



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 01:50 PM EDT

PDB ID : 2CB5
Title : HUMAN BLEOMYCIN HYDROLASE, C73S/DELE455 MUTANT
Authors : O'Farrell, P.A.; Gonzalez, F.; Zheng, W.; Johnston, S.A.; Joshua-Tor, L.
Deposited on : unknown
Resolution : 1.85 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

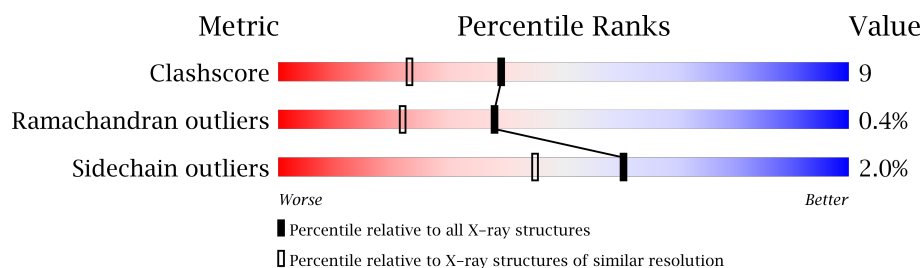
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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))
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	453	
1	B	453	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7953 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 PROTEIN (BLEOMYCIN HYDROLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	73	7	0
			3694	2354	629	684	27			
1	B	453	Total	C	N	O	S	68	8	0
			3695	2354	628	686	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	SER	CYS	ENGINEERED	UNP Q13867
A	280	HIS	TYR	SEE REMARK 999	UNP Q13867
B	73	SER	CYS	ENGINEERED	UNP Q13867
B	280	HIS	TYR	SEE REMARK 999	UNP Q13867

- Molecule 2 is water.

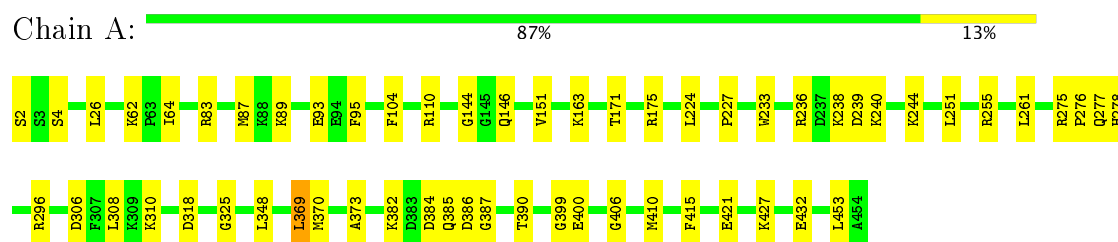
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	282	Total	O	0	0
			282	282		
2	B	282	Total	O	0	0
			282	282		

3 Residue-property plots

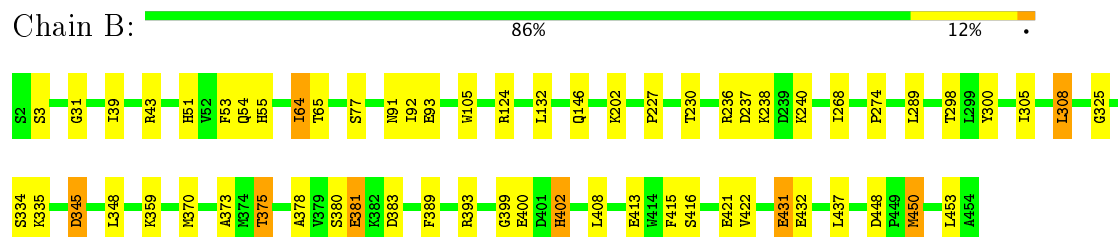
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (BLEOMYCIN HYDROLASE)



• Molecule 1: PROTEIN (BLEOMYCIN HYDROLASE)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	179.51Å 179.51Å 164.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.85	Depositor
% Data completeness (in resolution range)	89.9 (30.00-1.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	8.20	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.182 , 0.210	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7953	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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	0.58	0/3819	0.74	2/5159 (0.0%)
1	B	0.57	0/3819	0.72	0/5160
All	All	0.58	0/7638	0.73	2/10319 (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	410	MET	CG-SD-CE	-6.45	89.88	100.20
1	A	387	GLY	N-CA-C	-6.28	97.41	113.10

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	3694	0	3609	51	0
1	B	3695	0	3613	71	0
2	A	282	0	0	0	0
2	B	282	0	0	13	0
All	All	7953	0	7222	122	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 9.

All (122) 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:89:LYS:HD3	1:A:261:LEU:HD11	1.31	1.12
1:B:54:GLN:NE2	1:B:381:GLU:H	1.50	1.08
1:B:92:ILE:HA	1:B:238:LYS:HE3	1.38	1.01
1:B:93:GLU:HB2	1:B:238:LYS:HD2	1.38	1.00
1:B:431:GLU:CD	1:B:431:GLU:H	1.68	0.95
1:B:238:LYS:HE2	1:B:238:LYS:N	1.82	0.93
1:B:54:GLN:HE21	1:B:381:GLU:H	1.19	0.90
1:B:370:MET:SD	2:B:702:HOH:O	2.29	0.88
1:B:64:ILE:HD13	1:B:65:THR:N	1.89	0.87
1:A:93:GLU:HG2	1:A:238:LYS:HG2	1.56	0.87
1:B:237:ASP:C	1:B:238:LYS:HE2	1.99	0.83
1:A:370:MET:HE3	1:A:453:LEU:HD21	1.61	0.81
1:B:453:LEU:HD21	2:B:702:HOH:O	1.78	0.81
1:A:89:LYS:CD	1:A:261:LEU:HD11	2.11	0.80
1:A:370:MET:CE	1:A:453:LEU:HD21	2.12	0.79
1:B:236[B]:ARG:HG3	1:B:236[B]:ARG:HH11	1.47	0.78
1:B:93:GLU:CB	1:B:238:LYS:HD2	2.12	0.78
1:B:54:GLN:HG3	1:B:55:HIS:CD2	2.20	0.77
1:B:93:GLU:HB2	1:B:238:LYS:CD	2.15	0.76
1:A:64:ILE:HD12	1:A:406:GLY:HA3	1.70	0.71
1:B:54:GLN:NE2	1:B:381:GLU:N	2.34	0.70
1:A:64:ILE:CD1	1:A:406:GLY:HA3	2.19	0.70
1:B:93:GLU:N	1:B:238:LYS:HD2	2.05	0.70
1:B:54:GLN:HE21	1:B:381:GLU:N	1.89	0.70
1:B:54:GLN:HG2	1:B:380:SER:HA	1.75	0.69
1:B:64:ILE:HG21	1:B:400:GLU:HB2	1.73	0.69
1:B:124:ARG:HH11	1:B:124:ARG:HG2	1.59	0.67
1:B:450:MET:HB3	2:B:706:HOH:O	1.95	0.67
1:B:51:HIS:HD2	2:B:512:HOH:O	1.79	0.65
1:B:431:GLU:CD	1:B:431:GLU:N	2.49	0.65
1:B:453:LEU:HD11	2:B:702:HOH:O	1.97	0.64
1:A:163:LYS:HD2	1:A:233:TRP:HE1	1.62	0.63
1:A:370:MET:HB2	1:A:453:LEU:HD21	1.81	0.63
1:B:334[A]:SER:OG	1:B:402:HIS:HD2	1.82	0.61
1:A:83:ARG:O	1:A:87:MET:HG3	2.00	0.61
1:A:251:LEU:HD11	1:A:255:ARG:HD2	1.83	0.61
1:A:236[B]:ARG:HH11	1:A:236[B]:ARG:HG3	1.67	0.60
1:B:370:MET:HB2	1:B:453:LEU:HD21	1.84	0.60
1:A:104:PHE:CD1	1:A:227:PRO:HG2	2.36	0.60
1:B:236[B]:ARG:HG3	1:B:236[B]:ARG:NH1	2.11	0.60
1:B:92:ILE:CA	1:B:238:LYS:HE3	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306[B]:ASP:OD2	1:A:310:LYS:HE2	2.02	0.59
1:B:402:HIS:NE2	1:B:408:LEU:HD21	2.19	0.58
1:A:369:LEU:HD22	1:A:370:MET:O	2.04	0.57
1:B:375:THR:HG23	2:B:529:HOH:O	2.04	0.57
1:A:373:ALA:HB2	1:A:453:LEU:HD13	1.87	0.57
1:A:175:ARG:HH11	1:A:175:ARG:HG3	1.70	0.56
1:B:236[B]:ARG:HD3	1:B:240:LYS:O	2.05	0.56
1:B:77[B]:SER:HB3	1:B:375:THR:HG22	1.88	0.56
1:A:369:LEU:CD2	1:A:370:MET:O	2.54	0.55
1:A:370:MET:CE	1:A:453:LEU:HD11	2.37	0.55
1:B:413:GLU:HG3	2:B:580:HOH:O	2.06	0.55
1:B:300:TYR:CD2	1:B:450:MET:SD	3.00	0.54
1:A:348:LEU:O	1:A:348:LEU:HD23	2.07	0.54
1:A:64:ILE:HD13	1:A:399:GLY:C	2.27	0.54
1:A:2:SER:C	1:A:4:SER:H	2.11	0.53
1:A:110:ARG:NH2	1:A:144:GLY:O	2.41	0.53
1:B:450:MET:HG3	1:B:450:MET:O	2.09	0.53
1:B:373:ALA:HB2	1:B:453:LEU:HD13	1.91	0.53
1:B:325:GLY:HA3	2:B:702:HOH:O	2.07	0.53
1:B:236[B]:ARG:NH1	2:B:531:HOH:O	2.41	0.52
1:B:230[A]:THR:HG22	2:B:723:HOH:O	2.08	0.52
1:A:64:ILE:HD13	1:A:400:GLU:HA	1.91	0.52
1:B:202:LYS:HB2	1:B:202:LYS:NZ	2.25	0.52
1:B:105:TRP:CZ2	1:B:227:PRO:HG3	2.45	0.52
1:A:64:ILE:HG21	1:A:400:GLU:HB2	1.92	0.52
1:B:93:GLU:CA	1:B:238:LYS:HD2	2.39	0.52
1:A:325:GLY:HA3	1:A:370:MET:HE3	1.92	0.51
1:B:305:ILE:HG12	1:B:416:SER:HA	1.92	0.51
1:A:370:MET:HE2	1:A:453:LEU:CG	2.41	0.51
1:A:370:MET:HE2	1:A:453:LEU:HD21	1.92	0.51
1:A:277:GLN:HG2	1:A:278:HIS:CD2	2.46	0.51
1:A:62:LYS:HE2	1:A:93:GLU:O	2.11	0.51
1:A:163:LYS:HD2	1:A:233:TRP:NE1	2.26	0.50
1:A:251:LEU:HD13	1:A:251:LEU:C	2.32	0.50
1:B:64:ILE:HD13	1:B:64:ILE:C	2.32	0.50
1:B:91:ASN:O	1:B:238:LYS:HG2	2.12	0.50
1:B:93:GLU:H	1:B:238:LYS:CE	2.24	0.50
1:A:432:GLU:H	1:A:432:GLU:CD	2.14	0.49
1:A:251:LEU:CD1	1:A:255:ARG:HD2	2.42	0.49
1:B:64:ILE:CD1	1:B:65:THR:O	2.60	0.49
1:A:325:GLY:HA3	1:A:370:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:C	1:A:369:LEU:HD22	2.33	0.48
1:A:87:MET:HG2	1:A:95:PHE:HB3	1.94	0.48
1:A:26:LEU:HD23	1:A:26:LEU:O	2.14	0.48
1:B:93:GLU:N	1:B:238:LYS:CD	2.75	0.48
1:A:239:ASP:O	1:A:240:LYS:HB2	2.14	0.47
1:B:345:ASP:HB3	1:B:348:LEU:HB3	1.97	0.47
1:B:64:ILE:HD13	1:B:65:THR:O	2.15	0.47
1:B:448:ASP:OD1	1:B:450:MET:HG2	2.15	0.47
1:B:450:MET:HE1	2:B:707:HOH:O	2.15	0.46
1:B:64:ILE:HD12	1:B:399:GLY:CA	2.45	0.46
1:B:268:ILE:HD12	1:B:437:LEU:HD21	1.98	0.45
1:A:26:LEU:HD23	1:A:26:LEU:C	2.37	0.45
1:A:93:GLU:HG2	1:A:238:LYS:CG	2.39	0.45
1:B:432:GLU:HG3	1:B:432:GLU:H	1.43	0.45
1:B:335:LYS:HG3	2:B:573:HOH:O	2.17	0.44
1:A:171:THR:CG2	1:A:224:LEU:HD22	2.47	0.44
1:A:64:ILE:HD13	1:A:400:GLU:CA	2.48	0.44
1:A:64:ILE:HD13	1:A:400:GLU:N	2.33	0.44
1:A:318:ASP:OD2	1:A:427:LYS:HE3	2.17	0.43
1:B:124:ARG:NH1	1:B:124:ARG:HG2	2.29	0.43
1:B:238:LYS:HE2	1:B:238:LYS:CA	2.46	0.43
1:B:238:LYS:N	1:B:238:LYS:CE	2.69	0.42
1:B:274:PRO:HG3	1:B:359:LYS:HB3	2.01	0.42
1:B:289:LEU:O	1:B:298:THR:CG2	2.68	0.42
1:B:124:ARG:CG	1:B:124:ARG:HH11	2.30	0.41
1:B:31:GLY:HA2	1:B:39:ILE:HD13	2.02	0.41
1:B:450:MET:CE	2:B:707:HOH:O	2.68	0.41
1:B:93:GLU:H	1:B:238:LYS:HD2	1.82	0.41
1:A:275:ARG:HA	1:A:276:PRO:HD3	1.89	0.41
1:A:146:GLN:OE1	1:A:421:GLU:OE2	2.38	0.41
1:B:381:GLU:HA	1:B:389:PHE:HA	2.02	0.41
1:B:77[A]:SER:HB2	1:B:375:THR:HG22	2.02	0.41
1:B:308:LEU:HD13	1:B:422:VAL:HG22	2.01	0.41
1:A:370:MET:HE2	1:A:453:LEU:CD2	2.51	0.40
1:A:151:VAL:HG11	1:A:296:ARG:CZ	2.51	0.40
1:B:378:ALA:HB3	1:B:393:ARG:HB3	2.02	0.40
1:B:146:GLN:OE1	1:B:421:GLU:OE2	2.39	0.40
1:A:370:MET:HE2	1:A:453:LEU:HD11	2.02	0.40
1:B:53:PHE:N	1:B:53:PHE:CD1	2.89	0.40
1:A:382:LYS:HG2	1:A:390:THR:HG23	2.02	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	458/453 (101%)	446 (97%)	9 (2%)	3 (1%)	25	10
1	B	459/453 (101%)	449 (98%)	9 (2%)	1 (0%)	51	35
All	All	917/906 (101%)	895 (98%)	18 (2%)	4 (0%)	38	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	386	ASP
1	A	384	ASP
1	B	3	SER

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	412/405 (102%)	408 (99%)	4 (1%)	80	74
1	B	413/405 (102%)	401 (97%)	12 (3%)	48	30
All	All	825/810 (102%)	809 (98%)	16 (2%)	60	47

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	A	308	LEU

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Mol	Chain	Res	Type
1	A	369	LEU
1	A	415	PHE
1	B	43	ARG
1	B	64	ILE
1	B	132	LEU
1	B	308	LEU
1	B	345	ASP
1	B	375	THR
1	B	381	GLU
1	B	383	ASP
1	B	402	HIS
1	B	415	PHE
1	B	431	GLU
1	B	450	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	241	ASN
1	B	23	GLN
1	B	51	HIS
1	B	54	GLN
1	B	55	HIS
1	B	91	ASN
1	B	241	ASN
1	B	402	HIS

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 carbohydrates 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.