



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 02:43 am GMT

PDB ID : 4KTB  
Title : The crystal structure of possible asymmetric diadenosine tetraphosphate (Ap(4)A) hydrolases from *Jonesia denitrificans* DSM 20603  
Authors : Tan, K.; Kim, Y.; Wu, R.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2013-05-20  
Resolution : 1.94 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	:	1.7.2 (RC1), CSD as538be (2017)
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

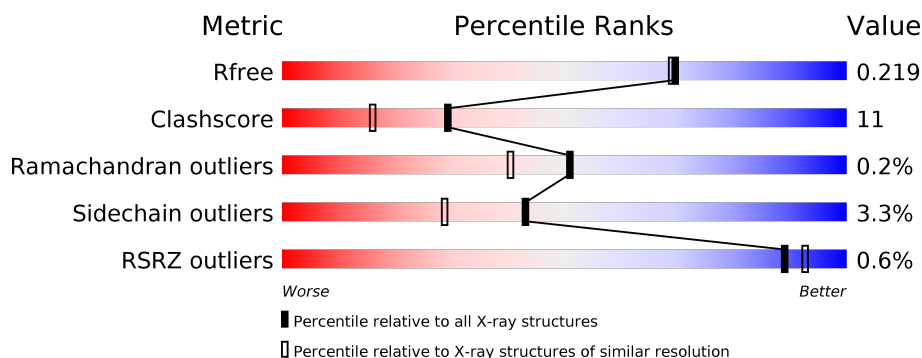
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	3233 (1.96-1.92)
Clashscore	112137	3430 (1.96-1.92)
Ramachandran outliers	110173	3395 (1.96-1.92)
Sidechain outliers	110143	3395 (1.96-1.92)
RSRZ outliers	101464	3250 (1.96-1.92)

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	194	 61% 22% 18%
1	B	194	 % 64% 15% • 19%
1	C	194	 % 58% 24% • 18%
1	D	194	 % 57% 25% • 18%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	204	-	-	X	X
3	CL	A	205	-	-	X	-
3	CL	A	208	-	-	X	X
3	CL	B	203	-	-	X	-
3	CL	D	202	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5516 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	Se	0	1	0
			1243	788	221	226	2	6			
1	B	158	Total	C	N	O	S	Se	0	2	0
			1237	784	219	225	2	7			
1	C	160	Total	C	N	O	S	Se	0	2	0
			1256	796	224	227	2	7			
1	D	159	Total	C	N	O	S	Se	0	2	0
			1243	788	221	226	2	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP C7R2I1
A	0	ASN	-	EXPRESSION TAG	UNP C7R2I1
A	1	ALA	-	EXPRESSION TAG	UNP C7R2I1
B	-1	SER	-	EXPRESSION TAG	UNP C7R2I1
B	0	ASN	-	EXPRESSION TAG	UNP C7R2I1
B	1	ALA	-	EXPRESSION TAG	UNP C7R2I1
C	-1	SER	-	EXPRESSION TAG	UNP C7R2I1
C	0	ASN	-	EXPRESSION TAG	UNP C7R2I1
C	1	ALA	-	EXPRESSION TAG	UNP C7R2I1
D	-1	SER	-	EXPRESSION TAG	UNP C7R2I1
D	0	ASN	-	EXPRESSION TAG	UNP C7R2I1
D	1	ALA	-	EXPRESSION TAG	UNP C7R2I1

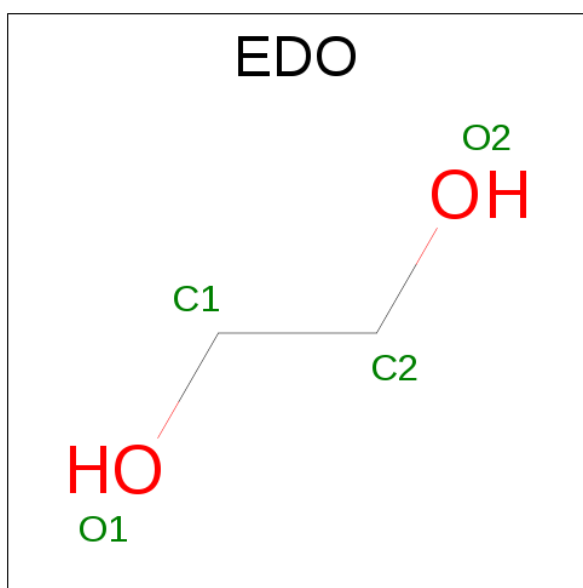
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	5	Total Cl 5 5	0	0
3	A	10	Total Cl 10 10	0	0
3	D	5	Total Cl 5 5	0	0
3	C	2	Total Cl 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

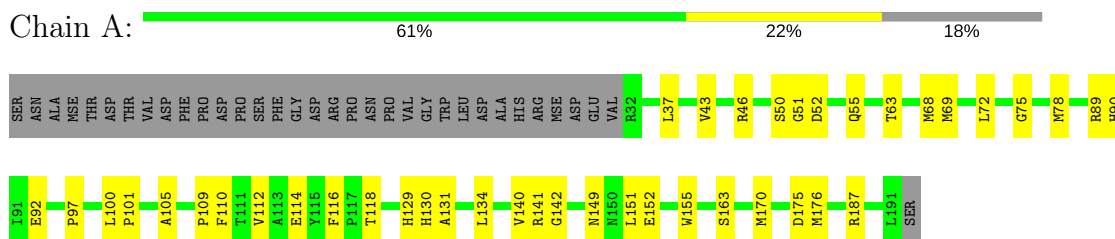
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	139	Total O 139 139	0	0
5	B	140	Total O 140 140	0	0
5	C	111	Total O 111 111	0	0
5	D	120	Total O 120 120	0	0

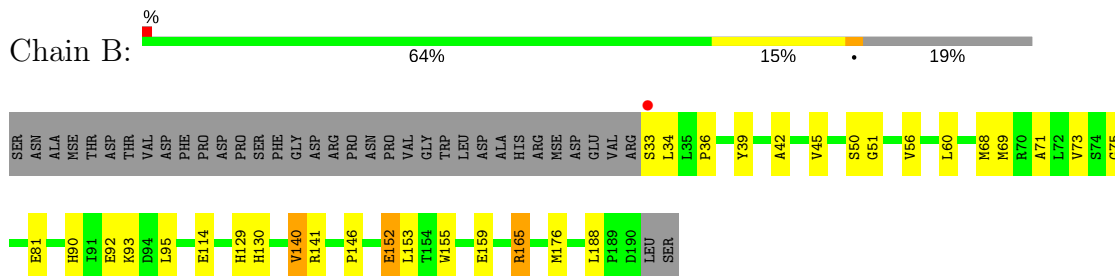
### 3 Residue-property plots

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.

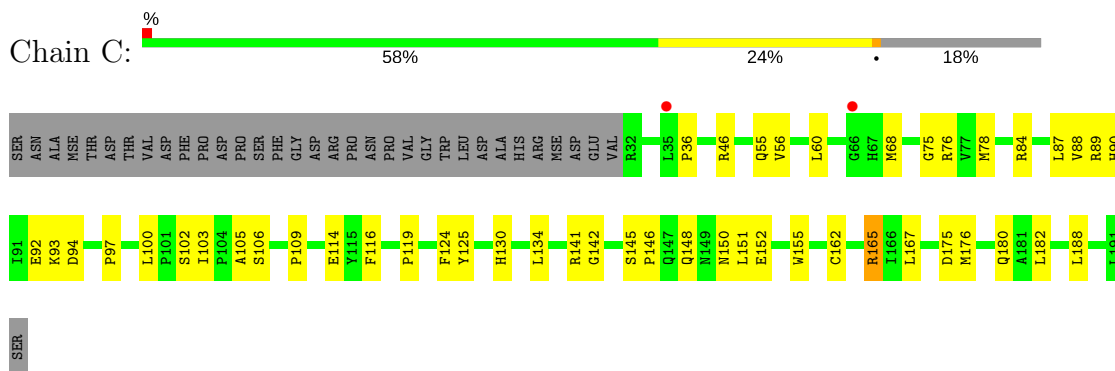
- Molecule 1: Putative uncharacterized protein



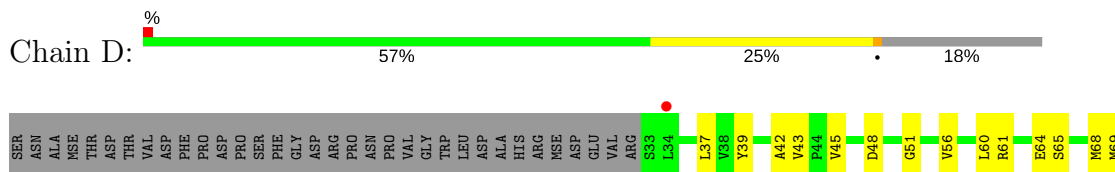
- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



R70	A71	L72	V73	S74	G75		W78	Y79	H80	E81	R82	Q83	R84	D85	A86	L87		H90	I91	E92	K93		P101	S102	I103	P104	A105		P117		D126	D127	R128	H129	H130		Y140		S145		Q148	N149		E152		W155		S163		I166		M176		L188		L191	SER
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.49Å 69.81Å 94.31Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	47.84 – 1.94 47.84 – 1.94	Depositor EDS
% Data completeness (in resolution range)	90.6 (47.84-1.94) 88.6 (47.84-1.94)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.173 , 0.224 0.171 , 0.219	Depositor DCC
$R_{free}$ test set	1953 reflections (4.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.437 for h,-k,-l	Xtriage
Reported twinning fraction	0.480 for h,-k,-l	Depositor
Outliers	0 of 48781 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 57.74 % 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 2.2663e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NA, EDO, 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	0.38	0/1268	0.60	0/1723
1	B	0.38	0/1262	0.58	0/1713
1	C	0.38	0/1282	0.58	0/1741
1	D	0.37	0/1268	0.59	0/1723
All	All	0.38	0/5080	0.59	0/6900

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	1243	0	1246	28	1
1	B	1237	0	1235	23	0
1	C	1256	0	1259	31	0
1	D	1243	0	1245	34	1
2	A	1	0	0	0	0
3	A	10	0	0	8	0
3	B	5	0	0	3	0
3	C	2	0	0	1	0
3	D	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	6	1	0
5	A	139	0	0	5	0
5	B	140	0	0	5	1
5	C	111	0	0	2	1
5	D	120	0	0	3	0
All	All	5516	0	4991	108	2

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 108 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:D:42:ALA:HB3	1:D:73:VAL:HB	1.70	0.72
1:D:61:ARG:NH1	5:D:417:HOH:O	2.25	0.68
1:B:176[B]:MSE:HE1	1:D:188:LEU:HB3	1.77	0.67
1:A:129:HIS:NE2	5:A:424:HOH:O	2.27	0.66
3:A:203:CL:CL	5:A:434:HOH:O	2.50	0.66

All (2) 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:D:149:ASN:O	5:C:359:HOH:O[2_646]	2.05	0.15
1:A:149:ASN:OD1	5:B:431:HOH:O[2_657]	2.19	0.01

## 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	159/194 (82%)	156 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	158/194 (81%)	154 (98%)	4 (2%)	0	100	100
1	C	160/194 (82%)	158 (99%)	2 (1%)	0	100	100
1	D	159/194 (82%)	154 (97%)	4 (2%)	1 (1%)	28	15
All	All	636/776 (82%)	622 (98%)	13 (2%)	1 (0%)	51	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	148	GLN

### 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	136/159 (86%)	134 (98%)	2 (2%)	70	63
1	B	136/159 (86%)	129 (95%)	7 (5%)	28	12
1	C	138/159 (87%)	134 (97%)	4 (3%)	48	34
1	D	136/159 (86%)	131 (96%)	5 (4%)	39	24
All	All	546/636 (86%)	528 (97%)	18 (3%)	43	29

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	165	ARG
1	C	56	VAL
1	D	65	SER
1	B	140	VAL
1	B	152	GLU

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

Mol	Chain	Res	Type
1	D	129	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 23 are monoatomic - leaving 1 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	$\# Z  > 2$
4	EDO	A	212	-	3,3,3	0.45	0	2,2,2	0.29	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
4	EDO	A	212	-	-	0/1/1/1	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	212	EDO	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 [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	155/194 (79%)	-0.44	0 100 100	7, 18, 38, 55	0
1	B	153/194 (78%)	-0.47	1 (0%) 87 91	6, 15, 40, 58	0
1	C	155/194 (79%)	-0.19	2 (1%) 77 83	9, 25, 51, 79	0
1	D	154/194 (79%)	-0.18	1 (0%) 89 92	12, 28, 57, 68	0
All	All	617/776 (79%)	-0.32	4 (0%) 89 92	6, 21, 48, 79	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	34	LEU	3.8
1	C	66	GLY	2.7
1	B	33	SER	2.4
1	C	35	LEU	2.1

### 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
3	CL	A	204	1/1	0.96	0.16	11.76	44,44,44,44	0
3	CL	D	202	1/1	0.96	0.12	5.82	29,29,29,29	0
3	CL	A	208	1/1	0.94	0.12	2.07	40,40,40,40	0
3	CL	D	203	1/1	0.99	0.09	-0.07	24,24,24,24	0
3	CL	A	203	1/1	0.99	0.07	-1.12	25,25,25,25	0
3	CL	D	204	1/1	0.99	0.07	-1.41	25,25,25,25	0
2	NA	A	201	1/1	0.98	0.06	-1.98	20,20,20,20	0
3	CL	A	206	1/1	0.99	0.05	-2.09	28,28,28,28	0
3	CL	A	205	1/1	0.99	0.06	-2.78	20,20,20,20	0
3	CL	B	205	1/1	1.00	0.06	-2.79	29,29,29,29	0
3	CL	C	201	1/1	0.98	0.05	-3.10	23,23,23,23	0
3	CL	B	201	1/1	0.99	0.05	-3.18	19,19,19,19	0
3	CL	B	203	1/1	0.99	0.05	-4.07	18,18,18,18	0
3	CL	A	211	1/1	0.99	0.04	-4.08	30,30,30,30	0
3	CL	A	207	1/1	0.98	0.05	-4.83	27,27,27,27	0
3	CL	D	201	1/1	0.98	0.04	-5.35	25,25,25,25	0
4	EDO	A	212	4/4	0.94	0.15	-	31,31,31,34	0
3	CL	A	209	1/1	0.99	0.09	-	22,22,22,22	0
3	CL	D	205	1/1	0.96	0.09	-	29,29,29,29	0
3	CL	A	210	1/1	0.97	0.06	-	29,29,29,29	0
3	CL	B	204	1/1	0.99	0.13	-	30,30,30,30	0
3	CL	A	202	1/1	0.99	0.06	-	25,25,25,25	0
3	CL	C	202	1/1	0.99	0.04	-	27,27,27,27	0
3	CL	B	202	1/1	0.99	0.05	-	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.