



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 06:19 am GMT

PDB ID : 5JSN
Title : Bcl2-inhibitor complex
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2016-05-09
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

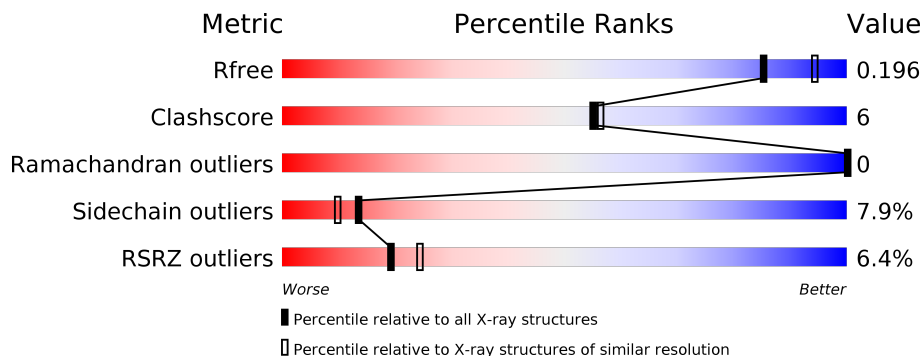
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (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 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	215	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>11%</div> <div>31%</div> </div> </div>
1	C	215	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>11%</div> <div>31%</div> </div> </div>
2	B	118	<div> <div>11%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• • •</div> </div> </div>
2	D	118	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>6% • • •</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4540 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 Apoptosis regulator Bcl-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1234	788	218	221	7			
1	C	149	Total	C	N	O	S	0	1	0
			1237	790	218	222	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	LEU	-	expression tag	UNP P10415
A	209	GLU	-	expression tag	UNP P10415
A	210	HIS	-	expression tag	UNP P10415
A	211	HIS	-	expression tag	UNP P10415
A	212	HIS	-	expression tag	UNP P10415
A	213	HIS	-	expression tag	UNP P10415
A	214	HIS	-	expression tag	UNP P10415
A	215	HIS	-	expression tag	UNP P10415
C	208	LEU	-	expression tag	UNP P10415
C	209	GLU	-	expression tag	UNP P10415
C	210	HIS	-	expression tag	UNP P10415
C	211	HIS	-	expression tag	UNP P10415
C	212	HIS	-	expression tag	UNP P10415
C	213	HIS	-	expression tag	UNP P10415
C	214	HIS	-	expression tag	UNP P10415
C	215	HIS	-	expression tag	UNP P10415

- Molecule 2 is a protein called Bcl2 inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			953	592	178	182	1			
2	D	115	Total	C	N	O	S	0	1	0
			964	598	182	183	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	19	Total 19	O 19	0	0
3	C	50	Total 50	O 50	0	0
3	D	33	Total 33	O 33	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	65.00Å 65.00Å 134.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.50 – 2.10 32.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.50-2.10) 99.0 (32.50-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.159 , 0.205 0.164 , 0.196	Depositor DCC
R_{free} test set	1650 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.305 for h,-k,-l	Xtriage
Reported twinning fraction	0.692 for H, K, L 0.308 for -H, K, -L	Depositor
Outliers	0 of 32173 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4540	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.04	0/1269	1.14	7/1719 (0.4%)
1	C	1.03	0/1275	1.08	9/1727 (0.5%)
2	B	0.96	1/958 (0.1%)	1.21	14/1273 (1.1%)
2	D	0.95	0/969	1.11	10/1287 (0.8%)
All	All	1.00	1/4471 (0.0%)	1.13	40/6006 (0.7%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	63	TYR	CB-CG	-6.17	1.42	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	67	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	A	146	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	B	67	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	A	181	LEU	CA-CB-CG	7.29	132.07	115.30
2	D	38	LEU	CA-CB-CG	7.23	131.94	115.30
2	D	101	ARG	NE-CZ-NH2	-7.23	116.68	120.30
2	B	18	ARG	NE-CZ-NH1	6.97	123.79	120.30
2	D	101	ARG	NE-CZ-NH1	6.69	123.64	120.30
2	B	112	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	D	51	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	C	146	ARG	NE-CZ-NH1	6.31	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	106	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	107	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	C	106	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	B	92	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	107	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	B	51	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	C	121	LEU	CA-CB-CG	5.85	128.75	115.30
1	C	109	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	D	51	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	110	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	D	18	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	D	108	ARG	NE-CZ-NH2	-5.65	117.48	120.30
2	B	18	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	D	115	LEU	CA-CB-CG	-5.57	102.48	115.30
1	C	111	ASP	CB-CG-OD1	5.53	123.28	118.30
2	D	60	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	183	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	B	92	ARG	NE-CZ-NH2	-5.41	117.59	120.30
2	B	108	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	D	108	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	C	98	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	139	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	B	101	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	B	112	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	109	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	B	20	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	B	77	LYS	CA-CB-CG	5.21	124.86	113.40
2	B	115	LEU	CB-CG-CD2	5.15	119.76	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	37	ASP	Peptide

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	1234	0	1172	11	0
1	C	1237	0	1177	13	0
2	B	953	0	995	13	0
2	D	964	0	1007	21	0
3	A	50	0	0	0	0
3	B	19	0	0	2	0
3	C	50	0	0	1	0
3	D	33	0	0	1	0
All	All	4540	0	4351	49	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 6.

All (49) 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)
2:D:39:THR:OG1	2:D:42:MET:HG3	1.79	0.80
2:B:24:GLN:OE1	2:D:20:ARG:NH1	2.17	0.78
2:B:43:ARG:HG3	2:B:115:LEU:HD23	1.65	0.77
2:D:43:ARG:HG3	2:D:115:LEU:HD23	1.72	0.70
2:B:18:ARG:NH2	2:B:56:GLN:HE21	1.90	0.69
1:C:208:LEU:HD21	2:D:90:LYS:HE2	1.76	0.68
2:D:18:ARG:NH2	2:D:56:GLN:OE1	2.27	0.67
2:D:102[A]:ARG:O	2:D:102[A]:ARG:HD2	1.98	0.64
2:B:18:ARG:HH21	2:B:56:GLN:HE21	1.46	0.61
2:D:33:ALA:HB2	2:D:46:LEU:HD13	1.81	0.61
1:A:175:LEU:O	1:A:179:GLU:HG3	2.02	0.59
2:D:102[A]:ARG:C	2:D:102[A]:ARG:HD2	2.25	0.57
2:B:56:GLN:NE2	3:B:201:HOH:O	2.28	0.56
1:C:105[B]:SER:OG	1:C:152:GLU:OE1	2.25	0.55
1:C:166:MET:HB3	1:C:169:LEU:HD13	1.89	0.54
1:C:183:ARG:NH2	3:C:302:HOH:O	2.33	0.54
2:B:106:LYS:HD2	3:B:205:HOH:O	2.07	0.54
2:B:40:GLN:HE22	2:B:43:ARG:NH1	2.07	0.53
1:A:167:SER:O	1:A:170:VAL:HG13	2.09	0.53
2:B:106:LYS:O	2:B:110:GLU:HG2	2.10	0.51
2:D:111:PHE:CZ	2:D:115:LEU:HD13	2.47	0.50
1:A:122:THR:OG1	1:A:125:THR:HB	2.13	0.49
1:A:107:ARG:HH11	2:B:62:PHE:HD1	1.61	0.48
1:C:204:PRO:O	1:C:208:LEU:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:THR:HG21	1:A:199:VAL:HA	1.96	0.47
1:C:122:THR:OG1	1:C:125:THR:HB	2.14	0.47
2:D:86:LEU:O	2:D:90:LYS:HG3	2.15	0.47
1:C:96:THR:HG21	1:C:199:VAL:HA	1.96	0.47
1:A:204:PRO:O	1:A:208:LEU:HD13	2.14	0.47
1:C:208:LEU:HD11	2:D:90:LYS:NZ	2.30	0.47
1:A:107:ARG:NH1	2:B:62:PHE:CD1	2.84	0.46
2:D:86:LEU:CD1	2:D:90:LYS:HE3	2.46	0.45
1:A:130:PHE:O	1:A:134:VAL:HG13	2.17	0.45
1:C:208:LEU:HD21	2:D:90:LYS:CE	2.43	0.45
2:D:106:LYS:HE3	3:D:232:HOH:O	2.16	0.45
2:D:102[A]:ARG:NH1	2:D:105:GLU:OE1	2.50	0.44
2:B:81:VAL:HG22	2:B:85:GLN:HB2	1.99	0.44
2:D:5:LYS:HD3	2:D:5:LYS:HA	1.91	0.44
2:D:91:ARG:NH1	2:D:95:GLU:OE2	2.51	0.43
1:A:21:TYR:CE2	1:A:98:ARG:HB2	2.54	0.42
2:D:88:GLU:OE2	2:D:91:ARG:NH2	2.45	0.42
1:C:208:LEU:HD11	2:D:90:LYS:HZ1	1.84	0.42
1:C:208:LEU:HD11	2:D:90:LYS:HE2	2.01	0.42
1:C:11:ASN:HD22	1:C:182:ASN:ND2	2.17	0.42
1:A:208:LEU:HD23	2:B:90:LYS:HD2	2.02	0.41
1:A:201:LEU:O	1:A:204:PRO:HD2	2.20	0.41
1:C:173:ILE:HD13	1:C:176:TRP:CZ3	2.55	0.41
2:B:88:GLU:O	2:B:92:ARG:HG2	2.20	0.41
2:D:30:TYR:N	2:D:111:PHE:HE1	2.19	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	145/215 (67%)	142 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	146/215 (68%)	142 (97%)	4 (3%)	0	100	100
2	B	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
2	D	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
All	All	518/666 (78%)	508 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	130/172 (76%)	122 (94%)	8 (6%)	20	17
1	C	131/172 (76%)	121 (92%)	10 (8%)	14	11
2	B	98/99 (99%)	90 (92%)	8 (8%)	12	9
2	D	99/99 (100%)	87 (88%)	12 (12%)	5	3
All	All	458/542 (84%)	420 (92%)	38 (8%)	13	8

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	87	SER
1	A	89	VAL
1	A	105	SER
1	A	109	ARG
1	A	125	THR
1	A	179	GLU
1	A	181	LEU
2	B	12	LYS
2	B	31	LYS
2	B	32	GLU
2	B	38	LEU
2	B	77	LYS

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Mol	Chain	Res	Type
2	B	99	GLU
2	B	112	ARG
2	B	115	LEU
1	C	7	THR
1	C	17	LYS
1	C	89	VAL
1	C	105[A]	SER
1	C	105[B]	SER
1	C	121	LEU
1	C	124	PHE
1	C	125	THR
1	C	160	GLU
1	C	209	GLU
2	D	5	LYS
2	D	29	LEU
2	D	31	LYS
2	D	32	GLU
2	D	38	LEU
2	D	39	THR
2	D	42	MET
2	D	83	SER
2	D	91	ARG
2	D	102[A]	ARG
2	D	102[B]	ARG
2	D	115	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	GLN
2	B	56	GLN
2	B	58	ASN
1	C	163	ASN
1	C	172	ASN
1	C	182	ASN
2	D	85	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](#)

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 ⓘ

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	149/215 (69%)	0.20	4 (2%) 54 61	30, 48, 73, 92	0
1	C	149/215 (69%)	0.41	9 (6%) 22 27	29, 48, 82, 109	0
2	B	115/118 (97%)	0.60	13 (11%) 5 6	32, 58, 92, 121	0
2	D	115/118 (97%)	0.37	8 (6%) 16 21	33, 52, 87, 112	0
All	All	528/666 (79%)	0.39	34 (6%) 19 24	29, 51, 87, 121	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	38	LEU	5.2
1	C	209	GLU	4.7
1	C	87	SER	4.4
2	B	3	ASP	4.3
1	C	120	HIS	4.3
1	C	32	ALA	4.1
2	B	36	LEU	4.1
1	C	208	LEU	4.0
2	B	117	TYR	3.9
2	D	111	PHE	3.9
2	B	4	PRO	3.6
2	B	86	LEU	3.0
2	D	42	MET	3.0
1	A	208	LEU	2.9
2	B	81	VAL	2.9
2	D	30	TYR	2.9
1	C	88	PRO	2.8
2	B	35	LYS	2.7
1	A	7	THR	2.7
2	B	89	LEU	2.5
2	D	115	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	38	LEU	2.5
2	D	34	ARG	2.5
1	C	169	LEU	2.4
1	C	7	THR	2.4
2	B	115	LEU	2.3
1	A	28	TYR	2.3
2	B	88	GLU	2.3
2	D	92	ARG	2.2
1	A	206	MET	2.2
1	C	124	PHE	2.2
2	B	42	MET	2.2
2	D	36	LEU	2.0
2	B	5	LYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.