



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:20 AM UTC

PDB ID : 2WK0 / pdb_00002wk0
Title : Crystal structure of the class A beta-lactamase BS3 inhibited by 6- beta-iodo penicillanate.
Authors : Sauvage, E.; Zervosen, A.; Dive, G.; Herman, R.; Kerff, F.; Amoroso, A.; Fonze, E.; Pratt, R.F.; Luxen, A.; Charlier, P.
Deposited on : 2009-06-03
Resolution : 1.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

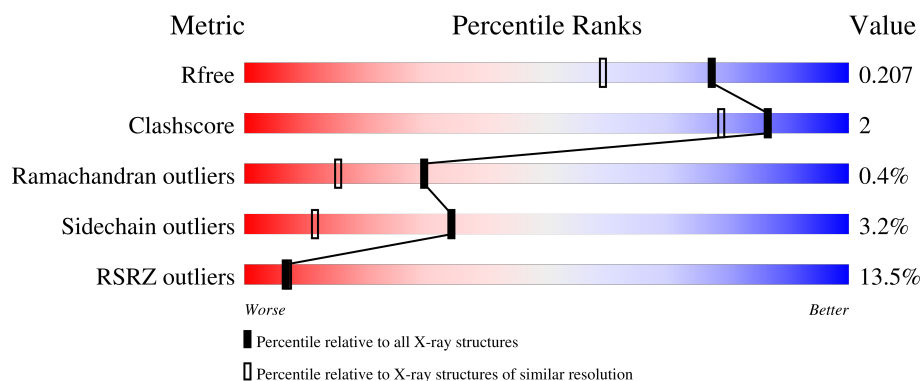
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

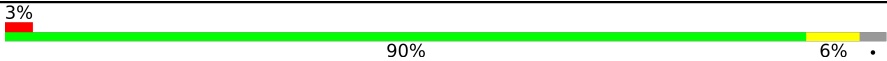
The reported resolution of this entry is 1.65 Å.

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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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 $\leq 5\%$. 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	265	
1	B	265	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EOH	B	1293	-	-	X	-

2 Entry composition [i](#)

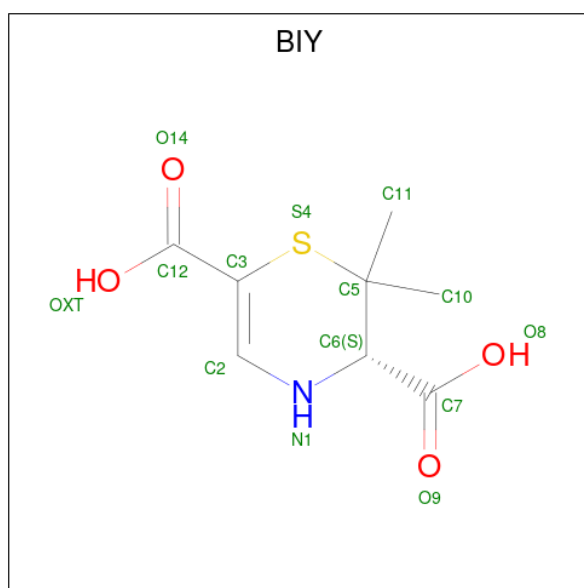
There are 7 unique types of molecules in this entry. The entry contains 4412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	256	Total	C	N	O	S	0	0	1
			1995	1251	343	399	2			
1	B	256	Total	C	N	O	S	0	0	1
			1995	1251	343	399	2			

- Molecule 2 is (3S)-2,2-dimethyl-3,4-dihydro-2H-1,4-thiazine-3,6-dicarboxylic acid (CCD ID: BIY) (formula: C₈H₁₁NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

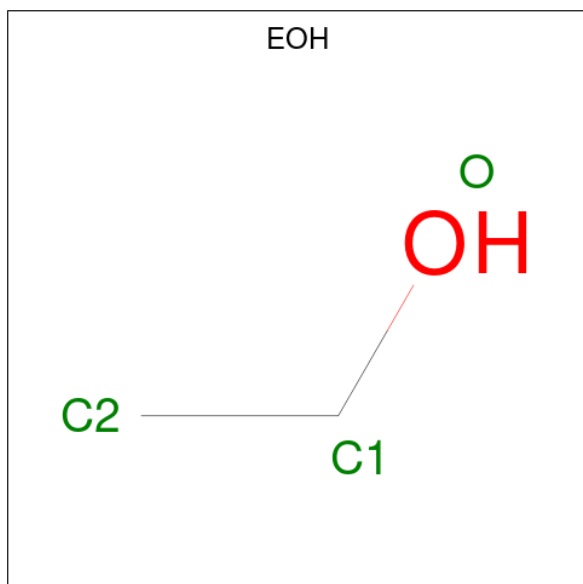
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



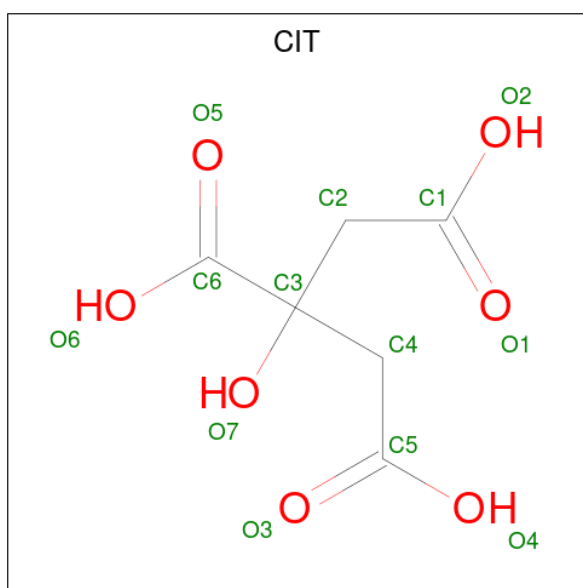
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	2	1		
5	A	1	Total	C	O	0	0
			3	2	1		
5	A	1	Total	C	O	0	0
			3	2	1		
5	B	1	Total	C	O	0	0
			3	2	1		

- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	204	Total	O	0	0
			204	204		
7	B	160	Total	O	0	0
			160	160		

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.

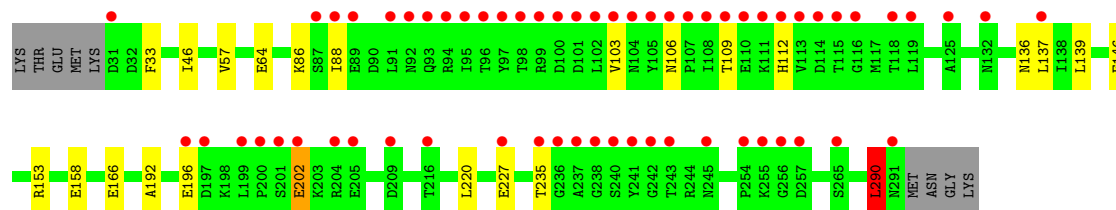
• Molecule 1: BETA-LACTAMASE

Chain A: 



• Molecule 1: BETA-LACTAMASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.99Å 104.48Å 63.74Å 90.00° 94.07° 90.00°	Depositor
Resolution (Å)	17.70 – 1.65 17.70 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.3 (17.70-1.65) 98.2 (17.70-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.211 0.185 , 0.207	Depositor DCC
R_{free} test set	3657 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4412	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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: BIY, CL, CIT, SO4, EOH

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	0.57	2/2025 (0.1%)	0.74	0/2744
1	B	0.57	2/2025 (0.1%)	0.74	0/2744
All	All	0.57	4/4050 (0.1%)	0.74	0/5488

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	VAL	C-N	7.17	1.43	1.33
1	B	290	LEU	C-N	-6.94	1.23	1.33
1	A	290	LEU	C-N	-6.72	1.24	1.33
1	B	112	HIS	C-N	6.22	1.40	1.34

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	1995	0	2004	6	0
1	B	1995	0	2004	9	0
2	A	13	0	8	0	0
2	B	13	0	8	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	5	0	0	1	0
5	A	9	0	18	1	0
5	B	3	0	6	2	0
6	B	13	0	5	0	0
7	A	204	0	0	1	0
7	B	160	0	0	3	0
All	All	4412	0	4053	17	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 (17) 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:146:GLU:HG2	7:B:2060:HOH:O	1.60	1.00
1:B:136:ASN:HD21	1:B:166:GLU:H	1.29	0.78
1:A:140:LYS:HG2	4:A:1292:SO4:O3	1.98	0.64
1:B:57:VAL:HG23	1:B:290:LEU:HD13	1.81	0.62
5:B:1293:EOH:H21	7:B:2084:HOH:O	2.02	0.58
1:A:119:LEU:HD21	1:A:141:GLN:HG3	1.88	0.56
1:A:32:ASP:HB3	5:A:1294:EOH:H11	1.90	0.52
1:B:106:ASN:HB3	1:B:109:THR:OG1	2.13	0.48
1:A:178:GLN:NE2	7:A:2120:HOH:O	2.23	0.48
1:B:220:LEU:HD12	1:B:235:THR:HG22	1.97	0.47
1:B:202:GLU:CD	1:B:202:GLU:H	2.24	0.45
1:A:169:LEU:C	1:A:169:LEU:HD12	2.42	0.44
1:B:33:PHE:CE1	1:B:46:ILE:HD13	2.53	0.43
1:B:192:ALA:HA	1:B:196:GLU:HG3	2.01	0.43
1:A:220:LEU:HD12	1:A:235:THR:HG22	2.01	0.42
1:B:153:ARG:HD3	1:B:158:GLU:HA	2.02	0.42
5:B:1293:EOH:H22	7:B:2035:HOH:O	2.21	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	254/265 (96%)	250 (98%)	3 (1%)	1 (0%)	30	15
1	B	254/265 (96%)	249 (98%)	4 (2%)	1 (0%)	30	15
All	All	508/530 (96%)	499 (98%)	7 (1%)	2 (0%)	30	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	B	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	216/225 (96%)	210 (97%)	6 (3%)	38	15
1	B	216/225 (96%)	208 (96%)	8 (4%)	30	8
All	All	432/450 (96%)	418 (97%)	14 (3%)	34	12

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	102	LEU
1	A	130	SER
1	A	139	LEU

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Mol	Chain	Res	Type
1	A	158	GLU
1	A	168	GLU
1	B	64	GLU
1	B	86	LYS
1	B	88	ILE
1	B	137	LEU
1	B	139	LEU
1	B	202	GLU
1	B	227	GLU
1	B	290	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	82	GLN
1	B	82	GLN
1	B	136	ASN
1	B	141	GLN
1	B	173	ASN
1	B	178	GLN
1	B	245	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
5	EOH	A	1294	-	2,2,2	0.38	0	1,1,1	0.18	0
2	BIY	B	300	1	11,13,14	4.07	5 (45%)	11,19,21	2.13	3 (27%)
5	EOH	B	1293	-	2,2,2	0.43	0	1,1,1	0.08	0
5	EOH	A	1293	-	2,2,2	0.47	0	1,1,1	0.10	0
2	BIY	A	300	1	11,13,14	3.84	5 (45%)	11,19,21	2.07	3 (27%)
4	SO4	A	1292	-	4,4,4	0.73	0	6,6,6	1.22	0
6	CIT	B	1292	-	12,12,12	1.09	0	17,17,17	1.36	1 (5%)
5	EOH	A	1295	-	2,2,2	0.47	0	1,1,1	0.11	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	BIY	A	300	1	-	0/3/22/24	0/1/1/1
6	CIT	B	1292	-	-	2/16/16/16	-
2	BIY	B	300	1	-	0/3/22/24	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	BIY	C2-N1	-8.23	1.21	1.34
2	B	300	BIY	C5-S4	-7.64	1.78	1.84
2	A	300	BIY	C2-N1	-7.56	1.22	1.34
2	A	300	BIY	C5-S4	-6.98	1.79	1.84
2	A	300	BIY	C2-C3	-6.29	1.24	1.35
2	B	300	BIY	C2-C3	-6.09	1.25	1.35
2	B	300	BIY	C3-S4	-2.94	1.66	1.73
2	A	300	BIY	C3-S4	-2.56	1.67	1.73
2	A	300	BIY	C6-N1	2.11	1.48	1.45
2	B	300	BIY	C12-C3	2.05	1.48	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	BIY	O14-C12-C3	-4.56	116.93	124.98
2	B	300	BIY	C12-C3-S4	3.70	121.99	112.53
2	A	300	BIY	O14-C12-C3	-3.53	118.75	124.98
6	B	1292	CIT	O6-C6-C3	3.16	119.21	113.14
2	A	300	BIY	C12-C3-S4	2.88	119.91	112.53
2	A	300	BIY	C10-C5-C11	-2.77	106.42	109.64
2	B	300	BIY	C10-C5-C11	-2.00	107.32	109.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1292	CIT	O2-C1-C2-C3
6	B	1292	CIT	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1294	EOH	1	0
5	B	1293	EOH	2	0
4	A	1292	SO4	1	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%)	0.21	8 (3%) 51 55	6, 12, 19, 26	0
1	B	256/265 (96%)	1.09	61 (23%) 2 2	8, 16, 32, 35	0
All	All	512/530 (96%)	0.65	69 (13%) 7 7	6, 13, 31, 35	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	ASN	9.7
1	B	113	VAL	6.8
1	B	105	TYR	6.8
1	B	103	VAL	6.6
1	B	255	LYS	6.2
1	B	104	ASN	6.1
1	B	97	TYR	5.9
1	B	115	THR	5.6
1	B	108	ILE	4.8
1	B	102	LEU	4.6
1	B	197	ASP	4.6
1	B	237	ALA	4.5
1	B	116	GLY	4.5
1	B	241	TYR	4.5
1	B	256	GLY	4.4
1	B	238	GLY	4.3
1	B	109	THR	4.3
1	B	112	HIS	4.2
1	B	236	GLY	4.1
1	B	243	THR	4.0
1	B	201	SER	3.9
1	B	114	ASP	3.7
1	B	106	ASN	3.7
1	B	98	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	202	GLU	3.5
1	A	255	LYS	3.4
1	B	107	PRO	3.4
1	B	257	ASP	3.4
1	B	240	SER	3.4
1	B	95	ILE	3.3
1	B	89	GLU	3.2
1	B	111	LYS	3.1
1	B	101	ASP	3.1
1	A	100	ASP	3.1
1	A	291	ASN	3.0
1	B	96	THR	3.0
1	B	110	GLU	2.9
1	B	100	ASP	2.8
1	B	119	LEU	2.8
1	B	204	ARG	2.8
1	B	227	GLU	2.7
1	B	88	ILE	2.7
1	B	265	SER	2.6
1	B	92	ASN	2.6
1	A	256	GLY	2.6
1	B	93	GLN	2.5
1	B	216	THR	2.5
1	B	242	GLY	2.5
1	B	205	GLU	2.5
1	A	99	ARG	2.4
1	B	196	GLU	2.4
1	B	245	ASN	2.3
1	B	91	LEU	2.3
1	B	200	PRO	2.2
1	B	209	ASP	2.2
1	A	205	GLU	2.2
1	B	137	LEU	2.2
1	B	235	THR	2.2
1	B	31	ASP	2.1
1	A	202	GLU	2.1
1	B	99	ARG	2.1
1	B	199	LEU	2.1
1	B	132	ASN	2.1
1	A	66	PHE	2.1
1	B	254	PRO	2.1
1	B	94	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	125	ALA	2.1
1	B	118	THR	2.1
1	B	87	SER	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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
5	EOH	A	1293	3/3	0.67	0.21	44,44,44,44	0
5	EOH	A	1295	3/3	0.67	0.21	42,42,42,43	0
6	CIT	B	1292	13/13	0.78	0.14	31,34,40,42	0
5	EOH	B	1293	3/3	0.82	0.16	21,21,21,22	0
5	EOH	A	1294	3/3	0.86	0.15	28,28,28,28	0
2	BIY	B	300	13/14	0.95	0.10	17,21,24,26	0
4	SO4	A	1292	5/5	0.96	0.18	7,16,26,26	0
2	BIY	A	300	13/14	0.97	0.09	11,14,19,19	0
3	CL	A	301	1/1	0.99	0.09	14,14,14,14	0
3	CL	B	301	1/1	0.99	0.09	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.