



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 11:14 pm GMT

PDB ID : 2VSA  
Title : Structure and mode of action of a mosquitocidal holotoxin  
Authors : Treiber, N.; Reinert, D.J.; Carpusca, I.; Aktories, K.; Schulz, G.E.  
Deposited on : 2008-04-22  
Resolution : 2.89 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 : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

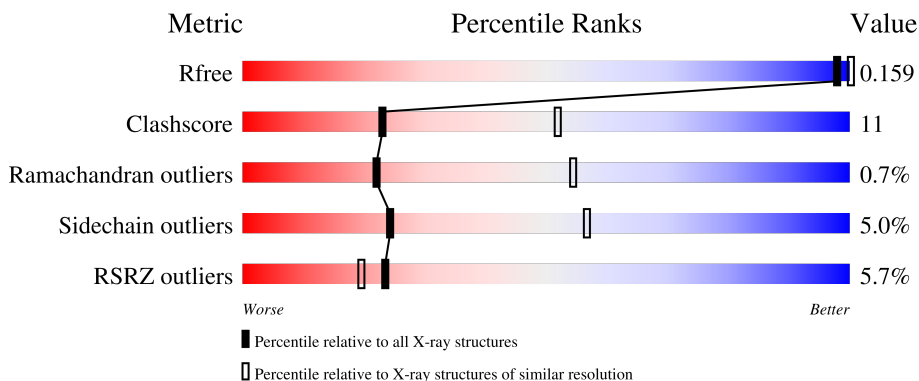
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

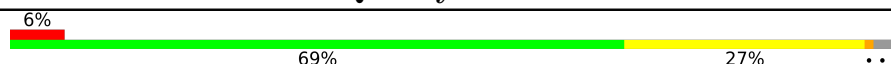
The reported resolution of this entry is 2.89 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	841	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6847 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 MOSQUITOCIDAL TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	822	6737	4255	1169	1305	8	0	0	0

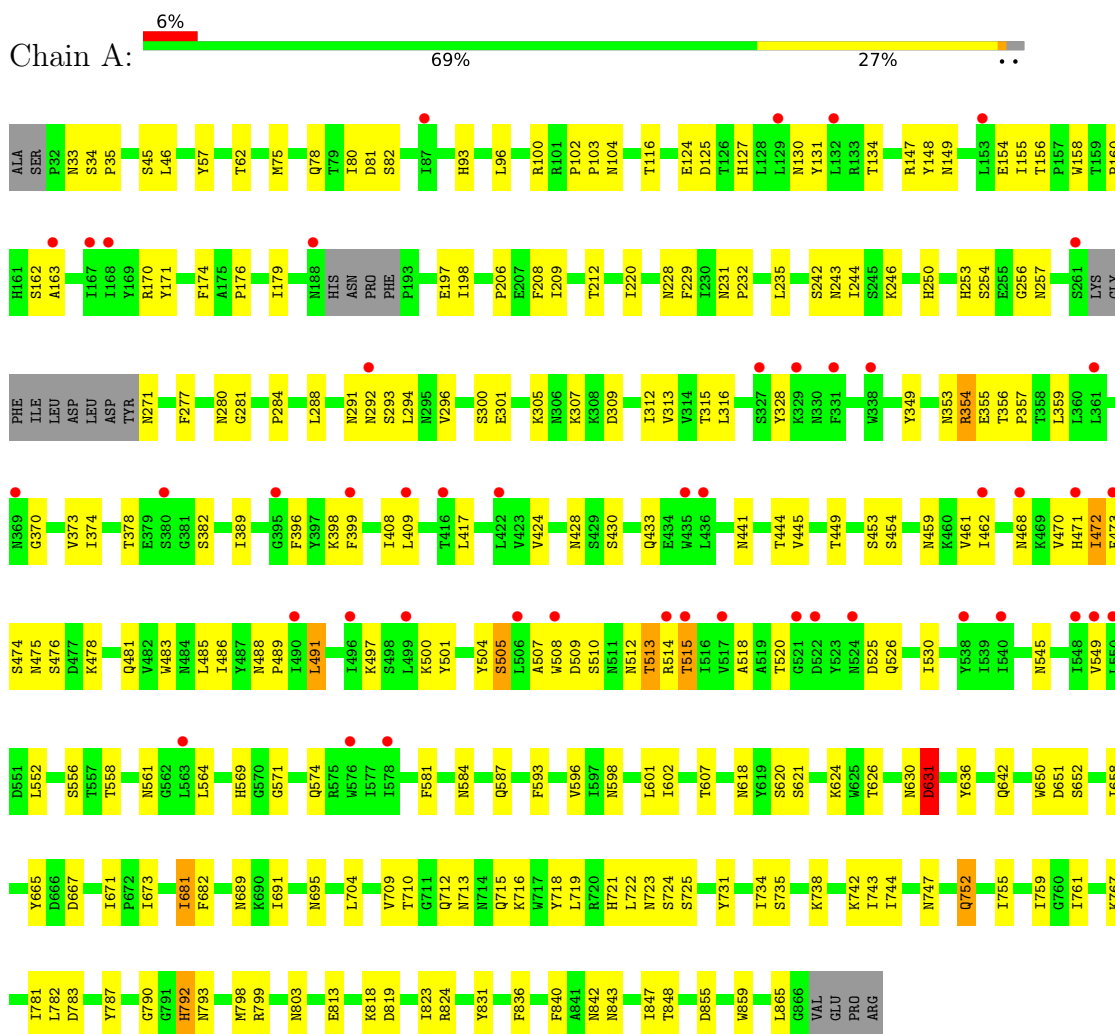
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		

### 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 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: MOSQUITOCIDAL TOXIN



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.97Å 129.97Å 68.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.89 64.99 – 2.89	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.89) 99.8 (64.99-2.89)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.187 , 0.239 0.153 , 0.159	Depositor DCC
$R_{free}$ test set	1453 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 70.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.078 for -h,-k,l 0.238 for h,-h-k,-l 0.088 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6847	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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	0.59	0/6907	0.69	0/9393

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	6737	0	6423	150	1
2	A	110	0	0	11	0
All	All	6847	0	6423	150	1

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 (150) 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:665:TYR:HD2	1:A:667:ASP:H	1.01	0.95
1:A:80:ILE:HD11	1:A:176:PRO:HB3	1.55	0.88
1:A:246:LYS:NZ	1:A:294:LEU:HD12	2.02	0.75
1:A:149:ASN:HB3	1:A:155:ILE:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HD21	1:A:116:THR:HG22	1.71	0.72
1:A:710:THR:HG22	1:A:715:GLN:NE2	2.05	0.72
1:A:242:SER:HB3	1:A:293:SER:HB3	1.71	0.72
1:A:759:ILE:HG13	1:A:761:ILE:HG23	1.74	0.69
1:A:507:ALA:HB2	1:A:526:GLN:HG2	1.73	0.69
1:A:783:ASP:O	1:A:799:ARG:HA	1.95	0.67
1:A:513:THR:OG1	1:A:515:THR:HG22	1.95	0.66
1:A:294:LEU:HB3	1:A:296:VAL:HG22	1.78	0.65
1:A:80:ILE:HD11	1:A:176:PRO:CB	2.27	0.65
1:A:747:ASN:ND2	1:A:752:GLN:HG3	2.12	0.64
1:A:444:THR:HG21	1:A:530:ILE:O	1.96	0.64
1:A:428:ASN:H	1:A:433:GLN:HE22	1.46	0.63
1:A:206:PRO:HA	1:A:209:ILE:HD12	1.80	0.62
1:A:747:ASN:HD21	1:A:752:GLN:HG3	1.63	0.62
1:A:624:LYS:HD3	1:A:722:LEU:CD1	2.29	0.62
1:A:710:THR:HG22	1:A:715:GLN:CD	2.20	0.62
1:A:587:GLN:HE21	1:A:721:HIS:HE1	1.47	0.62
1:A:398:LYS:NZ	1:A:433:GLN:HE21	1.98	0.61
1:A:428:ASN:H	1:A:433:GLN:NE2	1.98	0.61
1:A:35:PRO:HD3	1:A:57:TYR:CD1	2.34	0.61
1:A:171:TYR:CD1	1:A:212:THR:HB	2.36	0.60
1:A:472:ILE:HG13	1:A:552:LEU:HD13	1.83	0.60
1:A:508:TRP:HZ3	1:A:545:ASN:ND2	2.01	0.59
1:A:309:ASP:HB3	1:A:312:ILE:HG12	1.85	0.58
1:A:160:PRO:HG2	1:A:163:ALA:HB2	1.84	0.58
1:A:271:ASN:N	2:A:2034:HOH:O	2.35	0.58
1:A:104:ASN:HB2	1:A:257:ASN:HB3	1.86	0.57
1:A:497:LYS:HG2	1:A:505:SER:HB3	1.86	0.57
1:A:621:SER:HB2	1:A:642:GLN:HB2	1.85	0.57
1:A:399:PHE:HB2	1:A:409:LEU:HB3	1.87	0.57
1:A:710:THR:HG23	1:A:712:GLN:H	1.70	0.56
1:A:842:ASN:O	1:A:843:ASN:HB2	2.06	0.56
1:A:246:LYS:HZ1	1:A:294:LEU:HD12	1.70	0.55
1:A:831:TYR:HB3	1:A:848:THR:HB	1.89	0.54
1:A:459:ASN:ND2	2:A:2054:HOH:O	2.34	0.54
1:A:624:LYS:HD3	1:A:722:LEU:HD13	1.89	0.53
1:A:607:THR:HG22	2:A:2066:HOH:O	2.08	0.53
1:A:725:SER:HB3	2:A:2079:HOH:O	2.07	0.53
1:A:75:MET:SD	1:A:179:ILE:HG12	2.49	0.52
1:A:246:LYS:HZ2	1:A:294:LEU:HD12	1.74	0.52
1:A:671:ILE:HG22	1:A:673:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:TRP:CE2	1:A:652:SER:HA	2.45	0.51
1:A:658:ILE:HB	1:A:704:LEU:HB2	1.92	0.51
1:A:504:TYR:HB3	1:A:518:ALA:HB1	1.93	0.50
1:A:781:ILE:O	1:A:782:LEU:HB2	2.11	0.50
1:A:33:ASN:HB3	2:A:2001:HOH:O	2.11	0.50
1:A:475:ASN:HA	1:A:481:GLN:HE22	1.76	0.50
1:A:738:LYS:HB2	1:A:855:ASP:HB3	1.94	0.50
1:A:147:ARG:HD3	1:A:156:THR:O	2.11	0.50
1:A:174:PHE:O	1:A:208:PHE:HB3	2.12	0.50
1:A:453:SER:HB3	1:A:461:VAL:HG12	1.94	0.49
1:A:254:SER:HA	2:A:2031:HOH:O	2.11	0.49
1:A:787:TYR:CG	1:A:798:MET:HG3	2.47	0.49
1:A:292:ASN:HB3	2:A:2039:HOH:O	2.12	0.49
1:A:228:ASN:HA	1:A:441:ASN:ND2	2.28	0.49
1:A:445:VAL:HG21	1:A:485:LEU:HD23	1.94	0.49
1:A:818:LYS:O	1:A:819:ASP:HB3	2.12	0.49
1:A:156:THR:HG21	1:A:284:PRO:HG2	1.95	0.48
1:A:34:SER:HB2	1:A:35:PRO:HD2	1.95	0.48
1:A:449:THR:OG1	1:A:581:PHE:O	2.30	0.48
1:A:731:TYR:CZ	1:A:767:LYS:HD3	2.47	0.48
1:A:509:ASP:HA	2:A:2057:HOH:O	2.13	0.48
1:A:813:GLU:OE1	1:A:824:ARG:NH1	2.46	0.48
1:A:742:LYS:HE3	1:A:840:PHE:O	2.14	0.48
1:A:288:LEU:HB3	2:A:2036:HOH:O	2.13	0.48
1:A:428:ASN:C	1:A:430:SER:H	2.17	0.48
1:A:713:ASN:HA	1:A:716:LYS:HD3	1.96	0.48
1:A:96:LEU:HA	1:A:171:TYR:O	2.14	0.47
1:A:80:ILE:HG22	1:A:81:ASP:O	2.14	0.47
1:A:127:HIS:CE1	1:A:130:ASN:HB2	2.50	0.47
1:A:277:PHE:HB3	1:A:280:ASN:HD22	1.80	0.47
1:A:508:TRP:CE3	1:A:510:SER:HB3	2.49	0.47
1:A:593:PHE:HE1	1:A:682:PHE:CZ	2.31	0.47
1:A:621:SER:HB2	1:A:642:GLN:OE1	2.15	0.47
1:A:759:ILE:HD11	1:A:761:ILE:HD13	1.97	0.47
1:A:103:PRO:HD2	1:A:256:GLY:O	2.15	0.47
1:A:34:SER:HB2	1:A:35:PRO:CD	2.45	0.47
1:A:681:ILE:HG23	1:A:691:ILE:HG21	1.96	0.46
1:A:508:TRP:HZ3	1:A:545:ASN:HD22	1.62	0.46
1:A:78:GLN:HB2	1:A:93:HIS:NE2	2.31	0.46
1:A:682:PHE:HZ	1:A:719:LEU:HD21	1.80	0.46
1:A:787:TYR:CD2	1:A:798:MET:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:CD1	1:A:154:GLU:HA	2.51	0.45
1:A:408:ILE:O	1:A:424:VAL:HA	2.15	0.45
1:A:305:LYS:HG2	1:A:313:VAL:HG12	1.98	0.45
1:A:130:ASN:O	1:A:134:THR:HB	2.16	0.45
1:A:149:ASN:HB3	1:A:155:ILE:CD1	2.43	0.45
1:A:710:THR:HG23	1:A:712:GLN:HG2	1.98	0.45
1:A:100:ARG:HH21	1:A:162:SER:HB2	1.82	0.45
1:A:229:PHE:HB3	1:A:235:LEU:HD21	1.98	0.45
1:A:357:PRO:HD2	2:A:2045:HOH:O	2.17	0.44
1:A:102:PRO:HB2	1:A:257:ASN:HA	1.99	0.44
1:A:682:PHE:CZ	1:A:719:LEU:HD21	2.52	0.44
1:A:650:TRP:O	1:A:652:SER:N	2.46	0.44
1:A:149:ASN:HD22	1:A:155:ILE:HD11	1.81	0.44
1:A:569:HIS:CE1	1:A:571:GLY:HA3	2.51	0.44
1:A:220:ILE:HB	1:A:244:ILE:HD13	2.00	0.44
1:A:671:ILE:HG22	1:A:673:ILE:HD11	1.99	0.44
1:A:197:GLU:O	1:A:198:ILE:HD13	2.17	0.44
1:A:158:TRP:CZ2	1:A:281:GLY:HA3	2.52	0.44
1:A:78:GLN:HB2	1:A:93:HIS:CE1	2.53	0.43
1:A:468:ASN:OD1	1:A:468:ASN:N	2.46	0.43
1:A:512:ASN:HB3	1:A:513:THR:H	1.68	0.43
1:A:444:THR:HG23	1:A:445:VAL:HG13	1.99	0.43
1:A:472:ILE:HA	1:A:472:ILE:HD13	1.75	0.43
1:A:721:HIS:NE2	1:A:723:ASN:HB3	2.34	0.43
1:A:790:GLY:O	1:A:793:ASN:HB2	2.19	0.43
1:A:315:THR:HG21	1:A:328:TYR:HB2	2.01	0.43
1:A:349:TYR:CD2	1:A:389:ILE:HD12	2.54	0.43
1:A:353:ASN:OD1	1:A:355:GLU:HB3	2.19	0.43
1:A:374:ILE:HG13	1:A:409:LEU:CD1	2.49	0.43
1:A:584:ASN:HA	1:A:636:TYR:OH	2.19	0.43
1:A:596:VAL:HG22	1:A:718:TYR:CE2	2.54	0.43
1:A:462:ILE:HG22	1:A:483:TRP:CZ2	2.54	0.42
1:A:587:GLN:HE21	1:A:721:HIS:CE1	2.34	0.42
1:A:598:ASN:HB3	1:A:601:LEU:HD12	2.00	0.42
1:A:823:ILE:HD12	1:A:859:TRP:CD1	2.55	0.42
1:A:836:PHE:HB2	1:A:847:ILE:HG23	2.01	0.42
1:A:277:PHE:HB3	1:A:280:ASN:ND2	2.34	0.42
1:A:398:LYS:HZ1	1:A:433:GLN:HE21	1.65	0.42
1:A:398:LYS:HZ2	1:A:433:GLN:HE21	1.67	0.42
1:A:734:ILE:HG21	1:A:744:ILE:HD12	2.02	0.42
1:A:556:SER:OG	1:A:558:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ASN:O	1:A:631:ASP:C	2.57	0.42
1:A:307:LYS:HG3	1:A:396:PHE:CE1	2.54	0.42
1:A:549:VAL:HG23	1:A:574:GLN:HG2	2.02	0.42
1:A:556:SER:HB3	1:A:561:ASN:ND2	2.35	0.41
1:A:271:ASN:N	2:A:2033:HOH:O	2.52	0.41
1:A:316:LEU:HD21	1:A:359:LEU:HD13	2.02	0.41
1:A:691:ILE:O	1:A:691:ILE:HD12	2.20	0.41
1:A:102:PRO:CB	1:A:257:ASN:HA	2.50	0.41
1:A:513:THR:O	1:A:514:ARG:HB2	2.20	0.41
1:A:124:GLU:O	1:A:125:ASP:C	2.59	0.41
1:A:488:ASN:HA	1:A:489:PRO:HD3	1.86	0.41
1:A:671:ILE:HG22	1:A:673:ILE:HD12	2.03	0.41
1:A:689:ASN:O	1:A:709:VAL:HG23	2.21	0.41
1:A:491:LEU:HD12	1:A:491:LEU:HA	1.95	0.41
1:A:665:TYR:HD2	1:A:667:ASP:N	1.87	0.41
1:A:602:ILE:O	1:A:602:ILE:HD12	2.21	0.41
1:A:621:SER:CB	1:A:642:GLN:HB2	2.49	0.41
1:A:735:SER:HB3	1:A:743:ILE:HG22	2.03	0.41
1:A:231:ASN:HA	1:A:232:PRO:HD2	1.92	0.40
1:A:250:HIS:CE1	1:A:253:HIS:HA	2.57	0.40
1:A:742:LYS:HB3	1:A:755:ILE:HG13	2.03	0.40
1:A:500:LYS:HG3	1:A:501:TYR:CE2	2.56	0.40
1:A:301:GLU:HG3	1:A:354:ARG:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:HIS:NE2	1:A:792:HIS:NE2[2_655]	2.19	0.01

## 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	816/841 (97%)	741 (91%)	69 (8%)	6 (1%)	22 54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	695	ASN
1	A	724	SER
1	A	513	THR
1	A	631	ASP
1	A	651	ASP
1	A	370	GLY

### 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	755/772 (98%)	717 (95%)	38 (5%)	24 57

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	62	THR
1	A	82	SER
1	A	131	TYR
1	A	170	ARG
1	A	243	ASN
1	A	291	ASN
1	A	300	SER
1	A	354	ARG
1	A	356	THR
1	A	373	VAL
1	A	378	THR
1	A	382	SER
1	A	417	LEU
1	A	454	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	470	VAL
1	A	471	HIS
1	A	472	ILE
1	A	473	PHE
1	A	474	SER
1	A	476	SER
1	A	478	LYS
1	A	486	ILE
1	A	491	LEU
1	A	505	SER
1	A	515	THR
1	A	520	THR
1	A	525	ASP
1	A	564	LEU
1	A	618	ASN
1	A	620	SER
1	A	626	THR
1	A	631	ASP
1	A	681	ILE
1	A	752	GLN
1	A	792	HIS
1	A	803	ASN
1	A	865	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	42	GLN
1	A	58	GLN
1	A	86	GLN
1	A	88	GLN
1	A	91	ASN
1	A	161	HIS
1	A	291	ASN
1	A	292	ASN
1	A	298	GLN
1	A	415	ASN
1	A	433	GLN
1	A	536	ASN
1	A	545	ASN
1	A	587	GLN
1	A	792	HIS

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Mol	Chain	Res	Type
1	A	803	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](#)

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	822/841 (97%)	0.68	47 (5%) <b>23</b> <b>19</b>	47, 59, 66, 84	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	ASN	7.7
1	A	515	THR	5.2
1	A	399	PHE	4.3
1	A	550	LEU	4.1
1	A	163	ALA	4.1
1	A	380	SER	3.8
1	A	468	ASN	3.7
1	A	409	LEU	3.6
1	A	576	TRP	3.6
1	A	436	LEU	3.5
1	A	329	LYS	3.2
1	A	369	ASN	3.1
1	A	563	LEU	2.9
1	A	508	TRP	2.9
1	A	416	THR	2.9
1	A	422	LEU	2.9
1	A	578	ILE	2.8
1	A	521	GLY	2.7
1	A	473	PHE	2.7
1	A	540	ILE	2.7
1	A	87	ILE	2.6
1	A	292	ASN	2.5
1	A	471	HIS	2.5
1	A	522	ASP	2.4
1	A	524	ASN	2.4
1	A	167	ILE	2.4
1	A	435	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	490	ILE	2.3
1	A	395	GLY	2.3
1	A	548	ILE	2.3
1	A	499	LEU	2.2
1	A	514	ARG	2.2
1	A	462	ILE	2.2
1	A	538	TYR	2.2
1	A	496	ILE	2.2
1	A	153	LEU	2.2
1	A	132	LEU	2.1
1	A	168	ILE	2.1
1	A	327	SER	2.1
1	A	549	VAL	2.1
1	A	129	LEU	2.1
1	A	506	LEU	2.1
1	A	517	VAL	2.1
1	A	361	LEU	2.0
1	A	338	TRP	2.0
1	A	261	SER	2.0
1	A	331	PHE	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 monosaccharides 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.