



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 03:19 pm GMT

PDB ID : 2AD5
Title : Mechanisms of feedback regulation and drug resistance of CTP synthetases: structure of the E. coli CTPS/CTP complex at 2.8-Angstrom resolution.
Authors : Endrizzi, J.A.; Kim, H.; Anderson, P.M.; Baldwin, E.P.
Deposited on : 2005-07-19
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

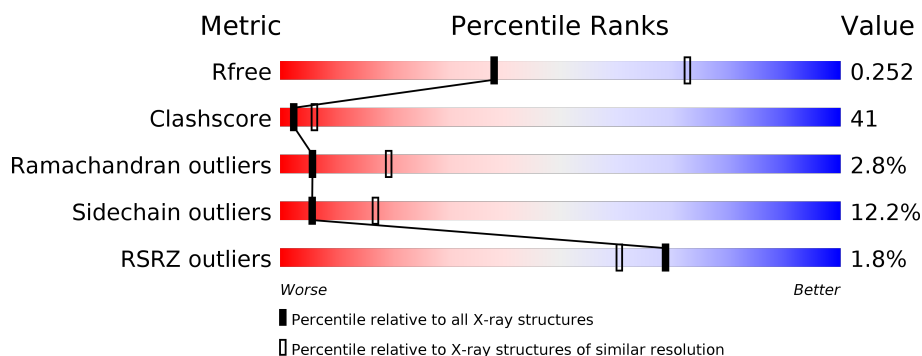
1 Overall quality at a glance

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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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	545	<div> <div>2%</div> <div> <div></div> <div>35%</div> <div>48%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	545	<div> <div>2%</div> <div> <div></div> <div>33%</div> <div>50%</div> <div>13%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8694 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 CTP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	16	0	0
			4156	2625	726	784	21			
1	B	536	Total	C	N	O	S	11	0	0
			4172	2636	729	786	21			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

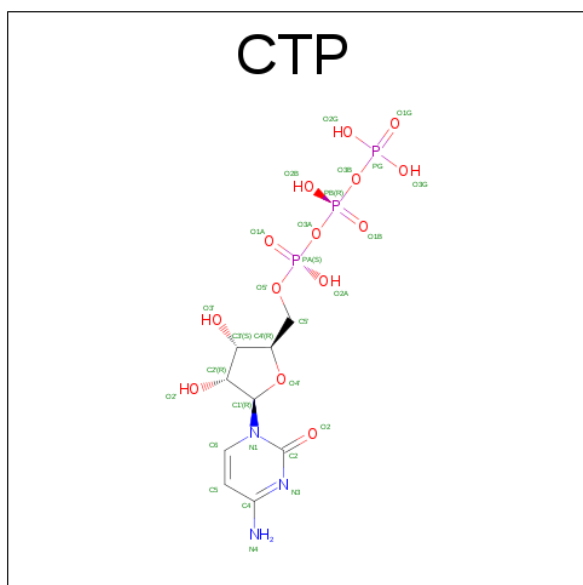
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



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

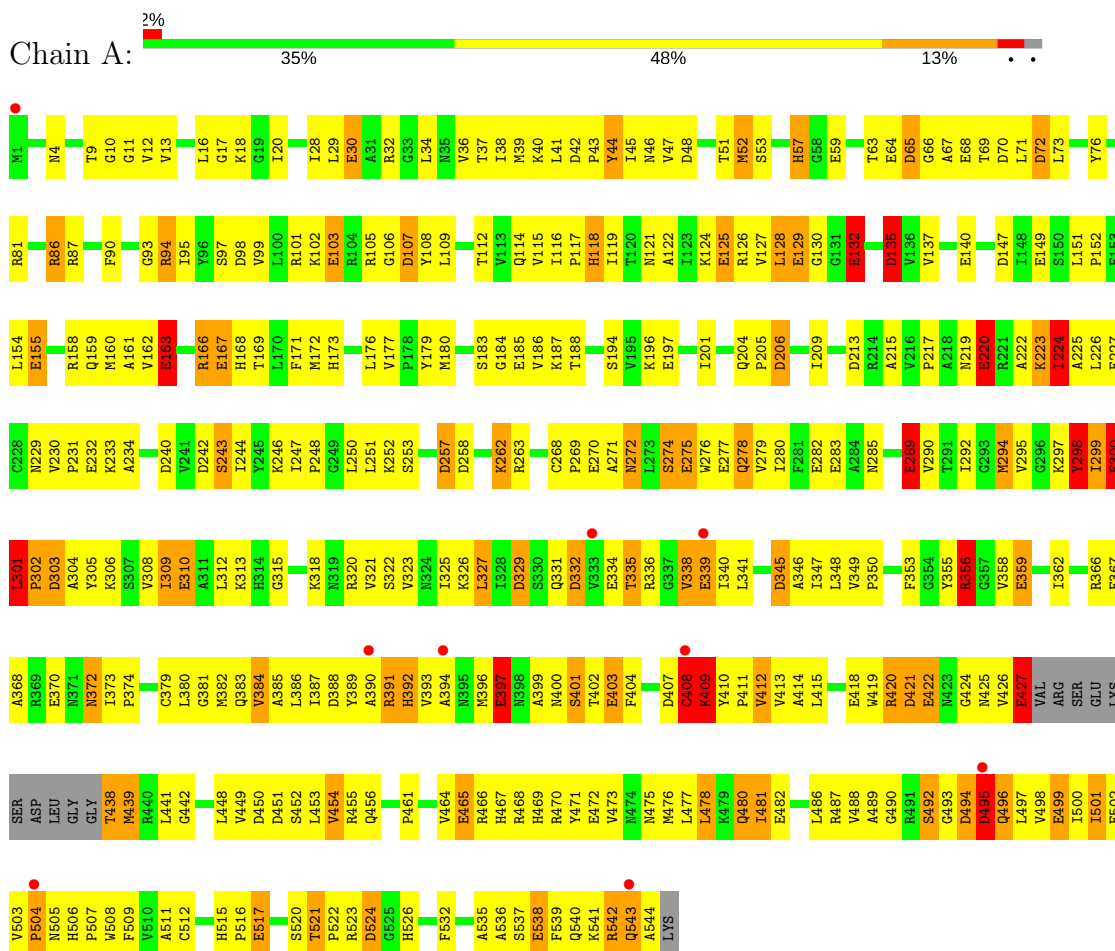
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	122	Total	O	0	0
			122	122		

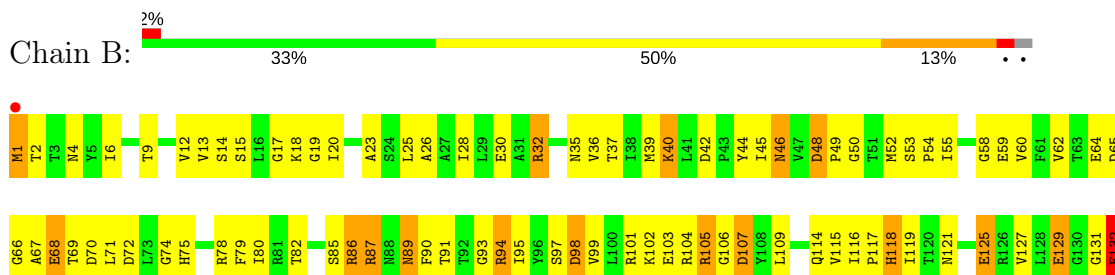
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: CTP synthase



• Molecule 1: CTP synthase



R487	G490	R491	S492	G493	D494	D495	Q496	L497	I500	I501	E502	V503	P504	N505	H506	P507	W508	F509	V510	A511	C512	Q513	F514	H515	P516	E517	F518	T519	S520	T521	P522	R523	D524	G525	H526	F527	L528	F529	A530	G531	F532	V533	K534	A535	A536	S537	E538	F539	Q540	K541	R542	Q543	A544	K545	
W419	R420	D421	R422	G423	G424	N425	V426	E427	V428	ARG	SER	GLU	LYS	SER	ASP	LEU	GLY	T438	M439	R440	L441	G442	A443	Q444	L448	V449	D450	D451	S452	L453	Y389	Y458	N459	A460	P461	E465	R466	H467	R468	H469	R470	Y471	E472	V473	N474	L477	L478	K479	Q480	I481	E482	D483	A484	G485	L486
G354	Y355	R356	G357	V358	E359	G360	R361	T362	T363	T364	A365	R366	F367	E370	N371	R372	T373	F374	Y375	C379	L380	G381	R382	Q383	V384	A385	L386	T387	D388	Y389	H392	V393	A394	R395	E397	N400	S401	T402	E403	F404	V405	P406	D407	C408	R409	Y410	P411	V412	V413	A414	L415	E418			
I280	F281	E282	E283	A284	N285	P286	V287	S288	E289	G293	M294	V295	G296	K297	E298	G299	I299	A234	L301	P302	D303	A304	Y305	K306	E310	K313	N319	R320	V321	S322	K326	L327	I328	D329	S330	Q331	D332	V333	E334	T335	R336	G337	V338	E339	I340	L341	K342	G343	L344	D345	A346	T347	L348	V349	P350
V216	P217	A218	N219	E220	R221	A222	K223	I224	A225	L226	F227	C228	L151	P152	M160	E163	I164	G165	R166	E167	H168	T169	L174	T175	L176	V177	P178	Y179	M180	A181	E185	V186	K187	T188	K189	P190	T191	Q192	H193	S194	E197	L198	I201	D206	I207	L208	N272	L273	I209	C210	R211	S212	D213	R214	A215

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.27Å 106.38Å 130.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 45.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 98.7 (45.42-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, R_{free}	0.202 , 0.277 0.195 , 0.252	Depositor DCC
R_{free} test set	1865 reflections (3.45%)	DCC
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 90.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8694	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, ADP

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	0.89	37/4232 (0.9%)	1.24	47/5734 (0.8%)
1	B	0.87	35/4248 (0.8%)	1.24	46/5755 (0.8%)
All	All	0.88	72/8480 (0.8%)	1.24	93/11489 (0.8%)

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	GLU	CD-OE2	6.69	1.33	1.25
1	A	499	GLU	CD-OE2	6.64	1.32	1.25
1	A	397	GLU	CD-OE2	6.59	1.32	1.25
1	A	300	GLU	CD-OE2	6.42	1.32	1.25
1	B	185	GLU	CD-OE2	6.14	1.32	1.25

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	LEU	C-N-CD	-11.39	95.53	120.60
1	B	107	ASP	CB-CG-OD1	-7.74	111.33	118.30
1	A	450	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	B	303	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	494	ASP	CB-CG-OD2	-7.21	111.81	118.30

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	4156	0	4162	362	0
1	B	4172	0	4184	327	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	5	0
3	B	27	0	12	4	0
4	A	29	0	12	5	0
4	B	29	0	12	6	0
5	A	130	0	0	11	0
5	B	122	0	0	12	1
All	All	8694	0	8394	690	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 41.

The worst 5 of 690 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:A:39:MET:HE1	1:A:130:GLY:HA3	1.35	1.09
1:A:301:LEU:HD12	1:A:302:PRO:HD2	1.36	1.06
1:A:396:MET:HE1	1:A:480:GLN:HB3	1.39	1.05
1:A:521:THR:HG22	1:A:524:ASP:H	1.27	0.99
1:A:521:THR:HG23	1:A:522:PRO:HD2	1.41	0.99

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)
5:B:1724:HOH:O	5:B:1724:HOH:O[2_555]	0.81	1.39

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	530/545 (97%)	445 (84%)	66 (12%)	19 (4%)	4	13
1	B	532/545 (98%)	461 (87%)	60 (11%)	11 (2%)	8	27
All	All	1062/1090 (97%)	906 (85%)	126 (12%)	30 (3%)	6	19

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	TYR
1	A	335	THR
1	A	356	ARG
1	A	391	ARG
1	A	392	HIS

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	
1	A	451/461 (98%)	396 (88%)	55 (12%)	6	17
1	B	453/461 (98%)	398 (88%)	55 (12%)	6	17
All	All	904/922 (98%)	794 (88%)	110 (12%)	6	17

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	GLN
1	B	86	ARG
1	B	428	VAL
1	A	495	ASP
1	B	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	B	134	HIS
1	B	425	ASN
1	A	469	HIS
1	A	506	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 6 ligands modelled in this entry, 2 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	$\# Z > 2$
3	ADP	A	601	2	25,29,29	0.89	2 (8%)	24,45,45	1.37	1 (4%)
4	CTP	A	602	-	24,30,30	1.60	4 (16%)	24,47,47	1.43	2 (8%)
3	ADP	B	1601	2	25,29,29	0.91	2 (8%)	24,45,45	0.90	1 (4%)
4	CTP	B	1602	-	24,30,30	1.43	3 (12%)	24,47,47	1.94	2 (8%)

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
3	ADP	A	601	2	-	0/12/32/32	0/3/3/3
4	CTP	A	602	-	-	0/18/38/38	0/2/2/2
3	ADP	B	1601	2	-	0/12/32/32	0/3/3/3
4	CTP	B	1602	-	-	0/18/38/38	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	CTP	C2'-C1'	-2.69	1.49	1.53
3	A	601	ADP	PA-O5'	-2.31	1.49	1.59
3	B	1601	ADP	PA-O5'	-2.20	1.49	1.59
4	B	1602	CTP	C5'-C4'	2.08	1.58	1.51
3	A	601	ADP	PB-O3A	2.10	1.63	1.60

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1602	CTP	O4'-C1'-N1	-7.00	94.05	108.08
3	A	601	ADP	C1'-N9-C4	-5.53	117.08	126.64
4	A	602	CTP	C4'-O4'-C1'	-5.47	103.95	109.77
4	B	1602	CTP	C4'-O4'-C1'	-4.62	104.85	109.77
4	A	602	CTP	O4'-C1'-N1	-2.42	103.23	108.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ADP	5	0
4	A	602	CTP	5	0
3	B	1601	ADP	4	0
4	B	1602	CTP	6	0

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 [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	534/545 (97%)	-0.14	9 (1%) 70 63	30, 58, 93, 99	5 (0%)
1	B	536/545 (98%)	-0.15	10 (1%) 67 58	25, 56, 92, 100	3 (0%)
All	All	1070/1090 (98%)	-0.14	19 (1%) 69 60	25, 57, 92, 100	8 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	545	LYS	4.6
1	B	1	MET	4.0
1	A	339	GLU	3.3
1	A	394	ALA	3.0
1	A	390	ALA	3.0

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	ADP	B	1601	27/27	0.94	0.18	-0.01	45,78,94,100	0
3	ADP	A	601	27/27	0.94	0.16	-0.18	38,72,98,100	0
4	CTP	A	602	29/29	0.97	0.15	-1.11	29,41,48,52	0
4	CTP	B	1602	29/29	0.97	0.15	-1.22	39,44,48,50	0
2	MG	A	701	1/1	0.99	0.10	-	32,32,32,32	0
2	MG	B	1701	1/1	0.96	0.19	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.