



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:11 PM UTC

PDB ID : 1OY6 / pdb_00001oy6
Title : Structural Basis of the Multiple Binding Capacity of the AcrB Multidrug Efflux Pump
Authors : Yu, E.W.; McDermott, G.; Zgurskaya, H.I.; Nikaido, H.; Koshland Jr., D.E.
Deposited on : 2003-04-03
Resolution : 3.68 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

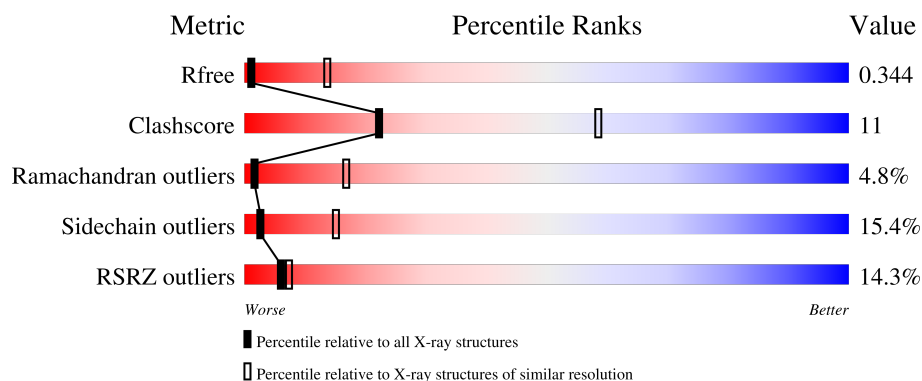
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

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	1049	14% 65% 26% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7639 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.

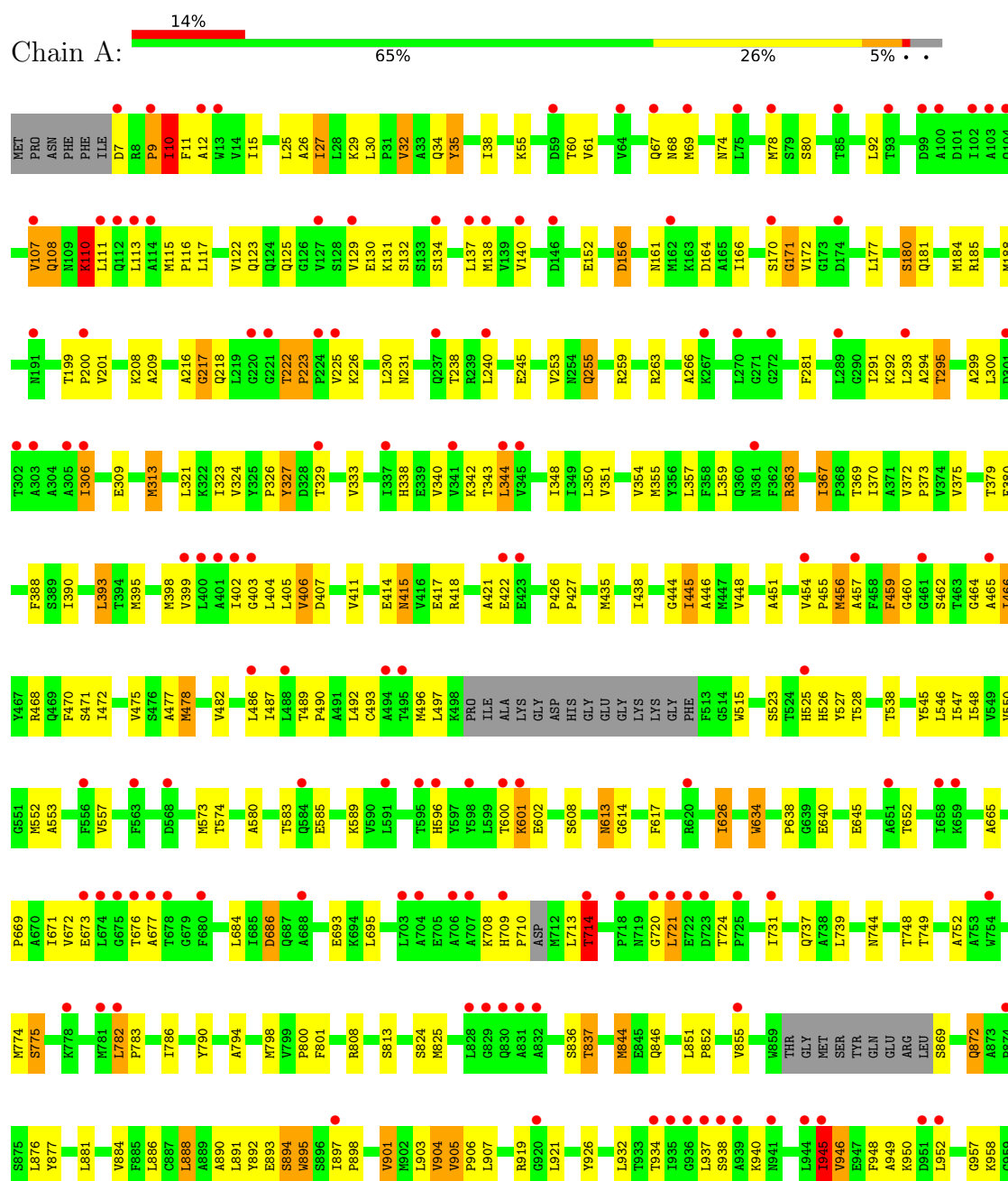
- Molecule 1 is a protein called Acriflavine resistance protein B.

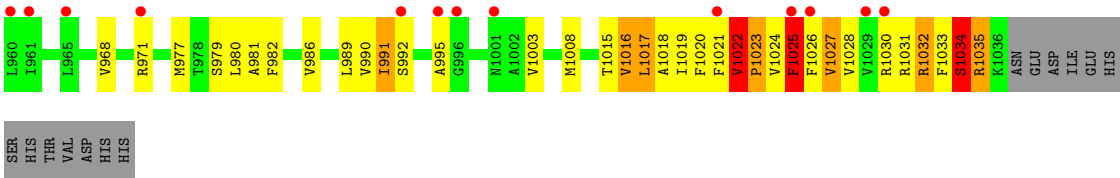
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1006	7639	4916	1262	1419	42	0	0	0

3 Residue-property plots [i](#)

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: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	143.56Å 143.56Å 519.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 3.68 46.00 – 3.68	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.00-3.68) 99.5 (46.00-3.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.272 , 0.330 0.351 , 0.344	Depositor DCC
R_{free} test set	1170 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	138.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7639	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.49	0/7779	0.83	2/10563 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	PRO	N-CA-C	7.91	120.35	110.70
1	A	10	ILE	N-CA-C	5.39	120.56	109.34

There are no chirality outliers.

There are no planarity outliers.

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	7639	0	7800	163	0
All	All	7639	0	7800	163	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 (163) 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:351:VAL:HG23	1:A:981:ALA:HB1	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ASN:HD22	1:A:613:ASN:C	1.88	0.81
1:A:721:LEU:HD22	1:A:825:MET:HE3	1.65	0.79
1:A:200:PRO:HD2	1:A:749:THR:HG22	1.69	0.72
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.71	0.71
1:A:596:HIS:O	1:A:600:THR:HG22	1.93	0.68
1:A:456:MET:SD	1:A:932:LEU:HD11	2.33	0.68
1:A:613:ASN:HD22	1:A:614:GLY:N	1.93	0.66
1:A:903:LEU:O	1:A:906:PRO:HD2	1.95	0.66
1:A:300:LEU:HD22	1:A:333:VAL:HG11	1.79	0.65
1:A:937:LEU:HD11	1:A:982:PHE:CE1	2.33	0.63
1:A:897:ILE:HG23	1:A:946:VAL:HG11	1.82	0.61
1:A:1027:VAL:HG23	1:A:1028:VAL:H	1.66	0.61
1:A:1022:VAL:O	1:A:1023:PRO:O	2.18	0.61
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.83	0.61
1:A:686:ASP:CB	1:A:695:LEU:HD12	2.33	0.59
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.83	0.59
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.85	0.59
1:A:950:LYS:NZ	1:A:1028:VAL:HG11	2.18	0.58
1:A:686:ASP:HB2	1:A:695:LEU:HD12	1.84	0.58
1:A:456:MET:HG2	1:A:876:LEU:HD13	1.86	0.57
1:A:894:SER:O	1:A:895:TRP:HB2	2.03	0.57
1:A:415:ASN:C	1:A:415:ASN:HD22	2.13	0.57
1:A:752:ALA:O	1:A:774:MET:HA	2.05	0.57
1:A:372:VAL:N	1:A:373:PRO:HD2	2.21	0.56
1:A:613:ASN:C	1:A:613:ASN:ND2	2.56	0.56
1:A:379:THR:HB	1:A:398:MET:HE1	1.88	0.55
1:A:32:VAL:HG23	1:A:300:LEU:CD2	2.37	0.55
1:A:291:ILE:HG21	1:A:306:ILE:HD11	1.87	0.55
1:A:354:VAL:HG13	1:A:980:LEU:HD23	1.89	0.55
1:A:454:VAL:N	1:A:455:PRO:HD2	2.21	0.55
1:A:525:HIS:O	1:A:527:TYR:N	2.39	0.55
1:A:359:LEU:HD21	1:A:977:MET:HE1	1.89	0.54
1:A:1018:ALA:CB	1:A:1024:VAL:HG21	2.38	0.54
1:A:240:LEU:HD12	1:A:245:GLU:HB3	1.89	0.54
1:A:326:PRO:O	1:A:327:TYR:C	2.50	0.54
1:A:393:LEU:HD11	1:A:466:ILE:HA	1.90	0.53
1:A:1016:VAL:O	1:A:1017:LEU:HB2	2.08	0.53
1:A:919:ARG:HB3	1:A:921:LEU:HD23	1.90	0.53
1:A:110:LYS:HZ2	1:A:113:LEU:HD12	1.74	0.52
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.90	0.52
1:A:926:TYR:HB3	1:A:1003:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:TRP:H	1:A:634:TRP:CD1	2.28	0.52
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.92	0.52
1:A:111:LEU:C	1:A:111:LEU:HD23	2.34	0.51
1:A:294:ALA:O	1:A:295:THR:C	2.52	0.51
1:A:950:LYS:HZ2	1:A:1028:VAL:HG11	1.75	0.51
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.92	0.51
1:A:390:ILE:HG23	1:A:395:MET:SD	2.51	0.51
1:A:580:ALA:HB1	1:A:724:THR:HG22	1.91	0.51
1:A:903:LEU:O	1:A:907:LEU:HD13	2.12	0.50
1:A:892:TYR:HB3	1:A:897:ILE:HG21	1.93	0.50
1:A:652:THR:HG23	1:A:665:ALA:HB3	1.94	0.50
1:A:1032:ARG:CG	1:A:1032:ARG:HH11	2.24	0.50
1:A:475:VAL:HA	1:A:478:MET:HE3	1.95	0.49
1:A:890:ALA:C	1:A:891:LEU:HD22	2.37	0.49
1:A:945:ILE:HG22	1:A:945:ILE:O	2.13	0.49
1:A:27:ILE:CD1	1:A:390:ILE:HD11	2.44	0.48
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.95	0.48
1:A:222:THR:HB	1:A:223:PRO:HD3	1.95	0.48
1:A:240:LEU:HD12	1:A:245:GLU:CB	2.42	0.48
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.96	0.48
1:A:774:MET:O	1:A:775:SER:HB3	2.14	0.48
1:A:34:GLN:HG2	1:A:333:VAL:HG22	1.96	0.47
1:A:950:LYS:N	1:A:950:LYS:HE2	2.30	0.47
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.15	0.47
1:A:32:VAL:HG23	1:A:300:LEU:HD21	1.96	0.47
1:A:188:MET:N	1:A:775:SER:HA	2.29	0.47
1:A:370:ILE:HG22	1:A:370:ILE:O	2.14	0.47
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.49	0.47
1:A:459:PHE:C	1:A:872:GLN:HE22	2.21	0.47
1:A:380:PHE:CE2	1:A:398:MET:HE2	2.50	0.47
1:A:546:LEU:O	1:A:550:VAL:HG23	2.15	0.47
1:A:950:LYS:HZ2	1:A:1028:VAL:CG1	2.28	0.47
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.50	0.47
1:A:523:SER:O	1:A:528:THR:OG1	2.23	0.46
1:A:388:PHE:HE1	1:A:472:ILE:HG21	1.81	0.46
1:A:489:THR:HB	1:A:490:PRO:HD3	1.95	0.46
1:A:527:TYR:OH	1:A:968:VAL:HG21	2.16	0.46
1:A:907:LEU:HD21	1:A:1022:VAL:HG12	1.95	0.46
1:A:309:GLU:HG3	1:A:313:MET:HE1	1.98	0.46
1:A:676:THR:O	1:A:677:ALA:HB3	2.16	0.46
1:A:201:VAL:HG22	1:A:748:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:HB1	1:A:487:ILE:HG22	1.97	0.46
1:A:367:ILE:HG12	1:A:492:LEU:HD22	1.98	0.46
1:A:897:ILE:N	1:A:898:PRO:CD	2.78	0.46
1:A:402:ILE:HA	1:A:405:LEU:HD12	1.97	0.45
1:A:444:GLY:HA2	1:A:891:LEU:HD23	1.98	0.45
1:A:684:LEU:HD11	1:A:855:VAL:CG1	2.45	0.45
1:A:1033:PHE:O	1:A:1034:SER:C	2.59	0.45
1:A:904:VAL:HG13	1:A:1024:VAL:HG22	1.98	0.45
1:A:709:HIS:O	1:A:709:HIS:CG	2.70	0.45
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.98	0.45
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.98	0.45
1:A:363:ARG:HB2	1:A:496:MET:HE1	1.99	0.44
1:A:713:LEU:C	1:A:714:THR:HG1	2.25	0.44
1:A:937:LEU:HD11	1:A:982:PHE:CZ	2.52	0.44
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.98	0.44
1:A:457:ALA:HB2	1:A:471:SER:OG	2.18	0.44
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.48	0.44
1:A:407:ASP:O	1:A:411:VAL:HG23	2.18	0.44
1:A:445:ILE:HD13	1:A:940:LYS:HD2	1.98	0.44
1:A:686:ASP:HB3	1:A:695:LEU:HD12	1.99	0.44
1:A:108:GLN:HB2	1:A:129:VAL:HG21	2.00	0.44
1:A:405:LEU:HD21	1:A:477:ALA:HB1	1.99	0.44
1:A:774:MET:O	1:A:775:SER:CB	2.66	0.44
1:A:465:ALA:HA	1:A:468:ARG:HB3	1.99	0.44
1:A:340:VAL:HG11	1:A:395:MET:HB3	2.00	0.43
1:A:493:CYS:SG	1:A:497:LEU:HD22	2.59	0.43
1:A:527:TYR:OH	1:A:1019:ILE:O	2.29	0.43
1:A:713:LEU:O	1:A:714:THR:HG23	2.17	0.43
1:A:790:TYR:HD1	1:A:800:PRO:HA	1.83	0.43
1:A:872:GLN:CG	1:A:876:LEU:HD11	2.48	0.43
1:A:573:MET:HE3	1:A:626:ILE:HD11	2.01	0.43
1:A:348:ILE:O	1:A:351:VAL:HG12	2.18	0.43
1:A:744:ASN:O	1:A:748:THR:HG22	2.18	0.43
1:A:600:THR:HG23	1:A:601:LYS:HG3	1.99	0.43
1:A:949:ALA:HA	1:A:952:LEU:HD12	2.00	0.43
1:A:1033:PHE:O	1:A:1035:ARG:N	2.51	0.43
1:A:888:LEU:HD11	1:A:901:VAL:CG1	2.49	0.43
1:A:344:LEU:C	1:A:344:LEU:HD13	2.44	0.43
1:A:986:VAL:O	1:A:990:VAL:HG23	2.19	0.43
1:A:456:MET:CE	1:A:932:LEU:HD11	2.49	0.42
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PHE:CZ	1:A:398:MET:HE2	2.55	0.42
1:A:888:LEU:O	1:A:892:TYR:HB2	2.19	0.42
1:A:10:ILE:CD1	1:A:10:ILE:N	2.82	0.42
1:A:363:ARG:HB2	1:A:496:MET:SD	2.59	0.42
1:A:710:PRO:C	1:A:713:LEU:HA	2.44	0.42
1:A:446:ALA:HB2	1:A:482:VAL:HG21	2.02	0.42
1:A:460:GLY:N	1:A:872:GLN:HE22	2.18	0.42
1:A:115:MET:N	1:A:116:PRO:CD	2.83	0.42
1:A:92:LEU:HD13	1:A:107:VAL:HG21	2.01	0.42
1:A:26:ALA:O	1:A:30:LEU:HB2	2.20	0.42
1:A:782:LEU:HB3	1:A:783:PRO:HD2	2.02	0.42
1:A:216:ALA:O	1:A:217:GLY:O	2.38	0.41
1:A:445:ILE:HD13	1:A:940:LYS:CD	2.50	0.41
1:A:986:VAL:HG12	1:A:990:VAL:CG2	2.51	0.41
1:A:414:GLU:CD	1:A:414:GLU:C	2.88	0.41
1:A:338:HIS:O	1:A:342:LYS:HB2	2.20	0.41
1:A:468:ARG:O	1:A:472:ILE:HG22	2.21	0.41
1:A:672:VAL:HG12	1:A:673:GLU:N	2.36	0.41
1:A:156:ASP:HA	1:A:181:GLN:HA	2.02	0.41
1:A:170:SER:O	1:A:171:GLY:C	2.64	0.41
1:A:1025:PHE:H	1:A:1027:VAL:HG22	1.85	0.41
1:A:399:VAL:HA	1:A:402:ILE:HD12	2.03	0.41
1:A:836:SER:O	1:A:837:THR:C	2.62	0.41
1:A:27:ILE:HD11	1:A:390:ILE:HD11	2.03	0.41
1:A:188:MET:HA	1:A:266:ALA:HB2	2.02	0.41
1:A:451:ALA:HB1	1:A:884:VAL:HA	2.02	0.41
1:A:482:VAL:O	1:A:486:LEU:HG	2.21	0.41
1:A:877:TYR:O	1:A:881:LEU:HG	2.21	0.41
1:A:32:VAL:HG23	1:A:300:LEU:HD23	2.02	0.41
1:A:435:MET:HA	1:A:438:ILE:HB	2.03	0.41
1:A:553:ALA:O	1:A:557:VAL:HG23	2.21	0.41
1:A:9:PRO:C	1:A:10:ILE:CD1	2.94	0.40
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.70	0.40
1:A:957:GLY:O	1:A:958:LYS:C	2.64	0.40
1:A:60:THR:HG23	1:A:61:VAL:HG23	2.03	0.40
1:A:177:LEU:HD12	1:A:180:SER:HA	2.03	0.40
1:A:10:ILE:HD13	1:A:11:PHE:H	1.86	0.40
1:A:327:TYR:C	1:A:327:TYR:CD2	2.99	0.40
1:A:414:GLU:O	1:A:417:GLU:HB2	2.21	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	998/1049 (95%)	834 (84%)	116 (12%)	48 (5%)	2	17

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	10	ILE
1	A	134	SER
1	A	217	GLY
1	A	255	GLN
1	A	427	PRO
1	A	459	PHE
1	A	526	HIS
1	A	671	ILE
1	A	775	SER
1	A	794	ALA
1	A	837	THR
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	1034	SER
1	A	152	GLU
1	A	209	ALA
1	A	295	THR
1	A	327	TYR
1	A	464	GLY
1	A	714	THR
1	A	894	SER
1	A	971	ARG
1	A	1025	PHE
1	A	1027	VAL
1	A	74	ASN
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	421	ALA
1	A	720	GLY
1	A	992	SER
1	A	1022	VAL
1	A	35	TYR
1	A	110	LYS
1	A	184	MET
1	A	844	MET
1	A	171	GLY
1	A	538	THR
1	A	669	PRO
1	A	995	ALA
1	A	299	ALA
1	A	945	ILE
1	A	946	VAL
1	A	991	ILE
1	A	223	PRO
1	A	1016	VAL
1	A	466	ILE
1	A	638	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	818/855 (96%)	692 (85%)	126 (15%)	2 15

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	ILE
1	A	15	ILE
1	A	25	LEU
1	A	27	ILE
1	A	29	LYS

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Mol	Chain	Res	Type
1	A	32	VAL
1	A	35	TYR
1	A	38	ILE
1	A	55	LYS
1	A	67	GLN
1	A	68	ASN
1	A	69	MET
1	A	78	MET
1	A	80	SER
1	A	107	VAL
1	A	108	GLN
1	A	110	LYS
1	A	117	LEU
1	A	122	VAL
1	A	123	GLN
1	A	125	GLN
1	A	130	GLU
1	A	131	LYS
1	A	132	SER
1	A	137	LEU
1	A	138	MET
1	A	140	VAL
1	A	156	ASP
1	A	164	ASP
1	A	166	ILE
1	A	180	SER
1	A	185	ARG
1	A	199	THR
1	A	208	LYS
1	A	222	THR
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	238	THR
1	A	253	VAL
1	A	255	GLN
1	A	259	ARG
1	A	263	ARG
1	A	292	LYS
1	A	293	LEU
1	A	306	ILE
1	A	313	MET

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Mol	Chain	Res	Type
1	A	321	LEU
1	A	323	ILE
1	A	329	THR
1	A	344	LEU
1	A	350	LEU
1	A	355	MET
1	A	357	LEU
1	A	363	ARG
1	A	367	ILE
1	A	369	THR
1	A	393	LEU
1	A	404	LEU
1	A	406	VAL
1	A	415	ASN
1	A	418	ARG
1	A	422	GLU
1	A	445	ILE
1	A	448	VAL
1	A	456	MET
1	A	462	SER
1	A	470	PHE
1	A	478	MET
1	A	515	TRP
1	A	547	ILE
1	A	552	MET
1	A	574	THR
1	A	583	THR
1	A	585	GLU
1	A	589	LYS
1	A	601	LYS
1	A	602	GLU
1	A	608	SER
1	A	613	ASN
1	A	617	PHE
1	A	626	ILE
1	A	634	TRP
1	A	640	GLU
1	A	645	GLU
1	A	686	ASP
1	A	693	GLU
1	A	708	LYS
1	A	714	THR

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Mol	Chain	Res	Type
1	A	721	LEU
1	A	731	ILE
1	A	737	GLN
1	A	739	LEU
1	A	782	LEU
1	A	786	ILE
1	A	798	MET
1	A	801	PHE
1	A	808	ARG
1	A	813	SER
1	A	824	SER
1	A	844	MET
1	A	846	GLN
1	A	869	SER
1	A	872	GLN
1	A	886	LEU
1	A	888	LEU
1	A	893	GLU
1	A	895	TRP
1	A	901	VAL
1	A	904	VAL
1	A	905	VAL
1	A	934	THR
1	A	938	SER
1	A	945	ILE
1	A	948	PHE
1	A	991	ILE
1	A	1008	MET
1	A	1020	PHE
1	A	1022	VAL
1	A	1025	PHE
1	A	1030	ARG
1	A	1031	ARG
1	A	1032	ARG
1	A	1034	SER
1	A	1035	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	68	ASN

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	151	GLN
1	A	181	GLN
1	A	189	ASN
1	A	194	ASN
1	A	228	GLN
1	A	229	GLN
1	A	231	ASN
1	A	237	GLN
1	A	274	ASN
1	A	282	ASN
1	A	284	GLN
1	A	338	HIS
1	A	391	ASN
1	A	439	GLN
1	A	588	GLN
1	A	604	ASN
1	A	605	ASN
1	A	613	ASN
1	A	623	ASN
1	A	667	ASN
1	A	700	ASN
1	A	701	GLN
1	A	747	ASN
1	A	820	ASN
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 oligosaccharides 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	1006/1049 (95%)	0.92	144 (14%) 6 7	73, 102, 121, 144	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	ALA	6.5
1	A	402	ILE	6.5
1	A	935	ILE	6.4
1	A	67	GLN	5.9
1	A	399	VAL	5.5
1	A	945	ILE	5.4
1	A	600	THR	5.4
1	A	723	ASP	5.2
1	A	401	ALA	5.1
1	A	782	LEU	5.1
1	A	1021	PHE	5.0
1	A	658	ILE	4.8
1	A	591	LEU	4.5
1	A	1029	VAL	4.5
1	A	952	LEU	4.3
1	A	829	GLY	4.2
1	A	146	ASP	4.1
1	A	676	THR	4.1
1	A	595	THR	4.0
1	A	494	ALA	3.9
1	A	828	LEU	3.9
1	A	1030	ARG	3.9
1	A	85	THR	3.8
1	A	960	LEU	3.8
1	A	403	GLY	3.8
1	A	99	ASP	3.7
1	A	422	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	3.7
1	A	965	LEU	3.7
1	A	556	PHE	3.6
1	A	714	THR	3.6
1	A	830	GLN	3.6
1	A	936	GLY	3.5
1	A	874	PRO	3.4
1	A	337	ILE	3.3
1	A	596	HIS	3.3
1	A	620	ARG	3.2
1	A	127	VAL	3.2
1	A	237	GLN	3.2
1	A	706	ALA	3.2
1	A	465	ALA	3.2
1	A	961	ILE	3.1
1	A	113	LEU	3.1
1	A	100	ALA	3.1
1	A	677	ALA	3.0
1	A	302	THR	3.0
1	A	461	GLY	3.0
1	A	69	MET	3.0
1	A	134	SER	3.0
1	A	293	LEU	2.9
1	A	937	LEU	2.9
1	A	345	VAL	2.9
1	A	138	MET	2.8
1	A	1025	PHE	2.8
1	A	174	ASP	2.8
1	A	129	VAL	2.8
1	A	93	THR	2.8
1	A	78	MET	2.8
1	A	1026	PHE	2.8
1	A	400	LEU	2.7
1	A	678	THR	2.7
1	A	525	HIS	2.7
1	A	996	GLY	2.7
1	A	495	THR	2.7
1	A	306	ILE	2.7
1	A	951	ASP	2.7
1	A	920	GLY	2.6
1	A	721	LEU	2.6
1	A	486	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	992	SER	2.6
1	A	568	ASP	2.5
1	A	9	PRO	2.5
1	A	102	ILE	2.5
1	A	941	ASN	2.5
1	A	270	LEU	2.5
1	A	674	LEU	2.5
1	A	680	PHE	2.5
1	A	170	SER	2.5
1	A	938	SER	2.5
1	A	59	ASP	2.5
1	A	488	LEU	2.5
1	A	454	VAL	2.5
1	A	855	VAL	2.5
1	A	457	ALA	2.4
1	A	831	ALA	2.4
1	A	725	PRO	2.4
1	A	114	ALA	2.4
1	A	305	ALA	2.4
1	A	224	PRO	2.4
1	A	423	GLU	2.4
1	A	651	ALA	2.4
1	A	272	GLY	2.4
1	A	781	MET	2.4
1	A	584	GLN	2.3
1	A	703	LEU	2.3
1	A	140	VAL	2.3
1	A	934	THR	2.3
1	A	971	ARG	2.3
1	A	267	LYS	2.3
1	A	200	PRO	2.3
1	A	944	LEU	2.3
1	A	704	ALA	2.3
1	A	718	PRO	2.3
1	A	137	LEU	2.3
1	A	341	VAL	2.3
1	A	107	VAL	2.3
1	A	720	GLY	2.3
1	A	754	TRP	2.3
1	A	778	LYS	2.3
1	A	12	ALA	2.2
1	A	240	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	13	TRP	2.2
1	A	995	ALA	2.2
1	A	64	VAL	2.2
1	A	601	LYS	2.2
1	A	7	ASP	2.2
1	A	301	ASP	2.2
1	A	344	LEU	2.2
1	A	361	ASN	2.2
1	A	112	GLN	2.1
1	A	75	LEU	2.1
1	A	191	ASN	2.1
1	A	707	ALA	2.1
1	A	1001	ASN	2.1
1	A	221	GLY	2.1
1	A	563	PHE	2.1
1	A	673	GLU	2.1
1	A	722	GLU	2.1
1	A	832	ALA	2.1
1	A	104	GLN	2.1
1	A	709	HIS	2.1
1	A	162	MET	2.1
1	A	897	ILE	2.1
1	A	220	GLY	2.1
1	A	329	THR	2.0
1	A	659	LYS	2.0
1	A	731	ILE	2.0
1	A	103	ALA	2.0
1	A	939	ALA	2.0
1	A	598	TYR	2.0
1	A	289	LEU	2.0
1	A	688	ALA	2.0
1	A	675	GLY	2.0
1	A	225	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.