WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 09:27 am GMT

PDB ID	:	2Y91
Title	:	Crystal structure of class A beta-lactamase from Bacillus licheniformis BS3 with clavulanic acid
Authors	:	Power, P.; Sauvage, E.; Herman, R.; Kerff, F.; Charlier, P.
Deposited on	:	2011-02-11
Resolution	:	2.00 Å(reported)

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

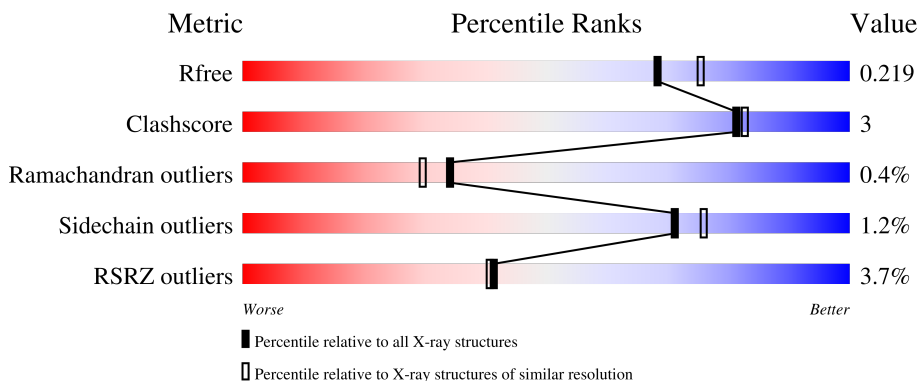|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	Percentile Ranks	Value
Rfree		0.219
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		1.2%
RSRZ outliers		3.7%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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
1	A	265	3% / 89% / 8% ·
1	B	265	4% / 90% / 6% ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4336 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 BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2016	1264	347	403	2			
1	B	257	Total	C	N	O	S	0	0	0
			2016	1264	347	403	2			

- Molecule 2 is 5-HYDROXY-3-OXOPENTANOIC ACID (three-letter code: 98J) (formula: $C_5H_8O_4$).
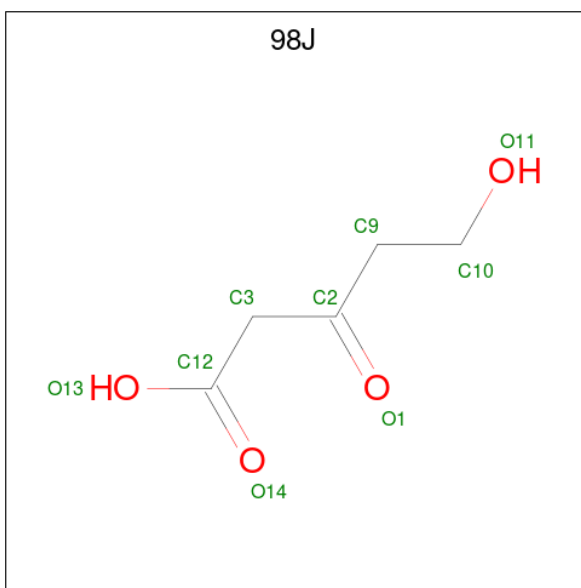
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	5	4		
2	B	1	Total	C	O	0	0
			9	5	4		
2	B	1	Total	C	O	0	0
			9	5	4		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 6	O 7	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 10	C 6	O 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	138	Total O 138 138	0	0
5	B	116	Total O 116 116	0	0

3 Residue-property plots ⓘ

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: BETA-LACTAMASE

Chain A:

• Molecule 1: BETA-LACTAMASE

Chain B:
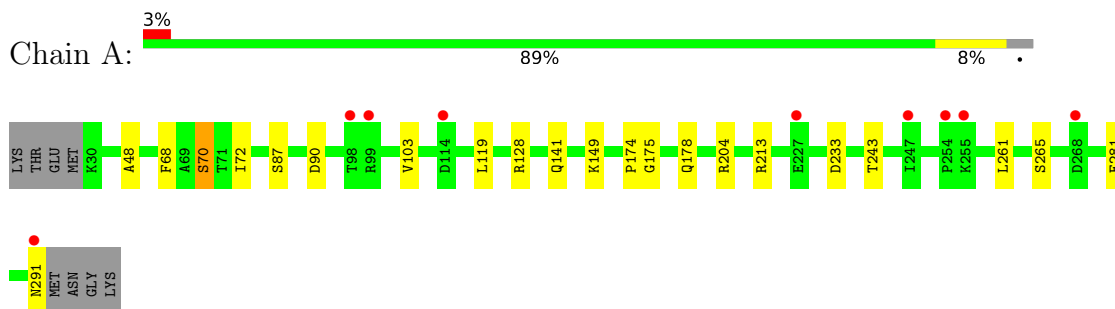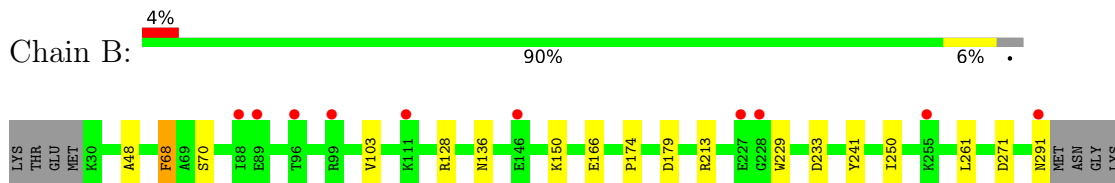
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.79Å 103.79Å 63.65Å 90.00° 94.82° 90.00°	Depositor
Resolution (Å)	34.13 – 2.00 34.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.13-2.00) 99.2 (34.13-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.179 , 0.219 0.178 , 0.219	Depositor DCC
R_{free} test set	2037 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4336	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

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: CIT, 98J, PGE, 1X6

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	0.52	0/2034	0.64	1/2753 (0.0%)
1	B	0.46	0/2034	0.59	0/2753
All	All	0.49	0/4068	0.61	1/5506 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	ARG	NE-CZ-NH2	-5.41	117.60	120.30

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	2016	0	2026	12	0
1	B	2016	0	2026	8	0
2	A	9	0	7	1	0
2	B	18	0	14	0	0
3	A	13	0	5	0	0
4	A	10	0	14	2	0
5	A	138	0	0	5	0
5	B	116	0	0	1	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4336	0	4092	21	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 3.

All (21) 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:B:136:ASN:HD21	1:B:166:GLU:H	1.20	0.86
1:A:178:GLN:NE2	5:A:2077:HOH:O	2.13	0.80
2:A:1293:98J:H102	5:A:2098:HOH:O	1.92	0.70
1:A:119:LEU:HD21	1:A:141:GLN:HG3	1.79	0.62
1:A:70:1X6:N4	5:A:2138:HOH:O	2.29	0.61
1:B:271:ASP:HB2	5:B:2102:HOH:O	2.01	0.59
1:A:175:GLY:H	4:A:1295:PGE:H62	1.72	0.53
1:A:174:PRO:HA	4:A:1295:PGE:H32	1.90	0.52
1:A:128:ARG:HD2	1:A:213:ARG:O	2.12	0.50
1:B:174:PRO:HD3	1:B:241:TYR:CZ	2.49	0.48
1:B:128:ARG:HD2	1:B:213:ARG:O	2.14	0.47
1:A:243:THR:HA	1:A:265:SER:O	2.13	0.47
1:B:150:LYS:HE2	1:B:150:LYS:HA	1.95	0.46
1:B:229:TRP:HE3	1:B:250:ILE:CG2	2.29	0.46
1:A:149:LYS:CE	5:A:2058:HOH:O	2.64	0.45
1:B:68:PHE:CZ	1:B:179:ASP:HA	2.52	0.44
1:A:281:GLU:OE2	5:A:2131:HOH:O	2.21	0.44
1:A:48:ALA:HB2	1:A:261:LEU:HD13	2.01	0.42
1:A:87:SER:O	1:A:90:ASP:HB2	2.21	0.41
1:A:68:PHE:CD1	1:A:72:ILE:HB	2.56	0.41
1:B:48:ALA:HB2	1:B:261:LEU:HD13	2.01	0.41

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	254/265 (96%)	249 (98%)	4 (2%)	1 (0%)	34	30
1	B	254/265 (96%)	249 (98%)	4 (2%)	1 (0%)	34	30
All	All	508/530 (96%)	498 (98%)	8 (2%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	VAL
1	A	103	VAL

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	217/224 (97%)	215 (99%)	2 (1%)	78	83
1	B	217/224 (97%)	214 (99%)	3 (1%)	67	72
All	All	434/448 (97%)	429 (99%)	5 (1%)	71	76

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	ASP
1	A	291	ASN
1	B	68	PHE
1	B	233	ASP
1	B	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	93	GLN
1	A	106	ASN
1	A	161	ASN
1	A	291	ASN
1	B	83	GLN
1	B	92	ASN
1	B	135	GLN
1	B	136	ASN
1	B	141	GLN
1	B	161	ASN
1	B	178	GLN
1	B	291	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	1X6	B	70	1	9,10,11	0.61	0	7,11,13	4.72	3 (42%)
1	1X6	A	70	1	9,10,11	0.63	0	7,11,13	2.39	4 (57%)

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
1	1X6	B	70	1	-	0/7/10/12	-
1	1X6	A	70	1	-	1/7/10/12	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	1X6	CB-OG-C7	8.44	130.96	116.60
1	B	70	1X6	OG-C7-C6	6.91	129.93	111.55
1	B	70	1X6	OG-C7-O8	-5.44	110.98	122.93
1	A	70	1X6	OG-C7-C6	3.68	121.34	111.55
1	A	70	1X6	C5-C6-C7	-3.33	112.82	119.81
1	A	70	1X6	CB-OG-C7	2.67	121.14	116.60
1	A	70	1X6	O8-C7-C6	-2.29	115.56	123.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	70	1X6	O8-C7-OG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	70	1X6	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	98J	B	1294	-	8,8,8	0.78	0	7,9,9	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	98J	A	1293	-	8,8,8	0.93	0	7,9,9	0.99	0
4	PGE	A	1295	-	9,9,9	0.57	0	8,8,8	0.32	0
3	CIT	A	1294	-	12,12,12	1.00	0	17,17,17	1.40	3 (17%)
2	98J	B	1293	-	8,8,8	0.86	0	7,9,9	0.91	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	98J	B	1294	-	-	5/7/7/7	-
2	98J	A	1293	-	-	7/7/7/7	-
4	PGE	A	1295	-	-	6/7/7/7	-
3	CIT	A	1294	-	-	1/16/16/16	-
2	98J	B	1293	-	-	7/7/7/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1294	CIT	O6-C6-C3	3.58	119.27	113.05
3	A	1294	CIT	O2-C1-C2	2.04	120.91	114.35
3	A	1294	CIT	O4-C5-O3	-2.02	118.26	123.30

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1293	98J	O13-C12-C3-C2
2	A	1293	98J	O1-C2-C3-C12
2	A	1293	98J	C9-C2-C3-C12
2	A	1293	98J	O11-C10-C9-C2
2	B	1293	98J	O1-C2-C3-C12
2	B	1293	98J	C9-C2-C3-C12
2	B	1293	98J	O11-C10-C9-C2
2	B	1294	98J	O11-C10-C9-C2
4	A	1295	PGE	O2-C3-C4-O3
4	A	1295	PGE	O1-C1-C2-O2
2	B	1293	98J	O14-C12-C3-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1295	PGE	O3-C5-C6-O4
2	B	1293	98J	C3-C2-C9-C10
4	A	1295	PGE	C4-C3-O2-C2
2	B	1293	98J	O13-C12-C3-C2
2	B	1294	98J	O13-C12-C3-C2
2	B	1293	98J	O1-C2-C9-C10
2	B	1294	98J	O1-C2-C3-C12
2	A	1293	98J	O14-C12-C3-C2
2	A	1293	98J	O1-C2-C9-C10
2	A	1293	98J	C3-C2-C9-C10
2	B	1294	98J	O14-C12-C3-C2
4	A	1295	PGE	C3-C4-O3-C5
3	A	1294	CIT	O1-C1-C2-C3
4	A	1295	PGE	C1-C2-O2-C3
2	B	1294	98J	O1-C2-C9-C10

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1293	98J	1	0
4	A	1295	PGE	2	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	256/265 (96%)	-0.05	9 (3%)	44	43	19, 28, 42, 57	0
1	B	256/265 (96%)	-0.05	10 (3%)	39	38	21, 34, 70, 94	0
All	All	512/530 (96%)	-0.05	19 (3%)	41	41	19, 31, 58, 94	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	LYS	4.7
1	A	291	ASN	4.3
1	B	99	ARG	4.2
1	B	88	ILE	3.9
1	B	89	GLU	3.7
1	A	247	ILE	3.0
1	A	99	ARG	3.0
1	B	291	ASN	2.9
1	B	228	GLY	2.6
1	A	227	GLU	2.6
1	A	98	THR	2.3
1	B	255	LYS	2.2
1	B	96	THR	2.2
1	B	227	GLU	2.2
1	B	111	LYS	2.2
1	A	114	ASP	2.1
1	B	146	GLU	2.1
1	A	254	PRO	2.1
1	A	268	ASP	2.1

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

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, 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	B-factors(Å^2)	Q<0.9
1	1X6	B	70	11/12	0.95	0.11	24,25,32,38	0
1	1X6	A	70	11/12	0.96	0.14	18,19,25,33	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 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	B-factors(Å^2)	Q<0.9
4	PGE	A	1295	10/10	0.83	0.15	42,44,48,48	0
2	98J	B	1294	9/9	0.85	0.16	39,45,49,51	0
3	CIT	A	1294	13/13	0.91	0.22	36,41,44,46	0
2	98J	B	1293	9/9	0.93	0.10	37,41,45,46	0
2	98J	A	1293	9/9	0.95	0.16	28,34,39,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.