



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 2VSE / pdb_00002vse
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 : 2.50 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

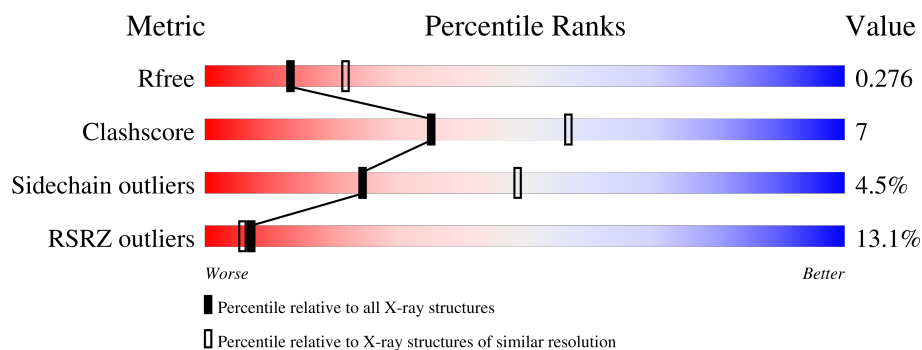
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	B	1868	X	-	-	-

2 Entry composition [i](#)

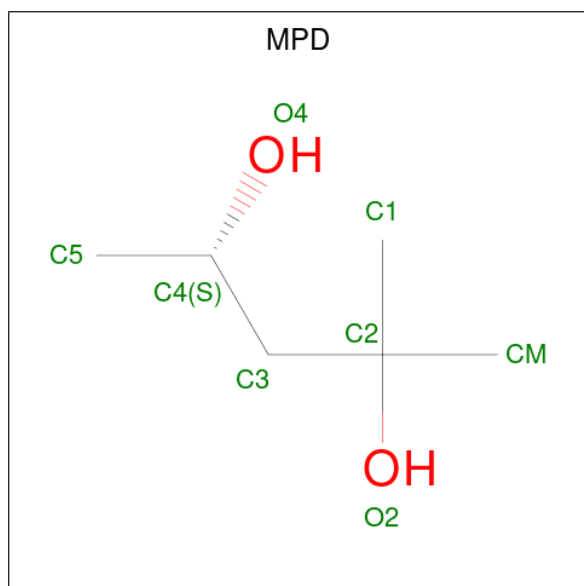
There are 4 unique types of molecules in this entry. The entry contains 14186 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

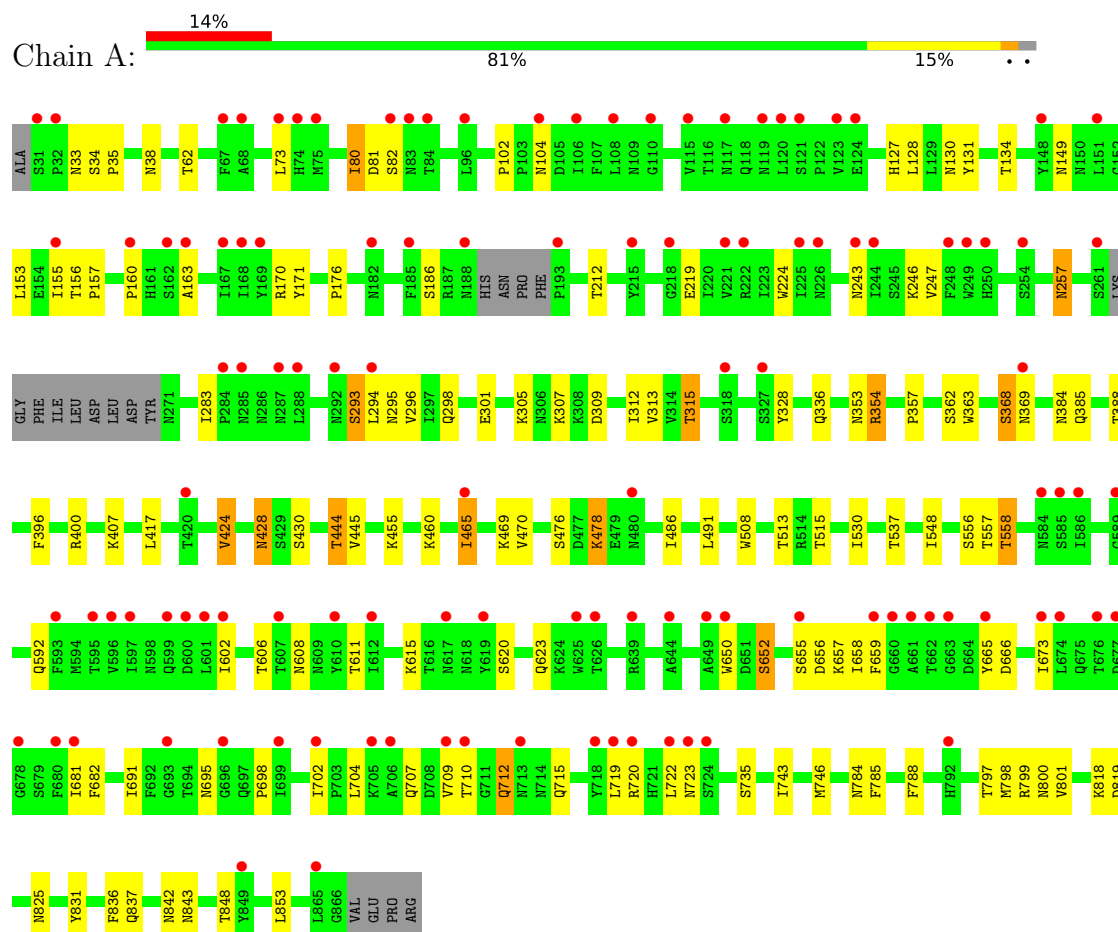
- Molecule 4 is water.

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

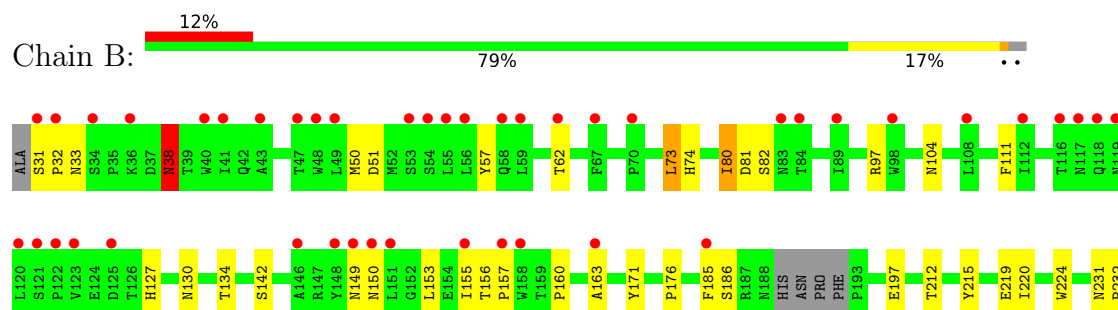
3 Residue-property plots

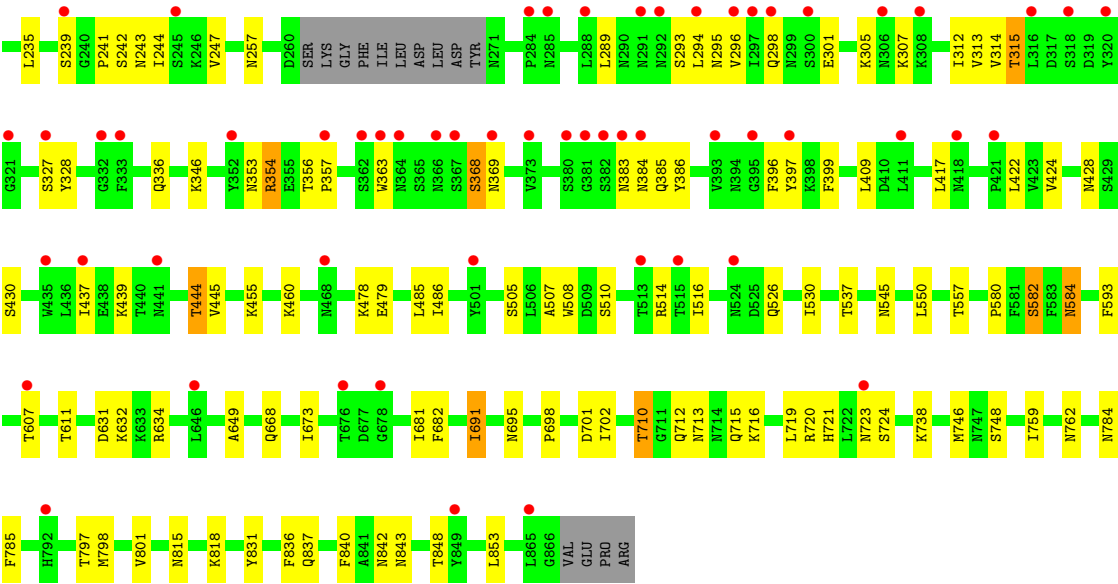
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: MOSQUITOCIDAL TOXIN





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 74.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.54-2.50) 99.9 (74.54-2.50)	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 (Not available) , 0.276	Depositor 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/Å ³), B_{sol} (Å ²)	0.35 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.89	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.59	1/6913 (0.0%)	0.83	2/9402 (0.0%)
1	B	0.57	0/6907	0.82	5/9394 (0.1%)
All	All	0.58	1/13820 (0.0%)	0.83	7/18796 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	ILE	CB-CG1	5.30	1.64	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASN	N-CA-C	5.38	118.64	111.75
1	B	38	ASN	N-CA-C	5.25	118.46	111.75
1	B	356	THR	CA-C-N	5.17	125.47	119.47
1	B	356	THR	C-N-CA	5.17	125.47	119.47
1	B	185	PHE	N-CA-C	5.14	117.48	109.52
1	A	368	SER	N-CA-C	-5.05	103.86	110.53
1	B	368	SER	N-CA-C	-5.01	103.79	110.55

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	94	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	194	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 7.

All (194) 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:HE1	1:A:784:ASN:CB	1.73	1.17
1:A:746:MET:HE1	1:A:784:ASN:HB3	1.30	1.09
1:B:746:MET:HE1	1:B:784:ASN:CB	1.92	0.98
1:B:746:MET:HE1	1:B:784:ASN:HB2	1.51	0.91
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:746:MET:HE1	1:A:784:ASN:HB2	1.56	0.83
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:691:ILE:HD11	1:A:715:GLN:CD	2.06	0.81
1:A:746:MET:HE2	1:A:797:THR:HB	1.64	0.79
1:B:746:MET:HE1	1:B:784:ASN:HB3	1.63	0.79
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:B:746:MET:HE2	1:B:797:THR:HB	1.66	0.77
1:A:315:THR:HB	1:A:336:GLN:HG2	1.68	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:B:215:TYR:CE1	1:B:220:ILE:HG12	2.25	0.71
1:A:80:ILE:HG22	1:A:81:ASP:O	1.89	0.71
1:A:746:MET:HE2	1:A:797:THR:CB	2.21	0.70
1:A:665:TYR:HD1	1:A:666:ASP:H	1.38	0.70
1:A:80:ILE:HD11	1:A:176:PRO:HB3	1.74	0.69
1:B:149:ASN:HD21	1:B:153:LEU:HB2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:746:MET:HE2	1:B:797:THR:CB	2.24	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
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: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: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: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:A:710:THR:HG22	1:A:715:GLN:CD	2.34	0.53
1:B:363:TRP:O	1:B:384:ASN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:368:SER:O	1:B:369:ASN:CB	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:MET:HB3	1:A:798:MET:HE3	1.76	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
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:B:691:ILE:HD11	1:B:715:GLN:CD	2.42	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: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: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: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: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:798:MET:HE3	1:B:798:MET:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:710:THR:HG22	1:B:715:GLN:CD	2.44	0.41
1:A:707:GLN:CD	1:A:715:GLN:HE21	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CZ	4:A:2126:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	756/772 (98%)	725 (96%)	31 (4%)	27	53
1	B	755/772 (98%)	718 (95%)	37 (5%)	22	45
All	All	1511/1544 (98%)	1443 (96%)	68 (4%)	24	49

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	73	LEU
1	A	80	ILE
1	A	134	THR
1	A	186	SER
1	A	219	GLU
1	A	243	ASN
1	A	247	VAL
1	A	257	ASN
1	A	293	SER

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Mol	Chain	Res	Type
1	A	295	ASN
1	A	315	THR
1	A	354	ARG
1	A	417	LEU
1	A	424	VAL
1	A	428	ASN
1	A	444	THR
1	A	465	ILE
1	A	470	VAL
1	A	478	LYS
1	A	486	ILE
1	A	491	LEU
1	A	558	THR
1	A	620	SER
1	A	652	SER
1	A	673	ILE
1	A	681	ILE
1	A	695	ASN
1	A	712	GLN
1	A	723	ASN
1	A	801	VAL
1	B	38	ASN
1	B	51	ASP
1	B	62	THR
1	B	73	LEU
1	B	80	ILE
1	B	134	THR
1	B	150	ASN
1	B	186	SER
1	B	219	GLU
1	B	239	SER
1	B	242	SER
1	B	243	ASN
1	B	247	VAL
1	B	289	LEU
1	B	293	SER
1	B	315	THR
1	B	354	ARG
1	B	417	LEU
1	B	424	VAL
1	B	444	THR
1	B	478	LYS

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Mol	Chain	Res	Type
1	B	486	ILE
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	673	ILE
1	B	681	ILE
1	B	691	ILE
1	B	695	ASN
1	B	701	ASP
1	B	710	THR
1	B	748	SER
1	B	762	ASN
1	B	801	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	42	GLN
1	A	58	GLN
1	A	86	GLN
1	A	88	GLN
1	A	91	ASN
1	A	127	HIS
1	A	135	ASN
1	A	149	ASN
1	A	165	ASN
1	A	291	ASN
1	A	298	GLN
1	A	339	ASN
1	A	347	ASN
1	A	415	ASN
1	A	418	ASN
1	A	428	ASN
1	A	441	ASN
1	A	512	ASN
1	A	536	ASN
1	A	561	ASN
1	A	712	GLN

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Mol	Chain	Res	Type
1	A	723	ASN
1	A	733	ASN
1	A	803	ASN
1	A	817	ASN
1	B	42	GLN
1	B	71	ASN
1	B	78	GLN
1	B	83	ASN
1	B	88	GLN
1	B	91	ASN
1	B	127	HIS
1	B	149	ASN
1	B	165	ASN
1	B	250	HIS
1	B	280	ASN
1	B	298	GLN
1	B	372	GLN
1	B	384	ASN
1	B	428	ASN
1	B	441	ASN
1	B	471	HIS
1	B	511	ASN
1	B	545	ASN
1	B	584	ASN
1	B	653	ASN
1	B	654	HIS
1	B	697	GLN
1	B	712	GLN
1	B	714	ASN
1	B	721	HIS
1	B	733	ASN
1	B	749	ASN
1	B	752	GLN
1	B	815	ASN

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 [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	GOL	B	1869	-	5,5,5	0.36	0	5,5,5	0.19	0
2	MPD	A	1867	-	7,7,7	0.24	0	9,10,10	0.71	0
2	MPD	B	1868	-	7,7,7	0.30	0	9,10,10	0.47	0
2	MPD	B	1867	-	7,7,7	0.36	0	9,10,10	1.26	1 (11%)

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	B	1869	-	-	2/4/4/4	-
2	MPD	A	1867	-	-	0/5/5/5	-
2	MPD	B	1868	-	1/1/2/2	4/5/5/5	-
2	MPD	B	1867	-	1/1/2/2	2/5/5/5	-

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	-2.45	105.13	110.63

All (2) chirality outliers are listed below:

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

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1867	MPD	C2-C3-C4-C5
2	B	1868	MPD	C2-C3-C4-C5
3	B	1869	GOL	O1-C1-C2-C3
3	B	1869	GOL	O1-C1-C2-O2
2	B	1868	MPD	C1-C2-C3-C4
2	B	1868	MPD	CM-C2-C3-C4
2	B	1868	MPD	O2-C2-C3-C4
2	B	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
3	B	1869	GOL	2	0
2	B	1867	MPD	4	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, 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%)	1.07	115 (13%) 6 5	45, 49, 52, 56	0
1	B	822/841 (97%)	1.02	101 (12%) 8 7	45, 49, 52, 58	0
All	All	1645/1682 (97%)	1.04	216 (13%) 7 6	45, 49, 52, 58	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	SER	5.4
1	A	67	PHE	4.7
1	B	120	LEU	4.5
1	A	31	SER	4.4
1	A	596	VAL	4.3
1	B	119	ASN	4.2
1	B	284	PRO	4.0
1	B	121	SER	4.0
1	A	292	ASN	3.9
1	B	67	PHE	3.8
1	A	676	THR	3.7
1	A	74	HIS	3.7
1	A	718	TYR	3.7
1	B	148	TYR	3.6
1	B	515	THR	3.6
1	A	369	ASN	3.5
1	A	865	LEU	3.5
1	B	117	ASN	3.5
1	A	82	SER	3.4
1	A	607	THR	3.4
1	B	373	VAL	3.4
1	A	724	SER	3.4
1	B	146	ALA	3.3
1	B	501	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	441	ASN	3.3
1	B	123	VAL	3.3
1	B	185	PHE	3.3
1	A	285	ASN	3.3
1	A	119	ASN	3.2
1	B	32	PRO	3.2
1	A	644	ALA	3.2
1	A	169	TYR	3.2
1	A	73	LEU	3.2
1	A	182	ASN	3.2
1	B	333	PHE	3.2
1	A	792	HIS	3.2
1	A	585	SER	3.1
1	B	792	HIS	3.1
1	B	292	ASN	3.1
1	A	168	ILE	3.1
1	B	380	SER	3.1
1	A	163	ALA	3.1
1	B	125	ASP	3.0
1	B	55	LEU	3.0
1	A	225	ILE	3.0
1	A	699	ILE	3.0
1	B	155	ILE	3.0
1	B	116	THR	2.9
1	A	720	ARG	2.9
1	B	294	LEU	2.9
1	A	148	TYR	2.9
1	A	600	ASP	2.9
1	B	58	GLN	2.9
1	B	239	SER	2.9
1	A	250	HIS	2.9
1	B	393	VAL	2.9
1	A	108	LEU	2.9
1	A	83	ASN	2.9
1	A	610	TYR	2.9
1	B	381	GLY	2.9
1	A	626	THR	2.8
1	B	382	SER	2.8
1	B	157	PRO	2.8
1	A	719	LEU	2.8
1	B	108	LEU	2.8
1	B	291	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	68	ALA	2.8
1	A	601	LEU	2.8
1	B	298	GLN	2.8
1	B	98	TRP	2.8
1	A	723	ASN	2.8
1	A	294	LEU	2.8
1	A	639	ARG	2.8
1	A	678	GLY	2.7
1	A	680	PHE	2.8
1	A	693	GLY	2.7
1	B	83	ASN	2.7
1	B	369	ASN	2.7
1	B	676	THR	2.7
1	A	673	ILE	2.7
1	B	70	PRO	2.7
1	B	437	ILE	2.7
1	B	36	LYS	2.7
1	B	363	TRP	2.7
1	A	167	ILE	2.7
1	A	185	PHE	2.7
1	A	84	THR	2.7
1	A	599	GLN	2.6
1	A	696	GLY	2.6
1	A	120	LEU	2.6
1	A	649	ALA	2.6
1	A	662	THR	2.6
1	B	118	GLN	2.6
1	B	320	TYR	2.6
1	A	284	PRO	2.6
1	B	366	ASN	2.6
1	B	158	TRP	2.6
1	B	288	LEU	2.6
1	B	34	SER	2.6
1	A	96	LEU	2.5
1	A	151	LEU	2.5
1	A	674	LEU	2.5
1	B	47	THR	2.5
1	A	659	PHE	2.5
1	B	49	LEU	2.5
1	B	607	THR	2.5
1	B	112	ILE	2.5
1	B	122	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	619	TYR	2.5
1	A	597	ILE	2.5
1	A	160	PRO	2.4
1	A	722	LEU	2.4
1	A	221	VAL	2.4
1	A	121	SER	2.4
1	A	193	PRO	2.4
1	B	357	PRO	2.4
1	A	677	ASP	2.4
1	A	288	LEU	2.4
1	B	332	GLY	2.4
1	B	59	LEU	2.4
1	B	316	LEU	2.4
1	A	249	TRP	2.4
1	A	612	ILE	2.4
1	A	75	MET	2.4
1	A	117	ASN	2.4
1	B	395	GLY	2.3
1	A	702	ILE	2.3
1	B	41	ILE	2.3
1	A	248	PHE	2.3
1	A	665	TYR	2.3
1	A	287	ASN	2.3
1	B	364	ASN	2.3
1	B	40	TRP	2.3
1	A	254	SER	2.3
1	B	367	SER	2.3
1	A	602	ILE	2.3
1	A	32	PRO	2.3
1	A	710	THR	2.3
1	A	589	GLY	2.3
1	A	681	ILE	2.3
1	B	306	ASN	2.3
1	B	31	SER	2.3
1	A	705	LYS	2.3
1	B	383	ASN	2.2
1	B	84	THR	2.2
1	A	110	GLY	2.2
1	A	124	GLU	2.2
1	A	222	ARG	2.2
1	A	661	ALA	2.2
1	B	524	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	849	TYR	2.2
1	A	420	THR	2.2
1	B	54	SER	2.2
1	A	123	VAL	2.2
1	A	188	ASN	2.2
1	A	244	ILE	2.2
1	B	297	ILE	2.2
1	A	115	VAL	2.2
1	B	296	VAL	2.2
1	A	215	TYR	2.2
1	B	308	LYS	2.2
1	A	104	ASN	2.1
1	A	226	ASN	2.1
1	B	43	ALA	2.1
1	B	468	ASN	2.1
1	B	151	LEU	2.1
1	B	321	GLY	2.1
1	B	865	LEU	2.1
1	A	655	SER	2.1
1	B	327	SER	2.1
1	B	421	PRO	2.1
1	A	584	ASN	2.1
1	A	617	ASN	2.1
1	B	62	THR	2.1
1	B	849	TYR	2.1
1	B	300	SER	2.1
1	A	625	TRP	2.1
1	A	650	TRP	2.1
1	A	706	ALA	2.1
1	A	243	ASN	2.1
1	A	480	ASN	2.1
1	B	150	ASN	2.1
1	B	513	THR	2.1
1	B	678	GLY	2.1
1	A	465	ILE	2.1
1	B	352	TYR	2.1
1	A	709	VAL	2.1
1	B	56	LEU	2.1
1	B	149	ASN	2.1
1	B	411	LEU	2.1
1	B	723	ASN	2.1
1	A	660	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	53	SER	2.1
1	B	285	ASN	2.0
1	A	663	GLY	2.0
1	A	106	ILE	2.0
1	A	155	ILE	2.0
1	A	586	ILE	2.0
1	A	595	THR	2.0
1	B	89	ILE	2.0
1	B	245	SER	2.0
1	B	318	SER	2.0
1	B	362	SER	2.0
1	A	593	PHE	2.0
1	B	163	ALA	2.0
1	B	646	LEU	2.0
1	A	218	GLY	2.0
1	A	713	ASN	2.0
1	B	384	ASN	2.0
1	B	418	ASN	2.0
1	B	48	TRP	2.0
1	B	435	TRP	2.0
1	A	162	SER	2.0
1	A	318	SER	2.0
1	A	327	SER	2.0
1	B	397	TYR	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MPD	B	1868	8/8	0.80	0.21	95,96,97,97	0
3	GOL	B	1869	6/6	0.84	0.28	70,72,72,73	0
2	MPD	B	1867	8/8	0.90	0.17	38,40,40,41	0
2	MPD	A	1867	8/8	0.96	0.13	36,38,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.