



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:27 pm GMT

PDB ID : 4DSF
Title : Ternary complex of Bacillus DNA Polymerase I Large Fragment F710Y, DNA duplex, and rCTP (paired with dG of template) in presence of Mn²⁺
Authors : Wang, W.; Beese, L.S.
Deposited on : 2012-02-18
Resolution : 1.66 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

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 : 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

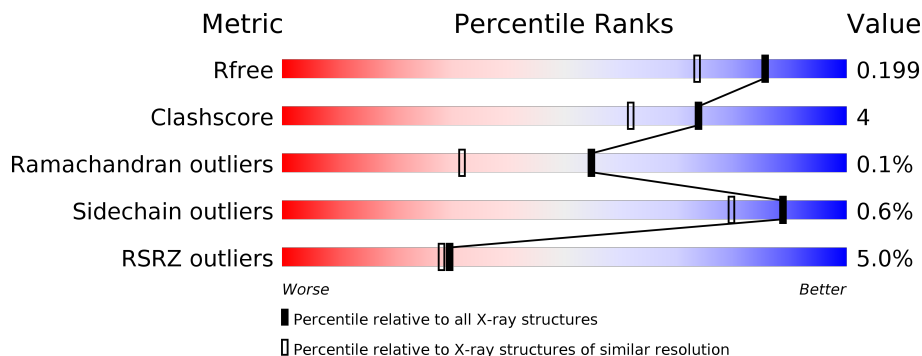
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

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	592	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>
1	D	592	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>•</div> </div> </div>
2	B	9	<div> <div></div> <div> <div>56%</div> <div>22%</div> <div>22%</div> </div> </div>
2	E	9	<div> <div></div> <div> <div>33%</div> <div>44%</div> <div>22%</div> </div> </div>
3	C	13	<div> <div></div> <div> <div>31%</div> <div>38%</div> <div>31%</div> </div> </div>
3	F	13	<div> <div>8%</div> <div> <div></div> <div>31%</div> <div>62%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20794 atoms, of which 9688 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 DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	546	Total	C	H	N	O	S	0	6	0
			8882	2803	4479	766	819	15			
1	D	579	Total	C	H	N	O	S	0	14	0
			9459	2984	4763	814	881	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
A	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
A	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1
D	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
D	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
D	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1

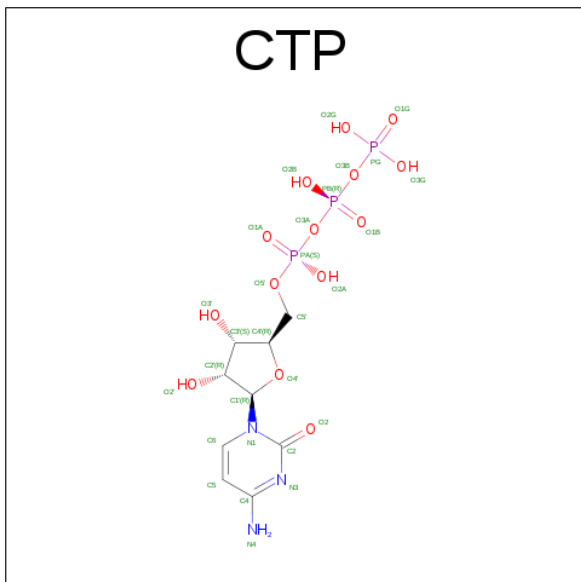
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3').

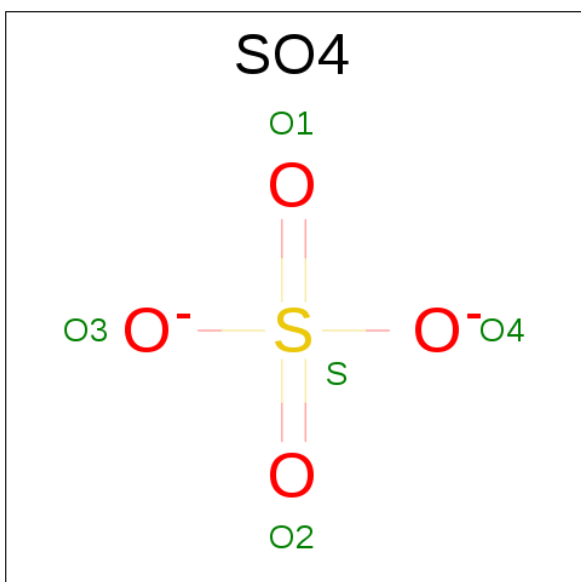
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O	P	0	0	0
			291	89	100	40	53	9			
3	F	12	Total	C	H	N	O	P	0	0	0
			385	119	134	52	69	11			

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	D	1	Total	C	H	N	O	P	0	0
			41	9	12	3	14	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		

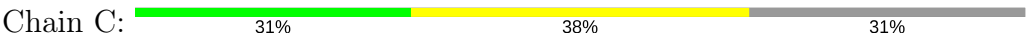
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	343	Total	O	0	0
			343	343		
6	D	659	Total	O	0	0
			659	659		
6	B	29	Total	O	0	0
			29	29		
6	C	48	Total	O	0	0
			48	48		
6	E	30	Total	O	0	0
			30	30		
6	F	59	Total	O	0	0
			59	59		



• Molecule 3: DNA (5'-D(*CP*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.68Å 109.06Å 150.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.06 – 1.66 71.06 – 1.66	Depositor EDS
% Data completeness (in resolution range)	86.5 (71.06-1.66) 86.5 (71.06-1.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, R_{free}	0.177 , 0.200 0.176 , 0.199	Depositor DCC
R_{free} test set	6759 reflections (4.32%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.5	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	0.96	EDS
Total number of atoms	20794	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: DOC, CTP, 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	0.43	0/4507	0.56	0/6085
1	D	0.62	1/4842 (0.0%)	0.71	2/6544 (0.0%)
2	B	1.02	0/173	1.92	9/264 (3.4%)
2	E	1.13	0/173	1.97	5/264 (1.9%)
3	C	1.22	1/215 (0.5%)	1.79	4/331 (1.2%)
3	F	1.24	1/283 (0.4%)	1.88	10/437 (2.3%)
All	All	0.62	3/10193 (0.0%)	0.84	30/13925 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	6	DA	N9-C4	-7.53	1.33	1.37
1	D	749	TYR	CB-CG	-5.29	1.43	1.51
3	C	6	DA	N9-C4	-5.00	1.34	1.37

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	8	DT	O4'-C1'-N1	-12.94	98.94	108.00
3	C	8	DT	O4'-C1'-N1	-9.12	101.61	108.00
2	E	23	DT	O4'-C1'-N1	-8.44	102.09	108.00
2	B	23	DT	O4'-C1'-N1	-7.86	102.50	108.00
2	B	25	DA	O4'-C4'-C3'	-7.33	101.57	104.50

There are no chirality outliers.

There are no planarity outliers.

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	4403	4479	4438	24	1
1	D	4696	4763	4688	43	1
2	B	174	100	103	3	0
2	E	174	100	103	5	0
3	C	191	100	101	0	0
3	F	251	134	136	1	0
4	D	29	12	12	4	0
5	D	20	0	0	0	0
6	A	343	0	0	13	1
6	B	29	0	0	1	0
6	C	48	0	0	0	0
6	D	659	0	0	20	1
6	E	30	0	0	0	0
6	F	59	0	0	0	0
All	All	11106	9688	9581	74	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 4.

The worst 5 of 74 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:845:CYS:SG	6:D:1411:HOH:O	2.30	0.88
1:D:705:ALA:N	6:D:1612:HOH:O	2.10	0.84
1:A:821:GLN:O	6:A:1183:HOH:O	2.01	0.79
1:A:676:ARG:HD2	6:A:1220:HOH:O	1.86	0.75
2:B:27:DT:OP1	6:B:128:HOH:O	2.07	0.72

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)
6:A:1027:HOH:O	6:D:1404:HOH:O[2_745]	1.88	0.32
1:A:505:LYS:HZ3	1:D:356:GLN:OE1[2_745]	1.57	0.03

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	546/592 (92%)	533 (98%)	13 (2%)	0	100	100
1	D	591/592 (100%)	576 (98%)	14 (2%)	1 (0%)	51	28
All	All	1137/1184 (96%)	1109 (98%)	27 (2%)	1 (0%)	55	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	628	ILE

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	470/507 (93%)	467 (99%)	3 (1%)	89	79
1	D	508/507 (100%)	505 (99%)	3 (1%)	89	79
All	All	978/1014 (96%)	972 (99%)	6 (1%)	89	79

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	LEU
1	D	728	SER
1	D	303	LEU
1	A	477	LEU
1	D	700	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are 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	DOC	B	29	3,2	13,19,20	1.11	1 (7%)	12,26,29	0.73	0
2	DOC	E	29	3,2	13,19,20	1.40	3 (23%)	12,26,29	1.20	1 (8%)

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	DOC	B	29	3,2	-	0/3/18/19	0/2/2/2
2	DOC	E	29	3,2	-	0/3/18/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	29	DOC	O5'-C5'	-3.10	1.40	1.44
2	E	29	DOC	C2-N3	-2.80	1.32	1.38
2	B	29	DOC	O5'-C5'	-2.65	1.41	1.44
2	E	29	DOC	C6-C5	-2.23	1.33	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DOC	O4'-C4'-C5'	-2.83	105.00	109.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	29	DOC	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 ligands are 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	$\# Z > 2$
4	CTP	D	901	-	24,30,30	1.48	4 (16%)	24,47,47	0.94	0
5	SO4	D	902	-	4,4,4	0.29	0	6,6,6	0.09	0
5	SO4	D	903	-	4,4,4	0.15	0	6,6,6	0.50	0
5	SO4	D	904	-	4,4,4	0.24	0	6,6,6	0.19	0
5	SO4	D	905	-	4,4,4	0.17	0	6,6,6	0.14	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	CTP	D	901	-	-	0/18/38/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	D	902	-	-	0/0/0/0	0/0/0/0
5	SO4	D	903	-	-	0/0/0/0	0/0/0/0
5	SO4	D	904	-	-	0/0/0/0	0/0/0/0
5	SO4	D	905	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	CTP	C2'-C1'	-3.20	1.48	1.53
4	D	901	CTP	C6-N1	2.25	1.38	1.35
4	D	901	CTP	C2-N3	2.28	1.42	1.38
4	D	901	CTP	C4-N4	2.59	1.43	1.35

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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	901	CTP	4	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, 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	546/592 (92%)	0.37	40 (7%) 16 15	21, 40, 67, 94	0
1	D	579/592 (97%)	0.10	17 (2%) 52 54	11, 24, 47, 79	0
2	B	8/9 (88%)	-0.40	0 100 100	27, 31, 42, 50	0
2	E	8/9 (88%)	-0.27	0 100 100	19, 25, 40, 50	0
3	C	9/13 (69%)	-0.57	0 100 100	21, 26, 34, 42	0
3	F	12/13 (92%)	0.12	1 (8%) 12 11	16, 25, 65, 76	0
All	All	1162/1228 (94%)	0.22	58 (4%) 30 28	11, 32, 61, 94	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	ALA	7.9
1	A	298	LYS	7.2
1	A	816	LYS	6.7
1	D	689	ILE	5.3
1	A	677	ARG	5.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	DOC	B	29	18/19	0.95	0.09	-	30,36,43,45	0
2	DOC	E	29	18/19	0.98	0.12	-	15,19,26,26	0

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
4	CTP	D	901	29/29	0.95	0.09	-0.42	21,28,42,50	0
5	SO4	D	903	5/5	0.98	0.08	-0.52	33,37,42,47	0
5	SO4	D	902	5/5	0.94	0.09	-0.59	40,40,45,46	0
5	SO4	D	905	5/5	0.96	0.18	-	62,67,69,69	0
5	SO4	D	904	5/5	0.93	0.24	-	59,67,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.