

Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2024 – 04:10 PM EDT

PDB ID : 8VXM

Title: Human Bcl-2/Bcl-xL Chimera Fused to MBP in Complex with Inhibitor

S55746

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Deposited on : 2024-02-05

Resolution : 2.10 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

Mogul : 2022.3.0, CSD as543be (2022)

Xtriage (Phenix) : 1.20.1

EDS : 3.0

buster-report : 1.1.7 (2018)

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.002 (Gargrove)

Density-Fitness : 1.0.11

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

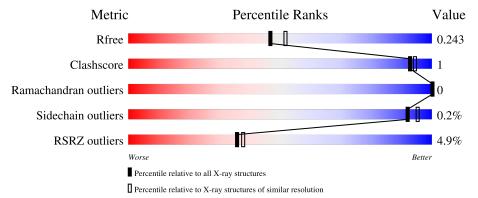
Validation Pipeline (wwPDB-VP) : 2.38.3

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 2.10 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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		
			5%		
1	Α	547	90%	•	6%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4179 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 Maltose/maltodextrin-binding periplasmic protein fused to apoptosis regulator Bcl-2/Bcl-xL chimera.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	515	Total 4051	C 2598	N 679	O 761	S 13	0	0	0

There are 29 discrepancies between the modelled and reference sequences:

C1 •	D • 1	2.6	A . 1	<u> </u>	D. C
Chain	Residue	Modelled	Actual	Comment	Reference
A	-380	MET	-	initiating methionine	UNP P0AEX9
A	-379	HIS	-	expression tag	UNP P0AEX9
A	-378	HIS	-	expression tag	UNP P0AEX9
A	-377	HIS	-	expression tag	UNP P0AEX9
A	-376	HIS	-	expression tag	UNP P0AEX9
A	-375	HIS	-	expression tag	UNP P0AEX9
A	-374	HIS	-	expression tag	UNP P0AEX9
A	-373	HIS	-	expression tag	UNP P0AEX9
A	-372	HIS	-	expression tag	UNP P0AEX9
A	-371	HIS	-	expression tag	UNP P0AEX9
A	-370	HIS	-	expression tag	UNP P0AEX9
A	-369	GLU	-	expression tag	UNP P0AEX9
A	-368	ASN	-	expression tag	UNP P0AEX9
A	-367	LEU	-	expression tag	UNP P0AEX9
A	-366	TYR	-	expression tag	UNP P0AEX9
A	-365	PHE	-	expression tag	UNP P0AEX9
A	-364	GLN	-	expression tag	UNP P0AEX9
A	-363	GLY	-	expression tag	UNP P0AEX9
A	-281	ALA	ASP	engineered mutation	UNP P0AEX9
A	-280	ALA	LYS	engineered mutation	UNP P0AEX9
A	-191	ALA	GLU	engineered mutation	UNP P0AEX9
A	-190	ALA	ASN	engineered mutation	UNP P0AEX9
A	-124	ALA	LYS	engineered mutation	UNP P0AEX9
A	4	ALA	-	linker	UNP P0AEX9
A	5	ALA	-	linker	UNP P0AEX9
A	6	ARG	-	linker	UNP P0AEX9
				~	1

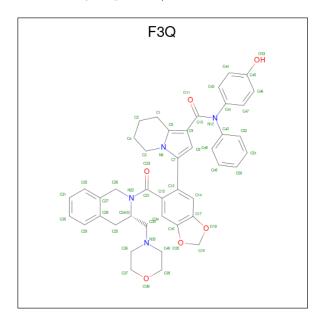
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Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	linker	UNP P0AEX9
A	8	ALA	-	linker	UNP P0AEX9
A	9	ALA	-	linker	UNP P0AEX9

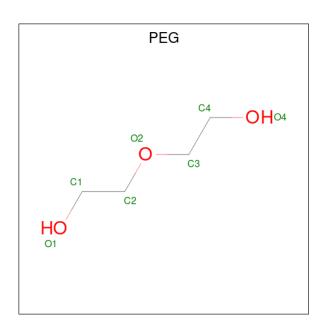
• Molecule 2 is $\{N\}$ -(4-hydroxyphenyl)-3-[6-[[(3 $\{S\})$)-3-(morpholin-4-ylmethyl)-3,4-dihydro-1 $\{H\}$ -isoquinolin-2-yl]carbonyl]-1,3-benzodioxol-5-yl]- $\{N\}$ -phenyl-5,6,7,8-tetrahydroindoli zine-1-carboxamide (three-letter code: F3Q) (formula: $C_{43}H_{42}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 53	C 43	N 4	O 6	0	0

• Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total 7	C 4	O 3	0	0

• Molecule 4 is water.

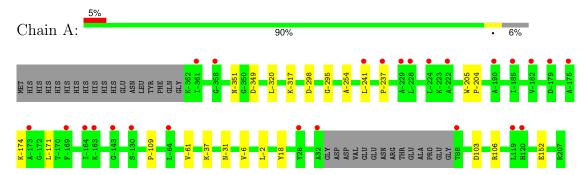
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	68	Total O 68 68	0	0



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 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: Maltose/maltodextrin-binding periplasmic protein fused to apoptosis regulator Bcl-2/Bcl-xL chimera





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	48.80Å 88.74Å 134.91Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.45 - 2.10	Depositor
Resolution (A)	67.45 - 2.10	EDS
% Data completeness	96.1 (67.45-2.10)	Depositor
(in resolution range)	96.4 (67.45-2.10)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.47 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.218 , 0.243	Depositor
R, R_{free}	0.219 , 0.243	DCC
R_{free} test set	1756 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 48.1	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	0.95	EDS
Total number of atoms	4179	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, F3Q

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).

ſ	Mal	Chain	Bond	lengths	Bond angles		
	IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
Ī	1	A	0.24	0/4152	0.43	0/5634	

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 (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	4051	0	3962	11	0
2	A	53	0	0	0	0
3	A	7	0	10	0	0
4	A	68	0	0	0	0
All	All	4179	0	3972	11	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 1.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:-171:LEU:HD23	1:A:-6:VAL:HG13	1.93	0.51
1:A:18:TYR:OH	1:A:152:GLU:OE2	2.30	0.49
1:A:-241:LEU:HD21	1:A:-237:PRO:HD3	1.94	0.49
1:A:-320:LEU:HA	1:A:-317:LYS:HB3	1.95	0.49
1:A:-109:PRO:HB3	1:A:-37:LYS:HD3	1.94	0.48
1:A:-351:ASN:ND2	1:A:-349:ASP:OD1	2.42	0.47
1:A:-295:GLY:HA3	1:A:-31:ASN:O	2.14	0.47
1:A:-205:TRP:N	1:A:-204:PRO:HD2	2.31	0.46
1:A:-254:ALA:HA	1:A:-61:VAL:HA	2.00	0.43
1:A:103:ASP:OD1	1:A:106:ARG:NH2	2.53	0.42
1:A:-174:LYS:HG2	1:A:-2:LEU:HD12	2.04	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	511/547 (93%)	504 (99%)	7 (1%)	0	100 100	

There are no Ramachandran outliers to report.

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	414/442 (94%)	413 (100%)	1 (0%)	92 95		



All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-298	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

	Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
						Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	2	F3Q	A	301	-	59,61,61	0.54	0	72,88,88	0.46	0
	3	PEG	A	302	-	6,6,6	0.50	0	5,5,5	0.28	0

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	F3Q	A	301	-	-	4/29/65/65	0/8/9/9
3	PEG	A	302	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

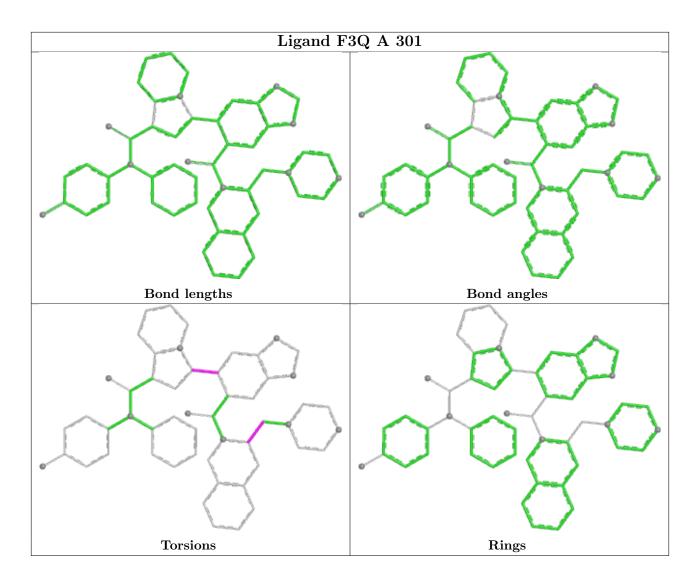
Mol	Chain	Res	Type	Atoms
2	A	301	F3Q	C25-C24-C33-N35
2	A	301	F3Q	C14-C13-C7-C8
3	A	302	PEG	C4-C3-O2-C2
2	A	301	F3Q	C14-C13-C7-N6
2	A	301	F3Q	N22-C24-C33-N35

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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)

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>	# RSRZ > 2		$OWAB(Å^2)$	Q<0.9	
1	A	515/547 (94%)	0.58	25 (4%)	36	38	39, 53, 79, 107	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	HIS	3.7
1	A	-222	ALA	3.2
1	A	-224	LEU	3.2
1	A	28	TYR	3.1
1	A	-228	LEU	2.8
1	A	32	ALA	2.7
1	A	-229	ALA	2.6
1	A	-185	ILE	2.6
1	A	-237	PRO	2.5
1	A	-190	ALA	2.4
1	A	88	THR	2.4
1	A	-241	LEU	2.3
1	A	-169	PHE	2.2
1	A	-358	GLY	2.2
1	A	-164	ILE	2.1
1	A	119	LEU	2.1
1	A	-361	ILE	2.1
1	A	-163	LYS	2.1
1	A	-130	SER	2.1
1	A	-175	ALA	2.1
1	A	-173	ALA	2.1
1	A	-143	GLY	2.1
1	A	-179	ASP	2.1
1	A	-64	LEU	2.0
1	A	-182	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.

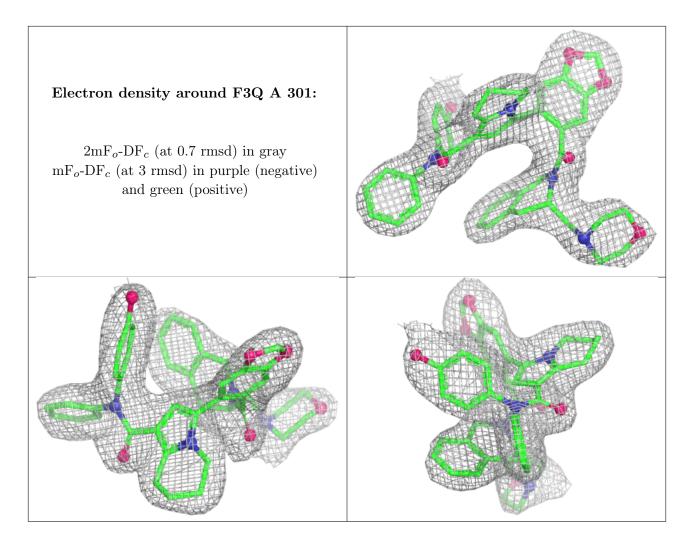
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	PEG	A	302	7/7	0.89	0.15	60,72,78,80	0
2	F3Q	A	301	53/53	0.92	0.10	46,56,67,75	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

