



Full wwPDB X-ray Structure Validation Report

Jul 30, 2014 – 05:09 PM EDT

PDB ID : 4MT1
Title : Crystal Structure of the Neisseria gonorrhoeae MtrD Inner Membrane Multidrug Efflux Pump
Authors : Su, C.-C.; Bolla, J.R.; Yu, E.W.
Deposited on : 2013-09-18
Resolution : 3.54 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

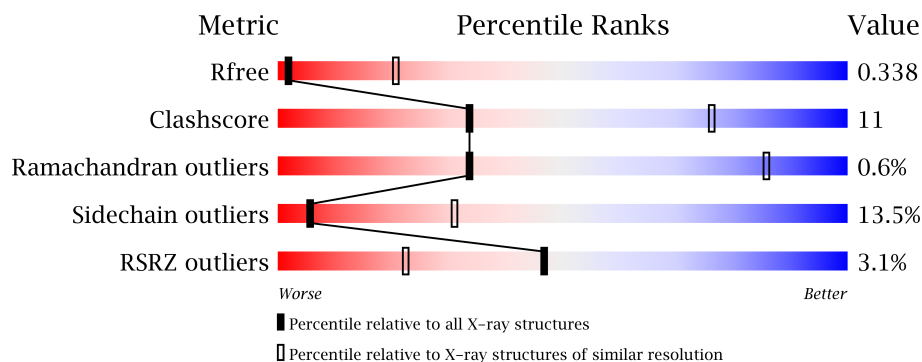
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.54 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}	66092	1270 (3.78-3.30)
Clashscore	79885	1033 (3.70-3.38)
Ramachandran outliers	78287	1067 (3.72-3.36)
Sidechain outliers	78261	1067 (3.72-3.36)
RSRZ outliers	66119	1270 (3.78-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1056	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7667 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Drug efflux protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1023	Total	C	N	O	S	0	0	0
			7667	4926	1268	1432	41			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	626	PHE	LEU	CONFLICT	UNP D1E405
A	839	GLU	ALA	CONFLICT	UNP D1E405
A	861	SER	ARG	CONFLICT	UNP D1E405

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	153.00Å 153.00Å 360.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.80 – 3.54 48.80 – 3.53	Depositor EDS
% Data completeness (in resolution range)	90.7 (48.80-3.54) 90.8 (48.80-3.53)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.280 , 0.333 0.281 , 0.338	Depositor DCC
R_{free} test set	953 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	127.3	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.7	EDS
Estimated twinning fraction	0.025 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.013 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.036 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 18421 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7667	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.23	0/7806	0.43	0/10594

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7667	0	7826	171	0
All	All	7667	0	7826	171	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (171) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:482:LEU:HG	1:A:486:LEU:HB3	1.69	0.75
1:A:365:ILE:HG23	1:A:366:PRO:HD3	1.73	0.70
1:A:885:LEU:HD23	1:A:895:PRO:HA	1.74	0.69
1:A:446:VAL:HG11	1:A:951:ILE:HG12	1.74	0.68
1:A:157:GLN:HG3	1:A:179:GLN:HB3	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:161:VAL:HG13	1:A:162:PRO:HD3	1.78	0.65
1:A:404:VAL:HG12	1:A:408:ILE:HG13	1.78	0.65
1:A:566:GLN:HG3	1:A:664:PRO:HG2	1.78	0.65
1:A:417:ILE:HG23	1:A:421:GLU:HB2	1.78	0.65
1:A:703:ARG:HG2	1:A:713:VAL:HG21	1.80	0.64
1:A:36:PRO:HG3	1:A:467:GLN:HE22	1.63	0.63
1:A:45:LEU:HG	1:A:90:VAL:HG13	1.80	0.63
1:A:140:VAL:HG11	1:A:308:LEU:HD13	1.81	0.63
1:A:954:ILE:HG23	1:A:1033:TYR:HD1	1.63	0.62
1:A:902:ILE:HG13	1:A:903:PRO:HD3	1.81	0.62
1:A:733:ALA:HA	1:A:737:GLY:HA3	1.83	0.60
1:A:698:LEU:HD12	1:A:848:LEU:HD11	1.82	0.60
1:A:530:LYS:HA	1:A:533:ARG:HD2	1.83	0.60
1:A:62:LEU:HD12	1:A:82:ALA:HB2	1.84	0.60
1:A:784:LEU:HA	1:A:798:LEU:HB2	1.84	0.59
1:A:574:GLN:NE2	1:A:619:MET:SD	2.76	0.59
1:A:408:ILE:HD13	1:A:984:MET:HG2	1.85	0.59
1:A:455:ALA:HB1	1:A:466:LYS:HG3	1.84	0.59
1:A:889:TYR:HB3	1:A:894:ILE:HD13	1.85	0.59
1:A:579:ALA:HB3	1:A:618:ASN:HB3	1.83	0.59
1:A:529:ALA:HB2	1:A:972:LEU:HD21	1.85	0.59
1:A:518:ASP:O	1:A:522:HIS:ND1	2.35	0.58
1:A:575:LEU:HD23	1:A:576:PRO:HD2	1.85	0.58
1:A:250:ARG:HB3	1:A:258:ILE:HD12	1.85	0.58
1:A:159:ASN:HB2	1:A:311:LEU:HD13	1.86	0.57
1:A:348:LEU:HD11	1:A:991:LEU:HB3	1.85	0.57
1:A:455:ALA:HA	1:A:466:LYS:HA	1.86	0.57
1:A:41:PRO:HG3	1:A:98:THR:HA	1.87	0.57
1:A:716:GLY:N	1:A:823:LYS:O	2.38	0.56
1:A:164:LEU:HD21	1:A:308:LEU:HD11	1.87	0.56
1:A:358:GLN:NE2	1:A:514:ASN:OD1	2.39	0.56
1:A:80:THR:HB	1:A:815:ARG:HB2	1.87	0.56
1:A:787:THR:HB	1:A:795:ALA:HB1	1.88	0.55
1:A:561:LEU:HG	1:A:934:TYR:HE2	1.71	0.55
1:A:885:LEU:HB3	1:A:895:PRO:HG3	1.87	0.55
1:A:276:SER:HB3	1:A:608:SER:HB3	1.88	0.55
1:A:348:LEU:HD21	1:A:991:LEU:HB3	1.89	0.55
1:A:618:ASN:ND2	1:A:719:GLU:OE1	2.40	0.54
1:A:395:ALA:O	1:A:399:VAL:N	2.25	0.54
1:A:699:ILE:HG12	1:A:824:LEU:HD13	1.89	0.54
1:A:408:ILE:HA	1:A:411:VAL:HG12	1.90	0.54
1:A:938:GLY:O	1:A:941:THR:OG1	2.23	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:400:ILE:O	1:A:404:VAL:HG23	2.08	0.53
1:A:454:LEU:HB3	1:A:469:ALA:HB2	1.90	0.53
1:A:668:LEU:HD12	1:A:860:SER:HA	1.90	0.53
1:A:392:THR:HB	1:A:471:THR:HG21	1.91	0.53
1:A:451:PHE:HZ	1:A:941:THR:HG22	1.74	0.53
1:A:349:VAL:HG11	1:A:404:VAL:HG21	1.91	0.53
1:A:531:VAL:HB	1:A:538:MET:HG3	1.91	0.53
1:A:695:ARG:HH11	1:A:699:ILE:HD12	1.73	0.52
1:A:302:LYS:HA	1:A:305:LYS:HE3	1.92	0.52
1:A:163:GLU:HG3	1:A:311:LEU:HD21	1.92	0.52
1:A:381:ILE:HD11	1:A:471:THR:HG22	1.90	0.52
1:A:916:ARG:HG2	1:A:929:PHE:HE2	1.75	0.52
1:A:389:ASN:ND2	1:A:467:GLN:OE1	2.43	0.52
1:A:442:GLY:O	1:A:446:VAL:HG13	2.09	0.52
1:A:761:ASN:HB3	1:A:766:GLN:HG3	1.92	0.51
1:A:953:ILE:HG12	1:A:1029:VAL:HG12	1.91	0.51
1:A:828:PRO:HG2	1:A:834:THR:HA	1.92	0.51
1:A:137:LEU:HD22	1:A:291:LEU:HD11	1.92	0.50
1:A:961:GLN:HG2	1:A:1037:ARG:HD2	1.92	0.50
1:A:571:VAL:HA	1:A:661:ALA:HA	1.93	0.50
1:A:527:ARG:HB3	1:A:1027:PHE:HE1	1.77	0.50
1:A:143:SER:HB3	1:A:322:LYS:HE2	1.92	0.50
1:A:703:ARG:HH21	1:A:711:SER:HA	1.77	0.49
1:A:916:ARG:HG2	1:A:929:PHE:CE2	2.47	0.49
1:A:360:ILE:HA	1:A:363:THR:HG22	1.95	0.49
1:A:164:LEU:HD11	1:A:308:LEU:HG	1.93	0.49
1:A:402:ILE:HD13	1:A:447:LEU:HD13	1.95	0.48
1:A:740:PHE:HD2	1:A:743:ILE:HD12	1.77	0.48
1:A:359:ASN:HB3	1:A:362:TYR:CD1	2.49	0.48
1:A:865:LYS:O	1:A:867:GLY:N	2.47	0.47
1:A:33:SER:OG	1:A:296:ASN:OD1	2.27	0.47
1:A:399:VAL:O	1:A:402:ILE:N	2.47	0.47
1:A:429:THR:HG21	1:A:491:CYS:HA	1.96	0.47
1:A:529:ALA:HB1	1:A:533:ARG:NH1	2.29	0.47
1:A:898:VAL:HG21	1:A:951:ILE:HD12	1.96	0.47
1:A:967:ALA:HB3	1:A:1038:LYS:HE2	1.97	0.47
1:A:412:GLU:OE1	1:A:980:ARG:NE	2.48	0.47
1:A:421:GLU:HG3	1:A:431:LYS:HG2	1.96	0.47
1:A:759:PHE:CE1	1:A:761:ASN:HB2	2.50	0.47
1:A:935:PHE:HA	1:A:1013:THR:HG21	1.96	0.47
1:A:186:VAL:HG12	1:A:264:ALA:HB2	1.97	0.47
1:A:885:LEU:HD11	1:A:951:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:413:ASN:O	1:A:416:ARG:NH2	2.48	0.46
1:A:529:ALA:HA	1:A:972:LEU:HD11	1.98	0.46
1:A:70:ASN:OD1	1:A:70:ASN:N	2.44	0.46
1:A:489:ALA:HA	1:A:492:ALA:HB3	1.98	0.46
1:A:277:THR:HG23	1:A:607:VAL:HG22	1.98	0.46
1:A:63:SER:O	1:A:67:ARG:HG3	2.16	0.46
1:A:532:LEU:HD13	1:A:1031:LEU:HD12	1.98	0.46
1:A:707:LEU:H	1:A:707:LEU:HD22	1.81	0.46
1:A:755:TYR:OH	1:A:758:ASP:OD1	2.27	0.46
1:A:449:SER:HB3	1:A:884:VAL:HG21	1.99	0.45
1:A:560:PHE:HB2	1:A:864:ALA:HB2	1.97	0.45
1:A:167:ILE:HD11	1:A:307:ARG:HG2	1.97	0.45
1:A:369:VAL:HG13	1:A:482:LEU:HD23	1.98	0.45
1:A:416:ARG:HH21	1:A:417:ILE:HG13	1.82	0.45
1:A:975:ALA:HB2	1:A:1030:PRO:HG3	1.97	0.45
1:A:956:PHE:HB2	1:A:978:ARG:HH11	1.82	0.45
1:A:891:SER:HB2	1:A:894:ILE:HD11	1.99	0.45
1:A:682:ASP:HB3	1:A:691:LEU:HD23	1.98	0.44
1:A:237:GLN:OE1	1:A:760:PRO:HD3	2.16	0.44
1:A:779:GLN:HB2	1:A:782:ASP:HB2	1.98	0.44
1:A:845:VAL:HG21	1:A:854:PHE:HB3	2.00	0.44
1:A:545:LEU:HD13	1:A:1024:LEU:HD13	1.99	0.44
1:A:575:LEU:HD22	1:A:579:ALA:HB2	1.98	0.44
1:A:137:LEU:HG	1:A:138:MET:HG2	1.98	0.44
1:A:65:ILE:HG23	1:A:111:LEU:HD13	2.00	0.44
1:A:681:GLN:HB2	1:A:681:GLN:HE21	1.64	0.43
1:A:960:LEU:HG	1:A:965:LYS:HD3	1.99	0.43
1:A:472:MET:O	1:A:476:ILE:HG22	2.18	0.43
1:A:626:PHE:HE2	1:A:642:VAL:HG11	1.84	0.43
1:A:598:ILE:HD13	1:A:642:VAL:HG13	1.99	0.43
1:A:843:LYS:O	1:A:847:GLU:HG3	2.18	0.43
1:A:20:ILE:HG21	1:A:372:ILE:HG13	2.00	0.43
1:A:282:VAL:HG23	1:A:284:THR:HG23	2.00	0.43
1:A:393:MET:O	1:A:397:ILE:HG12	2.19	0.43
1:A:538:MET:HA	1:A:541:VAL:HG12	2.00	0.43
1:A:405:ASP:OD1	1:A:985:THR:HB	2.18	0.43
1:A:181:ALA:HB2	1:A:271:GLU:HG2	2.00	0.43
1:A:922:LEU:HG	1:A:923:LEU:HD23	2.00	0.43
1:A:459:GLY:O	1:A:463:ASN:N	2.43	0.43
1:A:695:ARG:HG3	1:A:822:MET:HB3	2.00	0.43
1:A:185:TRP:HZ3	1:A:777:ARG:HH12	1.66	0.43
1:A:467:GLN:O	1:A:471:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:TYR:CE1	1:A:667:ILE:HG12	2.54	0.42
1:A:570:MET:HG3	1:A:623:PHE:CE1	2.55	0.42
1:A:678:ILE:O	1:A:823:LYS:HA	2.19	0.42
1:A:184:ILE:HG12	1:A:266:VAL:HG23	2.01	0.42
1:A:917:ASN:OD1	1:A:929:PHE:HB2	2.18	0.42
1:A:335:ILE:HA	1:A:338:VAL:HG12	2.01	0.42
1:A:535:THR:HA	1:A:1031:LEU:HD11	2.02	0.42
1:A:483:ALA:HA	1:A:487:THR:OG1	2.20	0.42
1:A:410:VAL:HA	1:A:436:ILE:HD12	2.01	0.42
1:A:16:SER:O	1:A:20:ILE:HG23	2.20	0.41
1:A:718:LEU:HB3	1:A:719:GLU:H	1.66	0.41
1:A:111:LEU:HD11	1:A:127:VAL:HG11	2.02	0.41
1:A:299:ALA:HA	1:A:302:LYS:HE3	2.02	0.41
1:A:416:ARG:NH2	1:A:417:ILE:HG13	2.35	0.41
1:A:575:LEU:HD23	1:A:576:PRO:CD	2.50	0.41
1:A:796:VAL:HA	1:A:797:PRO:HD3	1.88	0.41
1:A:954:ILE:HG23	1:A:1033:TYR:CD1	2.48	0.41
1:A:397:ILE:O	1:A:400:ILE:HG22	2.20	0.41
1:A:759:PHE:CE2	1:A:766:GLN:HB2	2.54	0.41
1:A:874:TYR:HA	1:A:877:ALA:HB3	2.02	0.41
1:A:34:GLN:HA	1:A:388:ILE:O	2.19	0.41
1:A:561:LEU:HG	1:A:934:TYR:CE2	2.54	0.41
1:A:592:THR:HA	1:A:604:ILE:HD13	2.02	0.41
1:A:937:VAL:O	1:A:941:THR:HG23	2.20	0.41
1:A:111:LEU:HD21	1:A:127:VAL:HG22	2.03	0.41
1:A:137:LEU:HB2	1:A:291:LEU:CD2	2.51	0.41
1:A:881:VAL:O	1:A:885:LEU:HD13	2.21	0.41
1:A:98:THR:OG1	1:A:100:GLU:OE1	2.25	0.41
1:A:97:ASP:N	1:A:97:ASP:OD1	2.54	0.41
1:A:209:ASN:HB2	1:A:238:LEU:HD22	2.02	0.41
1:A:827:SER:HA	1:A:828:PRO:HD3	1.76	0.41
1:A:457:PHE:HE1	1:A:873:LEU:HD12	1.86	0.41
1:A:43:ILE:HD12	1:A:94:PHE:CE2	2.56	0.41
1:A:423:LEU:HB3	1:A:424:PRO:HD2	2.03	0.40
1:A:709:ASP:HA	1:A:710:PRO:HD3	1.86	0.40
1:A:217:ILE:O	1:A:229:THR:HA	2.22	0.40
1:A:784:LEU:HD21	1:A:804:VAL:HG13	2.03	0.40
1:A:532:LEU:HD11	1:A:1031:LEU:HA	2.03	0.40
1:A:736:GLN:HB2	1:A:736:GLN:HE21	1.61	0.40
1:A:891:SER:HB2	1:A:894:ILE:CD1	2.51	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	1017/1056 (96%)	965 (95%)	46 (4%)	6 (1%)	33 86

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	828	PRO
1	A	866	GLY
1	A	777	ARG
1	A	395	ALA
1	A	831	GLY
1	A	36	PRO

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	820/848 (97%)	709 (86%)	111 (14%)	6 31

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	8	ARG
1	A	10	ILE
1	A	20	ILE
1	A	34	GLN
1	A	42	THR
1	A	45	LEU

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Mol	Chain	Res	Type
1	A	46	HIS
1	A	49	TYR
1	A	65	ILE
1	A	75	LEU
1	A	80	THR
1	A	90	VAL
1	A	98	THR
1	A	101	ASN
1	A	102	LEU
1	A	115	LEU
1	A	117	THR
1	A	121	THR
1	A	161	VAL
1	A	168	GLU
1	A	170	VAL
1	A	201	VAL
1	A	220	LEU
1	A	224	ARG
1	A	227	THR
1	A	232	VAL
1	A	233	THR
1	A	238	LEU
1	A	279	LEU
1	A	283	ASN
1	A	289	VAL
1	A	298	MET
1	A	310	VAL
1	A	321	TRP
1	A	335	ILE
1	A	337	LYS
1	A	352	VAL
1	A	357	LEU
1	A	365	ILE
1	A	367	THR
1	A	368	ILE
1	A	375	LEU
1	A	386	MET
1	A	390	VAL
1	A	400	ILE
1	A	402	ILE
1	A	418	MET
1	A	421	GLU

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Mol	Chain	Res	Type
1	A	433	MET
1	A	451	PHE
1	A	454	LEU
1	A	472	MET
1	A	509	PHE
1	A	517	PHE
1	A	521	THR
1	A	532	LEU
1	A	555	ARG
1	A	571	VAL
1	A	572	SER
1	A	574	GLN
1	A	612	PHE
1	A	625	ILE
1	A	628	ASP
1	A	630	ASN
1	A	651	MET
1	A	655	LYS
1	A	662	VAL
1	A	663	VAL
1	A	676	LEU
1	A	678	ILE
1	A	681	GLN
1	A	686	THR
1	A	688	HIS
1	A	698	LEU
1	A	703	ARG
1	A	712	THR
1	A	718	LEU
1	A	736	GLN
1	A	756	VAL
1	A	765	LEU
1	A	773	ASP
1	A	777	ARG
1	A	786	LEU
1	A	822	MET
1	A	824	LEU
1	A	832	VAL
1	A	839	GLU
1	A	848	LEU
1	A	856	TRP
1	A	869	GLN

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Mol	Chain	Res	Type
1	A	870	THR
1	A	872	ILE
1	A	881	VAL
1	A	883	LEU
1	A	894	ILE
1	A	900	LEU
1	A	901	VAL
1	A	907	ILE
1	A	916	ARG
1	A	919	PHE
1	A	923	LEU
1	A	945	LEU
1	A	951	ILE
1	A	953	ILE
1	A	969	GLU
1	A	972	LEU
1	A	977	LEU
1	A	978	ARG
1	A	1026	VAL
1	A	1037	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	ASN
1	A	467	GLN
1	A	736	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	1023/1056 (96%)	0.17	32 (3%)	47 22	44, 91, 145, 211	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	830	THR	4.0
1	A	712	THR	3.9
1	A	826	ALA	3.8
1	A	734	ALA	3.7
1	A	831	GLY	3.7
1	A	719	GLU	3.3
1	A	791	LYS	3.3
1	A	319	MET	3.2
1	A	766	GLN	3.2
1	A	287	MET	3.1
1	A	157	GLN	2.8
1	A	456	MET	2.8
1	A	869	GLN	2.7
1	A	271	GLU	2.7
1	A	308	LEU	2.7
1	A	403	VAL	2.6
1	A	689	THR	2.5
1	A	141	MET	2.4
1	A	458	SER	2.3
1	A	173	VAL	2.3
1	A	179	GLN	2.3
1	A	801	ILE	2.3
1	A	439	ALA	2.2
1	A	136	PHE	2.2
1	A	707	LEU	2.2
1	A	876	LEU	2.2
1	A	288	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	466	LYS	2.2
1	A	178	ALA	2.2
1	A	714	ARG	2.2
1	A	156	ALA	2.1
1	A	290	MET	2.1

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.