q03018
A	43	GLY	-	expression tag	UNP Q03018
A	44	GLY	-	expression tag	UNP Q03018
A	45	SER	-	expression tag	UNP Q03018
A	46	ARG	-	expression tag	UNP Q03018
A	47	SER	-	expression tag	UNP Q03018
A	48	GLU	-	expression tag	UNP Q03018
A	49	ALA	-	expression tag	UNP Q03018
A	50	HIS	-	expression tag	UNP Q03018

- Molecule 2 is a protein called Securin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	66	Total	C	N	O	S	0	0	0
			539	346	79	113	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	257	MET	-	initiating methionine	UNP P40316

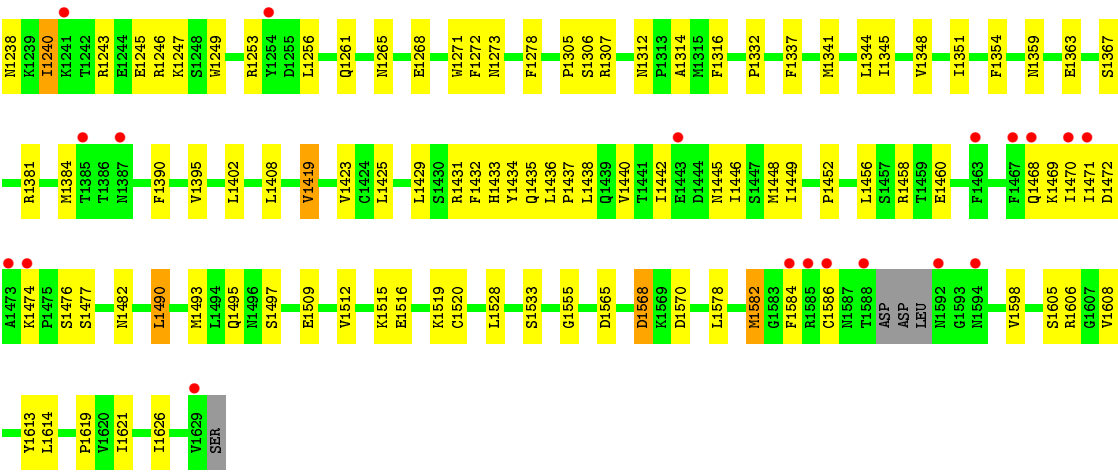
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0

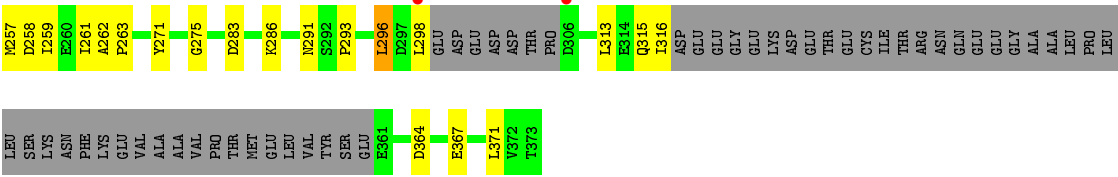
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

**Chain A:**

Position	Amino Acid(s)
I1143	K1054
S1144	M977
T1145	S978
S1149	G979
V1152	L980
Q1156	E981
M1160	K987
I1169	P996
T1170	G997
I1176	S998
R1179	V1002
L1180	I1003
L1181	P1004
L1182	S1005
K1184	L1006
L1185	D1007
R1187	N1008
R1192	L1009
L1195	L1010
L1197	L1011
P1198	L1012
L1199	L1013
I1200	L1014
S1201	L1015
S1202	L1016
S1203	L1017
S1204	L1018
S1205	L1019
S1206	L1020
S1207	L1021
S1208	L1022
S1209	L1023
S1210	L1024
S1211	L1025
S1212	L1026
S1213	L1027
S1214	L1028
S1215	L1029
S1216	L1030
S1217	L1031
S1218	L1032
S1219	L1033
S1220	L1034
S1221	L1035
S1222	L1036
S1223	L1037
S1224	L1038
S1225	L1039
S1226	L1040
S1227	L1041
S1228	L1042
S1229	L1043
S1230	L1044
S1231	L1045
S1232	L1046
S1233	L1047
S1234	L1048
S1235	L1049
S1236	L1050
S1237	L1051
S1238	L1052
S1239	L1053
S1240	L1054
S1241	L1055
S1242	L1056
S1243	L1057
S1244	L1058
S1245	L1059
S1246	L1060
S1247	L1061
S1248	L1062
S1249	L1063
S1250	L1064
S1251	L1065
S1252	L1066
S1253	L1067
S1254	L1068
S1255	L1069
S1256	L1070
S1257	L1071
S1258	L1072
S1259	L1073
S1260	L1074
S1261	L1075
S1262	L1076
S1263	L1077
S1264	L1078
S1265	L1079
S1266	L1080
S1267	L1081
S1268	L1082
S1269	L1083
S1270	L1084
S1271	L1085
S1272	L1086
S1273	L1087
S1274	L1088
S1275	L1089
S1276	L1090
S1277	L1091
S1278	L1092
S1279	L1093
S1280	L1094
S1281	L1095
S1282	L1096
S1283	L1097
S1284	L1098
S1285	L1099
S1286	L1100
S1287	L1101
S1288	L1102
S1289	L1103
S1290	L1104
S1291	L1105
S1292	L1106
S1293	L1107
S1294	L1108
S1295	L1109
S1296	L1110
S1297	L1111
S1298	L1112
S1299	L1113
S1300	L1114
S1301	L1115
S1302	L1116
S1303	L1117
S1304	L1118
S1305	L1119
S1306	L1120
S1307	L1121
S1308	L1122
S1309	L1123
S1310	L1124
S1311	L1125
S1312	L1126
S1313	L1127
S1314	L1128
S1315	L1129
S1316	L1130
S1317	L1131
S1318	L1132
S1319	L1133
S1320	L1134
S1321	L1135
S1322	L1136
S1323	L1137
S1324	L1138
S1325	L1139
S1326	L1140
S1327	L1141
S1328	L1142
S1329	L1143
S1330	L1144
S1331	L1145
S1332	L1146
S1333	L1147
S1334	L1148
S1335	L1149
S1336	L1150
S1337	L1151
S1338	L1152
S1339	L1153
S1340	L1154
S1341	L1155
S1342	L1156
S1343	L1157
S1344	L1158
S1345	L1159
S1346	L1160
S1347	L1161
S1348	L1



● Molecule 2: Securin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.86Å 125.86Å 271.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.67 – 2.60 48.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.67-2.60) 91.5 (48.67-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.221 , 0.264 0.220 , 0.261	Depositor DCC
$R_{free}$ test set	1836 reflections (2.59%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	0/12316	0.59	2/16621 (0.0%)
2	B	0.56	0/549	0.61	0/745
All	All	0.53	0/12865	0.59	2/17366 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	813	LYS	N-CA-C	-5.18	97.02	111.00
1	A	860	LEU	CB-CG-CD1	-5.11	102.31	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	996	ILE	Peptide

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

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12078	0	12320	325	0
2	B	539	0	518	21	0
3	A	16	0	0	1	0
All	All	12633	0	12838	333	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 13.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:CD1	1:A:395:SER:OG	1.66	1.43
1:A:734:LEU:HD11	1:A:738:GLN:NE2	1.42	1.33
1:A:353:ILE:HD12	1:A:395:SER:OG	1.12	1.28
1:A:591:GLU:OE2	1:A:595:ARG:NE	1.71	1.23
1:A:255:SER:HB3	1:A:290:ILE:HD11	1.15	1.12
1:A:860:LEU:HD12	1:A:861:GLU:H	1.22	1.00
1:A:255:SER:HB3	1:A:290:ILE:CD1	1.95	0.97
1:A:860:LEU:HD12	1:A:861:GLU:N	1.79	0.97
1:A:734:LEU:HD11	1:A:738:GLN:HE21	0.86	0.96
1:A:734:LEU:CD1	1:A:738:GLN:NE2	2.29	0.95
1:A:336:ASN:ND2	1:A:377:ASP:OD2	1.99	0.95
1:A:634:ILE:HG21	1:A:639:MET:CE	1.97	0.94
1:A:317:TYR:OH	1:A:341:ASN:ND2	2.01	0.93
1:A:494:ASN:HD21	1:A:532:ASN:HD22	1.14	0.93
1:A:255:SER:CB	1:A:290:ILE:HD11	1.99	0.93
1:A:356:THR:O	1:A:360:LEU:HD13	1.70	0.92
1:A:607:HIS:CD2	1:A:862:GLU:OE2	2.23	0.91
1:A:728:HIS:ND1	1:A:959:GLU:OE1	2.04	0.90
1:A:187:ILE:HD13	1:A:216:PHE:HE2	1.38	0.88
1:A:494:ASN:HD21	1:A:532:ASN:ND2	1.72	0.88
1:A:1446:ILE:HD11	1:A:1470:ILE:HG21	1.53	0.88
1:A:323:ASN:HD21	1:A:358:LYS:NZ	1.70	0.88
1:A:860:LEU:CD1	1:A:861:GLU:H	1.87	0.87
1:A:277:TYR:OH	1:A:289:LYS:CE	2.22	0.86
1:A:1446:ILE:HD11	1:A:1470:ILE:CG2	2.06	0.85
1:A:145:HIS:H	1:A:149:ASN:HD22	1.27	0.82
1:A:557:GLN:HG3	1:A:580:THR:OG1	1.79	0.81
1:A:634:ILE:HG21	1:A:639:MET:HE3	1.63	0.81
1:A:323:ASN:HD21	1:A:358:LYS:HZ2	1.27	0.79
1:A:277:TYR:OH	1:A:289:LYS:HE2	1.82	0.78
1:A:734:LEU:CD1	1:A:738:GLN:HE21	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1490:LEU:HD11	1:A:1512:VAL:HB	1.68	0.75
1:A:271:ILE:HD11	1:A:324:ARG:NH1	2.02	0.75
1:A:634:ILE:HG21	1:A:639:MET:HE2	1.66	0.75
2:B:316:ILE:N	2:B:316:ILE:HD12	2.02	0.74
1:A:323:ASN:ND2	1:A:358:LYS:NZ	2.35	0.73
1:A:303:GLU:HA	1:A:306:ARG:HB2	1.69	0.73
1:A:1490:LEU:HA	1:A:1493:MET:HB2	1.70	0.73
1:A:808:LEU:HD13	2:B:283:ASP:HB3	1.70	0.73
1:A:1046:ARG:NH2	1:A:1354:PHE:O	2.22	0.72
1:A:857:ILE:HD11	1:A:869:CYS:HB3	1.72	0.72
1:A:1268:GLU:HG3	1:A:1408:LEU:HD22	1.70	0.72
1:A:634:ILE:CG2	1:A:639:MET:HE2	2.20	0.71
1:A:1123:ASN:HD21	1:A:1519:LYS:HA	1.55	0.71
1:A:187:ILE:HD13	1:A:216:PHE:CE2	2.25	0.70
1:A:304:VAL:O	1:A:308:ILE:HG12	1.92	0.69
1:A:236:LYS:HG2	1:A:283:LEU:HB3	1.74	0.69
1:A:353:ILE:CD1	1:A:395:SER:CB	2.69	0.69
1:A:494:ASN:ND2	1:A:532:ASN:HD22	1.88	0.67
1:A:727:VAL:HG12	1:A:783:LEU:HG	1.77	0.67
1:A:353:ILE:HD13	1:A:395:SER:OG	1.84	0.67
1:A:258:LEU:HA	1:A:263:TYR:HD2	1.59	0.67
1:A:1432:PHE:CG	1:A:1438:LEU:HD11	2.30	0.66
1:A:267:GLY:O	1:A:270:LYS:HE2	1.95	0.66
1:A:806:SER:HA	1:A:809:LYS:HE2	1.77	0.66
1:A:1170:THR:HG22	1:A:1395:VAL:HB	1.76	0.66
1:A:1606:ARG:NH2	1:A:1619:PRO:O	2.29	0.65
1:A:382:PHE:HZ	1:A:428:ILE:HD11	1.61	0.65
1:A:494:ASN:ND2	1:A:532:ASN:ND2	2.42	0.65
1:A:634:ILE:CG2	1:A:639:MET:CE	2.73	0.65
1:A:356:THR:O	1:A:360:LEU:CD1	2.44	0.65
1:A:323:ASN:ND2	1:A:358:LYS:HZ1	1.95	0.65
1:A:421:GLU:HB3	1:A:424:ARG:HB2	1.78	0.64
1:A:998:SER:HB2	1:A:1351:ILE:HD13	1.79	0.64
1:A:860:LEU:CD1	1:A:861:GLU:N	2.53	0.64
1:A:946:HIS:HD2	1:A:963:LYS:HE2	1.62	0.64
1:A:1160:MET:HE3	1:A:1192:ARG:NH1	2.13	0.64
1:A:1470:ILE:HG13	1:A:1586:CYS:SG	2.38	0.64
1:A:492:LEU:HD13	1:A:492:LEU:C	2.19	0.63
1:A:1149:SER:O	1:A:1152:VAL:HG12	1.99	0.62
1:A:810:LYS:O	2:B:286:LYS:NZ	2.32	0.62
1:A:1431:ARG:NH2	1:A:1555:GLY:O	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:SER:O	1:A:1102:THR:HG23	1.98	0.62
1:A:237:GLN:CB	1:A:283:LEU:HD21	2.30	0.62
1:A:1232:THR:HG21	1:A:1565:ASP:HB3	1.83	0.61
1:A:713:LYS:HZ2	1:A:715:GLU:H	1.48	0.61
1:A:563:PHE:CZ	1:A:567:ARG:HD2	2.35	0.61
1:A:1470:ILE:HG23	1:A:1474:LYS:HD2	1.83	0.60
1:A:492:LEU:O	1:A:492:LEU:HD13	2.00	0.60
1:A:725:ILE:HG22	1:A:779:GLU:HG3	1.83	0.60
2:B:316:ILE:O	2:B:316:ILE:HG22	2.01	0.60
1:A:237:GLN:HB2	1:A:283:LEU:HD21	1.83	0.60
1:A:728:HIS:CE1	1:A:959:GLU:OE2	2.54	0.60
1:A:1306:SER:H	1:A:1359:ASN:HD21	1.48	0.60
1:A:617:LYS:HE2	1:A:657:LEU:HD21	1.84	0.60
1:A:1446:ILE:CD1	1:A:1470:ILE:HG21	2.28	0.59
1:A:311:LYS:HE2	1:A:317:TYR:HB3	1.84	0.59
1:A:591:GLU:OE2	1:A:595:ARG:CZ	2.46	0.59
1:A:1160:MET:HE2	1:A:1185:LEU:HD21	1.83	0.59
1:A:277:TYR:OH	1:A:289:LYS:HE3	2.01	0.59
1:A:1438:LEU:O	1:A:1440:VAL:HG23	2.02	0.59
1:A:607:HIS:HD2	1:A:862:GLU:OE2	1.85	0.58
1:A:1432:PHE:CD1	1:A:1438:LEU:HD11	2.38	0.58
1:A:972:MET:SD	1:A:1059:LEU:CD2	2.91	0.58
1:A:1341:MET:O	1:A:1345:ILE:HG12	2.04	0.58
1:A:353:ILE:HD11	1:A:395:SER:OG	1.92	0.58
1:A:249:ILE:HG22	1:A:250:THR:H	1.69	0.57
1:A:346:LEU:HD22	1:A:388:TYR:CD2	2.39	0.57
1:A:573:ASP:HB3	1:A:576:GLU:HG2	1.86	0.57
1:A:267:GLY:O	1:A:270:LYS:HG2	2.05	0.57
1:A:1433:HIS:O	1:A:1435:GLN:HG3	2.05	0.57
1:A:952:ASP:HB3	1:A:955:ILE:HG12	1.86	0.56
1:A:1442:ILE:HD11	1:A:1584:PHE:HD1	1.70	0.56
2:B:296:LEU:H	2:B:296:LEU:CD2	2.18	0.56
1:A:709:LEU:HD12	1:A:748:MET:HE3	1.87	0.56
1:A:972:MET:SD	1:A:1059:LEU:HD22	2.46	0.56
1:A:714:ILE:HD12	1:A:751:GLU:HG3	1.88	0.56
1:A:226:LEU:HD21	1:A:273:LEU:HA	1.88	0.56
1:A:684:LEU:HD13	1:A:699:MET:HB3	1.87	0.56
1:A:1182:LEU:HD12	1:A:1195:LEU:HD11	1.88	0.56
1:A:205:LYS:HG3	2:B:371:LEU:HD12	1.87	0.56
1:A:271:ILE:HG21	1:A:369:LEU:HD13	1.87	0.56
1:A:237:GLN:HB2	1:A:283:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:SER:H	1:A:1359:ASN:ND2	2.04	0.55
1:A:1232:THR:HG23	2:B:262:ALA:CB	2.37	0.55
1:A:570:PHE:HZ	1:A:601:ASN:HB3	1.71	0.55
1:A:727:VAL:N	1:A:779:GLU:OE2	2.40	0.55
1:A:1234:VAL:O	1:A:1238:ASN:HB2	2.07	0.55
1:A:996:ILE:HD12	1:A:1088:SER:OG	2.07	0.55
1:A:1179:ASN:HD22	1:A:1196:ARG:NH1	2.05	0.54
1:A:1442:ILE:HD11	1:A:1584:PHE:CD1	2.43	0.54
2:B:296:LEU:HD23	2:B:296:LEU:H	1.71	0.54
1:A:1445:ASN:ND2	1:A:1476:SER:OG	2.41	0.54
1:A:331:SER:HB2	1:A:334:ASP:HB2	1.88	0.54
1:A:725:ILE:HD12	1:A:775:LYS:HD3	1.90	0.54
1:A:236:LYS:HE2	1:A:283:LEU:O	2.08	0.54
1:A:727:VAL:HG13	1:A:779:GLU:OE2	2.07	0.54
1:A:79:ILE:HD13	1:A:85:VAL:HG21	1.90	0.54
1:A:1073:LEU:HD21	1:A:1109:LEU:HB3	1.89	0.53
1:A:294:ASP:N	1:A:294:ASP:OD1	2.42	0.53
2:B:315:GLN:C	2:B:316:ILE:HD12	2.29	0.53
1:A:1227:GLU:O	1:A:1230:GLN:HB3	2.09	0.53
1:A:1598:VAL:HG13	1:A:1621:ILE:HD13	1.90	0.53
1:A:308:ILE:HD12	1:A:338:ILE:HD11	1.90	0.53
1:A:574:PRO:HA	1:A:577:LEU:HD23	1.91	0.53
1:A:1246:ARG:HG2	2:B:257:MET:O	2.09	0.53
1:A:145:HIS:H	1:A:149:ASN:ND2	2.03	0.52
1:A:604:MET:HE2	1:A:648:TYR:CD1	2.44	0.52
1:A:681:ASN:ND2	1:A:723:SER:HB3	2.24	0.52
2:B:296:LEU:N	2:B:296:LEU:CD2	2.72	0.52
1:A:277:TYR:CZ	1:A:289:LYS:HE3	2.44	0.52
1:A:1180:LEU:HD23	1:A:1197:LEU:HD12	1.92	0.52
1:A:1169:ILE:HG12	1:A:1184:LYS:HG3	1.91	0.52
1:A:237:GLN:N	1:A:283:LEU:HD23	2.25	0.52
1:A:1449:ILE:HG22	1:A:1452:PRO:HG3	1.92	0.52
1:A:267:GLY:O	1:A:270:LYS:CG	2.58	0.52
1:A:364:TRP:CZ3	1:A:367:ILE:HD12	2.46	0.51
1:A:833:LEU:O	1:A:837:HIS:HD2	1.94	0.51
1:A:1495:GLN:NE2	1:A:1520:CYS:SG	2.83	0.51
1:A:1605:SER:O	1:A:1608:VAL:HG22	2.10	0.51
1:A:242:PHE:CD2	1:A:251:VAL:HB	2.46	0.51
1:A:1082:LEU:O	1:A:1086:ILE:HG12	2.11	0.51
1:A:257:ASN:O	1:A:263:TYR:CD2	2.64	0.51
1:A:1195:LEU:HD13	1:A:1197:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:NZ	2:B:367:GLU:OE1	2.40	0.50
1:A:1256:LEU:HB2	1:A:1614:LEU:HD11	1.93	0.50
1:A:924:GLN:O	1:A:927:VAL:HG22	2.12	0.50
1:A:979:GLN:HB3	1:A:1044:PHE:HE2	1.76	0.50
1:A:1446:ILE:HD11	1:A:1470:ILE:HG22	1.88	0.50
1:A:596:ILE:HD12	1:A:619:TYR:HB2	1.94	0.50
1:A:926:LEU:HD13	1:A:940:PRO:HA	1.94	0.50
1:A:323:ASN:HD21	1:A:358:LYS:HZ1	1.51	0.50
1:A:132:ILE:HG23	1:A:166:LEU:HD11	1.93	0.50
1:A:382:PHE:O	1:A:386:VAL:HG13	2.12	0.49
1:A:972:MET:SD	1:A:1059:LEU:HD23	2.52	0.49
1:A:116:ILE:HD13	1:A:132:ILE:HG12	1.93	0.49
1:A:589:LYS:HE2	1:A:590:TYR:OH	2.12	0.49
1:A:1073:LEU:HG	1:A:1110:PRO:HG3	1.94	0.49
1:A:460:ASN:HD22	1:A:499:LEU:HD13	1.77	0.49
1:A:860:LEU:CG	1:A:861:GLU:N	2.75	0.49
1:A:1419:VAL:HG11	1:A:1425:LEU:HB2	1.95	0.49
1:A:570:PHE:CZ	1:A:601:ASN:HB3	2.48	0.49
1:A:966:ILE:O	1:A:970:HIS:HD2	1.96	0.49
1:A:597:VAL:HG22	1:A:641:PHE:CD1	2.48	0.48
1:A:1515:LYS:HD3	2:B:271:TYR:CE1	2.48	0.48
1:A:1065:LEU:HB2	1:A:1145:THR:HG21	1.95	0.48
1:A:398:ASP:OD1	1:A:398:ASP:N	2.46	0.48
1:A:713:LYS:HZ1	1:A:715:GLU:HB2	1.78	0.48
1:A:791:ILE:HB	1:A:1142:ASN:OD1	2.13	0.48
1:A:1249:TRP:CZ2	1:A:1253:ARG:HD2	2.48	0.48
1:A:1307:ARG:HG2	1:A:1316:PHE:CE2	2.49	0.48
1:A:216:PHE:HB3	1:A:227:PHE:CE2	2.48	0.48
1:A:814:LEU:O	2:B:291:ASN:ND2	2.43	0.48
1:A:1436:LEU:HD12	1:A:1436:LEU:N	2.29	0.48
1:A:664:CYS:O	1:A:667:SER:HB3	2.14	0.48
1:A:1271:TRP:CD1	1:A:1271:TRP:N	2.80	0.48
2:B:316:ILE:CD1	2:B:316:ILE:N	2.72	0.48
1:A:1184:LYS:HE2	1:A:1278:PHE:O	2.13	0.47
1:A:1442:ILE:O	1:A:1474:LYS:HD3	2.14	0.47
1:A:300:GLU:O	1:A:304:VAL:HG23	2.15	0.47
1:A:934:LEU:HD11	1:A:940:PRO:HG3	1.96	0.47
2:B:364:ASP:OD1	2:B:367:GLU:HG3	2.14	0.47
1:A:1077:SER:CB	1:A:1106:LEU:HD22	2.44	0.47
1:A:1468:GLN:O	1:A:1471:ILE:HG12	2.14	0.47
1:A:242:PHE:CG	1:A:251:VAL:HB	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:ILE:HD13	1:A:966:ILE:HA	1.73	0.47
1:A:832:GLN:O	1:A:836:ILE:HG13	2.15	0.47
1:A:382:PHE:CZ	1:A:428:ILE:HD11	2.47	0.47
1:A:112:HIS:CG	1:A:135:LEU:HD12	2.50	0.47
1:A:233:GLN:O	1:A:283:LEU:HD22	2.14	0.47
1:A:790:VAL:HG11	1:A:840:ILE:HG21	1.97	0.47
1:A:708:ASN:HD21	1:A:711:THR:HG23	1.79	0.47
1:A:1469:LYS:O	1:A:1472:ASP:HB2	2.16	0.46
1:A:1509:GLU:H	1:A:1509:GLU:CD	2.19	0.46
1:A:1240:ILE:HG23	1:A:1245:GLU:HB3	1.97	0.46
1:A:895:LYS:HB2	1:A:895:LYS:HE3	1.55	0.46
1:A:1456:LEU:HD21	2:B:263:PRO:HD3	1.98	0.46
1:A:237:GLN:CA	1:A:283:LEU:HD21	2.46	0.46
1:A:757:ASN:HB2	1:A:766:TYR:CE1	2.51	0.46
1:A:1101:ILE:HG12	1:A:1192:ARG:NH2	2.31	0.46
1:A:1578:LEU:CD1	1:A:1582:MET:HE1	2.46	0.46
1:A:604:MET:CE	1:A:816:GLN:HE21	2.29	0.46
1:A:1105:SER:HB2	1:A:1152:VAL:HG13	1.98	0.46
1:A:1077:SER:HB2	1:A:1106:LEU:HD22	1.97	0.46
1:A:1515:LYS:O	1:A:1519:LYS:HG3	2.15	0.46
1:A:1578:LEU:HD13	1:A:1582:MET:CE	2.46	0.46
1:A:492:LEU:C	1:A:492:LEU:CD1	2.85	0.46
1:A:604:MET:HE3	1:A:648:TYR:HB2	1.98	0.45
1:A:114:MET:O	1:A:118:LYS:HG3	2.16	0.45
1:A:1179:ASN:HD22	1:A:1196:ARG:HH11	1.63	0.45
1:A:283:LEU:HD12	1:A:283:LEU:N	2.30	0.45
1:A:735:THR:O	1:A:739:ILE:HG12	2.16	0.45
1:A:702:GLN:O	1:A:706:THR:HG23	2.16	0.45
1:A:1160:MET:HE3	1:A:1192:ARG:HH11	1.80	0.45
1:A:1390:PHE:HZ	1:A:1437:PRO:HD3	1.81	0.45
1:A:1458:ARG:NH2	1:A:1568:ASP:OD2	2.48	0.45
1:A:190:LEU:HD11	1:A:198:LEU:HD23	1.99	0.45
1:A:409:LEU:HD11	1:A:431:VAL:HG12	1.98	0.45
1:A:857:ILE:CD1	1:A:869:CYS:HB3	2.44	0.45
1:A:1344:LEU:HA	1:A:1344:LEU:HD23	1.78	0.45
1:A:1429:LEU:HB3	1:A:1434:TYR:CD1	2.51	0.45
1:A:1460:GLU:OE1	1:A:1482:ASN:HB2	2.17	0.45
1:A:557:GLN:HG3	1:A:580:THR:HG1	1.79	0.45
1:A:635:SER:O	1:A:639:MET:HG2	2.16	0.45
1:A:977:MET:O	1:A:981:GLU:HB2	2.17	0.45
1:A:217:PHE:HB2	1:A:227:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LYS:NZ	1:A:715:GLU:HB2	2.31	0.45
1:A:353:ILE:HD13	1:A:395:SER:CB	2.44	0.45
1:A:966:ILE:HD11	1:A:1068:LEU:HD21	1.99	0.45
1:A:562:ILE:O	1:A:566:LEU:HD23	2.16	0.44
1:A:1104:PHE:HB2	1:A:1156:GLN:HE22	1.83	0.44
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.81	0.44
1:A:1221:LEU:HD23	1:A:1402:LEU:HD12	1.99	0.44
1:A:622:LYS:HD2	1:A:622:LYS:HA	1.80	0.44
1:A:325:LEU:HD11	1:A:363:LEU:HD12	1.98	0.44
1:A:1095:ASN:HB3	1:A:1098:SER:OG	2.17	0.44
1:A:1079:LEU:HD13	1:A:1176:ILE:HD13	1.98	0.44
1:A:634:ILE:HG22	1:A:639:MET:HE2	1.99	0.44
1:A:755:ILE:O	1:A:766:TYR:OH	2.24	0.44
1:A:938:PHE:CD2	1:A:957:LEU:HD12	2.52	0.44
1:A:1109:LEU:HA	1:A:1109:LEU:HD23	1.78	0.44
1:A:1232:THR:O	2:B:262:ALA:HB3	2.18	0.44
1:A:644:MET:HG2	2:B:293:PRO:HG3	1.99	0.44
1:A:1272:PHE:CD1	1:A:1272:PHE:N	2.86	0.44
1:A:1470:ILE:CG1	1:A:1586:CYS:SG	3.06	0.44
1:A:1446:ILE:HG13	1:A:1477:SER:OG	2.18	0.43
1:A:476:ILE:O	1:A:485:LYS:HG2	2.18	0.43
1:A:1493:MET:O	1:A:1497:SER:OG	2.26	0.43
1:A:494:ASN:O	1:A:497:CYS:HB2	2.18	0.43
1:A:1261:GLN:HB2	1:A:1613:TYR:CE1	2.54	0.43
1:A:906:ILE:HB	1:A:929:TYR:CD2	2.53	0.43
1:A:619:TYR:CZ	1:A:624:LEU:HD13	2.54	0.43
1:A:1528:LEU:HD23	1:A:1533:SER:HB2	2.00	0.43
1:A:396:ILE:HG23	1:A:401:ALA:HB3	2.01	0.43
1:A:807:LEU:HD23	1:A:807:LEU:O	2.18	0.43
1:A:1121:LEU:HD23	1:A:1124:ILE:HD11	2.00	0.43
1:A:1578:LEU:HD11	1:A:1582:MET:HE1	2.01	0.43
1:A:846:CYS:HB3	1:A:876:TYR:CE1	2.53	0.43
1:A:387:ILE:HD12	2:B:313:LEU:HD13	2.01	0.42
1:A:1438:LEU:HD12	1:A:1438:LEU:HA	1.84	0.42
1:A:182:GLU:OE2	1:A:182:GLU:N	2.47	0.42
1:A:421:GLU:OE1	1:A:424:ARG:NH1	2.51	0.42
1:A:1312:ASN:OD1	1:A:1314:ALA:N	2.48	0.42
1:A:237:GLN:CA	1:A:283:LEU:CD2	2.97	0.42
1:A:651:PHE:CD2	1:A:820:LEU:HB3	2.55	0.42
1:A:1243:ARG:HH12	1:A:1247:LYS:HZ2	1.65	0.42
1:A:190:LEU:HD11	1:A:198:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:LYS:HE2	1:A:809:LYS:HB2	1.84	0.42
1:A:823:LEU:HD23	1:A:823:LEU:HA	1.92	0.42
1:A:853:LEU:HD11	1:A:869:CYS:SG	2.60	0.42
1:A:251:VAL:O	1:A:251:VAL:HG22	2.17	0.42
1:A:589:LYS:HE2	1:A:590:TYR:CZ	2.55	0.42
1:A:1075:LYS:HB2	1:A:1075:LYS:HE3	1.93	0.42
1:A:1160:MET:HE2	1:A:1185:LEU:CD2	2.50	0.42
1:A:1104:PHE:HB3	1:A:1156:GLN:OE1	2.20	0.42
1:A:1381:ARG:O	1:A:1384:MET:HG2	2.20	0.42
1:A:1332:PRO:HA	1:A:1337:PHE:CD1	2.55	0.42
1:A:1185:LEU:O	1:A:1187:PRO:HD3	2.20	0.41
1:A:1197:LEU:HA	1:A:1198:PRO:HD3	1.80	0.41
1:A:946:HIS:CD2	1:A:963:LYS:HE2	2.48	0.41
1:A:1436:LEU:CD1	1:A:1436:LEU:N	2.84	0.41
1:A:515:PHE:HA	1:A:519:PHE:HB3	2.01	0.41
1:A:575:LEU:HA	1:A:575:LEU:HD12	1.89	0.41
1:A:1237:THR:HA	1:A:1240:ILE:HG13	2.02	0.41
1:A:1305:PRO:HD2	1:A:1359:ASN:ND2	2.35	0.41
1:A:1123:ASN:ND2	1:A:1519:LYS:HA	2.30	0.41
1:A:176:LYS:HA	1:A:176:LYS:HD2	1.65	0.41
1:A:557:GLN:CG	1:A:580:THR:OG1	2.62	0.41
1:A:1229:ASN:O	1:A:1232:THR:HB	2.20	0.41
1:A:1112:HIS:CE1	1:A:1423:VAL:HG11	2.56	0.41
1:A:170:ALA:O	1:A:174:ILE:HG13	2.21	0.41
1:A:336:ASN:HA	1:A:339:LEU:HB2	2.03	0.41
1:A:734:LEU:CG	1:A:738:GLN:NE2	2.83	0.41
1:A:1126:ASN:ND2	2:B:275:GLY:HA3	2.36	0.41
1:A:1256:LEU:CB	1:A:1614:LEU:HD11	2.51	0.41
1:A:726:ASN:O	1:A:729:LEU:HB2	2.20	0.41
1:A:921:LYS:HB2	1:A:921:LYS:HE2	1.78	0.41
1:A:1232:THR:HG21	1:A:1565:ASP:CB	2.49	0.41
1:A:1402:LEU:H	1:A:1402:LEU:HD23	1.86	0.41
1:A:348:ASN:HD22	1:A:348:ASN:N	2.19	0.41
1:A:1344:LEU:O	1:A:1348:VAL:HG23	2.21	0.41
1:A:1273:ASN:N	1:A:1273:ASN:OD1	2.52	0.41
1:A:323:ASN:HD22	1:A:323:ASN:HA	1.68	0.41
1:A:112:HIS:HB3	1:A:135:LEU:HD12	2.03	0.40
1:A:242:PHE:O	1:A:244:LYS:N	2.54	0.40
1:A:342:ALA:HA	1:A:345:PHE:HB2	2.04	0.40
1:A:561:MET:CE	1:A:595:ARG:HA	2.51	0.40
1:A:206:ALA:O	1:A:210:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PHE:CE2	1:A:412:LEU:HD22	2.55	0.40
1:A:642:VAL:HB	1:A:675:ILE:HD11	2.04	0.40
1:A:1099:SER:O	1:A:1103:ASN:HB2	2.21	0.40
1:A:90:ASN:ND2	1:A:138:GLU:OE2	2.52	0.40
1:A:1468:GLN:NE2	3:A:1701:HOH:O	2.54	0.40
1:A:304:VAL:HG22	1:A:327:TRP:HB3	2.02	0.40
1:A:364:TRP:CE3	1:A:367:ILE:HD12	2.57	0.40
1:A:433:PHE:O	1:A:437:VAL:HG23	2.21	0.40
1:A:715:GLU:HG3	1:A:765:LEU:HD21	2.04	0.40
1:A:1050:ILE:HG22	1:A:1054:LYS:HD2	2.04	0.40
1:A:1438:LEU:HB3	1:A:1626:ILE:HG22	2.03	0.40
1:A:150:ILE:O	1:A:167:LYS:HE2	2.22	0.40
1:A:194:ASP:OD1	1:A:195:LYS:N	2.55	0.40
1:A:383:ASP:O	1:A:387:ILE:HD13	2.21	0.40
1:A:734:LEU:HA	1:A:783:LEU:HD13	2.04	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	
1	A	1470/1596 (92%)	1394 (95%)	76 (5%)	0	100	100
2	B	60/117 (51%)	58 (97%)	2 (3%)	0	100	100
All	All	1530/1713 (89%)	1452 (95%)	78 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1391/1491 (93%)	1337 (96%)	54 (4%)	37	65
2	B	63/108 (58%)	58 (92%)	5 (8%)	14	28
All	All	1454/1599 (91%)	1395 (96%)	59 (4%)	35	63

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	95	LEU
1	A	127	LEU
1	A	182	GLU
1	A	225	VAL
1	A	250	THR
1	A	264	LEU
1	A	287	LEU
1	A	294	ASP
1	A	311	LYS
1	A	317	TYR
1	A	318	CYS
1	A	327	TRP
1	A	344	ASN
1	A	348	ASN
1	A	460	ASN
1	A	464	THR
1	A	490	SER
1	A	508	PHE
1	A	512	GLN
1	A	582	ASP
1	A	628	ASP
1	A	635	SER
1	A	707	MET
1	A	732	SER
1	A	760	ASN
1	A	797	CYS
1	A	810	LYS
1	A	825	SER
1	A	903	GLU
1	A	920	VAL

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Mol	Chain	Res	Type
1	A	987	LYS
1	A	1002	VAL
1	A	1066	ASP
1	A	1093	ILE
1	A	1103	ASN
1	A	1106	LEU
1	A	1109	LEU
1	A	1122	ASN
1	A	1143	ILE
1	A	1211	HIS
1	A	1212	LEU
1	A	1232	THR
1	A	1240	ILE
1	A	1265	ASN
1	A	1363	GLU
1	A	1367	SER
1	A	1419	VAL
1	A	1448	MET
1	A	1490	LEU
1	A	1516	GLU
1	A	1568	ASP
1	A	1570	ASP
1	A	1582	MET
2	B	258	ASP
2	B	259	ILE
2	B	261	ILE
2	B	296	LEU
2	B	298	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	143	GLN
1	A	149	ASN
1	A	323	ASN
1	A	341	ASN
1	A	348	ASN
1	A	392	ASN
1	A	442	HIS
1	A	460	ASN
1	A	466	HIS

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	532	ASN
1	A	578	ASN
1	A	601	ASN
1	A	607	HIS
1	A	625	GLN
1	A	708	ASN
1	A	720	HIS
1	A	738	GLN
1	A	773	ASN
1	A	837	HIS
1	A	882	GLN
1	A	886	GLN
1	A	946	HIS
1	A	1095	ASN
1	A	1123	ASN
1	A	1126	ASN
1	A	1128	ASN
1	A	1179	ASN
1	A	1261	GLN
1	A	1301	HIS
1	A	1359	ASN
1	A	1445	ASN
1	A	1495	GLN
1	A	1498	ASN
2	B	280	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 carbohydrates 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1486/1596 (93%)	0.13	55 (3%) 42 34	42, 67, 107, 139	0
2	B	66/117 (56%)	0.30	2 (3%) 51 43	57, 79, 101, 119	0
All	All	1552/1713 (90%)	0.14	57 (3%) 42 34	42, 68, 108, 139	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	ILE	6.6
1	A	245	PHE	5.5
1	A	348	ASN	5.3
1	A	1594	ASN	4.9
1	A	1471	ILE	4.8
1	A	311	LYS	4.5
1	A	73	ASN	4.2
1	A	347	GLN	4.1
1	A	337	VAL	3.9
1	A	298	TYR	3.5
1	A	334	ASP	3.5
1	A	345	PHE	3.4
1	A	306	ARG	3.3
1	A	628	ASP	3.1
1	A	303	GLU	3.1
1	A	310	SER	3.0
1	A	1586	CYS	3.0
1	A	1241	LYS	2.9
1	A	258	LEU	2.9
1	A	317	TYR	2.8
2	B	298	LEU	2.7
1	A	353	ILE	2.7
1	A	243	LYS	2.7
1	A	671	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	304	VAL	2.6
1	A	346	LEU	2.6
1	A	1470	ILE	2.6
1	A	325	LEU	2.5
1	A	256	LYS	2.5
1	A	811	LYS	2.5
1	A	1588	THR	2.5
1	A	339	LEU	2.5
1	A	1443	GLU	2.5
1	A	1467	PHE	2.5
1	A	1387	ASN	2.4
1	A	1592	ASN	2.4
1	A	462	SER	2.4
1	A	327	TRP	2.4
1	A	1585	ARG	2.4
1	A	1629	VAL	2.3
1	A	1385	THR	2.3
1	A	397	ASN	2.2
1	A	335	LEU	2.2
1	A	1473	ALA	2.2
1	A	331	SER	2.2
1	A	1584	PHE	2.2
1	A	77	LEU	2.2
1	A	344	ASN	2.2
1	A	1468	GLN	2.2
1	A	363	LEU	2.1
1	A	1474	LYS	2.1
1	A	1463	PHE	2.1
1	A	309	LYS	2.1
2	B	306	ASP	2.1
1	A	326	LEU	2.1
1	A	703	LEU	2.1
1	A	1254	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.