



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:59 PM UTC

PDB ID : 6UTY / pdb_00006uty
Title : E. coli sigma-S transcription initiation complex with a mismatching CTP
("Old" crystal soaked with CTP for 30 minutes)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 4.15 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

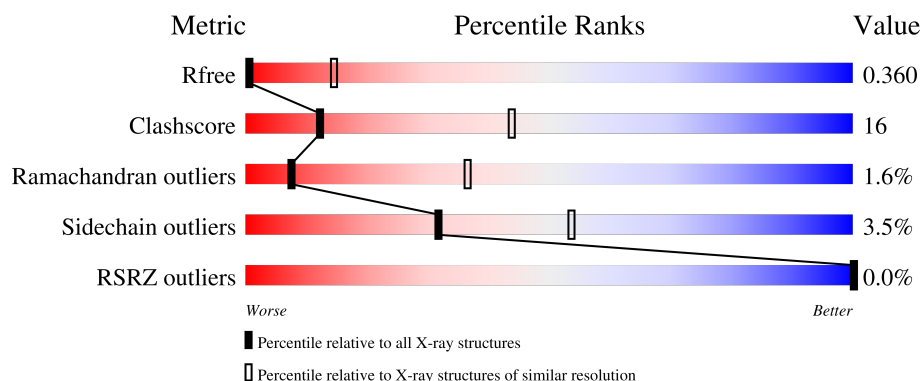
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.15 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}	180053	1077 (4.50-3.82)
Clashscore	190562	1019 (4.48-3.84)
Ramachandran outliers	187476	1035 (4.50-3.82)
Sidechain outliers	187428	1022 (4.50-3.82)
RSRZ outliers	180081	1074 (4.50-3.82)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	AAA	242	
1	BBB	242	
2	CCC	1342	
3	DDD	1407	
4	EEE	90	

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Mol	Chain	Length	Quality of chain
5	FFF	336	
6	111	50	
7	222	50	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	DDD	1502	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28961 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	BBB	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP P0A7Z4
AAA	-5	HIS	-	expression tag	UNP P0A7Z4
AAA	-4	HIS	-	expression tag	UNP P0A7Z4
AAA	-3	HIS	-	expression tag	UNP P0A7Z4
AAA	-2	HIS	-	expression tag	UNP P0A7Z4
AAA	-1	HIS	-	expression tag	UNP P0A7Z4
AAA	0	HIS	-	expression tag	UNP P0A7Z4
BBB	-6	ALA	-	expression tag	UNP P0A7Z4
BBB	-5	HIS	-	expression tag	UNP P0A7Z4
BBB	-4	HIS	-	expression tag	UNP P0A7Z4
BBB	-3	HIS	-	expression tag	UNP P0A7Z4
BBB	-2	HIS	-	expression tag	UNP P0A7Z4
BBB	-1	HIS	-	expression tag	UNP P0A7Z4
BBB	0	HIS	-	expression tag	UNP P0A7Z4

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	EEE	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	FFF	277	Total	C	N	O	S	0	0	0
			2253	1411	415	423	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	2	GLY	SER	conflict	UNP P13445
FFF	33	GLU	GLN	conflict	UNP P13445
FFF	329	LEU	-	expression tag	UNP P13445
FFF	330	GLU	-	expression tag	UNP P13445
FFF	331	HIS	-	expression tag	UNP P13445
FFF	332	HIS	-	expression tag	UNP P13445
FFF	333	HIS	-	expression tag	UNP P13445
FFF	334	HIS	-	expression tag	UNP P13445
FFF	335	HIS	-	expression tag	UNP P13445
FFF	336	HIS	-	expression tag	UNP P13445

- Molecule 6 is a DNA chain called Synthetic DNA 50-MER (promoter non-template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	32	Total	C	N	O	P	0	0	0
			661	314	121	194	32			

- Molecule 7 is a DNA chain called Synthetic DNA 50-MER (promoter DNA template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	34	Total	C	N	O	P	0	0	0
			695	332	127	203	33			

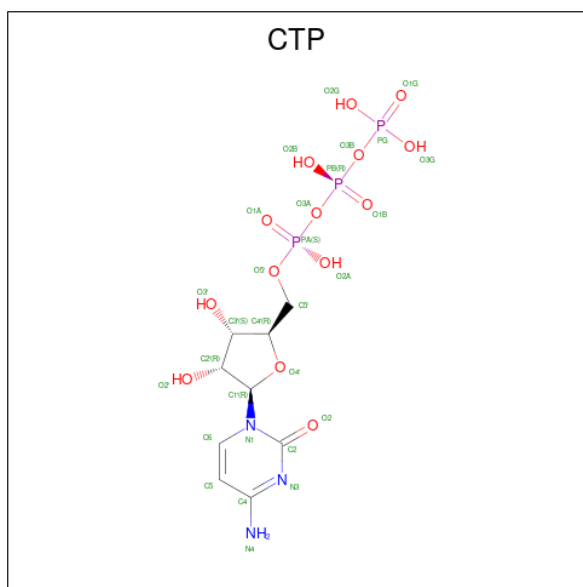
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	DDD	2	Total	Zn	0	0
			2	2		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	DDD	2	Total	Mg	0	0
			2	2		

- Molecule 10 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: C₉H₁₆N₃O₁₄P₃).

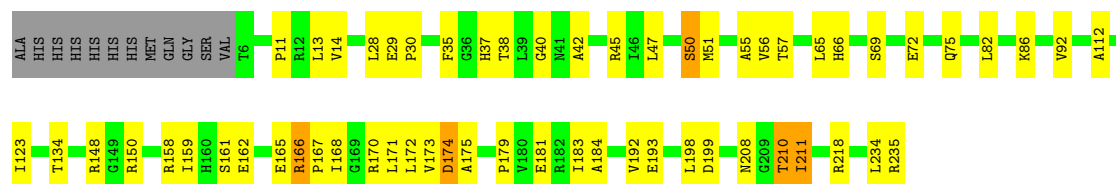


3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

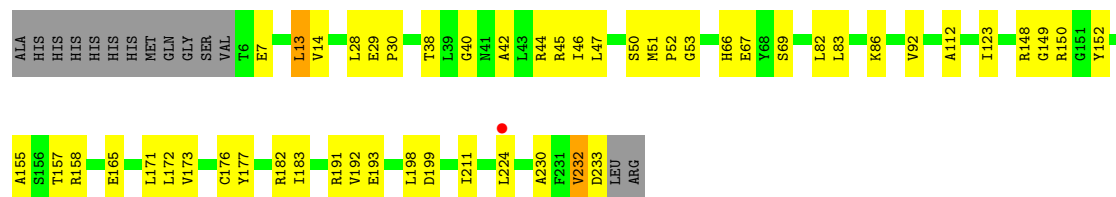
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain AAA: 



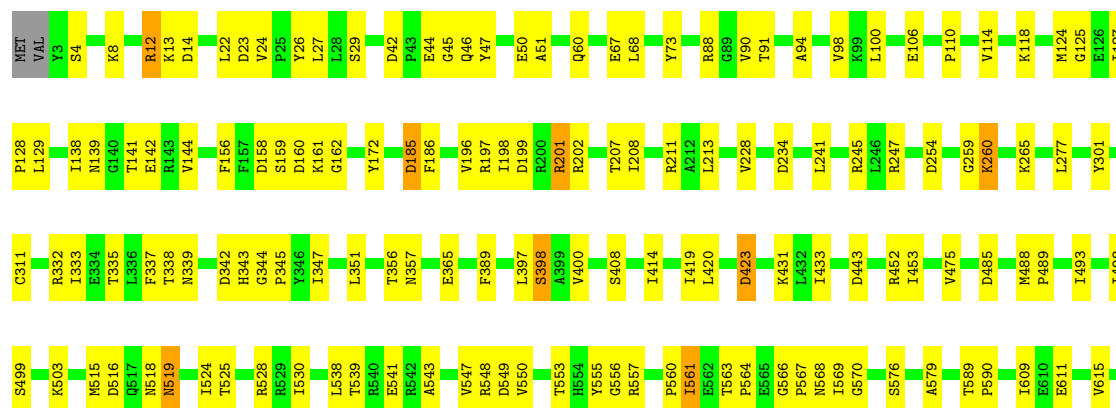
- Molecule 1: DNA-directed RNA polymerase subunit alpha

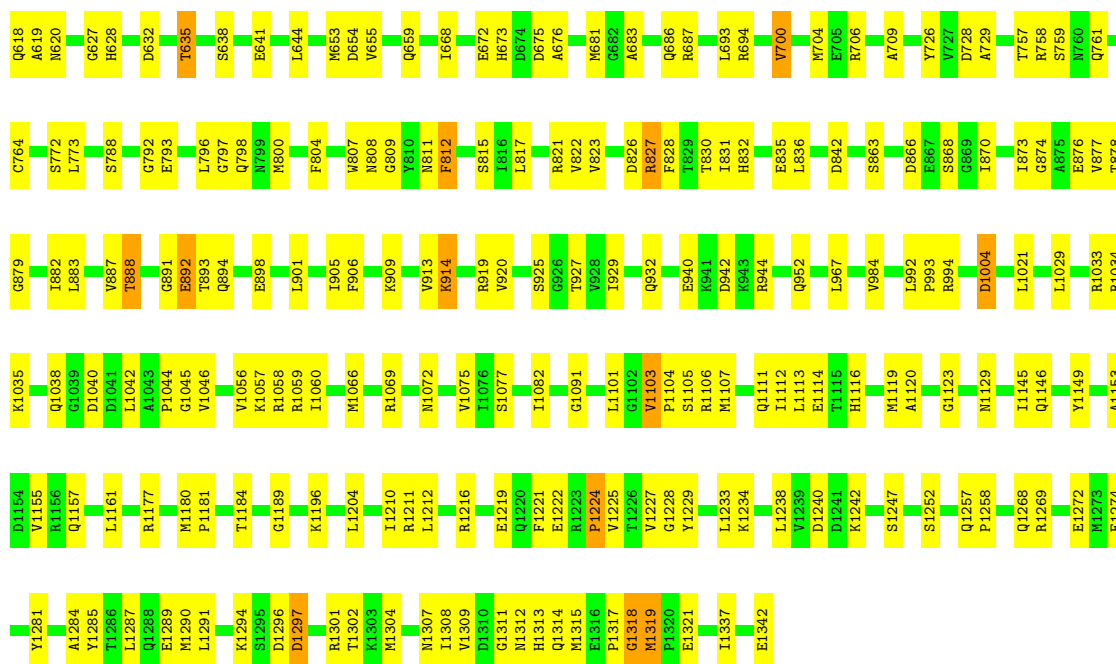
Chain BBB: 



- Molecule 2: DNA-directed RNA polymerase subunit beta

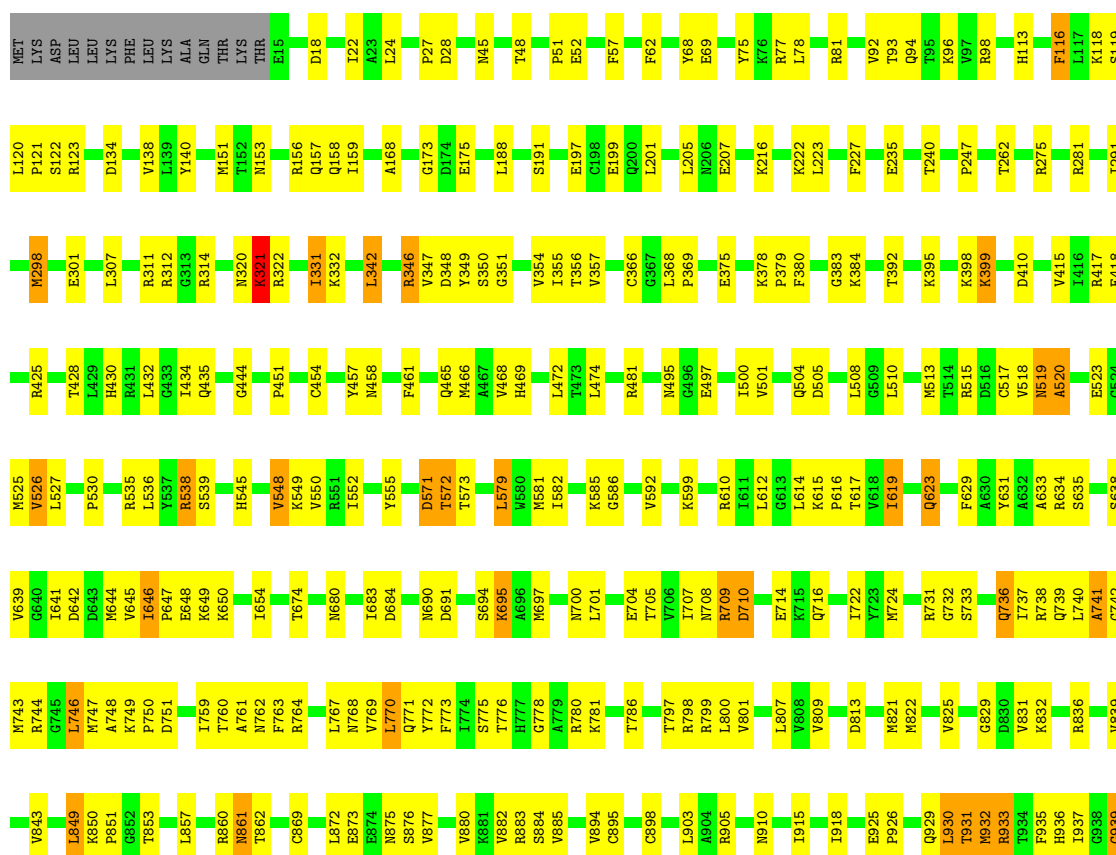
Chain CCC: 

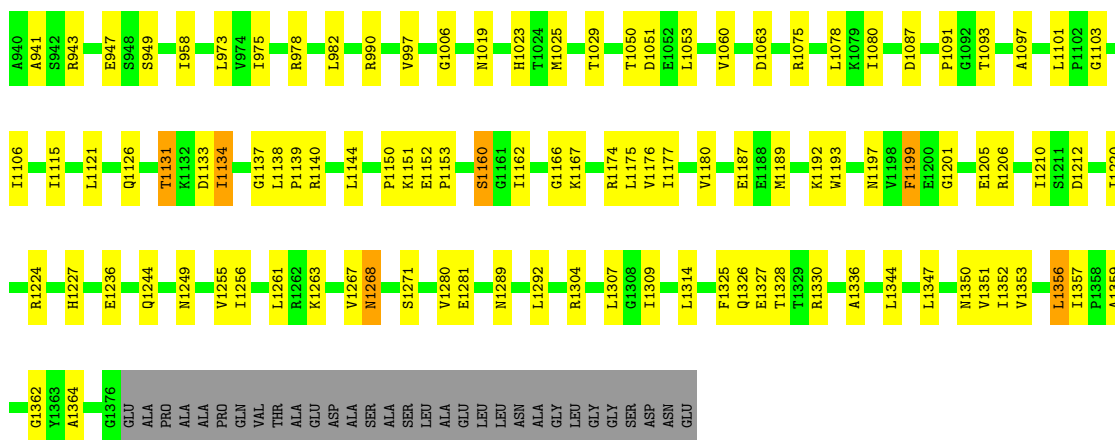




• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain DDD: 68% 26%





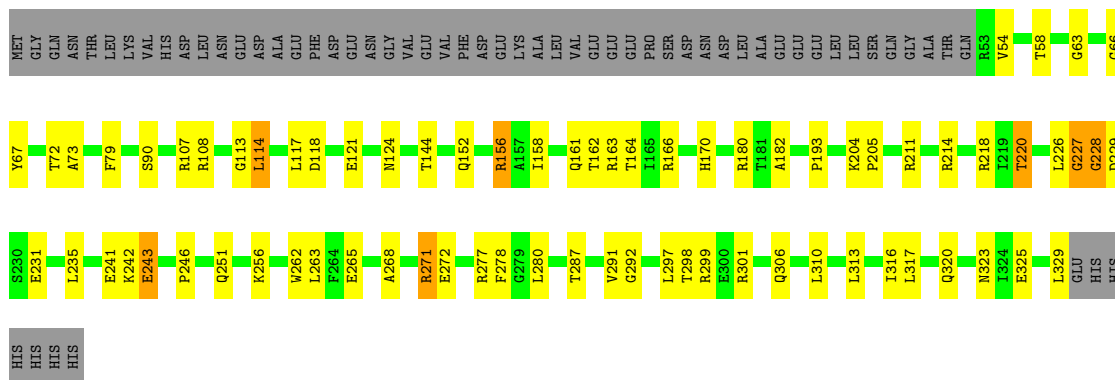
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain EEE:



- Molecule 5: RNA polymerase sigma factor RpoS

Chain FFF:



- Molecule 6: Synthetic DNA 50-MER (promoter non-template strand)

Chain 111:



- Molecule 7: Synthetic DNA 50-MER (promoter DNA template strand)

Chain 222:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.58Å 152.73Å 229.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 4.15 48.96 – 4.15	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.96-4.15) 98.1 (48.96-4.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.302 , 0.370 0.297 , 0.360	Depositor DCC
R_{free} test set	1698 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	166.4	Xtriage
Anisotropy	0.715	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 257.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28961	wwPDB-VP
Average B, all atoms (Å ²)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, ZN, 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	AAA	0.97	0/1809	1.16	0/2450
1	BBB	0.96	0/1789	1.16	1/2425 (0.0%)
2	CCC	0.92	0/10739	1.23	4/14489 (0.0%)
3	DDD	0.94	0/10729	1.23	4/14487 (0.0%)
4	EEE	0.92	0/629	1.31	0/847
5	FFF	0.99	0/2282	1.28	0/3076
6	111	0.30	0/741	0.61	1/1143 (0.1%)
7	222	0.29	0/779	0.52	0/1201
All	All	0.92	0/29497	1.20	10/40118 (0.0%)

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(°)
3	DDD	331	ILE	N-CA-C	-6.36	106.93	113.10
3	DDD	741	ALA	N-CA-C	-6.29	106.14	113.88
3	DDD	118	LYS	N-CA-C	-6.21	105.84	113.41
1	BBB	52	PRO	N-CA-C	5.66	122.42	112.01
2	CCC	414	ILE	N-CA-C	-5.50	106.33	111.45

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	AAA	1787	0	1813	79	0
1	BBB	1767	0	1789	73	0
2	CCC	10570	0	10582	339	0
3	DDD	10568	0	10779	479	0
4	EEE	627	0	634	10	0
5	FFF	2253	0	2298	84	1
6	111	661	0	362	18	0
7	222	695	0	385	25	0
8	DDD	2	0	0	2	0
9	DDD	2	0	0	0	0
10	DDD	29	0	12	7	0
All	All	28961	0	28654	891	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 16.

The worst 5 of 891 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)
3:DDD:690:ASN:ND2	3:DDD:738:ARG:HH12	1.30	1.28
2:CCC:549:ASP:CG	3:DDD:750:PRO:CG	2.06	1.26
2:CCC:549:ASP:OD2	3:DDD:750:PRO:HG2	1.18	1.26
3:DDD:646:ILE:HG22	3:DDD:647:PRO:CD	1.65	1.26
3:DDD:898:CYS:SG	8:DDD:1502:ZN:ZN	1.25	1.23

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:FFF:67:TYR:O	5:FFF:299:ARG:NH2[3_644]	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	AAA	228/242 (94%)	206 (90%)	15 (7%)	7 (3%)	3	22
1	BBB	226/242 (93%)	206 (91%)	17 (8%)	3 (1%)	9	41
2	CCC	1338/1342 (100%)	1191 (89%)	126 (9%)	21 (2%)	7	36
3	DDD	1360/1407 (97%)	1203 (88%)	135 (10%)	22 (2%)	7	36
4	EEE	77/90 (86%)	70 (91%)	7 (9%)	0	100	100
5	FFF	275/336 (82%)	247 (90%)	24 (9%)	4 (2%)	8	38
All	All	3504/3659 (96%)	3123 (89%)	324 (9%)	57 (2%)	7	36

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CCC	161	LYS
2	CCC	1319	MET
3	DDD	519	ASN
3	DDD	710	ASP
3	DDD	1053	LEU

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	AAA	198/208 (95%)	192 (97%)	6 (3%)	36	57
1	BBB	196/208 (94%)	192 (98%)	4 (2%)	48	65
2	CCC	1155/1157 (100%)	1124 (97%)	31 (3%)	39	60
3	DDD	1135/1168 (97%)	1083 (95%)	52 (5%)	24	46
4	EEE	67/74 (90%)	65 (97%)	2 (3%)	36	57
5	FFF	240/292 (82%)	231 (96%)	9 (4%)	29	51
All	All	2991/3107 (96%)	2887 (96%)	104 (4%)	32	54

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	DDD	505	ASP

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Mol	Chain	Res	Type
3	DDD	649	LYS
5	FFF	211	ARG
3	DDD	538	ARG
3	DDD	599	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 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	$\# Z > 2$
10	CTP	DDD	1505	9	29,30,30	0.82	1 (3%)	43,47,47	0.58	0

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
10	CTP	DDD	1505	9	-	4/22/38/38	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	DDD	1505	CTP	PA-O3A	2.83	1.62	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

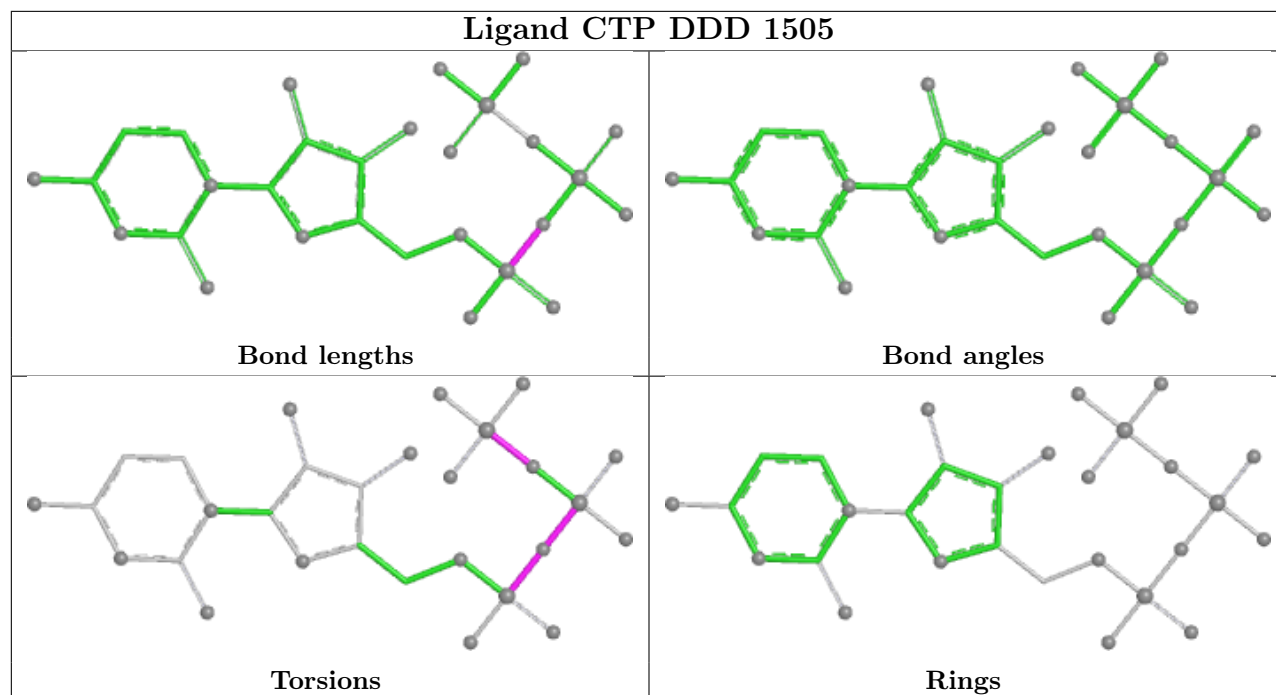
Mol	Chain	Res	Type	Atoms
10	DDD	1505	CTP	PB-O3B-PG-O3G
10	DDD	1505	CTP	PB-O3A-PA-O1A
10	DDD	1505	CTP	PB-O3A-PA-O2A
10	DDD	1505	CTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	DDD	1505	CTP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	AAA	230/242 (95%)	-0.82	0 100 100	216, 319, 398, 462	0
1	BBB	228/242 (94%)	-0.80	1 (0%) 88 76	213, 333, 449, 481	0
2	CCC	1340/1342 (99%)	-0.90	0 100 100	128, 257, 407, 557	0
3	DDD	1362/1407 (96%)	-0.89	0 100 100	123, 291, 435, 538	0
4	EEE	79/90 (87%)	-1.01	0 100 100	240, 334, 443, 501	0
5	FFF	277/336 (82%)	-0.91	0 100 100	222, 332, 581, 640	0
6	111	32/50 (64%)	-0.64	0 100 100	284, 355, 454, 489	0
7	222	34/50 (68%)	-0.51	0 100 100	277, 344, 462, 463	0
All	All	3582/3759 (95%)	-0.88	1 (0%) 100 100	123, 292, 446, 640	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	224	LEU	3.9

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 oligosaccharides in this entry.

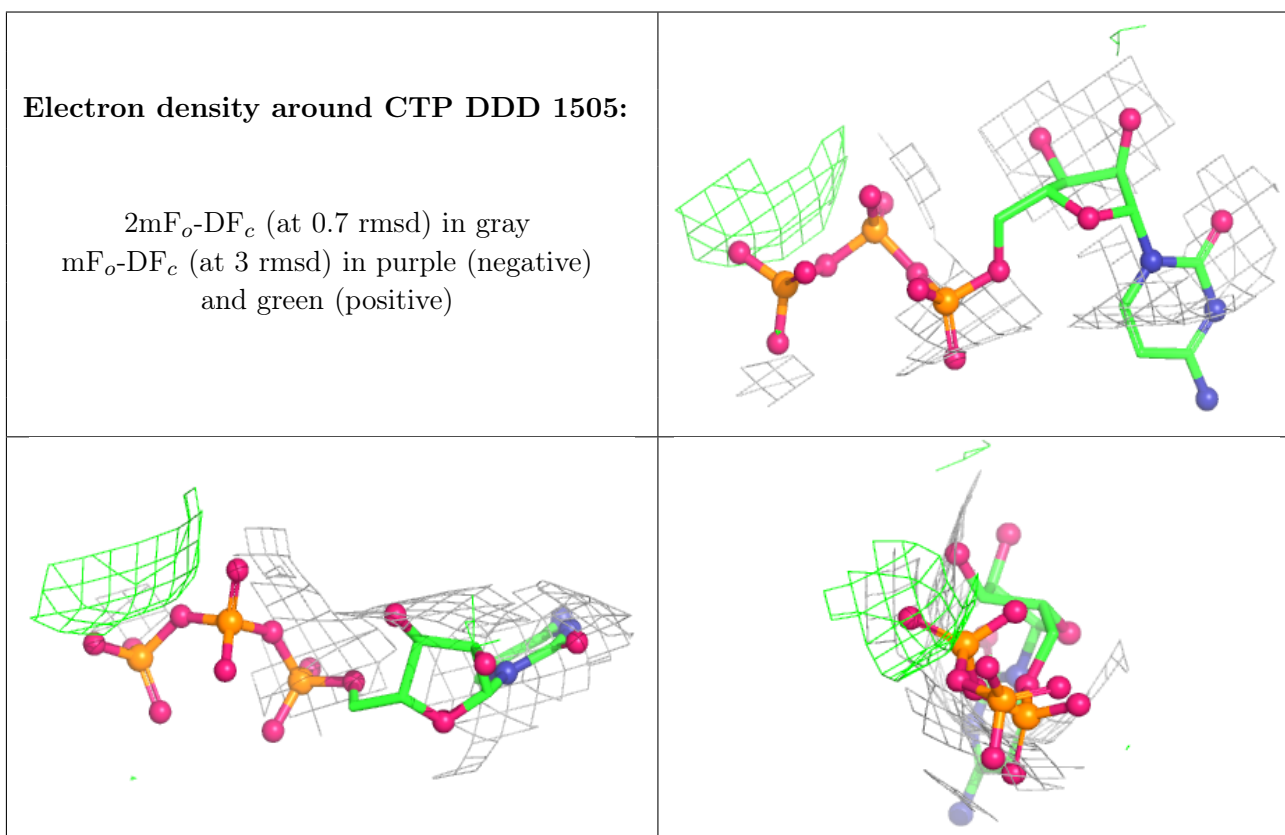
6.4 Ligands [i](#)

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. 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	B-factors(Å ²)	Q<0.9
9	MG	DDD	1504	1/1	0.89	0.06	150,150,150,150	0
10	CTP	DDD	1505	29/29	0.89	0.07	267,293,345,369	0
9	MG	DDD	1503	1/1	0.97	0.03	193,193,193,193	0
8	ZN	DDD	1501	1/1	0.98	0.04	375,375,375,375	0
8	ZN	DDD	1502	1/1	1.00	0.03	247,247,247,247	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.