



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2017 – 08:23 AM EDT

PDB ID : 2F78
Title : BenM effector binding domain with its effector benzoate
Authors : Clark, T.; Haddad, S.; Ezezika, O.; Neidle, E.; Momany, C.
Deposited on : unknown
Resolution : 2.05 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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

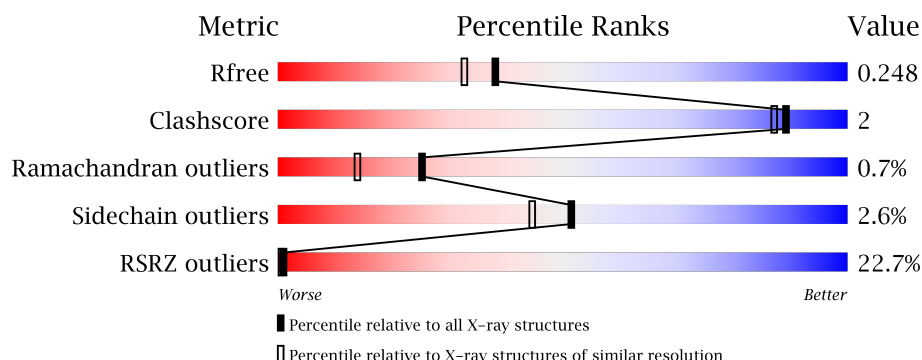
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	232	<div> <div>15%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>•</div> </div> </div>
1	B	232	<div> <div>28%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4189 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 HTH-type transcriptional regulator benM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	9	0
			1836	1183	319	329	5			
1	B	214	Total	C	N	O	S	0	3	0
			1720	1108	295	312	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	LEU	-	CLONING ARTIFACT	UNP O68014
A	306	GLU	-	CLONING ARTIFACT	UNP O68014
A	307	HIS	-	EXPRESSION TAG	UNP O68014
A	308	HIS	-	EXPRESSION TAG	UNP O68014
A	309	HIS	-	EXPRESSION TAG	UNP O68014
A	310	HIS	-	EXPRESSION TAG	UNP O68014
A	311	HIS	-	EXPRESSION TAG	UNP O68014
A	312	HIS	-	EXPRESSION TAG	UNP O68014
B	305	LEU	-	CLONING ARTIFACT	UNP O68014
B	306	GLU	-	CLONING ARTIFACT	UNP O68014
B	307	HIS	-	EXPRESSION TAG	UNP O68014
B	308	HIS	-	EXPRESSION TAG	UNP O68014
B	309	HIS	-	EXPRESSION TAG	UNP O68014
B	310	HIS	-	EXPRESSION TAG	UNP O68014
B	311	HIS	-	EXPRESSION TAG	UNP O68014
B	312	HIS	-	EXPRESSION TAG	UNP O68014

- Molecule 2 is BENZOIC ACID (three-letter code: BEZ) (formula: C₇H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	7	2		
2	A	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		

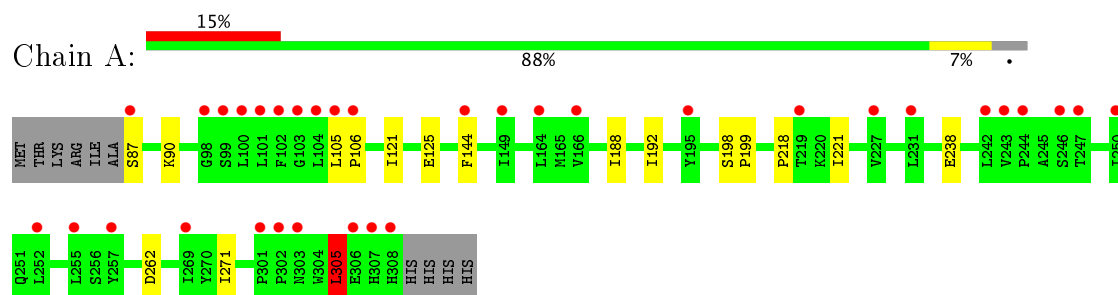
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	317	Total	O	0	0
			317	317		
3	B	271	Total	O	0	0
			271	271		

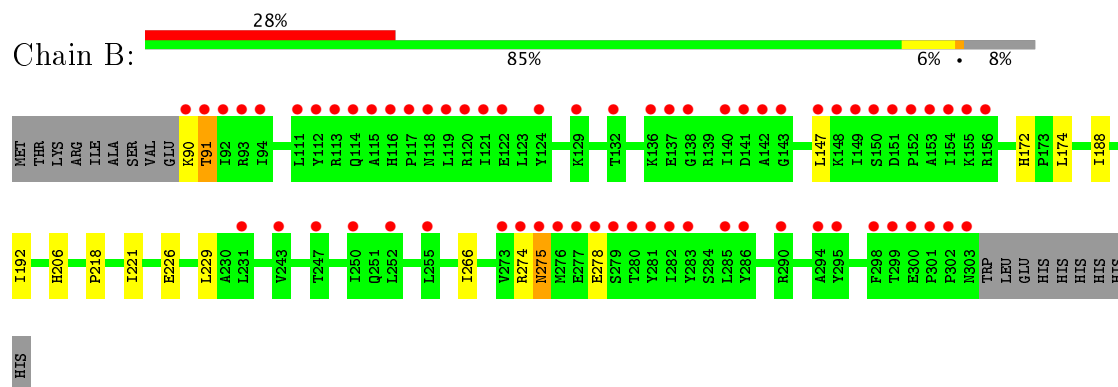
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: HTH-type transcriptional regulator benM



- Molecule 1: HTH-type transcriptional regulator benM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.39 Å 69.51 Å 116.86 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.76 – 2.05 44.73 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.7 (59.76-2.05) 95.7 (44.73-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.05 Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0005	Depositor
R, R_{free}	0.180 , 0.242 0.192 , 0.248	Depositor DCC
R_{free} test set	1635 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4189	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	0/1898	0.58	1/2574 (0.0%)
1	B	0.36	0/1763	0.56	0/2392
All	All	0.37	0/3661	0.57	1/4966 (0.0%)

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	A	1	0
1	B	1	0
All	All	2	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	305	LEU	N-CA-C	5.13	124.85	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	305	LEU	CA
1	B	275	ASN	CA

There are no planarity outliers.

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	1836	0	1891	9	0
1	B	1720	0	1769	8	0
2	A	18	0	10	0	0
2	B	27	0	15	0	0
3	A	317	0	0	1	0
3	B	271	0	0	2	0
All	All	4189	0	3685	16	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 2.

All (16) 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:188[B]:ILE:HD11	3:A:1060:HOH:O	1.97	0.64
1:B:226:GLU:HG2	1:B:229[B]:LEU:HD12	1.83	0.59
1:A:218:PRO:HB2	1:A:221:ILE:HD11	1.88	0.55
1:A:125:GLU:OE1	1:B:229[B]:LEU:HD11	2.09	0.53
1:B:192:ILE:HB	1:B:221[A]:ILE:HD13	1.92	0.50
1:A:105:LEU:HB3	1:A:106:PRO:HD3	1.94	0.48
1:A:144:PHE:CE1	1:A:271:ILE:HD12	2.49	0.48
1:B:206:HIS:HE1	1:B:266:ILE:O	1.98	0.47
1:B:192:ILE:HD12	1:B:218:PRO:HB3	1.98	0.46
1:B:91:THR:HG23	3:B:1138:HOH:O	2.16	0.44
1:B:147:LEU:HD21	3:B:1045:HOH:O	2.17	0.44
1:B:172:HIS:HD2	1:B:174:LEU:H	1.66	0.44
1:A:192:ILE:HB	1:A:221:ILE:HD13	2.00	0.44
1:A:198:SER:HB2	1:A:199:PRO:HD2	2.00	0.44

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	229/232 (99%)	226 (99%)	2 (1%)	1 (0%)	38	27
1	B	215/232 (93%)	212 (99%)	1 (0%)	2 (1%)	20	10
All	All	444/464 (96%)	438 (99%)	3 (1%)	3 (1%)	25	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	275	ASN
1	B	278	GLU
1	A	305	LEU

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	204/204 (100%)	199 (98%)	5 (2%)	53	46
1	B	190/204 (93%)	184 (97%)	6 (3%)	44	36
All	All	394/408 (97%)	383 (97%)	11 (3%)	51	42

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	90	LYS
1	A	238	GLU

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Mol	Chain	Res	Type
1	A	262	ASP
1	A	305	LEU
1	B	90	LYS
1	B	91	THR
1	B	188	ILE
1	B	274[A]	ARG
1	B	274[B]	ARG
1	B	275	ASN

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

Mol	Chain	Res	Type
1	B	161	ASN
1	B	172	HIS
1	B	206	HIS
1	B	291	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	BEZ	A	1001	-	6,9,9	0.24	0	8,11,11	0.96	0
2	BEZ	A	1003	-	6,9,9	0.64	0	8,11,11	0.35	0
2	BEZ	B	1002	-	6,9,9	0.40	0	8,11,11	0.66	0
2	BEZ	B	1004	-	6,9,9	0.67	0	8,11,11	0.42	0
2	BEZ	B	1005	-	6,9,9	0.53	0	8,11,11	0.46	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	BEZ	A	1001	-	-	0/0/4/4	0/1/1/1
2	BEZ	A	1003	-	-	0/0/4/4	0/1/1/1
2	BEZ	B	1002	-	-	0/0/4/4	0/1/1/1
2	BEZ	B	1004	-	-	0/0/4/4	0/1/1/1
2	BEZ	B	1005	-	-	0/0/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	222/232 (95%)	0.94	34 (15%)	2 2	21, 35, 46, 58	0
1	B	214/232 (92%)	1.56	65 (30%)	0 0	16, 33, 60, 74	0
All	All	436/464 (93%)	1.24	99 (22%)	1 0	16, 34, 49, 74	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	GLU	10.4
1	B	303	ASN	8.9
1	B	281	TYR	6.9
1	B	273	VAL	6.6
1	B	119	LEU	6.5
1	B	279	SER	6.3
1	B	92	ILE	6.2
1	B	283	TYR	6.0
1	B	276	MET	5.9
1	B	142	ALA	5.4
1	B	280	THR	5.3
1	B	302	PRO	5.2
1	B	149	ILE	5.2
1	B	154	ILE	5.1
1	B	120	ARG	5.0
1	B	155	LYS	4.9
1	B	277	GLU	4.8
1	B	121	ILE	4.8
1	B	286	TYR	4.7
1	B	90	LYS	4.7
1	B	93	ARG	4.6
1	A	303	ASN	4.6
1	A	227	VAL	4.5
1	B	141	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	140	ILE	4.4
1	A	308	HIS	4.3
1	A	302	PRO	4.1
1	B	299	THR	4.1
1	B	298	PHE	4.0
1	A	307	HIS	4.0
1	B	300	GLU	3.9
1	A	87	SER	3.8
1	B	91	THR	3.7
1	A	243	VAL	3.7
1	B	132	THR	3.7
1	B	274[A]	ARG	3.6
1	B	118	ASN	3.6
1	B	153	ALA	3.5
1	B	301	PRO	3.5
1	B	124	TYR	3.5
1	B	250	ILE	3.4
1	B	152	PRO	3.4
1	B	285	LEU	3.4
1	A	100	LEU	3.3
1	A	104	LEU	3.3
1	B	282	ILE	3.3
1	B	115	ALA	3.1
1	B	275	ASN	3.1
1	B	129	LYS	3.1
1	A	231	LEU	3.1
1	B	151	ASP	3.1
1	A	102	PHE	3.0
1	B	148	LYS	3.0
1	B	247	THR	3.0
1	B	252	LEU	3.0
1	A	301	PRO	2.9
1	A	149	ILE	2.9
1	B	143	GLY	2.9
1	A	164	LEU	2.9
1	A	250	ILE	2.8
1	B	94	ILE	2.8
1	B	114	GLN	2.8
1	B	117	PRO	2.8
1	B	156	ARG	2.7
1	B	112	TYR	2.7
1	B	113	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	247	THR	2.7
1	A	257	TYR	2.7
1	B	294	ALA	2.6
1	B	231	LEU	2.5
1	B	138	GLY	2.5
1	A	101	LEU	2.5
1	B	116	HIS	2.5
1	B	255	LEU	2.4
1	A	98	GLY	2.4
1	B	290	ARG	2.4
1	A	242	LEU	2.4
1	A	219	THR	2.4
1	B	147	LEU	2.4
1	B	150	SER	2.4
1	B	136	LYS	2.4
1	B	137	GLU	2.3
1	A	244	PRO	2.3
1	A	255	LEU	2.3
1	A	246	SER	2.3
1	B	243	VAL	2.2
1	A	306	GLU	2.2
1	A	269	ILE	2.2
1	B	122	GLU	2.2
1	A	103	GLY	2.1
1	A	105	LEU	2.1
1	A	166	VAL	2.1
1	A	252	LEU	2.1
1	B	111	LEU	2.1
1	A	99	SER	2.1
1	A	144	PHE	2.1
1	A	195	TYR	2.0
1	B	295	TYR	2.0
1	A	106	PRO	2.0

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 ⓘ

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(Å ²)	Q<0.9
2	BEZ	B	1005	9/9	0.78	0.19	1.76	55,55,55,56	0
2	BEZ	B	1004	9/9	0.91	0.15	0.23	30,30,31,32	0
2	BEZ	B	1002	9/9	0.91	0.14	-0.36	35,36,37,38	0
2	BEZ	A	1003	9/9	0.86	0.17	-0.58	30,31,31,32	0
2	BEZ	A	1001	9/9	0.95	0.12	-1.44	21,23,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.