



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 09:34 PM EDT

PDB ID : 1S0F  
Title : Crystal structure of botulinum neurotoxin type B at pH 7.0  
Authors : Eswaramoorthy, S.; Kumaran, D.; Keller, J.; Swaminathan, S.  
Deposited on : 2003-12-30  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Xtrriage (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

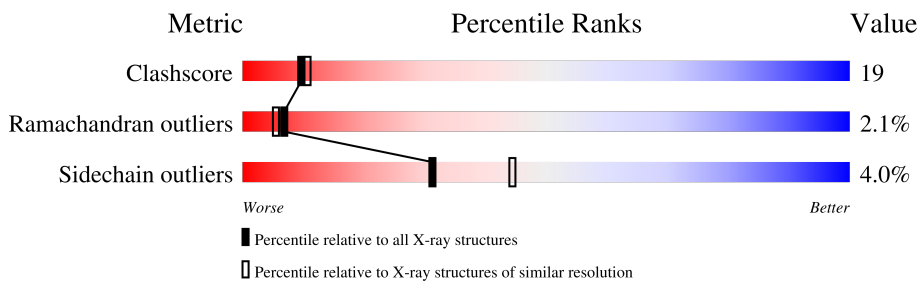
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1290	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10851 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 Botulinum neurotoxin type B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1276	10429	6719	1676	2001	33	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

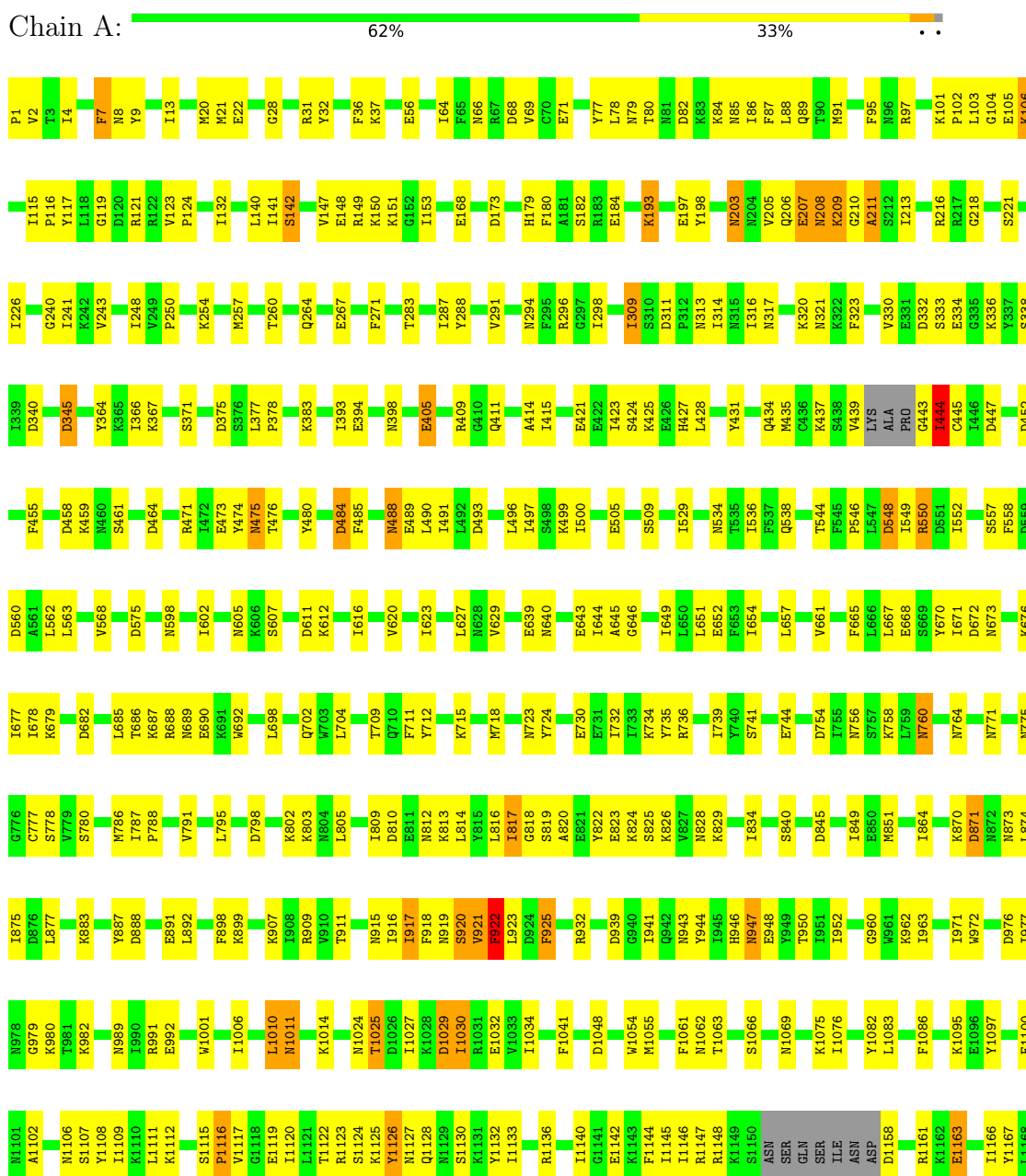
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	419	Total	O	0	0
			419	419		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Botulinum neurotoxin type B



D1169	Y1243
M1172	E1244
L1173	S1245
E1176	G1246
H1177	ILE
R1178	VAL
V1179	PHE
Y1180	GLU
T1181	E1251
Y1182	Y1252
K1183	K1253
Y1184	D1254
F1185	Y1255
K1186	E1256
K1187	C1257
E1188	I1258
E1189	Y1262
E1190	L1263
K1191	K1264
L1192	E1265
F1193	V1266
L1194	K1267
A1195	R1268
P1196	K1269
I1197	P1270
S1198	Y1271
D1199	M1272
S1200	L1275
D1201	G1276
E1202	C1277
F1203	M1278
Y1204	W1279
Q1208	Q1280
I1209	F1281
K1210	I1282
Q1215	E1290
C1220	
Q1221	
L1222	
L1223	
D1227	
E1228	
E1229	
S1230	
F1231	
D1232	
E1233	
L1236	
I1239	
H1240	
R1241	
F1242	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.60Å 122.85Å 93.41Å 90.00° 112.48° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	80.8 (50.00-2.30)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.227 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	0.41	0/10653	0.62	2/14403 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	661	VAL	N-CA-C	-5.06	97.33	111.00
1	A	193	LYS	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	10429	0	10182	399	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	419	0	0	19	0
All	All	10851	0	10182	399	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 19.

All (399) 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:1223:LEU:HB2	1:A:1236:LEU:HD23	1.28	1.10
1:A:834:ILE:HD11	1:A:917:ILE:HG13	1.44	0.99
1:A:946:HIS:O	1:A:947:ASN:HB2	1.65	0.96
1:A:1075:LYS:HE2	1:A:1215:GLN:HE22	1.31	0.95
1:A:142:SER:OG	1:A:148:GLU:HG2	1.68	0.93
1:A:309:ILE:HD13	1:A:309:ILE:H	1.36	0.91
1:A:367:LYS:H	1:A:411:GLN:HE22	0.91	0.90
1:A:1241:ARG:HH21	1:A:1252:TYR:H	1.15	0.90
1:A:367:LYS:H	1:A:411:GLN:NE2	1.71	0.89
1:A:142:SER:HB2	1:A:149:ARG:H	1.38	0.88
1:A:1192:LEU:HD21	1:A:1258:ILE:HB	1.55	0.88
1:A:1223:LEU:HB2	1:A:1236:LEU:CD2	2.03	0.88
1:A:826:LYS:HA	1:A:829:LYS:HE2	1.58	0.85
1:A:425:LYS:HD3	1:A:428:LEU:HD12	1.58	0.85
1:A:1115:SER:HB2	1:A:1116:PRO:HD2	1.60	0.84
1:A:1241:ARG:HH21	1:A:1252:TYR:N	1.76	0.83
1:A:1272:ASN:HD22	1:A:1275:LEU:HG	1.42	0.82
1:A:802:LYS:HE2	1:A:828:ASN:ND2	1.93	0.82
1:A:367:LYS:N	1:A:411:GLN:HE22	1.75	0.81
1:A:612:LYS:HB3	1:A:1076:ILE:HD13	1.62	0.81
1:A:640:ASN:HB2	4:A:1500:HOH:O	1.82	0.80
1:A:211:ALA:HB1	1:A:764:ASN:HD21	1.45	0.80
1:A:309:ILE:H	1:A:309:ILE:CD1	1.96	0.79
1:A:493:ASP:OD2	1:A:496:LEU:HB2	1.81	0.79
1:A:1106:ASN:ND2	1:A:1136:ARG:HE	1.82	0.78
1:A:140:LEU:HD11	1:A:147:VAL:HA	1.66	0.77
1:A:563:LEU:HG	4:A:1695:HOH:O	1.85	0.76
1:A:213:ILE:H	1:A:760:ASN:HD21	1.34	0.76
1:A:1241:ARG:HA	1:A:1254:ASP:HA	1.69	0.75
1:A:203:ASN:HB3	1:A:218:GLY:HA2	1.68	0.75
1:A:211:ALA:HB1	1:A:764:ASN:ND2	2.02	0.74
1:A:657:LEU:HD11	1:A:786:MET:HG2	1.68	0.74
1:A:977:ILE:HG21	1:A:1032:GLU:OE1	1.87	0.74
1:A:1125:LYS:HD3	1:A:1136:ARG:NH1	2.03	0.74
1:A:550:ARG:HH11	1:A:550:ARG:HB2	1.52	0.74
1:A:435:MET:HG2	1:A:529:ILE:HD11	1.71	0.73
1:A:1192:LEU:HG	1:A:1256:PHE:O	1.90	0.72
1:A:976:ASP:OD2	1:A:980:LYS:HB3	1.90	0.71
1:A:670:TYR:CD2	1:A:676:LYS:HB3	2.25	0.71
1:A:1181:THR:O	1:A:1203:PHE:HB3	1.91	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:TYR:O	1:A:1244:GLU:HG3	1.90	0.70
1:A:193:LYS:HD3	4:A:1404:HOH:O	1.89	0.70
1:A:1014:LYS:HE2	1:A:1024:ASN:ND2	2.07	0.70
1:A:802:LYS:HE3	1:A:828:ASN:HA	1.74	0.69
1:A:870:LYS:HG3	1:A:875:ILE:HD11	1.74	0.68
1:A:309:ILE:HD13	1:A:309:ILE:N	2.07	0.68
1:A:919:ASN:C	1:A:921:VAL:H	1.95	0.68
1:A:209:LYS:CB	1:A:218:GLY:H	2.07	0.67
1:A:1236:LEU:HD12	1:A:1262:TYR:CB	2.24	0.67
1:A:205:VAL:HA	4:A:1608:HOH:O	1.94	0.67
1:A:812:ASN:O	1:A:816:LEU:HG	1.95	0.67
1:A:4:ILE:HD12	1:A:95:PHE:HB3	1.76	0.67
1:A:32:TYR:OH	1:A:150:LYS:HE2	1.94	0.67
1:A:439:VAL:HB	1:A:443:GLY:HA2	1.77	0.67
1:A:330:VAL:HG23	1:A:338:SER:HB3	1.75	0.67
1:A:548:ASP:HA	4:A:1466:HOH:O	1.96	0.66
1:A:213:ILE:N	1:A:760:ASN:HD21	1.93	0.65
1:A:1115:SER:HB2	1:A:1116:PRO:CD	2.25	0.65
1:A:1197:ILE:HA	4:A:1354:HOH:O	1.94	0.65
1:A:812:ASN:HB3	1:A:816:LEU:HG	1.79	0.65
1:A:394:GLU:HB3	4:A:1666:HOH:O	1.97	0.64
1:A:1126:TYR:CE1	1:A:1128:GLN:HB2	2.33	0.64
1:A:1107:SER:HB3	1:A:1120:ILE:CG2	2.28	0.64
1:A:670:TYR:CD2	1:A:676:LYS:HD3	2.33	0.63
1:A:920:SER:HG	1:A:922:PHE:HE1	1.46	0.63
1:A:437:LYS:HD2	1:A:444:ILE:HG23	1.80	0.63
1:A:85:ASN:ND2	1:A:89:GLN:HE21	1.97	0.63
1:A:471:ARG:HH11	1:A:471:ARG:HG3	1.64	0.62
1:A:825:SER:O	1:A:829:LYS:HG2	1.98	0.62
1:A:1142:GLU:HB2	1:A:1144:PHE:CE1	2.33	0.62
1:A:13:ILE:HD13	1:A:20:MET:HG2	1.82	0.62
1:A:550:ARG:HH11	1:A:550:ARG:CB	2.12	0.61
1:A:1126:TYR:CZ	1:A:1128:GLN:HB2	2.36	0.61
1:A:7:PHE:HZ	1:A:37:LYS:O	1.83	0.61
1:A:685:LEU:O	1:A:688:ARG:HB3	2.01	0.61
1:A:982:LYS:HG2	1:A:1030:ILE:HD11	1.83	0.61
1:A:1111:LEU:HD23	1:A:1172:ASN:ND2	2.14	0.61
1:A:845:ASP:O	1:A:849:ILE:HG12	2.01	0.61
1:A:946:HIS:O	1:A:947:ASN:CB	2.43	0.61
1:A:1086:PHE:HB2	1:A:1282:ILE:HG12	1.81	0.60
1:A:1117:VAL:HG22	4:A:1668:HOH:O	2.00	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.65	0.60
1:A:816:LEU:HB2	1:A:820:ALA:HB2	1.83	0.60
1:A:802:LYS:HE2	1:A:828:ASN:CG	2.21	0.60
1:A:1241:ARG:NH2	1:A:1252:TYR:H	1.95	0.60
1:A:1:PRO:HB2	1:A:105:GLU:OE2	2.01	0.60
1:A:1236:LEU:HD12	1:A:1262:TYR:HB3	1.84	0.60
1:A:330:VAL:CG2	1:A:338:SER:HB3	2.32	0.60
1:A:646:GLY:O	1:A:649:ILE:HG12	2.01	0.60
1:A:667:LEU:HD11	1:A:805:LEU:HD23	1.84	0.60
1:A:206:GLN:HA	1:A:771:ASN:ND2	2.17	0.60
1:A:1189:GLU:N	1:A:1189:GLU:OE1	2.35	0.59
1:A:921:VAL:O	1:A:922:PHE:HB3	2.02	0.59
1:A:1268:ARG:HH11	1:A:1268:ARG:HG3	1.67	0.59
1:A:1111:LEU:HD13	1:A:1194:LEU:HD12	1.83	0.59
1:A:1148:ARG:NH2	1:A:1158:ASP:HB3	2.17	0.59
1:A:1183:LYS:HD2	1:A:1202:GLU:O	2.03	0.59
1:A:409:ARG:NH1	1:A:415:ILE:HD13	2.18	0.59
1:A:977:ILE:HD13	1:A:1032:GLU:HB3	1.84	0.59
1:A:1236:LEU:HD12	1:A:1262:TYR:HB2	1.84	0.59
1:A:817:ILE:HG22	1:A:818:GLY:H	1.68	0.58
1:A:1145:ILE:HD13	1:A:1147:ARG:NH2	2.18	0.58
1:A:1241:ARG:HB2	1:A:1254:ASP:OD2	2.04	0.58
1:A:1223:LEU:CB	1:A:1236:LEU:HD23	2.20	0.58
1:A:330:VAL:HG22	1:A:338:SER:O	2.04	0.58
1:A:1241:ARG:NH2	1:A:1251:GLU:HA	2.19	0.58
1:A:976:ASP:HB3	1:A:1030:ILE:HG23	1.86	0.57
1:A:826:LYS:HA	1:A:829:LYS:CE	2.33	0.57
1:A:243:VAL:CG2	1:A:287:ILE:HG23	2.34	0.57
1:A:645:ALA:HB3	1:A:649:ILE:HG23	1.87	0.57
1:A:213:ILE:H	1:A:760:ASN:ND2	2.00	0.57
1:A:670:TYR:HB2	1:A:677:ILE:HG13	1.87	0.57
1:A:899:LYS:HD2	1:A:1054:TRP:CZ2	2.40	0.57
1:A:645:ALA:HB3	1:A:649:ILE:CG2	2.35	0.56
1:A:1106:ASN:HD22	1:A:1136:ARG:HE	1.53	0.56
1:A:639:GLU:O	1:A:643:GLU:HG3	2.04	0.56
1:A:546:PRO:HB2	1:A:549:ILE:HG12	1.87	0.56
1:A:819:SER:O	1:A:822:TYR:HB3	2.05	0.56
1:A:1228:GLU:N	1:A:1228:GLU:OE1	2.38	0.56
1:A:101:LYS:HB2	1:A:364:TYR:CZ	2.40	0.56
1:A:332:ASP:OD2	1:A:336:LYS:HB3	2.06	0.56
1:A:670:TYR:CG	1:A:676:LYS:HB3	2.41	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:CD1	1:A:431:TYR:HB2	2.36	0.56
1:A:1147:ARG:O	1:A:1166:ILE:HB	2.06	0.56
1:A:730:GLU:OE1	1:A:756:ASN:OD1	2.23	0.56
1:A:80:THR:O	1:A:84:LYS:HG3	2.07	0.55
1:A:840:SER:HB3	1:A:849:ILE:HD12	1.88	0.55
1:A:311:ASP:HB3	1:A:314:ILE:HG12	1.88	0.55
1:A:1185:PHE:C	1:A:1187:LYS:H	2.10	0.55
1:A:909:ARG:HD2	4:A:1561:HOH:O	2.06	0.55
1:A:1181:THR:HG21	1:A:1258:ILE:HD13	1.88	0.55
1:A:499:LYS:O	1:A:500:ILE:HD13	2.07	0.55
1:A:892:LEU:HD23	1:A:898:PHE:HB3	1.89	0.55
1:A:1255:TYR:C	1:A:1257:CYS:H	2.10	0.54
1:A:1263:LEU:O	1:A:1266:VAL:HG22	2.06	0.54
1:A:1265:GLU:HA	1:A:1268:ARG:HH11	1.73	0.54
1:A:260:THR:HG21	1:A:455:PHE:HE1	1.72	0.54
1:A:787:ILE:HB	1:A:788:PRO:HD3	1.90	0.54
1:A:1182:TYR:C	1:A:1182:TYR:CD2	2.81	0.54
1:A:332:ASP:OD1	1:A:334:GLU:HB2	2.08	0.54
1:A:485:PHE:HE2	1:A:490:LEU:HB2	1.73	0.54
1:A:377:LEU:HB3	1:A:378:PRO:CD	2.38	0.54
1:A:698:LEU:O	1:A:702:GLN:HG3	2.08	0.54
1:A:1083:LEU:HD13	1:A:1209:ILE:CD1	2.38	0.54
1:A:692:TRP:CH2	1:A:834:ILE:HB	2.43	0.53
1:A:1208:GLN:OE1	1:A:1210:LYS:HD3	2.07	0.53
1:A:1199:ASP:O	1:A:1201:ASP:N	2.42	0.53
1:A:823:GLU:HA	1:A:826:LYS:HB2	1.89	0.53
1:A:1272:ASN:ND2	1:A:1275:LEU:HG	2.16	0.53
1:A:670:TYR:HD2	1:A:676:LYS:HD3	1.74	0.53
1:A:813:LYS:HG3	1:A:814:LEU:N	2.23	0.53
1:A:1268:ARG:HG3	1:A:1268:ARG:NH1	2.23	0.53
1:A:887:TYR:HD1	1:A:907:LYS:HG3	1.73	0.53
1:A:1180:TYR:HB3	1:A:1204:TYR:O	2.08	0.53
1:A:1265:GLU:HA	1:A:1268:ARG:NH1	2.23	0.53
1:A:31:ARG:HG3	1:A:32:TYR:N	2.24	0.53
1:A:817:ILE:HG22	1:A:818:GLY:N	2.24	0.53
1:A:1086:PHE:CB	1:A:1282:ILE:HG12	2.40	0.53
1:A:296:ARG:HG2	1:A:296:ARG:NH1	2.23	0.52
1:A:221:SER:HB2	1:A:226:ILE:HD11	1.90	0.52
1:A:1014:LYS:HE2	1:A:1024:ASN:HD21	1.74	0.52
1:A:907:LYS:HA	1:A:1041:PHE:O	2.08	0.52
1:A:1125:LYS:HB3	1:A:1136:ARG:HH11	1.74	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASP:O	1:A:86:ILE:HG13	2.10	0.52
1:A:887:TYR:CD1	1:A:907:LYS:HG3	2.44	0.52
1:A:1066:SER:H	1:A:1069:ASN:HD22	1.57	0.52
1:A:1191:LYS:HG3	1:A:1242:PHE:HE1	1.74	0.52
1:A:972:TRP:CD2	1:A:1006:ILE:HG21	2.44	0.52
1:A:1163:GLU:OE1	1:A:1210:LYS:HD2	2.10	0.52
1:A:1179:VAL:HG22	1:A:1194:LEU:HD22	1.92	0.51
1:A:1182:TYR:O	1:A:1183:LYS:CB	2.58	0.51
1:A:1230:SER:C	1:A:1232:ASP:N	2.62	0.51
1:A:64:ILE:HD11	1:A:431:TYR:CD1	2.45	0.51
1:A:864:ILE:HG21	1:A:916:ILE:HG21	1.91	0.51
1:A:241:ILE:HG22	1:A:291:VAL:HG13	1.91	0.51
1:A:102:PRO:O	1:A:106:LYS:HD2	2.10	0.51
1:A:932:ARG:HD3	1:A:1001:TRP:CD1	2.45	0.51
1:A:1010:LEU:HD13	1:A:1011:ASN:OD1	2.10	0.51
1:A:665:PHE:CZ	1:A:687:LYS:HG3	2.46	0.51
1:A:338:SER:HB2	4:A:1557:HOH:O	2.10	0.51
1:A:32:TYR:N	1:A:32:TYR:CD1	2.78	0.51
1:A:925:PHE:HB2	1:A:1061:PHE:O	2.11	0.51
1:A:1169:ASP:OD2	1:A:1176:GLU:OE2	2.29	0.50
1:A:1275:LEU:HD13	1:A:1277:CYS:SG	2.50	0.50
1:A:425:LYS:HB3	4:A:1468:HOH:O	2.11	0.50
1:A:826:LYS:CA	1:A:829:LYS:HE2	2.34	0.50
1:A:1262:TYR:O	1:A:1265:GLU:N	2.44	0.50
1:A:1272:ASN:HD22	1:A:1275:LEU:CG	2.20	0.50
1:A:444:ILE:O	1:A:444:ILE:HG13	2.11	0.50
1:A:819:SER:O	1:A:822:TYR:N	2.43	0.50
1:A:960:GLY:HA2	1:A:1034:ILE:O	2.11	0.50
1:A:22:GLU:CD	1:A:28:GLY:HA2	2.32	0.50
1:A:627:LEU:HD11	1:A:718:MET:HG2	1.94	0.50
1:A:66:ASN:OD1	1:A:69:VAL:HG23	2.12	0.50
1:A:775:ASN:HB3	1:A:851:MET:HG2	1.93	0.50
1:A:1215:GLN:HE21	1:A:1215:GLN:HA	1.76	0.49
1:A:1112:LYS:HA	1:A:1119:GLU:OE2	2.11	0.49
1:A:1253:LYS:CB	1:A:1255:TYR:HE1	2.24	0.49
1:A:1227:ASP:C	1:A:1229:GLU:H	2.16	0.49
1:A:439:VAL:HG12	1:A:439:VAL:O	2.12	0.49
1:A:817:ILE:CG2	1:A:818:GLY:H	2.25	0.49
1:A:976:ASP:HA	1:A:1032:GLU:O	2.12	0.49
1:A:142:SER:CB	1:A:148:GLU:HG2	2.42	0.49
1:A:989:ASN:HD22	1:A:992:GLU:HG3	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:ARG:HG2	1:A:1140:ILE:HD11	1.94	0.49
1:A:686:THR:HA	1:A:689:ASN:HD22	1.78	0.49
1:A:1025:THR:HG22	1:A:1027:ILE:HG23	1.95	0.49
1:A:103:LEU:HB2	1:A:491:ILE:HD11	1.95	0.49
1:A:791:VAL:HB	1:A:915:ASN:HB3	1.94	0.48
1:A:71:GLU:HG2	1:A:168:GLU:OE2	2.12	0.48
1:A:952:ILE:HD12	1:A:963:ILE:HD12	1.95	0.48
1:A:1265:GLU:O	1:A:1268:ARG:HB2	2.13	0.48
1:A:605:ASN:C	1:A:607:SER:H	2.15	0.48
1:A:809:ILE:HG23	1:A:816:LEU:HD12	1.96	0.48
1:A:260:THR:CG2	1:A:455:PHE:HE1	2.27	0.48
1:A:1272:ASN:HB3	1:A:1275:LEU:HG	1.96	0.48
1:A:182:SER:O	1:A:240:GLY:HA2	2.14	0.48
1:A:1191:LYS:CG	1:A:1242:PHE:HE1	2.27	0.48
1:A:1257:CYS:O	1:A:1257:CYS:SG	2.72	0.48
1:A:678:ILE:HG12	1:A:823:GLU:OE1	2.14	0.48
1:A:730:GLU:O	1:A:734:LYS:HG3	2.14	0.48
1:A:919:ASN:C	1:A:921:VAL:N	2.63	0.48
1:A:1111:LEU:HD23	1:A:1172:ASN:HD22	1.76	0.48
1:A:1111:LEU:CD2	1:A:1172:ASN:HD22	2.26	0.48
1:A:950:THR:OG1	1:A:962:LYS:HD2	2.14	0.48
1:A:678:ILE:HG22	1:A:682:ASP:OD2	2.14	0.48
1:A:1182:TYR:O	1:A:1183:LYS:HB2	2.14	0.48
1:A:1132:TYR:N	1:A:1132:TYR:CD1	2.82	0.47
1:A:497:ILE:HD13	4:A:1710:HOH:O	2.13	0.47
1:A:612:LYS:HE3	4:A:1463:HOH:O	2.14	0.47
1:A:670:TYR:O	1:A:677:ILE:HD11	2.14	0.47
1:A:802:LYS:CE	1:A:828:ASN:HA	2.44	0.47
1:A:1120:ILE:HD12	1:A:1239:ILE:HD13	1.96	0.47
1:A:474:TYR:HB2	1:A:679:LYS:HB2	1.97	0.47
1:A:645:ALA:CB	1:A:649:ILE:HG23	2.44	0.47
1:A:919:ASN:O	1:A:921:VAL:N	2.48	0.47
1:A:203:ASN:N	1:A:203:ASN:HD22	2.12	0.47
1:A:458:ASP:OD2	1:A:459:LYS:N	2.47	0.47
1:A:704:LEU:O	1:A:709:THR:HG23	2.13	0.47
1:A:1147:ARG:HB2	1:A:1167:TYR:HB2	1.96	0.47
1:A:21:MET:HG2	1:A:22:GLU:N	2.30	0.47
1:A:398:ASN:HD21	1:A:411:GLN:HE21	1.62	0.47
1:A:1082:TYR:HA	1:A:1161:ARG:HA	1.96	0.47
1:A:64:ILE:HD12	1:A:431:TYR:HB2	1.97	0.47
1:A:558:PHE:CZ	1:A:562:LEU:HD11	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:ASN:HD22	1:A:992:GLU:CG	2.28	0.47
1:A:1199:ASP:O	1:A:1199:ASP:OD1	2.33	0.47
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.79	0.47
1:A:216:ARG:O	1:A:414:ALA:HB2	2.14	0.47
1:A:405:GLU:C	1:A:405:GLU:OE1	2.54	0.46
1:A:1100:PHE:HD2	1:A:1280:GLN:HB2	1.80	0.46
1:A:1230:SER:C	1:A:1232:ASP:H	2.17	0.46
1:A:283:THR:HA	4:A:1638:HOH:O	2.15	0.46
1:A:1190:GLU:O	1:A:1258:ILE:HG22	2.16	0.46
1:A:1220:CYS:SG	1:A:1281:PHE:HE1	2.39	0.46
1:A:1241:ARG:HB2	1:A:1254:ASP:CG	2.35	0.46
1:A:85:ASN:HD21	1:A:89:GLN:HE21	1.64	0.46
1:A:434:GLN:HG2	1:A:445:CYS:HB3	1.97	0.46
1:A:552:ILE:HD12	1:A:568:VAL:HG21	1.98	0.46
1:A:892:LEU:HD23	1:A:898:PHE:CB	2.46	0.46
1:A:184:GLU:HA	1:A:294:ASN:ND2	2.31	0.46
1:A:377:LEU:HD23	1:A:377:LEU:N	2.29	0.46
1:A:921:VAL:O	1:A:922:PHE:CB	2.63	0.46
1:A:1227:ASP:O	1:A:1229:GLU:N	2.49	0.46
1:A:629:VAL:HG23	1:A:652:GLU:OE1	2.15	0.45
1:A:437:LYS:HD2	1:A:444:ILE:CG2	2.45	0.45
1:A:873:ASN:ND2	1:A:874:LEU:H	2.14	0.45
1:A:1233:GLU:HB2	4:A:1706:HOH:O	2.16	0.45
1:A:557:SER:HB3	1:A:560:ASP:HB2	1.98	0.45
1:A:671:ILE:O	1:A:672:ASP:HB2	2.17	0.45
1:A:1240:HIS:N	1:A:1257:CYS:SG	2.89	0.45
1:A:97:ARG:HA	1:A:393:ILE:HG23	1.99	0.45
1:A:316:ILE:O	1:A:320:LYS:HG3	2.16	0.45
1:A:434:GLN:HG3	1:A:447:ASP:OD1	2.16	0.45
1:A:711:PHE:CE1	1:A:778:SER:HA	2.51	0.45
1:A:31:ARG:HG3	1:A:32:TYR:H	1.80	0.45
1:A:1107:SER:HB3	1:A:1120:ILE:HG23	1.99	0.45
1:A:117:TYR:HA	1:A:323:PHE:CE2	2.52	0.45
1:A:141:ILE:CD1	1:A:151:LYS:HB2	2.47	0.45
1:A:529:ILE:HD12	1:A:529:ILE:C	2.37	0.45
1:A:317:ASN:O	1:A:321:ASN:ND2	2.47	0.44
1:A:651:LEU:HD12	1:A:654:ILE:HD13	1.99	0.44
1:A:1146:ILE:HG23	1:A:1166:ILE:HD12	1.99	0.44
1:A:22:GLU:OE2	1:A:28:GLY:HA2	2.17	0.44
1:A:85:ASN:HD21	1:A:89:GLN:NE2	2.14	0.44
1:A:119:GLY:HA2	1:A:132:ILE:HD13	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:HA	1:A:505:GLU:O	2.16	0.44
1:A:1185:PHE:CD2	1:A:1190:GLU:HG2	2.53	0.44
1:A:1269:LYS:HA	1:A:1270:PRO:C	2.37	0.44
1:A:216:ARG:HG2	4:A:1590:HOH:O	2.16	0.44
1:A:473:GLU:HB3	1:A:670:TYR:OH	2.17	0.44
1:A:489:GLU:O	1:A:493:ASP:HB2	2.17	0.44
1:A:1083:LEU:HD13	1:A:1209:ILE:HD13	1.99	0.44
1:A:1:PRO:HB2	1:A:2:VAL:H	1.66	0.44
1:A:754:ASP:OD2	1:A:758:LYS:HE3	2.17	0.44
1:A:208:ASN:O	1:A:210:GLY:N	2.51	0.44
1:A:1215:GLN:HA	1:A:1215:GLN:NE2	2.33	0.44
1:A:1220:CYS:C	1:A:1221:GLN:NE2	2.71	0.44
1:A:9:TYR:H	1:A:85:ASN:HD22	1.64	0.44
1:A:870:LYS:O	1:A:871:ASP:C	2.56	0.44
1:A:1169:ASP:HB3	1:A:1176:GLU:HG2	2.00	0.44
1:A:670:TYR:HB2	1:A:677:ILE:CG1	2.47	0.44
1:A:948:GLU:O	1:A:948:GLU:HG3	2.17	0.44
1:A:425:LYS:C	1:A:427:HIS:N	2.71	0.43
1:A:925:PHE:HA	1:A:1063:THR:N	2.33	0.43
1:A:198:TYR:HD2	1:A:423:ILE:HD11	1.83	0.43
1:A:544:THR:HG22	1:A:724:TYR:CE2	2.52	0.43
1:A:605:ASN:C	1:A:607:SER:N	2.72	0.43
1:A:1145:ILE:O	1:A:1145:ILE:HG23	2.16	0.43
1:A:471:ARG:HH11	1:A:471:ARG:CG	2.30	0.43
1:A:550:ARG:CB	1:A:550:ARG:NH1	2.79	0.43
1:A:787:ILE:O	1:A:791:VAL:HG23	2.18	0.43
1:A:963:ILE:HA	1:A:971:ILE:O	2.18	0.43
1:A:741:SER:OG	1:A:744:GLU:HG3	2.19	0.43
1:A:823:GLU:O	1:A:824:LYS:C	2.56	0.43
1:A:864:ILE:CG2	1:A:1062:ASN:HD22	2.32	0.43
1:A:980:LYS:HE2	1:A:1029:ASP:CG	2.38	0.43
1:A:1200:SER:C	1:A:1202:GLU:H	2.21	0.43
1:A:147:VAL:HG23	1:A:147:VAL:O	2.18	0.43
1:A:475:ASN:HD22	1:A:475:ASN:HA	1.53	0.43
1:A:813:LYS:HG3	1:A:814:LEU:H	1.82	0.43
1:A:1102:ALA:HB3	1:A:1278:ASN:HB2	2.01	0.43
1:A:97:ARG:NH2	1:A:366:ILE:HD11	2.34	0.43
1:A:243:VAL:HG21	1:A:287:ILE:HG23	1.99	0.43
1:A:271:PHE:CE2	1:A:371:SER:HA	2.53	0.43
1:A:1095:LYS:HD3	1:A:1097:TYR:OH	2.18	0.43
1:A:1108:TYR:HE2	1:A:1122:THR:O	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:LEU:HD11	1:A:805:LEU:CD2	2.48	0.43
1:A:977:ILE:CD1	1:A:1032:GLU:HB3	2.49	0.43
1:A:87:PHE:O	1:A:91:MET:HG2	2.19	0.43
1:A:711:PHE:O	1:A:715:LYS:HG3	2.18	0.43
1:A:735:TYR:O	1:A:739:ILE:HG12	2.19	0.43
1:A:777:CYS:O	1:A:780:SER:HB3	2.19	0.43
1:A:891:GLU:O	1:A:898:PHE:HA	2.19	0.43
1:A:330:VAL:HG11	1:A:340:ASP:HB2	2.01	0.42
1:A:488:ASN:HD22	1:A:488:ASN:HA	1.58	0.42
1:A:1083:LEU:HD22	1:A:1220:CYS:CB	2.48	0.42
1:A:943:ASN:O	1:A:946:HIS:O	2.37	0.42
1:A:104:GLY:HA3	1:A:364:TYR:OH	2.20	0.42
1:A:123:VAL:HA	1:A:124:PRO:HD3	1.90	0.42
1:A:267:GLU:HB2	4:A:1529:HOH:O	2.19	0.42
1:A:1192:LEU:CD2	1:A:1258:ILE:HB	2.37	0.42
1:A:536:ILE:HA	1:A:627:LEU:O	2.19	0.42
1:A:809:ILE:HG23	1:A:816:LEU:CD1	2.49	0.42
1:A:1014:LYS:HG2	1:A:1024:ASN:ND2	2.35	0.42
1:A:9:TYR:H	1:A:85:ASN:ND2	2.17	0.42
1:A:36:PHE:CD1	1:A:36:PHE:N	2.88	0.42
1:A:333:SER:O	1:A:334:GLU:HG2	2.20	0.42
1:A:732:ILE:O	1:A:736:ARG:HG2	2.19	0.42
1:A:1083:LEU:HD22	1:A:1220:CYS:HB2	2.00	0.42
1:A:920:SER:OG	1:A:922:PHE:HE1	2.02	0.42
1:A:56:GLU:HG3	4:A:1609:HOH:O	2.19	0.42
1:A:115:ILE:HA	1:A:116:PRO:HD3	1.90	0.42
1:A:101:LYS:HB2	1:A:364:TYR:OH	2.20	0.42
1:A:1178:ARG:HB3	1:A:1180:TYR:CE2	2.55	0.42
1:A:1236:LEU:HB2	1:A:1262:TYR:CD2	2.55	0.42
1:A:1242:PHE:N	1:A:1242:PHE:CD2	2.86	0.42
1:A:117:TYR:HA	1:A:323:PHE:CZ	2.55	0.42
1:A:254:LYS:HB2	1:A:257:MET:HG3	2.02	0.42
1:A:620:VAL:CG1	1:A:623:ILE:HG13	2.49	0.42
1:A:1130:SER:HB3	1:A:1133:ILE:HG12	2.02	0.42
1:A:207:GLU:O	1:A:208:ASN:CB	2.67	0.41
1:A:250:PRO:HB3	1:A:455:PHE:CE1	2.55	0.41
1:A:79:ASN:OD1	1:A:80:THR:HG23	2.20	0.41
1:A:288:TYR:OH	1:A:345:ASP:OD1	2.32	0.41
1:A:480:TYR:OH	1:A:690:GLU:HA	2.20	0.41
1:A:941:ILE:HD12	1:A:944:TYR:HB3	2.02	0.41
1:A:1201:ASP:CG	1:A:1201:ASP:O	2.58	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ASP:HB3	1:A:616:ILE:HB	2.01	0.41
1:A:644:ILE:HA	1:A:877:LEU:HD22	2.01	0.41
1:A:13:ILE:CD1	1:A:20:MET:HG2	2.50	0.41
1:A:248:ILE:HD13	1:A:461:SER:HB3	2.03	0.41
1:A:484:ASP:OD1	1:A:485:PHE:N	2.53	0.41
1:A:1185:PHE:C	1:A:1187:LYS:N	2.73	0.41
1:A:671:ILE:C	1:A:673:ASN:H	2.24	0.41
1:A:1182:TYR:O	1:A:1183:LYS:HG3	2.20	0.41
1:A:1189:GLU:HG3	1:A:1240:HIS:CD2	2.55	0.41
1:A:375:ASP:OD1	1:A:712:TYR:HE2	2.03	0.41
1:A:77:TYR:OH	1:A:197:GLU:OE1	2.24	0.41
1:A:264:GLN:O	1:A:267:GLU:HB3	2.20	0.41
1:A:383:LYS:NZ	1:A:421:GLU:HG2	2.36	0.41
1:A:424:SER:HB3	4:A:1423:HOH:O	2.21	0.41
1:A:898:PHE:CZ	1:A:1055:MET:HB3	2.56	0.41
1:A:598:ASN:O	1:A:602:ILE:HG13	2.21	0.41
1:A:173:ASP:HB2	1:A:182:SER:OG	2.22	0.40
1:A:260:THR:HG21	1:A:455:PHE:CE1	2.55	0.40
1:A:534:ASN:HA	1:A:538:GLN:HG2	2.03	0.40
1:A:294:ASN:O	1:A:298:ILE:HG12	2.22	0.40
1:A:668:GLU:HB3	1:A:670:TYR:CE1	2.57	0.40
1:A:883:LYS:HB2	1:A:911:THR:HB	2.04	0.40
1:A:141:ILE:HD11	1:A:151:LYS:HB2	2.03	0.40
1:A:1109:ILE:HD13	1:A:1256:PHE:CE2	2.56	0.40
1:A:77:TYR:CD2	1:A:78:LEU:HG	2.55	0.40
1:A:121:ARG:HD3	1:A:179:HIS:CG	2.57	0.40
1:A:180:PHE:O	1:A:184:GLU:HG3	2.22	0.40
1:A:475:ASN:O	1:A:476:THR:C	2.60	0.40
1:A:795:LEU:HD21	1:A:834:ILE:HG21	2.04	0.40
1:A:834:ILE:CD1	1:A:917:ILE:HG13	2.32	0.40
1:A:1111:LEU:CD2	1:A:1172:ASN:ND2	2.84	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
1	A	1268/1290 (98%)	1127 (89%)	115 (9%)	26 (2%)	7 5

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	208	ASN
1	A	444	ILE
1	A	922	PHE
1	A	1030	ILE
1	A	1183	LYS
1	A	142	SER
1	A	209	LYS
1	A	211	ALA
1	A	947	ASN
1	A	1029	ASP
1	A	1126	TYR
1	A	1200	SER
1	A	1228	GLU
1	A	1252	TYR
1	A	817	ILE
1	A	920	SER
1	A	1191	LYS
1	A	871	ASP
1	A	923	LEU
1	A	979	GLY
1	A	1173	LEU
1	A	1256	PHE
1	A	921	VAL
1	A	1116	PRO
1	A	1196	PRO

### 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	1150/1189 (97%)	1104 (96%)	46 (4%)	31 44

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	8	ASN
1	A	68	ASP
1	A	88	LEU
1	A	106	LYS
1	A	203	ASN
1	A	309	ILE
1	A	313	ASN
1	A	345	ASP
1	A	405	GLU
1	A	444	ILE
1	A	452	ASP
1	A	464	ASP
1	A	475	ASN
1	A	484	ASP
1	A	488	ASN
1	A	509	SER
1	A	548	ASP
1	A	550	ARG
1	A	575	ASP
1	A	723	ASN
1	A	760	ASN
1	A	798	ASP
1	A	803	LYS
1	A	810	ASP
1	A	888	ASP
1	A	917	ILE
1	A	918	PHE
1	A	922	PHE
1	A	925	PHE
1	A	939	ASP
1	A	991	ARG
1	A	1010	LEU
1	A	1011	ASN
1	A	1025	THR
1	A	1048	ASP
1	A	1124	SER
1	A	1127	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1163	GLU
1	A	1181	THR
1	A	1182	TYR
1	A	1190	GLU
1	A	1228	GLU
1	A	1254	ASP
1	A	1256	PHE
1	A	1257	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	16	ASN
1	A	85	ASN
1	A	411	GLN
1	A	475	ASN
1	A	488	ASN
1	A	523	GLN
1	A	605	ASN
1	A	683	ASN
1	A	689	ASN
1	A	723	ASN
1	A	727	GLN
1	A	753	ASN
1	A	760	ASN
1	A	764	ASN
1	A	873	ASN
1	A	946	HIS
1	A	989	ASN
1	A	999	ASN
1	A	1008	ASN
1	A	1024	ASN
1	A	1062	ASN
1	A	1069	ASN
1	A	1106	ASN
1	A	1215	GLN
1	A	1240	HIS
1	A	1272	ASN
1	A	1278	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.