wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 15, 2023 – 11:06 PM EDT

PDB ID	:	1TWG
Title	:	RNA polymerase II complexed with CTP
Authors	:	Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on	:	2004-06-30
Resolution	:	3.30 Å(reported)

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

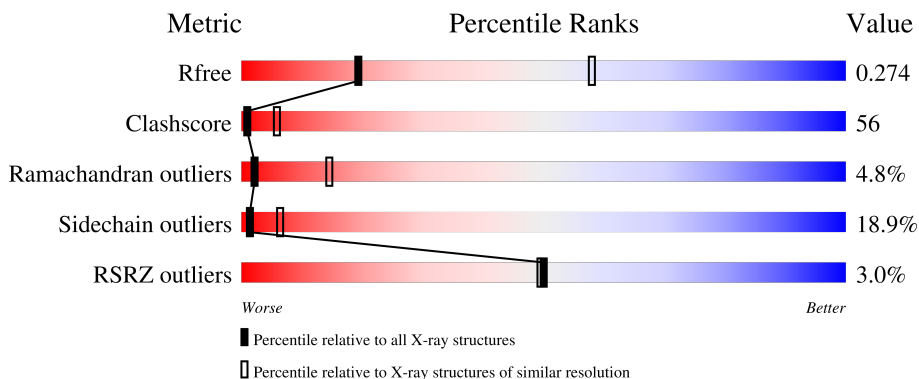|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.30 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	Percentile Ranks	Value
Rfree		0.274
Clashscore		56
Ramachandran outliers		4.8%
Sidechain outliers		18.9%
RSRZ outliers		3.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	1733	2% / 5% 34% 28% 11% 22%
2	B	1224	4% / 6% 36% 33% 14% 11%
3	C	318	% / • 27% 39% 13% 16%
4	E	215	2% / 7% 29% 46% 18%
5	F	155	% / • 24% 20% 6% 46%

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Mol	Chain	Length	Quality of chain
6	H	146	4% · 24% 30% 34% 9%
7	I	122	2% · 40% 42% 14% ·
8	J	70	· 37% 41% 10% 9%
9	K	120	5% 30% 44% 16% 5%
10	L	70	% · 9% 27% 29% 34%

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
12	ZN	J	3001	-	-	X	-
12	ZN	L	3005	-	-	X	-
13	CTP	B	3008	X	-	X	-

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 27731 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 II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1349	Total	C	N	O	S	0	0	0
			10606	6692	1839	2017	58			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1091	Total	C	N	O	S	0	0	0
			8690	5511	1516	1610	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	83	Total	C	N	O	S	0	0	0
			670	428	114	125	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total 1068	C 673	N 180	O 211	S 4	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	121	Total 990	C 610	N 181	O 188	S 11	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	64	Total 525	C 334	N 92	O 93	S 6	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total 919	C 590	N 156	O 171	S 2	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total 364	C 224	N 72	O 64	S 4	0	0	0

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total 2	Mn 2	0	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total 1	Zn 1	0	0
12	I	2	Total 2	Zn 2	0	0
12	J	1	Total 1	Zn 1	0	0
12	L	1	Total 1	Zn 1	0	0

- Molecule 13 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).
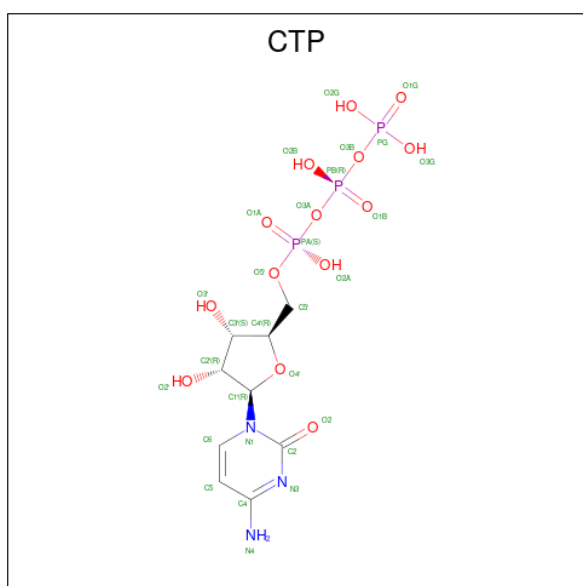
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total 29	C 9	N 3	O 14	P 3	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total 2	O 2	0	0
14	B	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

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 II largest subunit

SER PRO SER TYR SER PRO THR SER PRO ASN TYR SER ASP GLU ASP PRO TYR SER PRO SER PRO THR SER PRO SER PRO TYR SER PRO THR SER PRO GLY TYR SER PRO GLY SER PRO ALA TYR SER PRO LYS GLN ASP GLU GLN GLN LYS HIS ASN GLU ASN GLU ASN SER ARG

• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:

• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide
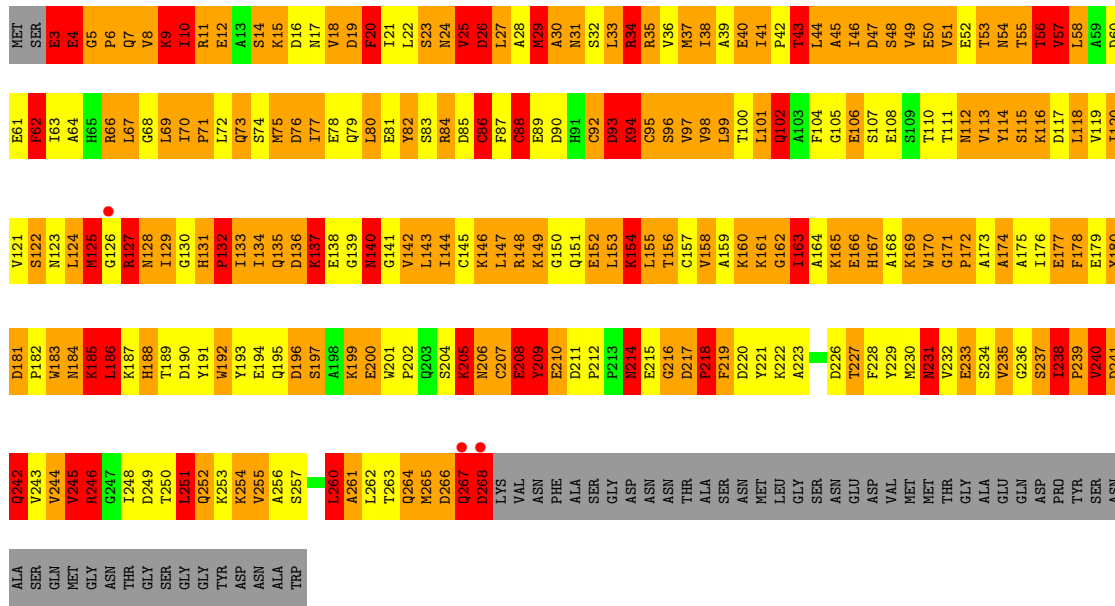
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide
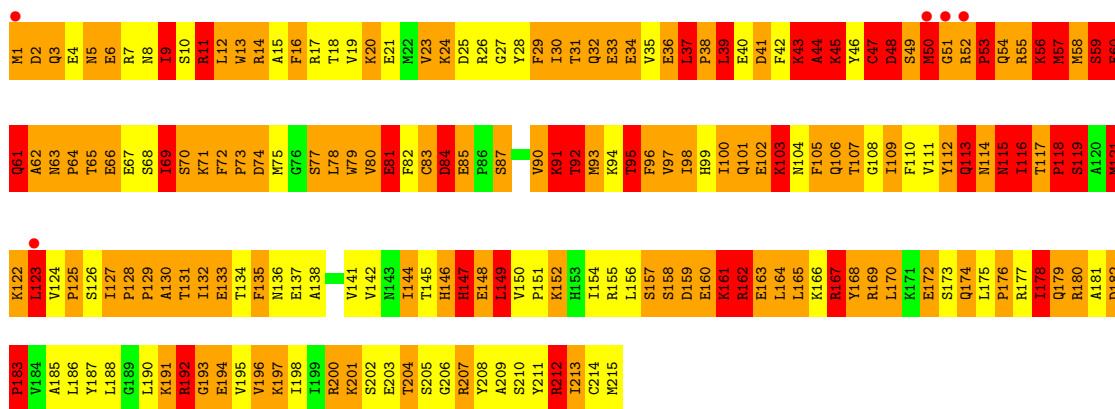
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide
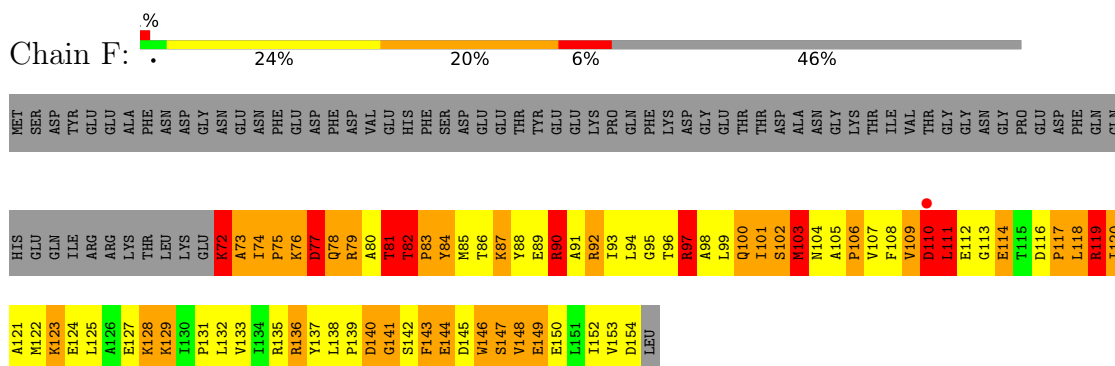
Chain F:

- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide
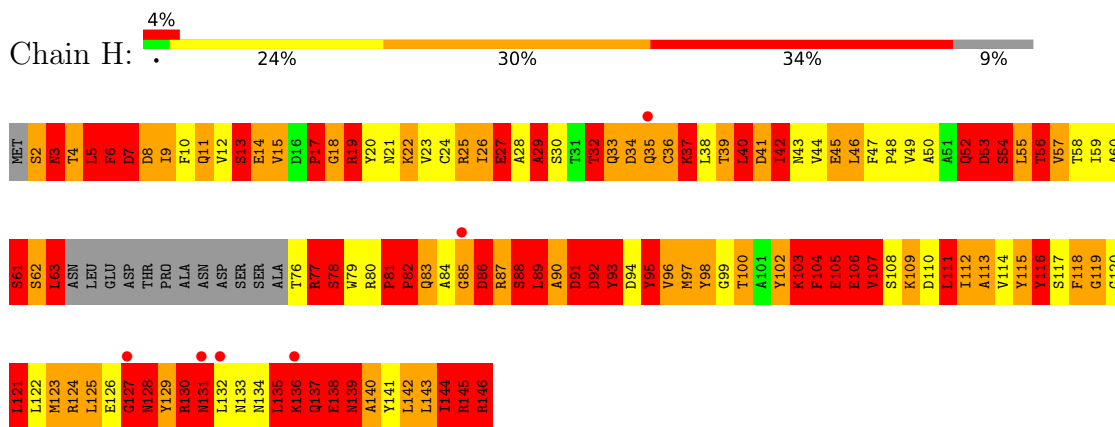
Chain H:

- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide
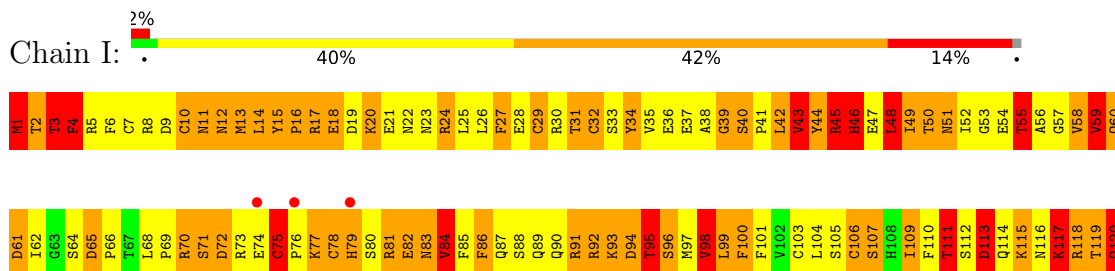
Chain I:

F121 SER

• Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J: 37%   41%   10%   9%

M1 I2 V3 P4 V5 R6 C7 F8 S9 C10 G11 K12 V13 V14 G15 D16 K17 W18 E19 S20 Y21 L22 N23 L24 L25 Q26 E27 D28 E29 L30 D31 E32 G33 T34 A35 L36 S37 R38 L39 G40 L41 K42 R43 Y44 C45 C46 R47 R48 M49 I50 L51 T52 H53 V54 D55 L56 I57 E58 K59 F60

L61 R62 Y63 N64 PRO LEU GLU LYS ARG ASP

• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 5%   30%   44%   16%   5%

M1 N2 A3 P4 D5 R6 F7 E8 L9 F10 L11 L12 G13 E14 G15 E16 S17 K18 L19 K20 I21 D22 P23 D24 T25 K26 A27 P28 N29 A30 V31 V32 I33 T34 F35 E36 K37 E38 D39 H40 T41 L42 G43 N44 L45 I46 R47 A48 E49 L50 L51 N52 D53 R54 K55 V56 L57 F58 Y61

K62 V63 E64 H65 P66 F67 F68 A69 R70 F71 K72 L73 R74 I75 Q76 T77 T78 E79 G80 Y81 D82 P83 K84 D85 A86 L87 K88 N89 A90 C91 N92 S93 I94 I95 N96 K97 L98 G99 A100 L101 K102 T103 N104 F105 E106 T107 E108 W109 N110 L111 Q112 T113 L114 ALA ALA ASP ASP ALA PHE

• Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L: %   9%   27%   29%   34%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ALA ARG THR A25 T26 L27 K28 Y29 I30 C31 A32 E33 C34 S35 S36 K37 L38 S39 L40 S41 R42 T43 D44 A45 V46 R47 C48 K49 D50 C51 G52 H53 R54 I55 L56 L57 K58 A59 R60

T61 K62 R63 L64 V65 Q66 F67 E68 A69 R70

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.00Å 223.00Å 374.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 39.42 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.30) 93.0 (39.42-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.281 0.214 , 0.274	Depositor DCC
R_{free} test set	2324 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 46.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	27731	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, CTP, MN

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	4.63	2498/10792 (23.1%)	3.14	1255/14601 (8.6%)
2	B	4.65	2069/8860 (23.4%)	3.12	1000/11945 (8.4%)
3	C	4.80	513/2133 (24.1%)	3.12	254/2891 (8.8%)
4	E	4.70	404/1796 (22.5%)	3.05	209/2416 (8.7%)
5	F	4.16	139/682 (20.4%)	2.87	60/922 (6.5%)
6	H	4.56	229/1086 (21.1%)	3.04	130/1470 (8.8%)
7	I	5.31	288/1009 (28.5%)	3.40	147/1357 (10.8%)
8	J	4.28	125/533 (23.5%)	3.41	78/715 (10.9%)
9	K	4.50	226/937 (24.1%)	3.21	126/1265 (10.0%)
10	L	5.07	98/366 (26.8%)	3.32	59/485 (12.2%)
All	All	4.66	6589/28194 (23.4%)	3.14	3318/38067 (8.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	69
2	B	0	59
3	C	0	19
4	E	0	9
6	H	0	15
7	I	0	9
8	J	0	2
9	K	0	5
10	L	0	4
All	All	0	191

The worst 5 of 6589 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	564	GLU	CD-OE1	30.56	1.59	1.25
7	I	34	TYR	CD1-CE1	-29.71	0.94	1.39
1	A	1234	GLU	CD-OE1	29.21	1.57	1.25
7	I	34	TYR	CE2-CZ	-28.02	1.02	1.38
1	A	728	LYS	CD-CE	27.41	2.19	1.51

The worst 5 of 3318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	774	ARG	NE-CZ-NH1	45.06	142.83	120.30
2	B	995	ARG	NE-CZ-NH2	-36.16	102.22	120.30
7	I	91	ARG	NE-CZ-NH1	32.74	136.67	120.30
2	B	995	ARG	NE-CZ-NH1	32.13	136.37	120.30
1	A	469	ARG	NE-CZ-NH1	31.48	136.04	120.30

There are no chirality outliers.

5 of 191 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	THR	Peptide
1	A	52	GLY	Peptide
1	A	60	SER	Peptide
1	A	65	LEU	Peptide
1	A	74	MET	Peptide

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	A	10606	0	10660	1097	0
2	B	8690	0	8709	1000	2
3	C	2095	0	2053	264	0
4	E	1760	0	1788	203	1
5	F	670	0	690	70	0
6	H	1068	0	1040	223	0
7	I	990	0	948	109	0
8	J	525	0	538	60	0
9	K	919	0	927	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L	364	0	389	108	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0
12	B	1	0	0	0	0
12	C	1	0	0	1	0
12	I	2	0	0	0	0
12	J	1	0	0	2	0
12	L	1	0	0	2	0
13	B	29	0	11	13	0
14	A	2	0	0	0	0
14	B	3	0	0	7	0
All	All	27731	0	27753	3079	2

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 56.

The worst 5 of 3079 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:226:PHE:CD1	2:B:226:PHE:CE1	1.77	1.67
2:B:370:PHE:CD1	2:B:370:PHE:CE1	1.78	1.67
3:C:165:LYS:CG	3:C:165:LYS:CD	1.74	1.65
2:B:18:PHE:CB	2:B:18:PHE:CG	1.79	1.65
4:E:79:TRP:CB	4:E:79:TRP:CG	1.78	1.65

All (2) 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)
2:B:434:ARG:O	2:B:465:ASN:ND2[2_655]	2.11	0.09
2:B:1223:ASP:OD1	4:E:1:MET:CE[8_455]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1332/1733 (77%)	1160 (87%)	113 (8%)	59 (4%)	2	16	
2	B	1071/1224 (88%)	897 (84%)	131 (12%)	43 (4%)	3	18	
3	C	264/318 (83%)	218 (83%)	36 (14%)	10 (4%)	3	19	
4	E	213/215 (99%)	180 (84%)	20 (9%)	13 (6%)	1	10	
5	F	81/155 (52%)	71 (88%)	8 (10%)	2 (2%)	5	27	
6	H	129/146 (88%)	85 (66%)	21 (16%)	23 (18%)	0	1	
7	I	119/122 (98%)	108 (91%)	8 (7%)	3 (2%)	5	27	
8	J	62/70 (89%)	58 (94%)	4 (6%)	0	100	100	
9	K	112/120 (93%)	98 (88%)	10 (9%)	4 (4%)	3	20	
10	L	44/70 (63%)	26 (59%)	11 (25%)	7 (16%)	0	1	
All	All	3427/4173 (82%)	2901 (85%)	362 (11%)	164 (5%)	2	14	

5 of 164 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	43	GLU
1	A	45	GLN
1	A	47	ARG
1	A	56	PRO

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	1181/1520 (78%)	984 (83%)	197 (17%)	2	10
2	B	947/1061 (89%)	795 (84%)	152 (16%)	2	10
3	C	234/274 (85%)	192 (82%)	42 (18%)	2	8
4	E	197/197 (100%)	147 (75%)	50 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	73/137 (53%)	61 (84%)	12 (16%)	2	10
6	H	117/128 (91%)	72 (62%)	45 (38%)	0	0
7	I	115/116 (99%)	88 (76%)	27 (24%)	1	3
8	J	59/65 (91%)	48 (81%)	11 (19%)	1	7
9	K	99/102 (97%)	77 (78%)	22 (22%)	1	3
10	L	40/57 (70%)	18 (45%)	22 (55%)	0	0
All	All	3062/3657 (84%)	2482 (81%)	580 (19%)	1	6

5 of 580 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	H	36	CYS
10	L	60	ARG
6	H	83	GLN
6	H	35	GLN
7	I	98	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	73	GLN
9	K	65	HIS
3	C	167	HIS
4	E	147	HIS
1	A	1173	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 10 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	#$|Z| > 2$
13	CTP	B	3008	11	26,30,30	2.77	5 (19%)	39,47,47	3.18	12 (30%)

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
13	CTP	B	3008	11	1/1/7/7	5/22/38/38	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3008	CTP	C2-N1	9.64	1.60	1.40
13	B	3008	CTP	C1'-N1	7.42	1.69	1.47
13	B	3008	CTP	C6-N1	4.62	1.49	1.38
13	B	3008	CTP	C6-C5	4.21	1.44	1.35
13	B	3008	CTP	C4-N3	2.18	1.39	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	3008	CTP	O4'-C1'-N1	11.29	134.17	108.36
13	B	3008	CTP	C1'-N1-C2	8.46	137.30	118.42
13	B	3008	CTP	C6-N1-C2	-7.44	107.58	120.49
13	B	3008	CTP	O2-C2-N3	-7.17	110.66	122.33
13	B	3008	CTP	PB-O3A-PA	-3.55	120.63	132.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	3008	CTP	C1'

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	3008	CTP	C3'-C4'-C5'-O5'
13	B	3008	CTP	O4'-C4'-C5'-O5'
13	B	3008	CTP	PB-O3B-PG-O2G
13	B	3008	CTP	C2'-C1'-N1-C2
13	B	3008	CTP	PB-O3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	3008	CTP	13	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 then 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.

Ligand CTP B 3008

Bond lengths

Bond angles

Torsions

Rings
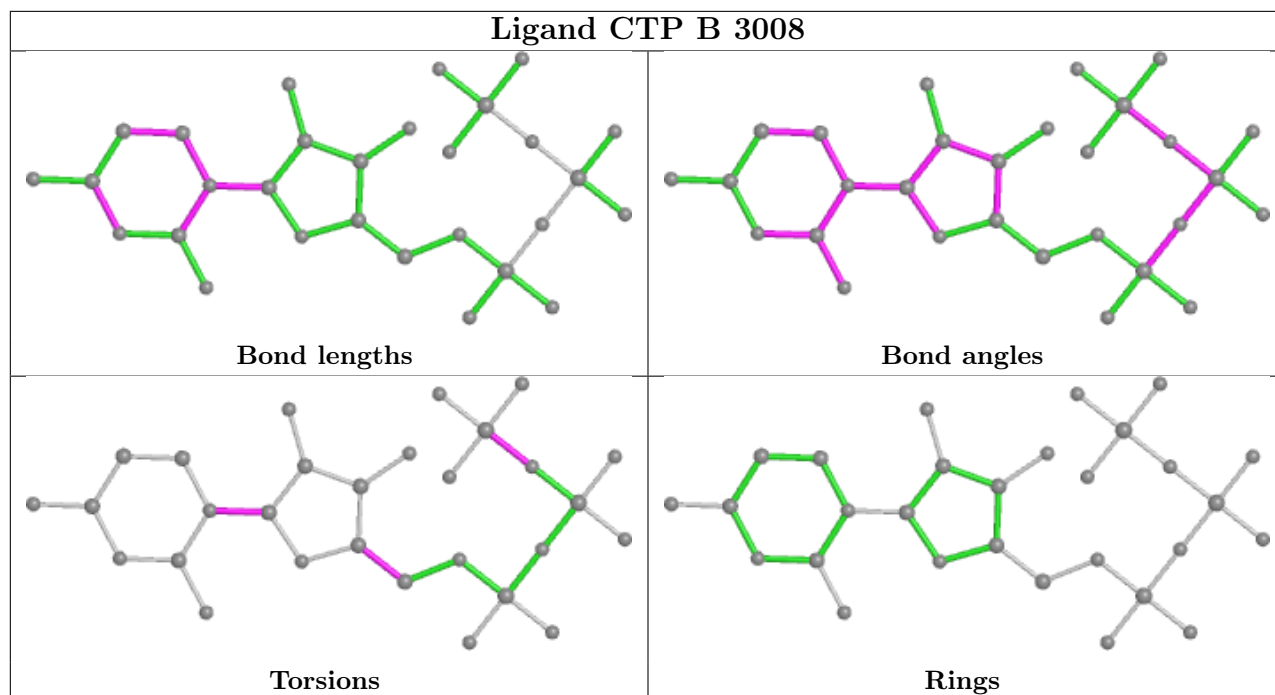
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	13
2	B	13
9	K	3
4	E	2
6	H	1
8	J	1
7	I	1

The worst 5 of 34 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1066:VAL	C	1067:LEU	N	1.20
1	A	1106:ASN	C	1107:VAL	N	1.20
1	A	1191:TRP	C	1192:LEU	N	1.20
1	A	1328:TYR	C	1329:THR	N	1.20
1	B	224:GLN	C	225:VAL	N	1.20

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	A	1349/1733 (77%)	-0.23	33 (2%)	59	56	1, 24, 101, 195	0
2	B	1091/1224 (89%)	-0.16	54 (4%)	29	27	1, 25, 114, 167	0
3	C	266/318 (83%)	-0.34	3 (1%)	80	81	1, 29, 77, 167	0
4	E	215/215 (100%)	-0.05	5 (2%)	60	59	1, 38, 111, 135	0
5	F	83/155 (53%)	-0.29	1 (1%)	79	78	1, 22, 64, 86	0
6	H	133/146 (91%)	0.17	6 (4%)	33	32	22, 68, 127, 188	0
7	I	121/122 (99%)	-0.03	3 (2%)	57	54	1, 31, 83, 100	0
8	J	64/70 (91%)	-0.37	0	100	100	3, 22, 76, 91	0
9	K	114/120 (95%)	-0.23	0	100	100	3, 36, 73, 99	0
10	L	46/70 (65%)	0.27	1 (2%)	62	60	24, 73, 133, 137	0
All	All	3482/4173 (83%)	-0.18	106 (3%)	50	49	1, 28, 108, 195	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	9.6
2	B	882	THR	9.3
1	A	69	THR	7.0
2	B	1109	GLY	6.9
2	B	1110	PRO	6.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.
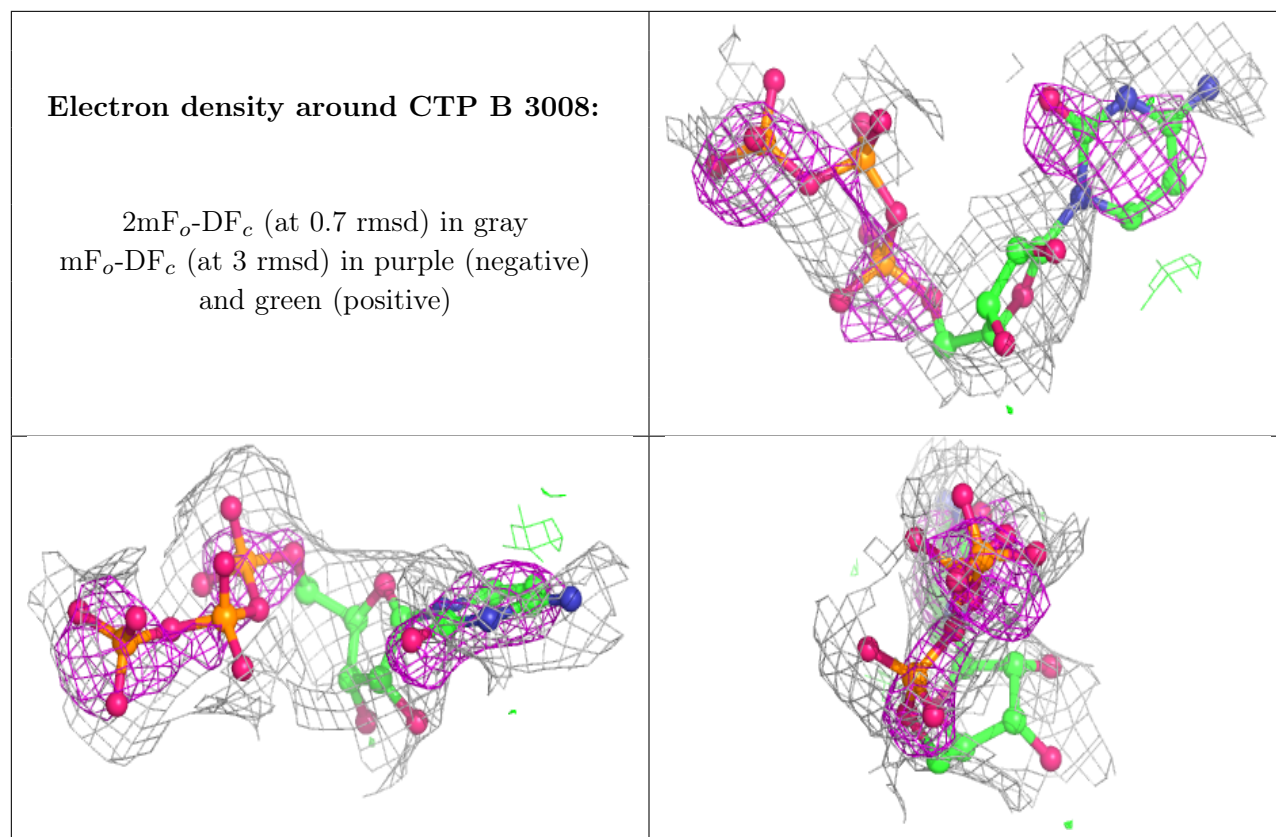
6.3　Carbohydrates (i)

There are no monosaccharides 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
13	CTP	B	3008	29/29	0.82	0.27	26,36,73,77	0
12	ZN	L	3005	1/1	0.89	0.08	84,84,84,84	0
12	ZN	I	3004	1/1	0.89	0.17	49,49,49,49	0
12	ZN	A	3006	1/1	0.92	0.07	48,48,48,48	0
12	ZN	C	3002	1/1	0.94	0.09	35,35,35,35	0
11	MN	A	3010	1/1	0.94	0.07	29,29,29,29	0
12	ZN	B	3007	1/1	0.97	0.08	37,37,37,37	0
11	MN	A	3009	1/1	0.97	0.12	15,15,15,15	0
12	ZN	I	3003	1/1	0.97	0.06	45,45,45,45	0
12	ZN	A	3008	1/1	0.98	0.06	87,87,87,87	0
12	ZN	J	3001	1/1	0.99	0.05	31,31,31,31	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.

Electron density around CTP B 3008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.