



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:47 PM UTC

PDB ID : 5UJD / pdb_00005ujd
Title : SbnI from Staphylococcus pseudintermedius
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Deposited on : 2017-01-17
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 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

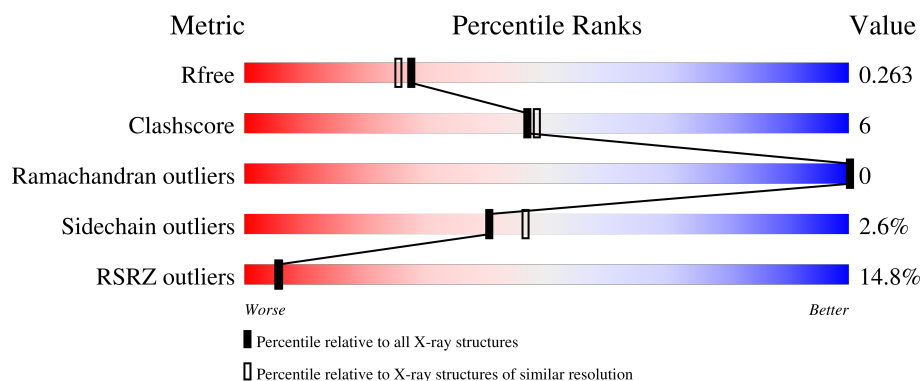
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	256	15% 81% 16% ..
1	B	256	14% 89% 9% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8415 atoms, of which 4148 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.

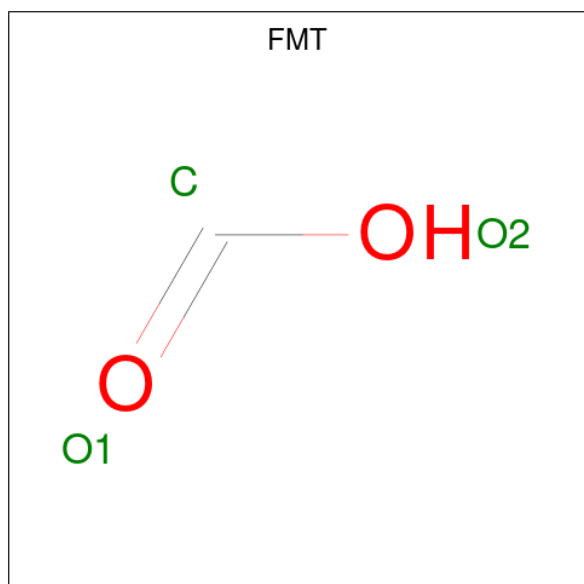
- Molecule 1 is a protein called Siderophore biosynthesis protein SbnI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	254	Total	C	H	N	O	S	0	2	0
			4135	1317	2068	356	380	14			
1	B	254	Total	C	H	N	O	S	0	4	0
			4154	1323	2077	359	381	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A166Q2C7
A	0	SER	-	expression tag	UNP A0A166Q2C7
B	-1	GLY	-	expression tag	UNP A0A166Q2C7
B	0	SER	-	expression tag	UNP A0A166Q2C7

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 4 1 1 2	0	0
2	A	1	Total C H O 4 1 1 2	0	0
2	B	1	Total C H O 4 1 1 2	0	0

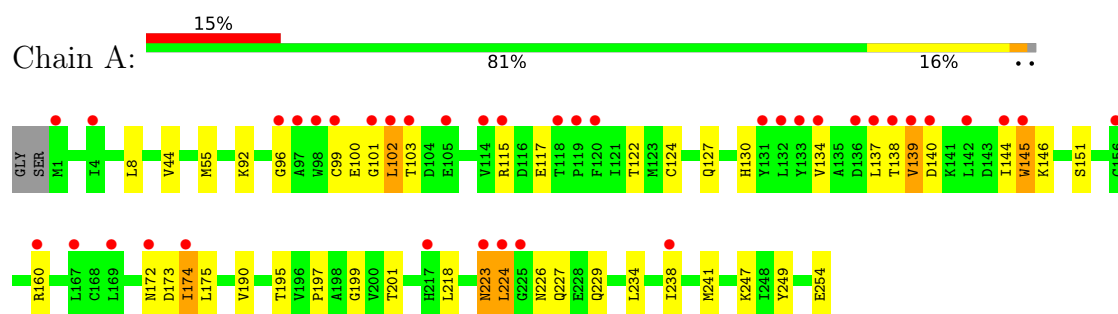
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total O 63 63	0	0
3	B	51	Total O 51 51	0	0

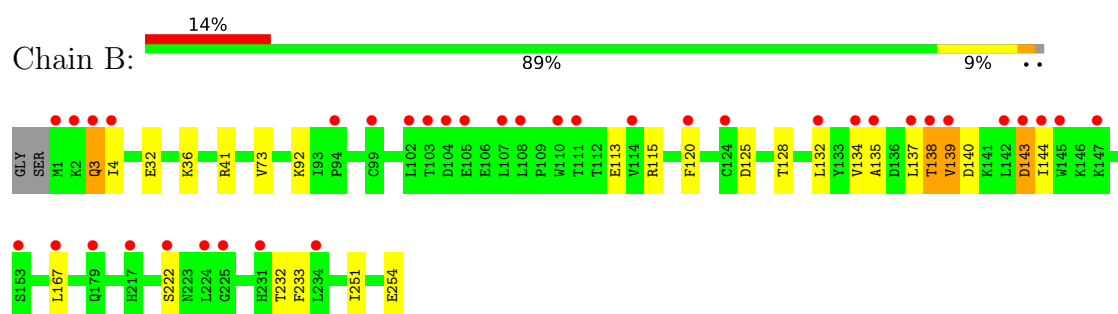
3 Residue-property plots [i](#)

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: Siderophore biosynthesis protein SbnI



- Molecule 1: Siderophore biosynthesis protein SbnI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.76Å 111.39Å 67.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.62 – 2.10 46.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.62-2.10) 99.8 (46.62-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.218 , 0.260 0.221 , 0.263	Depositor DCC
R_{free} test set	1770 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8415	wwPDB-VP
Average B, all atoms (Å ²)	67.0	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 41.46 % 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 2.3551e-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, 0.333 respectively for untwinned datasets, and 0.375, 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: FMT

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	0.23	0/2121	0.41	0/2878
1	B	0.19	0/2140	0.38	0/2904
All	All	0.21	0/4261	0.39	0/5782

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2067	2068	2060	32	1
1	B	2077	2077	2056	17	1
2	A	6	2	2	0	0
2	B	3	1	1	0	0
3	A	63	0	0	1	0
3	B	51	0	0	1	0
All	All	4267	4148	4119	47	1

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 (47) 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:41:ARG:NH2	1:B:254:GLU:OE1	2.04	0.91
1:A:99:CYS:O	1:A:103:THR:OG1	1.92	0.86
1:A:201:THR:OG1	3:A:401:HOH:O	2.01	0.77
1:B:134:VAL:O	3:B:401:HOH:O	2.09	0.69
1:A:117:GLU:N	1:A:117:GLU:OE1	2.27	0.67
1:B:120:PHE:CZ	1:B:134:VAL:HG12	2.32	0.65
1:A:99:CYS:SG	1:A:102:LEU:HD22	2.39	0.62
1:B:139:VAL:HG12	1:B:140:ASP:H	1.68	0.59
1:B:113:GLU:OE2	1:B:115:ARG:NE	2.34	0.57
1:A:146:LYS:NZ	1:A:195:THR:OG1	2.38	0.56
1:A:223:ASN:OD1	1:A:223:ASN:N	2.38	0.55
1:B:137:LEU:HD13	1:B:144:ILE:HD13	1.88	0.55
1:A:172:ASN:OD1	1:A:173:ASP:N	2.41	0.53
1:B:132:LEU:HB3	1:B:137:LEU:HD11	1.90	0.53
1:A:137:LEU:HD13	1:A:144:ILE:HG13	1.90	0.53
1:B:138:THR:HG23	1:B:139:VAL:HG23	1.92	0.52
1:A:247:LYS:NZ	1:A:249:TYR:OH	2.41	0.52
1:A:254:GLU:HG3	1:B:254:GLU:HG2	1.92	0.51
1:B:32:GLU:O	1:B:36:LYS:HG3	2.11	0.51
1:A:99:CYS:C	1:A:103:THR:OG1	2.55	0.50
1:A:55:MET:SD	1:A:190:VAL:HG21	2.52	0.49
1:A:127:GLN:OE1	1:A:127:GLN:N	2.45	0.49
1:B:73:VAL:HG13	1:B:222:SER:HB2	1.95	0.49
1:A:137:LEU:HD22	1:A:144:ILE:HD12	1.95	0.48
1:A:100:GLU:HA	1:A:103:THR:OG1	2.14	0.47
1:A:139:VAL:HG22	1:A:144:ILE:HD11	1.97	0.47
1:B:125:ASP:OD1	1:B:128:THR:HG22	2.15	0.47
1:A:241:MET:HE3	1:B:251:ILE:HD11	1.97	0.46
1:A:234:LEU:O	1:A:238:ILE:HG12	2.15	0.46
1:A:218:LEU:HD21	1:A:229:GLN:HB3	1.99	0.45
1:A:160:ARG:HE	1:A:199:GLY:HA3	1.82	0.45
1:B:232:THR:O	1:B:233:PHE:C	2.60	0.45
1:A:223:ASN:O	1:A:226:ASN:HB3	2.17	0.45
1:A:139:VAL:HG22	1:A:144:ILE:CD1	2.47	0.44
1:A:134:VAL:HA	1:A:137:LEU:HB2	1.99	0.44
1:B:3:GLN:OE1	1:B:4:ILE:HG12	2.18	0.44
1:A:224:LEU:HD13	1:A:227:GLN:HG3	1.99	0.43
1:A:101:GLY:HA3	1:A:151:SER:O	2.19	0.42
1:B:143:ASP:OD2	1:B:143:ASP:N	2.52	0.42
1:A:122:THR:HA	1:A:130:HIS:O	2.18	0.42
1:A:115:ARG:HB3	1:A:117:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLY:HA3	1:A:174:ILE:HD13	2.02	0.41
1:A:124:CYS:HB2	1:A:175:LEU:HB3	2.02	0.41
1:B:92:LYS:HD2	1:B:167:LEU:HD21	2.03	0.41
1:A:8:LEU:HB2	1:A:234:LEU:HD21	2.03	0.40
1:A:145:TRP:HB3	1:A:197:PRO:HG2	2.04	0.40
1:A:140:ASP:OD1	1:A:140:ASP:N	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:OG1	1:B:135:ALA:O[2_754]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	254/256 (99%)	246 (97%)	8 (3%)	0	100	100
1	B	256/256 (100%)	253 (99%)	3 (1%)	0	100	100
All	All	510/512 (100%)	499 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	234/233 (100%)	226 (97%)	8 (3%)	32	35
1	B	236/233 (101%)	232 (98%)	4 (2%)	53	62
All	All	470/466 (101%)	458 (97%)	12 (3%)	40	46

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	92	LYS
1	A	102	LEU
1	A	139	VAL
1	A	145	TRP
1	A	174	ILE
1	A	223	ASN
1	A	224	LEU
1	B	3	GLN
1	B	138	THR
1	B	139	VAL
1	B	143	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	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

3 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	FMT	A	302	-	2,2,2	0.77	0	1,1,1	0.54	0
2	FMT	A	301	-	2,2,2	0.73	0	1,1,1	0.51	0
2	FMT	B	301	-	2,2,2	0.77	0	1,1,1	0.46	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	254/256 (99%)	0.82	38 (14%)	5 5	19, 57, 131, 188	1 (0%)
1	B	254/256 (99%)	0.84	37 (14%)	6 6	24, 61, 117, 164	2 (0%)
All	All	508/512 (99%)	0.83	75 (14%)	5 6	19, 60, 123, 188	3 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TRP	7.0
1	A	145	TRP	5.7
1	A	134	VAL	5.5
1	A	114	VAL	5.0
1	A	120	PHE	4.9
1	B	4	ILE	4.4
1	A	224	LEU	4.4
1	B	224	LEU	4.2
1	B	1	MET	4.1
1	A	102	LEU	4.0
1	A	142	LEU	3.9
1	B	167	LEU	3.9
1	A	144	ILE	3.6
1	B	134	VAL	3.5
1	A	139	VAL	3.5
1	B	135	ALA	3.3
1	A	115	ARG	3.3
1	B	114	VAL	3.2
1	A	118	THR	3.2
1	A	1	MET	3.2
1	B	107	LEU	3.1
1	A	133	TYR	3.1
1	A	105	GLU	3.1
1	B	105	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	104	ASP	3.0
1	A	97	ALA	3.0
1	A	101	GLY	3.0
1	B	139	VAL	2.9
1	A	174	ILE	2.9
1	B	137	LEU	2.8
1	B	222	SER	2.8
1	B	120	PHE	2.8
1	B	2	LYS	2.8
1	B	99	CYS	2.7
1	A	99	CYS	2.7
1	A	238	ILE	2.6
1	A	156	CYS	2.6
1	A	169	LEU	2.6
1	A	4	ILE	2.6
1	A	96	GLY	2.6
1	B	225	GLY	2.6
1	A	217	HIS	2.6
1	A	119	PRO	2.6
1	B	102	LEU	2.6
1	A	136	ASP	2.5
1	A	172	ASN	2.4
1	A	132	LEU	2.4
1	B	3	GLN	2.4
1	A	167	LEU	2.4
1	B	147	LYS	2.4
1	A	138	THR	2.3
1	B	231	HIS	2.3
1	A	103	THR	2.3
1	B	94	PRO	2.3
1	B	142	LEU	2.2
1	B	234	LEU	2.2
1	B	110	TRP	2.2
1	B	138	THR	2.2
1	B	144	ILE	2.2
1	B	145	TRP	2.2
1	A	131	TYR	2.2
1	B	111	THR	2.2
1	B	179	GLN	2.1
1	B	217[A]	HIS	2.1
1	A	137	LEU	2.1
1	B	143	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	103	THR	2.1
1	A	160	ARG	2.1
1	A	225	GLY	2.1
1	B	153	SER	2.1
1	B	108	LEU	2.0
1	B	132	LEU	2.0
1	A	223	ASN	2.0
1	A	140	ASP	2.0
1	B	124	CYS	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(Å ²)	Q<0.9
2	FMT	A	302	3/3	0.77	0.17	40,61,73,73	0
2	FMT	A	301	3/3	0.95	0.10	37,41,45,54	0
2	FMT	B	301	3/3	0.96	0.08	43,50,55,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.