



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:14 AM GMT

PDB ID : 2O5E
Title : Structure of E. coli topoisomerase III in complex with an 8-base single stranded oligonucleotide. Frozen in glucose pH 7.0
Authors : Changela, A.; DiGate, R.J.; Mondragon, A.
Deposited on : 2006-12-05
Resolution : 2.50 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>

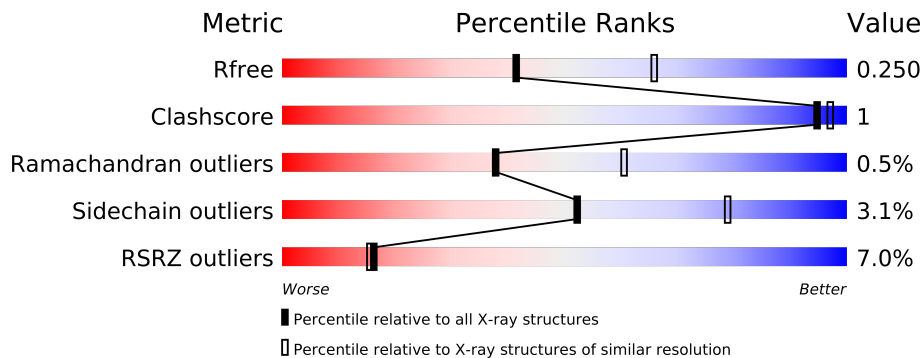
The following versions of software and data (see [references](#)) were used in the production of this report:

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


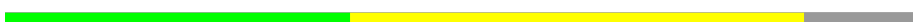

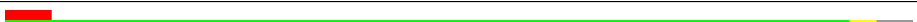
The reported resolution of this entry is 2.50 Å.

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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	TDR	D	9	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10496 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			

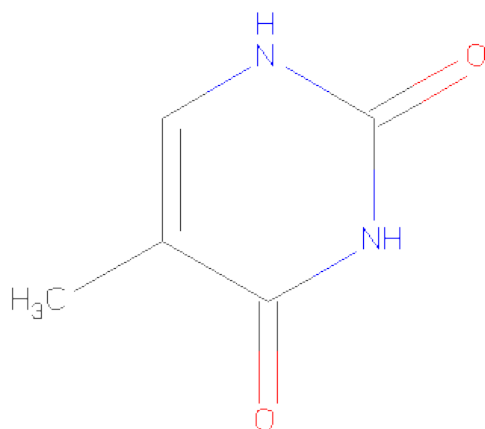
There are 12 discrepancies between the modelled and reference sequences:

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	85	Total	O	0	0
			85	85		
5	B	55	Total	O	0	0
			55	55		
5	C	3	Total	O	0	0
			3	3		
5	D	4	Total	O	0	0
			4	4		

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: 



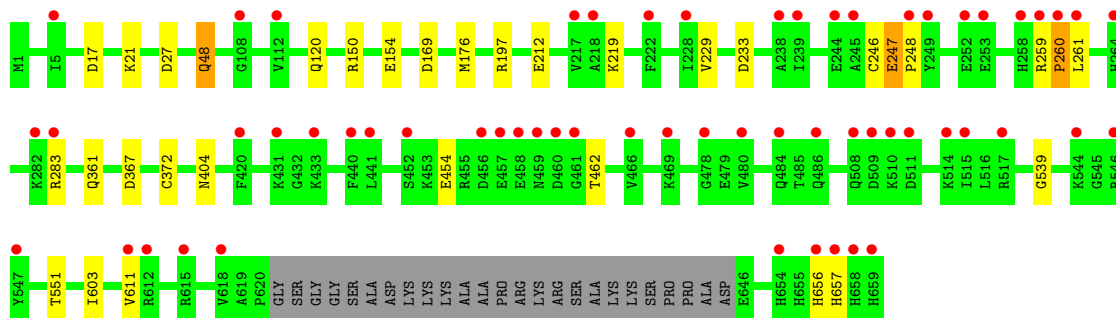
- Molecule 1: 5'-D(*CP*GP*CP*AP*AP*CP*TP*T)-3'

Chain D: 



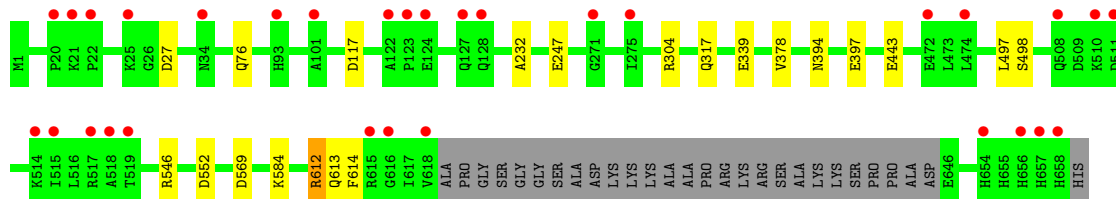
- Molecule 2: DNA topoisomerase 3

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	102.26Å 102.26Å 445.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.13 – 2.50 29.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (29.13-2.50) 95.8 (29.13-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.260 0.209 , 0.250	Depositor DCC
R_{free} test set	3992 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	3 of 79661 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10496	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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	1.11	0/154	1.61	3/235 (1.3%)
1	D	1.04	0/154	1.64	2/235 (0.9%)
2	A	0.52	0/5154	0.60	0/6989
2	B	0.50	0/5130	0.61	0/6955
All	All	0.53	0/10592	0.66	5/14414 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	DC	O4'-C1'-N1	7.48	113.24	108.00
1	C	5	DA	O4'-C1'-N9	5.80	112.06	108.00
1	C	1	DC	O4'-C1'-N1	5.65	111.96	108.00
1	C	4	DA	O4'-C1'-N9	-5.30	104.29	108.00
1	D	3	DC	O4'-C1'-N1	5.12	111.59	108.00

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	0	0
1	D	138	0	80	3	0
2	A	5042	0	0	11	0
2	B	5020	0	0	1	0
3	A	2	0	0	0	0
4	D	9	0	6	0	0
5	A	85	0	0	4	0
5	B	55	0	0	0	0
5	C	3	0	0	0	0
5	D	4	0	0	0	0
All	All	10496	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:A:21:LYS:O	5:A:806:HOH:O	2.04	0.75
2:A:656:HIS:CD2	5:A:850:HOH:O	2.55	0.58
1:D:6:DC:H4'	1:D:7:DT:C7	2.40	0.52
2:A:247:GLU:N	2:A:248:PRO:CD	2.74	0.51
2:A:361:GLN:NE2	5:A:838:HOH:O	2.47	0.48
2:A:150:ARG:NH1	2:A:154:GLU:OE1	2.48	0.45
2:A:169:ASP:OD1	2:A:197:ARG:NH1	2.49	0.45
2:B:612:ARG:O	2:B:614:PHE:N	2.50	0.45
2:A:539:GLY:O	2:A:551:THR:OG1	2.36	0.44
2:A:176:MET:CE	2:A:603:ILE:CD1	2.96	0.42
2:A:48:GLN:N	5:A:835:HOH:O	2.52	0.42
2:A:259:ARG:C	2:A:261:LEU:N	2.73	0.41
1:D:6:DC:H4'	1:D:7:DT:H72	2.03	0.41
2:A:259:ARG:N	2:A:260:PRO:CD	2.83	0.41
1:D:6:DC:H4'	1:D:7:DT:H71	2.03	0.41

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%)	600 (95%)	27 (4%)	3 (0%)	38	60
2	B	627/659 (95%)	606 (97%)	18 (3%)	3 (0%)	38	60
All	All	1257/1318 (95%)	1206 (96%)	45 (4%)	6 (0%)	38	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	247	GLU
2	B	612	ARG
2	B	613	GLN
2	B	232	ALA
2	A	260	PRO
2	A	120	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	
2	A	538/555 (97%)	522 (97%)	16 (3%)	53	80
2	B	536/555 (97%)	519 (97%)	17 (3%)	51	77
All	All	1074/1110 (97%)	1041 (97%)	33 (3%)	52	79

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	ASP
2	A	27	ASP
2	A	48	GLN
2	A	212	GLU
2	A	219	LYS
2	A	229	VAL
2	A	233	ASP
2	A	246	CYS
2	A	283	ARG

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Mol	Chain	Res	Type
2	A	367	ASP
2	A	372	CYS
2	A	404	ASN
2	A	454	GLU
2	A	462	THR
2	A	611	VAL
2	A	657	HIS
2	B	27	ASP
2	B	76	GLN
2	B	117	ASP
2	B	247	GLU
2	B	304	ARG
2	B	317	GLN
2	B	339	GLU
2	B	378	VAL
2	B	394	ASN
2	B	397	GLU
2	B	443	GLU
2	B	497	LEU
2	B	498	SER
2	B	546	ARG
2	B	552	ASP
2	B	569	ASP
2	B	584	LYS

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	9	-	9,9,9	1.70	2 (22%)	8,12,12	1.43	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	9	-	-	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	9	TDR	C4-C5	3.17	1.49	1.42
4	D	9	TDR	C6-N1	3.04	1.35	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	9	TDR	C5-C6-N1	-2.98	119.34	121.81
4	D	9	TDR	C4-N3-C2	-2.05	121.20	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%)	-0.17	0 100 100	39, 40, 50, 68	0
1	D	7/8 (87%)	-0.19	0 100 100	40, 44, 61, 78	0
2	A	634/659 (96%)	0.42	59 (9%) 9 8	34, 56, 109, 152	0
2	B	631/659 (95%)	0.26	31 (4%) 28 29	35, 61, 102, 128	0
All	All	1279/1334 (95%)	0.34	90 (7%) 16 15	34, 58, 105, 152	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	245	ALA	6.6
2	B	658	HIS	6.3
2	B	515	ILE	5.9
2	A	461	GLY	5.8
2	A	657	HIS	5.7
2	B	654	HIS	5.3
2	B	656	HIS	5.1
2	B	618	VAL	4.6
2	A	656	HIS	4.4
2	A	218	ALA	4.2
2	A	264	HIS	4.1
2	B	514	LYS	3.6
2	B	615	ARG	3.6
2	B	657	HIS	3.6
2	A	658	HIS	3.5
2	A	260	PRO	3.5
2	A	249	TYR	3.5
2	A	458	GLU	3.4
2	A	244	GLU	3.4
2	B	616	GLY	3.3
2	A	514	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	515	ILE	3.3
2	A	546	ARG	3.2
2	A	615	ARG	3.1
2	B	21	LYS	3.1
2	A	452	SER	3.1
2	A	547	TYR	3.1
2	A	460	ASP	3.0
2	A	456	ASP	3.0
2	B	93	HIS	3.0
2	A	618	VAL	3.0
2	A	654	HIS	2.9
2	B	508	GLN	2.9
2	A	486	GLN	2.9
2	A	508	GLN	2.9
2	A	459	ASN	2.9
2	A	440	PHE	2.8
2	A	252	GLU	2.8
2	B	474	LEU	2.8
2	B	517	ARG	2.8
2	A	433	LYS	2.8
2	A	659	HIS	2.7
2	A	510	LYS	2.6
2	A	283	ARG	2.6
2	A	478	GLY	2.6
2	A	222	PHE	2.6
2	B	22	PRO	2.6
2	B	127	GLN	2.6
2	A	248	PRO	2.6
2	A	258	HIS	2.6
2	A	544	LYS	2.6
2	B	519	THR	2.5
2	A	441	LEU	2.5
2	A	611	VAL	2.5
2	B	511	ASP	2.5
2	B	518	ALA	2.5
2	A	612	ARG	2.5
2	A	238	ALA	2.5
2	B	275	ILE	2.5
2	A	112	VAL	2.4
2	A	469	LYS	2.4
2	B	20	PRO	2.4
2	B	271	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	217	VAL	2.3
2	A	239	ILE	2.3
2	B	510	LYS	2.3
2	B	123	PRO	2.3
2	B	128	GLN	2.3
2	B	101	ALA	2.3
2	A	517	ARG	2.2
2	B	34	ASN	2.2
2	A	253	GLU	2.2
2	B	122	ALA	2.2
2	A	5	ILE	2.2
2	A	480	VAL	2.2
2	A	511	ASP	2.2
2	B	25	LYS	2.2
2	A	259	ARG	2.2
2	A	108	GLY	2.2
2	B	472	GLU	2.2
2	A	420	PHE	2.1
2	B	124	GLU	2.1
2	A	431	LYS	2.1
2	A	457	GLU	2.1
2	A	509	ASP	2.1
2	A	484	GLN	2.1
2	A	282	LYS	2.1
2	A	261	LEU	2.0
2	A	228	ILE	2.0
2	A	466	VAL	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	9	9/9	0.26	2.28	107,108,108,108	0
3	CL	A	801	1/1	0.14	0.40	52,52,52,52	0
3	CL	A	800	1/1	0.10	-2.32	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.