



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 08:43 AM JST

PDB ID : 5KZK
Title : Crystal Structure of rRNA methyltransferase from *Sinorhizobium meliloti*
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Deposited on : 2016-07-25
Resolution : 2.28 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

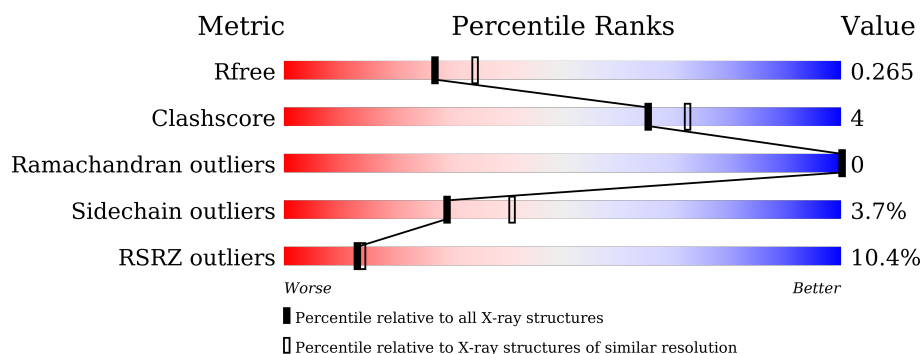
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	288	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>9%</div> </div> </div>
1	B	288	<div> <div>9%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>10%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3980 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.

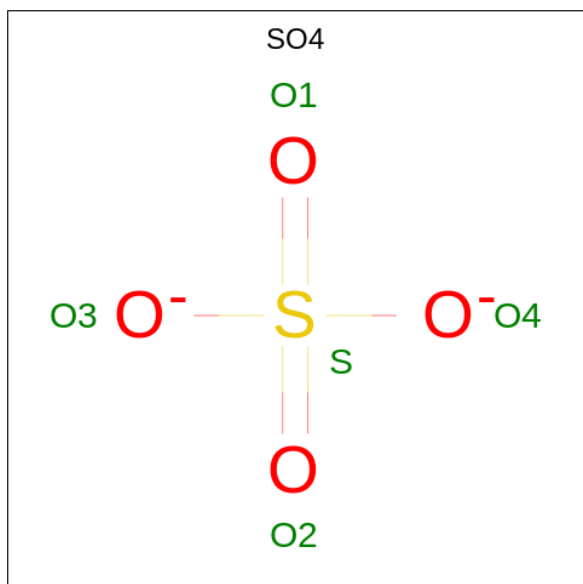
- Molecule 1 is a protein called Probable RNA methyltransferase, TrmH family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	Se	0	2	0
			1970	1249	348	368	5			
1	B	259	Total	C	N	O	Se	0	0	0
			1961	1239	351	366	5			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		
2	B	1	Total	Co	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

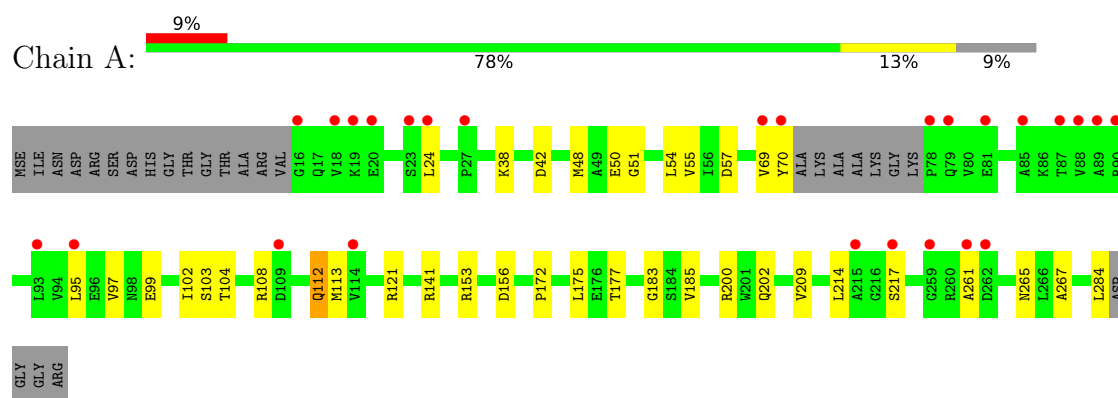
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	22	Total	O	0	0
			22	22		

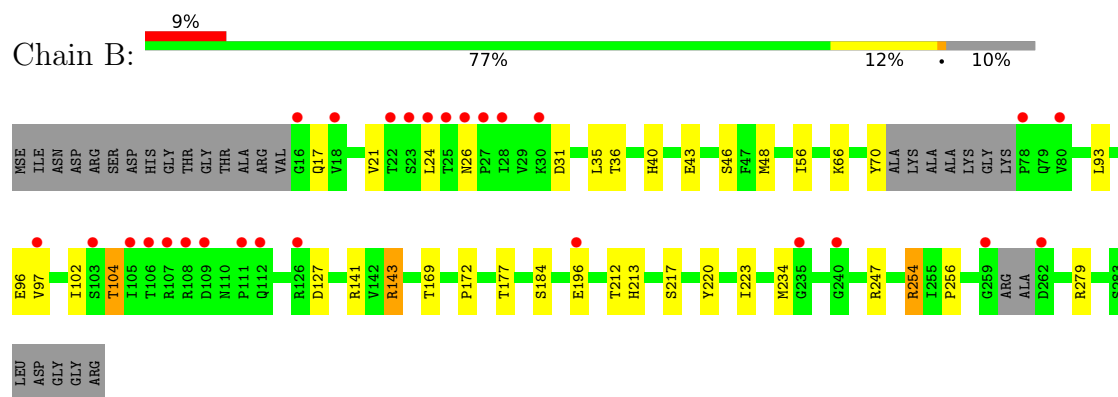
3 Residue-property plots [i](#)

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: Probable RNA methyltransferase, TrmH family



- Molecule 1: Probable RNA methyltransferase, TrmH family



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.82Å 84.30Å 112.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.36 – 2.28 67.36 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.0 (67.36-2.28) 96.4 (67.36-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.206 , 0.259 0.213 , 0.265	Depositor DCC
R_{free} test set	1384 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3980	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CO, SO4

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	1.07	0/1995	1.01	4/2704 (0.1%)
1	B	1.14	4/1983 (0.2%)	1.09	6/2683 (0.2%)
All	All	1.10	4/3978 (0.1%)	1.05	10/5387 (0.2%)

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	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	GLU	CD-OE1	5.55	1.31	1.25
1	B	184	SER	CB-OG	-5.29	1.35	1.42
1	B	43	GLU	CG-CD	5.17	1.59	1.51
1	B	43	GLU	CD-OE2	5.08	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	127	ASP	CB-CG-OD1	6.67	124.31	118.30
1	A	153	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	B	279	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	156	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	254	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	247	ARG	NE-CZ-NH2	5.96	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	196	GLU	N-CA-CB	-5.29	101.08	110.60
1	A	141	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	ALA	Peptide

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	1970	0	1994	16	0
1	B	1961	0	1998	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	15	0	0	0	0
4	B	22	0	0	0	0
All	All	3980	0	3992	29	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 4.

All (29) 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:202:GLN:HG3	1:A:209:VAL:HG21	1.78	0.65
1:B:46:SER:HB3	1:B:66:LYS:HE3	1.79	0.65
1:A:54:LEU:HD11	1:A:183:GLY:HA3	1.83	0.59
1:A:69:VAL:HG12	1:A:102:ILE:CD1	2.33	0.58
1:B:21:VAL:HG22	1:B:97:VAL:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:SER:HB2	1:A:108:ARG:O	2.05	0.57
1:B:21:VAL:HB	1:B:26:ASN:HD22	1.69	0.57
1:A:54:LEU:HD11	1:A:183:GLY:CA	2.34	0.57
1:B:35:LEU:HD23	1:B:40:HIS:CD2	2.42	0.55
1:B:213:HIS:O	1:B:217:SER:HB3	2.07	0.55
1:B:17:GLN:O	1:B:93:LEU:HD12	2.07	0.54
1:A:48:MSE:HE2	1:A:175:LEU:HD13	1.91	0.53
1:B:35:LEU:HD23	1:B:40:HIS:HD2	1.75	0.52
1:A:38:LYS:NZ	1:A:42:ASP:OD2	2.45	0.50
1:A:51:GLY:O	1:A:55:VAL:HG23	2.12	0.50
1:A:284:LEU:HD13	1:B:256:PRO:HG3	1.94	0.50
1:A:50:GLU:HB3	1:A:112:GLN:HG3	1.94	0.49
1:A:172:PRO:HA	1:A:177:THR:HG21	1.97	0.46
1:B:70:TYR:O	1:B:96:GLU:HA	2.16	0.45
1:A:265:ASN:OD1	1:A:267:ALA:HB3	2.17	0.45
1:A:185:VAL:HG22	1:A:185:VAL:O	2.17	0.45
1:B:24:LEU:HD23	1:B:104:THR:HG21	1.98	0.45
1:A:24:LEU:HD22	1:A:104:THR:HG21	1.98	0.44
1:B:141:ARG:HA	1:B:169:THR:HG22	2.00	0.43
1:B:172:PRO:HA	1:B:177:THR:HG21	1.99	0.43
1:B:212:THR:HG21	1:B:234:MSE:HE1	2.01	0.42
1:A:70:TYR:HA	1:A:113:MSE:O	2.20	0.41
1:B:220:TYR:HA	1:B:223:ILE:HD12	2.03	0.41
1:A:284:LEU:HD11	1:B:254:ARG:HD3	2.04	0.40

There are no symmetry-related clashes.

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	260/288 (90%)	249 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	253/288 (88%)	247 (98%)	6 (2%)	0	100	100
All	All	513/576 (89%)	496 (97%)	17 (3%)	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	201/224 (90%)	193 (96%)	8 (4%)	27	37
1	B	203/224 (91%)	196 (97%)	7 (3%)	32	45
All	All	404/448 (90%)	389 (96%)	15 (4%)	29	41

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	97	VAL
1	A	99	GLU
1	A	112	GLN
1	A	121	ARG
1	A	200	ARG
1	A	214	LEU
1	A	217	SER
1	B	31	ASP
1	B	36	THR
1	B	48	MSE
1	B	56	ILE
1	B	102	ILE
1	B	104	THR
1	B	143	ARG

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	40	HIS

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	SO4	A	302	-	4,4,4	0.90	0	6,6,6	1.49	2 (33%)
3	SO4	B	302	-	4,4,4	0.55	0	6,6,6	1.22	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	SO4	O4-S-O1	2.70	123.39	109.31
3	A	302	SO4	O3-S-O1	-2.16	98.05	109.31

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	257/288 (89%)	0.39	26 (10%)	14 15	7, 36, 79, 99	2 (0%)
1	B	254/288 (88%)	0.31	27 (10%)	13 13	12, 33, 85, 120	0
All	All	511/576 (88%)	0.35	53 (10%)	13 14	7, 35, 81, 120	2 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	PRO	6.0
1	B	23	SER	4.9
1	B	259	GLY	4.8
1	B	78	PRO	4.7
1	B	108	ARG	4.2
1	B	25	THR	4.2
1	A	88	VAL	3.8
1	B	24	LEU	3.8
1	B	22	THR	3.5
1	A	261	ALA	3.4
1	A	18	VAL	3.4
1	A	262	ASP	3.4
1	A	27	PRO	3.3
1	B	235	GLY	3.2
1	B	97	VAL	3.1
1	A	24	LEU	3.1
1	B	240	GLY	3.0
1	B	27	PRO	3.0
1	A	87	THR	2.9
1	A	95	LEU	2.9
1	A	20	GLU	2.9
1	A	93	LEU	2.8
1	A	70	TYR	2.7
1	B	16	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	16	GLY	2.6
1	A	89	ALA	2.6
1	B	109	ASP	2.6
1	A	109	ASP	2.5
1	B	103	SER	2.5
1	B	111	PRO	2.5
1	A	90	ARG	2.4
1	A	114	VAL	2.4
1	B	18	VAL	2.4
1	B	112	GLN	2.4
1	B	106	THR	2.4
1	A	81	GLU	2.4
1	A	85	ALA	2.3
1	B	26	ASN	2.2
1	B	107	ARG	2.2
1	A	79	GLN	2.2
1	B	80	VAL	2.2
1	A	19	LYS	2.2
1	A	217	SER	2.2
1	B	196	GLU	2.2
1	A	69	VAL	2.1
1	A	23	SER	2.1
1	B	105	ILE	2.1
1	B	30	LYS	2.1
1	A	215	ALA	2.1
1	A	259	GLY	2.1
1	B	262	ASP	2.0
1	B	28	ILE	2.0
1	B	126	ARG	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 monosaccharides 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
3	SO4	B	302	5/5	0.94	0.17	44,49,54,55	0
3	SO4	A	302	5/5	0.95	0.12	34,39,43,43	0
2	CO	A	301	1/1	0.96	0.07	44,44,44,44	0
2	CO	B	301	1/1	0.98	0.04	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.