



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 08:48 pm GMT

PDB ID : 1YSI

Title : Solution structure of the anti-apoptotic protein Bcl-xL in complex with an acyl-sulfonamide-based ligand

Authors : Oltersdorf, T.; Elmore, S.W.; Shoemaker, A.R.; Armstrong, R.C.; Augeri, D.J.; Belli, B.A.; Bruncko, M.; Deckwerth, T.L.; Dinges, J.; Hajduk, P.J.; Joseph, M.K.; Kitada, S.; Korsmeyer, S.J.; Kunzer, A.R.; Letai, A.; Li, C.; Mitten, M.J.; Nettesheim, D.G.; Ng, S.; Nimmer, P.M.; O'Connor, J.M.; Oleksijew, A.; Petros, A.M.; Reed, J.C.; Shen, W.; Tahir, S.K.; Thompson, C.B.; Tomaselli, K.J.; Wang, B.; Wendt, M.D.; Zhang, H.; Fesik, S.W.; Rosenberg, S.H.

Deposited on : 2005-02-08

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

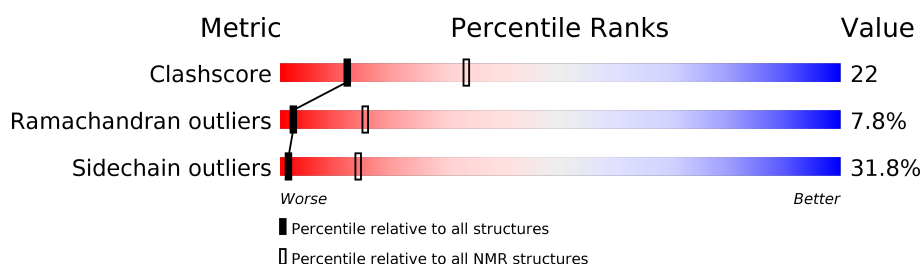
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	181	 42% 46% 10% •

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2893 atoms, of which 1388 are hydrogens and 0 are deuteriums.

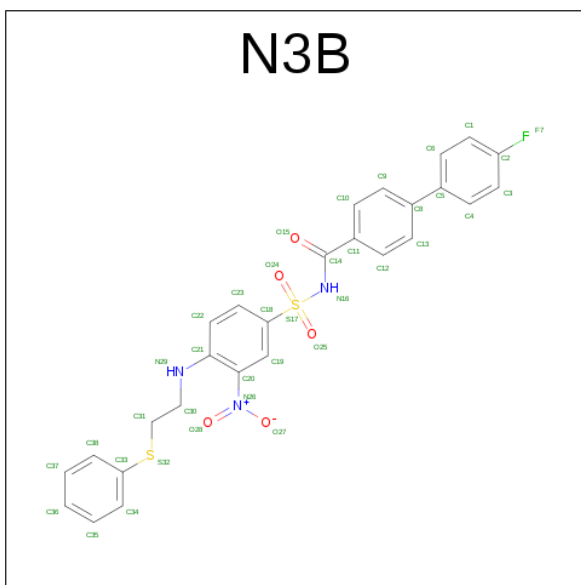
- Molecule 1 is a protein called Apoptosis regulator Bcl-X.

Mol	Chain	Residues	Atoms						Trace
1	A	181	Total	C	H	N	O	S	0
			2833	918	1366	258	285	6	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q07817
A	2	SER	-	EXPRESSION TAG	UNP Q07817
A	3	MET	-	EXPRESSION TAG	UNP Q07817
A	4	ALA	-	EXPRESSION TAG	UNP Q07817
A	214	LEU	-	EXPRESSION TAG	UNP Q07817
A	215	GLU	-	EXPRESSION TAG	UNP Q07817
A	216	HIS	-	EXPRESSION TAG	UNP Q07817
A	217	HIS	-	EXPRESSION TAG	UNP Q07817
A	218	HIS	-	EXPRESSION TAG	UNP Q07817
A	219	HIS	-	EXPRESSION TAG	UNP Q07817
A	220	HIS	-	EXPRESSION TAG	UNP Q07817
A	181	HIS	-	EXPRESSION TAG	UNP Q07817

- Molecule 2 is N-[(4'-FLUORO-1,1'-BIPHENYL-4-YL)CARBONYL]-3-NITRO-4-{[2-(PHENYLSULFANYL)ETHYL]AMINO}BENZENESULFONAMIDE (three-letter code: N3B) (formula: C₂₇H₂₂FN₃O₅S₂).



Mol	Chain	Residues	Atoms						
2	A	1	Total	C	F	H	N	O	S
			60	27	1	22	3	5	2

4 Residue-property plots [i](#)

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Apoptosis regulator Bcl-X



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: N3B

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0	11
All	All	0	11

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	95	ARG	Sidechain
1	A	38	ARG	Sidechain
1	A	136	ARG	Sidechain
1	A	104	ARG	Sidechain
1	A	107	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	213	ARG	Sidechain
1	A	143	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	106	ARG	Sidechain
1	A	10	ARG	Sidechain

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1467	1366	1366	63
2	A	38	22	22	3
All	All	1505	1388	1388	63

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 22.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:116:LEU:HD22	1:A:154:LEU:HD21	0.96	1.35
1:A:14:VAL:HG23	1:A:28:TRP:CZ2	0.75	2.16
1:A:198:LEU:HD23	1:A:199:TYR:CD1	0.71	2.20
1:A:147:PHE:CE2	1:A:174:MET:SD	0.70	2.85
1:A:13:VAL:CG1	1:A:171:ALA:HB1	0.68	2.18
1:A:123:ALA:HB1	1:A:173:TRP:CH2	0.67	2.24
1:A:3:MET:N	1:A:3:MET:SD	0.65	2.69
1:A:14:VAL:HG23	1:A:28:TRP:CE2	0.65	2.26
1:A:182:LEU:HD23	1:A:186:ILE:HD11	0.64	1.69
1:A:13:VAL:HG11	1:A:171:ALA:HB1	0.64	1.70
1:A:31:PHE:CD2	1:A:167:VAL:HG21	0.64	2.28
1:A:159:VAL:HG13	1:A:164:GLN:CG	0.61	2.24
1:A:90:VAL:HG13	1:A:192:TRP:CE3	0.61	2.31
1:A:90:VAL:HG13	1:A:192:TRP:CZ3	0.61	2.31
1:A:21:LEU:HD13	1:A:31:PHE:CZ	0.59	2.31
1:A:31:PHE:CE2	1:A:167:VAL:HG21	0.59	2.32
1:A:33:ASP:O	1:A:34:VAL:HG22	0.59	1.98
1:A:214:LEU:N	1:A:214:LEU:HD23	0.58	2.13
1:A:5:MET:SD	1:A:5:MET:N	0.58	2.76
1:A:159:VAL:HG13	1:A:164:GLN:HG2	0.58	1.75
1:A:2:SER:C	1:A:3:MET:SD	0.56	2.84
1:A:33:ASP:O	1:A:34:VAL:HG13	0.56	2.01
1:A:26:TYR:CD1	1:A:159:VAL:HG12	0.56	2.36
1:A:142:GLY:CA	2:A:1000:N3B:HG	0.56	2.31
1:A:97:ALA:HB1	1:A:145:VAL:CG1	0.55	2.30
1:A:33:ASP:C	1:A:34:VAL:HG13	0.55	2.21
1:A:123:ALA:HB1	1:A:173:TRP:CZ2	0.55	2.37
1:A:1:MET:C	1:A:3:MET:SD	0.54	2.86
1:A:31:PHE:CZ	1:A:159:VAL:HG11	0.54	2.38
1:A:94:LEU:HD21	1:A:148:PHE:CD2	0.54	2.38
1:A:17:LEU:HD13	1:A:28:TRP:CZ3	0.51	2.40
1:A:97:ALA:HB1	1:A:145:VAL:HG11	0.49	1.84
1:A:127:PHE:CE1	1:A:131:VAL:HG21	0.49	2.42
1:A:14:VAL:CG2	1:A:28:TRP:CE2	0.48	2.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:213:ARG:HB3	1:A:214:LEU:HD23	0.48	1.86
1:A:13:VAL:O	1:A:17:LEU:HD12	0.47	2.10
1:A:183:GLU:N	1:A:184:PRO:CD	0.47	2.78
1:A:213:ARG:NH1	1:A:214:LEU:HD22	0.46	2.26
1:A:198:LEU:CD2	1:A:199:TYR:CE1	0.45	2.98
1:A:14:VAL:HG23	1:A:28:TRP:CH2	0.45	2.45
1:A:90:VAL:CG1	1:A:192:TRP:CZ3	0.45	3.00
1:A:144:ILE:HG12	1:A:182:LEU:HD21	0.45	1.89
1:A:90:VAL:CG1	1:A:192:TRP:CE3	0.45	3.00
1:A:109:PHE:CD1	1:A:109:PHE:N	0.44	2.86
1:A:118:ILE:O	1:A:119:THR:HG23	0.44	2.12
1:A:17:LEU:HD21	1:A:155:CYS:SG	0.43	2.53
1:A:198:LEU:HD23	1:A:199:TYR:CE1	0.43	2.47
1:A:155:CYS:O	1:A:159:VAL:HG23	0.43	2.14
1:A:11:GLU:HA	1:A:14:VAL:HG12	0.43	1.90
1:A:192:TRP:O	1:A:196:VAL:HG23	0.43	2.14
1:A:105:TYR:OH	2:A:1000:N3B:HD1	0.42	2.14
1:A:214:LEU:CD2	1:A:214:LEU:N	0.42	2.82
1:A:13:VAL:HG13	1:A:17:LEU:HD12	0.42	1.91
1:A:13:VAL:HG11	1:A:171:ALA:CB	0.42	2.42
1:A:1:MET:HB2	1:A:3:MET:SD	0.42	2.55
1:A:109:PHE:HB3	1:A:112:LEU:HD12	0.41	1.91
1:A:94:LEU:HD21	1:A:148:PHE:CG	0.41	2.50
1:A:105:TYR:CE2	2:A:1000:N3B:HC1	0.41	2.51
1:A:12:LEU:HD13	1:A:148:PHE:HZ	0.41	1.75
1:A:119:THR:HG22	1:A:120:PRO:HD2	0.41	1.93
1:A:93:ALA:HB3	1:A:195:PHE:CE2	0.40	2.51
1:A:27:SER:O	1:A:31:PHE:CE1	0.40	2.74
1:A:139:VAL:O	1:A:185:TRP:CZ2	0.40	2.74

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	179/181 (99%)	137 (77%)	28 (16%)	14 (8%)	2 15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	179/181 (99%)	137 (77%)	28 (16%)	14 (8%)	2	15

All 14 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	121	GLY
1	A	200	GLY
1	A	123	ALA
1	A	162	GLU
1	A	46	GLU
1	A	45	THR
1	A	37	ASN
1	A	38	ARG
1	A	43	GLU
1	A	34	VAL
1	A	208	ARG
1	A	182	LEU
1	A	211	GLN
1	A	209	LYS

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	154/154 (100%)	105 (68%)	49 (32%)	1	14
All	All	154/154 (100%)	105 (68%)	49 (32%)	1	14

All 49 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	163	MET
1	A	193	ASP
1	A	124	TYR
1	A	114	SER
1	A	5	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	111	ASP
1	A	208	ARG
1	A	218	HIS
1	A	137	ASP
1	A	20	LYS
1	A	143	ARG
1	A	180	ASP
1	A	3	MET
1	A	8	SER
1	A	174	MET
1	A	7	GLN
1	A	116	LEU
1	A	38	ARG
1	A	202	ASN
1	A	110	SER
1	A	149	SER
1	A	103	LEU
1	A	23	GLN
1	A	109	PHE
1	A	117	HIS
1	A	216	HIS
1	A	148	PHE
1	A	40	GLU
1	A	189	ASN
1	A	209	LYS
1	A	178	LEU
1	A	158	SER
1	A	140	ASN
1	A	29	SER
1	A	157	GLU
1	A	94	LEU
1	A	164	GLN
1	A	39	THR
1	A	91	LYS
1	A	27	SER
1	A	119	THR
1	A	196	VAL
1	A	181	HIS
1	A	34	VAL
1	A	13	VAL
1	A	161	LYS
1	A	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	147	PHE
1	A	6	SER

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	N3B	A	1000	-	39,41,41	1.45	1 (2%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	N3B	A	1000	-	53,57,57	2.15	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	N3B	A	1000	-	-	0,28,30,30	0,4,4,4

All bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	N3B	S17-N16	6.69	1.78	1.64

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	N3B	C31-S32-C33	9.09	120.34	104.04
2	A	1000	N3B	O25-S17-O24	8.01	109.31	119.55
2	A	1000	N3B	C11-C14-N16	5.36	122.67	115.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided