



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:46 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 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

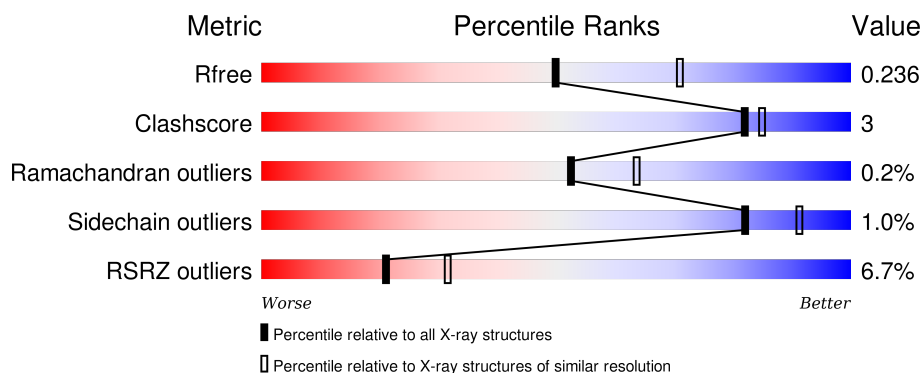
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	C	8	<div> <div>13%</div> <div>63%</div> <div>13%</div> <div>13%</div> </div>
1	D	8	<div> <div>38%</div> <div>38%</div> <div>13%</div> <div>13%</div> </div>
2	A	659	<div> <div>8%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>
2	B	659	<div> <div>5%</div> <div>86%</div> <div>9%</div> <div>•</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10705 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 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			

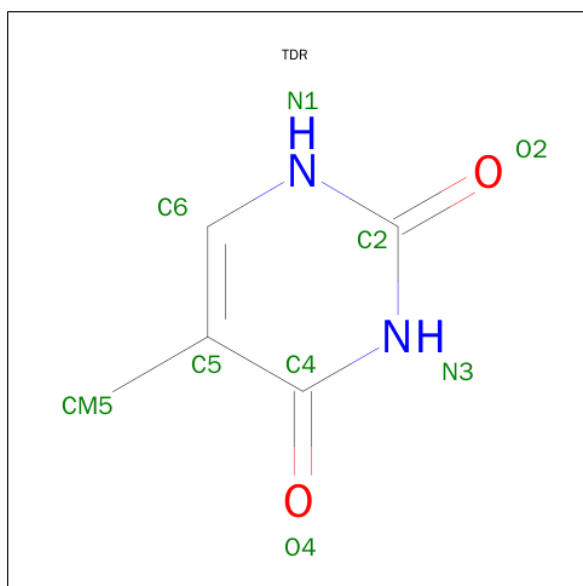
There are 12 discrepancies between the modelled and reference sequences:

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 2 2	0	0

- Molecule 4 is THYMINE (three-letter code: TDR) (formula: $C_5H_6N_2O_2$).



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

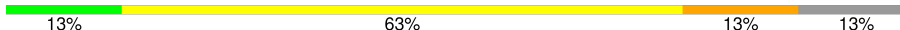
- Molecule 5 is water.

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

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 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: 




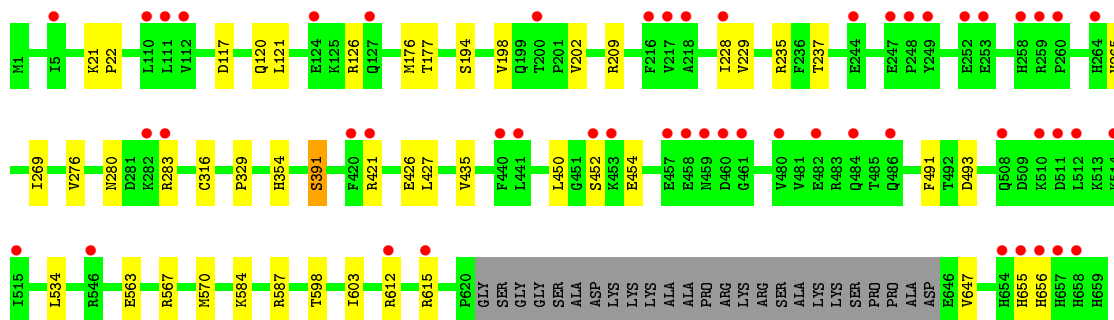
- Molecule 1: 5'-D(*CP*GP*CP*AP*AP*CP*TP*T)-3'

Chain D: 




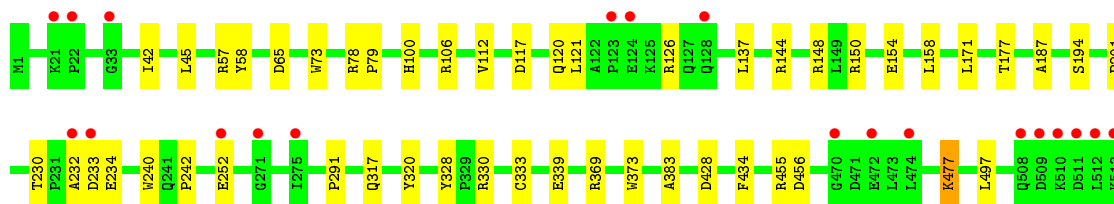
- Molecule 2: DNA topoisomerase 3

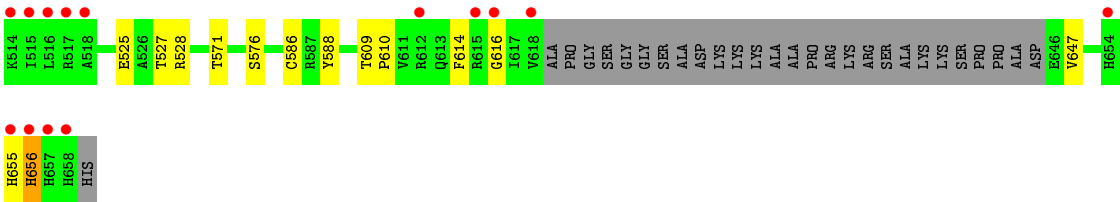
Chain A: 



- 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	102.21Å 102.21Å 443.75Å 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 2.36Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.245 0.200 , 0.236	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)	0.34 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 95012 reflections	Xtriage
F_o, F_c correlation	0.95	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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 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	C	138	0	80	1	0
1	D	138	0	80	2	0
2	A	5042	0	5042	28	0
2	B	5020	0	5023	36	0
3	A	2	0	0	0	0
4	D	9	0	6	0	0
5	A	176	0	0	2	0
5	B	158	0	0	0	0
5	C	13	0	0	1	0
5	D	9	0	0	0	0
All	All	10705	0	10231	66	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 3.

All (66) 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:B:477:LYS:NZ	2:B:477:LYS:CE	1.76	1.47
2:A:176:MET:CE	2:A:603:ILE:HD13	2.16	0.76
2:A:121:LEU:HD21	2:A:126:ARG:HD3	1.68	0.74
2:B:477:LYS:CD	2:B:477:LYS:NZ	2.53	0.72
2:A:117:ASP:HB3	2:A:647:VAL:HG13	1.72	0.71
2:B:230:THR:HG22	2:B:232:ALA:H	1.58	0.68
2:B:588:TYR:HB3	2:B:656:HIS:HE1	1.59	0.66
2:B:201:PRO:HG2	2:B:571:THR:HG21	1.80	0.63
2:A:209:ARG:HG3	2:A:491:PHE:CE2	2.34	0.62
2:A:283:ARG:HG3	2:A:421:ARG:HE	1.65	0.62
2:B:588:TYR:HB3	2:B:656:HIS:CE1	2.36	0.61
2:B:586:CYS:O	2:B:655:HIS:HE1	1.86	0.58
2:B:106:ARG:HG3	2:B:158:LEU:HG	1.86	0.57
2:B:317:GLN:HE22	2:B:330:ARG:HH11	1.54	0.55
2:A:176:MET:HE2	2:A:603:ILE:CD1	2.36	0.55
2:A:584:LYS:HA	2:A:655:HIS:HE1	1.73	0.54
2:B:144:ARG:O	2:B:148:ARG:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:ASP:HB3	2:B:647:VAL:HG13	1.91	0.52
2:A:450:LEU:HB3	2:A:454:GLU:HG3	1.93	0.50
2:A:656:HIS:CD2	5:A:863:HOH:O	2.63	0.50
2:B:42:ILE:H	2:B:45:LEU:HD21	1.76	0.50
2:B:73:TRP:HH2	2:B:171:LEU:HG	1.77	0.50
2:B:240:TRP:HB2	2:B:434:PHE:CE2	2.46	0.50
2:B:100:HIS:CE1	2:B:112:VAL:HB	2.46	0.49
2:B:230:THR:HB	2:B:234:GLU:HB2	1.95	0.49
2:B:137:LEU:HD13	2:B:320:TYR:CZ	2.47	0.49
2:B:525:GLU:HG2	2:B:528:ARG:NH1	2.27	0.49
2:B:317:GLN:NE2	2:B:330:ARG:HH11	2.10	0.49
5:C:10:HOH:O	2:A:534:LEU:HD13	2.13	0.49
2:A:229:VAL:HG21	2:A:235:ARG:HH21	1.77	0.49
2:B:177:THR:HG23	2:B:194:SER:HA	1.94	0.48
2:A:354:HIS:HE1	2:A:391:SER:O	1.96	0.47
2:A:587:ARG:HD2	5:A:871:HOH:O	2.15	0.47
2:B:333:CYS:O	2:B:383:ALA:HA	2.13	0.47
2:A:587:ARG:HD2	2:A:656:HIS:CD2	2.48	0.47
2:B:328:TYR:CZ	2:B:330:ARG:HB2	2.50	0.47
2:A:177:THR:HG23	2:A:194:SER:HA	1.98	0.46
2:B:455:ARG:NH1	2:B:456:ASP:OD1	2.49	0.46
2:A:176:MET:CE	2:A:603:ILE:CD1	2.87	0.45
2:B:252:GLU:H	2:B:252:GLU:CD	2.19	0.45
2:B:240:TRP:O	2:B:242:PRO:HD3	2.18	0.44
2:B:57:ARG:NH1	2:B:65:ASP:OD1	2.51	0.44
2:B:187:ALA:CB	2:B:614:PHE:HB2	2.47	0.44
1:D:5:DA:C6	1:D:7:DT:H1'	2.52	0.43
2:B:121:LEU:HD23	2:B:126:ARG:HG2	2.00	0.43
2:A:426:GLU:HG2	2:A:435:VAL:HG22	2.00	0.43
2:A:316:CYS:HB3	2:A:329:PRO:CB	2.48	0.43
2:A:612:ARG:HA	2:A:615:ARG:HE	1.83	0.43
2:B:588:TYR:H	2:B:656:HIS:HE1	1.67	0.43
2:A:570:MET:SD	2:A:598:THR:HG21	2.58	0.43
1:C:1:DC:H2''	1:C:2:DG:H5'	2.00	0.42
2:B:291:PRO:HB2	2:B:383:ALA:HB1	2.02	0.42
2:A:563:GLU:HG2	2:A:567:ARG:HG2	2.02	0.42
2:A:265:VAL:O	2:A:269:ILE:HG12	2.19	0.42
2:B:150:ARG:HD2	2:B:154:GLU:OE1	2.20	0.42
2:B:369:ARG:HG3	2:B:373:TRP:CD1	2.55	0.42
1:D:5:DA:C2'	2:B:527:THR:HG21	2.50	0.41
2:B:78:ARG:HA	2:B:79:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:THR:HA	2:B:610:PRO:HD3	1.88	0.41
2:A:21:LYS:HB3	2:A:22:PRO:HA	2.02	0.41
2:A:121:LEU:H	2:A:121:LEU:HD23	1.86	0.41
2:A:587:ARG:HB3	2:A:656:HIS:CD2	2.55	0.41
2:B:57:ARG:NH1	2:B:58:TYR:HE1	2.18	0.41
2:A:276:VAL:HA	2:A:427:LEU:HD23	2.03	0.41
2:A:198:VAL:O	2:A:202:VAL:HG23	2.21	0.41
2:A:228:ILE:HD13	2:A:427:LEU:HD13	2.04	0.40

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	
2	A	630/659 (96%)	618 (98%)	10 (2%)	2 (0%)	46	55
2	B	627/659 (95%)	614 (98%)	12 (2%)	1 (0%)	52	63
All	All	1257/1318 (95%)	1232 (98%)	22 (2%)	3 (0%)	52	63

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 [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	
2	A	538/555 (97%)	534 (99%)	4 (1%)	88	95
2	B	536/555 (97%)	529 (99%)	7 (1%)	76	87
All	All	1074/1110 (97%)	1063 (99%)	11 (1%)	82	91

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
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. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	655	HIS
2	B	317	GLN
2	B	655	HIS
2	B	656	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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	-	5,9,9	0.49	0	7,12,12	5.98	5 (71%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	799	TDR	N1-C2-N3	-10.26	121.79	128.33
4	D	799	TDR	C5-C6-N1	-6.45	119.47	125.23
4	D	799	TDR	C5-C4-N3	-6.32	118.10	125.14
4	D	799	TDR	C6-N1-C2	4.07	122.02	115.47
4	D	799	TDR	C4-N3-C2	6.59	120.94	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	-0.33	0 100 100	26, 28, 38, 51	0
1	D	7/8 (87%)	-0.23	0 100 100	29, 34, 46, 62	0
2	A	634/659 (96%)	0.32	52 (8%) 14 23	26, 43, 95, 139	0
2	B	631/659 (95%)	0.22	34 (5%) 29 44	27, 49, 95, 140	0
All	All	1279/1334 (95%)	0.26	86 (6%) 21 31	26, 46, 95, 140	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	657	HIS	9.5
2	A	657	HIS	6.3
2	A	656	HIS	6.2
2	B	515	ILE	5.8
2	B	656	HIS	5.8
2	A	658	HIS	5.6
2	B	654	HIS	5.5
2	B	514	LYS	5.0
2	A	249	TYR	4.8
2	B	124	GLU	4.5
2	B	508	GLN	4.5
2	A	452	SER	4.4
2	A	440	PHE	4.3
2	B	618	VAL	4.3
2	A	515	ILE	4.2
2	B	512	LEU	3.9
2	B	612	ARG	3.9
2	A	264	HIS	3.8
2	A	460	ASP	3.7
2	A	248	PRO	3.7
2	B	123	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	517	ARG	3.6
2	A	252	GLU	3.6
2	B	615	ARG	3.5
2	A	514	LYS	3.5
2	A	258	HIS	3.3
2	A	457	GLU	3.3
2	A	453	LYS	3.2
2	A	512	LEU	3.2
2	A	546	ARG	3.1
2	B	22	PRO	3.1
2	B	511	ASP	3.1
2	B	271	GLY	3.1
2	B	518	ALA	3.1
2	A	461	GLY	3.0
2	A	486	GLN	3.0
2	A	260	PRO	3.0
2	A	124	GLU	3.0
2	A	253	GLU	2.9
2	B	472	GLU	2.9
2	B	513	LYS	2.9
2	B	509	ASP	2.9
2	B	474	LEU	2.8
2	A	511	ASP	2.8
2	A	482	GLU	2.8
2	A	216	PHE	2.7
2	A	612	ARG	2.7
2	A	218	ALA	2.6
2	A	441	LEU	2.6
2	A	508	GLN	2.6
2	A	283	ARG	2.6
2	A	421	ARG	2.6
2	B	128	GLN	2.6
2	A	458	GLU	2.5
2	B	616	GLY	2.5
2	B	655	HIS	2.5
2	A	615	ARG	2.5
2	A	654	HIS	2.5
2	B	21	LYS	2.5
2	A	480	VAL	2.5
2	A	459	ASN	2.5
2	B	510	LYS	2.4
2	A	127	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	510	LYS	2.4
2	A	420	PHE	2.4
2	A	484	GLN	2.4
2	B	470	GLY	2.3
2	A	5	ILE	2.3
2	A	244	GLU	2.3
2	A	200	THR	2.3
2	B	275	ILE	2.3
2	B	658	HIS	2.2
2	A	247	GLU	2.2
2	B	252	GLU	2.2
2	B	516	LEU	2.2
2	B	233	ASP	2.2
2	A	217	VAL	2.2
2	A	259	ARG	2.2
2	A	110	LEU	2.1
2	B	33	GLY	2.1
2	A	112	VAL	2.1
2	A	655	HIS	2.1
2	A	111	LEU	2.1
2	A	228	ILE	2.1
2	B	232	ALA	2.0
2	A	282	LYS	2.0

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, 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
3	CL	A	800	1/1	0.99	0.11	-0.80	34,34,34,34	0
3	CL	A	801	1/1	0.99	0.10	-1.13	40,40,40,40	0
4	TDR	D	799	9/9	0.61	0.23	-	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.