



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 04:49 PM EST

PDB ID : 5XGE
Title : Crystal structure of the PAS-GGDEF-EAL domain of PA0861 from *Pseudomonas aeruginosa* in complex with cyclic di-GMP
Authors : Liu, C.; Liew, C.W.; Sreekanth, R.; Lescar, J.
Deposited on : 2017-04-13
Resolution : 3.31 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : rb-20030736
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) : rb-20030736

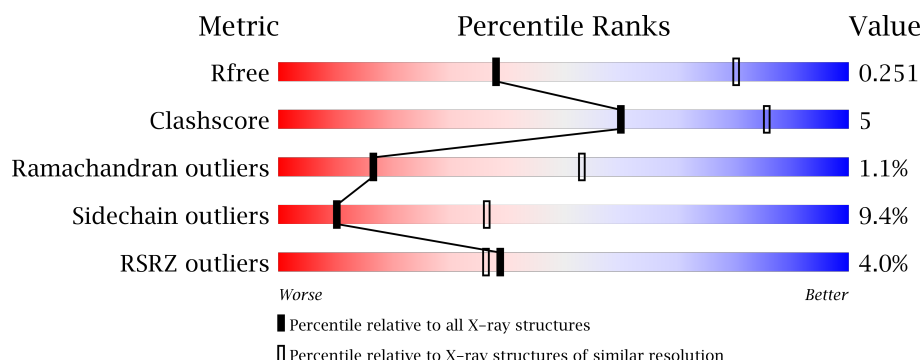
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1002 (3.38-3.26)
Clashscore	112137	1066 (3.38-3.26)
Ramachandran outliers	110173	1048 (3.38-3.26)
Sidechain outliers	110143	1047 (3.38-3.26)
RSRZ outliers	101464	1007 (3.38-3.26)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	568	<div> <div>4%</div> <div>77%</div> <div>18%</div> <div>••</div> </div>

2 Entry composition [i](#)

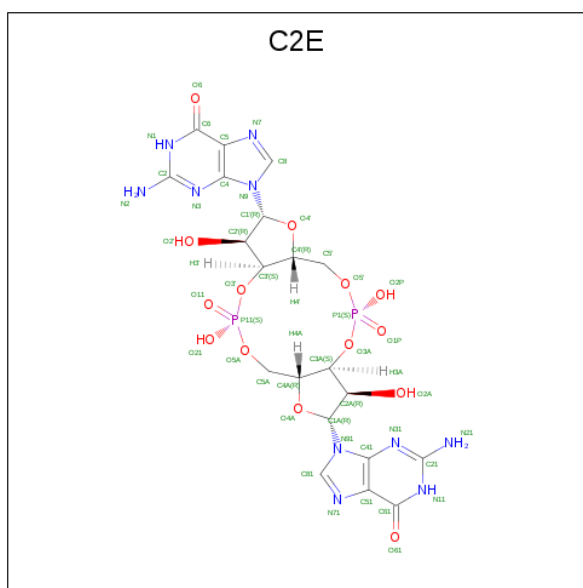
There are 3 unique types of molecules in this entry. The entry contains 4482 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PA0861.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4295	2709	758	805	23			

- Molecule 2 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

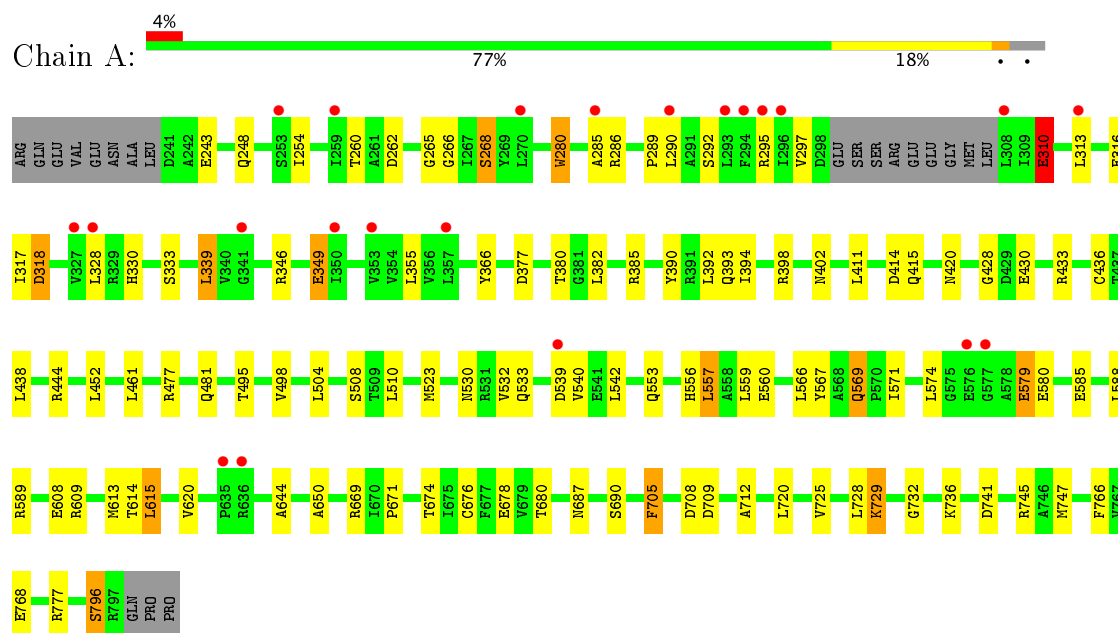
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		

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 PA0861



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	134.88Å 134.88Å 211.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.12 – 3.31 48.12 – 3.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.12-3.31) 100.0 (48.12-3.31)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.180 , 0.255 0.175 , 0.251	Depositor DCC
R_{free} test set	565 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 88.8	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	0.93	EDS
Total number of atoms	4482	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C2E

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	0.46	0/4372	0.68	0/5919

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	4295	0	4281	45	0
2	A	46	0	22	2	0
3	A	141	0	0	0	0
All	All	4482	0	4303	46	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 5.

All (46) 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:A:901:C2E:H512	2:A:901:C2E:H81	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLN:HE22	1:A:495:THR:HG22	1.53	0.72
1:A:556:HIS:HA	1:A:559:LEU:HD12	1.78	0.66
1:A:289:PRO:HG2	1:A:292:SER:HB2	1.81	0.63
1:A:553:GLN:HG3	1:A:557:LEU:HD12	1.86	0.56
1:A:574:LEU:HB3	1:A:777:ARG:HG3	1.87	0.56
1:A:720:LEU:HD11	1:A:728:LEU:HD11	1.88	0.55
1:A:420:ASN:HD22	1:A:428:GLY:HA3	1.73	0.54
1:A:393:GLN:HG2	1:A:510:LEU:HD13	1.90	0.54
1:A:290:LEU:HD22	1:A:310:GLU:HG2	1.90	0.54
1:A:567:TYR:CD1	1:A:589:ARG:HG3	2.44	0.52
1:A:705:PHE:HB3	1:A:725:VAL:HG12	1.92	0.52
1:A:585:GLU:HA	1:A:644:ALA:HB3	1.92	0.51
1:A:614:THR:HG23	1:A:650:ALA:HB1	1.92	0.51
1:A:566:LEU:HB2	1:A:796:SER:HB3	1.92	0.51
1:A:579:GLU:CD	1:A:580:GLU:H	2.14	0.51
1:A:569:GLN:OE1	2:A:901:C2E:H8	2.11	0.50
1:A:380:THR:HG23	1:A:382:LEU:H	1.77	0.50
1:A:481:GLN:HE21	1:A:530:ASN:HD21	1.61	0.49
1:A:260:THR:HG22	1:A:268:SER:HB2	1.94	0.49
1:A:708:ASP:HA	1:A:729:LYS:HB2	1.94	0.49
1:A:411:LEU:HG	1:A:498:VAL:HG13	1.95	0.49
1:A:732:GLY:HA3	1:A:766:PHE:CD1	2.48	0.48
1:A:588:LEU:HD13	1:A:620:VAL:HG22	1.96	0.47
1:A:678:GLU:HG2	1:A:708:ASP:HB2	1.96	0.47
1:A:644:ALA:HA	1:A:676:CYS:O	2.16	0.45
1:A:390:TYR:CZ	1:A:394:ILE:HD11	2.52	0.45
1:A:539:ASP:HA	1:A:542:LEU:HD12	1.99	0.45
1:A:385:ARG:HG3	1:A:452:LEU:HD22	1.99	0.44
1:A:415:GLN:NE2	1:A:495:THR:HG22	2.27	0.44
1:A:392:LEU:HD23	1:A:510:LEU:HD12	1.99	0.44
1:A:523:MET:HB3	1:A:533:GLN:HG2	1.98	0.44
1:A:346:ARG:HB3	1:A:349:GLU:HB3	2.00	0.44
1:A:680:THR:HG22	1:A:708:ASP:HB3	1.99	0.44
1:A:571:ILE:HD11	1:A:585:GLU:HB2	2.00	0.43
1:A:556:HIS:CE1	1:A:615:LEU:HD11	2.54	0.43
1:A:712:ALA:HB3	1:A:747:MET:SD	2.59	0.43
1:A:736:LYS:HE2	1:A:768:GLU:OE1	2.19	0.42
1:A:671:PRO:HG2	1:A:674:THR:OG1	2.19	0.42
1:A:608:GLU:HG3	1:A:613:MET:HG3	2.01	0.42
1:A:339:LEU:HD21	1:A:355:LEU:HD22	2.02	0.42
1:A:477:ARG:HD3	1:A:532:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TRP:CD1	1:A:285:ALA:HB2	2.56	0.41
1:A:377:ASP:OD2	1:A:380:THR:HG22	2.19	0.41
1:A:394:ILE:O	1:A:398:ARG:HB2	2.21	0.41
1:A:414:ASP:OD2	1:A:495:THR:HG23	2.20	0.41

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	544/568 (96%)	496 (91%)	42 (8%)	6 (1%)	17	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	A	366	TYR
1	A	265	GLY
1	A	266	GLY
1	A	310	GLU
1	A	318	ASP

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	458/476 (96%)	415 (91%)	43 (9%)	10	36

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	GLU
1	A	248	GLN
1	A	254	ILE
1	A	262	ASP
1	A	268	SER
1	A	280	TRP
1	A	286	ARG
1	A	295	ARG
1	A	297	VAL
1	A	310	GLU
1	A	313	LEU
1	A	316	GLU
1	A	317	ILE
1	A	318	ASP
1	A	328	LEU
1	A	330	HIS
1	A	339	LEU
1	A	349	GLU
1	A	402	ASN
1	A	430	GLU
1	A	433	ARG
1	A	436	CYS
1	A	438	LEU
1	A	444	ARG
1	A	461	LEU
1	A	504	LEU
1	A	508	SER
1	A	540	VAL
1	A	557	LEU
1	A	560	GLU
1	A	569	GLN
1	A	579	GLU
1	A	609	ARG
1	A	615	LEU
1	A	669	ARG
1	A	687	ASN
1	A	690	SER
1	A	705	PHE

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Mol	Chain	Res	Type
1	A	709	ASP
1	A	729	LYS
1	A	741	ASP
1	A	745	ARG
1	A	796	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	GLN
1	A	402	ASN
1	A	420	ASN
1	A	481	GLN
1	A	536	HIS
1	A	749	GLN

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](#)

1 ligand is 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	C2E	A	901	-	44,52,52	1.70	10 (22%)	50,82,82	1.99	10 (20%)

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
2	C2E	A	901	-	-	0/22/62/62	0/6/7/7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	C2E	C61-C51	-3.77	1.34	1.41
2	A	901	C2E	C6-C5	-3.60	1.34	1.41
2	A	901	C2E	C51-C41	-2.74	1.34	1.40
2	A	901	C2E	C5-C4	-2.34	1.35	1.40
2	A	901	C2E	O4'-C1'	2.20	1.44	1.41
2	A	901	C2E	C21-N11	2.73	1.40	1.35
2	A	901	C2E	O4A-C1A	2.96	1.45	1.41
2	A	901	C2E	C2-N1	3.39	1.41	1.35
2	A	901	C2E	C61-N11	4.39	1.41	1.33
2	A	901	C2E	C6-N1	4.55	1.41	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	C2E	N3-C2-N1	-6.10	118.56	127.46
2	A	901	C2E	N31-C21-N11	-5.99	118.71	127.46
2	A	901	C2E	C5-C6-N1	-3.02	119.19	123.48
2	A	901	C2E	C51-C61-N11	-2.11	120.48	123.48
2	A	901	C2E	C5A-C4A-C3A	-2.09	107.21	114.30
2	A	901	C2E	C6-N1-C2	2.02	118.97	116.06
2	A	901	C2E	N21-C21-N11	2.27	120.88	117.24
2	A	901	C2E	N2-C2-N1	2.70	121.55	117.24
2	A	901	C2E	C2-N3-C4	5.29	121.34	115.16
2	A	901	C2E	C21-N31-C41	5.84	121.97	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	C2E	2	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 ⓘ

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	548/568 (96%)	0.15	22 (4%) 39 36	25, 53, 102, 145	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	LEU	4.1
1	A	577	GLY	4.0
1	A	576	GLU	3.0
1	A	327	VAL	2.7
1	A	253	SER	2.7
1	A	539	ASP	2.6
1	A	296	ILE	2.6
1	A	259	ILE	2.6
1	A	350	ILE	2.5
1	A	285	ALA	2.5
1	A	353	VAL	2.4
1	A	295	ARG	2.4
1	A	328	LEU	2.4
1	A	636	ARG	2.3
1	A	357	LEU	2.2
1	A	313	LEU	2.2
1	A	341	GLY	2.1
1	A	308	LEU	2.1
1	A	293	LEU	2.1
1	A	294	PHE	2.1
1	A	635	PRO	2.1
1	A	270	LEU	2.1

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 [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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	C2E	A	901	46/46	0.93	0.19	-0.27	68,80,86,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.