



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TFY
Title : How CCA is added to the 3' end of immature tRNA without the use of an oligonucleotide template
Authors : Xiong, Y.; Steitz, T.A.
Deposited on : 2004-05-27
Resolution : 3.20 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 (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

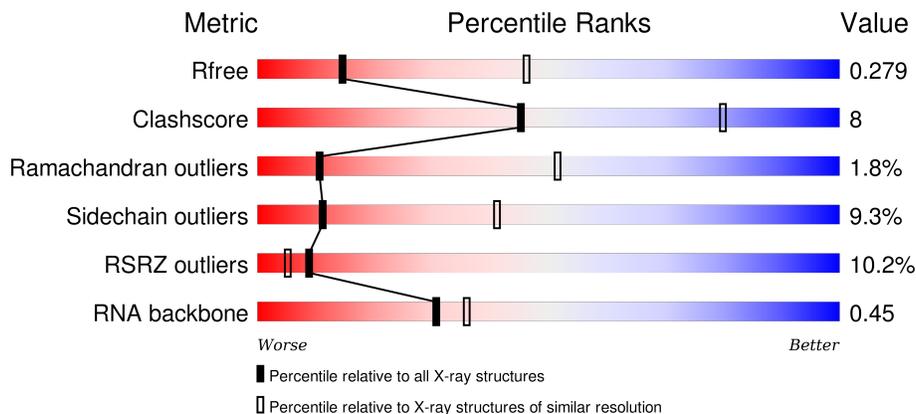
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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	E	13	Upper red bar: 23% Lower bar: 62% (green), 31% (yellow), 8% (red)
1	F	13	Lower bar: 46% (green), 54% (yellow)
2	H	14	Upper red bar: 29% Lower bar: 57% (green), 21% (yellow), 7% (orange), 14% (red)
2	I	14	Upper red bar: 14% Lower bar: 36% (green), 57% (yellow), 7% (orange)

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Mol	Chain	Length	Quality of chain
3	G	11	<p>9% 27% 27% 36%</p>
4	J	8	<p>13% 63% 75% 13%</p>
5	A	437	<p>7% 79% 17% .</p>
5	B	437	<p>14% 76% 21% .</p>
5	C	437	<p>6% 72% 23% . .</p>
5	D	437	<p>10% 75% 22% .</p>

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 16180 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 RNA chain called 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	13	Total	C	N	O	P	0	0	0
			276	124	51	89	12			
1	F	13	Total	C	N	O	P	0	0	0
			276	124	51	89	12			

- Molecule 2 is a RNA chain called 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*P*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	H	14	Total	C	N	O	P	0	0	0
			295	133	54	95	13			
2	I	14	Total	C	N	O	P	0	0	0
			295	133	54	95	13			

- Molecule 3 is a RNA chain called 5'-R(*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	G	11	Total	C	N	O	P	0	0	0
			230	104	42	74	10			

- Molecule 4 is a RNA chain called 5'-R(*CP*GP*CP*GP*GP*AP*UP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	J	8	Total	C	N	O	P	0	0	0
			168	76	31	54	7			

- Molecule 5 is a protein called tRNA nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	A	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			

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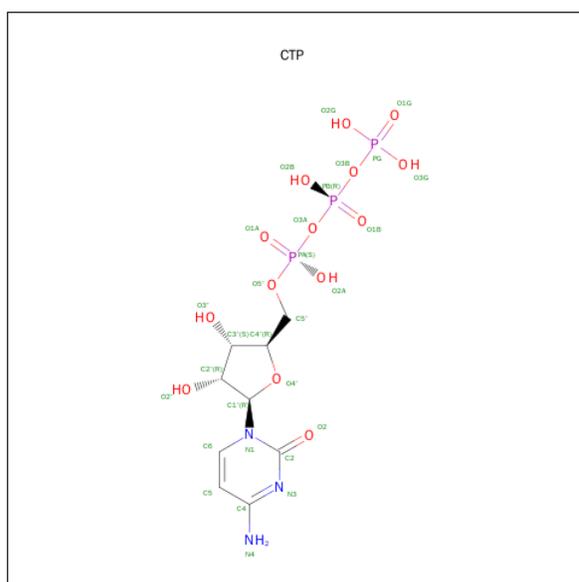
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	C	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	D	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: C₉H₁₆N₃O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
7	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
7	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

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.

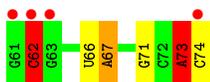
- Molecule 1: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*G)-3'



- Molecule 1: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*G)-3'



- Molecule 2: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*AP*C)-3'



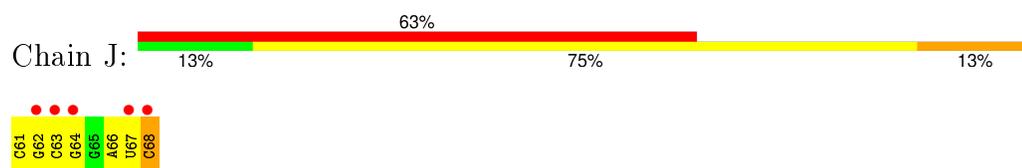
- Molecule 2: 5'-R(*GP*CP*GP*GP*AP*UP*AP*UP*CP*CP*GP*CP*AP*C)-3'



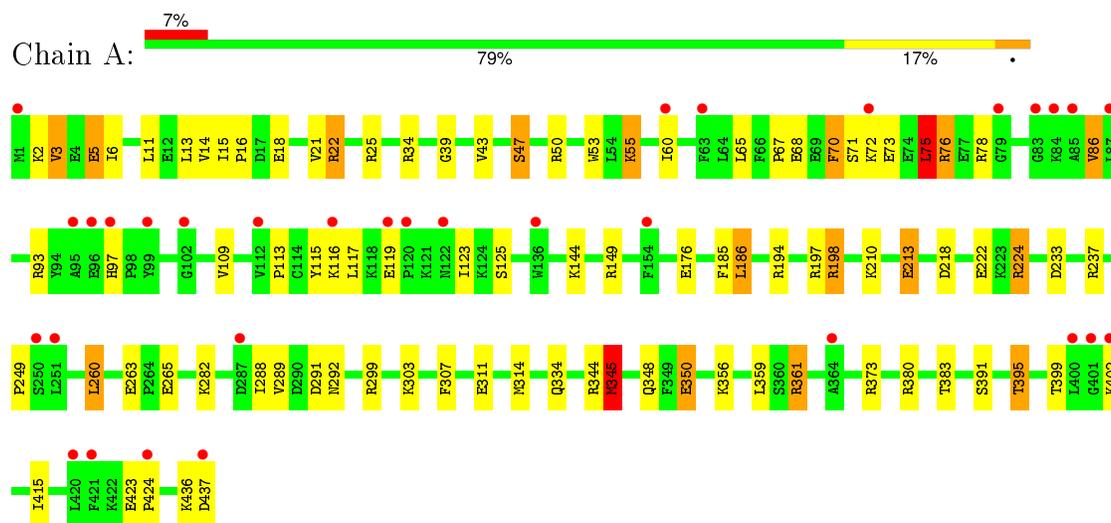
- Molecule 3: 5'-R(*CP*GP*GP*AP*UP*CP*CP*GP*CP*AP*C)-3'



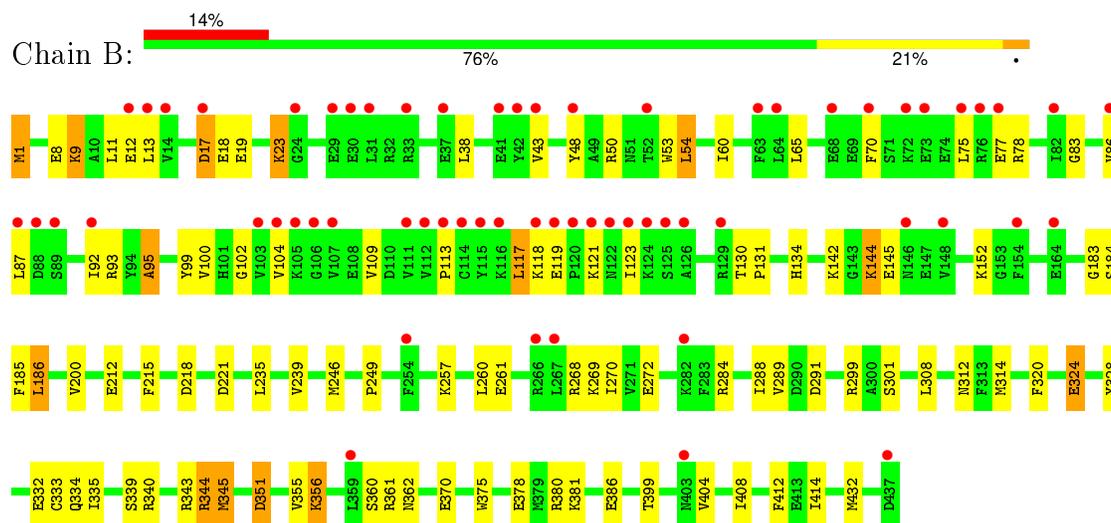
- Molecule 4: 5'-R(*CP*GP*CP*GP*GP*AP*UP*C)-3'



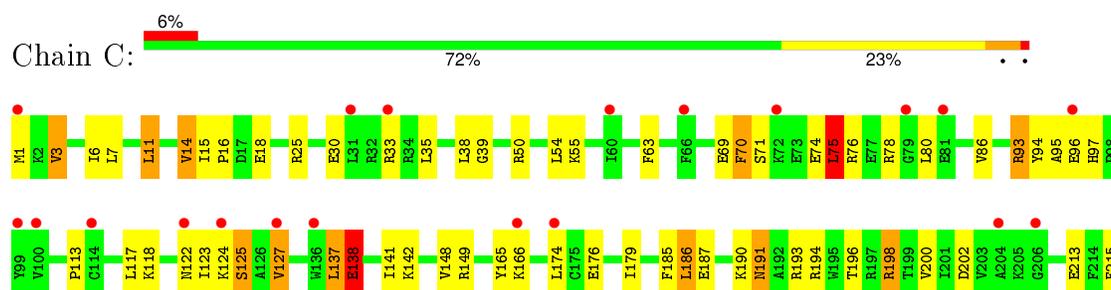
- Molecule 5: tRNA nucleotidyltransferase

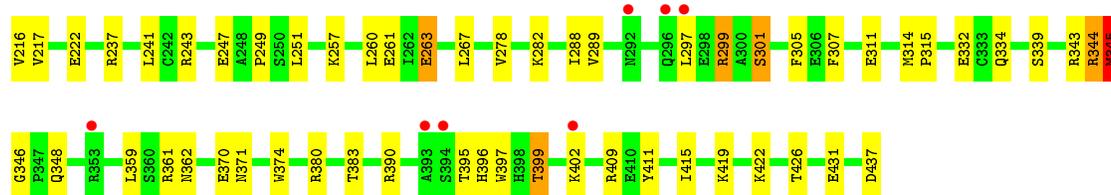


- Molecule 5: tRNA nucleotidyltransferase

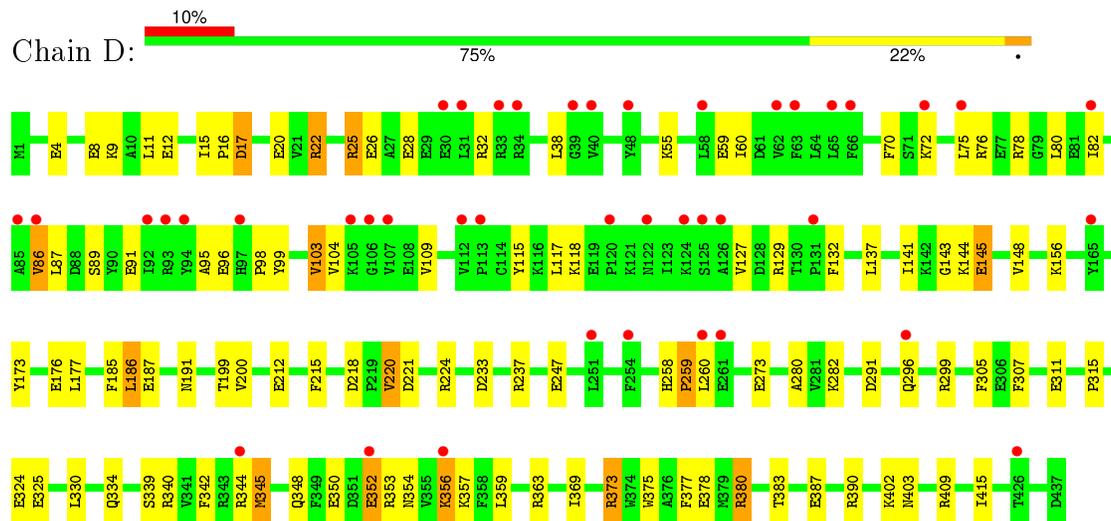


- Molecule 5: tRNA nucleotidyltransferase





• Molecule 5: tRNA nucleotidyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.09Å 84.02Å 134.56Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	44.28 – 3.20 44.18 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.28-3.20) 98.8 (44.18-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.235 , 0.290 0.226 , 0.279	Depositor DCC
R_{free} test set	2053 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	103.6	Xtrriage
Anisotropy	0.098	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 124.1	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Outliers	0 of 40914 reflections	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16180	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	E	0.67	0/308	1.26	2/479 (0.4%)
1	F	0.72	0/308	1.17	0/479
2	H	0.78	0/329	1.39	3/511 (0.6%)
2	I	0.77	0/329	1.40	3/511 (0.6%)
3	G	0.99	1/256 (0.4%)	1.95	12/397 (3.0%)
4	J	0.77	0/187	1.46	1/290 (0.3%)
5	A	0.35	0/3713	0.52	1/4987 (0.0%)
5	B	0.36	0/3713	0.51	0/4987
5	C	0.36	0/3713	0.53	1/4987 (0.0%)
5	D	0.38	0/3713	0.53	0/4987
All	All	0.43	1/16569 (0.0%)	0.70	23/22615 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	13	C	C1'-N1	5.26	1.56	1.48

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5	G	P-O3'-C3'	-11.56	105.83	119.70
3	G	8	C	P-O3'-C3'	-9.96	107.75	119.70
3	G	6	A	P-O3'-C3'	-6.96	111.35	119.70
3	G	7	U	C5'-C4'-O4'	6.75	117.20	109.10
4	J	68	C	O4'-C1'-N1	6.46	113.37	108.20

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	E	276	0	143	4	0
1	F	276	0	143	3	0
2	H	295	0	154	3	0
2	I	295	0	154	2	0
3	G	230	0	122	12	0
4	J	168	0	89	11	0
5	A	3630	0	3633	60	0
5	B	3630	0	3633	55	0
5	C	3630	0	3633	71	0
5	D	3630	0	3633	60	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	29	0	12	0	0
7	B	29	0	12	0	0
7	C	29	0	12	0	0
7	D	29	0	12	1	0
All	All	16180	0	15385	244	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 8.

The worst 5 of 244 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)
5:A:198:ARG:HH11	5:A:198:ARG:HG2	1.02	1.11
5:A:198:ARG:NH1	5:A:198:ARG:HG2	1.78	0.89
5:C:395:THR:HG23	5:C:396:HIS:HD2	1.40	0.87
5:D:132:PHE:HB3	5:D:220:VAL:HG21	1.55	0.87
5:D:22:ARG:HE	5:D:25:ARG:HG2	1.39	0.87

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	
5	A	435/437 (100%)	404 (93%)	23 (5%)	8 (2%)	11	51
5	B	435/437 (100%)	395 (91%)	32 (7%)	8 (2%)	11	51
5	C	435/437 (100%)	403 (93%)	23 (5%)	9 (2%)	9	46
5	D	435/437 (100%)	390 (90%)	39 (9%)	6 (1%)	14	57
All	All	1740/1748 (100%)	1592 (92%)	117 (7%)	31 (2%)	11	51

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	72	LYS
5	A	186	LEU
5	B	186	LEU
5	C	70	PHE
5	C	117	LEU

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	
5	A	387/387 (100%)	355 (92%)	32 (8%)	14	49
5	B	387/387 (100%)	354 (92%)	33 (8%)	13	47
5	C	387/387 (100%)	341 (88%)	46 (12%)	6	28
5	D	387/387 (100%)	354 (92%)	33 (8%)	13	47
All	All	1548/1548 (100%)	1404 (91%)	144 (9%)	11	41

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	1	MET
5	C	127	VAL
5	D	299	ARG
5	C	11	LEU
5	C	75	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	97	HIS
5	B	312	ASN
5	C	362	ASN
5	A	396	HIS
5	C	334	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	12/13 (92%)	1 (8%)	0
1	F	12/13 (92%)	3 (25%)	0
2	H	13/14 (92%)	4 (30%)	1 (7%)
2	I	13/14 (92%)	4 (30%)	1 (7%)
3	G	10/11 (90%)	6 (60%)	0
4	J	7/8 (87%)	1 (14%)	0
All	All	67/73 (91%)	19 (28%)	2 (2%)

5 of 19 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	12	C
2	H	62	C
2	H	67	A
2	H	71	G
2	H	74	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	73	A

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Mol	Chain	Res	Type
2	I	73	A

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
7	CTP	A	501	6	21,30,30	0.81	0	31,47,47	1.18	3 (9%)
7	CTP	B	502	6	21,30,30	0.69	0	31,47,47	1.29	3 (9%)
7	CTP	C	503	6	21,30,30	0.86	2 (9%)	31,47,47	1.44	5 (16%)
7	CTP	D	504	6	21,30,30	0.75	0	31,47,47	1.30	3 (9%)

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
7	CTP	A	501	6	-	0/18/38/38	0/2/2/2
7	CTP	B	502	6	-	0/18/38/38	0/2/2/2
7	CTP	C	503	6	-	0/18/38/38	0/2/2/2
7	CTP	D	504	6	-	0/18/38/38	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	503	CTP	C6-N1	2.00	1.38	1.35
7	C	503	CTP	O4'-C1'	2.09	1.43	1.41

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	504	CTP	PB-O3B-PG	-3.84	119.80	132.67
7	D	504	CTP	PB-O3A-PA	-3.64	122.50	132.73
7	B	502	CTP	PB-O3B-PG	-3.32	121.55	132.67
7	A	501	CTP	PB-O3A-PA	-2.98	124.36	132.73
7	B	502	CTP	PB-O3A-PA	-2.71	125.12	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	504	CTP	1	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	E	13/13 (100%)	1.24	3 (23%) 1 1	130, 131, 132, 132	0
1	F	13/13 (100%)	1.83	6 (46%) 0 0	130, 131, 131, 132	0
2	H	14/14 (100%)	1.42	4 (28%) 1 0	129, 131, 133, 134	0
2	I	14/14 (100%)	1.56	2 (14%) 4 2	130, 131, 133, 133	0
3	G	11/11 (100%)	1.63	3 (27%) 1 0	130, 131, 132, 132	0
4	J	8/8 (100%)	2.17	5 (62%) 0 0	129, 130, 131, 131	0
5	A	437/437 (100%)	0.41	32 (7%) 18 10	130, 131, 132, 133	0
5	B	437/437 (100%)	0.76	62 (14%) 4 2	130, 131, 132, 132	0
5	C	437/437 (100%)	0.40	27 (6%) 24 13	130, 131, 132, 133	0
5	D	437/437 (100%)	0.65	42 (9%) 10 6	130, 131, 132, 132	0
All	All	1821/1821 (100%)	0.60	186 (10%) 9 5	129, 131, 132, 134	0

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	61	G	8.7
5	D	92	ILE	7.6
5	C	72	LYS	7.2
5	B	107	VAL	7.1
5	D	94	TYR	7.0

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(Å ²)	Q<0.9
7	CTP	C	503	29/29	0.75	0.29	0.28	134,135,137,138	0
7	CTP	A	501	29/29	0.73	0.30	0.12	134,135,138,138	0
7	CTP	B	502	29/29	0.90	0.21	-0.72	132,132,133,133	0
7	CTP	D	504	29/29	0.91	0.24	-0.74	131,131,132,132	0
6	MG	C	603	1/1	0.87	0.16	-	109,109,109,109	0
6	MG	A	601	1/1	0.64	0.33	-	117,117,117,117	0
6	MG	B	602	1/1	0.82	0.22	-	95,95,95,95	0
6	MG	D	604	1/1	0.90	0.19	-	102,102,102,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.