



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:36 PM UTC

PDB ID : 4MT1 / pdb_00004mt1
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

<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
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

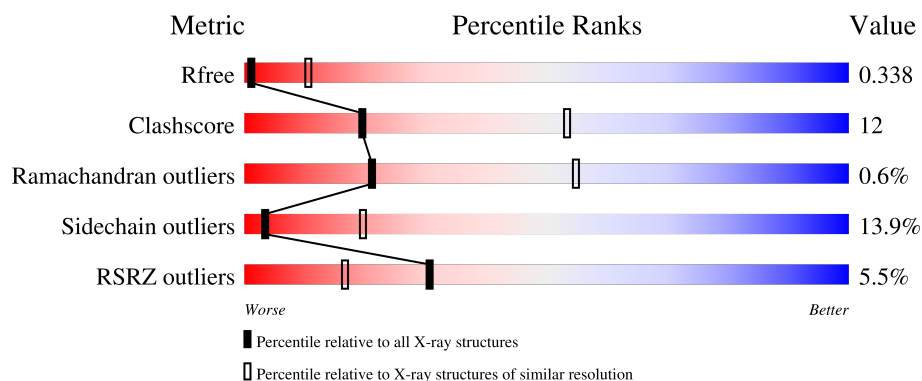
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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	1056	5% 65% 27% 5%

2 Entry composition

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
1	A	1023	Total	C	N	O	S	0	0	0
			7667	4926	1268	1432	41			

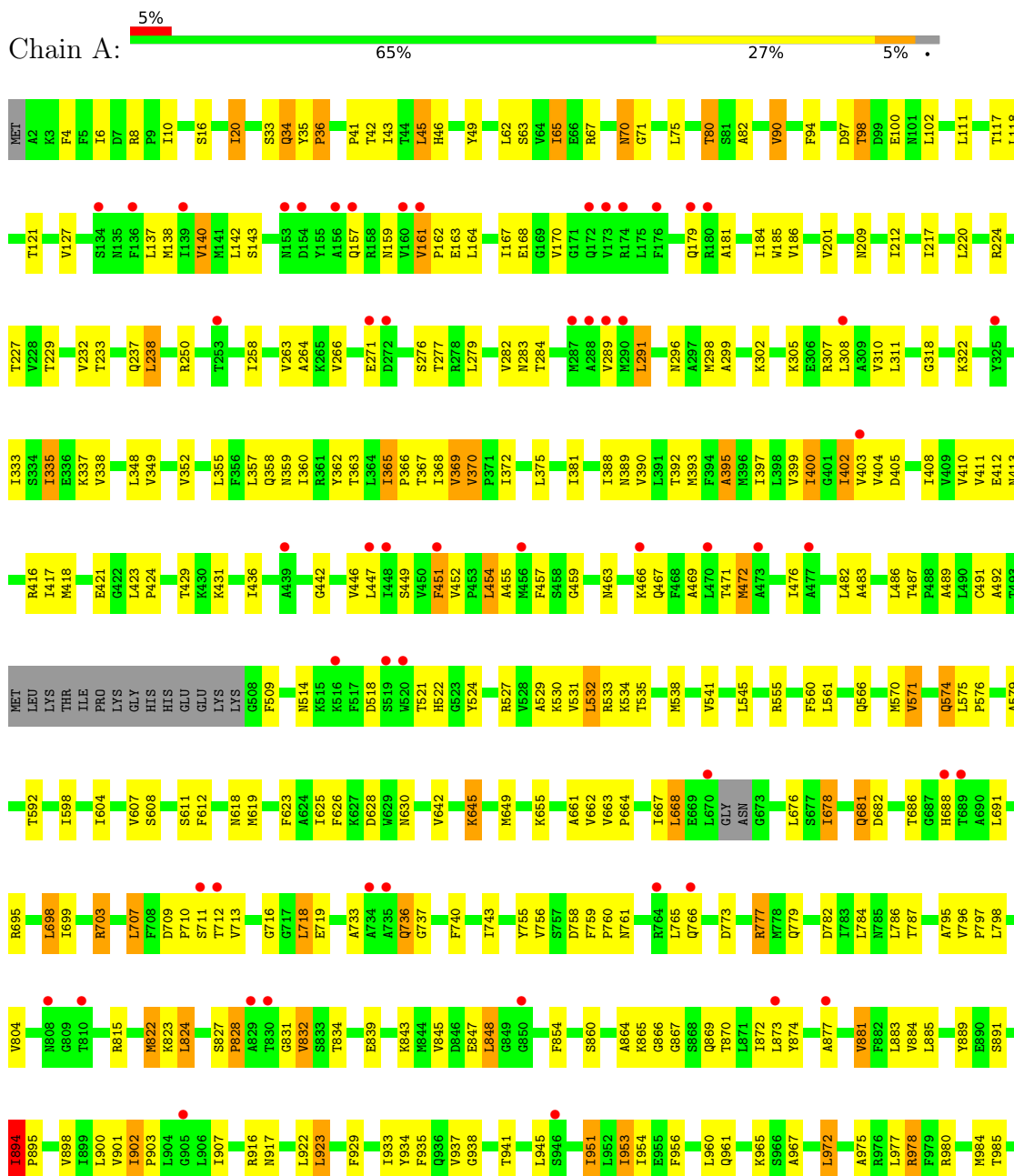
There are 3 discrepancies between the modelled and reference sequences:

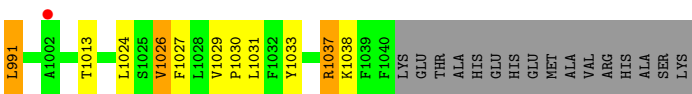
Chain	Residue	Modelled	Actual	Comment	Reference
A	626	PHE	LEU	conflict	UNP D1E405
A	839	GLU	ALA	conflict	UNP D1E405
A	861	SER	ARG	conflict	UNP D1E405

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: Drug efflux protein





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 – 3.54	Depositor EDS
% Data completeness (in resolution range)	90.7 (48.80-3.54) 90.7 (48.80-3.54)	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 1.8.1_1168	Depositor
R, R_{free}	0.280 , 0.333 0.283 , 0.338	Depositor DCC
R_{free} test set	962 reflections (4.59%)	wwPDB-VP
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 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
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
F_o, F_c correlation	0.89	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.

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

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	0.32	0/7806	0.79	11/10594 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	902	ILE	CA-C-N	-5.68	113.90	119.64
1	A	902	ILE	C-N-CA	-5.68	113.90	119.64
1	A	49	TYR	CA-C-N	5.66	126.91	119.84
1	A	49	TYR	C-N-CA	5.66	126.91	119.84
1	A	894	ILE	CB-CA-C	-5.55	108.47	114.35
1	A	318	GLY	N-CA-C	-5.45	107.58	115.27
1	A	370	VAL	CA-C-N	-5.39	113.47	119.19
1	A	370	VAL	C-N-CA	-5.39	113.47	119.19
1	A	452	VAL	CA-C-N	-5.32	114.55	120.45
1	A	452	VAL	C-N-CA	-5.32	114.55	120.45
1	A	71	GLY	N-CA-C	-5.10	106.73	115.61

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	180	0
All	All	7667	0	7826	180	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 12.

All (180) 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:611:SER:HB3	1:A:619:MET:HE3	1.74	0.70
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
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:645:LYS:HD2	1:A:649:MET:HE3	1.81	0.62
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:531:VAL:HG12	1:A:538:MET:HE3	1.91	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:524:TYR:OH	1:A:1026:VAL:O	2.24	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:98:THR:OG1	1:A:100:GLU:OE1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:413:ASN:O	1:A:416:ARG:NH2	2.48	0.46
1:A:70:ASN:OD1	1:A:70:ASN:N	2.44	0.46
1:A:529:ALA:HA	1:A:972:LEU:HD11	1.98	0.46
1:A:63:SER:O	1:A:67:ARG:HG3	2.16	0.46
1:A:277:THR:HG23	1:A:607:VAL:HG22	1.98	0.46
1:A:489:ALA:HA	1:A:492:ALA:HB3	1.98	0.46
1:A:532:LEU:HD13	1:A:1031:LEU:HD12	1.98	0.46
1:A:707:LEU:HD22	1:A:707:LEU:H	1.81	0.46
1:A:755:TYR:OH	1:A:758:ASP:OD1	2.27	0.46
1:A:399:VAL:HG22	1:A:472:MET:HE2	1.99	0.45
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:65:ILE:HG23	1:A:111:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HG	1:A:138:MET:HG2	1.98	0.44
1:A:681:GLN:HE21	1:A:681:GLN:HB2	1.64	0.43
1:A:709:ASP:CG	1:A:832:VAL:HG21	2.43	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:598:ILE:HD13	1:A:642:VAL:HG13	1.99	0.43
1:A:626:PHE:HE2	1:A:642:VAL:HG11	1.84	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:402:ILE:HA	1:A:405:ASP:CG	2.43	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
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:534:LYS:HD2	1:A:538:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLN:HA	1:A:388:ILE:O	2.19	0.41
1:A:100:GLU:H	1:A:100:GLU:CD	2.29	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:97:ASP:OD1	1:A:97:ASP:N	2.54	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:457:PHE:HE1	1:A:873:LEU:HD12	1.86	0.41
1:A:827:SER:HA	1:A:828:PRO:HD3	1.76	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:HE21	1:A:736:GLN:HB2	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 [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%)	21 55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	828	PRO

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Mol	Chain	Res	Type
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%)	706 (86%)	114 (14%)	3 19

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	6	ILE
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	65	ILE
1	A	70	ASN
1	A	75	LEU
1	A	80	THR
1	A	90	VAL
1	A	98	THR
1	A	102	LEU
1	A	117	THR
1	A	118	LEU
1	A	121	THR
1	A	140	VAL
1	A	142	LEU

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Mol	Chain	Res	Type
1	A	161	VAL
1	A	168	GLU
1	A	170	VAL
1	A	201	VAL
1	A	212	ILE
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	263	VAL
1	A	279	LEU
1	A	283	ASN
1	A	289	VAL
1	A	291	LEU
1	A	298	MET
1	A	310	VAL
1	A	333	ILE
1	A	335	ILE
1	A	337	LYS
1	A	352	VAL
1	A	355	LEU
1	A	357	LEU
1	A	365	ILE
1	A	367	THR
1	A	368	ILE
1	A	369	VAL
1	A	370	VAL
1	A	375	LEU
1	A	390	VAL
1	A	400	ILE
1	A	402	ILE
1	A	403	VAL
1	A	418	MET
1	A	451	PHE
1	A	454	LEU
1	A	472	MET
1	A	509	PHE
1	A	521	THR
1	A	532	LEU
1	A	555	ARG

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Mol	Chain	Res	Type
1	A	571	VAL
1	A	574	GLN
1	A	612	PHE
1	A	625	ILE
1	A	628	ASP
1	A	630	ASN
1	A	645	LYS
1	A	655	LYS
1	A	662	VAL
1	A	663	VAL
1	A	668	LEU
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	707	LEU
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	786	LEU
1	A	822	MET
1	A	824	LEU
1	A	832	VAL
1	A	839	GLU
1	A	848	LEU
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	923	LEU
1	A	933	ILE

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Mol	Chain	Res	Type
1	A	945	LEU
1	A	951	ILE
1	A	953	ILE
1	A	972	LEU
1	A	977	LEU
1	A	978	ARG
1	A	991	LEU
1	A	1026	VAL
1	A	1037	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	283	ASN
1	A	389	ASN
1	A	467	GLN
1	A	566	GLN
1	A	630	ASN
1	A	681	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1023/1056 (96%)	0.14	56 (5%) 30 16	44, 91, 145, 211	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	ALA	6.5
1	A	154	ASP	6.5
1	A	157	GLN	6.4
1	A	174	ARG	5.9
1	A	272	ASP	5.9
1	A	136	PHE	5.5
1	A	160	VAL	5.2
1	A	173	VAL	5.0
1	A	734	ALA	4.6
1	A	271	GLU	4.3
1	A	153	ASN	4.2
1	A	766	GLN	4.2
1	A	288	ALA	4.0
1	A	439	ALA	3.9
1	A	905	GLY	3.7
1	A	403	VAL	3.6
1	A	176	PHE	3.4
1	A	712	THR	3.4
1	A	520	TRP	3.3
1	A	179	GLN	3.3
1	A	516	LYS	3.3
1	A	161	VAL	3.1
1	A	253	THR	3.0
1	A	287	MET	2.9
1	A	290	MET	2.9
1	A	808	ASN	2.9
1	A	451	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	139	ILE	2.7
1	A	764	ARG	2.7
1	A	873	LEU	2.5
1	A	325	TYR	2.5
1	A	447	LEU	2.5
1	A	877	ALA	2.5
1	A	448	ILE	2.4
1	A	180	ARG	2.4
1	A	1002	ALA	2.4
1	A	308	LEU	2.3
1	A	670	LEU	2.3
1	A	946	SER	2.3
1	A	830	THR	2.3
1	A	829	ALA	2.3
1	A	470	LEU	2.3
1	A	134	SER	2.2
1	A	456	MET	2.2
1	A	172	GLN	2.2
1	A	711	SER	2.2
1	A	810	THR	2.2
1	A	477	ALA	2.2
1	A	519	SER	2.2
1	A	466	LYS	2.2
1	A	735	ALA	2.1
1	A	689	THR	2.1
1	A	473	ALA	2.1
1	A	688	HIS	2.1
1	A	850	GLY	2.0
1	A	289	VAL	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.