Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 08:55 AM EDT

PDB ID	:	4ZLN
Title	:	Crystal structure of transporter AcrB deletion mutant
Authors	:	Ababou, A.; Koronakis, V.
Deposited on	:	2015-05-01
Resolution	:	3.56 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:

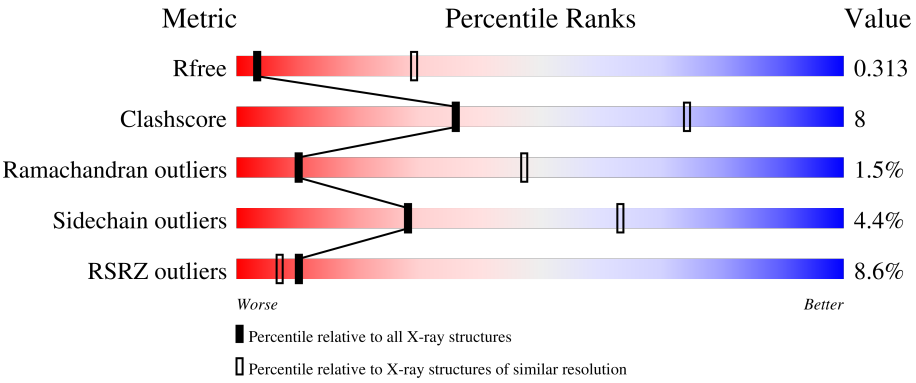
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.56 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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	1044	9% 76% 21%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7813 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	1029	7813	5026	1288	1455	44	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

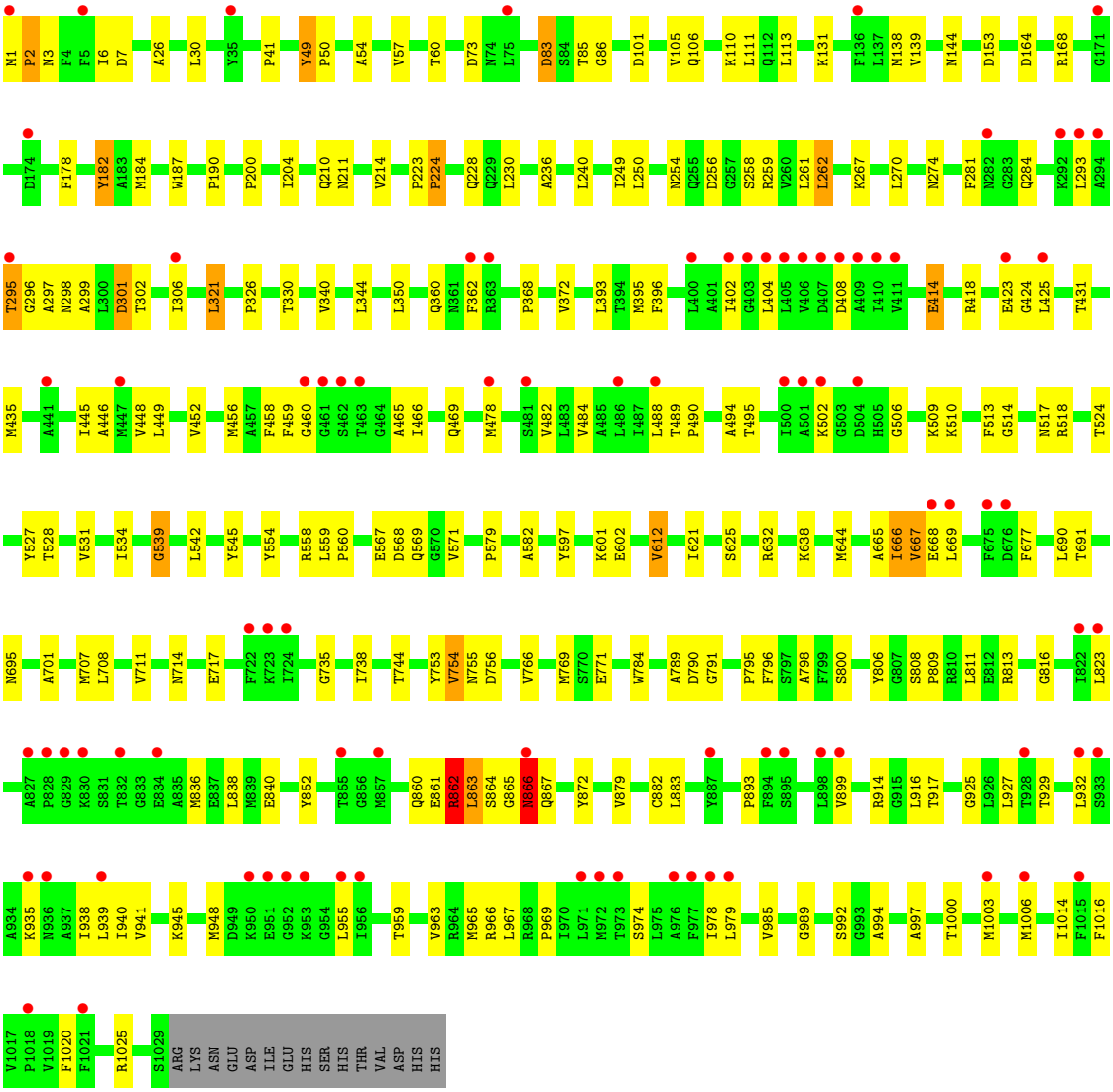
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224

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	143.85Å 143.85Å 519.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 3.56 112.34 – 3.56	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.95-3.56) 98.5 (112.34-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.269 , 0.303 0.280 , 0.313	Depositor DCC
R_{free} test set	1262 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	98.2	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.68	EDS
Total number of atoms	7813	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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	0.24	0/7961	0.42	0/10813

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	7813	0	7967	126	0
All	All	7813	0	7967	126	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 (126) 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:862:ARG:HB2	1:A:863:LEU:HG	1.58	0.84
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.66	0.78
1:A:666:ILE:HG12	1:A:667:VAL:HG23	1.69	0.73
1:A:612:VAL:HG23	1:A:621:ILE:HG23	1.72	0.72
1:A:414:GLU:HG2	1:A:969:PRO:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLU:HB3	1:A:425:LEU:HD13	1.75	0.69
1:A:524:THR:HG22	1:A:967:LEU:HD12	1.76	0.68
1:A:985:VAL:HG23	1:A:1000:THR:HG22	1.75	0.67
1:A:200:PRO:HD2	1:A:744:THR:HG22	1.76	0.67
1:A:297:ALA:HA	1:A:298:ASN:HB2	1.82	0.61
1:A:210:GLN:NE2	1:A:250:LEU:O	2.33	0.61
1:A:83:ASP:OD2	1:A:83:ASP:N	2.33	0.61
1:A:254:ASN:HB2	1:A:258:SER:HB2	1.83	0.61
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.83	0.61
1:A:860:GLN:HB3	1:A:861:GLU:HA	1.84	0.60
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.84	0.59
1:A:567:GLU:OE2	1:A:994:ALA:N	2.36	0.59
1:A:484:VAL:HG13	1:A:488:LEU:HB3	1.84	0.58
1:A:144:ASN:O	1:A:284:GLN:NE2	2.36	0.58
1:A:571:VAL:HG12	1:A:625:SER:HA	1.86	0.58
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.36	0.58
1:A:568:ASP:OD2	1:A:632:ARG:NH2	2.30	0.57
1:A:701:ALA:HB1	1:A:711:VAL:HG11	1.86	0.57
1:A:813:ARG:NH2	1:A:816:GLY:O	2.36	0.57
1:A:925:GLY:O	1:A:929:THR:OG1	2.21	0.57
1:A:211:ASN:O	1:A:755:ASN:ND2	2.38	0.57
1:A:527:TYR:OH	1:A:1014:ILE:O	2.17	0.57
1:A:707:MET:HG3	1:A:838:LEU:HD22	1.85	0.56
1:A:863:LEU:HD13	1:A:867:GLN:HB2	1.88	0.56
1:A:790:ASP:OD1	1:A:791:GLY:N	2.37	0.55
1:A:360:GLN:NE2	1:A:517:ASN:OD1	2.37	0.55
1:A:408:ASP:OD1	1:A:935:LYS:NZ	2.36	0.54
1:A:452:VAL:HG12	1:A:879:VAL:HG21	1.90	0.54
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.90	0.54
1:A:101:ASP:OD1	1:A:131:LYS:NZ	2.41	0.54
1:A:666:ILE:HG23	1:A:669:LEU:HB3	1.90	0.54
1:A:301:ASP:OD1	1:A:301:ASP:N	2.29	0.53
1:A:863:LEU:HB2	1:A:866:ASN:HB3	1.90	0.53
1:A:101:ASP:O	1:A:105:VAL:HG23	2.09	0.53
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.91	0.53
1:A:153:ASP:OD1	1:A:182:TYR:OH	2.27	0.53
1:A:228:GLN:NE2	1:A:230:LEU:O	2.38	0.52
1:A:404:LEU:HD22	1:A:478:MET:HE1	1.92	0.52
1:A:959:THR:O	1:A:963:VAL:HG23	2.10	0.52
1:A:940:ILE:HG12	1:A:966:ARG:HG2	1.92	0.51
1:A:256:ASP:OD1	1:A:258:SER:OG	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:TYR:OH	1:A:558:ARG:NH1	2.45	0.50
1:A:883:LEU:HB3	1:A:893:PRO:HB3	1.95	0.49
1:A:418:ARG:HD3	1:A:965:MET:HG3	1.94	0.49
1:A:569:GLN:NE2	1:A:665:ALA:O	2.46	0.48
1:A:539:GLY:HA2	1:A:542:LEU:HB2	1.95	0.48
1:A:978:ILE:HG23	1:A:1003:MET:HG3	1.95	0.48
1:A:54:ALA:HB1	1:A:811:LEU:HD13	1.96	0.48
1:A:281:PHE:HE1	1:A:326:PRO:HB3	1.77	0.48
1:A:484:VAL:HG12	1:A:489:THR:HG23	1.96	0.48
1:A:714:ASN:HB2	1:A:823:LEU:HD13	1.95	0.47
1:A:187:TRP:HB2	1:A:267:LYS:HB2	1.96	0.47
1:A:945:LYS:HA	1:A:948:MET:HE2	1.96	0.47
1:A:3:ASN:HA	1:A:6:ILE:HB	1.97	0.47
1:A:350:LEU:HD23	1:A:979:LEU:HB3	1.97	0.47
1:A:691:THR:O	1:A:695:ASN:ND2	2.30	0.47
1:A:974:SER:HA	1:A:1006:MET:HE3	1.95	0.47
1:A:738:ILE:H	1:A:738:ILE:HD12	1.80	0.47
1:A:424:GLY:HA3	1:A:502:LYS:HB2	1.97	0.46
1:A:41:PRO:HA	1:A:295:THR:HG21	1.98	0.46
1:A:735:GLY:O	1:A:789:ALA:N	2.46	0.46
1:A:456:MET:HE3	1:A:927:LEU:HD21	1.97	0.46
1:A:916:LEU:HD21	1:A:997:ALA:HA	1.98	0.46
1:A:435:MET:HG3	1:A:490:PRO:HB3	1.98	0.46
1:A:753:TYR:OH	1:A:756:ASP:OD1	2.22	0.45
1:A:259:ARG:HD3	1:A:261:LEU:HD21	1.99	0.45
1:A:632:ARG:O	1:A:638:LYS:NZ	2.43	0.45
1:A:465:ALA:O	1:A:469:GLN:HG2	2.17	0.45
1:A:360:GLN:HG2	1:A:513:PHE:CG	2.52	0.45
1:A:939:LEU:HB3	1:A:966:ARG:HD3	1.98	0.45
1:A:164:ASP:O	1:A:168:ARG:NH2	2.50	0.45
1:A:1:MET:H2	1:A:2:PRO:HD3	1.81	0.44
1:A:667:VAL:HG12	1:A:668:GLU:HG2	1.99	0.44
1:A:190:PRO:HB3	1:A:784:TRP:CE3	2.53	0.44
1:A:445:ILE:HD13	1:A:935:LYS:HZ3	1.82	0.44
1:A:184:MET:HB3	1:A:766:VAL:HG22	1.99	0.44
1:A:396:PHE:HE1	1:A:994:ALA:HB1	1.81	0.44
1:A:861:GLU:O	1:A:862:ARG:HG3	2.17	0.44
1:A:423:GLU:HA	1:A:502:LYS:HE3	1.99	0.43
1:A:597:TYR:HD1	1:A:601:LYS:HD2	1.83	0.43
1:A:808:SER:HA	1:A:809:PRO:HD3	1.88	0.43
1:A:448:VAL:O	1:A:452:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLY:O	1:A:518:ARG:HG3	2.18	0.43
1:A:49:TYR:HD2	1:A:50:PRO:HD2	1.83	0.43
1:A:864:SER:HA	1:A:865:GLY:HA2	1.83	0.43
1:A:449:LEU:O	1:A:452:VAL:HG22	2.19	0.42
1:A:545:TYR:HB2	1:A:1016:PHE:CE1	2.54	0.42
1:A:677:PHE:CZ	1:A:852:TYR:HB2	2.54	0.42
1:A:26:ALA:O	1:A:30:LEU:HB2	2.19	0.42
1:A:254:ASN:HD22	1:A:258:SER:HB2	1.85	0.42
1:A:466:ILE:H	1:A:466:ILE:HD12	1.83	0.42
1:A:524:THR:O	1:A:528:THR:HG23	2.19	0.42
1:A:448:VAL:HG12	1:A:882:CYS:HB2	2.01	0.42
1:A:83:ASP:HB2	1:A:85:THR:HG22	2.01	0.42
1:A:559:LEU:HD12	1:A:560:PRO:HD2	2.01	0.42
1:A:110:LYS:HD3	1:A:110:LYS:HA	1.82	0.42
1:A:249:ILE:HD12	1:A:262:LEU:HD12	2.01	0.42
1:A:1016:PHE:HB3	1:A:1020:PHE:CZ	2.55	0.42
1:A:506:GLY:HA2	1:A:509:LYS:HD2	2.02	0.41
1:A:708:LEU:HB2	1:A:838:LEU:HD23	2.02	0.41
1:A:204:ILE:HD13	1:A:754:VAL:HG22	2.01	0.41
1:A:531:VAL:HA	1:A:534:ILE:HG12	2.02	0.41
1:A:836:MET:O	1:A:840:GLU:HG3	2.21	0.41
1:A:396:PHE:CE1	1:A:994:ALA:HB1	2.56	0.41
1:A:431:THR:HG21	1:A:494:ALA:HB2	2.02	0.41
1:A:211:ASN:HA	1:A:240:LEU:HD13	2.03	0.41
1:A:458:PHE:HA	1:A:459:PHE:HA	1.81	0.41
1:A:139:VAL:O	1:A:326:PRO:HD2	2.21	0.41
1:A:989:GLY:N	1:A:992:SER:OG	2.54	0.41
1:A:795:PRO:HG2	1:A:798:ALA:HB2	2.03	0.41
1:A:883:LEU:HD21	1:A:938:ILE:HD11	2.03	0.41
1:A:302:THR:O	1:A:306:ILE:HG12	2.21	0.41
1:A:527:TYR:OH	1:A:1014:ILE:HG13	2.21	0.41
1:A:872:TYR:CE2	1:A:927:LEU:HD11	2.56	0.41
1:A:178:PHE:CD1	1:A:612:VAL:HG11	2.56	0.40
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.82	0.40
1:A:214:VAL:HG23	1:A:236:ALA:HB3	2.01	0.40
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.90	0.40
1:A:368:PRO:O	1:A:372:VAL:HG23	2.21	0.40
1:A:862:ARG:HA	1:A:863:LEU:HA	1.76	0.40
1:A:187:TRP:HA	1:A:769:MET:O	2.21	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	1027/1044 (98%)	933 (91%)	79 (8%)	15 (2%)	10 47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	ALA
1	A	2	PRO
1	A	579	PRO
1	A	862	ARG
1	A	295	THR
1	A	510	LYS
1	A	582	ALA
1	A	667	VAL
1	A	330	THR
1	A	460	GLY
1	A	866	ASN
1	A	754	VAL
1	A	296	GLY
1	A	224	PRO
1	A	539	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	837/852 (98%)	800 (96%)	37 (4%)	28 63

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	49	TYR
1	A	60	THR
1	A	83	ASP
1	A	111	LEU
1	A	113	LEU
1	A	138	MET
1	A	182	TYR
1	A	262	LEU
1	A	270	LEU
1	A	274	ASN
1	A	293	LEU
1	A	301	ASP
1	A	321	LEU
1	A	362	PHE
1	A	414	GLU
1	A	495	THR
1	A	602	GLU
1	A	612	VAL
1	A	644	MET
1	A	666	ILE
1	A	690	LEU
1	A	717	GLU
1	A	771	GLU
1	A	796	PHE
1	A	800	SER
1	A	806	TYR
1	A	862	ARG
1	A	863	LEU
1	A	866	ASN
1	A	899	VAL
1	A	914	ARG
1	A	917	THR
1	A	932	LEU
1	A	941	VAL
1	A	955	LEU
1	A	1025	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	517	ASN

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	1029/1044 (98%)	0.45	89 (8%) 10 7	31, 87, 140, 169	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	ASP	5.8
1	A	404	LEU	5.4
1	A	410	ILE	5.0
1	A	408	ASP	5.0
1	A	977	PHE	5.0
1	A	830	LYS	4.7
1	A	461	GLY	4.6
1	A	676	ASP	4.4
1	A	953	LYS	4.4
1	A	292	LYS	4.3
1	A	502	LYS	4.0
1	A	486	LEU	4.0
1	A	936	ASN	3.7
1	A	939	LEU	3.7
1	A	405	LEU	3.7
1	A	462	SER	3.6
1	A	136	PHE	3.6
1	A	406	VAL	3.5
1	A	956	ILE	3.5
1	A	295	THR	3.4
1	A	935	LYS	3.4
1	A	1021	PHE	3.4
1	A	500	ILE	3.3
1	A	976	ALA	3.3
1	A	669	LEU	3.3
1	A	971	LEU	3.2
1	A	478	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	501	ALA	3.1
1	A	832	THR	3.1
1	A	1006	MET	3.0
1	A	951	GLU	3.0
1	A	1	MET	3.0
1	A	1003	MET	3.0
1	A	828	PRO	2.9
1	A	866	ASN	2.9
1	A	827	ALA	2.9
1	A	362	PHE	2.9
1	A	1015	PHE	2.9
1	A	894	PHE	2.8
1	A	460	GLY	2.8
1	A	35	TYR	2.8
1	A	978	ILE	2.7
1	A	973	THR	2.7
1	A	409	ALA	2.7
1	A	402	ILE	2.6
1	A	855	THR	2.6
1	A	174	ASP	2.6
1	A	834	GLU	2.5
1	A	425	LEU	2.5
1	A	75	LEU	2.5
1	A	932	LEU	2.5
1	A	955	LEU	2.5
1	A	282	ASN	2.5
1	A	895	SER	2.5
1	A	403	GLY	2.5
1	A	887	TYR	2.4
1	A	5	PHE	2.4
1	A	463	THR	2.4
1	A	722	PHE	2.4
1	A	933	SER	2.4
1	A	423	GLU	2.3
1	A	829	GLY	2.3
1	A	1018	PRO	2.3
1	A	724	ILE	2.3
1	A	400	LEU	2.3
1	A	488	LEU	2.3
1	A	411	VAL	2.3
1	A	928	THR	2.3
1	A	972	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	723	LYS	2.2
1	A	857	MET	2.2
1	A	504	ASP	2.2
1	A	171	GLY	2.2
1	A	822	ILE	2.2
1	A	979	LEU	2.2
1	A	293	LEU	2.2
1	A	447	MET	2.1
1	A	668	GLU	2.1
1	A	441	ALA	2.1
1	A	823	LEU	2.1
1	A	950	LYS	2.1
1	A	899	VAL	2.1
1	A	306	ILE	2.1
1	A	294	ALA	2.1
1	A	898	LEU	2.1
1	A	481	SER	2.0
1	A	952	GLY	2.0
1	A	675	PHE	2.0
1	A	363	ARG	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.