



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID : 3N7K
Title : Crystal structure of botulinum neurotoxin serotype C1 binding domain
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Deposited on : 2010-05-27
Resolution : 2.50 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

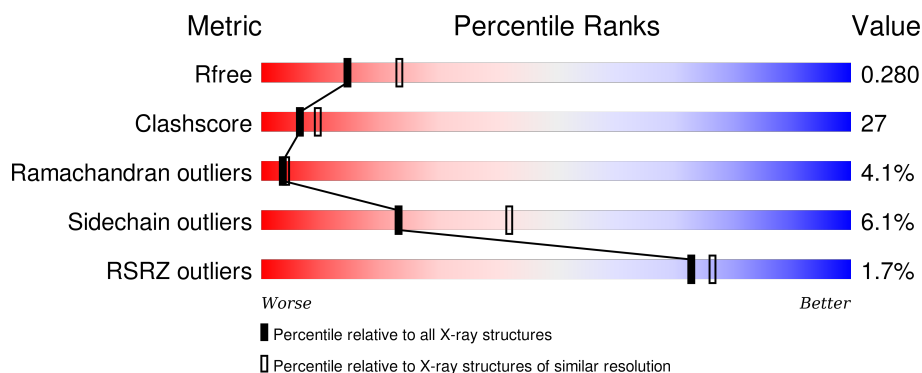
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	426	<div> <div>2%</div> <div>51%</div> <div>42%</div> <div>5%</div> </div>
1	B	426	<div> <div>%</div> <div>54%</div> <div>39%</div> <div>6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7035 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 C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3466	2207	580	667	12			
1	B	421	Total	C	N	O	S	0	0	0
			3459	2203	579	665	12			

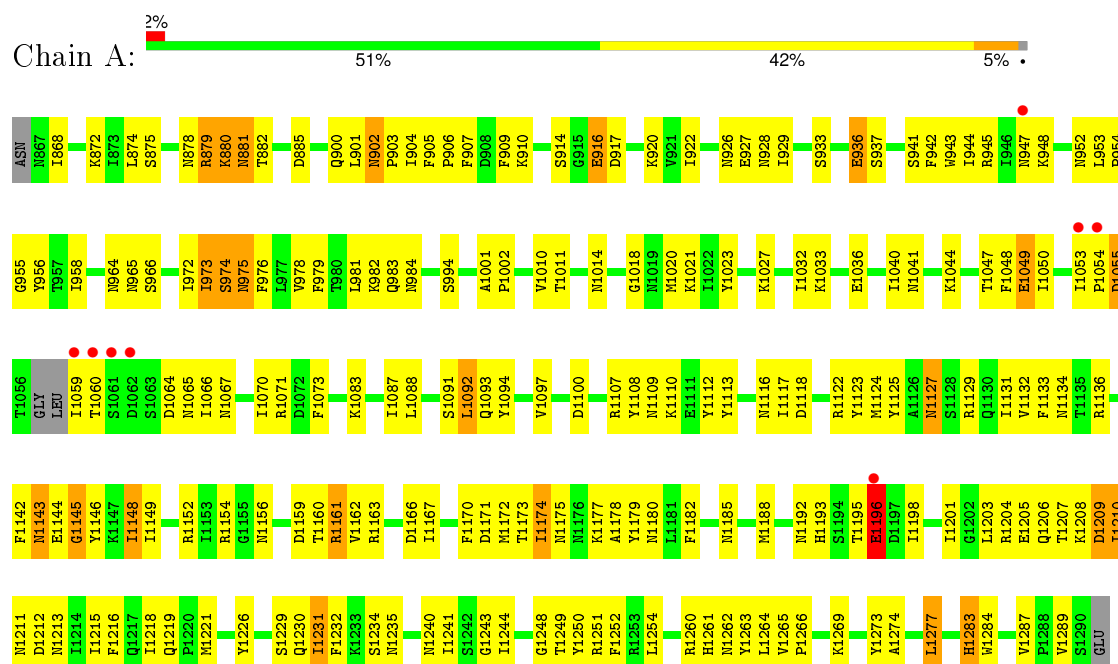
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	O	0	0
			51	51		
2	B	59	Total	O	0	0
			59	59		

3 Residue-property plots

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

• Molecule 1: Botulinum neurotoxin type C1





V1289
S1290
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.18Å 77.35Å 107.39Å 90.00° 116.36° 90.00°	Depositor
Resolution (Å)	29.84 – 2.50 29.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.4 (29.84-2.50) 87.5 (29.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.281 0.223 , 0.280	Depositor DCC
R_{free} test set	2085 reflections (4.55%)	DCC
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.8	EDS
Estimated twinning fraction	0.113 for -H,-K,H+L 0.046 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.113 for -H,-K,H+L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 45891 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7035	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/3543	0.69	1/4797 (0.0%)
1	B	0.43	0/3536	0.67	0/4787
All	All	0.43	0/7079	0.68	1/9584 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	881	ASN	N-CA-C	-5.28	96.73	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1161	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3466	0	3339	176	0
1	B	3459	0	3332	197	0
2	A	51	0	0	1	0
2	B	59	0	0	10	0
All	All	7035	0	6671	373	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 27.

All (373) 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:B:947:ASN:HB2	1:B:1067:ASN:H	1.12	1.11
1:B:953:LEU:HD12	1:B:954:PRO:HD2	1.42	1.02
1:A:975:ASN:HD22	1:A:975:ASN:H	1.02	0.99
1:A:879:ARG:HE	1:A:879:ARG:HA	1.30	0.97
1:A:880:LYS:HB3	1:A:882:THR:HG22	1.44	0.96
1:A:947:ASN:CB	1:A:1067:ASN:H	1.79	0.96
1:A:947:ASN:HB2	1:A:1067:ASN:H	1.31	0.94
1:B:1188:MET:HB2	1:B:1195:THR:HG23	1.50	0.91
1:A:973:ILE:HG23	1:A:974:SER:H	1.39	0.87
1:A:1156:ASN:HB3	1:A:1163:ARG:HH21	1.40	0.86
1:A:973:ILE:HG23	1:A:974:SER:N	1.92	0.84
1:A:1154:ARG:HH21	1:A:1154:ARG:HG2	1.43	0.82
1:B:1274:ALA:HA	1:B:1277:LEU:HD23	1.59	0.82
1:B:1201:ILE:HD11	1:B:1268:VAL:HG23	1.61	0.81
1:B:947:ASN:HB2	1:B:1067:ASN:N	1.95	0.81
1:B:947:ASN:CB	1:B:1067:ASN:H	1.92	0.80
1:A:973:ILE:HG22	1:A:976:PHE:HB2	1.64	0.80
1:B:1234:SER:HB3	1:B:1241:ILE:HD13	1.63	0.80
1:A:975:ASN:HD22	1:A:975:ASN:N	1.80	0.78
1:B:975:ASN:HD22	1:B:975:ASN:H	1.29	0.78
1:A:1274:ALA:HA	1:A:1277:LEU:HD22	1.66	0.78
1:A:1129:ARG:HH11	1:A:1205:GLU:HG3	1.48	0.77
1:B:902:ASN:HD22	1:B:903:PRO:HD2	1.48	0.76
1:B:1204:ARG:HH11	1:B:1213:ASN:HD21	1.33	0.75
1:B:1252:PHE:HB2	1:B:1263:TYR:CD2	2.21	0.75
1:A:1182:PHE:HB2	1:A:1213:ASN:OD1	1.87	0.75
1:B:868:ILE:H	1:B:868:ILE:HD13	1.50	0.74
1:B:1234:SER:CB	1:B:1241:ILE:HD13	2.17	0.73
1:B:1253:ARG:HB2	1:B:1260:ARG:HA	1.70	0.73
1:A:1243:GLY:HA2	1:A:1273:TYR:CD2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:ASN:ND2	1:A:965:ASN:H	1.88	0.72
1:B:973:ILE:HG23	1:B:974:SER:H	1.55	0.72
1:B:1126:ALA:HB2	1:B:1172:MET:HE1	1.71	0.71
1:B:954:PRO:HB3	1:B:1059:ILE:HG21	1.72	0.70
1:B:1252:PHE:HB2	1:B:1263:TYR:HD2	1.57	0.70
1:B:1083:LYS:HB3	1:B:1083:LYS:NZ	2.07	0.69
1:B:1170:PHE:HB2	1:B:1181:LEU:HD12	1.74	0.69
1:A:1148:ILE:HD12	1:A:1170:PHE:HB3	1.74	0.69
1:A:964:ASN:CG	1:A:965:ASN:H	1.95	0.69
1:B:1053:ILE:HG23	1:B:1054:PRO:HD2	1.75	0.68
1:B:1088:LEU:O	1:B:1092:LEU:HD22	1.93	0.68
1:A:1032:ILE:HD12	1:A:1033:LYS:H	1.57	0.68
1:A:975:ASN:H	1:A:975:ASN:ND2	1.83	0.68
1:B:955:GLY:CA	1:B:973:ILE:HD12	2.23	0.68
1:A:1174:ILE:HG22	1:A:1175:ASN:N	2.07	0.67
1:B:1143:ASN:OD1	1:B:1144:GLU:HG3	1.95	0.67
1:A:948:LYS:HE2	1:A:1002:PRO:O	1.95	0.67
1:B:975:ASN:HD22	1:B:975:ASN:N	1.87	0.67
1:B:926:ASN:HB3	1:B:929:ILE:CD1	2.25	0.67
1:B:1159:ASP:HB3	1:B:1161:ARG:HG3	1.77	0.67
1:A:902:ASN:HD22	1:A:903:PRO:N	1.94	0.66
1:B:966:SER:HA	1:B:982:LYS:O	1.96	0.66
1:B:1237:ASN:OD1	1:B:1239:GLU:HG2	1.94	0.66
1:A:1172:MET:HE1	1:A:1203:LEU:HD11	1.77	0.66
1:A:879:ARG:HA	1:A:879:ARG:NE	2.04	0.66
1:B:976:PHE:CD2	1:B:994:SER:HB3	2.31	0.66
1:A:1159:ASP:HB3	1:A:1161:ARG:H	1.60	0.65
1:A:902:ASN:HD22	1:A:903:PRO:CD	2.10	0.64
1:A:1249:THR:HG22	1:A:1264:LEU:HD13	1.79	0.64
1:A:976:PHE:CE2	1:A:994:SER:HB3	2.33	0.64
1:A:1053:ILE:HG23	1:A:1054:PRO:HD2	1.79	0.63
1:B:975:ASN:ND2	1:B:975:ASN:H	1.96	0.63
1:A:1167:ILE:HD12	1:A:1167:ILE:N	2.13	0.63
1:A:920:LYS:HD3	1:A:922:ILE:HD11	1.79	0.63
1:A:1094:TYR:HB3	1:A:1097:VAL:HG13	1.81	0.63
1:A:947:ASN:ND2	1:A:948:LYS:HB2	2.14	0.62
1:A:1212:ASP:HA	1:A:1215:ILE:HD12	1.80	0.62
1:A:1108:TYR:CE2	1:A:1152:ARG:HB2	2.33	0.62
1:A:947:ASN:HB2	1:A:1067:ASN:N	2.09	0.62
1:B:906:PRO:HB2	1:B:1071:ARG:HD2	1.81	0.62
1:B:902:ASN:HD22	1:B:903:PRO:CD	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:ASN:O	1:A:929:ILE:HG22	1.99	0.62
1:B:974:SER:N	2:B:50:HOH:O	2.32	0.61
1:B:953:LEU:HD12	1:B:954:PRO:CD	2.26	0.61
1:B:1234:SER:HB3	1:B:1241:ILE:CD1	2.30	0.61
1:A:1001:ALA:HB3	1:A:1002:PRO:HD3	1.83	0.61
1:A:947:ASN:HB3	1:A:1067:ASN:H	1.64	0.61
1:B:955:GLY:HA2	1:B:973:ILE:HA	1.81	0.61
1:A:902:ASN:ND2	1:A:904:ILE:H	1.98	0.61
1:B:955:GLY:N	1:B:973:ILE:HD12	2.15	0.61
1:A:973:ILE:CG2	1:A:976:PHE:HB2	2.32	0.60
1:B:1159:ASP:HB2	1:B:1163:ARG:NH1	2.17	0.60
1:B:1071:ARG:NH1	1:B:1092:LEU:O	2.30	0.60
1:B:904:ILE:HG22	1:B:905:PHE:N	2.17	0.60
1:B:1181:LEU:HD23	1:B:1203:LEU:HD23	1.82	0.60
1:B:1119:TYR:HB3	1:B:1122:ARG:HG3	1.84	0.60
1:B:1148:ILE:HD12	1:B:1181:LEU:HD11	1.83	0.60
1:B:1212:ASP:HA	1:B:1215:ILE:HD12	1.84	0.59
1:B:1182:PHE:HB2	1:B:1213:ASN:HD22	1.67	0.59
1:A:1088:LEU:O	1:A:1091:SER:HB3	2.03	0.59
1:B:965:ASN:ND2	1:B:985:GLU:HB3	2.18	0.59
1:A:1195:THR:O	1:A:1196:GLU:O	2.20	0.59
1:A:1136:ARG:HB2	1:A:1144:GLU:OE1	2.03	0.58
1:A:1154:ARG:NH2	1:A:1154:ARG:HG2	2.13	0.58
1:A:880:LYS:HG2	1:A:881:ASN:N	2.18	0.58
1:B:868:ILE:H	1:B:868:ILE:CD1	2.17	0.58
1:B:1136:ARG:HB2	1:B:1144:GLU:OE1	2.04	0.58
1:A:1092:LEU:N	1:A:1092:LEU:HD13	2.19	0.58
1:A:1172:MET:CE	1:A:1203:LEU:HD11	2.34	0.57
1:A:1251:ARG:HH11	1:A:1261:HIS:HA	1.68	0.57
1:A:1211:ASN:OD1	1:A:1213:ASN:HB3	2.04	0.57
1:A:902:ASN:C	1:A:902:ASN:HD22	2.06	0.57
1:A:902:ASN:HD22	1:A:903:PRO:HD2	1.70	0.57
1:B:1150:ILE:CG2	1:B:1168:LEU:HD22	2.35	0.57
1:B:1123:TYR:HD2	1:B:1136:ARG:HA	1.70	0.57
1:B:1172:MET:CE	1:B:1174:ILE:HD11	2.35	0.56
1:B:1250:TYR:HB2	1:B:1252:PHE:HE1	1.71	0.56
1:A:1252:PHE:HB2	1:A:1263:TYR:HD2	1.71	0.56
1:B:1170:PHE:CB	1:B:1181:LEU:HD12	2.36	0.55
1:A:1244:ILE:HG22	1:A:1273:TYR:HB2	1.88	0.55
1:B:1251:ARG:HH11	1:B:1261:HIS:HA	1.70	0.55
1:B:1182:PHE:CZ	1:B:1184:LYS:HG2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:GLN:O	1:B:1044:LYS:HE3	2.06	0.55
1:A:872:LYS:HD3	1:A:875:SER:HB2	1.87	0.55
1:B:1159:ASP:HB3	1:B:1161:ARG:H	1.72	0.55
1:B:926:ASN:HB3	1:B:929:ILE:HD12	1.89	0.55
1:A:1146:TYR:HD1	1:A:1172:MET:HE3	1.71	0.55
1:B:954:PRO:HB2	1:B:1052:LYS:NZ	2.23	0.54
1:B:1188:MET:H	1:B:1195:THR:HG21	1.73	0.54
1:B:926:ASN:HB3	1:B:929:ILE:HD11	1.90	0.54
1:B:1146:TYR:CD1	1:B:1172:MET:HE3	2.43	0.54
1:B:976:PHE:CE2	1:B:994:SER:HB3	2.43	0.54
1:A:1251:ARG:HD3	1:A:1262:ASN:ND2	2.22	0.54
1:B:1249:THR:HG23	1:B:1264:LEU:HD13	1.90	0.54
1:B:1195:THR:O	1:B:1196:GLU:C	2.46	0.53
1:B:1123:TYR:CZ	1:B:1134:ASN:HB2	2.44	0.53
1:A:1252:PHE:HB2	1:A:1263:TYR:CD2	2.43	0.53
1:B:1250:TYR:HB2	1:B:1252:PHE:CE1	2.44	0.53
1:A:1172:MET:CE	1:A:1174:ILE:HD11	2.39	0.53
1:A:1226:TYR:OH	1:A:1283:HIS:HD2	1.91	0.53
1:B:989:GLN:HE21	1:B:1032:ILE:HD12	1.74	0.53
1:B:876:LEU:O	1:B:877:GLN:HG3	2.09	0.53
1:A:1144:GLU:O	1:A:1145:GLY:O	2.27	0.53
1:B:973:ILE:HG23	1:B:974:SER:N	2.22	0.53
1:B:1083:LYS:HB3	1:B:1083:LYS:HZ3	1.74	0.52
1:A:1132:VAL:HA	1:A:1265:VAL:HG12	1.89	0.52
1:B:1195:THR:HG22	1:B:1195:THR:O	2.09	0.52
1:A:952:ASN:O	1:A:1059:ILE:HD11	2.09	0.52
1:A:1235:ASN:OD1	1:A:1240:ASN:HB3	2.10	0.52
1:A:927:GLU:HG3	1:A:928:ASN:N	2.24	0.52
1:B:1124:MET:HE3	1:B:1148:ILE:HD11	1.91	0.52
1:A:1018:GLY:O	1:A:1033:LYS:HD2	2.09	0.52
1:B:889:TYR:HB3	1:B:929:ILE:HD13	1.91	0.52
1:A:1178:ALA:O	1:A:1206:GLN:HG3	2.09	0.52
1:B:1110:LYS:NZ	1:B:1290:SER:OG	2.42	0.52
1:B:1185:ASN:HB3	2:B:104:HOH:O	2.09	0.52
1:A:1154:ARG:NH1	1:A:1167:ILE:HD11	2.25	0.52
1:B:924:THR:HG22	1:B:1044:LYS:HE2	1.91	0.52
1:A:976:PHE:CD2	1:A:994:SER:HB3	2.45	0.52
1:A:944:ILE:HG12	1:A:945:ARG:N	2.24	0.52
1:A:983:GLN:HG3	1:A:984:ASN:ND2	2.25	0.52
1:A:1289:VAL:O	1:A:1289:VAL:HG23	2.09	0.51
1:B:972:ILE:HG22	1:B:977:LEU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:ASN:OD1	1:A:1118:ASP:HB2	2.10	0.51
1:A:1172:MET:HE3	1:A:1174:ILE:HD11	1.92	0.51
1:A:1221:MET:HB3	1:A:1229:SER:HA	1.92	0.51
1:B:1167:ILE:HD12	1:B:1167:ILE:N	2.25	0.51
1:A:906:PRO:HB2	1:A:1071:ARG:HD2	1.91	0.51
1:B:1099:LYS:HD2	1:B:1103:GLY:O	2.11	0.51
1:B:1252:PHE:O	1:B:1253:ARG:HB3	2.11	0.51
1:A:1162:VAL:CG1	1:A:1218:ILE:HG21	2.41	0.51
1:B:1127:ASN:O	1:B:1129:ARG:N	2.42	0.51
1:B:1172:MET:CE	1:B:1203:LEU:HD11	2.40	0.51
1:A:1131:ILE:CD1	1:A:1172:MET:HE1	2.40	0.51
1:A:1054:PRO:O	1:A:1055:ASP:O	2.29	0.51
1:B:1093:GLN:HG3	2:B:42:HOH:O	2.10	0.50
1:A:973:ILE:CG2	1:A:974:SER:N	2.65	0.50
1:B:1126:ALA:HB2	1:B:1172:MET:CE	2.38	0.50
1:A:1148:ILE:HD13	1:A:1171:ASP:O	2.11	0.50
1:A:1113:TYR:HB2	1:A:1287:VAL:HB	1.92	0.50
1:A:1124:MET:HG3	1:A:1133:PHE:CE2	2.47	0.50
1:A:1010:VAL:HG12	1:A:1011:THR:N	2.26	0.50
1:B:1113:TYR:HB2	1:B:1287:VAL:HB	1.93	0.50
1:B:1001:ALA:HB3	1:B:1002:PRO:HD3	1.92	0.50
1:B:1234:SER:HB2	1:B:1241:ILE:HD13	1.93	0.50
1:A:979:PHE:CE1	1:A:981:LEU:HD13	2.47	0.50
1:A:1071:ARG:HH11	1:A:1092:LEU:HB2	1.77	0.50
1:B:1277:LEU:HD12	2:B:89:HOH:O	2.12	0.49
1:B:872:LYS:HD3	1:B:875:SER:HB2	1.93	0.49
1:B:1159:ASP:HB2	1:B:1163:ARG:HH12	1.78	0.49
1:A:922:ILE:HG12	1:A:1047:THR:HG23	1.94	0.49
1:B:909:PHE:CZ	1:B:1070:ILE:HB	2.47	0.49
1:B:989:GLN:NE2	1:B:1032:ILE:HD12	2.27	0.49
1:A:947:ASN:HB2	1:A:1067:ASN:HB2	1.94	0.49
1:A:1195:THR:O	1:A:1195:THR:HG23	2.11	0.49
1:A:914:SER:OG	1:A:916:GLU:HG2	2.13	0.49
1:B:1193:HIS:N	1:B:1193:HIS:ND1	2.59	0.49
1:B:965:ASN:CG	1:B:985:GLU:HB3	2.33	0.49
1:B:983:GLN:NE2	1:B:1037:LEU:HA	2.28	0.49
1:B:1011:THR:HB	1:B:1023:TYR:HB2	1.95	0.48
1:B:1117:ILE:HG12	1:B:1226:TYR:CE2	2.47	0.48
1:A:1156:ASN:HB3	1:A:1163:ARG:NH2	2.19	0.48
1:A:880:LYS:CG	1:A:881:ASN:N	2.76	0.48
1:B:1172:MET:HE2	1:B:1203:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ILE:C	2:B:50:HOH:O	2.51	0.48
1:A:900:GLN:O	1:A:910:LYS:N	2.46	0.48
1:A:1234:SER:HB3	1:A:1241:ILE:CD1	2.44	0.48
1:B:926:ASN:HA	2:B:44:HOH:O	2.14	0.48
1:B:1116:ASN:OD1	1:B:1118:ASP:HB2	2.13	0.48
1:A:1071:ARG:NH1	1:A:1092:LEU:O	2.45	0.48
1:A:900:GLN:O	1:A:909:PHE:HA	2.14	0.48
1:B:979:PHE:CE1	1:B:981:LEU:HD13	2.49	0.48
1:A:1116:ASN:HB2	1:A:1284:TRP:CZ3	2.49	0.47
1:B:1093:GLN:NE2	2:B:72:HOH:O	2.47	0.47
1:A:1216:PHE:HB3	1:A:1231:ILE:HG22	1.96	0.47
1:B:1207:THR:O	1:B:1208:LYS:HB2	2.14	0.47
1:B:957:THR:OG1	1:B:1053:ILE:HD11	2.14	0.47
1:B:1243:GLY:HA2	1:B:1273:TYR:CD2	2.49	0.47
1:A:1180:ASN:HB2	1:A:1204:ARG:HG2	1.95	0.47
1:B:868:ILE:N	1:B:868:ILE:HD13	2.24	0.47
1:A:965:ASN:O	1:A:982:LYS:HG2	2.13	0.47
1:B:904:ILE:CG2	1:B:905:PHE:N	2.77	0.47
1:B:1081:ASP:O	1:B:1085:ILE:HG13	2.15	0.47
1:A:880:LYS:CG	1:A:881:ASN:H	2.26	0.47
1:B:876:LEU:C	1:B:877:GLN:HG3	2.35	0.47
1:A:1201:ILE:HD12	1:A:1266:PRO:HB2	1.97	0.47
1:B:1133:PHE:CE1	1:B:1266:PRO:HD3	2.50	0.47
1:B:1231:ILE:N	1:B:1231:ILE:HD12	2.30	0.47
1:B:1179:TYR:HB3	1:B:1204:ARG:O	2.16	0.46
1:B:1092:LEU:CD2	1:B:1092:LEU:H	2.28	0.46
1:A:1146:TYR:CD1	1:A:1172:MET:HE3	2.50	0.46
1:A:983:GLN:HA	1:A:1040:ILE:HG13	1.97	0.46
1:A:874:LEU:HD12	1:A:885:ASP:OD2	2.14	0.46
1:A:902:ASN:O	1:A:907:PHE:HA	2.16	0.46
1:A:1251:ARG:NH1	1:A:1261:HIS:HA	2.31	0.46
1:A:1182:PHE:CD2	1:A:1204:ARG:HB3	2.50	0.46
1:B:924:THR:CG2	1:B:1044:LYS:HE2	2.46	0.46
1:A:1230:GLN:HB3	1:A:1232:PHE:CE2	2.50	0.46
1:B:1053:ILE:HG23	1:B:1054:PRO:CD	2.45	0.46
1:B:1110:LYS:HD3	1:B:1112:TYR:CZ	2.51	0.46
1:B:929:ILE:H	1:B:929:ILE:HG13	1.60	0.46
1:A:1108:TYR:CZ	1:A:1152:ARG:HB2	2.51	0.46
1:B:1269:LYS:HE2	1:B:1270:GLN:O	2.16	0.46
1:B:1143:ASN:OD1	1:B:1144:GLU:N	2.49	0.46
1:A:1083:LYS:O	1:A:1087:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:MET:HG3	1:A:1198:ILE:HG22	1.98	0.46
1:B:1016:MET:HG2	2:B:1:HOH:O	2.16	0.45
1:B:1196:GLU:HG2	1:B:1269:LYS:HE3	1.98	0.45
1:A:1108:TYR:CZ	1:A:1162:VAL:HG22	2.51	0.45
1:B:983:GLN:HG2	1:B:984:ASN:ND2	2.31	0.45
1:A:966:SER:HA	1:A:982:LYS:O	2.17	0.45
1:A:905:PHE:CG	1:A:906:PRO:HA	2.52	0.45
1:A:1252:PHE:O	1:A:1260:ARG:HA	2.16	0.45
1:A:1123:TYR:CZ	1:A:1134:ASN:HB2	2.50	0.45
1:B:1182:PHE:HB2	1:B:1213:ASN:ND2	2.30	0.45
1:B:978:VAL:HB	1:B:992:ASN:HB3	1.98	0.45
1:B:958:ILE:HG13	1:B:959:ILE:H	1.80	0.45
1:B:879:ARG:HG2	1:B:884:VAL:CG2	2.45	0.45
1:A:964:ASN:CG	1:A:965:ASN:N	2.65	0.45
1:B:1119:TYR:HB3	1:B:1122:ARG:CG	2.47	0.45
1:B:944:ILE:HG12	1:B:945:ARG:N	2.32	0.45
1:A:955:GLY:HA2	1:A:973:ILE:HD12	1.99	0.45
1:A:1167:ILE:CD1	1:A:1167:ILE:N	2.80	0.45
1:B:1204:ARG:NH1	1:B:1213:ASN:HD21	2.06	0.45
1:B:959:ILE:N	1:B:959:ILE:HD12	2.32	0.45
1:B:966:SER:HG	1:B:1041:ASN:H	1.61	0.45
1:B:1207:THR:O	1:B:1208:LYS:CB	2.65	0.45
1:A:1122:ARG:HA	1:A:1134:ASN:O	2.17	0.45
1:A:941:SER:O	1:A:942:PHE:HB3	2.17	0.45
1:A:1171:ASP:OD2	1:A:1180:ASN:ND2	2.49	0.45
1:B:1113:TYR:CE1	1:B:1143:ASN:HA	2.52	0.45
1:A:1110:LYS:HD3	1:A:1112:TYR:CZ	2.52	0.45
1:A:1100:ASP:OD2	1:A:1100:ASP:C	2.55	0.45
1:A:1177:LYS:HB3	1:A:1177:LYS:NZ	2.33	0.44
1:B:1179:TYR:HB2	1:B:1203:LEU:HD22	1.98	0.44
1:A:943:TRP:HE1	1:A:1092:LEU:HD23	1.82	0.44
1:A:920:LYS:HE3	1:A:1049:GLU:OE2	2.17	0.44
1:B:996:ASP:OD2	1:B:999:ASN:ND2	2.50	0.44
1:B:1253:ARG:CB	1:B:1260:ARG:HA	2.45	0.44
1:B:1001:ALA:N	1:B:1002:PRO:CD	2.81	0.44
1:B:1073:PHE:C	1:B:1074:TYR:HD2	2.21	0.44
1:A:1248:GLY:C	1:A:1264:LEU:HD12	2.39	0.43
1:A:902:ASN:C	1:A:902:ASN:ND2	2.71	0.43
1:A:902:ASN:ND2	1:A:903:PRO:HD2	2.33	0.43
1:B:1108:TYR:CZ	1:B:1162:VAL:HG22	2.53	0.43
1:B:928:ASN:O	1:B:932:ASN:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:LEU:O	1:A:1092:LEU:CD2	2.66	0.43
1:A:1127:ASN:HA	1:A:1127:ASN:HD22	1.49	0.43
1:B:1129:ARG:NH1	1:B:1205:GLU:HG3	2.33	0.43
1:B:1003:GLY:O	1:B:1005:ASN:N	2.51	0.43
1:A:1066:ILE:O	1:A:1066:ILE:HG13	2.17	0.43
1:B:1092:LEU:HD23	1:B:1092:LEU:H	1.83	0.43
1:B:1161:ARG:NH1	2:B:48:HOH:O	2.52	0.43
1:B:1188:MET:H	1:B:1195:THR:CG2	2.32	0.43
1:A:904:ILE:HG22	1:A:905:PHE:N	2.34	0.43
1:B:965:ASN:O	1:B:982:LYS:HG2	2.19	0.43
1:A:937:SER:HA	1:A:1014:ASN:O	2.18	0.43
1:B:871:SER:O	1:B:1076:PHE:HA	2.18	0.43
1:A:1163:ARG:O	1:A:1166:ASP:HB2	2.18	0.43
1:A:1179:TYR:N	1:A:1179:TYR:CD1	2.87	0.43
1:A:954:PRO:HG2	1:A:956:TYR:CE2	2.54	0.43
1:A:942:PHE:HB3	1:A:1073:PHE:HA	2.00	0.43
1:B:1147:LYS:HD3	1:B:1289:VAL:HG11	2.00	0.43
1:A:1159:ASP:HB2	1:A:1163:ARG:NH2	2.34	0.43
1:B:905:PHE:CG	1:B:906:PRO:HA	2.53	0.43
1:B:1123:TYR:CD1	1:B:1145:GLY:HA2	2.54	0.43
1:A:958:ILE:HG22	1:A:1050:ILE:HD13	1.99	0.43
1:B:1052:LYS:HD3	1:B:1053:ILE:N	2.33	0.43
1:A:1173:THR:HA	1:A:1177:LYS:O	2.19	0.43
1:B:1097:VAL:HG23	1:B:1097:VAL:O	2.18	0.43
1:A:1249:THR:HG22	1:A:1264:LEU:CD1	2.48	0.42
1:A:1162:VAL:HG11	1:A:1218:ILE:HD13	2.00	0.42
1:B:954:PRO:HB2	1:B:1052:LYS:HZ2	1.84	0.42
1:B:1274:ALA:HA	1:B:1277:LEU:CD2	2.41	0.42
1:B:902:ASN:HB3	1:B:907:PHE:HA	2.01	0.42
1:B:1108:TYR:CE2	1:B:1152:ARG:HB2	2.54	0.42
1:B:939:SER:HA	1:B:1012:VAL:O	2.19	0.42
1:A:1109:ASN:HA	1:A:1149:ILE:CG2	2.49	0.42
1:B:1177:LYS:O	1:B:1179:TYR:CE1	2.72	0.42
1:A:1133:PHE:CE1	1:A:1266:PRO:HD3	2.54	0.42
1:B:1182:PHE:HD1	1:B:1213:ASN:HD22	1.67	0.42
1:B:1204:ARG:HH11	1:B:1213:ASN:ND2	2.07	0.42
1:B:981:LEU:HA	1:B:981:LEU:HD12	1.78	0.42
1:B:914:SER:C	1:B:916:GLU:H	2.22	0.42
1:A:1211:ASN:C	1:A:1213:ASN:N	2.70	0.42
1:B:1144:GLU:O	1:B:1145:GLY:O	2.37	0.42
1:A:1053:ILE:HG23	1:A:1054:PRO:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:PHE:O	1:A:1049:GLU:HB2	2.19	0.42
1:B:1020:MET:HE3	1:B:1032:ILE:HD11	2.02	0.42
1:A:944:ILE:CG1	1:A:945:ARG:N	2.81	0.42
1:A:901:LEU:HD23	1:A:909:PHE:HB3	2.02	0.42
1:B:1231:ILE:HD13	1:B:1284:TRP:CD1	2.54	0.42
1:B:918:ARG:HG2	1:B:918:ARG:HH11	1.83	0.42
1:B:973:ILE:HG23	2:B:50:HOH:O	2.20	0.42
1:A:1032:ILE:HD12	1:A:1033:LYS:N	2.32	0.42
1:B:976:PHE:HD2	1:B:992:ASN:ND2	2.17	0.42
1:B:942:PHE:HB3	1:B:1073:PHE:HA	2.02	0.42
1:B:1148:ILE:CD1	1:B:1181:LEU:HD11	2.48	0.42
1:B:1249:THR:HA	1:B:1263:TYR:O	2.20	0.42
1:A:927:GLU:HB3	1:A:1044:LYS:HD3	2.00	0.42
1:B:1207:THR:C	1:B:1209:ASP:H	2.23	0.42
1:A:1127:ASN:O	1:A:1129:ARG:N	2.52	0.42
1:A:956:TYR:HB2	1:A:972:ILE:HG13	2.01	0.42
1:B:1151:LYS:O	1:B:1168:LEU:HB2	2.19	0.42
1:A:1250:TYR:HB2	1:A:1252:PHE:HE1	1.85	0.42
1:B:1207:THR:OG1	1:B:1209:ASP:O	2.38	0.42
1:B:939:SER:O	1:B:1075:ILE:HA	2.20	0.42
1:B:1174:ILE:HG22	1:B:1175:ASN:N	2.34	0.41
1:A:956:TYR:N	1:A:1053:ILE:HD13	2.34	0.41
1:B:948:LYS:HG2	1:B:950:VAL:CG1	2.50	0.41
1:A:1143:ASN:HB2	1:A:1144:GLU:H	1.65	0.41
1:A:914:SER:HA	1:A:1065:ASN:HD22	1.85	0.41
1:A:1174:ILE:O	1:A:1175:ASN:C	2.58	0.41
1:A:1210:ILE:HG22	1:A:1215:ILE:HD11	2.02	0.41
1:A:1216:PHE:HA	1:A:1232:PHE:O	2.20	0.41
1:B:916:GLU:HB3	1:B:917:ASP:H	1.66	0.41
1:A:933:SER:O	1:A:936:GLU:HG3	2.20	0.41
1:B:1201:ILE:HD11	1:B:1268:VAL:CG2	2.41	0.41
1:A:1125:TYR:CE1	1:A:1146:TYR:CZ	3.09	0.41
1:A:868:ILE:HG22	2:A:63:HOH:O	2.21	0.41
1:B:926:ASN:HD21	1:B:928:ASN:ND2	2.19	0.41
1:B:917:ASP:O	1:B:918:ARG:C	2.59	0.41
1:B:1124:MET:HE1	1:B:1148:ILE:HG12	2.03	0.41
1:A:981:LEU:HB2	1:A:1020:MET:HE1	2.03	0.41
1:B:901:LEU:HD23	1:B:909:PHE:HB3	2.03	0.41
1:A:973:ILE:O	1:A:974:SER:O	2.39	0.41
1:B:902:ASN:HA	1:B:903:PRO:HD2	1.88	0.41
1:A:1232:PHE:HB3	1:A:1241:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1207:THR:O	1:A:1208:LYS:C	2.59	0.41
1:A:1092:LEU:O	1:A:1093:GLN:HB2	2.21	0.40
1:B:972:ILE:O	1:B:972:ILE:HG13	2.21	0.40
1:B:1108:TYR:CZ	1:B:1152:ARG:HB2	2.55	0.40
1:A:1107:ARG:HA	1:A:1160:THR:O	2.21	0.40
1:B:1172:MET:HB3	1:B:1203:LEU:CD2	2.52	0.40
1:A:909:PHE:CZ	1:A:1070:ILE:HB	2.56	0.40
1:B:991:ILE:HG12	1:B:1030:ASP:HB3	2.03	0.40
1:A:1179:TYR:HB2	1:A:1203:LEU:HD22	2.03	0.40
1:B:959:ILE:HG13	1:B:1048:PHE:CD1	2.56	0.40
1:B:1088:LEU:O	1:B:1092:LEU:CD2	2.64	0.40
1:B:961:SER:HB3	1:B:968:TRP:CE2	2.56	0.40
1:B:1052:LYS:HD3	1:B:1053:ILE:H	1.86	0.40
1:B:1195:THR:CG2	1:B:1195:THR:O	2.69	0.40
1:A:1198:ILE:HD13	1:A:1269:LYS:HA	2.02	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	418/426 (98%)	352 (84%)	49 (12%)	17 (4%)	3	4
1	B	417/426 (98%)	357 (86%)	43 (10%)	17 (4%)	3	4
All	All	835/852 (98%)	709 (85%)	92 (11%)	34 (4%)	3	4

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	974	SER
1	A	1055	ASP
1	A	1145	GLY

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Mol	Chain	Res	Type
1	A	1193	HIS
1	A	1196	GLU
1	B	916	GLU
1	B	1196	GLU
1	A	880	LYS
1	A	916	GLU
1	B	880	LYS
1	B	918	ARG
1	B	974	SER
1	B	1145	GLY
1	B	1191	ASP
1	B	1255	GLY
1	A	973	ILE
1	A	1036	GLU
1	A	1209	ASP
1	B	1004	TYR
1	B	1144	GLU
1	B	1193	HIS
1	A	1049	GLU
1	A	1254	LEU
1	B	879	ARG
1	B	914	SER
1	B	964	ASN
1	B	947	ASN
1	B	1054	PRO
1	A	1060	THR
1	A	1210	ILE
1	B	973	ILE
1	A	953	LEU
1	A	1174	ILE
1	A	1117	ILE

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/390 (99%)	362 (94%)	25 (6%)	21	39
1	B	386/390 (99%)	364 (94%)	22 (6%)	25	46
All	All	773/780 (99%)	726 (94%)	47 (6%)	23	42

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	878	ASN
1	A	879	ARG
1	A	902	ASN
1	A	917	ASP
1	A	936	GLU
1	A	975	ASN
1	A	978	VAL
1	A	1021	LYS
1	A	1023	TYR
1	A	1027	LYS
1	A	1041	ASN
1	A	1064	ASP
1	A	1092	LEU
1	A	1127	ASN
1	A	1142	PHE
1	A	1143	ASN
1	A	1148	ILE
1	A	1185	ASN
1	A	1192	ASN
1	A	1196	GLU
1	A	1209	ASP
1	A	1219	GLN
1	A	1231	ILE
1	A	1277	LEU
1	A	1283	HIS
1	B	868	ILE
1	B	878	ASN
1	B	902	ASN
1	B	917	ASP
1	B	926	ASN
1	B	927	GLU
1	B	975	ASN

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Mol	Chain	Res	Type
1	B	978	VAL
1	B	981	LEU
1	B	1021	LYS
1	B	1030	ASP
1	B	1041	ASN
1	B	1066	ILE
1	B	1083	LYS
1	B	1092	LEU
1	B	1117	ILE
1	B	1127	ASN
1	B	1142	PHE
1	B	1154	ARG
1	B	1156	ASN
1	B	1193	HIS
1	B	1290	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	878	ASN
1	A	900	GLN
1	A	902	ASN
1	A	932	ASN
1	A	947	ASN
1	A	975	ASN
1	A	983	GLN
1	A	992	ASN
1	A	1067	ASN
1	A	1086	ASN
1	A	1127	ASN
1	A	1130	GLN
1	A	1180	ASN
1	A	1185	ASN
1	A	1206	GLN
1	A	1213	ASN
1	A	1230	GLN
1	A	1240	ASN
1	A	1261	HIS
1	A	1262	ASN
1	A	1270	GLN
1	A	1283	HIS
1	B	867	ASN

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Mol	Chain	Res	Type
1	B	877	GLN
1	B	878	ASN
1	B	900	GLN
1	B	902	ASN
1	B	926	ASN
1	B	928	ASN
1	B	932	ASN
1	B	965	ASN
1	B	975	ASN
1	B	992	ASN
1	B	999	ASN
1	B	1041	ASN
1	B	1065	ASN
1	B	1090	ASN
1	B	1093	GLN
1	B	1127	ASN
1	B	1130	GLN
1	B	1134	ASN
1	B	1140	ASN
1	B	1156	ASN
1	B	1158	ASN
1	B	1180	ASN
1	B	1206	GLN
1	B	1213	ASN
1	B	1230	GLN
1	B	1262	ASN
1	B	1270	GLN
1	B	1283	HIS

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, 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	A	422/426 (99%)	-0.22	8 (1%) 70 73	9, 27, 54, 84	0
1	B	421/426 (98%)	-0.21	6 (1%) 78 80	11, 28, 55, 76	0
All	All	843/852 (98%)	-0.22	14 (1%) 73 76	9, 28, 55, 84	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1059	ILE	7.1
1	A	1059	ILE	6.2
1	A	1061	SER	5.3
1	A	1060	THR	4.3
1	B	1060	THR	3.6
1	B	1061	SER	2.5
1	A	1062	ASP	2.5
1	A	1054	PRO	2.4
1	B	1290	SER	2.3
1	B	1062	ASP	2.3
1	B	947	ASN	2.2
1	A	1196	GLU	2.2
1	A	947	ASN	2.1
1	A	1053	ILE	2.1

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.