



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 01:38 am GMT

PDB ID : 2PHP  
Title : Crystal structure of the C-terminal domain of protein MJ0236 (Y236\_METJA)  
Authors : Eswaramoorthy, S.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-04-11  
Resolution : 2.03 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

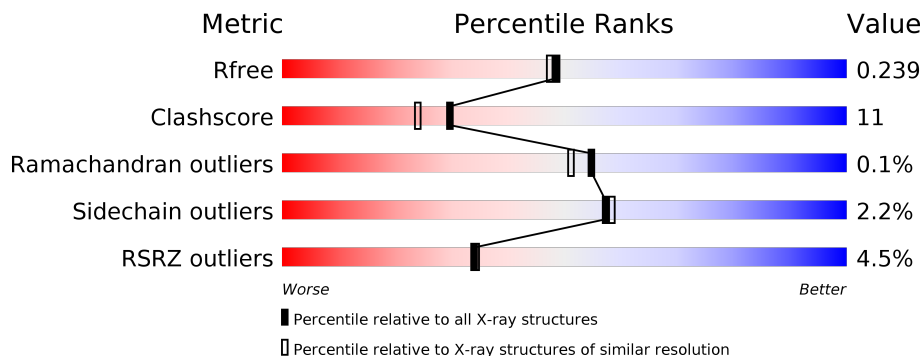
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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))
$R_{free}$	100719	8396 (2.04-2.00)
Clashscore	112137	9678 (2.04-2.00)
Ramachandran outliers	110173	9566 (2.04-2.00)
Sidechain outliers	110143	9565 (2.04-2.00)
RSRZ outliers	101464	8490 (2.04-2.00)

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 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	192	<div> <div> <div></div> <div>74%</div> <div>20%</div> <div>6%</div> </div> <div> <div>9%</div> <div>64%</div> <div>31%</div> <div>5%</div> </div> </div>
1	B	192	<div> <div>3%</div> <div>76%</div> <div>19%</div> <div>2%</div> </div> <div> <div>3%</div> <div>76%</div> <div>19%</div> <div>2%</div> </div>
1	D	192	<div> <div>9%</div> <div>64%</div> <div>31%</div> <div>5%</div> </div> <div> <div>9%</div> <div>64%</div> <div>31%</div> <div>5%</div> </div>
1	E	192	<div> <div>4%</div> <div>76%</div> <div>20%</div> <div>5%</div> </div> <div> <div>4%</div> <div>76%</div> <div>20%</div> <div>5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6109 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 Uncharacterized protein MJ0236.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	Se	0	0	0
			1423	925	234	258	2	4			
1	B	186	Total	C	N	O	S	Se	0	0	0
			1462	948	241	267	2	4			
1	D	184	Total	C	N	O	S	Se	0	0	0
			1444	938	237	263	2	4			
1	E	183	Total	C	N	O	S	Se	0	0	0
			1441	935	238	262	2	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	MSE	-	CLONING ARTIFACT	UNP Q57688
A	238	SER	-	CLONING ARTIFACT	UNP Q57688
A	239	LEU	-	CLONING ARTIFACT	UNP Q57688
A	261	MSE	MET	MODIFIED RESIDUE	UNP Q57688
A	333	MSE	MET	MODIFIED RESIDUE	UNP Q57688
A	366	MSE	MET	MODIFIED RESIDUE	UNP Q57688
A	395	MSE	MET	MODIFIED RESIDUE	UNP Q57688
A	421	GLU	-	CLONING ARTIFACT	UNP Q57688
A	422	GLY	-	CLONING ARTIFACT	UNP Q57688
A	423	HIS	-	CLONING ARTIFACT	UNP Q57688
A	424	HIS	-	CLONING ARTIFACT	UNP Q57688
A	425	HIS	-	CLONING ARTIFACT	UNP Q57688
A	426	HIS	-	CLONING ARTIFACT	UNP Q57688
A	427	HIS	-	CLONING ARTIFACT	UNP Q57688
A	428	HIS	-	CLONING ARTIFACT	UNP Q57688
B	237	MSE	-	CLONING ARTIFACT	UNP Q57688
B	238	SER	-	CLONING ARTIFACT	UNP Q57688
B	239	LEU	-	CLONING ARTIFACT	UNP Q57688
B	261	MSE	MET	MODIFIED RESIDUE	UNP Q57688
B	333	MSE	MET	MODIFIED RESIDUE	UNP Q57688
B	366	MSE	MET	MODIFIED RESIDUE	UNP Q57688

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Chain	Residue	Modelled	Actual	Comment	Reference
B	395	MSE	MET	MODIFIED RESIDUE	UNP Q57688
B	421	GLU	-	CLONING ARTIFACT	UNP Q57688
B	422	GLY	-	CLONING ARTIFACT	UNP Q57688
B	423	HIS	-	CLONING ARTIFACT	UNP Q57688
B	424	HIS	-	CLONING ARTIFACT	UNP Q57688
B	425	HIS	-	CLONING ARTIFACT	UNP Q57688
B	426	HIS	-	CLONING ARTIFACT	UNP Q57688
B	427	HIS	-	CLONING ARTIFACT	UNP Q57688
B	428	HIS	-	CLONING ARTIFACT	UNP Q57688
D	237	MSE	-	CLONING ARTIFACT	UNP Q57688
D	238	SER	-	CLONING ARTIFACT	UNP Q57688
D	239	LEU	-	CLONING ARTIFACT	UNP Q57688
D	261	MSE	MET	MODIFIED RESIDUE	UNP Q57688
D	333	MSE	MET	MODIFIED RESIDUE	UNP Q57688
D	366	MSE	MET	MODIFIED RESIDUE	UNP Q57688
D	395	MSE	MET	MODIFIED RESIDUE	UNP Q57688
D	421	GLU	-	CLONING ARTIFACT	UNP Q57688
D	422	GLY	-	CLONING ARTIFACT	UNP Q57688
D	423	HIS	-	CLONING ARTIFACT	UNP Q57688
D	424	HIS	-	CLONING ARTIFACT	UNP Q57688
D	425	HIS	-	CLONING ARTIFACT	UNP Q57688
D	426	HIS	-	CLONING ARTIFACT	UNP Q57688
D	427	HIS	-	CLONING ARTIFACT	UNP Q57688
D	428	HIS	-	CLONING ARTIFACT	UNP Q57688
E	237	MSE	-	CLONING ARTIFACT	UNP Q57688
E	238	SER	-	CLONING ARTIFACT	UNP Q57688
E	239	LEU	-	CLONING ARTIFACT	UNP Q57688
E	261	MSE	MET	MODIFIED RESIDUE	UNP Q57688
E	333	MSE	MET	MODIFIED RESIDUE	UNP Q57688
E	366	MSE	MET	MODIFIED RESIDUE	UNP Q57688
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E	421	GLU	-	CLONING ARTIFACT	UNP Q57688
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E	423	HIS	-	CLONING ARTIFACT	UNP Q57688
E	424	HIS	-	CLONING ARTIFACT	UNP Q57688
E	425	HIS	-	CLONING ARTIFACT	UNP Q57688
E	426	HIS	-	CLONING ARTIFACT	UNP Q57688
E	427	HIS	-	CLONING ARTIFACT	UNP Q57688
E	428	HIS	-	CLONING ARTIFACT	UNP Q57688

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Cl 3	0	0
2	A	3	Total 3	Cl 3	0	0
2	D	1	Total 1	Cl 1	0	0
2	E	2	Total 2	Cl 2	0	0

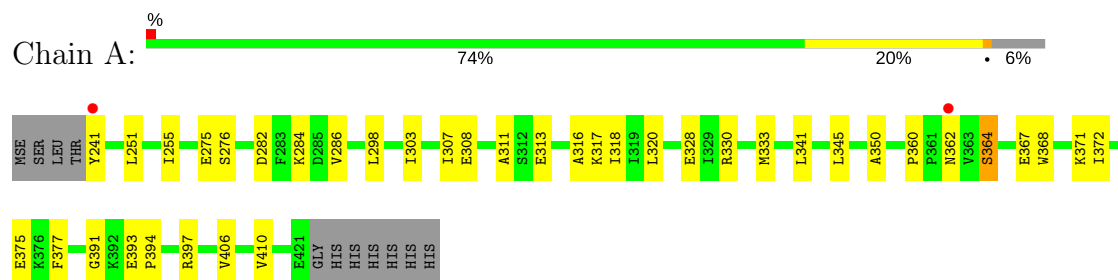
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total 90	O 90	0	0
3	B	91	Total 91	O 91	0	0
3	D	57	Total 57	O 57	0	0
3	E	92	Total 92	O 92	0	0

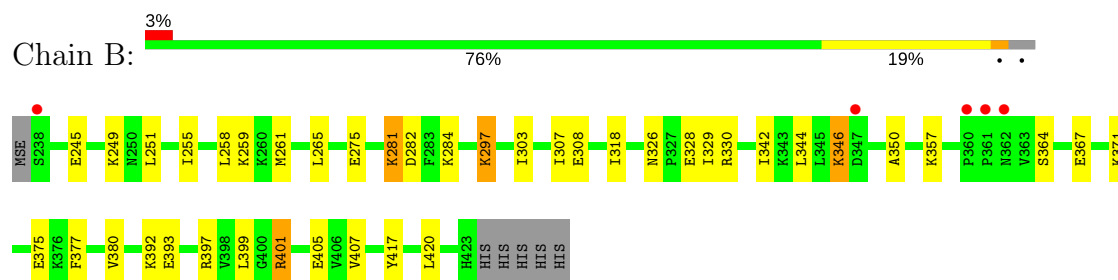
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

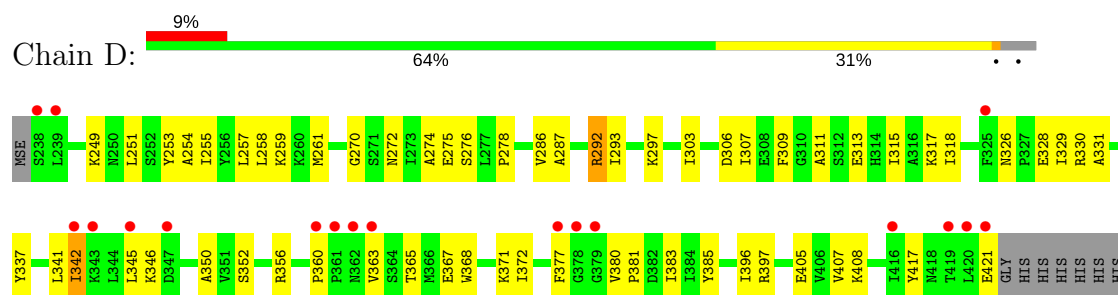
- Molecule 1: Uncharacterized protein MJ0236



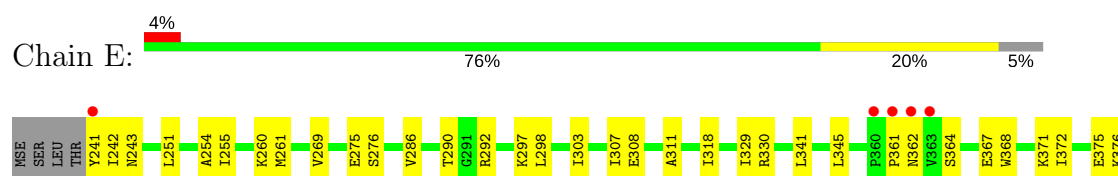
- Molecule 1: Uncharacterized protein MJ0236

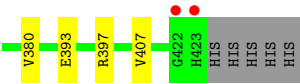


- Molecule 1: Uncharacterized protein MJ0236



- Molecule 1: Uncharacterized protein MJ0236





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.08Å 112.14Å 67.25Å 90.00° 109.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.03 36.09 – 2.04	Depositor EDS
% Data completeness (in resolution range)	89.6 (50.00-2.03) 90.4 (36.09-2.04)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.03Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.216 , 0.238 0.217 , 0.239	Depositor DCC
$R_{free}$ test set	2397 reflections (4.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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:  
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	0.37	0/1445	0.59	0/1935
1	B	0.36	0/1485	0.59	0/1989
1	D	0.35	0/1466	0.58	0/1964
1	E	0.34	0/1464	0.58	0/1960
All	All	0.36	0/5860	0.58	0/7848

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 [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	1423	0	1483	26	0
1	B	1462	0	1520	37	0
1	D	1444	0	1506	49	0
1	E	1441	0	1497	26	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
3	A	90	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	91	0	0	0	0
3	D	57	0	0	4	0
3	E	92	0	0	1	0
All	All	6109	0	6006	126	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 11.

The worst 5 of 126 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:241:TYR:HB3	3:A:485:HOH:O	1.50	1.10
1:D:259:LYS:HG2	1:D:303:ILE:HD12	1.55	0.86
1:B:401:ARG:HG3	1:B:401:ARG:HH11	1.48	0.78
1:B:281:LYS:HE2	1:B:281:LYS:HA	1.70	0.74
1:B:401:ARG:NH1	1:B:401:ARG:HG3	2.01	0.73

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	179/192 (93%)	175 (98%)	4 (2%)	0	100	100
1	B	184/192 (96%)	180 (98%)	3 (2%)	1 (0%)	32	25
1	D	182/192 (95%)	172 (94%)	10 (6%)	0	100	100
1	E	181/192 (94%)	176 (97%)	5 (3%)	0	100	100
All	All	726/768 (94%)	703 (97%)	22 (3%)	1 (0%)	55	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	346	LYS

### 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	154/160 (96%)	150 (97%)	4 (3%)	51	51
1	B	159/160 (99%)	154 (97%)	5 (3%)	45	43
1	D	157/160 (98%)	154 (98%)	3 (2%)	62	64
1	E	156/160 (98%)	154 (99%)	2 (1%)	73	77
All	All	626/640 (98%)	612 (98%)	14 (2%)	57	58

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	297	LYS
1	B	393	GLU
1	D	405	GLU
1	B	281	LYS
1	D	342	ILE

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

Mol	Chain	Res	Type
1	A	362	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [i](#)

There are no chain breaks in this entry.

## 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	177/192 (92%)	-0.04	2 (1%) 80 80	22, 34, 50, 58	0
1	B	182/192 (94%)	-0.15	5 (2%) 55 55	23, 36, 50, 60	0
1	D	180/192 (93%)	0.43	18 (10%) 8 8	27, 46, 57, 63	0
1	E	179/192 (93%)	0.15	7 (3%) 40 41	24, 38, 54, 60	0
All	All	718/768 (93%)	0.10	32 (4%) 34 34	22, 38, 55, 63	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	378	GLY	5.2
1	E	362	ASN	4.2
1	D	362	ASN	4.0
1	A	362	ASN	3.8
1	E	361	PRO	3.7

### 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 [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. 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( $\text{\AA}^2$ )	Q<0.9
2	CL	E	7	1/1	0.93	0.14	-0.26	64,64,64,64	0
2	CL	B	5	1/1	0.97	0.11	-0.58	50,50,50,50	0
2	CL	A	6	1/1	0.97	0.11	-0.79	49,49,49,49	0
2	CL	A	8	1/1	0.95	0.06	-	48,48,48,48	0
2	CL	B	1	1/1	0.98	0.10	-	44,44,44,44	0
2	CL	B	9	1/1	0.97	0.10	-	46,46,46,46	0
2	CL	D	4	1/1	0.95	0.14	-	54,54,54,54	0
2	CL	A	2	1/1	0.97	0.16	-	42,42,42,42	0
2	CL	E	3	1/1	0.96	0.11	-	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.