



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:31 am BST

PDB ID : 3N7L  
Title : Crystal structure of botulinum neurotoxin serotype D/C VPI 5993 binding domain  
Authors : Fu, Z.; Karalewitz, A.; Kroken, A.; Baldwin, M.R.; Barbieri, J.T.; Kim, J.-J.P.  
Deposited on : 2010-05-27  
Resolution : 2.00 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

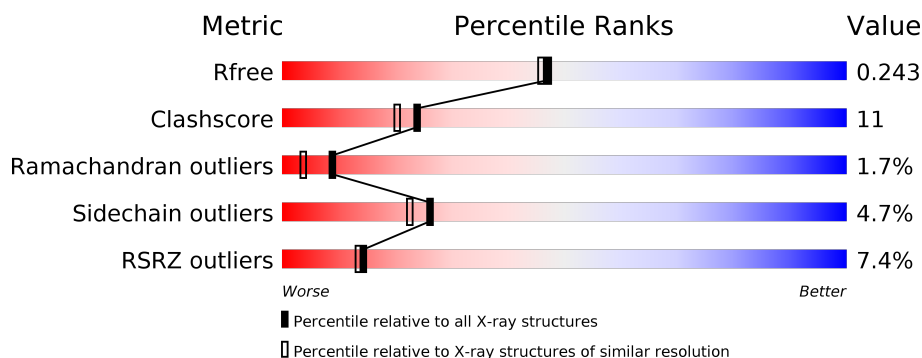
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\leq 5\%$ . 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	424	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3632 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 Neurotoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	418	3412	2190	564	644	14	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

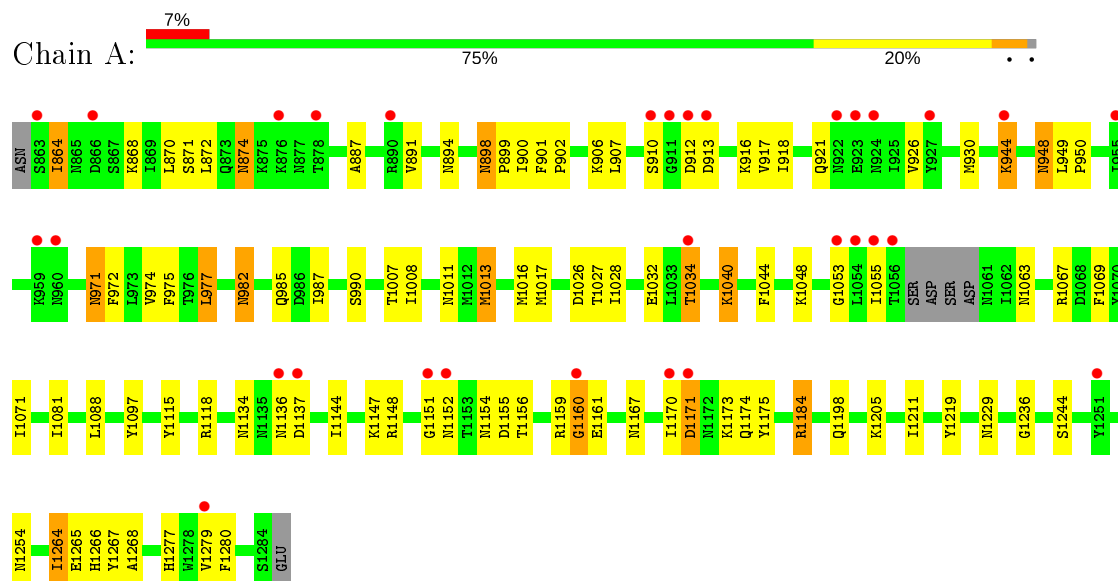
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total	O	0	0
			169	169		

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

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.29Å 57.81Å 184.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.91 – 2.00 28.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (28.91-2.00) 92.2 (28.90-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.216 , 0.257 0.205 , 0.243	Depositor DCC
$R_{free}$ test set	1960 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3632	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.36	0/3489	0.65	0/4722

There are no bond length outliers.

There are no bond angle outliers.

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	3412	0	3345	76	0
2	A	15	0	0	1	0
3	A	36	0	48	5	0
4	A	169	0	0	3	0
All	All	3632	0	3393	76	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 11.

All (76) 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:971:ASN:H	1:A:971:ASN:HD22	1.09	0.99
1:A:1097:TYR:CD1	1:A:1279:VAL:HG11	2.10	0.86
1:A:902:PRO:HB2	1:A:1067:ARG:HD2	1.63	0.79
1:A:1266:HIS:HB3	3:A:1405:GOL:H2	1.64	0.79
1:A:864:ILE:H	1:A:864:ILE:HD13	1.51	0.75
1:A:868:LYS:HD3	1:A:871:SER:HB2	1.71	0.72
1:A:898:ASN:HD22	1:A:899:PRO:HD2	1.53	0.71
1:A:916:LYS:HE2	1:A:918:ILE:HD11	1.72	0.70
1:A:1032:GLU:OE1	1:A:1034:THR:HG23	1.92	0.69
1:A:1067:ARG:NH1	1:A:1088:LEU:O	2.17	0.69
1:A:971:ASN:ND2	1:A:971:ASN:H	1.89	0.67
1:A:1174:GLN:OE1	3:A:1403:GOL:H11	1.96	0.66
1:A:950:PRO:HB2	1:A:1048:LYS:HE2	1.79	0.65
1:A:1148:ARG:HH12	1:A:1151:GLY:HA3	1.62	0.65
1:A:948:ASN:HD22	1:A:948:ASN:H	1.45	0.64
1:A:1264:ILE:HG22	1:A:1265:GLU:N	2.12	0.64
1:A:1007:THR:HG21	1:A:1081:ILE:HG12	1.80	0.63
1:A:1067:ARG:NH1	1:A:1088:LEU:HB3	2.14	0.62
1:A:898:ASN:HD22	1:A:899:PRO:CD	2.11	0.62
1:A:1160:GLY:O	1:A:1211:ILE:O	2.21	0.59
1:A:1254:ASN:HB2	3:A:1401:GOL:H2	1.85	0.59
1:A:1017:MET:HE2	4:A:1480:HOH:O	2.02	0.59
1:A:1219:TYR:OH	1:A:1277:HIS:HD2	1.86	0.59
1:A:1147:LYS:HE2	3:A:1404:GOL:H12	1.86	0.58
1:A:1268:ALA:HB3	3:A:1405:GOL:H12	1.86	0.58
1:A:926:VAL:HG13	1:A:930:MET:HG3	1.86	0.56
1:A:917:VAL:HB	1:A:1044:PHE:HB2	1.88	0.56
1:A:864:ILE:H	1:A:864:ILE:CD1	2.17	0.56
1:A:1053:GLY:O	1:A:1055:ILE:HG13	2.07	0.54
1:A:1144:ILE:C	1:A:1144:ILE:HD12	2.29	0.53
1:A:1173:LYS:NZ	1:A:1173:LYS:HB3	2.25	0.52
1:A:1155:ASP:O	1:A:1156:THR:HB	2.10	0.51
1:A:1170:ILE:HG22	1:A:1171:ASP:N	2.26	0.51
1:A:1236:GLY:HA2	1:A:1267:TYR:CE2	2.46	0.51
1:A:987:ILE:HG13	1:A:1026:ASP:OD2	2.10	0.51
1:A:971:ASN:N	1:A:971:ASN:HD22	1.88	0.50
1:A:1205:LYS:HG2	1:A:1229:ASN:ND2	2.26	0.50
1:A:1184:ARG:HD2	1:A:1244:SER:O	2.12	0.49
1:A:1159:ARG:HD3	2:A:1302:SO4:O3	2.11	0.49
1:A:949:LEU:HD12	1:A:950:PRO:HD2	1.95	0.48
1:A:972:PHE:CE2	1:A:990:SER:HB3	2.49	0.48
1:A:864:ILE:HD13	1:A:864:ILE:N	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:ASN:OD1	1:A:1013:MET:HG2	2.15	0.47
1:A:921:GLN:HG2	1:A:1040:LYS:O	2.14	0.46
1:A:1016:MET:HE3	1:A:1028:ILE:HD11	1.97	0.46
1:A:950:PRO:CB	1:A:1048:LYS:HE2	2.46	0.46
1:A:1279:VAL:CG1	1:A:1280:PHE:N	2.79	0.46
1:A:874:ASN:ND2	1:A:874:ASN:C	2.70	0.45
1:A:985:GLN:HG2	1:A:1016:MET:HE1	1.98	0.45
1:A:1279:VAL:HG12	1:A:1280:PHE:N	2.31	0.45
1:A:874:ASN:HD22	1:A:874:ASN:C	2.19	0.45
1:A:887:ALA:HB2	4:A:1519:HOH:O	2.16	0.45
1:A:982:ASN:O	1:A:982:ASN:ND2	2.50	0.44
1:A:975:PHE:CD2	1:A:1008:ILE:HD13	2.52	0.44
1:A:1148:ARG:HH12	1:A:1151:GLY:CA	2.30	0.44
1:A:972:PHE:CD2	1:A:990:SER:HB3	2.52	0.44
1:A:1136:ASN:O	1:A:1137:ASP:OD2	2.35	0.44
1:A:898:ASN:HD22	1:A:899:PRO:N	2.15	0.44
1:A:891:VAL:HG13	1:A:891:VAL:O	2.18	0.44
1:A:944:LYS:HD2	1:A:944:LYS:HA	1.82	0.44
1:A:921:GLN:HG3	1:A:926:VAL:CG2	2.48	0.43
1:A:1167:ASN:HD22	1:A:1167:ASN:HA	1.65	0.43
1:A:1173:LYS:HE3	1:A:1175:TYR:OH	2.17	0.43
1:A:902:PRO:CB	1:A:1067:ARG:HD2	2.42	0.42
1:A:1159:ARG:O	1:A:1160:GLY:O	2.38	0.42
1:A:1115:TYR:HB3	1:A:1118:ARG:HG3	2.01	0.42
1:A:1144:ILE:O	1:A:1144:ILE:HD12	2.19	0.42
1:A:1097:TYR:CD1	1:A:1279:VAL:CG1	2.93	0.41
1:A:870:LEU:HB3	1:A:1071:ILE:HB	2.03	0.41
1:A:906:LYS:HE2	1:A:1063:ASN:ND2	2.36	0.41
1:A:901:PHE:CG	1:A:902:PRO:HA	2.56	0.41
1:A:975:PHE:CE1	1:A:977:LEU:HD13	2.56	0.40
1:A:1198:GLN:NE2	4:A:1479:HOH:O	2.55	0.40
1:A:906:LYS:C	1:A:907:LEU:HD12	2.41	0.40
1:A:872:LEU:HB3	1:A:1069:PHE:HB3	2.04	0.40
1:A:898:ASN:ND2	1:A:900:ILE:H	2.19	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	414/424 (98%)	379 (92%)	28 (7%)	7 (2%)	9 4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	910	SER
1	A	912	ASP
1	A	1160	GLY
1	A	1161	GLU
1	A	1264	ILE
1	A	944	LYS
1	A	1152	ASN

### 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	382/388 (98%)	364 (95%)	18 (5%)	26 22

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	864	ILE
1	A	874	ASN
1	A	894	ASN
1	A	898	ASN

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Mol	Chain	Res	Type
1	A	913	ASP
1	A	948	ASN
1	A	971	ASN
1	A	974	VAL
1	A	977	LEU
1	A	982	ASN
1	A	1013	MET
1	A	1027	THR
1	A	1034	THR
1	A	1040	LYS
1	A	1134	ASN
1	A	1154	ASN
1	A	1171	ASP
1	A	1184	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	873	GLN
1	A	874	ASN
1	A	894	ASN
1	A	896	GLN
1	A	898	ASN
1	A	948	ASN
1	A	971	ASN
1	A	979	GLN
1	A	982	ASN
1	A	988	ASN
1	A	1061	ASN
1	A	1063	ASN
1	A	1117	ASN
1	A	1134	ASN
1	A	1135	ASN
1	A	1154	ASN
1	A	1162	ASN
1	A	1167	ASN
1	A	1198	GLN
1	A	1212	GLN
1	A	1215	ASN
1	A	1223	GLN
1	A	1229	ASN
1	A	1277	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 ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	1406	-	5,5,5	0.39	0	5,5,5	0.39	0
3	GOL	A	1402	-	5,5,5	0.39	0	5,5,5	0.41	0
2	SO4	A	1302	-	4,4,4	0.21	0	6,6,6	0.18	0
2	SO4	A	1301	-	4,4,4	0.19	0	6,6,6	0.11	0
3	GOL	A	1404	-	5,5,5	0.47	0	5,5,5	0.50	0
3	GOL	A	1403	-	5,5,5	0.32	0	5,5,5	0.42	0
3	GOL	A	1405	-	5,5,5	0.27	0	5,5,5	0.39	0
2	SO4	A	1303	-	4,4,4	0.25	0	6,6,6	0.15	0
3	GOL	A	1401	-	5,5,5	0.30	0	5,5,5	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1406	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1402	-	-	0/4/4/4	-
3	GOL	A	1404	-	-	0/4/4/4	-
3	GOL	A	1403	-	-	0/4/4/4	-
3	GOL	A	1405	-	-	0/4/4/4	-
3	GOL	A	1401	-	-	0/4/4/4	-

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.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1302	SO4	1	0
3	A	1404	GOL	1	0
3	A	1403	GOL	1	0
3	A	1405	GOL	2	0
3	A	1401	GOL	1	0

## 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	418/424 (98%)	0.34	31 (7%) 14 13	17, 29, 49, 73	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1055	ILE	7.3
1	A	1056	THR	6.7
1	A	1054	LEU	6.0
1	A	911	GLY	4.9
1	A	912	ASP	4.4
1	A	1251	TYR	4.0
1	A	876	LYS	4.0
1	A	1170	ILE	3.7
1	A	927	TYR	3.7
1	A	913	ASP	3.3
1	A	1152	ASN	3.1
1	A	910	SER	3.1
1	A	890	ARG	3.0
1	A	1160	GLY	3.0
1	A	1053	GLY	3.0
1	A	1171	ASP	3.0
1	A	1034	THR	2.9
1	A	1151	GLY	2.9
1	A	878	THR	2.8
1	A	1279	VAL	2.6
1	A	866	ASP	2.6
1	A	955	ILE	2.5
1	A	863	SER	2.4
1	A	923	GLU	2.4
1	A	922	ASN	2.4
1	A	960	ASN	2.3
1	A	924	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1136	ASN	2.3
1	A	944	LYS	2.2
1	A	959	LYS	2.1
1	A	1137	ASP	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	1405	6/6	0.69	0.24	50,52,53,54	0
3	GOL	A	1404	6/6	0.83	0.19	46,47,48,51	0
3	GOL	A	1406	6/6	0.83	0.30	48,53,54,56	0
3	GOL	A	1401	6/6	0.86	0.16	37,40,41,41	0
3	GOL	A	1403	6/6	0.88	0.22	43,47,48,49	0
3	GOL	A	1402	6/6	0.94	0.14	31,35,37,38	0
2	SO4	A	1302	5/5	0.95	0.14	65,66,67,67	0
2	SO4	A	1303	5/5	0.97	0.31	60,60,61,61	0
2	SO4	A	1301	5/5	0.98	0.10	34,34,37,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.