

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2VSE
Title	:	Structure and mode of action of a mosquitocidal holotoxin
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Deposited on	:	2008-04-22
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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (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 (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	А	841	8%	15%	••		
1	В	841	80%	17%	••		

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	MPD	В	1867	Х	-	-	-
2	MPD	В	1868	Х	_	-	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14186 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	
1	А	823	Total 6743	C 4258	N 1170	O 1307	S 8	0	0	0
1	В	822	Total 6737	$\begin{array}{c} \mathrm{C} \\ 4255 \end{array}$	N 1169	O 1305	S 8	0	0	0

• Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	В	1	Total 6	${ m C} { m 3}$	O 3	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	367	Total O 367 367	0	0
4	В	309	Total O 309 309	0	0



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: MOSQUITOCIDAL TOXIN

T444 V445 G448 <mark>S365</mark> N366 <mark>S367</mark> S368 N369 T557 F568 K500 Y501 P502 N503 Y504 S505 F581 S582 F583 N584 T513 R514 T515 I516 Y523 N524 E479 **A507** D701 1702 L7 19 R7 20 H7 21 N7 23 S7 24 V7 95 A7 96 T710 G711 Q712 N713 N713 Q715 Q715 K716 N7 84 F7 85 1747 3748 F840 A841 N842 N843 N843 1847 T848 Y849 N850 L853 C866 VAL GLU PRO ARG F836 0837 <mark>7831</mark>



4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	130.96Å 130.96Å 396.06Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	74.54 - 2.50	Depositor
Resolution (A)	$74.59 \ - \ 2.50$	EDS
% Data completeness	$100.0 \ (74.54-2.50)$	Depositor
(in resolution range)	99.9(74.59-2.50)	EDS
R _{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	$2.74 (at 2.51 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.192 , 0.234	Depositor
Π, Π_{free}	0.188 , 0.228	DCC
R_{free} test set	4379 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	43.5	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.30 , 64.0	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.033 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14186	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: MPD, GOL

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).

Mal	Chain	Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.50	0/6913	0.60	0/9402	
1	В	0.49	1/6907~(0.0%)	0.59	0/9394	
All	All	0.49	1/13820~(0.0%)	0.60	0/18796	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	В	365	SER	CB-OG	5.89	1.50	1.42

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	А	6743	0	6427	99	0
1	В	6737	0	6422	97	0
2	А	8	0	14	0	0
2	В	16	0	28	4	0
3	В	6	0	8	2	0
4	А	367	0	0	4	0
4	В	309	0	0	7	0
All	All	14186	0	12899	199	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 8.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:746:MET:HE2	1:A:784:ASN:HB3	1.53	0.90
1:B:710:THR:HG23	1:B:712:GLN:HG2	1.53	0.87
1:A:746:MET:CE	1:A:784:ASN:HB3	2.06	0.85
1:B:80:ILE:HD11	1:B:176:PRO:HB3	1.57	0.85
1:A:62:THR:CG2	1:A:819:ASP:OD1	2.25	0.83
1:A:149:ASN:HD21	1:A:153:LEU:HB2	1.43	0.81
1:A:301:GLU:OE2	1:A:354:ARG:HD3	1.83	0.78
2:B:1867:MPD:HM1	2:B:1867:MPD:H52	1.66	0.78
1:B:80:ILE:HG22	1:B:81:ASP:O	1.85	0.77
1:A:315:THR:HB	1:A:336:GLN:HG2	1.68	0.76
1:A:691:ILE:HD11	1:A:715:GLN:CD	2.06	0.76
1:A:294:LEU:HB3	1:A:296:VAL:HG22	1.69	0.75
1:A:428:ASN:HB3	1:A:430:SER:H	1.52	0.74
1:B:815:ASN:HD22	1:B:818:LYS:H	1.35	0.72
1:A:746:MET:CE	1:A:784:ASN:CB	2.67	0.72
1:B:746:MET:HE1	1:B:784:ASN:HB2	1.72	0.71
1:B:215:TYR:CE1	1:B:220:ILE:HG12	2.25	0.71
1:A:746:MET:HE1	1:A:784:ASN:CB	2.20	0.71
1:A:80:ILE:HG22	1:A:81:ASP:O	1.89	0.71
1:A:665:TYR:HD1	1:A:666:ASP:H	1.38	0.70
1:B:746:MET:HE2	1:B:784:ASN:HB3	1.73	0.70
1:A:80:ILE:HD11	1:A:176:PRO:HB3	1.74	0.69
1:A:746:MET:HE1	1:A:784:ASN:HB2	1.75	0.69
1:B:149:ASN:HD21	1:B:153:LEU:HB2	1.58	0.68
1:A:62:THR:HG23	1:A:819:ASP:OD1	1.92	0.68
1:A:293:SER:O	1:A:294:LEU:HD23	1.94	0.67
1:B:815:ASN:ND2	1:B:818:LYS:H	1.93	0.67
1:A:712:GLN:HE21	1:A:712:GLN:HA	1.60	0.66
1:A:62:THR:HG21	1:A:819:ASP:OD1	1.97	0.65
1:A:556:SER:OG	1:A:558:THR:HG22	1.95	0.65
1:B:584:ASN:H	1:B:584:ASN:HD22	1.46	0.63
1:B:368:SER:O	1:B:369:ASN:HB2	2.00	0.62
1:A:104:ASN:HB2	1:A:257:ASN:HB3	1.82	0.62
1:B:241:PRO:HB2	1:B:244:ILE:HD12	1.83	0.61
1:B:580:PRO:HB2	3:B:1869:GOL:H31	1.82	0.61
1:B:746:MET:CE	1:B:784:ASN:HB3	2.31	0.61
1:B:582:SER:HB2	3:B:1869:GOL:H2	1.82	0.60



	At and 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:127:HIS:CD2	1:A:130:ASN:HB2	2.37	0.60
1:B:746:MET:HE2	1:B:797:THR:HB	1.82	0.60
1:B:294:LEU:HB3	1:B:296:VAL:HG22	1.82	0.60
1:B:746:MET:HE1	1:B:784:ASN:CB	2.32	0.59
1:A:313:VAL:O	1:A:315:THR:HG22	2.03	0.59
1:A:650:TRP:CE2	1:A:652:SER:HA	2.38	0.59
1:A:691:ILE:HD11	1:A:715:GLN:NE2	2.17	0.59
1:A:710:THR:HG22	1:A:715:GLN:OE1	2.01	0.59
1:B:160:PRO:HG2	1:B:163:ALA:HB2	1.84	0.58
1:B:831:TYR:HB3	1:B:848:THR:HB	1.84	0.58
1:B:312:ILE:HD12	1:B:327:SER:HB2	1.86	0.58
1:B:127:HIS:CD2	1:B:130:ASN:HB2	2.37	0.58
1:B:746:MET:CE	1:B:784:ASN:CB	2.82	0.58
1:B:428:ASN:HB3	1:B:430:SER:H	1.69	0.57
1:B:80:ILE:HD11	1:B:176:PRO:CB	2.30	0.57
1:B:682:PHE:HZ	1:B:719:LEU:HD21	1.70	0.57
1:B:759:ILE:HG21	2:B:1867:MPD:H13	1.87	0.56
1:A:746:MET:CE	1:A:797:THR:HB	2.35	0.56
1:A:818:LYS:HG3	1:A:853:LEU:HB3	1.88	0.55
1:B:444:THR:HG23	1:B:445:VAL:HG13	1.89	0.55
2:B:1867:MPD:H52	2:B:1867:MPD:CM	2.35	0.55
1:A:710:THR:HG23	1:A:712:GLN:HG2	1.88	0.55
1:A:138:SER:HG	1:A:140:PHE:HD2	1.54	0.54
1:A:831:TYR:HB3	1:A:848:THR:HB	1.90	0.54
1:B:721:HIS:CD2	1:B:724:SER:HB3	2.43	0.54
1:B:315:THR:HG21	1:B:328:TYR:CB	2.38	0.54
1:A:444:THR:HG23	1:A:445:VAL:HG13	1.90	0.53
1:B:713:ASN:HA	1:B:716:LYS:HD3	1.90	0.53
1:A:691:ILE:HD13	1:A:709:VAL:HG12	1.91	0.53
1:B:363:TRP:O	1:B:384:ASN:HB2	2.09	0.53
1:B:305:LYS:HG2	1:B:313:VAL:HG12	1.90	0.52
1:B:479:GLU:OE2	1:B:634:ARG:HD2	2.10	0.52
1:A:513:THR:OG1	1:A:515:THR:HB	2.10	0.52
1:A:460:LYS:HE2	1:A:557:THR:O	2.11	0.51
1:A:309:ASP:O	1:A:312:ILE:HG12	2.11	0.51
1:A:608:ASN:O	1:A:611:THR:HG23	2.10	0.51
1:B:307:LYS:HG3	1:B:396:PHE:CE1	2.45	0.51
1:A:315:THR:HG21	1:A:328:TYR:CB	2.41	0.50
1:B:746:MET:HE3	1:B:797:THR:HG21	1.93	0.50
1:A:157:PRO:HG2	1:A:170:ARG:HH21	1.76	0.50
1:B:74:HIS:HD2	4:B:2021:HOH:O	1.93	0.50



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:631:ASP:N	4:B:2169:HOH:O	2.43	0.49	
1:A:34:SER:HB2	1:A:35:PRO:CD	2.43	0.49	
1:A:160:PRO:HG2	1:A:163:ALA:HB2	1.94	0.49	
1:A:657:LYS:HD3	1:A:659:PHE:HB3	1.94	0.49	
1:B:315:THR:HG21	1:B:328:TYR:HB3	1.94	0.49	
1:B:383:ASN:O	1:B:386:TYR:N	2.41	0.49	
1:A:710:THR:HG23	1:A:712:GLN:H	1.77	0.49	
1:A:602:ILE:HD13	1:A:623:GLN:HB3	1.93	0.49	
1:B:710:THR:CG2	1:B:712:GLN:HG2	2.34	0.49	
1:A:460:LYS:HG3	1:A:557:THR:HB	1.95	0.49	
1:B:212:THR:HG22	1:B:224:TRP:HB2	1.94	0.49	
1:B:710:THR:HG21	4:B:2202:HOH:O	2.11	0.49	
1:A:212:THR:HG22	1:A:224:TRP:HB2	1.94	0.49	
1:A:606:THR:HG22	1:A:615:LYS:HD2	1.94	0.49	
1:B:171:TYR:CD1	1:B:212:THR:HB	2.48	0.49	
1:A:655:SER:OG	1:A:656:ASP:N	2.44	0.49	
1:B:397:TYR:CD2	1:B:437:ILE:HG12	2.48	0.49	
1:B:455:LYS:HD3	1:B:537:THR:HG21	1.95	0.49	
1:B:81:ASP:OD1	1:B:82:SER:N	2.46	0.48	
1:B:649:ALA:HB2	1:B:668:GLN:HG2	1.95	0.48	
1:B:505:SER:HB2	4:B:2119:HOH:O	2.11	0.48	
1:B:460:LYS:HE2	1:B:557:THR:O	2.14	0.48	
1:A:710:THR:HG22	1:A:715:GLN:CD	2.34	0.48	
1:B:368:SER:O	1:B:369:ASN:CB	2.61	0.48	
1:A:746:MET:HE3	1:A:797:THR:HG21	1.96	0.48	
1:A:155:ILE:HG22	1:A:156:THR:N	2.28	0.48	
1:A:407:LYS:HB3	1:A:424:VAL:CG2	2.44	0.47	
1:B:314:VAL:HG22	1:B:422:LEU:HD21	1.96	0.47	
1:A:476:SER:OG	1:A:478:LYS:HD3	2.15	0.47	
1:A:658:ILE:HB	1:A:704:LEU:HB2	1.96	0.47	
1:A:80:ILE:CG2	1:A:81:ASP:O	2.61	0.47	
1:A:294:LEU:CD1	1:A:298:GLN:HE22	2.28	0.47	
1:A:799:ARG:O	1:A:800:ASN:HB2	2.15	0.47	
1:A:691:ILE:HD12	1:A:715:GLN:HB3	1.97	0.47	
1:A:465:ILE:CG2	1:A:469:LYS:HE2	2.45	0.47	
1:B:301:GLU:OE2	1:B:354:ARG:HD3	2.14	0.47	
1:A:294:LEU:HD13	1:A:298:GLN:HE22	1.81	0.46	
1:B:220:ILE:HD12	1:B:241:PRO:HG2	1.97	0.46	
1:A:354:ARG:NE	4:A:2126:HOH:O	2.48	0.46	
1:B:399:PHE:HB2	1:B:409:LEU:HB3	1.98	0.46	
1:B:383:ASN:O	1:B:385:GLN:N	2.48	0.46	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:682:PHE:HZ	1:A:719:LEU:HD21	1.81	0.46
1:B:315:THR:HB	1:B:336:GLN:HG2	1.98	0.46
1:A:315:THR:HG21	1:A:328:TYR:HB3	1.98	0.45
1:B:295:ASN:HA	4:B:2065:HOH:O	2.16	0.45
1:A:362:SER:OG	1:A:385:GLN:HG2	2.16	0.45
1:A:785:PHE:O	1:A:797:THR:HA	2.16	0.45
1:A:305:LYS:HG2	1:A:313:VAL:HG12	1.98	0.45
1:A:720:ARG:HD3	4:A:2264:HOH:O	2.17	0.45
1:B:632:LYS:H	1:B:632:LYS:HD2	1.82	0.45
1:A:34:SER:HB2	1:A:35:PRO:HD2	1.99	0.45
1:B:818:LYS:HG3	1:B:853:LEU:HB3	1.99	0.45
1:A:368:SER:O	1:A:369:ASN:HB2	2.17	0.45
1:B:632:LYS:HD2	1:B:632:LYS:N	2.32	0.45
2:B:1867:MPD:HM1	2:B:1867:MPD:C5	2.37	0.45
1:A:157:PRO:CG	1:A:170:ARG:HH21	2.31	0.44
1:A:746:MET:HE2	1:A:797:THR:HB	2.00	0.44
1:B:235:LEU:HD12	1:B:439:LYS:HB3	1.99	0.44
1:B:710:THR:HG23	1:B:712:GLN:H	1.83	0.44
1:A:746:MET:HE2	1:A:784:ASN:CB	2.33	0.44
1:A:746:MET:HE3	1:A:797:THR:HB	1.97	0.44
1:B:57:TYR:HE1	1:B:73:LEU:HD12	1.82	0.44
1:B:97:ARG:HD3	1:B:111:PHE:CZ	2.53	0.44
1:B:516:ILE:HG13	1:B:550:LEU:HD12	2.00	0.44
1:A:592:GLN:HG3	1:A:722:LEU:HD11	1.99	0.44
1:A:746:MET:HE1	1:A:784:ASN:HB3	1.88	0.44
1:A:149:ASN:ND2	1:A:153:LEU:HB2	2.21	0.43
1:A:508:TRP:CH2	1:A:548:ILE:HG13	2.54	0.43
1:A:102:PRO:HB2	1:A:257:ASN:HA	2.01	0.43
1:A:746:MET:HE3	1:A:797:THR:CG2	2.48	0.43
1:B:104:ASN:HB2	1:B:257:ASN:HB3	2.00	0.43
1:A:444:THR:HG21	1:A:530:ILE:HG22	2.00	0.43
1:B:593:PHE:HE1	1:B:682:PHE:CZ	2.37	0.43
1:B:508:TRP:CE3	1:B:510:SER:HB3	2.54	0.43
1:B:738:LYS:HG2	1:B:840:PHE:CE2	2.54	0.42
1:A:81:ASP:OD1	1:A:82:SER:N	2.51	0.42
1:A:788:PHE:HB2	1:A:825:ASN:ND2	2.34	0.42
1:B:445:VAL:HG21	1:B:485:LEU:HD23	2.00	0.42
1:A:353:ASN:O	1:A:357:PRO:HA	2.19	0.42
1:A:836:PHE:CE1	1:A:837:GLN:HG3	2.54	0.42
1:B:33:ASN:HB3	4:B:2001:HOH:O	2.20	0.42
1:B:315:THR:HG21	1:B:328:TYR:HB2	2.00	0.42



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:388:THR:OG1	1:A:400:ARG:HG2	2.20	0.42	
1:A:455:LYS:HD3	1:A:537:THR:HG21	2.01	0.42	
1:A:698:PRO:HA	1:A:702:ILE:HD11	2.00	0.42	
1:A:746:MET:HE3	1:A:797:THR:CB	2.50	0.42	
1:B:142:SER:OG	1:B:197:GLU:OE2	2.31	0.42	
1:A:407:LYS:HB3	1:A:424:VAL:HG22	2.02	0.42	
1:B:294:LEU:CD1	1:B:298:GLN:HE22	2.32	0.42	
1:B:720:ARG:HD3	4:B:2209:HOH:O	2.20	0.42	
1:B:353:ASN:O	1:B:357:PRO:HA	2.20	0.42	
1:B:31:SER:HA	1:B:32:PRO:HD3	1.93	0.42	
1:B:97:ARG:HD3	1:B:111:PHE:CE1	2.55	0.42	
1:B:507:ALA:HB2	1:B:526:GLN:HG2	2.01	0.42	
1:B:746:MET:CE	1:B:797:THR:HB	2.49	0.42	
1:B:785:PHE:O	1:B:797:THR:HA	2.20	0.42	
1:B:836:PHE:CE1	1:B:837:GLN:HG3	2.55	0.42	
1:B:721:HIS:CE1	1:B:723:ASN:HB3	2.55	0.41	
1:B:842:ASN:O	1:B:843:ASN:HB2	2.20	0.41	
1:A:307:LYS:HG3	1:A:396:PHE:CE1	2.56	0.41	
1:A:363:TRP:O	1:A:384:ASN:HB2	2.20	0.41	
1:B:156:THR:HA	1:B:157:PRO:HD3	1.78	0.41	
1:B:444:THR:HG21	1:B:530:ILE:O	2.21	0.41	
1:B:698:PRO:HA	1:B:702:ILE:HD11	2.01	0.41	
1:B:721:HIS:CG	1:B:724:SER:HB3	2.55	0.41	
1:B:38:ASN:ND2	1:B:50:MET:O	2.54	0.41	
1:A:354:ARG:NH2	4:A:2126:HOH:O	2.52	0.41	
1:A:842:ASN:O	1:A:843:ASN:HB2	2.21	0.41	
1:B:155:ILE:CG2	1:B:156:THR:N	2.84	0.41	
1:B:155:ILE:HG22	1:B:156:THR:N	2.35	0.41	
1:B:231:ASN:HA	1:B:232:PRO:HD2	1.91	0.41	
1:B:346:LYS:HE2	1:B:386:TYR:CE2	2.55	0.41	
1:B:460:LYS:HG3	1:B:557:THR:HB	2.03	0.41	
1:A:460:LYS:HA	1:A:460:LYS:HD2	1.88	0.41	
1:B:294:LEU:HD13	1:B:298:GLN:HE22	1.86	0.41	
1:A:735:SER:CB	1:A:743:ILE:HG22	2.51	0.40	
1:A:128:LEU:O	1:A:131:TYR:HB3	2.21	0.40	
1:A:171:TYR:CD1	1:A:212:THR:HB	2.56	0.40	
1:A:246:LYS:NZ	1:A:294:LEU:HD12	2.36	0.40	
$1:A:354:ARG:C\overline{Z}$	4:A:2126:HOH:O	2.69	0.40	
1:B:691:ILE:HD11	1:B:715:GLN:CD	2.42	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	Perce	ntiles
1	А	817/841~(97%)	780~(96%)	37~(4%)	0	100	100
1	В	816/841~(97%)	779~(96%)	36~(4%)	1 (0%)	51	73
All	All	1633/1682~(97%)	1559 (96%)	73 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	384	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	А	756/772~(98%)	723~(96%)	33~(4%)	28 52
1	В	755/772~(98%)	723~(96%)	32~(4%)	30 54
All	All	1511/1544~(98%)	1446 (96%)	65~(4%)	29 53

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	33	ASN
1	А	51	ASP
1	А	73	LEU
1	А	80	ILE
1	А	186	SER



Mol	Chain	Res	Type
1	А	187	ARG
1	А	243	ASN
1	А	247	VAL
1	А	257	ASN
1	А	293	SER
1	А	295	ASN
1	А	315	THR
1	А	354	ARG
1	А	394	ASN
1	А	417	LEU
1	А	424	VAL
1	А	428	ASN
1	А	444	THR
1	А	465	ILE
1	А	471	HIS
1	А	473	PHE
1	А	478	LYS
1	А	486	ILE
1	А	491	LEU
1	А	558	THR
1	А	620	SER
1	А	632	LYS
1	А	652	SER
1	А	665	TYR
1	А	681	ILE
1	А	695	ASN
1	А	701	ASP
1	А	712	GLN
1	В	51	ASP
1	В	62	THR
1	В	73	LEU
1	В	127	HIS
1	В	134	THR
1	В	150	ASN
1	В	186	SER
1	В	187	ARG
1	В	242	SER
1	В	243	ASN
1	В	247	VAL
1	В	273	ASP
1	В	293	SER
1	В	315	THR



Mol	Chain	Res	Type
1	В	354	ARG
1	В	417	LEU
1	В	424	VAL
1	В	444	THR
1	В	473	PHE
1	В	478	LYS
1	В	514	ARG
1	В	545	ASN
1	В	582	SER
1	В	584	ASN
1	В	607	THR
1	В	611	THR
1	В	632	LYS
1	В	681	ILE
1	В	695	ASN
1	В	701	ASP
1	В	710	THR
1	В	748	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	42	GLN
1	А	86	GLN
1	А	88	GLN
1	А	91	ASN
1	А	127	HIS
1	А	130	ASN
1	А	135	ASN
1	А	149	ASN
1	А	165	ASN
1	А	298	GLN
1	А	339	ASN
1	А	418	ASN
1	А	428	ASN
1	А	512	ASN
1	А	697	GLN
1	А	712	GLN
1	А	817	ASN
1	В	42	GLN
1	В	71	ASN
1	В	83	ASN



Mol	Chain	Res	Type
1	В	88	GLN
1	В	91	ASN
1	В	127	HIS
1	В	149	ASN
1	В	165	ASN
1	В	280	ASN
1	В	298	GLN
1	В	339	ASN
1	В	415	ASN
1	В	428	ASN
1	В	545	ASN
1	В	584	ASN
1	В	697	GLN
1	В	712	GLN
1	В	721	HIS
1	В	749	ASN
1	В	752	GLN
1	В	815	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)

4 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



Mal Truna Chain		Chain		Dog	Dec	Dog	Dec	Dec	Dec	Dog	Dec	Dec	Dec	Tink	B	ond leng	gths	E	Bond ang	gles
	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2										
2	MPD	В	1867	-	7,7,7	0.34	0	9,10,10	1.26	1 (11%)										
3	GOL	В	1869	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	0.18	0										
2	MPD	В	1868	-	7,7,7	0.30	0	9,10,10	0.44	0										
2	MPD	А	1867	-	7,7,7	0.21	0	9,10,10	0.71	0										

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).

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
2	MPD	В	1867	-	1/1/2/2	1/5/5/5	-
3	GOL	В	1869	-	-	2/4/4/4	-
2	MPD	В	1868	-	1/1/2/2	3/5/5/5	-
2	MPD	А	1867	-	-	0/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1867	MPD	CM-C2-C1	-2.61	105.13	110.57

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	В	1867	MPD	C4
2	В	1868	MPD	C4

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	1869	GOL	O1-C1-C2-C3
3	В	1869	GOL	O1-C1-C2-O2
2	В	1868	MPD	O2-C2-C3-C4
2	В	1868	MPD	C1-C2-C3-C4
2	В	1868	MPD	CM-C2-C3-C4
2	В	1867	MPD	C2-C3-C4-O4



There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1867	MPD	4	0
3	В	1869	GOL	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	А	823/841~(97%)	0.97	71 (8%) 10	0	10	45, 49, 52, 56	0
1	В	822/841~(97%)	1.18	120 (14%)	2	2	45, 49, 52, 58	0
All	All	1645/1682~(97%)	1.07	191 (11%)	4	4	45, 49, 52, 58	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	284	PRO	6.4
1	В	408	ILE	6.2
1	В	396	PHE	6.1
1	В	411	LEU	6.0
1	В	395	GLY	6.0
1	А	31	SER	5.9
1	А	82	SER	5.7
1	В	31	SER	5.2
1	В	89	ILE	5.1
1	А	292	ASN	5.1
1	В	84	THR	5.0
1	В	393	VAL	5.0
1	В	240	GLY	4.9
1	В	424	VAL	4.7
1	А	151	LEU	4.7
1	А	74	HIS	4.5
1	В	83	ASN	4.5
1	В	82	SER	4.4
1	В	363	TRP	4.4
1	В	394	ASN	4.3
1	А	83	ASN	4.3
1	В	373	VAL	4.2
1	В	515	THR	4.2
1	В	366	ASN	4.1



2	V	S	E
2	V	S	E

Mol	Chain	Res	Type	RSRZ
1	А	393	VAL	4.1
1	В	397	TYR	4.0
1	В	98	TRP	4.0
1	В	307	LYS	4.0
1	В	414	GLY	3.9
1	В	328	TYR	3.9
1	А	98	TRP	3.7
1	А	67	PHE	3.6
1	В	524	ASN	3.6
1	В	158	TRP	3.6
1	А	86	GLN	3.6
1	В	501	TYR	3.5
1	В	67	PHE	3.4
1	А	84	THR	3.4
1	А	96	LEU	3.4
1	В	177	GLY	3.4
1	В	32	PRO	3.4
1	В	415	ASN	3.3
1	В	364	ASN	3.3
1	А	32	PRO	3.3
1	А	185	PHE	3.3
1	А	163	ALA	3.3
1	В	239	SER	3.2
1	В	312	ILE	3.2
1	В	374	ILE	3.2
1	А	289	LEU	3.2
1	В	399	PHE	3.1
1	В	306	ASN	3.1
1	А	284	PRO	3.1
1	А	665	TYR	3.1
1	В	146	ALA	3.0
1	А	81	ASP	3.0
1	В	320	TYR	3.0
1	А	369	ASN	3.0
1	А	646	LEU	3.0
1	В	157	PRO	3.0
1	В	435	TRP	3.0
1	В	465	ILE	2.9
1	В	81	ASP	2.9
1	А	78	GLN	2.9
1	В	291	ASN	2.9
1	В	436	LEU	2.9



2VSE

Mol	Chain	Res	Type	RSRZ
1	А	396	PHE	2.9
1	А	285	ASN	2.9
1	В	241	PRO	2.9
1	А	225	ILE	2.9
1	А	72	GLY	2.8
1	В	426	SER	2.8
1	А	168	ILE	2.8
1	В	150	ASN	2.8
1	В	292	ASN	2.8
1	В	34	SER	2.8
1	В	96	LEU	2.8
1	В	74	HIS	2.8
1	В	421	PRO	2.8
1	А	283	ILE	2.7
1	В	568	PHE	2.7
1	А	92	GLU	2.7
1	В	448	GLY	2.7
1	В	68	ALA	2.7
1	А	153	LEU	2.7
1	В	423	VAL	2.7
1	В	72	GLY	2.7
1	В	148	TYR	2.7
1	В	792	HIS	2.6
1	В	305	LYS	2.6
1	В	392	ASN	2.6
1	В	369	ASN	2.6
1	В	329	LYS	2.6
1	В	149	ASN	2.6
1	А	625	TRP	2.6
1	А	71	ASN	2.6
1	В	155	ILE	2.6
1	А	792	HIS	2.6
1	В	377	TYR	2.6
1	А	294	LEU	2.5
1	В	401	ASN	2.5
1	В	367	SER	2.5
1	В	294	LEU	2.5
1	В	422	LEU	2.5
1	В	71	ASN	2.5
1	В	185	PHE	2.5
1	В	223	ILE	2.5
1	В	78	GLN	2.5



2VS	SE
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Mol	Chain	Res	Type	RSRZ	
1	В	153	LEU	2.5	
1	А	241	PRO	2.5	
1	А	167	ILE	2.5	
1	В	75	MET	2.5	
1	В	513	THR	2.5	
1	В	313	VAL	2.5	
1	В	428	ASN	2.5	
1	В	365	SER	2.4	
1	А	91	ASN	2.4	
1	В	289	LEU	2.4	
1	В	309	ASP	2.4	
1	В	849	TYR	2.4	
1	В	283	ILE	2.4	
1	В	316	LEU	2.4	
1	А	196	ASP	2.4	
1	А	103	PRO	2.4	
1	В	88	GLN	2.4	
1	А	791	GLY	2.3	
1	А	424	VAL	2.3	
1	А	650	TRP	2.3	
1	В	293	SER	2.3	
1	А	149	ASN	2.3	
1	В	247	VAL	2.3	
1	А	146	ALA	2.3	
1	В	91	ASN	2.3	
1	В	510	SER	2.3	
1	А	421	PRO	2.3	
1	В	92	GLU	2.3	
1	В	429	SER	2.2	
1	В	431	SER	2.2	
1	В	238	VAL	2.2	
1	В	503	ASN	2.2	
1	A	162	SER	2.2	
1	В	87	ILE	2.2	
1	В	847	ILE	2.2	
1	A	558	THR	2.2	
1	В	499	LEU	2.2	
1	A	810	TRP	2.2	
1	В	398	LYS	2.2	
1	В	413	ASP	2.2	
1	В	311	ASN	2.2	
1	А	73	LEU	2.2	



Mol	Chain	Res	Type	RSRZ
1	В	235	LEU	2.2
1	А	34	SER	2.2
1	А	148	TYR	2.1
1	А	182	ASN	2.1
1	А	177	GLY	2.1
1	А	611	THR	2.1
1	В	639	ARG	2.1
1	А	846	ILE	2.1
1	А	160	PRO	2.1
1	В	215	TYR	2.1
1	А	219	GLU	2.1
1	А	370	GLY	2.1
1	А	849	TYR	2.1
1	В	795	VAL	2.1
1	А	223	ILE	2.1
1	В	543	TYR	2.1
1	В	850	GLN	2.1
1	В	219	GLU	2.1
1	А	644	ALA	2.1
1	В	244	ILE	2.1
1	А	655	SER	2.1
1	А	861	PHE	2.1
1	В	468	ASN	2.1
1	В	848	THR	2.0
1	В	211	SER	2.0
1	В	425	SER	2.0
1	В	523	TYR	2.0
1	В	831	TYR	2.0
1	А	277	PHE	2.0
1	А	420	THR	2.0
1	А	515	THR	2.0
1	А	831	TYR	2.0
1	В	168	ILE	2.0
1	А	659	PHE	2.0
1	В	509	ASP	2.0
1	В	576	TRP	2.0
1	А	339	ASN	2.0
1	А	790	GLY	2.0
1	В	437	ILE	2.0
1	А	852	TYR	2.0
1	В	746	MET	2.0

Continued from previous page...



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)

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^{th} 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	${f B}$ -factors(Å ²)	Q<0.9
2	MPD	В	1868	8/8	0.88	0.36	$95,\!96,\!97,\!97$	0
3	GOL	В	1869	6/6	0.88	0.41	70,72,72,73	0
2	MPD	В	1867	8/8	0.93	0.19	38,40,40,41	0
2	MPD	А	1867	8/8	0.99	0.18	36,38,40,42	0

6.5 Other polymers (i)

There are no such residues in this entry.

