



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 03:17 pm BST

PDB ID : 1YXW  
Title : A common binding site for disialyllactose and a tri-peptide in the C-fragment of tetanus neurotoxin  
Authors : Jayaraman, S.; Eswaramoorthy, S.; Kumaran, D.; Swaminathan, S.  
Deposited on : 2005-02-22  
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (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) : 2.11

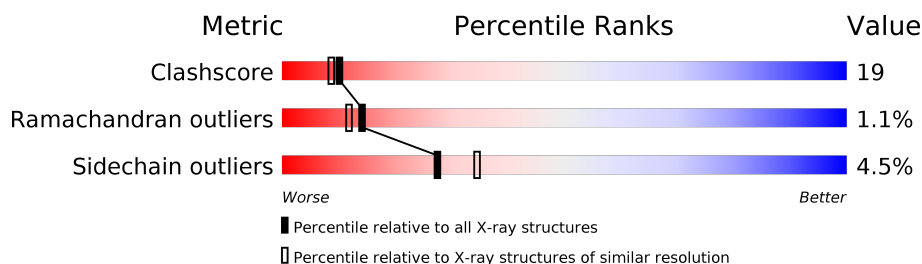
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 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	441	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TYR	A	5292	-	-	X	-
3	GLU	A	5293	-	-	X	-

## 2 Entry composition [i](#)

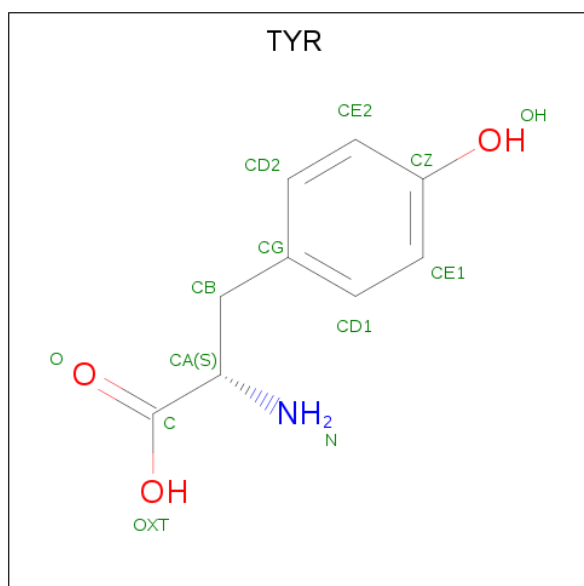
There are 5 unique types of molecules in this entry. The entry contains 3802 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tetanus toxin (Tentoxylisin).

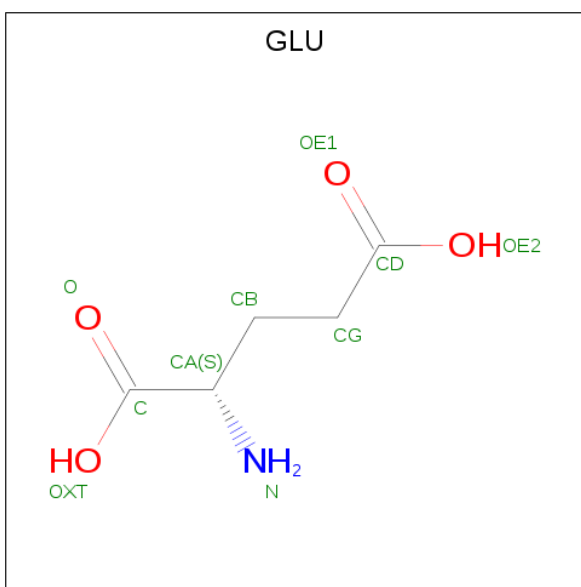
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3564	2282	597	676	9			

- Molecule 2 is TYROSINE (three-letter code: TYR) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub>).



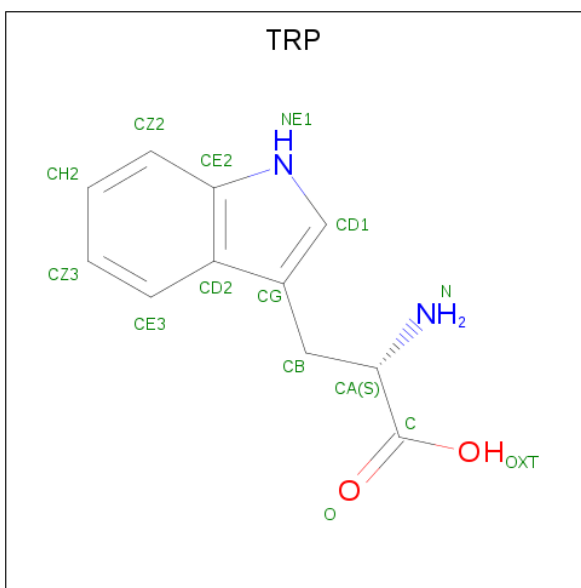
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 4 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is water.

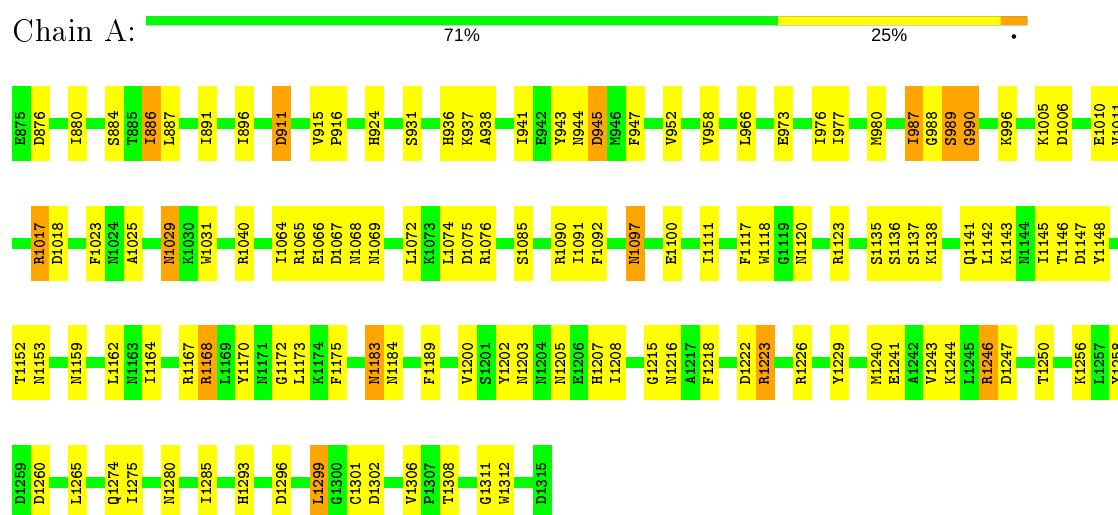
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	202	Total 202	O 202	0	0

### 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 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 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. 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: Tetanus toxin (Tentoxylisin)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.76 Å 79.18 Å 90.27 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.59 – 2.20	Depositor
% Data completeness (in resolution range)	91.7 (39.59-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

## 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	0.38	1/3645 (0.0%)	0.66	3/4945 (0.1%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1183	ASN	C-N	-7.80	1.16	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1183	ASN	O-C-N	-10.50	105.90	122.70
1	A	1183	ASN	C-N-CA	8.16	142.11	121.70
1	A	1183	ASN	CA-C-N	5.63	129.58	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1183	ASN	Mainchain,Peptide



## 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	3564	0	3515	127	0
2	A	12	0	8	6	0
3	A	9	0	6	14	0
4	A	15	0	10	4	0
5	A	202	0	0	3	0
All	All	3802	0	3539	135	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 (135) 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:1216:ASN:H	3:A:5293:GLU:HG3	1.20	1.02
1:A:980:MET:HA	1:A:989:SER:HB2	1.45	0.98
1:A:989:SER:HB3	1:A:1066:GLU:HA	1.50	0.93
1:A:1216:ASN:N	3:A:5293:GLU:HG3	1.84	0.92
1:A:1143:LYS:HZ3	4:A:5294:TRP:HH2	1.22	0.86
1:A:987:ILE:HD13	1:A:987:ILE:H	1.40	0.86
1:A:938:ALA:O	1:A:941:ILE:HG22	1.77	0.84
1:A:1274:GLN:NE2	1:A:1280:ASN:HD22	1.76	0.83
1:A:1274:GLN:HE22	1:A:1280:ASN:HD22	1.24	0.83
1:A:1216:ASN:H	3:A:5293:GLU:CG	1.95	0.80
1:A:988:GLY:HA3	1:A:1005:LYS:HD3	1.66	0.78
1:A:1215:GLY:HA2	3:A:5293:GLU:HG3	1.66	0.77
1:A:1223:ARG:HG2	1:A:1223:ARG:HH11	1.52	0.74
1:A:1203:ASN:HD22	1:A:1205:ASN:HD21	1.35	0.74
1:A:886:ILE:HD11	1:A:1091:ILE:HG22	1.70	0.72
1:A:1138:LYS:NZ	1:A:1153:ASN:HD21	1.87	0.72
1:A:1223:ARG:HD2	1:A:1223:ARG:H	1.54	0.72
1:A:1031:TRP:HE1	1:A:1120:ASN:HD21	1.37	0.72
2:A:5292:TYR:CD1	3:A:5293:GLU:N	2.58	0.72
1:A:1274:GLN:HE21	1:A:1280:ASN:HB2	1.55	0.71
1:A:1111:ILE:HD11	1:A:1244:LYS:HB3	1.70	0.70
1:A:1146:THR:O	1:A:1226:ARG:NH1	2.24	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:HIS:CE1	1:A:1068:ASN:HD22	2.10	0.70
1:A:1143:LYS:NZ	4:A:5294:TRP:HH2	1.89	0.70
1:A:1017:ARG:HH11	1:A:1017:ARG:HB3	1.58	0.69
1:A:1097:ASN:ND2	1:A:1100:GLU:H	1.90	0.68
1:A:1097:ASN:ND2	1:A:1100:GLU:HG3	2.10	0.66
1:A:1138:LYS:HZ3	1:A:1153:ASN:HD21	1.45	0.65
1:A:966:LEU:HD22	1:A:1162:LEU:HD22	1.79	0.65
1:A:1241:GLU:HG2	1:A:1243:VAL:HG13	1.79	0.64
1:A:1018:ASP:OD2	1:A:1025:ALA:HB1	1.99	0.62
1:A:1215:GLY:CA	3:A:5293:GLU:HG3	2.29	0.62
1:A:1260:ASP:HB2	5:A:203:HOH:O	1.99	0.62
1:A:1205:ASN:HB2	1:A:1207:HIS:CE1	2.36	0.60
1:A:1293:HIS:HB3	1:A:1296:ASP:OD2	2.01	0.60
1:A:987:ILE:H	1:A:987:ILE:CD1	2.10	0.60
1:A:1215:GLY:HA2	3:A:5293:GLU:CG	2.32	0.60
2:A:5292:TYR:O	3:A:5293:GLU:HB2	1.99	0.60
1:A:1274:GLN:HE21	1:A:1280:ASN:CB	2.16	0.59
1:A:987:ILE:HD13	1:A:987:ILE:N	2.14	0.59
1:A:1247:ASP:OD1	1:A:1250:THR:HG23	2.03	0.59
1:A:1168:ARG:HB3	1:A:1168:ARG:HH11	1.68	0.59
1:A:1031:TRP:HE1	1:A:1120:ASN:ND2	2.02	0.57
1:A:1023:PHE:CE2	1:A:1136:SER:HB2	2.40	0.57
1:A:1138:LYS:NZ	1:A:1153:ASN:ND2	2.52	0.56
2:A:5292:TYR:HD1	3:A:5293:GLU:N	2.01	0.56
1:A:1067:ASP:OD2	1:A:1069:ASN:HB2	2.06	0.56
1:A:1076:ARG:CZ	1:A:1076:ARG:HA	2.35	0.56
1:A:1097:ASN:HD21	1:A:1100:GLU:HG3	1.70	0.56
1:A:1285:ILE:C	1:A:1285:ILE:HD12	2.28	0.54
1:A:887:LEU:O	1:A:1090:ARG:HG2	2.07	0.54
1:A:988:GLY:CA	1:A:1005:LYS:HD3	2.35	0.54
1:A:1274:GLN:NE2	1:A:1280:ASN:HB2	2.21	0.54
1:A:936:HIS:HE1	1:A:1068:ASN:HD22	1.55	0.54
1:A:1017:ARG:CB	1:A:1017:ARG:HH11	2.21	0.54
1:A:1159:ASN:HB3	1:A:1164:ILE:HG23	1.90	0.54
1:A:1111:ILE:O	1:A:1111:ILE:HG12	2.08	0.53
1:A:988:GLY:HA3	1:A:1005:LYS:CD	2.38	0.53
1:A:1005:LYS:HA	1:A:1010:GLU:O	2.09	0.53
1:A:887:LEU:HD23	1:A:1091:ILE:HD12	1.90	0.52
1:A:1168:ARG:HB3	1:A:1168:ARG:NH1	2.25	0.52
1:A:1226:ARG:NH2	3:A:5293:GLU:OE2	2.42	0.52
1:A:944:ASN:HD22	1:A:1066:GLU:CD	2.13	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1223:ARG:NH1	1:A:1223:ARG:HG2	2.23	0.51
1:A:941:ILE:O	1:A:941:ILE:HG23	2.10	0.51
1:A:886:ILE:HD13	1:A:1091:ILE:O	2.09	0.51
1:A:1090:ARG:HD2	1:A:1092:PHE:CZ	2.45	0.51
1:A:1175:PHE:CE2	1:A:1200:VAL:HG12	2.46	0.51
3:A:5293:GLU:OE1	4:A:5294:TRP:HD1	1.93	0.51
1:A:973:GLU:HB2	1:A:996:LYS:HD2	1.92	0.51
1:A:976:ILE:HG22	1:A:1074:LEU:CD2	2.41	0.50
1:A:1312:TRP:CD1	1:A:1312:TRP:C	2.85	0.50
1:A:1226:ARG:CZ	3:A:5293:GLU:OE2	2.60	0.50
1:A:947:PHE:HA	1:A:1040:ARG:NH1	2.27	0.50
2:A:5292:TYR:C	2:A:5292:TYR:CD1	2.86	0.50
1:A:1170:TYR:CE1	1:A:1308:THR:HA	2.48	0.49
1:A:1168:ARG:HH11	1:A:1168:ARG:CB	2.26	0.49
2:A:5292:TYR:O	3:A:5293:GLU:CB	2.60	0.49
1:A:891:ILE:HD12	1:A:896:ILE:HG12	1.94	0.48
1:A:1223:ARG:N	1:A:1223:ARG:HD2	2.26	0.48
1:A:1123:ARG:HH11	1:A:1189:PHE:HE1	1.61	0.48
4:A:5294:TRP:CG	4:A:5294:TRP:O	2.66	0.48
1:A:976:ILE:HG22	1:A:1074:LEU:HD22	1.96	0.48
1:A:1218:PHE:HB2	1:A:1222:ASP:HB2	1.96	0.48
2:A:5292:TYR:C	2:A:5292:TYR:HD1	2.16	0.48
1:A:1246:ARG:NH2	1:A:1296:ASP:O	2.47	0.47
1:A:1005:LYS:HG3	1:A:1011:VAL:HG12	1.96	0.47
1:A:952:VAL:HG22	1:A:1091:ILE:HG12	1.97	0.47
1:A:1138:LYS:HZ2	1:A:1153:ASN:ND2	2.13	0.47
1:A:1223:ARG:CG	1:A:1223:ARG:HH11	2.25	0.47
1:A:1006:ASP:OD2	1:A:1010:GLU:HB2	2.16	0.46
1:A:1029:ASN:HB3	1:A:1118:TRP:CZ3	2.51	0.46
1:A:1226:ARG:NH1	1:A:1229:TYR:HD1	2.13	0.46
1:A:1141:GLN:NE2	1:A:1172:GLY:HA2	2.30	0.46
1:A:891:ILE:CD1	1:A:896:ILE:HG12	2.46	0.46
1:A:1097:ASN:HD21	1:A:1100:GLU:H	1.62	0.45
1:A:1142:LEU:HB2	1:A:1173:LEU:HD21	1.98	0.45
1:A:988:GLY:O	1:A:989:SER:O	2.34	0.45
1:A:944:ASN:ND2	1:A:1066:GLU:OE2	2.50	0.45
1:A:990:GLY:HA2	1:A:1064:ILE:HG23	1.98	0.45
1:A:1141:GLN:HA	1:A:1173:LEU:HD13	1.97	0.45
1:A:1256:LYS:HD3	1:A:1258:TYR:OH	2.17	0.44
1:A:1029:ASN:ND2	1:A:1311:GLY:HA3	2.31	0.44
1:A:1075:ASP:O	1:A:1076:ARG:HB2	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1136:SER:O	1:A:1167:ARG:HD2	2.16	0.44
1:A:1299:LEU:HD13	1:A:1301:CYS:SG	2.57	0.44
1:A:1246:ARG:HD2	1:A:1302:ASP:OD1	2.17	0.44
1:A:876:ASP:O	1:A:880:ILE:HG13	2.17	0.44
1:A:911:ASP:HB3	1:A:931:SER:HB2	2.00	0.44
1:A:937:LYS:HB3	1:A:941:ILE:HG23	1.99	0.44
1:A:1175:PHE:CD2	1:A:1200:VAL:HG12	2.54	0.43
1:A:936:HIS:HE1	1:A:1068:ASN:ND2	2.17	0.43
1:A:1148:TYR:CE2	1:A:1275:ILE:HD12	2.53	0.43
1:A:915:VAL:HB	1:A:916:PRO:CD	2.48	0.43
1:A:976:ILE:HG13	1:A:977:ILE:HG13	1.99	0.43
1:A:947:PHE:HA	1:A:1040:ARG:HG3	2.00	0.43
1:A:884:SER:O	1:A:1092:PHE:HA	2.19	0.43
1:A:1135:SER:C	1:A:1137:SER:H	2.23	0.43
1:A:1240:MET:HA	1:A:1256:LYS:O	2.19	0.43
1:A:886:ILE:H	1:A:886:ILE:HD13	1.84	0.42
1:A:1215:GLY:C	3:A:5293:GLU:HG3	2.38	0.42
1:A:1137:SER:HA	5:A:201:HOH:O	2.19	0.42
1:A:1117:PHE:HB2	1:A:1306:VAL:HG22	2.01	0.42
1:A:924:HIS:HD2	1:A:1085:SER:OG	2.03	0.42
1:A:943:TYR:CD1	1:A:943:TYR:N	2.83	0.42
1:A:1274:GLN:NE2	1:A:1280:ASN:ND2	2.56	0.42
1:A:958:VAL:HG23	1:A:958:VAL:O	2.20	0.42
1:A:1097:ASN:C	1:A:1097:ASN:HD22	2.24	0.41
1:A:1202:TYR:O	1:A:1203:ASN:HB3	2.20	0.41
1:A:1223:ARG:NH1	1:A:1265:LEU:HD22	2.35	0.41
1:A:1029:ASN:HD21	1:A:1311:GLY:HA3	1.85	0.41
1:A:1145:ILE:HG22	5:A:137:HOH:O	2.20	0.41
1:A:1152:THR:HG22	1:A:1153:ASN:N	2.35	0.41
1:A:886:ILE:O	1:A:941:ILE:HD12	2.21	0.41
1:A:1274:GLN:NE2	1:A:1280:ASN:CB	2.83	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	439/441 (100%)	403 (92%)	32 (7%)	4 (1%)	17	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	945	ASP
1	A	989	SER
1	A	1184	ASN
1	A	990	GLY

### 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/397 (100%)	382 (96%)	15 (4%)	33	42

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	886	ILE
1	A	911	ASP
1	A	945	ASP
1	A	987	ILE
1	A	1017	ARG
1	A	1029	ASN
1	A	1065	ARG
1	A	1072	LEU
1	A	1097	ASN
1	A	1147	ASP
1	A	1168	ARG
1	A	1208	ILE
1	A	1223	ARG
1	A	1246	ARG
1	A	1299	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	924	HIS
1	A	936	HIS
1	A	944	ASN
1	A	998	ASN
1	A	1013	GLN
1	A	1029	ASN
1	A	1097	ASN
1	A	1120	ASN
1	A	1141	GLN
1	A	1153	ASN
1	A	1203	ASN
1	A	1207	HIS
1	A	1274	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 ⓘ

3 ligands are modelled in this entry.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1183:ASN	C	1184:ASN	N	1.16

## 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.