Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:21 PM GMT

PDB ID	:	1T9T
Title	:	Structural Basis of Multidrug transport by the AcrB Multidrug Efflux Pump
Authors	:	Yu, E.W.; McDermott, G.; Nikaido, H.
Deposited on	:	2004-05-18
Resolution	:	3.23 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:

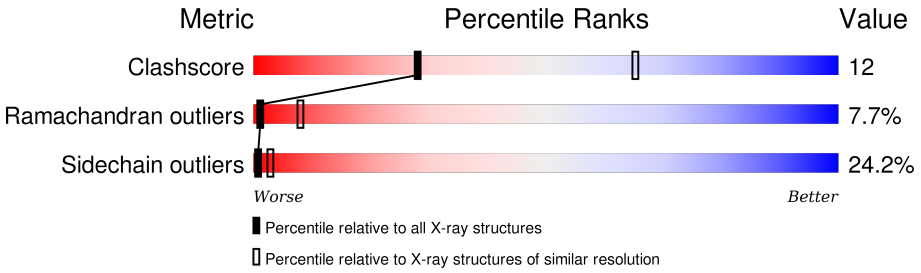
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.23 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))
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1049	55% 33% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7699 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1014	7699	4950	1273	1434	42	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ALA	ASN	ENGINEERED	UNP P31224

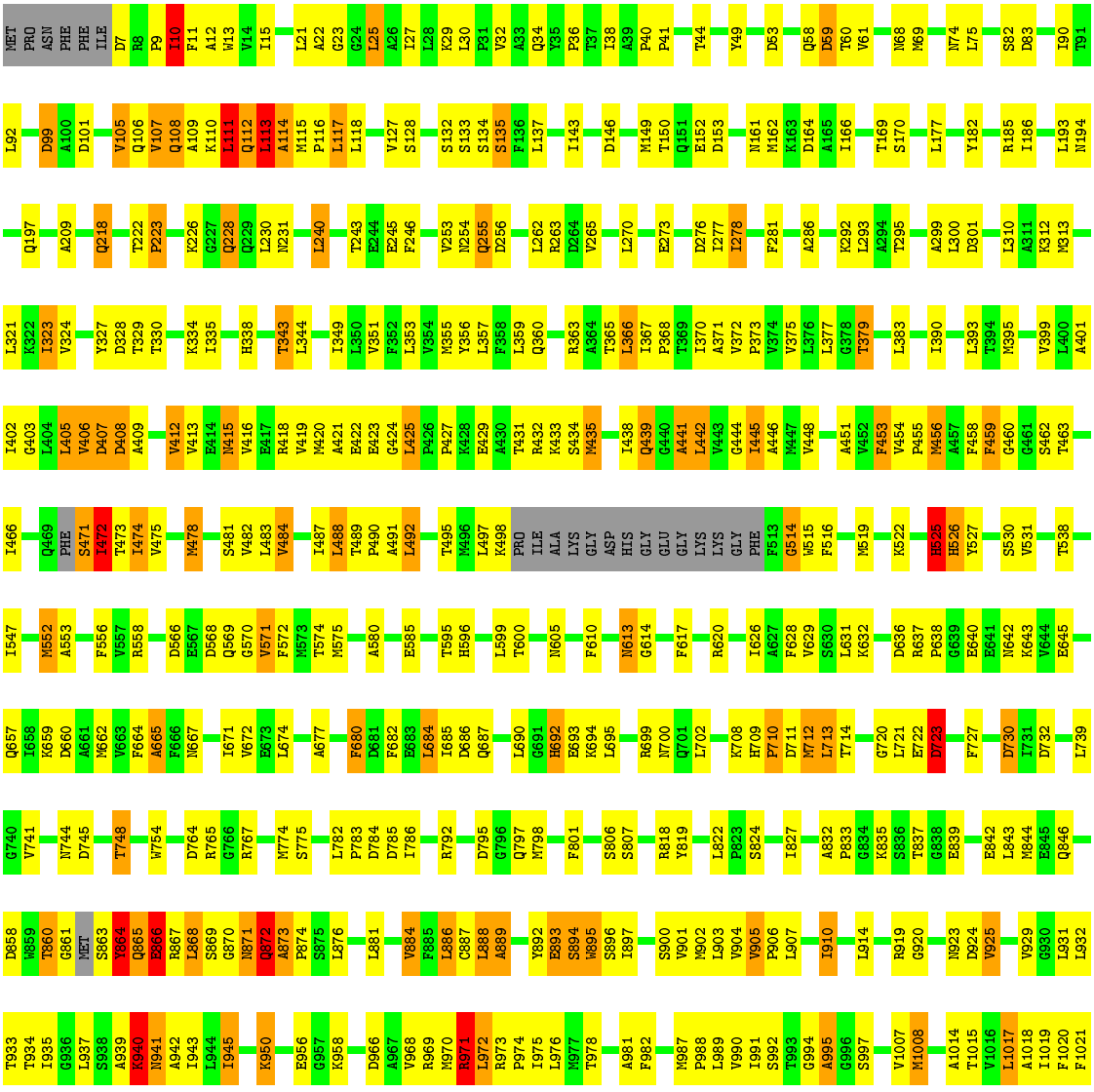
3 Residue-property plots (i)

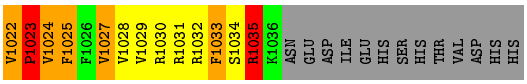
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: Acriflavine resistance protein B

Chain A:




V1022
P1023
V1024
F1025
F1026
V1027
V1028
V1029
R1030
R1031
R1032
F1033
S1034
R1035
K1036
ASN
GLU
ASP
ILE
GLU
HIS
SER
HIS
THR
VAL
ASP
HIS
HIS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	144.37Å 144.37Å 518.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	182.57 – 3.23	Depositor
% Data completeness (in resolution range)	(Not available) (182.57-3.23)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.275 , 0.338	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7699	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

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	0.35	0/7839	0.73	32/10644 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	723	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	971	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	680	PHE	N-CA-C	5.91	126.95	111.00
1	A	924	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	568	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	795	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	153	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	966	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	276	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	59	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	785	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	858	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	660	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	711	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	53	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	101	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	146	ASP	CB-CG-OD2	5.24	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	764	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	566	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	7	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	83	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	732	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	745	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	730	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	784	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	636	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	301	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	408	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	256	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	99	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	686	ASP	CB-CG-OD2	5.02	122.82	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	474	ILE	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	LEU	Peptide
1	A	525	HIS	Peptide
1	A	712	MET	Peptide

5.2 Too-close contacts (i)

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	7699	0	7856	182	1
All	All	7699	0	7856	182	1

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 (182) 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:613:ASN:HD22	1:A:613:ASN:C	1.82	0.83
1:A:950:LYS:HZ2	1:A:1028:VAL:HG11	1.45	0.81
1:A:525:HIS:HB2	1:A:526:HIS:HB2	1.64	0.80
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.70	0.73
1:A:950:LYS:NZ	1:A:1028:VAL:HG11	2.06	0.71
1:A:471:SER:O	1:A:473:THR:N	2.27	0.68
1:A:415:ASN:HB3	1:A:438:ILE:HD11	1.76	0.68
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.77	0.65
1:A:721:LEU:O	1:A:723:ASP:N	2.31	0.64
1:A:613:ASN:HD22	1:A:614:GLY:N	1.96	0.63
1:A:21:LEU:O	1:A:23:GLY:N	2.33	0.61
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.85	0.59
1:A:25:LEU:O	1:A:25:LEU:HD22	2.03	0.59
1:A:111:LEU:O	1:A:113:LEU:N	2.36	0.58
1:A:929:VAL:HA	1:A:932:LEU:HD12	1.83	0.58
1:A:864:TYR:O	1:A:865:GLN:HB2	2.04	0.58
1:A:454:VAL:N	1:A:455:PRO:HD2	2.19	0.58
1:A:525:HIS:HB2	1:A:526:HIS:CB	2.35	0.57
1:A:401:ALA:HB2	1:A:474:ILE:HG23	1.85	0.56
1:A:105:VAL:O	1:A:107:VAL:N	2.37	0.56
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.36	0.56
1:A:710:PRO:HB2	1:A:713:LEU:HA	1.87	0.56
1:A:613:ASN:C	1:A:613:ASN:ND2	2.54	0.56
1:A:13:TRP:HE1	1:A:492:LEU:HD12	1.69	0.56
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.86	0.56
1:A:68:ASN:ND2	1:A:111:LEU:O	2.38	0.56
1:A:525:HIS:CB	1:A:526:HIS:HB2	2.35	0.56
1:A:10:ILE:N	1:A:10:ILE:CD1	2.69	0.55
1:A:865:GLN:O	1:A:866:GLU:HB2	2.06	0.55
1:A:483:LEU:O	1:A:487:ILE:HD12	2.07	0.55
1:A:971:ARG:CG	1:A:971:ARG:HH11	2.19	0.55
1:A:971:ARG:C	1:A:971:ARG:HD2	2.28	0.54
1:A:372:VAL:N	1:A:373:PRO:HD2	2.23	0.54
1:A:338:HIS:ND1	1:A:338:HIS:O	2.41	0.54
1:A:1027:VAL:HG23	1:A:1028:VAL:H	1.72	0.54
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.90	0.54
1:A:278:ILE:HD12	1:A:613:ASN:HB3	1.88	0.54
1:A:860:THR:HG22	1:A:861:GLY:HA3	1.90	0.53
1:A:709:HIS:N	1:A:710:PRO:HD3	2.23	0.53
1:A:897:ILE:O	1:A:900:SER:OG	2.24	0.53
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:N	1:A:90:ILE:HD12	2.23	0.53
1:A:310:LEU:HD21	1:A:323:ILE:HD12	1.90	0.53
1:A:692:HIS:ND1	1:A:692:HIS:O	2.39	0.53
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.08	0.53
1:A:186:ILE:HD13	1:A:262:LEU:HD21	1.91	0.52
1:A:412:VAL:O	1:A:416:VAL:HG23	2.09	0.52
1:A:12:ALA:HB1	1:A:487:ILE:HG22	1.92	0.52
1:A:893:GLU:O	1:A:894:SER:CB	2.57	0.52
1:A:463:THR:HG23	1:A:466:ILE:HG21	1.92	0.52
1:A:905:VAL:HG23	1:A:906:PRO:HD3	1.90	0.52
1:A:888:LEU:HD21	1:A:943:ILE:HD11	1.91	0.52
1:A:10:ILE:HD13	1:A:11:PHE:H	1.75	0.52
1:A:664:PHE:O	1:A:665:ALA:CB	2.58	0.52
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.63	0.51
1:A:36:PRO:O	1:A:38:ILE:HG13	2.11	0.51
1:A:405:LEU:HD23	1:A:481:SER:HB3	1.92	0.51
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.93	0.51
1:A:41:PRO:HB3	1:A:295:THR:HG22	1.92	0.51
1:A:407:ASP:CG	1:A:978:THR:HG21	2.31	0.51
1:A:863:SER:O	1:A:865:GLN:NE2	2.45	0.50
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.46	0.50
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.92	0.50
1:A:893:GLU:O	1:A:894:SER:HB3	2.12	0.50
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.93	0.49
1:A:338:HIS:O	1:A:338:HIS:CG	2.65	0.49
1:A:895:TRP:CE3	1:A:895:TRP:HA	2.47	0.49
1:A:939:ALA:O	1:A:940:LYS:O	2.30	0.49
1:A:117:LEU:N	1:A:117:LEU:HD23	2.28	0.49
1:A:108:GLN:O	1:A:109:ALA:HB3	2.12	0.49
1:A:987:MET:N	1:A:988:PRO:HD2	2.27	0.49
1:A:458:PHE:O	1:A:459:PHE:O	2.30	0.49
1:A:409:ALA:O	1:A:413:VAL:HG23	2.13	0.49
1:A:439:GLN:CD	1:A:439:GLN:C	2.71	0.49
1:A:870:GLY:CA	1:A:871:ASN:C	2.82	0.49
1:A:870:GLY:HA2	1:A:872:GLN:N	2.28	0.49
1:A:425:LEU:C	1:A:427:PRO:HD2	2.33	0.48
1:A:475:VAL:HG13	1:A:478:MET:CE	2.43	0.48
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.96	0.48
1:A:435:MET:HA	1:A:438:ILE:HB	1.95	0.48
1:A:894:SER:O	1:A:895:TRP:CE3	2.66	0.48
1:A:870:GLY:HA3	1:A:871:ASN:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HA	1:A:445:ILE:HD11	1.94	0.48
1:A:108:GLN:C	1:A:110:LYS:H	2.17	0.48
1:A:886:LEU:O	1:A:889:ALA:HB3	2.13	0.48
1:A:487:ILE:HG22	1:A:488:LEU:N	2.29	0.48
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.95	0.48
1:A:570:GLY:O	1:A:571:VAL:HG23	2.14	0.48
1:A:727:PHE:CZ	1:A:783:PRO:HB3	2.49	0.47
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.48	0.47
1:A:527:TYR:O	1:A:531:VAL:HG23	2.14	0.47
1:A:133:SER:O	1:A:135:SER:N	2.47	0.47
1:A:10:ILE:N	1:A:10:ILE:HD12	2.29	0.47
1:A:940:LYS:O	1:A:942:ALA:N	2.47	0.47
1:A:441:ALA:O	1:A:444:GLY:N	2.48	0.47
1:A:105:VAL:O	1:A:108:GLN:N	2.48	0.47
1:A:895:TRP:HA	1:A:895:TRP:HE3	1.80	0.47
1:A:420:MET:HG2	1:A:425:LEU:O	2.14	0.46
1:A:685:ILE:HD11	1:A:819:TYR:CD2	2.50	0.46
1:A:514:GLY:O	1:A:516:PHE:N	2.48	0.46
1:A:971:ARG:HH11	1:A:971:ARG:HG2	1.81	0.46
1:A:870:GLY:CA	1:A:872:GLN:N	2.79	0.46
1:A:222:THR:HB	1:A:223:PRO:HD3	1.98	0.46
1:A:68:ASN:HD21	1:A:113:LEU:HD12	1.81	0.46
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.50	0.46
1:A:240:LEU:HD12	1:A:245:GLU:HB3	1.97	0.46
1:A:92:LEU:HD22	1:A:107:VAL:CG2	2.45	0.45
1:A:460:GLY:N	1:A:872:GLN:HE22	2.14	0.45
1:A:904:VAL:HA	1:A:907:LEU:HD13	1.98	0.45
1:A:931:LEU:O	1:A:935:ILE:HD12	2.16	0.45
1:A:373:PRO:O	1:A:377:LEU:HG	2.16	0.45
1:A:940:LYS:O	1:A:941:ASN:C	2.54	0.45
1:A:383:LEU:HD11	1:A:473:THR:HG23	1.99	0.45
1:A:471:SER:OG	1:A:472:ILE:N	2.49	0.45
1:A:112:GLN:C	1:A:114:ALA:H	2.19	0.45
1:A:832:ALA:HB1	1:A:833:PRO:HD2	1.99	0.45
1:A:712:MET:O	1:A:713:LEU:O	2.35	0.45
1:A:682:PHE:HB3	1:A:827:ILE:HB	1.99	0.45
1:A:475:VAL:HG13	1:A:478:MET:HE3	1.99	0.45
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.99	0.44
1:A:572:PHE:CE2	1:A:629:VAL:HG11	2.52	0.44
1:A:867:ARG:HB3	1:A:868:LEU:HG	1.99	0.44
1:A:489:THR:HB	1:A:490:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:TYR:CG	1:A:865:GLN:N	2.86	0.44
1:A:401:ALA:HB2	1:A:474:ILE:CG2	2.46	0.44
1:A:484:VAL:HG22	1:A:488:LEU:HD23	1.99	0.44
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.99	0.44
1:A:453:PHE:CE2	1:A:474:ILE:HB	2.53	0.44
1:A:68:ASN:ND2	1:A:113:LEU:HD12	2.33	0.44
1:A:970:MET:O	1:A:971:ARG:HB3	2.17	0.43
1:A:975:ILE:HD12	1:A:1019:ILE:HD13	2.00	0.43
1:A:448:VAL:HA	1:A:451:ALA:HB3	2.00	0.43
1:A:685:ILE:HD11	1:A:819:TYR:HD2	1.82	0.43
1:A:892:TYR:CD2	1:A:897:ILE:HG21	2.53	0.43
1:A:277:ILE:O	1:A:277:ILE:HD12	2.19	0.43
1:A:1033:PHE:O	1:A:1035:ARG:N	2.49	0.43
1:A:674:LEU:HD12	1:A:867:ARG:NH1	2.33	0.43
1:A:228:GLN:HE21	1:A:228:GLN:HA	1.82	0.43
1:A:925:VAL:O	1:A:929:VAL:HG23	2.18	0.43
1:A:488:LEU:O	1:A:491:ALA:N	2.51	0.43
1:A:379:THR:O	1:A:383:LEU:HG	2.19	0.43
1:A:835:LYS:HD3	1:A:839:GLU:HB3	2.01	0.43
1:A:972:LEU:C	1:A:972:LEU:HD13	2.39	0.43
1:A:973:ARG:HB3	1:A:974:PRO:HD3	2.01	0.43
1:A:552:MET:HA	1:A:910:ILE:HD12	2.00	0.42
1:A:945:ILE:HA	1:A:971:ARG:CZ	2.49	0.42
1:A:117:LEU:N	1:A:117:LEU:CD2	2.82	0.42
1:A:1014:ALA:O	1:A:1018:ALA:HB3	2.19	0.42
1:A:873:ALA:O	1:A:874:PRO:C	2.58	0.42
1:A:371:ALA:O	1:A:375:VAL:HG23	2.20	0.42
1:A:886:LEU:O	1:A:888:LEU:N	2.53	0.42
1:A:605:ASN:HD21	1:A:642:ASN:ND2	2.17	0.42
1:A:631:LEU:HD13	1:A:637:ARG:NH1	2.35	0.42
1:A:351:VAL:CG2	1:A:981:ALA:HB1	2.47	0.42
1:A:744:ASN:O	1:A:748:THR:HG22	2.19	0.42
1:A:246:PHE:O	1:A:262:LEU:HD23	2.20	0.42
1:A:1024:VAL:N	1:A:1027:VAL:HG22	2.35	0.41
1:A:525:HIS:CA	1:A:526:HIS:HB2	2.51	0.41
1:A:112:GLN:C	1:A:114:ALA:N	2.73	0.41
1:A:937:LEU:HD11	1:A:982:PHE:CE1	2.55	0.41
1:A:1027:VAL:O	1:A:1028:VAL:C	2.59	0.41
1:A:525:HIS:HB2	1:A:526:HIS:CG	2.55	0.41
1:A:968:VAL:HA	1:A:971:ARG:NE	2.34	0.41
1:A:61:VAL:HA	1:A:118:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:HIS:O	1:A:600:THR:HG22	2.20	0.41
1:A:994:GLY:O	1:A:995:ALA:HB2	2.21	0.41
1:A:115:MET:N	1:A:116:PRO:CD	2.84	0.41
1:A:111:LEU:HD23	1:A:112:GLN:H	1.85	0.41
1:A:343:THR:CG2	1:A:989:LEU:HD21	2.50	0.41
1:A:356:TYR:HD1	1:A:365:THR:HG21	1.86	0.41
1:A:684:LEU:HD12	1:A:685:ILE:N	2.36	0.41
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.69	0.41
1:A:367:ILE:N	1:A:368:PRO:HD2	2.35	0.41
1:A:553:ALA:O	1:A:556:PHE:HB3	2.21	0.41
1:A:40:PRO:HA	1:A:41:PRO:HD3	1.93	0.41
1:A:456:MET:HA	1:A:876:LEU:HB3	2.03	0.41
1:A:390:ILE:HG23	1:A:395:MET:SD	2.61	0.40
1:A:990:VAL:HG21	1:A:1008:MET:SD	2.61	0.40
1:A:610:PHE:HB3	1:A:628:PHE:HB2	2.03	0.40
1:A:448:VAL:HG11	1:A:888:LEU:HD23	2.02	0.40
1:A:365:THR:HG23	1:A:365:THR:O	2.21	0.40
1:A:1024:VAL:H	1:A:1027:VAL:HG22	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:O	1:A:596:HIS:NE2[10_445]	1.55	0.65

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	1006/1049 (96%)	809 (80%)	120 (12%)	77 (8%)	1 8

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ALA
1	A	106	GLN
1	A	112	GLN
1	A	134	SER
1	A	135	SER
1	A	255	GLN
1	A	424	GLY
1	A	442	LEU
1	A	459	PHE
1	A	515	TRP
1	A	665	ALA
1	A	713	LEU
1	A	722	GLU
1	A	864	TYR
1	A	866	GLU
1	A	887	CYS
1	A	889	ALA
1	A	894	SER
1	A	940	LYS
1	A	941	ASN
1	A	971	ARG
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	1034	SER
1	A	9	PRO
1	A	10	ILE
1	A	105	VAL
1	A	114	ALA
1	A	152	GLU
1	A	161	ASN
1	A	170	SER
1	A	209	ALA
1	A	327	TYR
1	A	472	ILE
1	A	488	LEU
1	A	525	HIS
1	A	580	ALA
1	A	638	PRO
1	A	671	ILE
1	A	720	GLY
1	A	775	SER
1	A	871	ASN

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Mol	Chain	Res	Type
1	A	872	GLN
1	A	920	GLY
1	A	995	ALA
1	A	1025	PHE
1	A	1027	VAL
1	A	1033	PHE
1	A	74	ASN
1	A	113	LEU
1	A	299	ALA
1	A	405	LEU
1	A	421	ALA
1	A	710	PRO
1	A	723	ASP
1	A	886	LEU
1	A	893	GLU
1	A	896	SER
1	A	1035	ARG
1	A	34	GLN
1	A	75	LEU
1	A	366	LEU
1	A	571	VAL
1	A	677	ALA
1	A	837	THR
1	A	956	GLU
1	A	441	ALA
1	A	495	THR
1	A	538	THR
1	A	672	VAL
1	A	884	VAL
1	A	223	PRO
1	A	514	GLY
1	A	1029	VAL
1	A	626	ILE
1	A	873	ALA

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	824/854 (96%)	625 (76%)	199 (24%)	1 3

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	15	ILE
1	A	25	LEU
1	A	27	ILE
1	A	29	LYS
1	A	30	LEU
1	A	32	VAL
1	A	44	THR
1	A	49	TYR
1	A	58	GLN
1	A	59	ASP
1	A	69	MET
1	A	82	SER
1	A	99	ASP
1	A	107	VAL
1	A	108	GLN
1	A	111	LEU
1	A	113	LEU
1	A	117	LEU
1	A	127	VAL
1	A	128	SER
1	A	132	SER
1	A	137	LEU
1	A	149	MET
1	A	150	THR
1	A	162	MET
1	A	164	ASP
1	A	166	ILE
1	A	169	THR
1	A	177	LEU
1	A	182	TYR
1	A	185	ARG
1	A	193	LEU
1	A	194	ASN
1	A	197	GLN
1	A	218	GLN
1	A	228	GLN
1	A	230	LEU

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Mol	Chain	Res	Type
1	A	240	LEU
1	A	243	THR
1	A	253	VAL
1	A	254	ASN
1	A	255	GLN
1	A	263	ARG
1	A	265	VAL
1	A	270	LEU
1	A	273	GLU
1	A	278	ILE
1	A	292	LYS
1	A	293	LEU
1	A	300	LEU
1	A	312	LYS
1	A	313	MET
1	A	321	LEU
1	A	323	ILE
1	A	328	ASP
1	A	329	THR
1	A	330	THR
1	A	334	LYS
1	A	335	ILE
1	A	343	THR
1	A	349	ILE
1	A	353	LEU
1	A	355	MET
1	A	357	LEU
1	A	359	LEU
1	A	360	GLN
1	A	363	ARG
1	A	366	LEU
1	A	370	ILE
1	A	379	THR
1	A	393	LEU
1	A	406	VAL
1	A	408	ASP
1	A	412	VAL
1	A	415	ASN
1	A	418	ARG
1	A	419	VAL
1	A	422	GLU
1	A	423	GLU

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Mol	Chain	Res	Type
1	A	425	LEU
1	A	429	GLU
1	A	431	THR
1	A	432	ARG
1	A	433	LYS
1	A	434	SER
1	A	435	MET
1	A	439	GLN
1	A	445	ILE
1	A	453	PHE
1	A	456	MET
1	A	462	SER
1	A	471	SER
1	A	472	ILE
1	A	474	ILE
1	A	478	MET
1	A	484	VAL
1	A	492	LEU
1	A	497	LEU
1	A	498	LYS
1	A	519	MET
1	A	522	LYS
1	A	526	HIS
1	A	530	SER
1	A	547	ILE
1	A	552	MET
1	A	558	ARG
1	A	569	GLN
1	A	574	THR
1	A	575	MET
1	A	585	GLU
1	A	613	ASN
1	A	617	PHE
1	A	620	ARG
1	A	632	LYS
1	A	640	GLU
1	A	643	LYS
1	A	645	GLU
1	A	657	GLN
1	A	659	LYS
1	A	662	MET
1	A	667	ASN

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Mol	Chain	Res	Type
1	A	680	PHE
1	A	684	LEU
1	A	687	GLN
1	A	690	LEU
1	A	692	HIS
1	A	693	GLU
1	A	694	LYS
1	A	695	LEU
1	A	699	ARG
1	A	700	ASN
1	A	702	LEU
1	A	708	LYS
1	A	714	THR
1	A	730	ASP
1	A	739	LEU
1	A	741	VAL
1	A	748	THR
1	A	765	ARG
1	A	767	ARG
1	A	774	MET
1	A	782	LEU
1	A	792	ARG
1	A	797	GLN
1	A	798	MET
1	A	801	PHE
1	A	806	SER
1	A	807	SER
1	A	818	ARG
1	A	822	LEU
1	A	824	SER
1	A	842	GLU
1	A	843	LEU
1	A	844	MET
1	A	846	GLN
1	A	860	THR
1	A	864	TYR
1	A	865	GLN
1	A	866	GLU
1	A	868	LEU
1	A	869	SER
1	A	872	GLN
1	A	881	LEU

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Mol	Chain	Res	Type
1	A	884	VAL
1	A	888	LEU
1	A	895	TRP
1	A	902	MET
1	A	903	LEU
1	A	905	VAL
1	A	910	ILE
1	A	914	LEU
1	A	919	ARG
1	A	923	ASN
1	A	925	VAL
1	A	933	THR
1	A	934	THR
1	A	940	LYS
1	A	945	ILE
1	A	950	LYS
1	A	958	LYS
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU
1	A	991	ILE
1	A	992	SER
1	A	997	SER
1	A	1007	VAL
1	A	1008	MET
1	A	1017	LEU
1	A	1020	PHE
1	A	1022	VAL
1	A	1023	PRO
1	A	1024	VAL
1	A	1030	ARG
1	A	1031	ARG
1	A	1032	ARG
1	A	1035	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	68	ASN
1	A	125	GLN

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Mol	Chain	Res	Type
1	A	161	ASN
1	A	181	GLN
1	A	194	ASN
1	A	213	GLN
1	A	218	GLN
1	A	228	GLN
1	A	254	ASN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	657	GLN
1	A	760	ASN
1	A	797	GLN
1	A	872	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.