Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 04:11 pm BST

PDB ID	:	8PX7
Title	:	Structure of Bacterial Multidrug Efflux transporter AcrB, solved at wavelength 3.02 A
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:

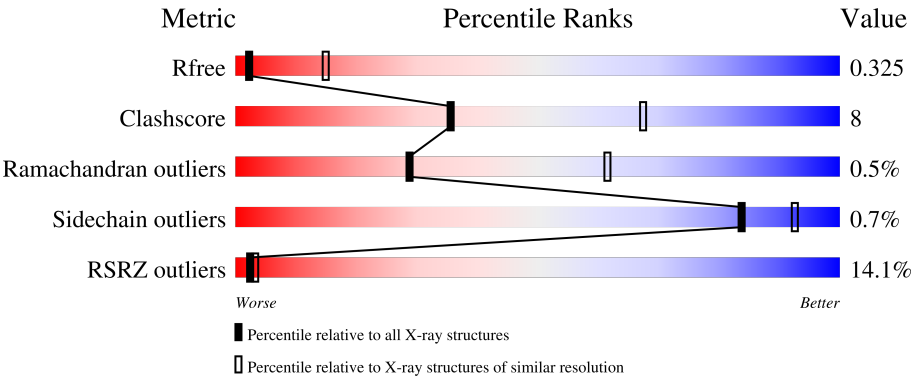
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	14% 81% 17% .

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	1034	7854	5055	1296	1459	44	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

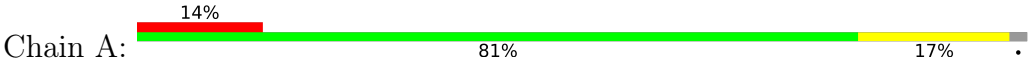
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224

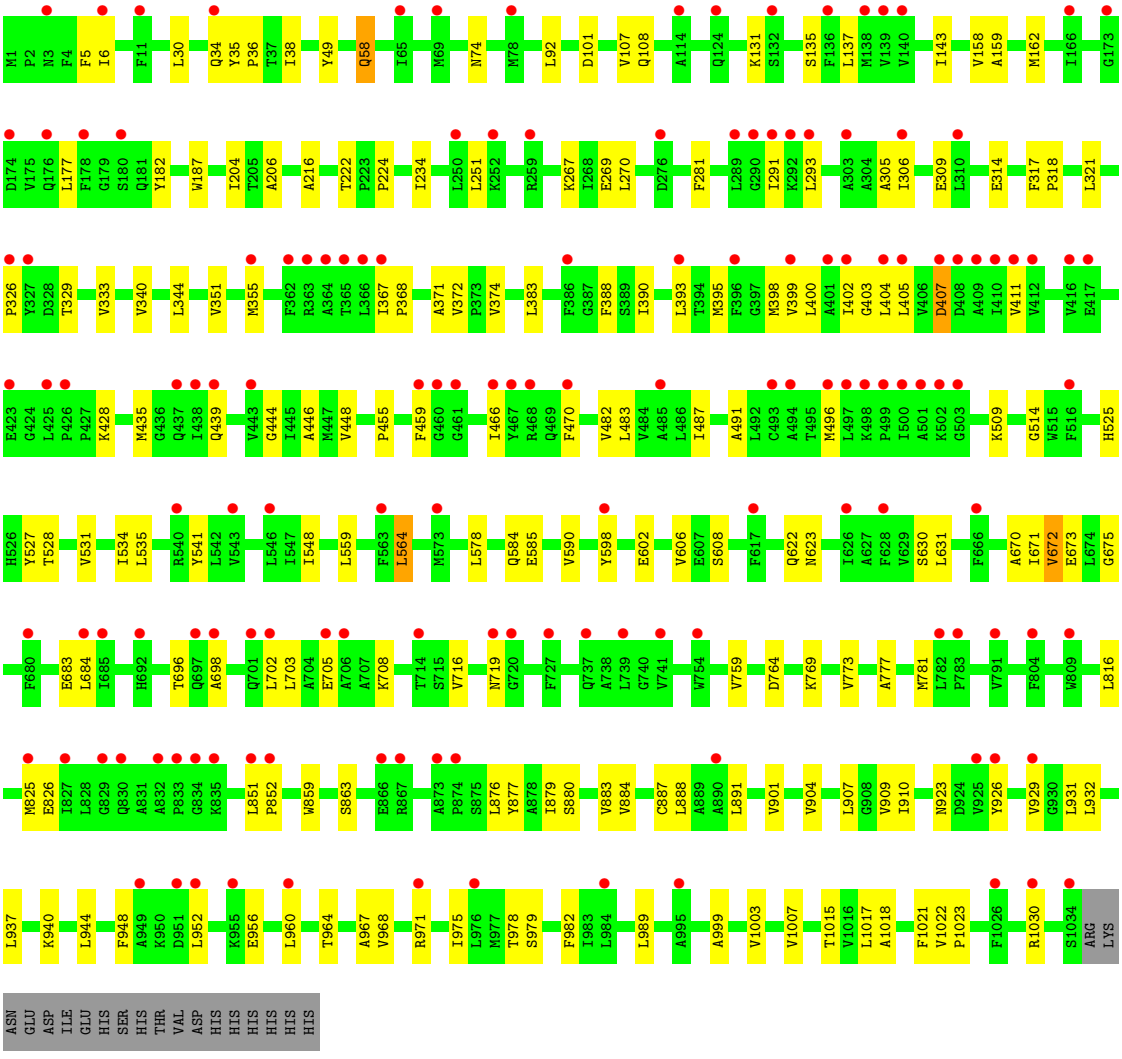
3 Residue-property plots (i)

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: Multidrug efflux pump subunit AcrB

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	145.30Å 145.30Å 516.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.94 – 3.40 47.89 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.94-3.40) 99.9 (47.89-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.301 , 0.310 0.316 , 0.325	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)	0.28 , 107.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.42	0/8004	0.60	0/10870

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	7854	0	8003	128	0
All	All	7854	0	8003	128	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 (128) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.66	0.76
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
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:696:THR:HG22	1:A:825:MET:CE	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:696:THR:HG22	1:A:825:MET:HE3	1.94	0.48
1:A:696:THR:HG22	1:A:825:MET:HE1	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	29 61

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 (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	839/859 (98%)	833 (99%)	6 (1%)	84 92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TYR
1	A	58	GLN
1	A	108	GLN

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Mol	Chain	Res	Type
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	622	GLN
1	A	701	GLN
1	A	928	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 monosaccharides 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	1034/1053 (98%)	0.76	146 (14%)	2	3	85, 174, 252, 271	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	GLY	8.8
1	A	496	MET	8.3
1	A	833	PRO	8.3
1	A	408	ASP	8.2
1	A	425	LEU	7.4
1	A	410	ILE	7.1
1	A	493	CYS	7.0
1	A	874	PRO	6.7
1	A	497	LEU	6.5
1	A	995	ALA	6.4
1	A	500	ILE	5.9
1	A	499	PRO	5.9
1	A	502	LYS	5.8
1	A	461	GLY	5.6
1	A	501	ALA	5.5
1	A	832	ALA	5.4
1	A	706	ALA	5.3
1	A	494	ALA	5.2
1	A	411	VAL	5.1
1	A	407	ASP	5.0
1	A	173	GLY	5.0
1	A	405	LEU	5.0
1	A	367	ILE	4.9
1	A	409	ALA	4.9
1	A	174	ASP	4.8
1	A	460	GLY	4.8
1	A	543	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	498	LYS	4.5
1	A	714	THR	4.3
1	A	292	LYS	4.3
1	A	468	ARG	4.2
1	A	366	LEU	4.2
1	A	470	PHE	4.1
1	A	327	TYR	4.1
1	A	834	GLY	4.1
1	A	363	ARG	4.0
1	A	851	LEU	3.9
1	A	362	PHE	3.8
1	A	3	ASN	3.8
1	A	804	PHE	3.8
1	A	365	THR	3.8
1	A	873	ALA	3.8
1	A	467	TYR	3.7
1	A	563	PHE	3.5
1	A	291	ILE	3.5
1	A	386	PHE	3.4
1	A	364	ALA	3.3
1	A	503	GLY	3.3
1	A	754	TRP	3.3
1	A	69	MET	3.3
1	A	719	ASN	3.3
1	A	401	ALA	3.3
1	A	867	ARG	3.2
1	A	11	PHE	3.2
1	A	65	ILE	3.1
1	A	835	LYS	3.1
1	A	827	ILE	3.1
1	A	78	MET	3.1
1	A	404	LEU	3.1
1	A	1026	PHE	3.0
1	A	136	PHE	3.0
1	A	459	PHE	3.0
1	A	540	ARG	3.0
1	A	355	MET	3.0
1	A	176	GLN	2.9
1	A	1030	ARG	2.9
1	A	443	VAL	2.9
1	A	114	ALA	2.9
1	A	737	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	951	ASP	2.8
1	A	485	ALA	2.8
1	A	132	SER	2.8
1	A	303	ALA	2.8
1	A	617	PHE	2.8
1	A	701	GLN	2.7
1	A	412	VAL	2.7
1	A	416	VAL	2.7
1	A	702	LEU	2.7
1	A	971	ARG	2.7
1	A	393	LEU	2.7
1	A	926	TYR	2.7
1	A	439	GLN	2.7
1	A	783	PRO	2.7
1	A	684	LEU	2.6
1	A	178	PHE	2.6
1	A	516	PHE	2.6
1	A	829	GLY	2.6
1	A	698	ALA	2.6
1	A	925	VAL	2.6
1	A	984	LEU	2.5
1	A	438	ILE	2.5
1	A	705	GLU	2.5
1	A	139	VAL	2.5
1	A	890	ALA	2.5
1	A	402	ILE	2.5
1	A	825	MET	2.5
1	A	423	GLU	2.5
1	A	417	GLU	2.5
1	A	289	LEU	2.4
1	A	976	LEU	2.4
1	A	310	LEU	2.4
1	A	396	PHE	2.4
1	A	180	SER	2.4
1	A	952	LEU	2.4
1	A	326	PRO	2.3
1	A	830	GLN	2.3
1	A	426	PRO	2.3
1	A	259	ARG	2.3
1	A	929	VAL	2.3
1	A	252	LYS	2.3
1	A	546	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	680	PHE	2.3
1	A	466	ILE	2.3
1	A	628	PHE	2.3
1	A	437	GLN	2.3
1	A	666	PHE	2.3
1	A	791	VAL	2.3
1	A	866	GLU	2.3
1	A	949	ALA	2.3
1	A	6	ILE	2.3
1	A	293	LEU	2.3
1	A	955	LYS	2.3
1	A	598	TYR	2.3
1	A	34	GLN	2.2
1	A	720	GLY	2.2
1	A	124	GLN	2.2
1	A	685	ILE	2.2
1	A	692	HIS	2.2
1	A	138	MET	2.2
1	A	739	LEU	2.2
1	A	626	ILE	2.1
1	A	1034	SER	2.1
1	A	727	PHE	2.1
1	A	809	TRP	2.1
1	A	276	ASP	2.1
1	A	140	VAL	2.1
1	A	741	VAL	2.1
1	A	697	GLN	2.0
1	A	782	LEU	2.0
1	A	166	ILE	2.0
1	A	250	LEU	2.0
1	A	573	MET	2.0
1	A	306	ILE	2.0
1	A	960	LEU	2.0
1	A	852	PRO	2.0
1	A	399	VAL	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 monosaccharides 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.