Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:37 AM EDT

PDB ID	:	1OY6
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 (i) 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 (1)) were used in the production of this report:

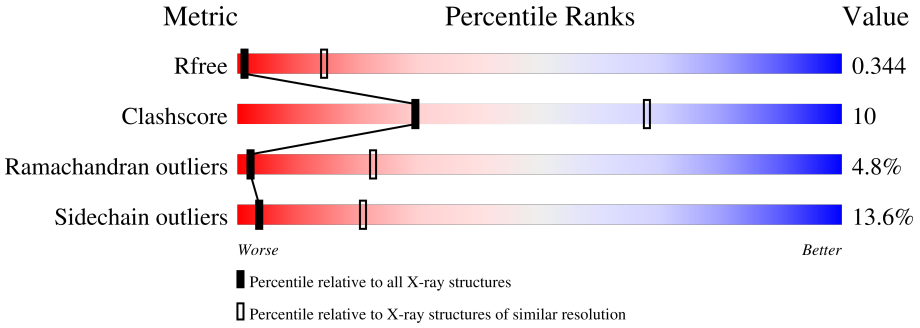
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.68 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}	130704	1013 (3.84-3.52)
Clashscore	141614	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)

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%

Mol	Chain	Length	Quality of chain
1	A	1049	64% 26% . . .

2 Entry composition (i)

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.

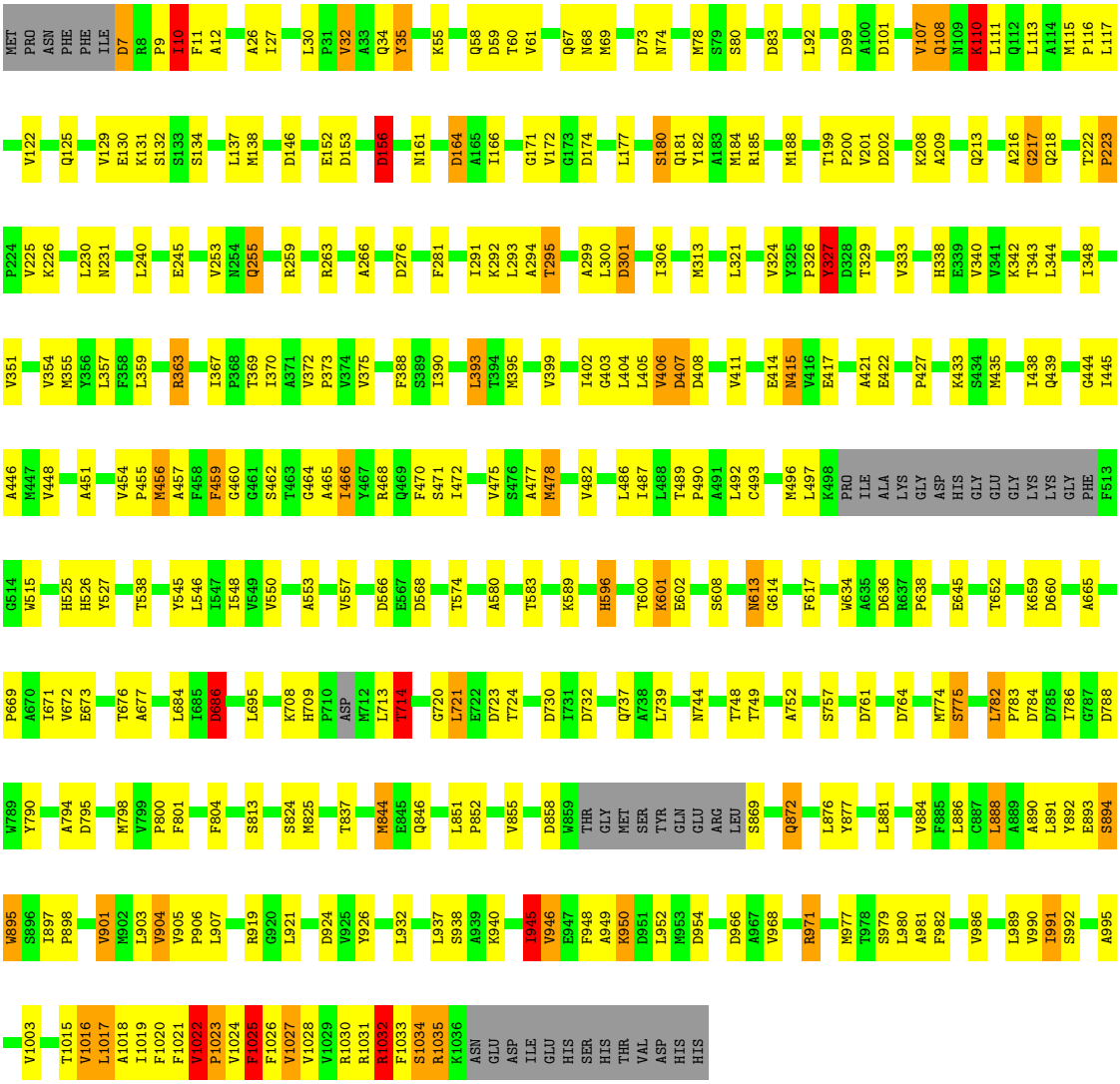
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1006	7639	4916	1262	1419	42	0	0	0

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. 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. 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

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	143.56Å 143.56Å 519.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 3.68 46.24 – 3.68	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.00-3.68) 99.6 (46.24-3.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.26 , 32.1	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	0.83	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.*

[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 (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	0.32	0/7779	0.67	34/10563 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	1032	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	795	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	858	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	723	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	568	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	59	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	146	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	174	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	7	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	408	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	83	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	764	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	153	ASP	CB-CG-OD2	5.22	122.99	118.30
1	A	276	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	966	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	101	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	202	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	636	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	660	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	730	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	732	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	301	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	954	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	566	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	924	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	784	ASP	CB-CG-OD2	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	156	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	788	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	99	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	761	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	164	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	686	ASP	CB-CG-OD2	5.01	122.81	118.30

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	147	0
All	All	7639	0	7800	147	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 10.

All (147) 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
1:A:613:ASN:HD22	1:A:613:ASN:C	1.88	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:613:ASN:C	1:A:613:ASN:ND2	2.56	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: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
1:A:415:ASN:C	1:A:415:ASN:HD22	2.13	0.52
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.92	0.52
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:950:LYS:HZ3	1:A:1028:VAL:HG11	1.77	0.49
1:A:326:PRO:O	1:A:327:TYR:C	2.50	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:359:LEU:HD21	1:A:977:MET:HE1	1.95	0.48
1:A:240:LEU:HD12	1:A:245:GLU:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.96	0.48
1:A:721:LEU:HD22	1:A:825:MET:CE	2.43	0.48
1:A:774:MET:O	1:A:775:SER:HB3	2.14	0.48
1:A:294:ALA:O	1:A:295:THR:C	2.52	0.47
1:A:111:LEU:C	1:A:111:LEU:HD23	2.34	0.47
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:546:LEU:O	1:A:550:VAL:HG23	2.15	0.47
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.50	0.47
1:A:475:VAL:HA	1:A:478:MET:HE3	1.97	0.47
1:A:721:LEU:HD13	1:A:825:MET:HE2	1.97	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: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
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:721:LEU:HD22	1:A:825:MET:HE2	1.99	0.45
1:A:890:ALA:C	1:A:891:LEU:HD22	2.37	0.45
1:A:904:VAL:HG13	1:A:1024:VAL:HG22	1.98	0.45
1:A:709:HIS:CG	1:A:709:HIS:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:110:LYS:HZ2	1:A:113:LEU:HD12	1.82	0.43
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: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: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:459:PHE:C	1:A:872:GLN:HE22	2.21	0.42
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	2.00	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1033:PHE:O	1:A:1034:SER:C	2.59	0.40
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.70	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:414:GLU:O	1:A:417:GLU:HB2	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	998/1049 (95%)	834 (84%)	116 (12%)	48 (5%)	2 22

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

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Mol	Chain	Res	Type
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
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 (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	818/855 (96%)	707 (86%)	111 (14%)	3 21

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	ILE
1	A	32	VAL
1	A	35	TYR
1	A	55	LYS
1	A	58	GLN
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	125	GLN
1	A	130	GLU
1	A	131	LYS
1	A	132	SER
1	A	137	LEU
1	A	138	MET
1	A	156	ASP
1	A	164	ASP
1	A	166	ILE
1	A	180	SER
1	A	182	TYR
1	A	185	ARG
1	A	199	THR
1	A	208	LYS

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Mol	Chain	Res	Type
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
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	301	ASP
1	A	313	MET
1	A	321	LEU
1	A	327	TYR
1	A	329	THR
1	A	355	MET
1	A	357	LEU
1	A	363	ARG
1	A	369	THR
1	A	393	LEU
1	A	404	LEU
1	A	406	VAL
1	A	415	ASN
1	A	422	GLU
1	A	433	LYS
1	A	439	GLN
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	574	THR
1	A	583	THR
1	A	589	LYS
1	A	596	HIS
1	A	601	LYS
1	A	602	GLU
1	A	608	SER
1	A	613	ASN
1	A	617	PHE
1	A	634	TRP

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Mol	Chain	Res	Type
1	A	645	GLU
1	A	659	LYS
1	A	686	ASP
1	A	708	LYS
1	A	714	THR
1	A	721	LEU
1	A	737	GLN
1	A	739	LEU
1	A	757	SER
1	A	782	LEU
1	A	786	ILE
1	A	798	MET
1	A	801	PHE
1	A	804	PHE
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	938	SER
1	A	945	ILE
1	A	948	PHE
1	A	950	LYS
1	A	971	ARG
1	A	991	ILE
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	1035	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	68	ASN
1	A	124	GLN
1	A	181	GLN
1	A	194	ASN
1	A	218	GLN
1	A	228	GLN
1	A	284	GLN
1	A	338	HIS
1	A	391	ASN
1	A	592	ASN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	667	ASN
1	A	700	ASN
1	A	747	ASN
1	A	872	GLN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.