



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:58 AM UTC

PDB ID : 2NM1 / pdb\_00002nm1  
Title : Structure of BoNT/B in complex with its protein receptor  
Authors : Jin, R.; Rummel, A.; Binz, T.; Brunger, A.T.  
Deposited on : 2006-10-20  
Resolution : 2.15 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

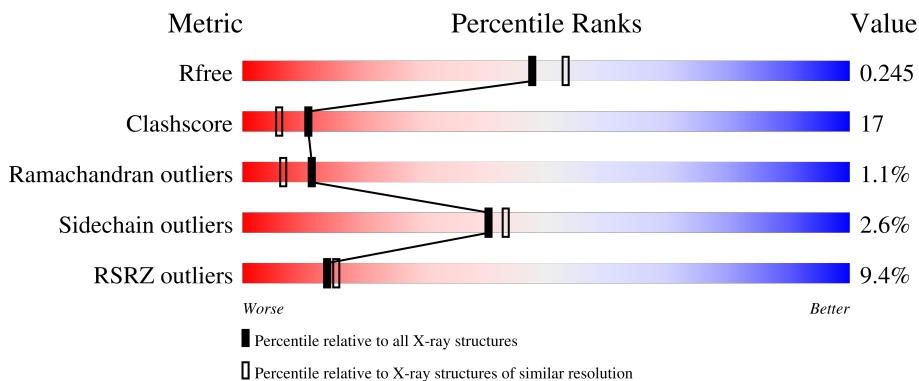
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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  $\leq 5\%$ . 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	436	
2	B	17	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3941 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	430	3663	2371	596	688	8	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1292	PRO	-	cloning artifact	UNP P10844
A	1293	PRO	-	cloning artifact	UNP P10844

- Molecule 2 is a protein called Synaptotagmin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	17	149	97	23	28	1	10	0	0

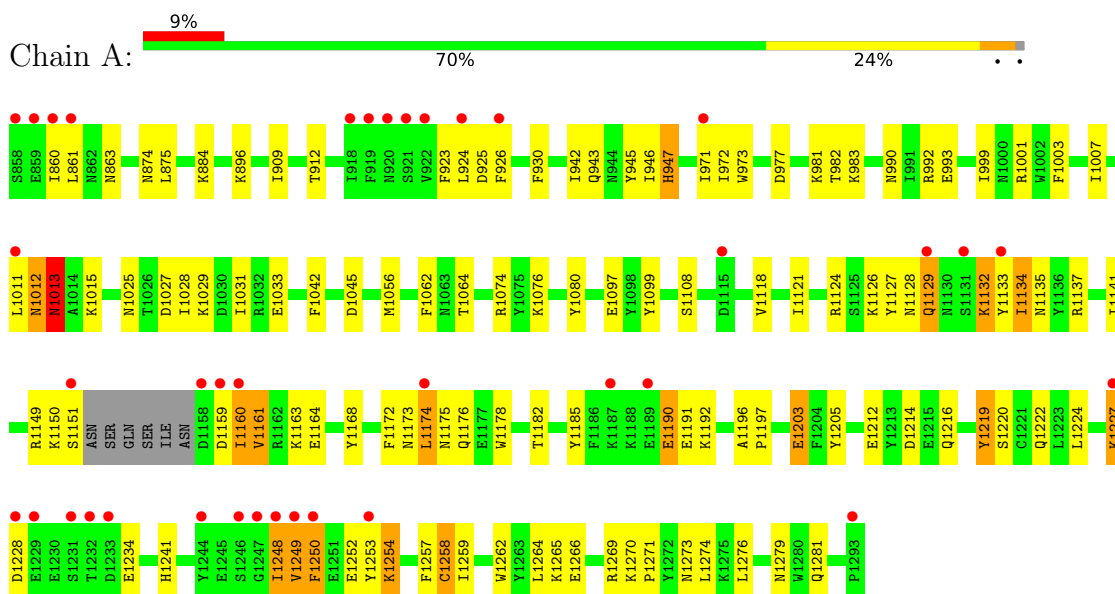
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		

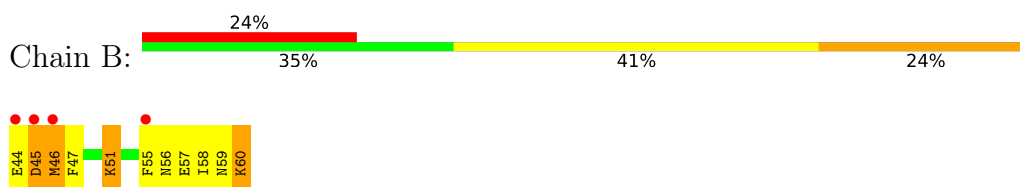
### 3 Residue-property plots [i](#)

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



- Molecule 2: Synaptotagmin-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.82Å 97.52Å 113.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 2.15 39.81 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.81-2.15) 94.4 (39.81-2.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.16Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.199 , 0.246 0.199 , 0.245	Depositor DCC
$R_{free}$ test set	1550 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtrriage
Anisotropy	0.698	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3941	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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	0.52	0/3752	0.95	16/5059 (0.3%)
2	B	0.47	0/151	1.05	2/196 (1.0%)
All	All	0.52	0/3903	0.95	18/5255 (0.3%)

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 (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1160	ILE	N-CA-C	8.09	126.16	109.34
1	A	1012	ASN	N-CA-C	7.32	122.49	112.90
1	A	1099	TYR	N-CA-C	-7.29	99.73	110.52
1	A	1227	LYS	N-CA-C	-6.95	103.32	111.03
1	A	1258	CYS	N-CA-C	6.82	118.47	108.86
2	B	46	MET	N-CA-C	-6.46	105.39	113.20
1	A	1257	PHE	N-CA-C	-6.46	100.10	109.59
1	A	972	ILE	N-CA-C	6.39	117.06	108.11
1	A	1013	ASN	N-CA-C	6.35	118.20	108.42
1	A	896	LYS	N-CA-C	-6.12	105.75	112.72
1	A	1168	TYR	N-CA-C	-5.70	100.11	109.40
1	A	1259	ILE	N-CA-C	-5.41	100.70	108.48
1	A	1185	TYR	N-CA-C	5.36	117.73	110.88
1	A	947	HIS	N-CA-C	5.31	119.89	113.41
1	A	1134	ILE	N-CA-C	5.19	117.32	108.86
1	A	1203	GLU	N-CA-C	5.16	119.26	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1219	TYR	N-CA-C	-5.13	106.26	112.88
2	B	47	PHE	N-CA-C	-5.08	105.24	111.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1080	TYR	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	A	3663	0	3575	116	0
2	B	149	0	146	9	0
3	A	129	0	0	4	0
All	All	3941	0	3721	124	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 17.

All (124) 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:1249:VAL:HG13	1:A:1250:PHE:H	1.33	0.94
1:A:1161:VAL:N	3:A:123:HOH:O	2.07	0.86
1:A:1013:ASN:HA	1:A:1028:ILE:HG12	1.59	0.83
1:A:1248:ILE:HD12	1:A:1249:VAL:H	1.44	0.83
1:A:1160:ILE:O	1:A:1160:ILE:HG22	1.84	0.76
1:A:1012:ASN:ND2	1:A:1029:LYS:HE2	2.03	0.74
2:B:44:GLU:HG3	2:B:45:ASP:N	2.02	0.74
1:A:860:ILE:HG13	1:A:861:LEU:HD22	1.69	0.73
1:A:923:PHE:HB3	1:A:1011:LEU:HD13	1.70	0.73
1:A:1150:LYS:O	1:A:1151:SER:HB3	1.89	0.73
1:A:1132:LYS:CE	1:A:1132:LYS:H	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:TYR:HD2	1:A:946:ILE:HD12	1.54	0.72
1:A:1160:ILE:O	1:A:1160:ILE:CG2	2.39	0.70
1:A:990:ASN:HD22	1:A:993:GLU:HG3	1.54	0.70
1:A:1175:ASN:N	3:A:117:HOH:O	2.21	0.69
1:A:1126:LYS:HB3	1:A:1137:ARG:HD3	1.76	0.68
2:B:44:GLU:HG3	2:B:45:ASP:H	1.61	0.65
1:A:1132:LYS:H	1:A:1132:LYS:HE3	1.61	0.65
1:A:1262:TRP:CH2	1:A:1266:GLU:HG3	2.32	0.64
1:A:992:ARG:HG2	1:A:992:ARG:HH11	1.62	0.64
1:A:942:ILE:HD11	1:A:1134:ILE:HD13	1.80	0.63
1:A:1160:ILE:C	3:A:123:HOH:O	2.38	0.63
1:A:1205:TYR:OH	1:A:1227:LYS:HG2	1.99	0.62
1:A:946:ILE:HG22	1:A:947:HIS:CD2	2.34	0.62
1:A:1128:ASN:HB2	1:A:1129:GLN:NE2	2.15	0.61
1:A:942:ILE:CD1	1:A:1134:ILE:HD13	2.31	0.61
1:A:1149:ARG:HH21	1:A:1159:ASP:CB	2.15	0.60
1:A:943:GLN:HE22	1:A:1133:TYR:HE1	1.50	0.60
1:A:874:ASN:HD22	1:A:875:LEU:H	1.49	0.59
1:A:1173:ASN:OD1	1:A:1174:LEU:HD13	2.02	0.59
1:A:912:THR:HG23	3:A:18:HOH:O	2.03	0.58
1:A:1249:VAL:HG13	1:A:1250:PHE:N	2.10	0.58
1:A:1108:SER:HB3	1:A:1121:ILE:CG2	2.34	0.58
1:A:884:LYS:HB3	1:A:912:THR:OG1	2.04	0.57
1:A:971:ILE:HD11	1:A:1003:PHE:HZ	1.68	0.57
1:A:1127:TYR:CZ	1:A:1129:GLN:HB2	2.39	0.56
1:A:990:ASN:ND2	1:A:993:GLU:HG3	2.20	0.56
1:A:1076:LYS:HE2	1:A:1216:GLN:HE22	1.71	0.56
1:A:1262:TRP:CZ3	1:A:1266:GLU:HG3	2.41	0.55
1:A:1129:GLN:NE2	1:A:1129:GLN:H	2.04	0.55
1:A:1273:ASN:HB3	1:A:1276:LEU:HG	1.89	0.55
1:A:1128:ASN:O	1:A:1129:GLN:C	2.50	0.55
1:A:923:PHE:CE2	1:A:925:ASP:HB2	2.42	0.55
1:A:942:ILE:O	1:A:946:ILE:HD13	2.07	0.54
1:A:1227:LYS:HE2	1:A:1228:ASP:HB2	1.89	0.54
1:A:1160:ILE:O	1:A:1161:VAL:O	2.26	0.54
2:B:56:ASN:O	2:B:60:LYS:HG3	2.07	0.53
1:A:982:THR:HG22	1:A:983:LYS:N	2.23	0.53
1:A:1254:LYS:HB2	1:A:1254:LYS:NZ	2.24	0.53
1:A:990:ASN:ND2	1:A:992:ARG:H	2.07	0.53
1:A:1262:TRP:CD1	1:A:1265:LYS:HE3	2.43	0.52
1:A:1149:ARG:HH21	1:A:1159:ASP:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:GLN:HE21	1:A:1279:ASN:HD22	1.58	0.52
2:B:44:GLU:CG	2:B:45:ASP:N	2.68	0.52
1:A:863:ASN:ND2	1:A:1064:THR:HG21	2.24	0.51
1:A:1132:LYS:H	1:A:1132:LYS:CD	2.23	0.51
1:A:1224:LEU:HD21	1:A:1234:GLU:HG2	1.93	0.51
1:A:1190:GLU:HG3	1:A:1241:HIS:CD2	2.46	0.51
1:A:860:ILE:C	1:A:861:LEU:HD22	2.36	0.50
1:A:1227:LYS:CE	1:A:1228:ASP:HB2	2.42	0.50
1:A:1128:ASN:HB2	1:A:1129:GLN:HE21	1.76	0.50
1:A:992:ARG:HG2	1:A:992:ARG:NH1	2.26	0.50
1:A:1269:ARG:HH11	1:A:1269:ARG:HG3	1.77	0.49
1:A:1128:ASN:O	1:A:1129:GLN:O	2.31	0.49
1:A:1196:ALA:HB1	1:A:1197:PRO:CD	2.42	0.49
1:A:1205:TYR:CE1	1:A:1227:LYS:HA	2.48	0.49
1:A:924:LEU:HD21	1:A:926:PHE:HE2	1.78	0.49
1:A:977:ASP:HB3	1:A:1031:ILE:HG23	1.94	0.49
1:A:1214:ASP:OD2	1:A:1274:LEU:HD11	2.13	0.49
1:A:930:PHE:CD1	1:A:1056:MET:HE3	2.48	0.48
1:A:926:PHE:HB2	1:A:1062:PHE:O	2.13	0.48
1:A:1249:VAL:HG22	1:A:1250:PHE:N	2.29	0.48
1:A:1127:TYR:OH	1:A:1129:GLN:HB2	2.13	0.48
1:A:874:ASN:ND2	1:A:875:LEU:H	2.12	0.47
1:A:971:ILE:HD11	1:A:1003:PHE:CZ	2.49	0.47
1:A:884:LYS:HE2	1:A:912:THR:OG1	2.14	0.47
1:A:1126:LYS:HD3	1:A:1135:ASN:HD21	1.79	0.47
1:A:1149:ARG:NH2	1:A:1159:ASP:CB	2.78	0.47
1:A:1248:ILE:CD1	1:A:1249:VAL:H	2.23	0.46
1:A:1227:LYS:HE2	1:A:1228:ASP:CB	2.46	0.46
2:B:51:LYS:HG2	2:B:55:PHE:CE2	2.51	0.46
1:A:1270:LYS:HA	1:A:1271:PRO:C	2.41	0.46
1:A:909:ILE:HB	1:A:1042:PHE:HB2	1.96	0.46
1:A:1234:GLU:OE1	1:A:1264:LEU:HD22	2.16	0.45
1:A:1205:TYR:CZ	1:A:1227:LYS:HG2	2.51	0.45
1:A:1027:ASP:OD1	1:A:1029:LYS:HG3	2.16	0.45
1:A:1212:GLU:OE1	1:A:1220:SER:O	2.34	0.45
1:A:1265:LYS:HG3	1:A:1266:GLU:N	2.31	0.45
1:A:983:LYS:HB2	1:A:1031:ILE:HD11	1.98	0.45
1:A:1196:ALA:HB1	1:A:1197:PRO:HD2	2.00	0.44
1:A:1252:GLU:C	1:A:1253:TYR:HD2	2.24	0.44
1:A:999:ILE:O	1:A:1001:ARG:HG3	2.17	0.44
1:A:1132:LYS:CD	1:A:1132:LYS:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:LYS:O	1:A:1164:GLU:HB2	2.17	0.44
1:A:1219:TYR:O	1:A:1281:GLN:HG2	2.18	0.44
1:A:1150:LYS:O	1:A:1151:SER:CB	2.61	0.44
1:A:884:LYS:HB3	1:A:884:LYS:HE2	1.76	0.43
1:A:1191:GLU:HG3	1:A:1192:LYS:N	2.33	0.43
1:A:1191:GLU:O	1:A:1258:CYS:HB2	2.19	0.43
2:B:44:GLU:O	2:B:45:ASP:C	2.62	0.43
1:A:1097:GLU:HG2	1:A:1172:PHE:HE2	1.84	0.43
1:A:1222:GLN:HE21	1:A:1279:ASN:ND2	2.17	0.43
1:A:1129:GLN:H	1:A:1129:GLN:CD	2.26	0.43
1:A:1132:LYS:N	1:A:1132:LYS:HD2	2.34	0.43
2:B:58:ILE:HG13	2:B:59:ASN:N	2.33	0.42
1:A:1250:PHE:HD2	1:A:1250:PHE:HA	1.72	0.42
1:A:973:TRP:CD2	1:A:1007:ILE:HG21	2.55	0.42
1:A:977:ASP:HB2	1:A:1033:GLU:O	2.19	0.42
1:A:1265:LYS:HG3	1:A:1265:LYS:HZ2	1.65	0.42
1:A:1160:ILE:O	1:A:1161:VAL:C	2.63	0.42
1:A:860:ILE:HG13	1:A:861:LEU:CD2	2.43	0.42
1:A:875:LEU:HD23	1:A:875:LEU:HA	1.93	0.42
2:B:44:GLU:CG	2:B:45:ASP:H	2.27	0.42
1:A:1015:LYS:HG2	1:A:1025:ASN:HD22	1.85	0.41
1:A:1182:THR:CG2	1:A:1205:TYR:HB2	2.50	0.41
1:A:1190:GLU:HG3	1:A:1241:HIS:CG	2.55	0.41
1:A:982:THR:CG2	1:A:983:LYS:N	2.83	0.41
1:A:1118:VAL:HG11	2:B:57:GLU:HG2	2.03	0.41
1:A:1254:LYS:HB2	1:A:1254:LYS:HZ2	1.84	0.41
1:A:1124:ARG:HG2	1:A:1141:ILE:HD11	2.02	0.41
1:A:942:ILE:HG22	1:A:946:ILE:HD13	2.03	0.40
1:A:860:ILE:HA	1:A:1074:ARG:NH2	2.37	0.40
1:A:981:LYS:HE3	1:A:981:LYS:HB2	1.92	0.40
1:A:1176:GLN:NE2	1:A:1178:TRP:HE1	2.20	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	426/436 (98%)	403 (95%)	19 (4%)	4 (1%)	14	9
2	B	15/17 (88%)	14 (93%)	0	1 (7%)	1	0
All	All	441/453 (97%)	417 (95%)	19 (4%)	5 (1%)	11	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1129	GLN
1	A	1161	VAL
1	A	1249	VAL
2	B	45	ASP
1	A	1174	LEU

### 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	405/411 (98%)	397 (98%)	8 (2%)	48	54
2	B	16/16 (100%)	13 (81%)	3 (19%)	1	0
All	All	421/427 (99%)	410 (97%)	11 (3%)	40	43

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1013	ASN
1	A	1045	ASP
1	A	1132	LYS
1	A	1190	GLU
1	A	1203	GLU
1	A	1248	ILE
1	A	1250	PHE
1	A	1254	LYS

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Mol	Chain	Res	Type
2	B	46	MET
2	B	51	LYS
2	B	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	862	ASN
1	A	863	ASN
1	A	867	ASN
1	A	873	ASN
1	A	874	ASN
1	A	913	GLN
1	A	915	GLN
1	A	943	GLN
1	A	947	HIS
1	A	954	ASN
1	A	979	ASN
1	A	990	ASN
1	A	1000	ASN
1	A	1012	ASN
1	A	1013	ASN
1	A	1025	ASN
1	A	1037	ASN
1	A	1105	ASN
1	A	1129	GLN
1	A	1130	ASN
1	A	1135	ASN
1	A	1176	GLN
1	A	1216	GLN
1	A	1241	HIS
1	A	1279	ASN
2	B	59	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 oligosaccharides 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

### 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	430/436 (98%)	0.31	38 (8%) <b>15</b> <b>17</b>	23, 38, 79, 124	1 (0%)
2	B	17/17 (100%)	1.37	4 (23%) <b>2</b> <b>2</b>	31, 61, 93, 100	3 (17%)
All	All	447/453 (98%)	0.35	42 (9%) <b>14</b> <b>15</b>	23, 39, 92, 124	4 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1248	ILE	8.1
1	A	860	ILE	7.7
1	A	1244	TYR	7.1
1	A	1250	PHE	6.5
1	A	1249	VAL	6.4
1	A	1174	LEU	4.8
1	A	859	GLU	4.5
1	A	1253	TYR	4.3
1	A	1158	ASP	4.2
1	A	1227	LYS	4.0
1	A	861	LEU	3.8
1	A	858	SER	3.7
1	A	922	VAL	3.5
1	A	1151	SER	3.5
1	A	1228	ASP	3.5
1	A	1233	ASP	3.2
1	A	1293	PRO	3.0
1	A	1247	GLY	2.9
1	A	1229	GLU	2.9
1	A	1231	SER	2.9
2	B	46	MET	2.9
1	A	1160	ILE	2.9
2	B	44	GLU	2.8
1	A	926	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1246	SER	2.7
1	A	1133	TYR	2.6
2	B	45	ASP	2.6
1	A	921	SER	2.6
1	A	1187	LYS	2.5
2	B	55	PHE	2.5
1	A	920	ASN	2.4
1	A	971	ILE	2.4
1	A	1115	ASP	2.3
1	A	1232	THR	2.3
1	A	1131	SER	2.3
1	A	919	PHE	2.3
1	A	1189	GLU	2.3
1	A	918	ILE	2.2
1	A	1011	LEU	2.2
1	A	1159	ASP	2.1
1	A	1129	GLN	2.0
1	A	924	LEU	2.0

## 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 oligosaccharides 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.