



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:04 AM GMT

PDB ID : 3H3A
Title : The complex structure of CCA-adding enzyme with CTP
Authors : Toh, Y.; Tomita, K.
Deposited on : 2009-04-16
Resolution : 2.80 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

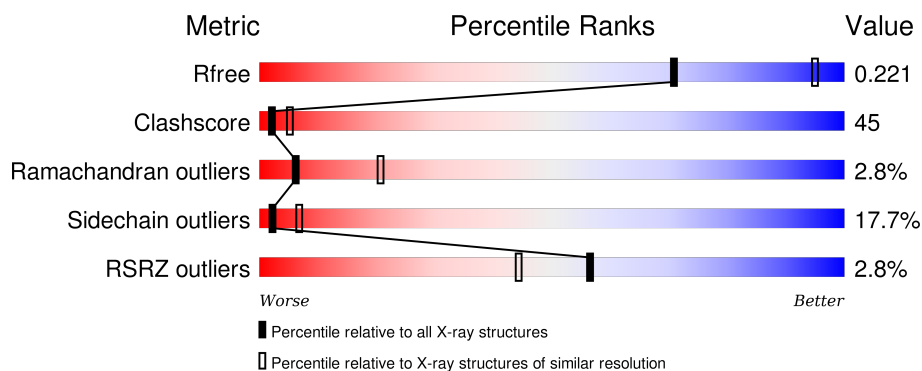
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	441	<div> <div>37%</div> <div>44%</div> <div>13%</div> <div>• 5%</div> </div>
1	B	441	<div> <div>4%</div> <div>43%</div> <div>39%</div> <div>12%</div> <div>• 5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6942 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 protein called TRNA nucleotidyl transferase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3426	2213	580	622	11			
1	B	418	Total	C	N	O	S	0	0	0
			3441	2222	583	625	11			

There are 28 discrepancies between the modelled and reference sequences:

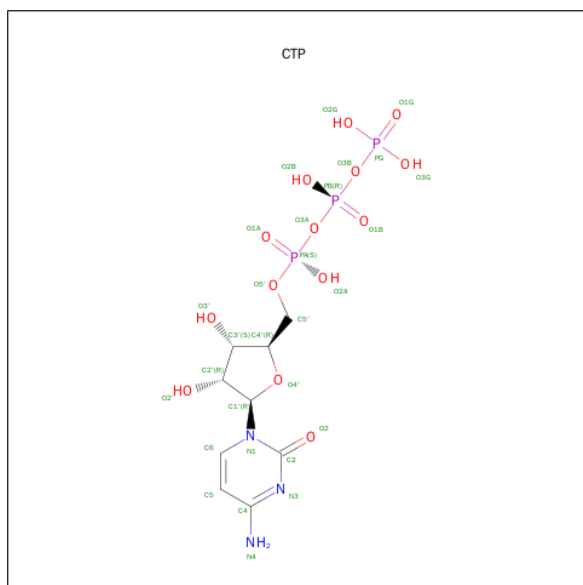
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9WZH4
A	429	LYS	-	EXPRESSION TAG	UNP Q9WZH4
A	430	LEU	-	EXPRESSION TAG	UNP Q9WZH4
A	431	ALA	-	EXPRESSION TAG	UNP Q9WZH4
A	432	ALA	-	EXPRESSION TAG	UNP Q9WZH4
A	433	ALA	-	EXPRESSION TAG	UNP Q9WZH4
A	434	LEU	-	EXPRESSION TAG	UNP Q9WZH4
A	435	GLU	-	EXPRESSION TAG	UNP Q9WZH4
A	436	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	437	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	438	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	439	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	440	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	441	HIS	-	EXPRESSION TAG	UNP Q9WZH4
B	1	MET	-	EXPRESSION TAG	UNP Q9WZH4
B	429	LYS	-	EXPRESSION TAG	UNP Q9WZH4
B	430	LEU	-	EXPRESSION TAG	UNP Q9WZH4
B	431	ALA	-	EXPRESSION TAG	UNP Q9WZH4
B	432	ALA	-	EXPRESSION TAG	UNP Q9WZH4
B	433	ALA	-	EXPRESSION TAG	UNP Q9WZH4
B	434	LEU	-	EXPRESSION TAG	UNP Q9WZH4
B	435	GLU	-	EXPRESSION TAG	UNP Q9WZH4
B	436	HIS	-	EXPRESSION TAG	UNP Q9WZH4
B	437	HIS	-	EXPRESSION TAG	UNP Q9WZH4
B	438	HIS	-	EXPRESSION TAG	UNP Q9WZH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	439	HIS	-	EXPRESSION TAG	UNP Q9WZH4
B	440	HIS	-	EXPRESSION TAG	UNP Q9WZH4
B	441	HIS	-	EXPRESSION TAG	UNP Q9WZH4

- Molecule 2 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



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

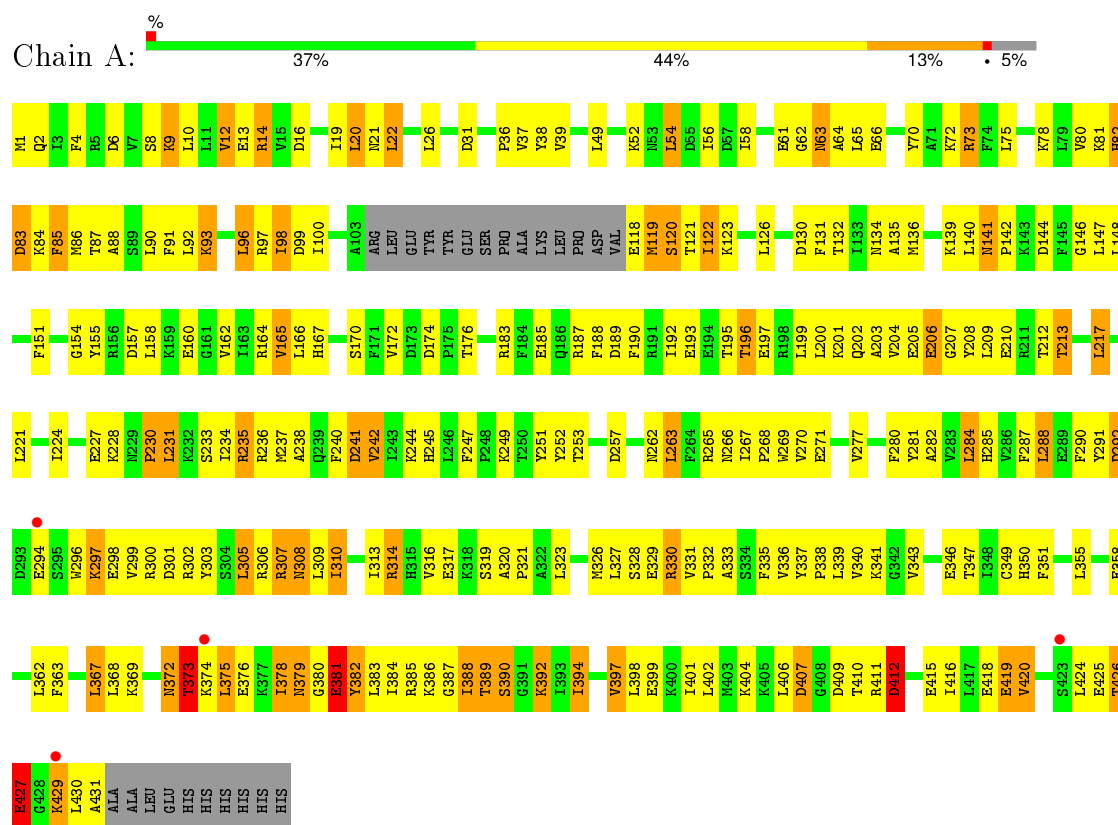
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	11	Total	O	0	0
			11	11		

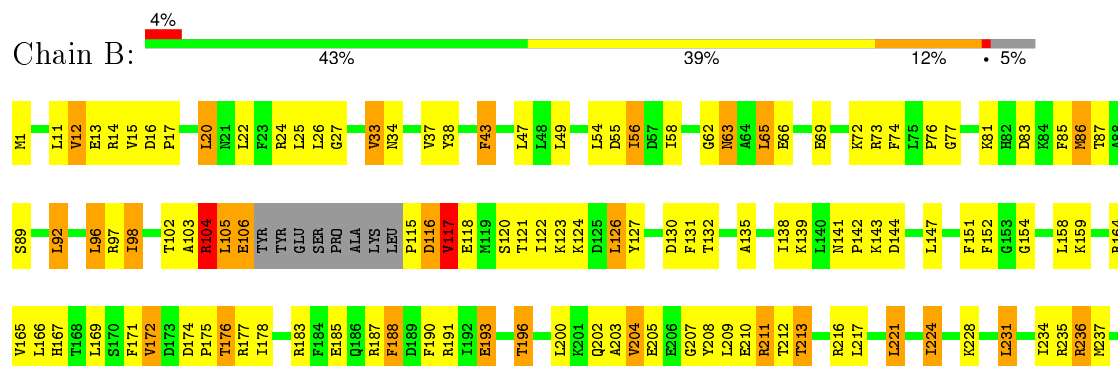
3 Residue-property plots

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: TRNA nucleotidyl transferase-related protein



- Molecule 1: TRNA nucleotidyl transferase-related protein



I394	S328	F240
I398	E329	D241
E399	R330	
K400	V331	H245
I401	P332	L246
L402	F335	F247
M403	V336	P248
	Y337	K249
L406	P338	T250
	I339	T253
T410	V340	P254
R411	K341	
D412	G342	D257
E413	V343	
E414	S344	L267
E415	R345	P268
I416	E346	W269
I417	T347	
E418	I348	E272
E419	G349	N273
V420	R350	F274
L421	F351	G275
A422	L352	E276
S423	A353	
L424	Y354	L284
E425	L355	H285
T426	E360	V286
GLU		F287
GLY	G361	L288
LYS		E289
LEU	K364	F290
ALA	S365	
ALA	Y366	D293
ALA	L367	E294
LEU	L368	S295
GLU	K369	W296
HIS		K297
HIS	N372	E298
HIS	T373	V299
HIS	K374	R300
HIS	L375	
HIS	E376	R307
HIS	K377	I308
	I378	L309
	N379	I310
	G380	
	E381	R314
	Y382	H315
	L383	Y316
	I384	E317
	R385	
	K386	A320
	G387	P321
	I388	A322
	T389	L323
	S390	L324
	G391	E325
	K392	H326
	I393	L327

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.45Å 63.59Å 152.58Å 90.00° 103.31° 90.00°	Depositor
Resolution (Å)	31.79 – 2.80 31.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (31.79-2.80) 95.4 (31.79-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.234 , 0.269 0.227 , 0.221	Depositor DCC
R_{free} test set	2100 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42184 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6942	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: 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	A	0.47	0/3487	0.74	6/4684 (0.1%)
1	B	0.47	0/3503	0.70	4/4707 (0.1%)
All	All	0.47	0/6990	0.72	10/9391 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ASP	CB-CA-C	-9.88	90.64	110.40
1	A	373	THR	CB-CA-C	-9.25	86.62	111.60
1	B	331	VAL	CB-CA-C	-8.81	94.65	111.40
1	A	381	GLU	N-CA-C	8.54	134.05	111.00
1	A	381	GLU	CB-CA-C	-6.98	96.45	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3426	0	3525	345	1
1	B	3441	0	3538	286	0
2	A	29	0	12	1	0
2	B	29	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	0	0	0
3	B	11	0	0	0	0
All	All	6942	0	7087	630	1

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 45.

The worst 5 of 630 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:B:272:GLU:C	1:B:273:ASN:HD22	1.33	1.28
1:B:401:ILE:CD1	1:B:416:ILE:HG12	1.72	1.20
1:A:90:LEU:HB3	1:A:98:ILE:HD11	1.23	1.18
1:B:375:LEU:N	1:B:375:LEU:HD23	1.59	1.18
1:A:90:LEU:CB	1:A:98:ILE:HD11	1.73	1.17

All (1) 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)
1:A:281:TYR:OH	1:A:382:TYR:OH[4_546]	2.08	0.12

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	
1	A	413/441 (94%)	356 (86%)	43 (10%)	14 (3%)	5	16
1	B	414/441 (94%)	371 (90%)	34 (8%)	9 (2%)	8	28
All	All	827/882 (94%)	727 (88%)	77 (9%)	23 (3%)	6	21

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	SER
1	A	373	THR
1	A	381	GLU
1	A	388	ILE
1	B	341	LYS

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	374/395 (95%)	308 (82%)	66 (18%)	2	7
1	B	377/395 (95%)	310 (82%)	67 (18%)	2	6
All	All	751/790 (95%)	618 (82%)	133 (18%)	2	7

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	ASP
1	B	63	ASN
1	B	375	LEU
1	A	409	ASP
1	B	12	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	ASN
1	B	82	HIS
1	B	266	ASN
1	A	266	ASN
1	A	350	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 ⓘ

2 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	$\# Z > 2$
2	CTP	A	501	-	21,30,30	0.79	0	31,47,47	1.60	3 (9%)
2	CTP	B	502	-	21,30,30	0.79	0	31,47,47	1.60	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
2	CTP	A	501	-	-	0/18/38/38	0/2/2/2
2	CTP	B	502	-	-	0/18/38/38	0/2/2/2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	CTP	PB-O3B-PG	-5.01	115.86	132.67
2	B	502	CTP	PB-O3B-PG	-5.00	115.89	132.67
2	B	502	CTP	PB-O3A-PA	-3.96	121.61	132.73
2	A	501	CTP	PB-O3A-PA	-3.95	121.64	132.73
2	B	502	CTP	C2-N3-C4	2.63	119.32	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CTP	1	0
2	B	502	CTP	2	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	417/441 (94%)	-0.31	4 (0%) 84 77	50, 121, 169, 215	0
1	B	418/441 (94%)	-0.17	19 (4%) 37 26	55, 94, 213, 319	0
All	All	835/882 (94%)	-0.24	23 (2%) 56 44	50, 109, 187, 319	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	6.3
1	B	414	GLU	4.6
1	B	426	THR	4.3
1	B	387	GLY	4.3
1	B	388	ILE	4.3

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
2	CTP	A	501	29/29	0.86	0.19	0.32	90,111,159,387	0
2	CTP	B	502	29/29	0.93	0.18	-0.16	90,111,159,387	0

6.5 Other polymers [i](#)

There are no such residues in this entry.