



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 AM GMT

PDB ID : 2VSE
Title : STRUCTURE AND MODE OF ACTION OF A MOSQUITOCIDAL HOLO-TOXIN
Authors : Treiber, N.; Reinert, D.J.; Carpusca, I.; Aktories, K.; Schulz, G.E.
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

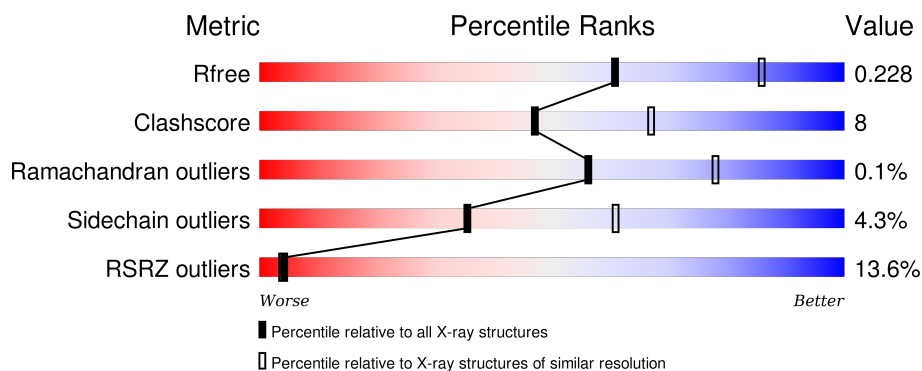
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	841	

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	B	1867	X	-	-	-
2	MPD	B	1868	X	-	-	X
3	GOL	B	1869	-	-	-	X

2 Entry composition [i](#)

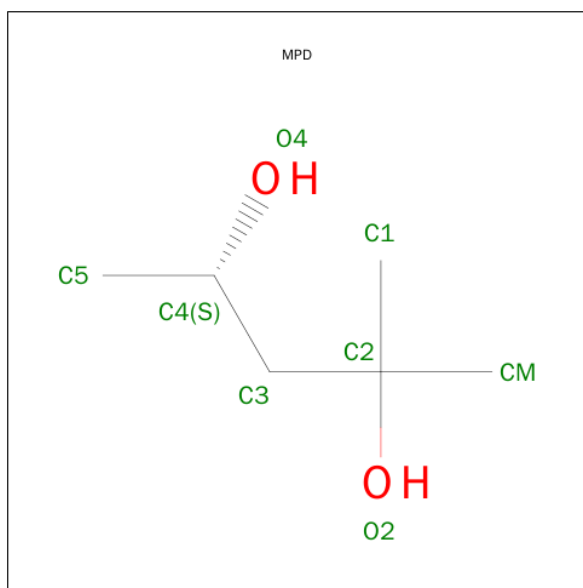
There are 4 unique types of molecules in this entry. The entry contains 14186 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	A	823	Total	C	N	O	S	0	0	0
			6743	4258	1170	1307	8			
1	B	822	Total	C	N	O	S	0	0	0
			6737	4255	1169	1305	8			

- 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	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		

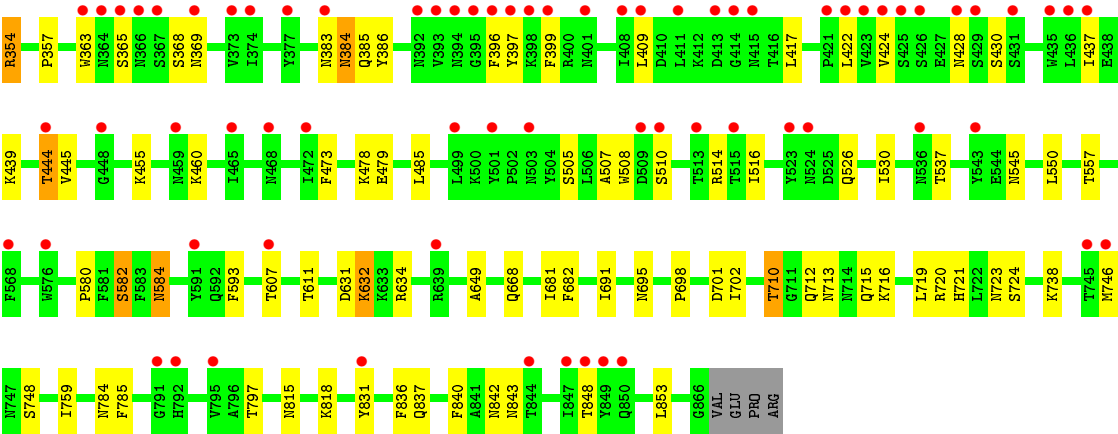
- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	367	Total	O	0	0
			367	367		
4	B	309	Total	O	0	0
			309	309		



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	130.96Å 130.96Å 396.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.54 – 2.50 74.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.54-2.50) 99.9 (74.59-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.234 0.188 , 0.228	Depositor DCC
R_{free} test set	4379 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.2	EDS
Estimated twinning fraction	0.033 for -h-k,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 87588 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.50	0/6913	0.60	0/9402
1	B	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	Z	Observed(Å)	Ideal(Å)
1	B	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

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	6743	0	6427	99	0
1	B	6737	0	6422	97	0
2	A	8	0	14	0	0
2	B	16	0	28	4	0
3	B	6	0	8	2	0
4	A	367	0	0	4	0
4	B	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 distance (Å)	Clash 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:HD22	1:B:584:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:MET:HE2	1:B:797:THR:HB	1.82	0.60
1:A:127:HIS:CD2	1:A:130:ASN:HB2	2.37	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:831:TYR:HB3	1:B:848:THR:HB	1.84	0.58
1:B:160:PRO:HG2	1:B:163:ALA:HB2	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:CM	2:B:1867:MPD:H52	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:B:74:HIS:HD2	4:B:2021:HOH:O	1.93	0.50
1:A:157:PRO:HG2	1:A:170:ARG:HH21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:ASP:N	4:B:2169:HOH:O	2.43	0.49
1:A:160:PRO:HG2	1:A:163:ALA:HB2	1.94	0.49
1:A:34:SER:HB2	1:A:35:PRO:CD	2.43	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:B:710:THR:CG2	1:B:712:GLN:HG2	2.34	0.49
1:A:602:ILE:HD13	1:A:623:GLN:HB3	1.93	0.49
1:B:710:THR:HG21	4:B:2202:HOH:O	2.11	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:171:TYR:CD1	1:B:212:THR:HB	2.48	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: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:658:ILE:HB	1:A:704:LEU:HB2	1.96	0.47
1:A:476:SER:OG	1:A:478:LYS:HD3	2.15	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:B:301:GLU:OE2	1:B:354:ARG:HD3	2.14	0.47
1:A:465:ILE:CG2	1:A:469:LYS:HE2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:THR:HB	1:B:336:GLN:HG2	1.98	0.46
1:A:682:PHE:HZ	1:A:719:LEU:HD21	1.81	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:785:PHE:O	1:A:797:THR:HA	2.16	0.45
1:A:362:SER:OG	1:A:385:GLN:HG2	2.16	0.45
1:A:305:LYS:HG2	1:A:313:VAL:HG12	1.98	0.45
1:B:632:LYS:H	1:B:632:LYS:HD2	1.82	0.45
1:A:720:ARG:HD3	4:A:2264:HOH:O	2.17	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
2:B:1867:MPD:HM1	2:B:1867:MPD:C5	2.37	0.45
1:B:632:LYS:N	1:B:632:LYS:HD2	2.32	0.45
1:A:368:SER:O	1:A:369:ASN:HB2	2.17	0.45
1:A:746:MET:HE2	1:A:797:THR:HB	2.00	0.44
1:B:710:THR:HG23	1:B:712:GLN:H	1.83	0.44
1:A:157:PRO:CG	1:A:170:ARG:HH21	2.31	0.44
1:B:235:LEU:HD12	1:B:439:LYS:HB3	1.99	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:746:MET:HE1	1:A:784:ASN:HB3	1.88	0.44
1:A:592:GLN:HG3	1:A:722:LEU:HD11	1.99	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:B:445:VAL:HG21	1:B:485:LEU:HD23	2.00	0.42
1:A:788:PHE:HB2	1:A:825:ASN:ND2	2.34	0.42
1:B:315:THR:HG21	1:B:328:TYR:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:698:PRO:HA	1:A:702:ILE:HD11	2.00	0.42
1:B:294:LEU:CD1	1:B:298:GLN:HE22	2.32	0.42
1:A:407:LYS:HB3	1:A:424:VAL:HG22	2.02	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:785:PHE:O	1:B:797:THR:HA	2.20	0.42
1:B:746:MET:CE	1:B:797:THR:HB	2.49	0.42
1:B:97:ARG:HD3	1:B:111:PHE:CE1	2.55	0.42
1:B:836:PHE:CE1	1:B:837:GLN:HG3	2.55	0.42
1:B:507:ALA:HB2	1:B:526:GLN:HG2	2.01	0.42
1:B:31:SER:HA	1:B:32:PRO:HD3	1.93	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: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:156:THR:HA	1:B:157:PRO:HD3	1.78	0.41
1:A:363:TRP:O	1:A:384:ASN:HB2	2.20	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: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: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:A:842:ASN:O	1:A:843:ASN:HB2	2.21	0.41
1:B:294:LEU:HD13	1:B:298:GLN:HE22	1.86	0.41
1:A:460:LYS:HD2	1:A:460:LYS:HA	1.88	0.41
1:A:735:SER:CB	1:A:743:ILE:HG22	2.51	0.40
1:A:354:ARG:CZ	4:A:2126:HOH:O	2.69	0.40
1:A:246:LYS:NZ	1:A:294:LEU:HD12	2.36	0.40
1:A:171:TYR:CD1	1:A:212:THR:HB	2.56	0.40
1:A:128:LEU:O	1:A:131:TYR:HB3	2.21	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

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	817/841 (97%)	780 (96%)	37 (4%)	0	100	100
1	B	816/841 (97%)	779 (96%)	36 (4%)	1 (0%)	56	78
All	All	1633/1682 (97%)	1559 (96%)	73 (4%)	1 (0%)	56	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	384	ASN

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	756/772 (98%)	723 (96%)	33 (4%)	35	60
1	B	755/772 (98%)	723 (96%)	32 (4%)	36	62
All	All	1511/1544 (98%)	1446 (96%)	65 (4%)	35	61

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

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

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

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

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

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

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Mol	Chain	Res	Type
1	B	88	GLN
1	B	91	ASN
1	B	127	HIS
1	B	149	ASN
1	B	165	ASN
1	B	280	ASN
1	B	298	GLN
1	B	339	ASN
1	B	415	ASN
1	B	428	ASN
1	B	545	ASN
1	B	584	ASN
1	B	697	GLN
1	B	712	GLN
1	B	721	HIS
1	B	749	ASN
1	B	752	GLN
1	B	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 carbohydrates 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 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	$\# Z > 2$
2	MPD	A	1867	-	6,7,7	0.19	0	7,10,10	0.65	0
2	MPD	B	1867	-	6,7,7	0.34	0	7,10,10	1.26	1 (14%)
2	MPD	B	1868	-	6,7,7	0.30	0	7,10,10	0.36	0
3	GOL	B	1869	-	5,5,5	0.31	0	5,5,5	0.19	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
2	MPD	A	1867	-	-	0/5/5/5	0/0/0/0
2	MPD	B	1867	-	1/1/2/2	0/5/5/5	0/0/0/0
2	MPD	B	1868	-	1/1/2/2	0/5/5/5	0/0/0/0
3	GOL	B	1869	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1867	MPD	CM-C2-C1	-2.34	105.13	110.24

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1867	MPD	4	0
3	B	1869	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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	A	823/841 (97%)	1.05	85 (10%) 9 9	45, 49, 52, 56	0
1	B	822/841 (97%)	1.26	139 (16%) 2 2	45, 49, 52, 58	0
All	All	1645/1682 (97%)	1.15	224 (13%) 4 4	45, 49, 52, 58	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	PRO	6.7
1	B	408	ILE	6.4
1	B	396	PHE	6.3
1	B	395	GLY	6.3
1	B	411	LEU	6.2
1	A	31	SER	6.1
1	A	82	SER	5.9
1	B	89	ILE	5.4
1	B	31	SER	5.4
1	B	393	VAL	5.3
1	A	292	ASN	5.2
1	B	84	THR	5.2
1	B	240	GLY	5.1
1	B	424	VAL	4.9
1	A	151	LEU	4.8
1	A	74	HIS	4.6
1	B	83	ASN	4.6
1	B	82	SER	4.6
1	B	363	TRP	4.5
1	B	394	ASN	4.5
1	A	83	ASN	4.4
1	B	373	VAL	4.4
1	B	515	THR	4.3
1	A	393	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	366	ASN	4.2
1	B	397	TYR	4.2
1	B	98	TRP	4.1
1	B	414	GLY	4.1
1	B	307	LYS	4.1
1	B	328	TYR	4.0
1	A	98	TRP	3.8
1	A	67	PHE	3.8
1	B	524	ASN	3.7
1	B	158	TRP	3.7
1	A	86	GLN	3.7
1	B	501	TYR	3.6
1	B	177	GLY	3.6
1	A	84	THR	3.6
1	B	67	PHE	3.6
1	B	32	PRO	3.5
1	A	96	LEU	3.5
1	A	163	ALA	3.5
1	B	415	ASN	3.5
1	A	32	PRO	3.5
1	B	364	ASN	3.5
1	A	185	PHE	3.4
1	B	312	ILE	3.4
1	B	239	SER	3.4
1	B	374	ILE	3.4
1	A	289	LEU	3.3
1	A	284	PRO	3.3
1	B	399	PHE	3.3
1	A	665	TYR	3.2
1	B	146	ALA	3.2
1	B	306	ASN	3.2
1	A	81	ASP	3.2
1	B	157	PRO	3.1
1	A	369	ASN	3.1
1	B	320	TYR	3.1
1	B	435	TRP	3.1
1	B	465	ILE	3.1
1	A	646	LEU	3.1
1	B	436	LEU	3.1
1	B	81	ASP	3.1
1	B	241	PRO	3.0
1	A	396	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	78	GLN	3.0
1	A	225	ILE	3.0
1	A	285	ASN	3.0
1	B	291	ASN	3.0
1	A	72	GLY	3.0
1	A	168	ILE	3.0
1	B	150	ASN	2.9
1	B	292	ASN	2.9
1	B	96	LEU	2.9
1	B	426	SER	2.9
1	B	448	GLY	2.9
1	B	34	SER	2.9
1	B	74	HIS	2.9
1	B	421	PRO	2.9
1	B	68	ALA	2.9
1	A	283	ILE	2.9
1	B	568	PHE	2.9
1	A	153	LEU	2.8
1	A	92	GLU	2.8
1	B	72	GLY	2.8
1	B	423	VAL	2.8
1	B	148	TYR	2.8
1	B	392	ASN	2.8
1	B	792	HIS	2.8
1	B	369	ASN	2.7
1	B	305	LYS	2.7
1	B	149	ASN	2.7
1	B	155	ILE	2.7
1	A	71	ASN	2.7
1	A	625	TRP	2.7
1	B	329	LYS	2.7
1	B	377	TYR	2.7
1	A	294	LEU	2.7
1	B	422	LEU	2.7
1	A	792	HIS	2.7
1	B	367	SER	2.7
1	B	294	LEU	2.6
1	A	241	PRO	2.6
1	B	185	PHE	2.6
1	B	401	ASN	2.6
1	B	153	LEU	2.6
1	B	75	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	313	VAL	2.6
1	A	167	ILE	2.6
1	B	223	ILE	2.6
1	B	78	GLN	2.6
1	B	513	THR	2.6
1	B	71	ASN	2.6
1	B	289	LEU	2.6
1	B	309	ASP	2.6
1	A	196	ASP	2.5
1	A	91	ASN	2.5
1	B	428	ASN	2.5
1	B	365	SER	2.5
1	B	283	ILE	2.5
1	B	316	LEU	2.5
1	B	849	TYR	2.5
1	A	791	GLY	2.5
1	A	424	VAL	2.5
1	A	103	PRO	2.5
1	A	149	ASN	2.4
1	A	146	ALA	2.4
1	B	247	VAL	2.4
1	B	88	GLN	2.4
1	A	650	TRP	2.4
1	B	91	ASN	2.4
1	B	293	SER	2.4
1	B	510	SER	2.4
1	A	421	PRO	2.4
1	B	238	VAL	2.4
1	B	92	GLU	2.4
1	B	429	SER	2.3
1	B	87	ILE	2.3
1	B	847	ILE	2.3
1	B	413	ASP	2.3
1	B	499	LEU	2.3
1	A	162	SER	2.3
1	B	431	SER	2.3
1	A	558	THR	2.3
1	A	160	PRO	2.3
1	B	398	LYS	2.3
1	A	810	TRP	2.3
1	B	503	ASN	2.3
1	A	177	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	2.3
1	B	235	LEU	2.3
1	B	311	ASN	2.3
1	A	846	ILE	2.3
1	A	148	TYR	2.3
1	A	611	THR	2.3
1	B	639	ARG	2.3
1	A	182	ASN	2.2
1	B	795	VAL	2.2
1	A	34	SER	2.2
1	B	215	TYR	2.2
1	A	370	GLY	2.2
1	A	219	GLU	2.2
1	A	644	ALA	2.2
1	A	223	ILE	2.2
1	A	849	TYR	2.2
1	B	219	GLU	2.2
1	B	848	THR	2.2
1	B	543	TYR	2.2
1	B	244	ILE	2.2
1	B	850	GLN	2.2
1	B	468	ASN	2.2
1	B	746	MET	2.1
1	B	831	TYR	2.1
1	B	168	ILE	2.1
1	B	437	ILE	2.1
1	A	861	PHE	2.1
1	B	509	ASP	2.1
1	A	420	THR	2.1
1	A	515	THR	2.1
1	B	234	THR	2.1
1	A	655	SER	2.1
1	A	790	GLY	2.1
1	B	211	SER	2.1
1	A	831	TYR	2.1
1	B	523	TYR	2.1
1	A	277	PHE	2.1
1	A	659	PHE	2.1
1	B	844	THR	2.1
1	B	576	TRP	2.1
1	B	425	SER	2.1
1	A	852	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	188	ASN	2.1
1	A	339	ASN	2.1
1	A	145	ARG	2.1
1	A	661	ALA	2.1
1	A	612	ILE	2.1
1	B	220	ILE	2.1
1	B	288	LEU	2.1
1	B	444	THR	2.1
1	B	175	ALA	2.1
1	B	459	ASN	2.1
1	B	536	ASN	2.1
1	B	591	TYR	2.1
1	A	491	LEU	2.1
1	A	186	SER	2.1
1	A	158	TRP	2.0
1	A	670	TRP	2.0
1	B	308	LYS	2.0
1	B	791	GLY	2.0
1	A	217	ASN	2.0
1	B	383	ASN	2.0
1	B	216	HIS	2.0
1	B	256	GLY	2.0
1	A	304	ILE	2.0
1	A	408	ILE	2.0
1	A	743	ILE	2.0
1	B	472	ILE	2.0
1	A	745	THR	2.0
1	B	86	GLN	2.0
1	B	409	LEU	2.0
1	B	745	THR	2.0
1	A	746	MET	2.0
1	B	607	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	B	1869	6/6	0.88	0.41	8.79	70,72,72,73	0
2	MPD	B	1868	8/8	0.88	0.36	5.83	95,96,97,97	0
2	MPD	B	1867	8/8	0.93	0.19	-3.22	38,40,40,41	0
2	MPD	A	1867	8/8	0.99	0.18	-4.00	36,38,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.