



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 6, 2016 – 12:55 AM EDT

PDB ID : 5DAR  
Title : CRYSTAL STRUCTURE OF THE BASE OF THE RIBOSOMAL P STALK  
FROM METHANOCOCCUS JANNASCHII  
Authors : Gabdulkhakov, A.G.; Mitroshin, I.V.; Garber, M.B.  
Deposited on : 2015-08-20  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027939

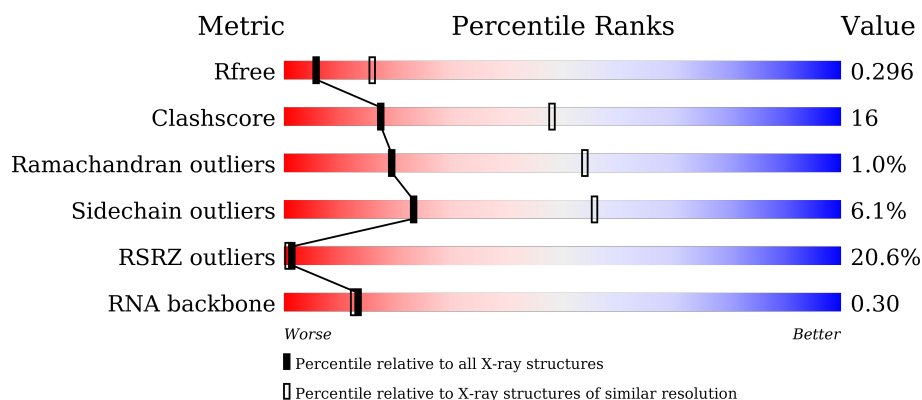
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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  $\geq 3$ , 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	74	<div> <div>3%</div> <div>32% 47% 18% .</div> </div>
1	D	74	<div> <div>5%</div> <div>35% 46% 16% .</div> </div>
2	B	213	<div> <div>11%</div> <div>46% 24% . 25%</div> </div>
2	E	213	<div> <div>19%</div> <div>65% 31% .</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	161	
3	F	161	

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
4	MG	A	1301	-	-	-	X
4	MG	A	1304	-	-	-	X
4	MG	D	1302	-	-	-	X
5	CL	A	1306	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8414 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 RNA chain called 74 nt fragment of 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	P	0	0	0
			1588	708	293	513	74			
1	D	74	Total	C	N	O	P	0	0	0
			1588	708	293	513	74			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	C	U	conflict	GB 470491724
D	1224	C	U	conflict	GB 470491724

- Molecule 2 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1243	802	213	222	6			
2	E	205	Total	C	N	O	S	0	0	0
			1571	1014	266	284	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	VAL	conflict	UNP P54049
E	9	MET	VAL	conflict	UNP P54049

- Molecule 3 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	158	Total	C	N	O	S	0	0	0
			1197	762	197	232	6			
3	F	158	Total	C	N	O	S	0	0	0
			1197	762	197	232	6			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	D	3	Total	Mg	0	0
			3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

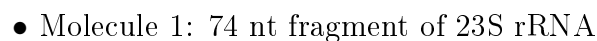
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	K	0	0
			2	2		
6	D	1	Total	K	0	0
			1	1		
6	C	1	Total	K	0	0
			1	1		
6	F	1	Total	K	0	0
			1	1		

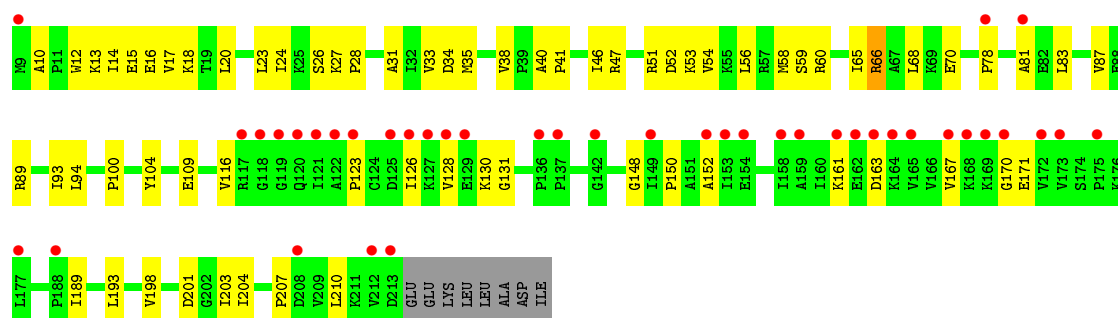
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	O	0	0
			5	5		
7	C	1	Total	O	0	0
			1	1		
7	D	7	Total	O	0	0
			7	7		
7	E	1	Total	O	0	0
			1	1		

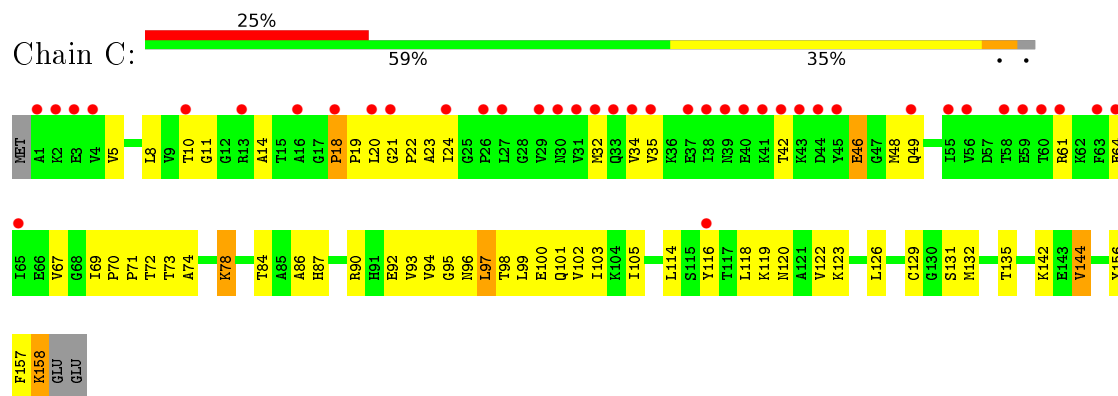


- Molecule 1: 74 nt fragment of 23S rRNA

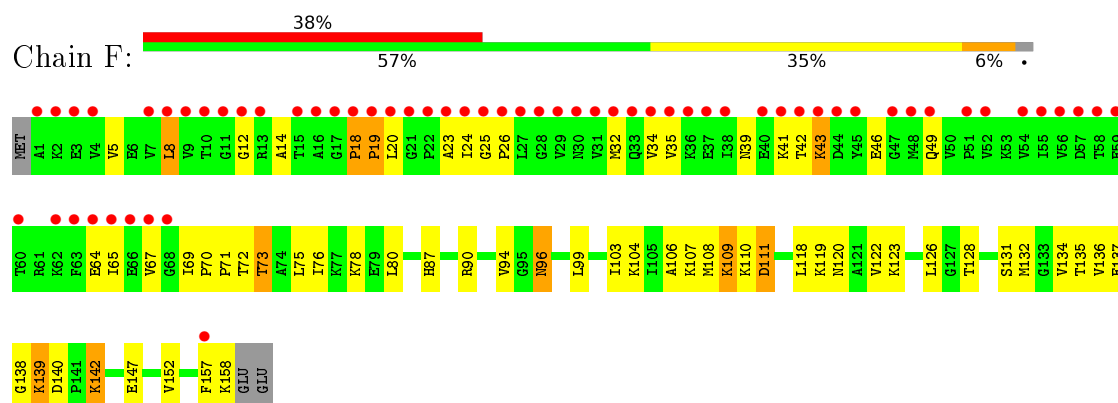




- Molecule 3: 50S ribosomal protein L11



- Molecule 3: 50S ribosomal protein L11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.40Å 88.45Å 95.23Å 90.00° 102.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 28.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.90) 97.5 (28.11-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.264 , 0.297 0.266 , 0.296	Depositor DCC
$R_{free}$ test set	1293 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 35.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	8414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: K, MG, CL

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	0.69	2/1777 (0.1%)	0.97	6/2768 (0.2%)
1	D	0.67	4/1777 (0.2%)	0.90	5/2768 (0.2%)
2	B	0.77	0/1259	0.83	1/1699 (0.1%)
2	E	0.52	0/1593	0.74	0/2149
3	C	0.64	0/1213	0.83	1/1639 (0.1%)
3	F	0.57	0/1213	0.75	0/1639
All	All	0.65	6/8832 (0.1%)	0.86	13/12662 (0.1%)

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
3	F	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1151	G	OP3-P	-10.13	1.49	1.61
1	A	1151	G	OP3-P	-10.00	1.49	1.61
1	A	1161	G	O3'-P	-5.71	1.54	1.61
1	D	1161	G	O3'-P	-5.61	1.54	1.61
1	D	1211	U	O3'-P	-5.56	1.54	1.61

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	97	LEU	CB-CA-C	7.68	124.80	110.20
1	D	1195	A	C2'-C3'-O3'	7.44	125.87	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1173	G	O5'-P-OP2	-7.15	99.27	105.70
1	A	1195	A	C2'-C3'-O3'	6.66	124.36	113.70
1	D	1180	A	O5'-P-OP1	-6.15	100.16	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	138	GLY	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	1588	0	802	35	0
1	D	1588	0	801	37	0
2	B	1243	0	1347	60	0
2	E	1571	0	1707	42	0
3	C	1197	0	1256	52	0
3	F	1197	0	1256	48	0
4	A	5	0	0	0	0
4	D	3	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	5	0	0	3	0
7	C	1	0	0	0	0
7	D	7	0	0	1	0
7	E	1	0	0	0	0
All	All	8414	0	7169	248	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 16.

The worst 5 of 248 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)
2:E:207:PRO:HA	2:E:210:LEU:HG	1.32	1.07
2:B:115:PRO:O	2:B:116:VAL:N	1.89	1.06
1:D:1170:U:OP2	3:F:109:LYS:NZ	1.89	1.04
2:B:104:TYR:OH	2:B:211:LYS:NZ	1.91	1.02
1:D:1151:G:H2'	1:D:1152:C:O5'	1.65	0.95

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	
2	B	154/213 (72%)	131 (85%)	21 (14%)	2 (1%)	15	46
2	E	201/213 (94%)	179 (89%)	21 (10%)	1 (0%)	34	71
3	C	156/161 (97%)	131 (84%)	23 (15%)	2 (1%)	15	46
3	F	156/161 (97%)	140 (90%)	14 (9%)	2 (1%)	15	46
All	All	667/748 (89%)	581 (87%)	79 (12%)	7 (1%)	19	54

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	18	PRO
3	F	18	PRO
3	F	19	PRO
2	B	11	PRO
3	C	19	PRO

### 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	
2	B	137/180 (76%)	128 (93%)	9 (7%)	21	51
2	E	173/180 (96%)	169 (98%)	4 (2%)	58	87
3	C	132/135 (98%)	123 (93%)	9 (7%)	20	49
3	F	132/135 (98%)	119 (90%)	13 (10%)	10	30
All	All	574/630 (91%)	539 (94%)	35 (6%)	23	56

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	142	LYS
2	E	66	ARG
3	F	139	LYS
3	C	144	VAL
3	C	158	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	49	GLN
3	F	96	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	73/74 (98%)	23 (31%)	2 (2%)
1	D	73/74 (98%)	19 (26%)	3 (4%)
All	All	146/148 (98%)	42 (28%)	5 (3%)

5 of 42 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1153	C
1	A	1155	A
1	A	1158	A
1	A	1161	G
1	A	1169	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1180	A
1	A	1195	A
1	D	1195	A
1	D	1214	C
1	D	1220	G

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	170:GLY	C	171:GLU	N	2.81
1	B	115:PRO	C	116:VAL	N	2.26

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	74/74 (100%)	0.35	2 (2%) 58 52	7, 12, 45, 85	0
1	D	74/74 (100%)	0.40	4 (5%) 29 23	10, 15, 66, 102	0
2	B	160/213 (75%)	0.66	23 (14%) 3 2	13, 30, 74, 91	1 (0%)
2	E	205/213 (96%)	0.99	41 (20%) 1 1	16, 41, 102, 132	1 (0%)
3	C	158/161 (98%)	1.42	40 (25%) 1 0	9, 31, 128, 160	0
3	F	158/161 (98%)	2.53	61 (38%) 0 0	18, 42, 178, 209	0
All	All	829/896 (92%)	1.19	171 (20%) 1 1	7, 32, 134, 209	2 (0%)

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	24	ILE	21.3
3	F	17	GLY	13.6
3	F	64	GLU	12.3
3	F	34	VAL	12.0
3	F	33	GLN	11.4

### 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 carbohydrates 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MG	D	1302	1/1	0.94	0.25	7.22	17,17,17,17	0
4	MG	A	1301	1/1	0.93	0.32	5.02	2,2,2,2	0
4	MG	A	1304	1/1	0.90	0.26	4.23	4,4,4,4	0
5	CL	A	1306	1/1	0.87	0.25	3.65	9,9,9,9	0
5	CL	F	201	1/1	0.95	0.25	0.75	38,38,38,38	0
6	K	A	1308	1/1	0.88	0.20	0.19	30,30,30,30	0
6	K	F	202	1/1	0.90	0.10	-2.06	49,49,49,49	0
6	K	C	201	1/1	0.94	0.09	-2.28	23,23,23,23	0
4	MG	A	1305	1/1	0.96	0.10	-3.61	30,30,30,30	0
6	K	D	1304	1/1	0.95	0.09	-3.84	11,11,11,11	0
4	MG	D	1301	1/1	0.96	0.07	-4.15	2,2,2,2	0
4	MG	A	1303	1/1	0.89	0.09	-5.42	5,5,5,5	0
6	K	A	1307	1/1	0.88	0.20	-	18,18,18,18	0
4	MG	A	1302	1/1	0.80	0.23	-	7,7,7,7	0
4	MG	D	1303	1/1	0.98	0.06	-	20,20,20,20	0
5	CL	B	301	1/1	0.75	0.23	-	43,43,43,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.