



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:43 PM UTC

PDB ID : 8PX7 / pdb_00008px7
Title : Structure of Bacterial Multidrug Efflux transporter AcrB, solved at wavelength 3.02 Å
Authors : El Omari, K.; Duman, R.; Mykhaylyk, V.; Orr, C.; Qu, F.; Beis, K.; Wagner, A.
Deposited on : 2023-07-22
Resolution : 3.40 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

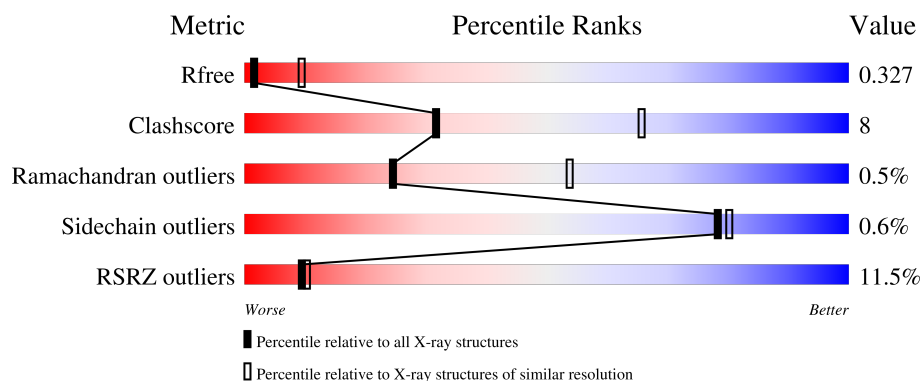
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	1053	11% 80% 17% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7854 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1034	Total	C	N	O	S	0	0	0
			7854	5055	1296	1459	44			

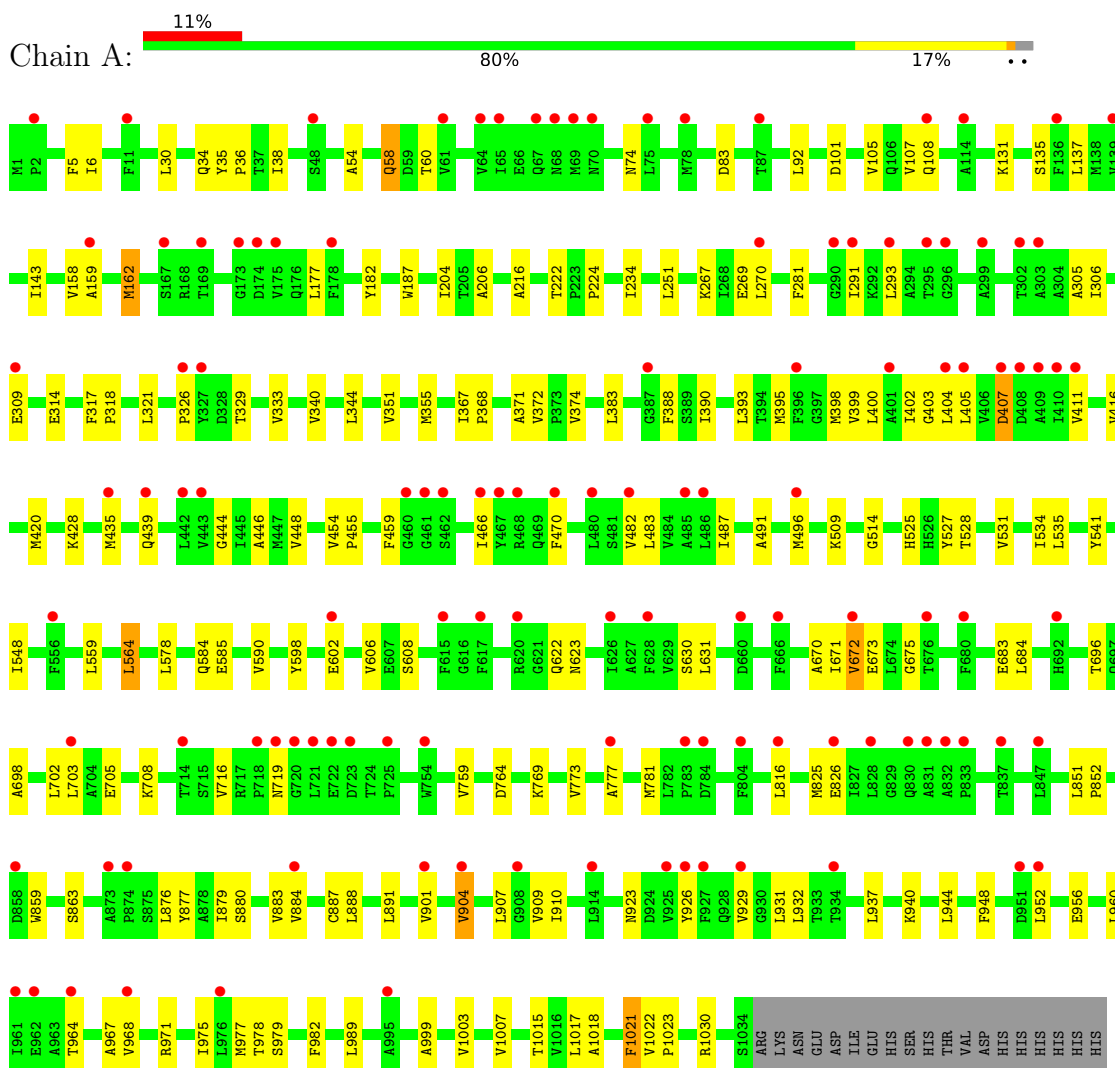
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224

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: Multidrug efflux pump subunit AcrB



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	145.30Å 145.30Å 516.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.94 – 3.40 28.94 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.94-3.40) 99.8 (28.94-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.301 , 0.310 0.315 , 0.327	Depositor DCC
R_{free} test set	1503 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	146.4	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 93.5	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	0.90	EDS
Total number of atoms	7854	wwPDB-VP
Average B, all atoms (Å ²)	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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	0.78	1/8004 (0.0%)	1.32	16/10870 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	VAL	CA-CB	5.39	1.56	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	904	VAL	CA-C-N	6.79	125.76	120.33
1	A	904	VAL	C-N-CA	6.79	125.76	120.33
1	A	105	VAL	CA-C-N	5.69	128.17	120.38
1	A	105	VAL	C-N-CA	5.69	128.17	120.38
1	A	977	MET	CA-C-N	5.66	128.12	120.65
1	A	977	MET	C-N-CA	5.66	128.12	120.65
1	A	54	ALA	CA-C-N	5.60	127.78	120.28
1	A	54	ALA	C-N-CA	5.60	127.78	120.28
1	A	60	THR	CA-C-N	5.59	127.54	120.72
1	A	60	THR	C-N-CA	5.59	127.54	120.72
1	A	1021	PHE	CA-C-N	5.57	124.79	120.33
1	A	1021	PHE	C-N-CA	5.57	124.79	120.33
1	A	83	ASP	CA-C-N	5.48	129.46	120.63
1	A	83	ASP	C-N-CA	5.48	129.46	120.63
1	A	162	MET	CA-C-N	5.07	127.07	120.28
1	A	162	MET	C-N-CA	5.07	127.07	120.28

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	7854	0	8003	129	0
All	All	7854	0	8003	129	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 8.

All (129) 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:696:THR:HG22	1:A:825:MET:HE1	1.37	1.06
1:A:143:ILE:HD11	1:A:281:PHE:CD2	2.04	0.92
1:A:135:SER:HB3	1:A:672:VAL:HG13	1.57	0.85
1:A:703:LEU:HD23	1:A:716:VAL:HG12	1.59	0.84
1:A:344:LEU:HD23	1:A:402:ILE:CD1	2.10	0.81
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.64	0.80
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.66	0.76
1:A:355:MET:HE2	1:A:368:PRO:HG2	1.69	0.74
1:A:444:GLY:CA	1:A:891:LEU:HD11	2.18	0.74
1:A:58:GLN:NE2	1:A:816:LEU:HD12	2.03	0.73
1:A:672:VAL:HG12	1:A:673:GLU:H	1.54	0.71
1:A:999:ALA:O	1:A:1003:VAL:HG23	1.92	0.70
1:A:6:ILE:HD13	1:A:428:LYS:HA	1.74	0.70
1:A:448:VAL:HG11	1:A:888:LEU:HG	1.76	0.68
1:A:371:ALA:O	1:A:374:VAL:HG12	1.94	0.67
1:A:305:ALA:O	1:A:309:GLU:HG2	1.95	0.67
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.25	0.67
1:A:531:VAL:O	1:A:535:LEU:HG	1.96	0.65
1:A:143:ILE:CD1	1:A:281:PHE:CD2	2.77	0.64
1:A:444:GLY:HA3	1:A:891:LEU:HD11	1.78	0.64
1:A:672:VAL:HG12	1:A:673:GLU:N	2.12	0.64
1:A:143:ILE:HD11	1:A:281:PHE:HD2	1.60	0.64
1:A:444:GLY:HA2	1:A:891:LEU:HD11	1.80	0.63
1:A:344:LEU:HD23	1:A:402:ILE:HD12	1.80	0.63
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.80	0.63
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:THR:CG2	1:A:825:MET:HE1	2.22	0.62
1:A:459:PHE:CE1	1:A:876:LEU:HD12	2.33	0.62
1:A:527:TYR:HE2	1:A:968:VAL:HG12	1.62	0.62
1:A:944:LEU:HB3	1:A:971:ARG:CZ	2.29	0.62
1:A:368:PRO:O	1:A:372:VAL:HG23	1.99	0.62
1:A:135:SER:HB2	1:A:673:GLU:HG2	1.81	0.62
1:A:351:VAL:O	1:A:355:MET:HG2	2.00	0.62
1:A:444:GLY:HA3	1:A:891:LEU:CD1	2.30	0.61
1:A:859:TRP:HB3	1:A:863:SER:HB3	1.82	0.60
1:A:926:TYR:HB3	1:A:1003:VAL:HG22	1.82	0.60
1:A:880:SER:O	1:A:884:VAL:HG23	2.02	0.59
1:A:527:TYR:CZ	1:A:531:VAL:HG21	2.38	0.59
1:A:367:ILE:HD11	1:A:496:MET:HB3	1.84	0.58
1:A:598:TYR:HD1	1:A:602:GLU:OE1	1.85	0.58
1:A:509:LYS:HA	1:A:514:GLY:HA3	1.86	0.57
1:A:448:VAL:CG1	1:A:888:LEU:HG	2.34	0.57
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.06	0.56
1:A:684:LEU:HD11	1:A:702:LEU:HD12	1.88	0.55
1:A:851:LEU:HD12	1:A:852:PRO:HD2	1.88	0.55
1:A:948:PHE:CE1	1:A:971:ARG:NH2	2.75	0.54
1:A:979:SER:HB3	1:A:1015:THR:HG21	1.90	0.54
1:A:34:GLN:HB3	1:A:333:VAL:HG22	1.91	0.53
1:A:206:ALA:CB	1:A:251:LEU:HD23	2.39	0.52
1:A:584:GLN:H	1:A:622:GLN:HE21	1.56	0.52
1:A:135:SER:CB	1:A:672:VAL:HG13	2.36	0.52
1:A:929:VAL:HA	1:A:932:LEU:HD12	1.91	0.51
1:A:909:VAL:HG22	1:A:931:LEU:HD11	1.91	0.51
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.92	0.51
1:A:372:VAL:HG13	1:A:405:LEU:HD11	1.93	0.50
1:A:314:GLU:HA	1:A:317:PHE:CE2	2.46	0.50
1:A:1017:LEU:HB3	1:A:1021:PHE:CE2	2.46	0.50
1:A:416:VAL:HG12	1:A:420:MET:HE2	1.93	0.50
1:A:698:ALA:HB1	1:A:851:LEU:HD11	1.94	0.50
1:A:952:LEU:O	1:A:956:GLU:HB2	2.12	0.50
1:A:159:ALA:HB2	1:A:177:LEU:HD21	1.94	0.50
1:A:948:PHE:HB3	1:A:967:ALA:HB1	1.93	0.49
1:A:964:THR:O	1:A:968:VAL:HG23	2.11	0.49
1:A:960:LEU:HD13	1:A:1030:ARG:HG2	1.93	0.49
1:A:971:ARG:HG3	1:A:975:ILE:HD12	1.95	0.49
1:A:455:PRO:HG2	1:A:880:SER:HB2	1.94	0.49
1:A:683:GLU:OE2	1:A:826:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:HB2	1:A:623:ASN:HB2	1.96	0.48
1:A:598:TYR:HB3	1:A:606:VAL:HG21	1.94	0.48
1:A:393:LEU:HD22	1:A:470:PHE:HE2	1.79	0.48
1:A:483:LEU:HG	1:A:487:ILE:HD12	1.95	0.48
1:A:143:ILE:CD1	1:A:281:PHE:HD2	2.23	0.47
1:A:314:GLU:HA	1:A:317:PHE:CD2	2.50	0.47
1:A:329:THR:O	1:A:333:VAL:HG23	2.15	0.47
1:A:326:PRO:O	1:A:630:SER:HB2	2.15	0.47
1:A:598:TYR:CD1	1:A:602:GLU:OE1	2.67	0.47
1:A:777:ALA:O	1:A:781:MET:HG2	2.15	0.47
1:A:383:LEU:HG	1:A:388:PHE:HB2	1.96	0.46
1:A:92:LEU:HD12	1:A:107:VAL:HG22	1.97	0.46
1:A:705:GLU:HA	1:A:708:LYS:HE3	1.96	0.46
1:A:216:ALA:HB1	1:A:234:ILE:HG22	1.98	0.46
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.50	0.46
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.98	0.46
1:A:58:GLN:HE21	1:A:816:LEU:HD12	1.78	0.46
1:A:159:ALA:HB2	1:A:177:LEU:CD2	2.46	0.46
1:A:548:ILE:HG23	1:A:910:ILE:HG13	1.98	0.46
1:A:187:TRP:HB2	1:A:267:LYS:HB3	1.98	0.46
1:A:877:TYR:HE1	1:A:932:LEU:HD21	1.80	0.46
1:A:38:ILE:HD13	1:A:466:ILE:HG12	1.97	0.45
1:A:404:LEU:HD23	1:A:937:LEU:HD13	1.98	0.45
1:A:143:ILE:HD11	1:A:281:PHE:HB3	1.98	0.45
1:A:158:VAL:O	1:A:162:MET:HB2	2.16	0.45
1:A:535:LEU:HD21	1:A:1023:PRO:HB2	1.99	0.45
1:A:435:MET:O	1:A:439:GLN:HB2	2.17	0.45
1:A:759:VAL:HG21	1:A:773:VAL:CG2	2.47	0.45
1:A:759:VAL:HG21	1:A:773:VAL:HG23	1.99	0.45
1:A:398:MET:O	1:A:402:ILE:HG13	2.18	0.44
1:A:407:ASP:OD1	1:A:978:THR:HG23	2.16	0.44
1:A:466:ILE:HD13	1:A:564:LEU:HD11	2.00	0.44
1:A:884:VAL:HA	1:A:887:CYS:SG	2.58	0.44
1:A:559:LEU:HD23	1:A:923:ASN:HB2	2.00	0.43
1:A:393:LEU:HD22	1:A:470:PHE:CE2	2.53	0.43
1:A:606:VAL:HA	1:A:631:LEU:HD23	2.00	0.43
1:A:411:VAL:HG13	1:A:971:ARG:HH12	1.84	0.43
1:A:584:GLN:N	1:A:622:GLN:HG2	2.33	0.43
1:A:907:LEU:HD22	1:A:1021:PHE:CD2	2.54	0.43
1:A:36:PRO:CD	1:A:393:LEU:HD12	2.49	0.43
1:A:982:PHE:CE2	1:A:1007:VAL:HG12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.55	0.42
1:A:534:ILE:HG23	1:A:541:TYR:CE2	2.55	0.42
1:A:944:LEU:HB3	1:A:971:ARG:NH2	2.35	0.42
1:A:101:ASP:OD1	1:A:131:LYS:HE2	2.20	0.42
1:A:407:ASP:HB3	1:A:940:LYS:CE	2.50	0.42
1:A:446:ALA:HB2	1:A:482:VAL:HG11	2.01	0.42
1:A:719:ASN:HB3	1:A:826:GLU:HB3	2.02	0.42
1:A:182:TYR:HB3	1:A:270:LEU:HD22	2.02	0.41
1:A:35:TYR:CD2	1:A:671:ILE:HG12	2.55	0.41
1:A:926:TYR:CD1	1:A:1003:VAL:HG22	2.55	0.41
1:A:982:PHE:CZ	1:A:1007:VAL:CG1	3.04	0.41
1:A:400:LEU:CD2	1:A:1007:VAL:HG21	2.51	0.41
1:A:318:PRO:HD2	1:A:321:LEU:HD22	2.03	0.41
1:A:525:HIS:HA	1:A:528:THR:HG22	2.03	0.41
1:A:901:VAL:O	1:A:904:VAL:HG22	2.20	0.41
1:A:137:LEU:HD13	1:A:293:LEU:HD11	2.03	0.41
1:A:5:PHE:HB3	1:A:491:ALA:HB2	2.02	0.40
1:A:222:THR:HA	1:A:224:PRO:HD3	2.03	0.40
1:A:879:ILE:O	1:A:883:VAL:HG23	2.21	0.40
1:A:204:ILE:HG23	1:A:759:VAL:HG13	2.03	0.40
1:A:764:ASP:HB3	1:A:769:LYS:HD2	2.03	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	1032/1053 (98%)	993 (96%)	34 (3%)	5 (0%)	24 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	670	ALA
1	A	672	VAL
1	A	564	LEU
1	A	74	ASN
1	A	675	GLY

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	839/859 (98%)	834 (99%)	5 (1%)	78 80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	108	GLN
1	A	269	GLU
1	A	407	ASP
1	A	585	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	68	ASN
1	A	189	ASN
1	A	194	ASN
1	A	197	GLN
1	A	254	ASN
1	A	298	ASN
1	A	360	GLN
1	A	517	ASN
1	A	622	GLN
1	A	687	GLN
1	A	701	GLN

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Mol	Chain	Res	Type
1	A	797	GLN
1	A	928	GLN
1	A	1001	ASN

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	1034/1053 (98%)	0.78	119 (11%) 9 10	85, 174, 252, 271	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	VAL	10.0
1	A	401	ALA	7.4
1	A	470	PHE	5.7
1	A	114	ALA	5.7
1	A	65	ILE	5.5
1	A	408	ASP	5.4
1	A	833	PRO	5.1
1	A	411	VAL	4.8
1	A	720	GLY	4.7
1	A	874	PRO	4.6
1	A	719	ASN	4.6
1	A	290	GLY	4.3
1	A	295	THR	4.2
1	A	722	GLU	4.1
1	A	832	ALA	4.1
1	A	672	VAL	4.0
1	A	327	TYR	3.9
1	A	442	LEU	3.8
1	A	407	ASP	3.7
1	A	925	VAL	3.7
1	A	291	ILE	3.7
1	A	714	THR	3.6
1	A	405	LEU	3.6
1	A	777	ALA	3.6
1	A	908	GLY	3.5
1	A	831	ALA	3.5
1	A	934	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	486	LEU	3.3
1	A	69	MET	3.3
1	A	410	ILE	3.3
1	A	626	ILE	3.3
1	A	303	ALA	3.3
1	A	387	GLY	3.2
1	A	326	PRO	3.2
1	A	929	VAL	3.2
1	A	67	GLN	3.2
1	A	293	LEU	3.2
1	A	901	VAL	3.1
1	A	461	GLY	3.1
1	A	858	ASP	3.1
1	A	951	ASP	3.1
1	A	75	LEU	3.0
1	A	816	LEU	3.0
1	A	837	THR	3.0
1	A	660	ASP	3.0
1	A	139	VAL	3.0
1	A	617	PHE	3.0
1	A	995	ALA	3.0
1	A	439	GLN	3.0
1	A	404	LEU	2.9
1	A	721	LEU	2.9
1	A	178	PHE	2.9
1	A	2	PRO	2.8
1	A	847	LEU	2.8
1	A	783	PRO	2.8
1	A	11	PHE	2.8
1	A	468	ARG	2.8
1	A	628	PHE	2.8
1	A	78	MET	2.7
1	A	467	TYR	2.7
1	A	692	HIS	2.7
1	A	602	GLU	2.7
1	A	169	THR	2.6
1	A	61	VAL	2.6
1	A	174	ASP	2.6
1	A	676	THR	2.6
1	A	723	ASP	2.5
1	A	873	ALA	2.5
1	A	173	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	64	VAL	2.5
1	A	826	GLU	2.5
1	A	496	MET	2.5
1	A	480	LEU	2.5
1	A	620	ARG	2.5
1	A	830	GLN	2.5
1	A	409	ALA	2.4
1	A	462	SER	2.4
1	A	926	TYR	2.4
1	A	952	LEU	2.4
1	A	296	GLY	2.4
1	A	804	PHE	2.4
1	A	270	LEU	2.4
1	A	914	LEU	2.4
1	A	754	TRP	2.4
1	A	784	ASP	2.3
1	A	680	PHE	2.3
1	A	968	VAL	2.3
1	A	460	GLY	2.3
1	A	615	PHE	2.3
1	A	435	MET	2.3
1	A	466	ILE	2.2
1	A	70	ASN	2.2
1	A	556	PHE	2.2
1	A	167	SER	2.2
1	A	703	LEU	2.2
1	A	136	PHE	2.2
1	A	108	GLN	2.2
1	A	961	ILE	2.2
1	A	485	ALA	2.2
1	A	964	THR	2.2
1	A	482	VAL	2.2
1	A	175	VAL	2.1
1	A	666	PHE	2.1
1	A	87	THR	2.1
1	A	309	GLU	2.1
1	A	884	VAL	2.1
1	A	904	VAL	2.1
1	A	159	ALA	2.1
1	A	962	GLU	2.1
1	A	48	SER	2.0
1	A	68	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	299	ALA	2.0
1	A	302	THR	2.0
1	A	396	PHE	2.0
1	A	725	PRO	2.0
1	A	927	PHE	2.0
1	A	976	LEU	2.0
1	A	718	PRO	2.0
1	A	828	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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.