



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:18 PM GMT

PDB ID : 4QNQ
Title : Crystal Structure Analysis of full-length Bcl-XL in complex with the inhibitor ABT-263
Authors : Korste, A.; Vetter, I.R.; Stoll, R.
Deposited on : 2014-06-18
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

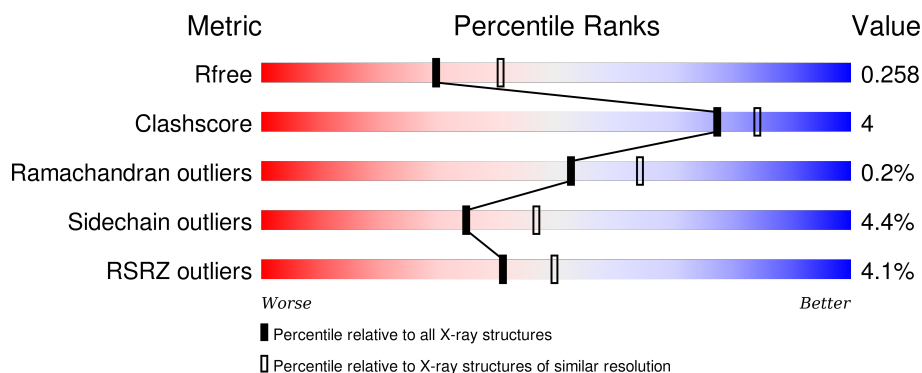
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>54%</div> <div>5% •</div> <div>40%</div> </div>
1	B	240	<div> <div>54%</div> <div>6%</div> <div>40%</div> </div>
1	C	240	<div> <div>55%</div> <div>5%</div> <div>40%</div> </div>
1	D	240	<div> <div>54%</div> <div>•</div> <div>41%</div> </div>
1	E	240	<div> <div>55%</div> <div>5% •</div> <div>38%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	240	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>57%</div><div>5%</div><div>38%</div></div></div>
1	G	240	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>51%</div><div>7%</div><div>42%</div></div></div>
1	H	240	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>52%</div><div>7%</div><div>41%</div></div></div>
1	I	240	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>56%</div><div>5%</div><div>39%</div></div></div>
1	J	240	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>55%</div><div>6%</div><div>38%</div></div></div>
1	K	240	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>55%</div><div></div><div>40%</div></div></div>
1	L	240	<div><div><div></div><div></div><div></div></div><div><div>6%</div><div>50%</div><div>8%</div><div>41%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14929 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 Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1169	749	196	219	5			
1	B	144	Total	C	N	O	S	0	0	0
			1167	745	196	222	4			
1	C	144	Total	C	N	O	S	0	0	0
			1167	748	195	219	5			
1	D	141	Total	C	N	O	S	0	0	0
			1143	730	193	215	5			
1	E	148	Total	C	N	O	S	0	0	0
			1199	771	199	224	5			
1	F	149	Total	C	N	O	S	0	0	0
			1207	775	201	226	5			
1	G	140	Total	C	N	O	S	0	0	0
			1135	726	191	213	5			
1	H	142	Total	C	N	O	S	0	0	0
			1150	734	194	217	5			
1	I	147	Total	C	N	O	S	0	0	0
			1188	762	198	223	5			
1	J	149	Total	C	N	O	S	0	0	0
			1207	775	201	226	5			
1	K	143	Total	C	N	O	S	0	0	0
			1161	742	196	219	4			
1	L	142	Total	C	N	O	S	0	0	0
			1150	734	194	217	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P53563
A	-5	SER	-	EXPRESSION TAG	UNP P53563
A	-4	PRO	-	EXPRESSION TAG	UNP P53563
A	-3	GLU	-	EXPRESSION TAG	UNP P53563
A	-2	PHE	-	EXPRESSION TAG	UNP P53563

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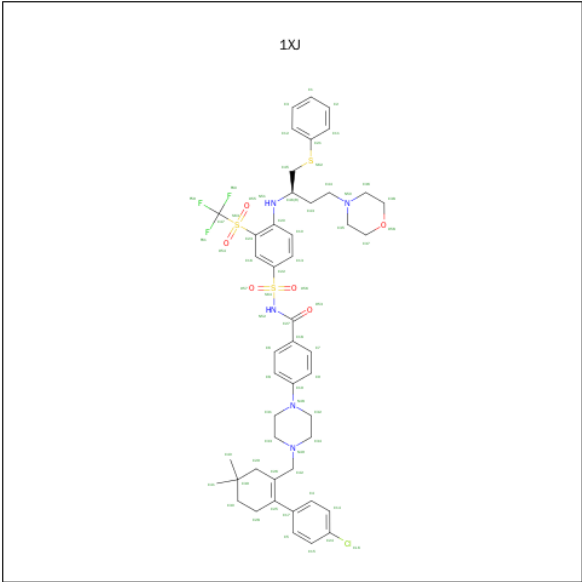
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PRO	-	EXPRESSION TAG	UNP P53563
A	0	GLY	-	EXPRESSION TAG	UNP P53563
B	-6	GLY	-	EXPRESSION TAG	UNP P53563
B	-5	SER	-	EXPRESSION TAG	UNP P53563
B	-4	PRO	-	EXPRESSION TAG	UNP P53563
B	-3	GLU	-	EXPRESSION TAG	UNP P53563
B	-2	PHE	-	EXPRESSION TAG	UNP P53563
B	-1	PRO	-	EXPRESSION TAG	UNP P53563
B	0	GLY	-	EXPRESSION TAG	UNP P53563
C	-6	GLY	-	EXPRESSION TAG	UNP P53563
C	-5	SER	-	EXPRESSION TAG	UNP P53563
C	-4	PRO	-	EXPRESSION TAG	UNP P53563
C	-3	GLU	-	EXPRESSION TAG	UNP P53563
C	-2	PHE	-	EXPRESSION TAG	UNP P53563
C	-1	PRO	-	EXPRESSION TAG	UNP P53563
C	0	GLY	-	EXPRESSION TAG	UNP P53563
D	-6	GLY	-	EXPRESSION TAG	UNP P53563
D	-5	SER	-	EXPRESSION TAG	UNP P53563
D	-4	PRO	-	EXPRESSION TAG	UNP P53563
D	-3	GLU	-	EXPRESSION TAG	UNP P53563
D	-2	PHE	-	EXPRESSION TAG	UNP P53563
D	-1	PRO	-	EXPRESSION TAG	UNP P53563
D	0	GLY	-	EXPRESSION TAG	UNP P53563
E	-6	GLY	-	EXPRESSION TAG	UNP P53563
E	-5	SER	-	EXPRESSION TAG	UNP P53563
E	-4	PRO	-	EXPRESSION TAG	UNP P53563
E	-3	GLU	-	EXPRESSION TAG	UNP P53563
E	-2	PHE	-	EXPRESSION TAG	UNP P53563
E	-1	PRO	-	EXPRESSION TAG	UNP P53563
E	0	GLY	-	EXPRESSION TAG	UNP P53563
F	-6	GLY	-	EXPRESSION TAG	UNP P53563
F	-5	SER	-	EXPRESSION TAG	UNP P53563
F	-4	PRO	-	EXPRESSION TAG	UNP P53563
F	-3	GLU	-	EXPRESSION TAG	UNP P53563
F	-2	PHE	-	EXPRESSION TAG	UNP P53563
F	-1	PRO	-	EXPRESSION TAG	UNP P53563
F	0	GLY	-	EXPRESSION TAG	UNP P53563
G	-6	GLY	-	EXPRESSION TAG	UNP P53563
G	-5	SER	-	EXPRESSION TAG	UNP P53563
G	-4	PRO	-	EXPRESSION TAG	UNP P53563
G	-3	GLU	-	EXPRESSION TAG	UNP P53563
G	-2	PHE	-	EXPRESSION TAG	UNP P53563

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	PRO	-	EXPRESSION TAG	UNP P53563
G	0	GLY	-	EXPRESSION TAG	UNP P53563
H	-6	GLY	-	EXPRESSION TAG	UNP P53563
H	-5	SER	-	EXPRESSION TAG	UNP P53563
H	-4	PRO	-	EXPRESSION TAG	UNP P53563
H	-3	GLU	-	EXPRESSION TAG	UNP P53563
H	-2	PHE	-	EXPRESSION TAG	UNP P53563
H	-1	PRO	-	EXPRESSION TAG	UNP P53563
H	0	GLY	-	EXPRESSION TAG	UNP P53563
I	-6	GLY	-	EXPRESSION TAG	UNP P53563
I	-5	SER	-	EXPRESSION TAG	UNP P53563
I	-4	PRO	-	EXPRESSION TAG	UNP P53563
I	-3	GLU	-	EXPRESSION TAG	UNP P53563
I	-2	PHE	-	EXPRESSION TAG	UNP P53563
I	-1	PRO	-	EXPRESSION TAG	UNP P53563
I	0	GLY	-	EXPRESSION TAG	UNP P53563
J	-6	GLY	-	EXPRESSION TAG	UNP P53563
J	-5	SER	-	EXPRESSION TAG	UNP P53563
J	-4	PRO	-	EXPRESSION TAG	UNP P53563
J	-3	GLU	-	EXPRESSION TAG	UNP P53563
J	-2	PHE	-	EXPRESSION TAG	UNP P53563
J	-1	PRO	-	EXPRESSION TAG	UNP P53563
J	0	GLY	-	EXPRESSION TAG	UNP P53563
K	-6	GLY	-	EXPRESSION TAG	UNP P53563
K	-5	SER	-	EXPRESSION TAG	UNP P53563
K	-4	PRO	-	EXPRESSION TAG	UNP P53563
K	-3	GLU	-	EXPRESSION TAG	UNP P53563
K	-2	PHE	-	EXPRESSION TAG	UNP P53563
K	-1	PRO	-	EXPRESSION TAG	UNP P53563
K	0	GLY	-	EXPRESSION TAG	UNP P53563
L	-6	GLY	-	EXPRESSION TAG	UNP P53563
L	-5	SER	-	EXPRESSION TAG	UNP P53563
L	-4	PRO	-	EXPRESSION TAG	UNP P53563
L	-3	GLU	-	EXPRESSION TAG	UNP P53563
L	-2	PHE	-	EXPRESSION TAG	UNP P53563
L	-1	PRO	-	EXPRESSION TAG	UNP P53563
L	0	GLY	-	EXPRESSION TAG	UNP P53563

- Molecule 2 is 4-(4-([2-(4-CHLOROPHENYL)-5,5-DIMETHYLCYCLOHEX-1-EN-1-YL]METHYL)PIPERAZIN-1-YL)-N-[(4-([2R]-4-(MORPHOLIN-4-YL)-1-(PHENYLSULFANYL)BUTAN-2-YL)AMINO)-3-[(TRIFLUOROMETHYL)SULFONYL]PHENYL)SULFONYL]BENZAMIDE (three-letter code: 1XJ) (formula: C₄₇H₅₅ClF₃N₅O₆S₃).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	C	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	D	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	E	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	F	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	G	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	H	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	I	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	J	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	K	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	L	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		

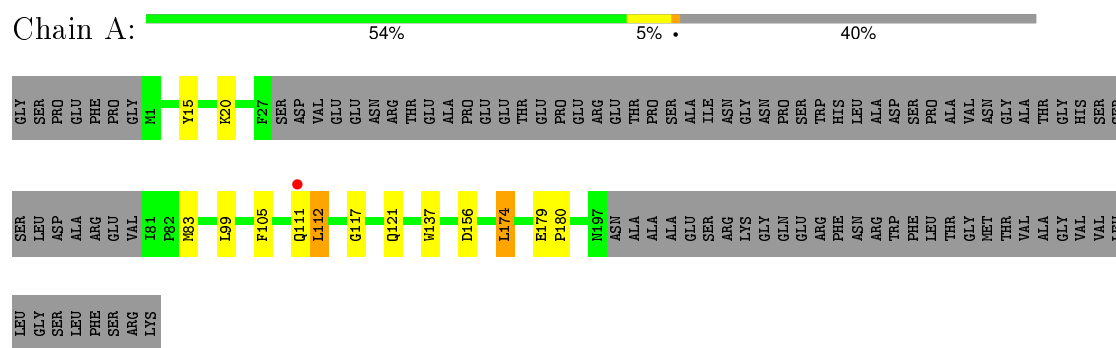
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	7	Total O 7 7	0	0
3	C	10	Total O 10 10	0	0
3	D	6	Total O 6 6	0	0
3	E	9	Total O 9 9	0	0
3	F	11	Total O 11 11	0	0
3	G	6	Total O 6 6	0	0
3	H	11	Total O 11 11	0	0
3	I	8	Total O 8 8	0	0
3	J	10	Total O 10 10	0	0
3	K	9	Total O 9 9	0	0
3	L	6	Total O 6 6	0	0

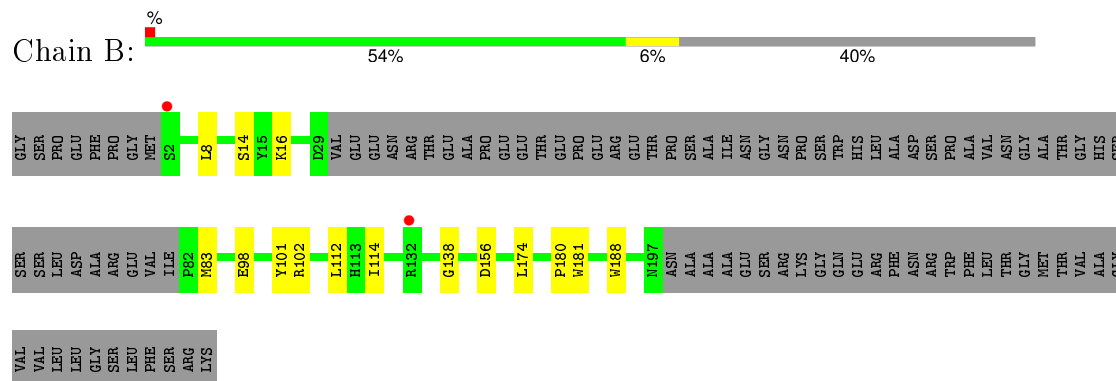
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

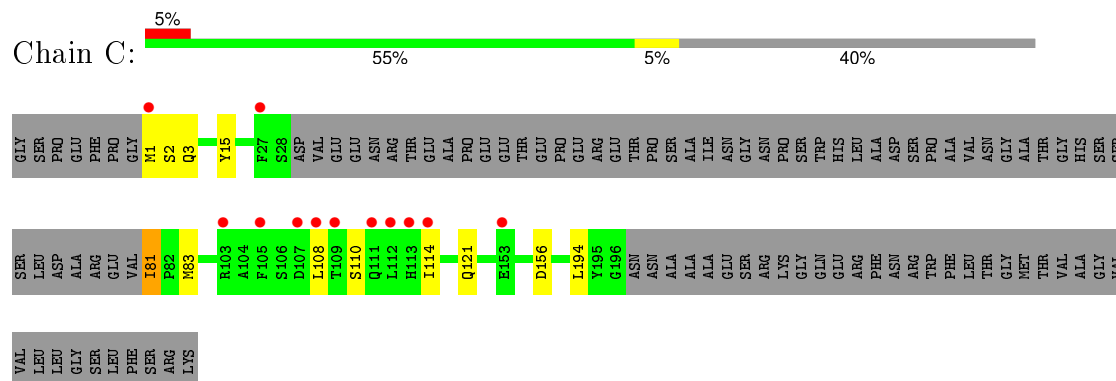
• Molecule 1: Bcl-2-like protein 1



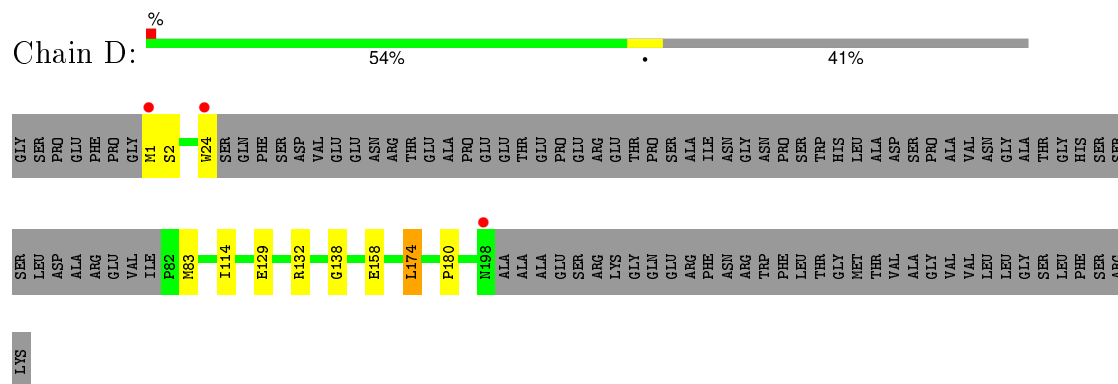
• Molecule 1: Bcl-2-like protein 1



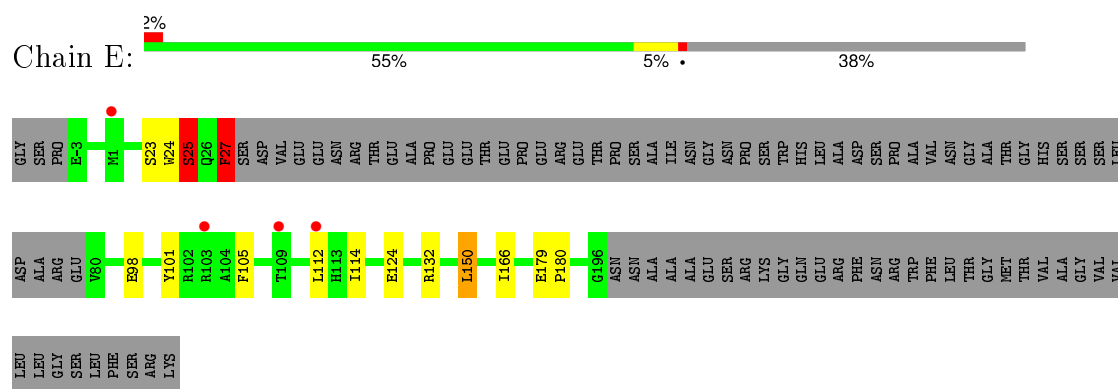
• Molecule 1: Bcl-2-like protein 1



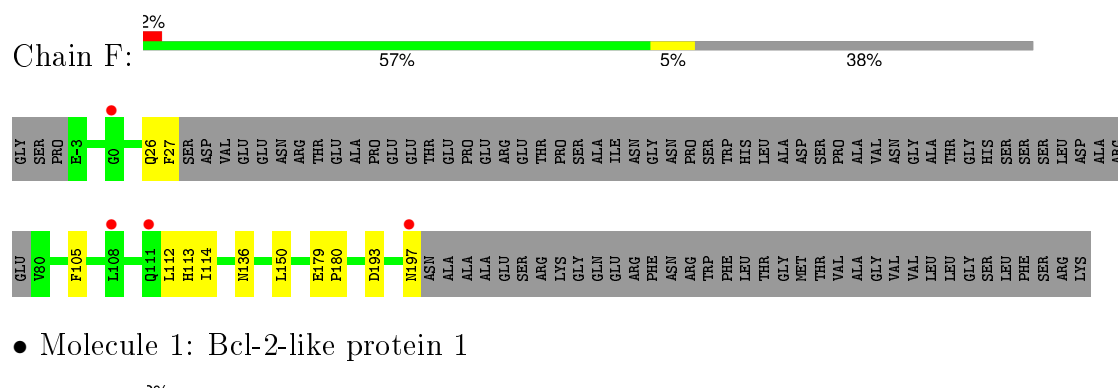
- Molecule 1: Bcl-2-like protein 1



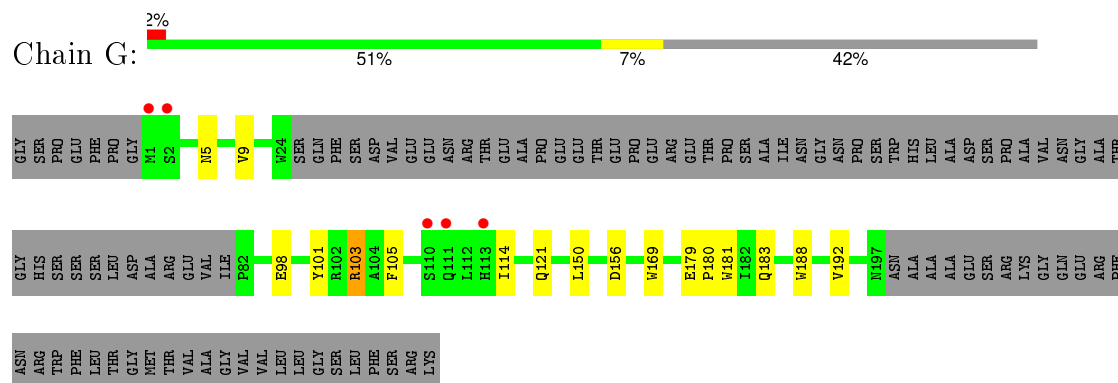
- Molecule 1: Bcl-2-like protein 1



- Molecule 1: Bcl-2-like protein 1



- Molecule 1: Bcl-2-like protein 1



VAL
ALA
GLY
VAL
VAL
LEU
LEU
GLY
SER
PHE
PHE
SER
ARG
LYS

● Molecule 1: Bcl-2-like protein 1



GLY
SER
PRO
GLU
PHE
PRO
GLY
M1
S2
Q3
S4
M5
L8
V9
Y22
S23
W24
S25
Q26
PHE
SER
ASP
VAL
GLU
GLU
ASN
ARG
THR
GLU
ALA
PRO
GLU
GLU
THR
GLU
PRO
GLU
ARG
THR
PRO
SER
ALA
ILE
ASN
GLY
ASN
PRO
SER
TRP
HIS
LEU
ALA
ASP
SER
PRO
ALA
VAL

ASN
GLY
ALA
THR
GLY
HIS
SER
SER
SER
LEU
ASP
ALA
ARG
GLU
VAL
ILE
P82
M83
Q88
E96
L99
R103
A104
F105
S106
D107
L108
T109
S110
Q111
L112
H113
I114
W137
G138
L150
E158
R165
L174
W181
W188
N197
ASN
ALA
ALA
ALA
GLU
SER

ARG
LYS
GLY
GLN
ARG
PHE
ASN
TRP
PHE
LEU
THR
GLY
MET
THR
VAL
VAL
ALA
GLY
VAL
VAL
LEU
LEU
GLY
SER
LEU
PHE
SER
ARG
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 85.81Å 93.64Å 72.94° 67.42° 69.38°	Depositor
Resolution (Å)	85.00 – 2.30 47.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (85.00-2.30) 92.1 (47.03-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.206 , 0.253 0.211 , 0.258	Depositor DCC
R_{free} test set	4444 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 89548 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14929	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.63 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2962e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1XJ

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	0.90	1/1198 (0.1%)	0.84	2/1621 (0.1%)
1	B	0.83	2/1196 (0.2%)	0.80	0/1618
1	C	0.77	0/1196	0.75	0/1618
1	D	0.93	0/1171	0.84	1/1584 (0.1%)
1	E	0.80	0/1230	0.77	1/1665 (0.1%)
1	F	0.84	0/1238	0.79	0/1676
1	G	0.84	2/1163 (0.2%)	0.75	0/1573
1	H	0.91	2/1178 (0.2%)	0.85	2/1593 (0.1%)
1	I	0.78	0/1218	0.74	1/1649 (0.1%)
1	J	0.85	0/1238	0.77	0/1676
1	K	0.76	0/1190	0.77	2/1610 (0.1%)
1	L	0.75	3/1178 (0.3%)	0.75	1/1593 (0.1%)
All	All	0.83	10/14394 (0.1%)	0.79	10/19476 (0.1%)

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 outliers	#Planarity outliers
1	E	0	1
1	H	0	1
1	J	0	1
1	K	0	1
All	All	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	24	TRP	CD2-CE2	6.40	1.49	1.41
1	G	169	TRP	CD2-CE2	5.54	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	TRP	CD2-CE2	5.50	1.48	1.41
1	H	181	TRP	CD2-CE2	5.46	1.48	1.41
1	L	181	TRP	CD2-CE2	5.41	1.47	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	165	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	D	174	LEU	CA-CB-CG	6.58	130.45	115.30
1	H	174	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	174	LEU	CB-CG-CD2	-6.02	100.77	111.00
1	K	139	ARG	NE-CZ-NH1	5.76	123.18	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	25	SER	Peptide
1	H	24	TRP	Peptide
1	J	25	SER	Peptide
1	K	25	SER	Peptide

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	1169	0	1113	8	0
1	B	1167	0	1100	8	0
1	C	1167	0	1112	6	0
1	D	1143	0	1087	6	0
1	E	1199	0	1141	10	0
1	F	1207	0	1147	6	0
1	G	1135	0	1081	9	0
1	H	1150	0	1094	9	0
1	I	1188	0	1132	10	0
1	J	1207	0	1147	14	0
1	K	1161	0	1097	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1150	0	1094	11	0
2	A	65	0	55	4	0
2	B	65	0	55	2	0
2	C	65	0	55	4	0
2	D	65	0	55	2	0
2	E	65	0	55	2	0
2	F	65	0	55	4	0
2	G	65	0	55	3	0
2	H	65	0	55	1	0
2	I	65	0	55	3	0
2	J	65	0	55	6	0
2	K	65	0	55	3	0
2	L	65	0	55	3	0
3	A	13	0	0	0	0
3	B	7	0	0	0	0
3	C	10	0	0	0	0
3	D	6	0	0	0	0
3	E	9	0	0	2	0
3	F	11	0	0	0	0
3	G	6	0	0	0	0
3	H	11	0	0	0	0
3	I	8	0	0	0	0
3	J	10	0	0	0	0
3	K	9	0	0	1	0
3	L	6	0	0	0	0
All	All	14929	0	14005	106	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 4.

The worst 5 of 106 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:I:105:PHE:O	1:I:108:LEU:HD12	1.46	1.12
1:D:129:GLU:OE2	1:D:132:ARG:NH1	2.10	0.85
1:I:108:LEU:HD13	1:I:109:THR:N	1.96	0.79
2:G:301:1XJ:C25	2:G:301:1XJ:H44	2.15	0.74
1:C:81:ILE:HG23	1:L:99:LEU:HD22	1.79	0.65

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	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
1	B	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
1	C	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
1	D	137/240 (57%)	134 (98%)	3 (2%)	0	100	100
1	E	144/240 (60%)	139 (96%)	5 (4%)	0	100	100
1	F	145/240 (60%)	144 (99%)	1 (1%)	0	100	100
1	G	136/240 (57%)	134 (98%)	2 (2%)	0	100	100
1	H	138/240 (58%)	134 (97%)	3 (2%)	1 (1%)	26	31
1	I	143/240 (60%)	140 (98%)	3 (2%)	0	100	100
1	J	145/240 (60%)	139 (96%)	5 (3%)	1 (1%)	26	31
1	K	139/240 (58%)	137 (99%)	2 (1%)	0	100	100
1	L	138/240 (58%)	136 (99%)	1 (1%)	1 (1%)	26	31
All	All	1685/2880 (58%)	1652 (98%)	30 (2%)	3 (0%)	52	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	25	SER
1	H	24	TRP
1	J	25	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	124/201 (62%)	118 (95%)	6 (5%)	31	42
1	B	124/201 (62%)	119 (96%)	5 (4%)	38	52
1	C	124/201 (62%)	117 (94%)	7 (6%)	26	35
1	D	121/201 (60%)	116 (96%)	5 (4%)	37	50
1	E	127/201 (63%)	121 (95%)	6 (5%)	32	43
1	F	128/201 (64%)	122 (95%)	6 (5%)	32	43
1	G	120/201 (60%)	116 (97%)	4 (3%)	45	61
1	H	122/201 (61%)	117 (96%)	5 (4%)	37	50
1	I	126/201 (63%)	119 (94%)	7 (6%)	26	35
1	J	128/201 (64%)	124 (97%)	4 (3%)	47	64
1	K	123/201 (61%)	118 (96%)	5 (4%)	37	50
1	L	122/201 (61%)	116 (95%)	6 (5%)	31	41
All	All	1489/2412 (62%)	1423 (96%)	66 (4%)	35	46

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	26	GLN
1	G	114	ILE
1	L	8	LEU
1	F	27	PHE
1	F	114	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	121	GLN
1	E	185	ASN
1	G	185	ASN
1	K	160	GLN

5.3.3 RNA ⓘ

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 [i](#)

12 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	1XJ	A	301	-	65,71,71	1.79	14 (21%)	85,104,104	2.90	31 (36%)
2	1XJ	B	301	-	65,71,71	1.27	8 (12%)	85,104,104	2.97	31 (36%)
2	1XJ	C	301	-	65,71,71	1.29	8 (12%)	85,104,104	3.26	28 (32%)
2	1XJ	D	301	-	65,71,71	1.57	9 (13%)	85,104,104	2.43	22 (25%)
2	1XJ	E	301	-	65,71,71	1.21	8 (12%)	85,104,104	3.10	27 (31%)
2	1XJ	F	301	-	65,71,71	1.42	10 (15%)	85,104,104	3.29	37 (43%)
2	1XJ	G	301	-	65,71,71	1.27	6 (9%)	85,104,104	3.40	33 (38%)
2	1XJ	H	301	-	65,71,71	1.37	13 (20%)	85,104,104	3.10	27 (31%)
2	1XJ	I	301	-	65,71,71	1.51	12 (18%)	85,104,104	3.18	33 (38%)
2	1XJ	J	301	-	65,71,71	1.36	10 (15%)	85,104,104	3.26	26 (30%)
2	1XJ	K	301	-	65,71,71	1.29	8 (12%)	85,104,104	3.11	38 (44%)
2	1XJ	L	301	-	65,71,71	1.30	9 (13%)	85,104,104	2.95	36 (42%)

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	1XJ	A	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	B	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	C	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	D	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	E	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	F	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	G	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	H	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	I	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	J	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	K	301	-	-	0/45/89/89	0/7/7/7
2	1XJ	L	301	-	-	0/45/89/89	0/7/7/7

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	1XJ	C23-S63	-5.05	1.73	1.79
2	D	301	1XJ	S64-N52	-4.83	1.54	1.64
2	J	301	1XJ	C45-S62	-4.68	1.71	1.81
2	F	301	1XJ	C45-S62	-4.43	1.71	1.81
2	A	301	1XJ	C23-S63	-4.43	1.74	1.79

The worst 5 of 369 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	1XJ	C28-C25-C17	-14.17	94.95	115.70
2	C	301	1XJ	O54-S63-O55	-13.89	105.34	118.71
2	G	301	1XJ	O54-S63-O55	-13.56	105.66	118.71
2	G	301	1XJ	C28-C25-C17	-13.32	96.20	115.70
2	J	301	1XJ	O56-S64-O57	-13.20	102.04	119.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	1XJ	4	0
2	B	301	1XJ	2	0
2	C	301	1XJ	4	0
2	D	301	1XJ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	1XJ	2	0
2	F	301	1XJ	4	0
2	G	301	1XJ	3	0
2	H	301	1XJ	1	0
2	I	301	1XJ	3	0
2	J	301	1XJ	6	0
2	K	301	1XJ	3	0
2	L	301	1XJ	3	0

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 ⓘ

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, 95th 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	144/240 (60%)	0.03	1 (0%) 89 92	26, 40, 75, 98	0
1	B	144/240 (60%)	0.19	2 (1%) 78 83	29, 44, 86, 108	0
1	C	144/240 (60%)	0.32	12 (8%) 14 20	33, 51, 95, 111	0
1	D	141/240 (58%)	0.21	3 (2%) 67 74	23, 39, 83, 105	0
1	E	148/240 (61%)	0.17	4 (2%) 58 67	31, 49, 98, 122	0
1	F	149/240 (62%)	0.13	4 (2%) 58 67	27, 44, 98, 117	0
1	G	140/240 (58%)	0.34	5 (3%) 46 55	34, 53, 93, 114	0
1	H	142/240 (59%)	0.20	4 (2%) 56 66	25, 42, 81, 113	0
1	I	147/240 (61%)	0.20	6 (4%) 41 50	32, 51, 101, 142	0
1	J	149/240 (62%)	0.16	8 (5%) 29 38	22, 43, 98, 123	0
1	K	143/240 (59%)	0.24	8 (5%) 28 36	29, 51, 94, 121	0
1	L	142/240 (59%)	0.46	14 (9%) 9 14	34, 56, 108, 134	0
All	All	1733/2880 (60%)	0.22	71 (4%) 41 50	22, 48, 97, 142	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	108	LEU	6.9
1	C	111	GLN	6.1
1	C	112	LEU	6.0
1	K	109	THR	5.9
1	C	105	PHE	5.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
2	1XJ	A	301	65/65	0.97	0.14	0.35	24,31,61,63	0
2	1XJ	I	301	65/65	0.96	0.15	0.04	36,49,68,80	0
2	1XJ	J	301	65/65	0.96	0.15	0.04	33,46,70,80	0
2	1XJ	L	301	65/65	0.96	0.14	-0.03	34,44,76,81	0
2	1XJ	C	301	65/65	0.96	0.15	-0.09	32,47,62,66	0
2	1XJ	D	301	65/65	0.98	0.13	-0.10	25,32,69,74	0
2	1XJ	E	301	65/65	0.97	0.14	-0.17	36,48,77,79	0
2	1XJ	F	301	65/65	0.96	0.14	-0.23	30,42,63,64	0
2	1XJ	H	301	65/65	0.97	0.14	-0.24	26,32,72,80	0
2	1XJ	K	301	65/65	0.97	0.13	-0.28	31,39,61,67	0
2	1XJ	B	301	65/65	0.98	0.13	-0.50	28,37,67,72	0
2	1XJ	G	301	65/65	0.97	0.13	-0.52	33,42,72,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.