Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:48 PM GMT

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 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 (i) symbol.

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

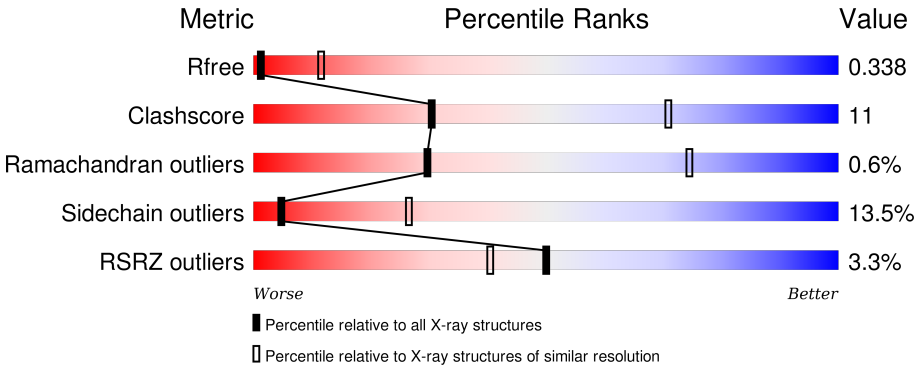
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	1136 (3.68-3.40)
Clashscore	102246	1248 (3.68-3.40)
Ramachandran outliers	100387	1208 (3.68-3.40)
Sidechain outliers	100360	1208 (3.68-3.40)
RSRZ outliers	91569	1143 (3.68-3.40)

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 <=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	1056	3% 65% 28%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7667 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 Drug efflux protein.

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

There are 3 discrepancies between the modelled and reference sequences:

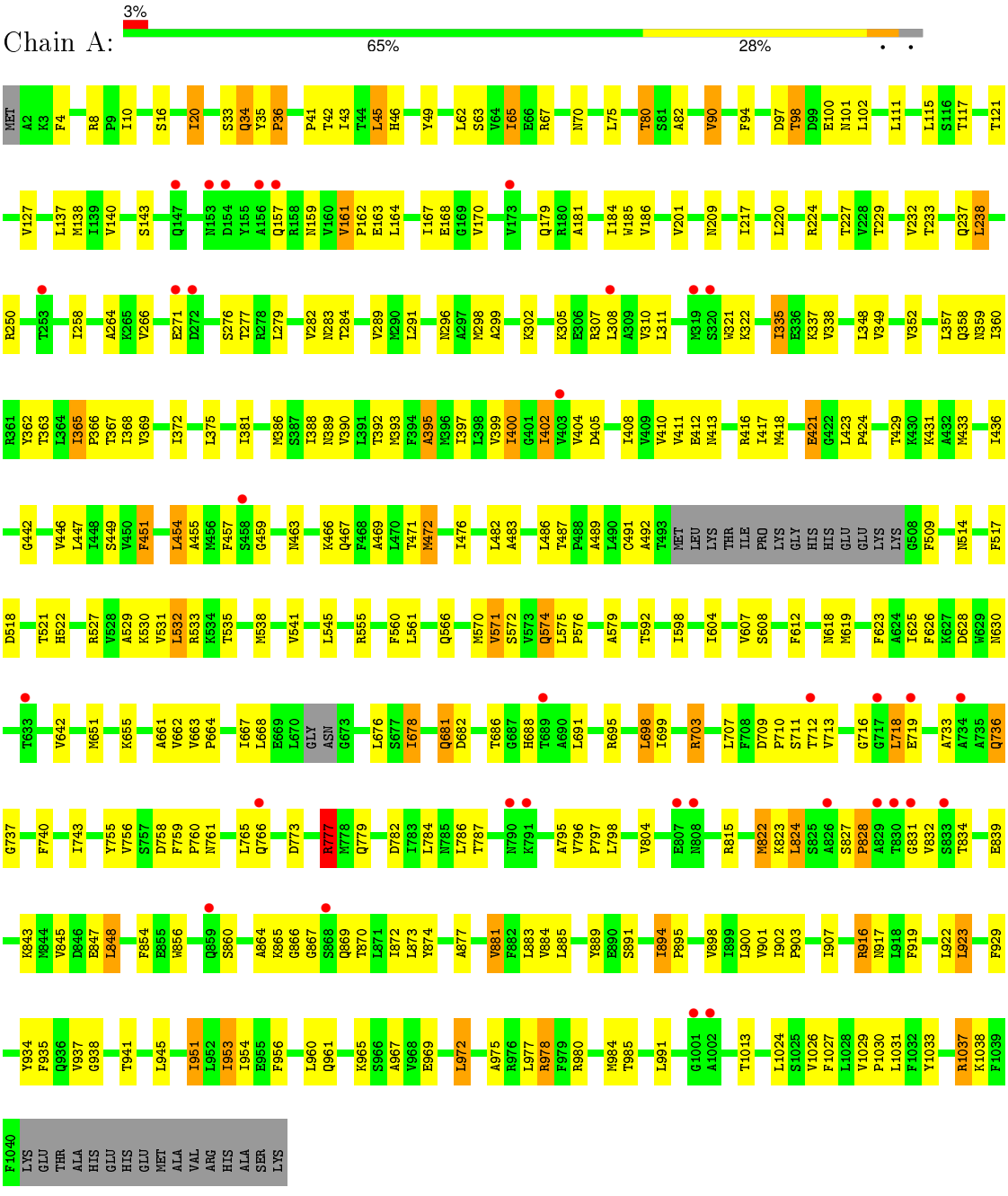
Chain	Residue	Modelled	Actual	Comment	Reference
A	626	PHE	LEU	CONFLICT	UNP D1E405
A	839	GLU	ALA	CONFLICT	UNP D1E405
A	861	SER	ARG	CONFLICT	UNP D1E405

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Drug efflux protein

Chain A:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 70.6	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[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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 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	7667	0	7826	171	0
All	All	7667	0	7826	171	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 11.

All (171) 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: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	Interatomic distance (Å)	Clash overlap (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:45:LEU:HG	1:A:90:VAL:HG13	1.80	0.63
1:A:36:PRO:HG3	1:A:467:GLN:HE22	1.63	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:62:LEU:HD12	1:A:82:ALA:HB2	1.84	0.60
1:A:530:LYS:HA	1:A:533:ARG:HD2	1.83	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:529:ALA:HB2	1:A:972:LEU:HD21	1.85	0.59
1:A:579:ALA:HB3	1:A:618:ASN:HB3	1.83	0.59
1:A:575:LEU:HD23	1:A:576:PRO:HD2	1.85	0.58
1:A:518:ASP:O	1:A:522:HIS:ND1	2.35	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:80:THR:HB	1:A:815:ARG:HB2	1.87	0.56
1:A:358:GLN:NE2	1:A:514:ASN:OD1	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:GLY:O	1:A:941:THR:OG1	2.23	0.54
1:A:400:ILE:O	1:A:404:VAL:HG23	2.08	0.53
1:A:668:LEU:HD12	1:A:860:SER:HA	1.90	0.53
1:A:454:LEU:HB3	1:A:469:ALA:HB2	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:442:GLY:O	1:A:446:VAL:HG13	2.09	0.52
1:A:389:ASN:ND2	1:A:467:GLN:OE1	2.43	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:898:VAL:HG21	1:A:951:ILE:HD12	1.96	0.47
1:A:529:ALA:HB1	1:A:533:ARG:NH1	2.29	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:967:ALA:HB3	1:A:1038:LYS:HE2	1.97	0.47
1:A:33:SER:OG	1:A:296:ASN:OD1	2.27	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:412:GLU:OE1	1:A:980:ARG:NE	2.48	0.47
1:A:935:PHE:HA	1:A:1013:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:LEU:HD11	1:A:951:ILE:HD11	1.97	0.47
1:A:186:VAL:HG12	1:A:264:ALA:HB2	1.97	0.47
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:707:LEU:H	1:A:707:LEU:HD22	1.81	0.46
1:A:532:LEU:HD13	1:A:1031:LEU:HD12	1.98	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:369:VAL:HG13	1:A:482:LEU:HD23	1.98	0.45
1:A:167:ILE:HD11	1:A:307:ARG:HG2	1.97	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:575:LEU:HD22	1:A:579:ALA:HB2	1.98	0.44
1:A:545:LEU:HD13	1:A:1024:LEU:HD13	1.99	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: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:472:MET:O	1:A:476:ILE:HG22	2.18	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: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:282:VAL:HG23	1:A:284:THR:HG23	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:695:ARG:HG3	1:A:822:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:GLY:O	1:A:463:ASN:N	2.43	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
1:A:35:TYR:CE1	1:A:667:ILE:HG12	2.54	0.42
1:A:678:ILE:O	1:A:823:LYS:HA	2.19	0.42
1:A:570:MET:HG3	1:A:623:PHE:CE1	2.55	0.42
1:A:917:ASN:OD1	1:A:929:PHE:HB2	2.18	0.42
1:A:184:ILE:HG12	1:A:266:VAL:HG23	2.01	0.42
1:A:535:THR:HA	1:A:1031:LEU:HD11	2.02	0.42
1:A:335:ILE:HA	1:A:338:VAL:HG12	2.01	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:718:LEU:HB3	1:A:719:GLU:H	1.66	0.41
1:A:16:SER:O	1:A:20:ILE:HG23	2.20	0.41
1:A:416:ARG:NH2	1:A:417:ILE:HG13	2.35	0.41
1:A:954:ILE:HG23	1:A:1033:TYR:CD1	2.48	0.41
1:A:575:LEU:HD23	1:A:576:PRO:CD	2.50	0.41
1:A:299:ALA:HA	1:A:302:LYS:HE3	2.02	0.41
1:A:111:LEU:HD11	1:A:127:VAL:HG11	2.02	0.41
1:A:796:VAL:HA	1:A:797:PRO:HD3	1.88	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:561:LEU:HG	1:A:934:TYR:CE2	2.54	0.41
1:A:937:VAL:O	1:A:941:THR:HG23	2.20	0.41
1:A:592:THR:HA	1:A:604:ILE:HD13	2.02	0.41
1:A:34:GLN:HA	1:A:388:ILE:O	2.19	0.41
1:A:111:LEU:HD21	1:A:127:VAL:HG22	2.03	0.41
1:A:881:VAL:O	1:A:885:LEU:HD13	2.21	0.41
1:A:137:LEU:HB2	1:A:291:LEU:CD2	2.51	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: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:209:ASN:HB2	1:A:238:LEU:HD22	2.02	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:784:LEU:HD21	1:A:804:VAL:HG13	2.03	0.40
1:A:217:ILE:O	1:A:229:THR:HA	2.22	0.40
1:A:532:LEU:HD11	1:A:1031:LEU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:SER:HB2	1:A:894:ILE:CD1	2.51	0.40
1:A:736:GLN:HB2	1:A:736:GLN:HE21	1.61	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	Percentiles
1	A	1017/1056 (96%)	965 (95%)	46 (4%)	6 (1%)	30 74

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 (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	820/848 (97%)	709 (86%)	111 (14%)	5 26

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 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

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, 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	A	1023/1056 (96%)	-0.03	34 (3%) 50 40	44, 91, 145, 211	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	831	GLY	8.5
1	A	830	THR	8.2
1	A	712	THR	6.0
1	A	826	ALA	5.6
1	A	734	ALA	4.4
1	A	719	GLU	4.4
1	A	319	MET	4.1
1	A	766	GLN	3.8
1	A	868	SER	3.6
1	A	791	LYS	3.6
1	A	1002	ALA	3.5
1	A	403	VAL	3.3
1	A	308	LEU	3.0
1	A	157	GLN	3.0
1	A	458	SER	3.0
1	A	859	GLN	2.9
1	A	147	GLN	2.8
1	A	154	ASP	2.8
1	A	689	THR	2.6
1	A	320	SER	2.6
1	A	717	GLY	2.6
1	A	173	VAL	2.5
1	A	807	GLU	2.5
1	A	156	ALA	2.5
1	A	829	ALA	2.5
1	A	633	THR	2.4
1	A	253	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	833	SER	2.4
1	A	808	ASN	2.4
1	A	272	ASP	2.3
1	A	1001	GLY	2.3
1	A	153	ASN	2.3
1	A	790	ASN	2.2
1	A	271	GLU	2.2

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.