



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:14 AM GMT

PDB ID : 2O5C
Title : Structure of E. coli topoisomerase III in complex with an 8-base single stranded oligonucleotide. Frozen in glucose pH 5.5
Authors : Changela, A.; DiGate, R.J.; Mondragon, A.
Deposited on : 2006-12-05
Resolution : 2.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

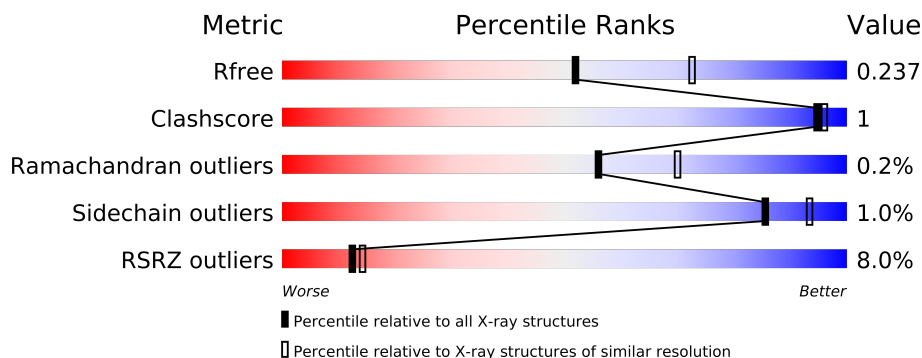
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	8	
1	D	8	
2	A	659	
2	B	659	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10705 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA chain called 5'-D(*CP*GP*CP*AP*AP*CP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	7	Total	C	N	O	P	0	0	0
			138	67	26	39	6			
1	D	7	Total	C	N	O	P	0	0	0
			138	67	26	39	6			

- Molecule 2 is a protein called DNA topoisomerase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	634	Total	C	N	O	S	0	0	0
			5042	3184	918	920	20			
2	B	631	Total	C	N	O	S	0	0	0
			5020	3170	913	917	20			

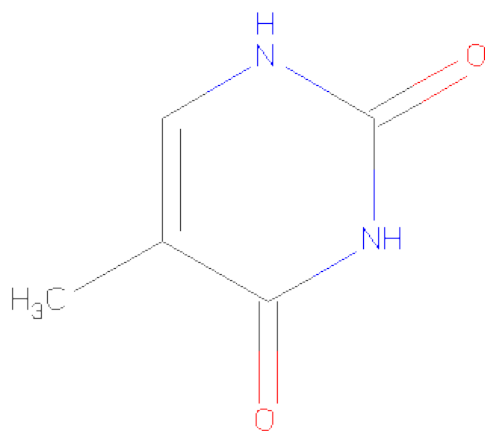
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	654	HIS	-	EXPRESSION TAG	UNP P14294
A	655	HIS	-	EXPRESSION TAG	UNP P14294
A	656	HIS	-	EXPRESSION TAG	UNP P14294
A	657	HIS	-	EXPRESSION TAG	UNP P14294
A	658	HIS	-	EXPRESSION TAG	UNP P14294
A	659	HIS	-	EXPRESSION TAG	UNP P14294
B	654	HIS	-	EXPRESSION TAG	UNP P14294
B	655	HIS	-	EXPRESSION TAG	UNP P14294
B	656	HIS	-	EXPRESSION TAG	UNP P14294
B	657	HIS	-	EXPRESSION TAG	UNP P14294
B	658	HIS	-	EXPRESSION TAG	UNP P14294
B	659	HIS	-	EXPRESSION TAG	UNP P14294

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is THYMINE (three-letter code: TDR) (formula: C₅H₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	176	Total	O	0	0
			176	176		
5	B	158	Total	O	0	0
			158	158		
5	C	13	Total	O	0	0
			13	13		
5	D	9	Total	O	0	0
			9	9		

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 errors 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: 5'-D(*CP*GP*CP*AP*AP*CP*TP*T)-3'

Chain C: 



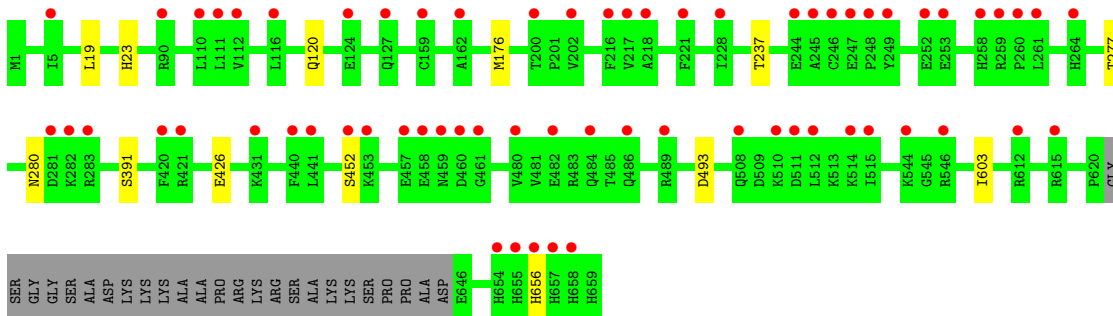
- Molecule 1: 5'-D(*CP*GP*CP*AP*AP*CP*TP*T)-3'

Chain D: 



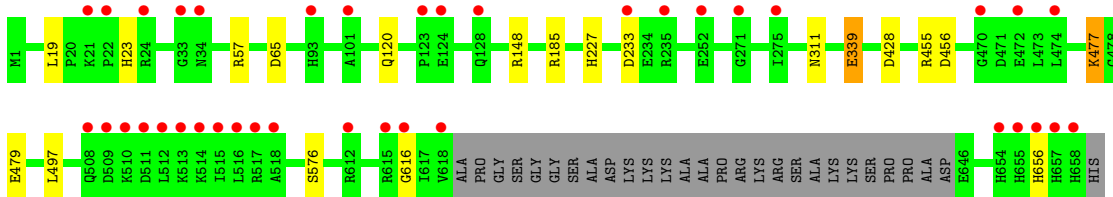
- Molecule 2: DNA topoisomerase 3

Chain A: 



- Molecule 2: DNA topoisomerase 3

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.21 Å 102.21 Å 443.75 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.15 – 2.35 29.15 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.15-2.35) 95.7 (29.15-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.36 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.245 0.203 , 0.237	Depositor DCC
R_{free} test set	4758 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 95012 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10705	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TDR, 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	C	0.95	0/154	1.63	6/235 (2.6%)
1	D	0.87	0/154	1.49	3/235 (1.3%)
2	A	0.46	0/5154	0.56	0/6989
2	B	0.48	2/5130 (0.0%)	0.58	1/6955 (0.0%)
All	All	0.49	2/10592 (0.0%)	0.63	10/14414 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	477	LYS	CE-NZ	10.86	1.76	1.49
2	B	477	LYS	CD-CE	5.25	1.64	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	DC	O4'-C1'-N1	7.00	112.90	108.00
1	C	1	DC	O4'-C1'-N1	6.94	112.86	108.00
2	B	477	LYS	CD-CE-NZ	-6.81	96.04	111.70
1	C	4	DA	O4'-C1'-N9	-6.48	103.47	108.00
1	C	6	DC	O4'-C1'-N1	6.40	112.48	108.00
1	D	5	DA	O4'-C1'-N9	5.98	112.19	108.00
1	C	5	DA	O4'-C1'-N9	5.89	112.13	108.00
1	D	6	DC	O4'-C1'-N1	5.34	111.74	108.00
1	C	7	DT	C3'-C2'-C1'	-5.31	96.13	102.50
1	C	4	DA	P-O3'-C3'	5.20	125.94	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	138	0	80	1	0
1	D	138	0	80	2	0
2	A	5042	0	0	4	0
2	B	5020	0	0	9	0
3	A	2	0	0	0	0
4	D	9	0	6	0	0
5	A	176	0	0	1	0
5	B	158	0	0	1	0
5	C	13	0	0	0	0
5	D	9	0	0	0	0
All	All	10705	0	166	15	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (15) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:477:LYS:NZ	2:B:477:LYS:CE	1.76	1.47
2:B:477:LYS:CD	2:B:477:LYS:NZ	2.53	0.72
2:A:176:MET:CE	2:A:603:ILE:CD1	2.87	0.52
2:A:656:HIS:CD2	5:A:863:HOH:O	2.63	0.50
2:B:227:HIS:NE2	2:B:479:GLU:OE1	2.45	0.49
2:B:455:ARG:NH1	2:B:456:ASP:OD1	2.49	0.46
2:B:311:ASN:ND2	5:B:678:HOH:O	2.48	0.45
2:B:57:ARG:NH1	2:B:65:ASP:OD1	2.51	0.44
1:D:5:DA:C6	1:D:7:DT:H1'	2.52	0.43
2:B:148:ARG:NH1	2:B:339:GLU:OE1	2.52	0.43
1:C:1:DC:H2''	1:C:2:DG:H5'	2.00	0.42
2:A:19:LEU:O	2:A:23:HIS:NE2	2.53	0.42
1:D:1:DC:O2	2:B:185:ARG:NH2	2.53	0.42
2:A:277:THR:N	2:A:426:GLU:O	2.54	0.40
2:B:19:LEU:O	2:B:23:HIS:NE2	2.54	0.40

There are no symmetry-related clashes.

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	
2	A	630/659 (96%)	618 (98%)	10 (2%)	2 (0%)	50	62
2	B	627/659 (95%)	614 (98%)	12 (2%)	1 (0%)	56	70
All	All	1257/1318 (95%)	1232 (98%)	22 (2%)	3 (0%)	56	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	452	SER
2	A	120	GLN
2	B	616	GLY

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	A	538/555 (97%)	534 (99%)	4 (1%)	91	96
2	B	536/555 (97%)	529 (99%)	7 (1%)	80	90
All	All	1074/1110 (97%)	1063 (99%)	11 (1%)	85	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	237	THR
2	A	280	ASN
2	A	391	SER
2	A	493	ASP
2	B	120	GLN
2	B	233	ASP

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Mol	Chain	Res	Type
2	B	339	GLU
2	B	428	ASP
2	B	497	LEU
2	B	576	SER
2	B	656	HIS

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 chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 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	TDR	D	799	-	9,9,9	1.62	2 (22%)	8,12,12	1.38	2 (25%)

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	TDR	D	799	-	-	0/0/0/0	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	799	TDR	C4-C5	3.14	1.49	1.42
4	D	799	TDR	C6-N1	2.77	1.34	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	799	TDR	C5-C6-N1	-2.82	119.47	121.81
4	D	799	TDR	C4-N3-C2	-2.18	120.94	125.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	C	7/8 (87%)	-0.26	0	100	100	26, 28, 38, 51	0
1	D	7/8 (87%)	-0.19	0	100	100	29, 34, 46, 62	0
2	A	634/659 (96%)	0.42	65 (10%)	7	8	26, 43, 95, 139	0
2	B	631/659 (95%)	0.30	38 (6%)	21	24	27, 49, 95, 140	0
All	All	1279/1334 (95%)	0.36	103 (8%)	12	14	26, 46, 95, 140	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	657	HIS	9.6
2	A	657	HIS	6.7
2	A	249	TYR	5.8
2	B	515	ILE	5.7
2	A	656	HIS	5.6
2	B	656	HIS	5.4
2	B	654	HIS	5.3
2	A	658	HIS	5.2
2	B	508	GLN	5.0
2	B	514	LYS	5.0
2	A	515	ILE	4.5
2	B	511	ASP	4.4
2	A	440	PHE	4.3
2	B	612	ARG	4.1
2	A	248	PRO	4.1
2	A	452	SER	3.9
2	B	124	GLU	3.9
2	B	509	ASP	3.8
2	B	22	PRO	3.8
2	A	252	GLU	3.7
2	B	615	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	512	LEU	3.5
2	B	128	GLN	3.5
2	A	218	ALA	3.5
2	B	472	GLU	3.5
2	A	514	LYS	3.5
2	B	474	LEU	3.4
2	B	21	LYS	3.3
2	A	258	HIS	3.3
2	A	482	GLU	3.3
2	A	484	GLN	3.3
2	B	510	LYS	3.3
2	A	260	PRO	3.2
2	B	517	ARG	3.2
2	A	264	HIS	3.1
2	A	612	ARG	3.1
2	A	253	GLU	3.1
2	A	461	GLY	3.0
2	A	546	ARG	3.0
2	A	453	LYS	3.0
2	B	618	VAL	3.0
2	A	460	ASP	3.0
2	A	457	GLU	3.0
2	A	259	ARG	2.9
2	A	200	THR	2.9
2	A	510	LYS	2.9
2	B	513	LYS	2.9
2	B	123	PRO	2.8
2	A	421	ARG	2.8
2	B	516	LEU	2.8
2	A	247	GLU	2.8
2	B	33	GLY	2.8
2	A	512	LEU	2.8
2	A	441	LEU	2.7
2	B	616	GLY	2.6
2	A	458	GLU	2.6
2	B	252	GLU	2.6
2	A	127	GLN	2.6
2	A	459	ASN	2.6
2	B	518	ALA	2.6
2	A	420	PHE	2.6
2	A	486	GLN	2.6
2	A	124	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	654	HIS	2.5
2	A	244	GLU	2.5
2	A	283	ARG	2.5
2	A	615	ARG	2.5
2	A	202	VAL	2.5
2	A	112	VAL	2.4
2	B	655	HIS	2.4
2	A	508	GLN	2.4
2	A	221	PHE	2.3
2	B	34	ASN	2.3
2	A	5	ILE	2.3
2	B	24	ARG	2.3
2	A	281	ASP	2.3
2	A	245	ALA	2.3
2	B	470	GLY	2.2
2	B	233	ASP	2.2
2	B	275	ILE	2.2
2	A	544	LYS	2.2
2	A	261	LEU	2.2
2	A	90	ARG	2.2
2	B	271	GLY	2.2
2	A	282	LYS	2.2
2	A	655	HIS	2.2
2	A	246	CYS	2.2
2	A	489	ARG	2.1
2	A	511	ASP	2.1
2	B	93	HIS	2.1
2	A	110	LEU	2.1
2	B	658	HIS	2.1
2	A	216	PHE	2.1
2	A	116	LEU	2.1
2	A	480	VAL	2.1
2	B	101	ALA	2.1
2	A	431	LYS	2.0
2	A	162	ALA	2.0
2	A	159	CYS	2.0
2	A	217	VAL	2.0
2	A	228	ILE	2.0
2	A	111	LEU	2.0
2	B	235	ARG	2.0

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

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	TDR	D	799	9/9	0.23	1.88	107,107,107,107	0
3	CL	A	800	1/1	0.11	-1.09	34,34,34,34	0
3	CL	A	801	1/1	0.09	-1.39	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.