W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 09:33 PM EDT

PDB ID	:	3OLB
Title	:	Poliovirus polymerase elongation complex with 2',3'-dideoxy-ctp
Authors	:	Gong, P.; Peersen, O.B.
Deposited on	:	2010-08-25
Resolution	:	2.41 Å(reported)

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

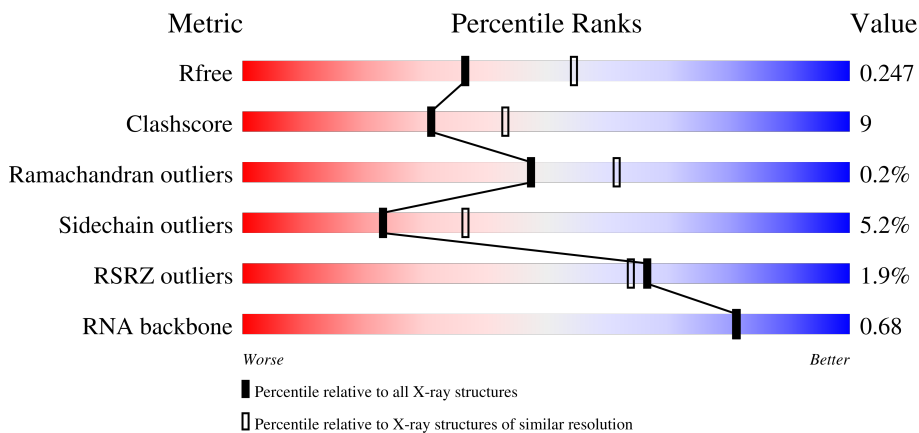|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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:
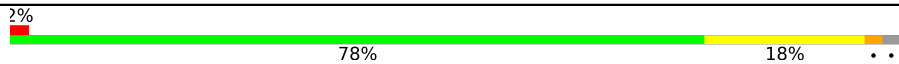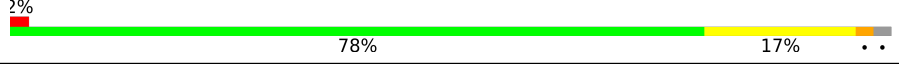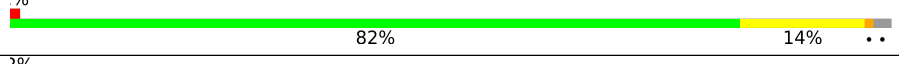*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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		0.247
Clashscore		9
Ramachandran outliers		0.2%
Sidechain outliers		5.2%
RSRZ outliers		1.9%
RNA backbone		0.68

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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)
RNA backbone	3102	1080 (2.80-2.04)

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	471	2% 78% 18% • •
1	E	471	2% 78% 17% • •
1	I	471	% 82% 14% • •
1	M	471	2% 82% 14% • •

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Mol	Chain	Length	Quality of chain
2	B	26	12% 46% 12% 31%
2	F	26	15% 46% 8% 31%
2	J	26	4% 38% 35% 27%
2	N	26	38% 35% 27%
3	C	14	79% 21%
3	G	14	86% 14%
3	K	14	79% 21%
3	O	14	71% 29%
4	D	9	22% 11% 67%
4	H	9	11% 22% 11% 67%
4	L	9	44% 56%
4	P	9	44% 56%

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
7	IPA	A	6032	-	-	X	-
7	IPA	M	6025	-	-	X	-
7	IPA	M	6031	-	-	X	-

2   Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 18860 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 Polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total 3697	C 2370	N 610	O 695	S 22	0	0	0
1	E	461	Total 3697	C 2370	N 610	O 695	S 22	0	0	0
1	I	461	Total 3697	C 2370	N 610	O 695	S 22	0	0	0
1	M	461	Total 3697	C 2370	N 610	O 695	S 22	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	ASP	LEU	engineered mutation	UNP B3VQP5
A	462	GLY	-	expression tag	UNP B3VQP5
A	463	SER	-	expression tag	UNP B3VQP5
A	464	SER	-	expression tag	UNP B3VQP5
A	465	SER	-	expression tag	UNP B3VQP5
A	466	HIS	-	expression tag	UNP B3VQP5
A	467	HIS	-	expression tag	UNP B3VQP5
A	468	HIS	-	expression tag	UNP B3VQP5
A	469	HIS	-	expression tag	UNP B3VQP5
A	470	HIS	-	expression tag	UNP B3VQP5
A	471	HIS	-	expression tag	UNP B3VQP5
E	446	ASP	LEU	engineered mutation	UNP B3VQP5
E	462	GLY	-	expression tag	UNP B3VQP5
E	463	SER	-	expression tag	UNP B3VQP5
E	464	SER	-	expression tag	UNP B3VQP5
E	465	SER	-	expression tag	UNP B3VQP5
E	466	HIS	-	expression tag	UNP B3VQP5
E	467	HIS	-	expression tag	UNP B3VQP5
E	468	HIS	-	expression tag	UNP B3VQP5
E	469	HIS	-	expression tag	UNP B3VQP5
E	470	HIS	-	expression tag	UNP B3VQP5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	471	HIS	-	expression tag	UNP B3VQP5
I	446	ASP	LEU	engineered mutation	UNP B3VQP5
I	462	GLY	-	expression tag	UNP B3VQP5
I	463	SER	-	expression tag	UNP B3VQP5
I	464	SER	-	expression tag	UNP B3VQP5
I	465	SER	-	expression tag	UNP B3VQP5
I	466	HIS	-	expression tag	UNP B3VQP5
I	467	HIS	-	expression tag	UNP B3VQP5
I	468	HIS	-	expression tag	UNP B3VQP5
I	469	HIS	-	expression tag	UNP B3VQP5
I	470	HIS	-	expression tag	UNP B3VQP5
I	471	HIS	-	expression tag	UNP B3VQP5
M	446	ASP	LEU	engineered mutation	UNP B3VQP5
M	462	GLY	-	expression tag	UNP B3VQP5
M	463	SER	-	expression tag	UNP B3VQP5
M	464	SER	-	expression tag	UNP B3VQP5
M	465	SER	-	expression tag	UNP B3VQP5
M	466	HIS	-	expression tag	UNP B3VQP5
M	467	HIS	-	expression tag	UNP B3VQP5
M	468	HIS	-	expression tag	UNP B3VQP5
M	469	HIS	-	expression tag	UNP B3VQP5
M	470	HIS	-	expression tag	UNP B3VQP5
M	471	HIS	-	expression tag	UNP B3VQP5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	P	0	0	0
			361	159	59	125	18			
2	F	18	Total	C	N	O	P	0	0	0
			361	159	59	125	18			
2	J	19	Total	C	N	O	P	0	0	0
			381	168	61	133	19			
2	N	19	Total	C	N	O	P	0	0	0
			381	168	61	133	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	14	Total 303	C 136	N 62	O 92	P 13	0	0	0
3	G	14	Total 303	C 136	N 62	O 92	P 13	0	0	0
3	K	14	Total 303	C 136	N 62	O 92	P 13	0	0	0
3	O	14	Total 303	C 136	N 62	O 92	P 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	3	Total 68	C 30	N 15	O 20	P 3	0	0	0
4	H	3	Total 68	C 30	N 15	O 20	P 3	0	0	0
4	L	4	Total 91	C 40	N 20	O 27	P 4	0	0	0
4	P	4	Total 91	C 40	N 20	O 27	P 4	0	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Zn 1	0	0
5	E	1	Total 1	Zn 1	0	0
5	I	1	Total 1	Zn 1	0	0
5	M	1	Total 1	Zn 1	0	0

- Molecule 6 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: $C_9H_{16}N_3O_{12}P_3$).

DCT
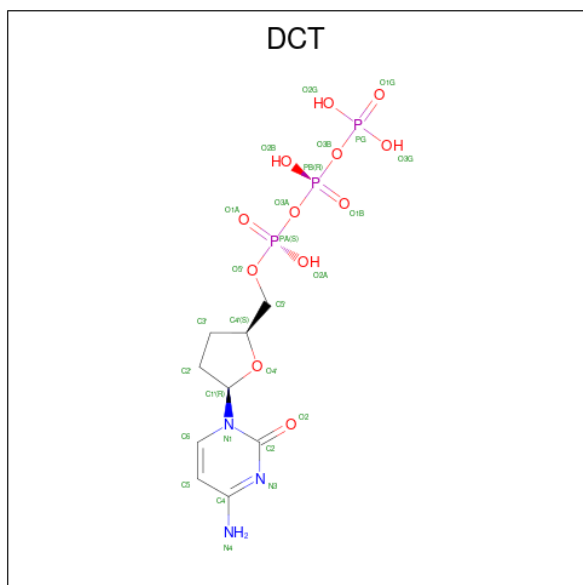
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	9	3	12	3		
6	E	1	Total	C	N	O	P	0	0
			27	9	3	12	3		
6	I	1	Total	C	N	O	P	0	0
			27	9	3	12	3		
6	M	1	Total	C	N	O	P	0	0
			27	9	3	12	3		

- Molecule 7 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).

IPA
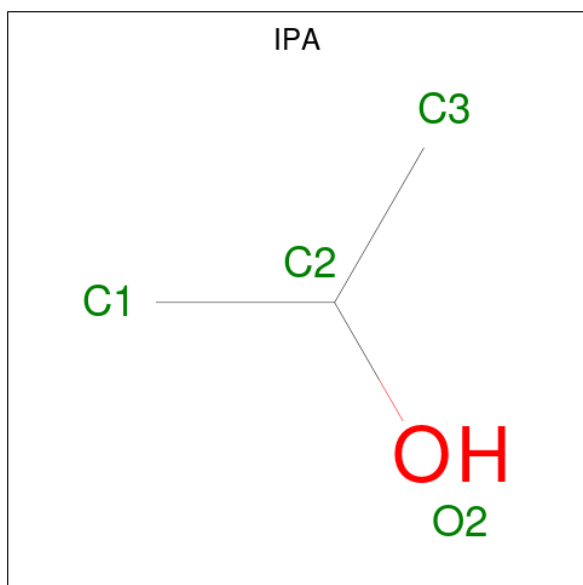
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 3	O 1	0	0
7	A	1	Total 4	C 3	O 1	0	0
7	E	1	Total 4	C 3	O 1	0	0
7	E	1	Total 4	C 3	O 1	0	0
7	E	1	Total 4	C 3	O 1	0	0
7	E	1	Total 4	C 3	O 1	0	0
7	I	1	Total 4	C 3	O 1	0	0
7	I	1	Total 4	C 3	O 1	0	0
7	I	1	Total 4	C 3	O 1	0	0
7	M	1	Total 4	C 3	O 1	0	0
7	M	1	Total 4	C 3	O 1	0	0
7	O	1	Total 4	C 3	O 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	163	Total 163	O 163	0	0
8	B	32	Total 32	O 32	0	0
8	C	34	Total 34	O 34	0	0
8	D	3	Total 3	O 3	0	0
8	E	180	Total 180	O 180	0	0
8	F	27	Total 27	O 27	0	0
8	G	19	Total 19	O 19	0	0
8	H	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	156	Total 156	O 156	0	0
8	J	29	Total 29	O 29	0	0
8	K	24	Total 24	O 24	0	0
8	L	1	Total 1	O 1	0	0
8	M	169	Total 169	O 169	0	0
8	N	29	Total 29	O 29	0	0
8	O	25	Total 25	O 25	0	0
8	P	5	Total 5	O 5	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.
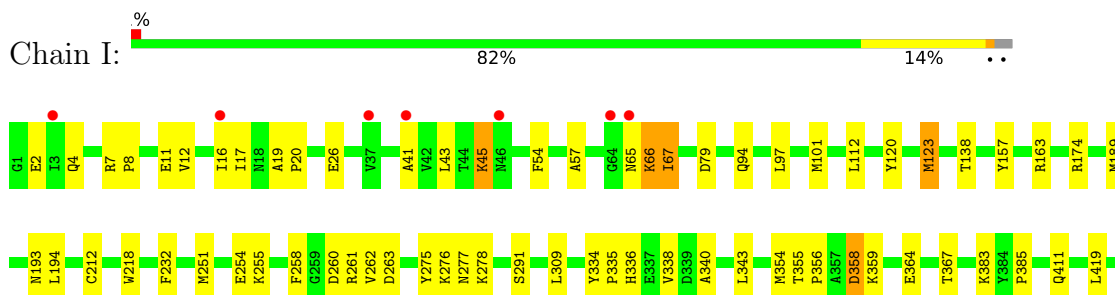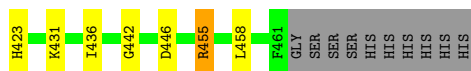
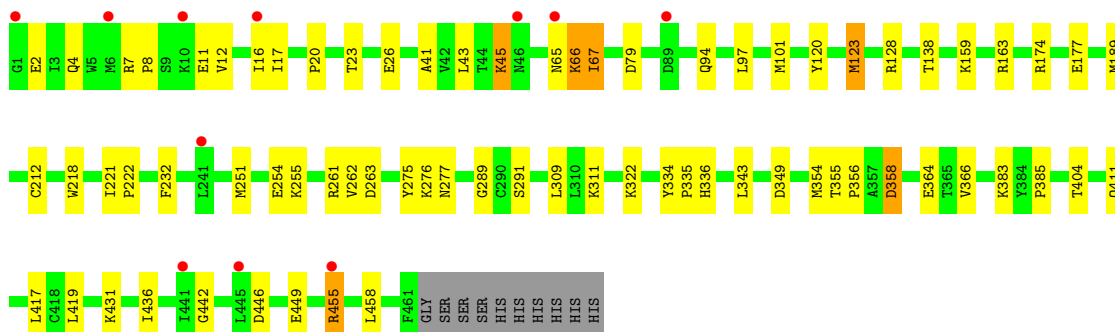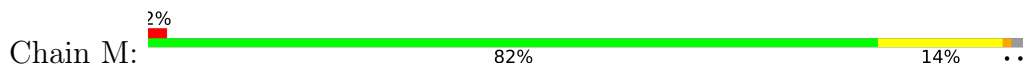- Molecule 1: Polymerase
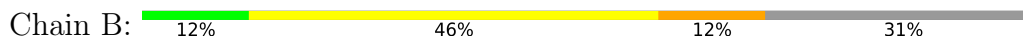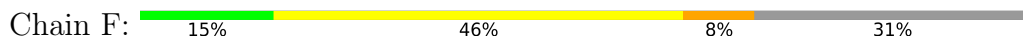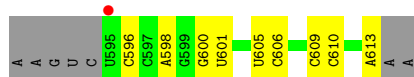

- Molecule 1: Polymerase

- Molecule 1: Polymerase

H423 K431 I436 G442 D446 R455 L458 F461 GLY SER SER HIS HIS HIS HIS HIS

• Molecule 1: Polymerase

Chain M:

2%

82%   14%

G1 E2 I3 Q4 W5 M6 R7 P8 S9 K10 E11 V12 I16 I17 P20 T23 E26 A41 V42 L43 T44 K45 N46 N65 K66 I67 D79 D89 Q94 L97 M101 Y120 M123 R128 T138 K159 R163 R174 E177 M189

C212 W218 I221 P222 F232 L241 M251 E254 K255 R261 V262 D263 Y275 K276 N277 G289 C290 S291 L309 L310 K311 K322 Y334 P335 H336 L343 D349 M354 T355 P356 A357 D358 E364 T365 V366 K383 Y384 P385 T404 Q411

L417 C418 L419 K431 I436 I441 G442 L445 D446 E449 R455 L458 F461 GLY SER SER SER HIS HIS HIS HIS HIS

• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*U*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

Chain B:

12%   46%   12%   31%

A A G U C U C596 C597 A598 G599 G600 U601 C602 U603 C604 U605 C606 G607 U608 C609 C610 A613 A A

• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*U*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

Chain F:

15%   46%   8%   31%

A A G U C C596 C597 A598 G599 G600 U601 C602 U603 C604 U605 C606 G607 U608 C609 C610 A613 A A

• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*U*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

Chain J:

4%

38%   35%   27%

A A G U C U595 C596 C597 A598 G599 G600 U601 U605 C606 C609 C610 A613 A A

• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*U*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

Chain N:

38%   35%   27%

A A G U C U595 C596 C597 A598 G599 G600 U601 U605 C606 C609 C610 A613 A A

• Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')

Chain C:

• Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')

Chain G:

• Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')

Chain K:

• Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')
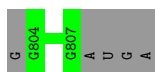
Chain O:

• Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')
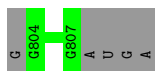
Chain D:

• Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

Chain H:

• Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

Chain L:

• Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

Chain P:

44%   56%

G G804 G807 A U G A

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.53Å 60.54Å 192.94Å 83.82° 83.84° 77.35°	Depositor
Resolution (Å)	45.23 – 2.41 45.22 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.23-2.41) 96.7 (45.22-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.217 , 0.261 0.199 , 0.247	Depositor DCC
R_{free} test set	7555 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.63$, $< L^2 > = 0.50$	Xtriage
Estimated twinning fraction	0.430 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18860	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7521e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: IPA, ZN, DCT

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	0.43	0/3787	0.56	0/5122
1	E	0.44	0/3787	0.56	0/5122
1	I	0.44	0/3787	0.56	0/5122
1	M	0.44	0/3787	0.57	0/5122
2	B	0.63	0/400	1.00	1/621 (0.2%)
2	F	0.66	0/400	0.98	0/621
2	J	0.63	0/422	0.93	0/655
2	N	0.62	0/422	0.94	0/655
3	C	0.65	0/340	0.97	0/530
3	G	0.68	0/340	1.00	0/530
3	K	0.60	0/340	0.93	0/530
3	O	0.59	0/340	1.03	0/530
4	D	0.25	0/76	0.58	0/117
4	H	0.24	0/76	0.54	0/117
4	L	0.26	0/102	0.47	0/158
4	P	0.24	0/102	0.48	0/158
All	All	0.47	0/18508	0.65	1/25710 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	608	U	N1-C2-O2	-5.25	119.12	122.80

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	3697	0	3658	67	0
1	E	3697	0	3658	71	0
1	I	3697	0	3658	56	0
1	M	3697	0	3658	55	0
2	B	361	0	183	20	0
2	F	361	0	183	20	0
2	J	381	0	193	5	0
2	N	381	0	193	6	0
3	C	303	0	156	5	0
3	G	303	0	156	4	0
3	K	303	0	156	5	0
3	O	303	0	156	7	0
4	D	68	0	34	0	0
4	H	68	0	34	0	0
4	L	91	0	45	0	0
4	P	91	0	45	0	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
5	M	1	0	0	0	0
6	A	27	0	12	2	0
6	E	27	0	12	3	0
6	I	27	0	12	1	0
6	M	27	0	12	3	0
7	A	8	0	16	7	0
7	E	16	0	32	6	0
7	I	12	0	24	7	0
7	M	8	0	16	9	0
7	O	4	0	8	1	0
8	A	163	0	0	5	0
8	B	32	0	0	1	0
8	C	34	0	0	0	0
8	D	3	0	0	0	0
8	E	180	0	0	7	0
8	F	27	0	0	2	0
8	G	19	0	0	0	0
8	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	156	0	0	8	0
8	J	29	0	0	0	0
8	K	24	0	0	0	0
8	L	1	0	0	0	0
8	M	169	0	0	6	0
8	N	29	0	0	0	0
8	O	25	0	0	1	0
8	P	5	0	0	0	0
All	All	18860	0	16310	310	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 9.

The worst 5 of 310 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:M:364:GLU:H	7:M:6025:IPA:H13	1.05	1.07
1:E:404:THR:HA	7:E:6010:IPA:H12	1.48	0.96
1:I:336:HIS:HB2	7:I:6023:IPA:H33	1.44	0.95
1:M:336:HIS:HB2	7:M:6031:IPA:C1	1.98	0.94
1:M:364:GLU:N	7:M:6025:IPA:H13	1.90	0.87

There are no symmetry-related clashes.

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	459/471 (98%)	443 (96%)	15 (3%)	1 (0%)	47	61
1	E	459/471 (98%)	445 (97%)	13 (3%)	1 (0%)	47	61
1	I	459/471 (98%)	447 (97%)	11 (2%)	1 (0%)	47	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	459/471 (98%)	446 (97%)	12 (3%)	1 (0%)	47	61
All	All	1836/1884 (98%)	1781 (97%)	51 (3%)	4 (0%)	47	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	66	LYS
1	M	66	LYS
1	A	285	GLY
1	E	285	GLY

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	403/412 (98%)	378 (94%)	25 (6%)	18	28
1	E	403/412 (98%)	377 (94%)	26 (6%)	17	26
1	I	403/412 (98%)	386 (96%)	17 (4%)	30	46
1	M	403/412 (98%)	387 (96%)	16 (4%)	31	48
All	All	1612/1648 (98%)	1528 (95%)	84 (5%)	23	37

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	174	ARG
1	M	45	LYS
1	I	218	TRP
1	I	419	LEU
1	M	212	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	269	ASN
1	M	4	GLN
1	E	320	HIS
1	I	411	GLN
1	E	170	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	16/26 (61%)	2 (12%)	0
2	F	16/26 (61%)	2 (12%)	0
2	J	17/26 (65%)	1 (5%)	0
2	N	17/26 (65%)	1 (5%)	0
3	C	13/14 (92%)	0	0
3	G	13/14 (92%)	0	0
3	K	13/14 (92%)	0	0
3	O	13/14 (92%)	0	0
4	D	2/9 (22%)	1 (50%)	0
4	H	2/9 (22%)	1 (50%)	0
4	L	3/9 (33%)	0	0
4	P	3/9 (33%)	0	0
All	All	128/196 (65%)	8 (6%)	0

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	597	C
2	B	598	A
4	D	806	A
2	F	597	C
2	F	598	A

There are no RNA pucker outliers to report.

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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	IPA	I	6015	-	3,3,3	0.54	0	3,3,3	0.37	0
7	IPA	A	6032	-	3,3,3	0.39	0	3,3,3	0.56	0
7	IPA	E	6027	-	3,3,3	0.53	0	3,3,3	0.35	0
7	IPA	O	6009	-	3,3,3	0.58	0	3,3,3	0.42	0
7	IPA	M	6031	-	3,3,3	0.30	0	3,3,3	0.60	0
7	IPA	E	6028	-	3,3,3	0.55	0	3,3,3	0.34	0
7	IPA	A	6008	-	3,3,3	0.62	0	3,3,3	0.35	0
7	IPA	E	6010	-	3,3,3	0.47	0	3,3,3	0.42	0
7	IPA	I	6023	-	3,3,3	0.50	0	3,3,3	0.43	0
6	DCT	E	4003	-	24,28,28	1.77	2 (8%)	33,43,43	1.43	3 (9%)
7	IPA	E	6007	-	3,3,3	0.62	0	3,3,3	0.36	0
7	IPA	M	6025	-	3,3,3	0.54	0	3,3,3	0.26	0
6	DCT	I	4002	-	24,28,28	1.82	2 (8%)	33,43,43	1.58	7 (21%)
6	DCT	A	4004	-	24,28,28	1.80	2 (8%)	33,43,43	1.52	6 (18%)
7	IPA	I	6026	-	3,3,3	0.63	0	3,3,3	0.29	0
6	DCT	M	4001	-	24,28,28	1.79	2 (8%)	33,43,43	1.31	5 (15%)

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
6	DCT	A	4004	-	-	3/22/31/31	0/2/2/2
6	DCT	E	4003	-	-	3/22/31/31	0/2/2/2
6	DCT	M	4001	-	-	2/22/31/31	0/2/2/2
6	DCT	I	4002	-	-	5/22/31/31	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	4002	DCT	O2-C2	7.17	1.37	1.23
6	M	4001	DCT	O2-C2	7.08	1.36	1.23
6	A	4004	DCT	O2-C2	6.96	1.36	1.23
6	E	4003	DCT	O2-C2	6.81	1.36	1.23
6	E	4003	DCT	C2-N1	-2.65	1.34	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	4002	DCT	C2'-C1'-N1	-4.11	104.61	112.40
6	I	4002	DCT	PB-O3B-PG	-4.10	118.74	132.83
6	A	4004	DCT	PB-O3B-PG	-3.98	119.19	132.83
6	E	4003	DCT	PB-O3B-PG	-3.81	119.76	132.83
6	A	4004	DCT	C2'-C1'-N1	-3.58	105.61	112.40

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4004	DCT	C5'-O5'-PA-O1A
6	A	4004	DCT	C5'-O5'-PA-O2A
6	E	4003	DCT	C5'-O5'-PA-O1A
6	E	4003	DCT	C5'-O5'-PA-O3A
6	I	4002	DCT	C3'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	6015	IPA	1	0
7	A	6032	IPA	7	0
7	O	6009	IPA	1	0
7	M	6031	IPA	4	0
7	E	6028	IPA	3	0
7	E	6010	IPA	3	0
7	I	6023	IPA	3	0
6	E	4003	DCT	3	0
7	M	6025	IPA	5	0
6	I	4002	DCT	1	0
6	A	4004	DCT	2	0
7	I	6026	IPA	3	0
6	M	4001	DCT	3	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 DCT E 4003

Bond lengths   Bond angles

Torsions   Rings

Ligand DCT I 4002

Bond lengths

Bond angles

Torsions

Rings

Ligand DCT A 4004

Bond lengths

Bond angles

Torsions

Rings

Ligand DCT M 4001

Bond lengths

Bond angles

Torsions

Rings
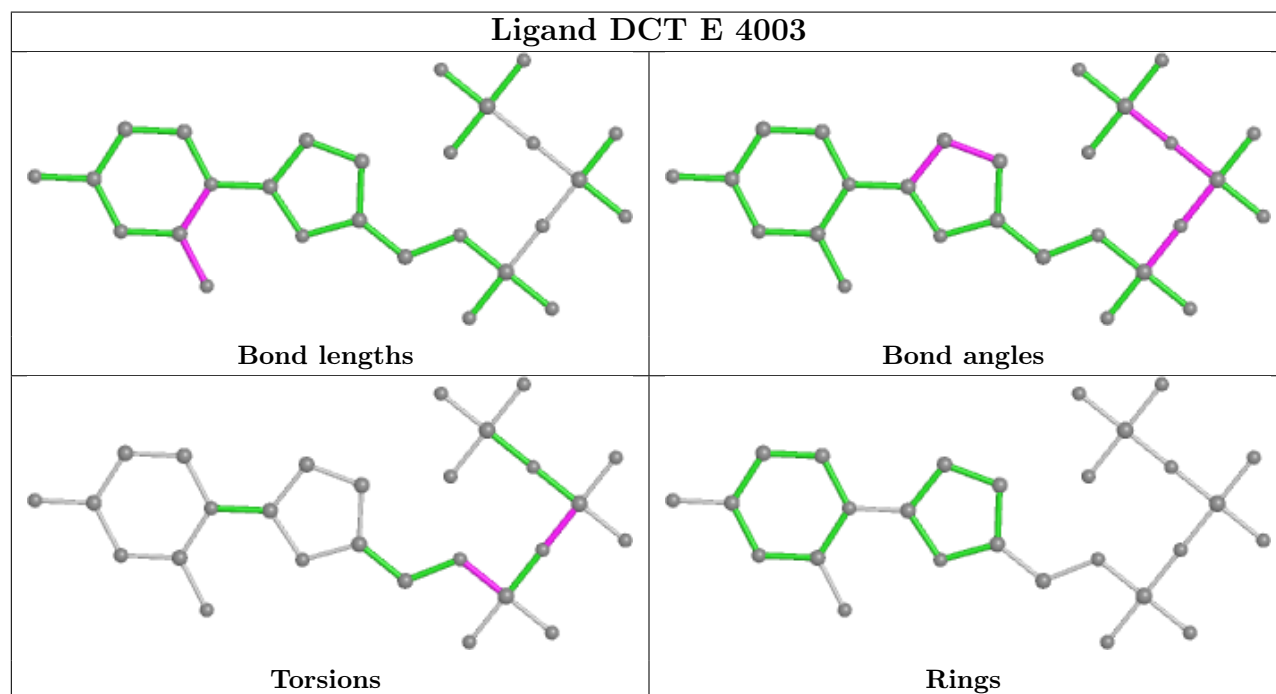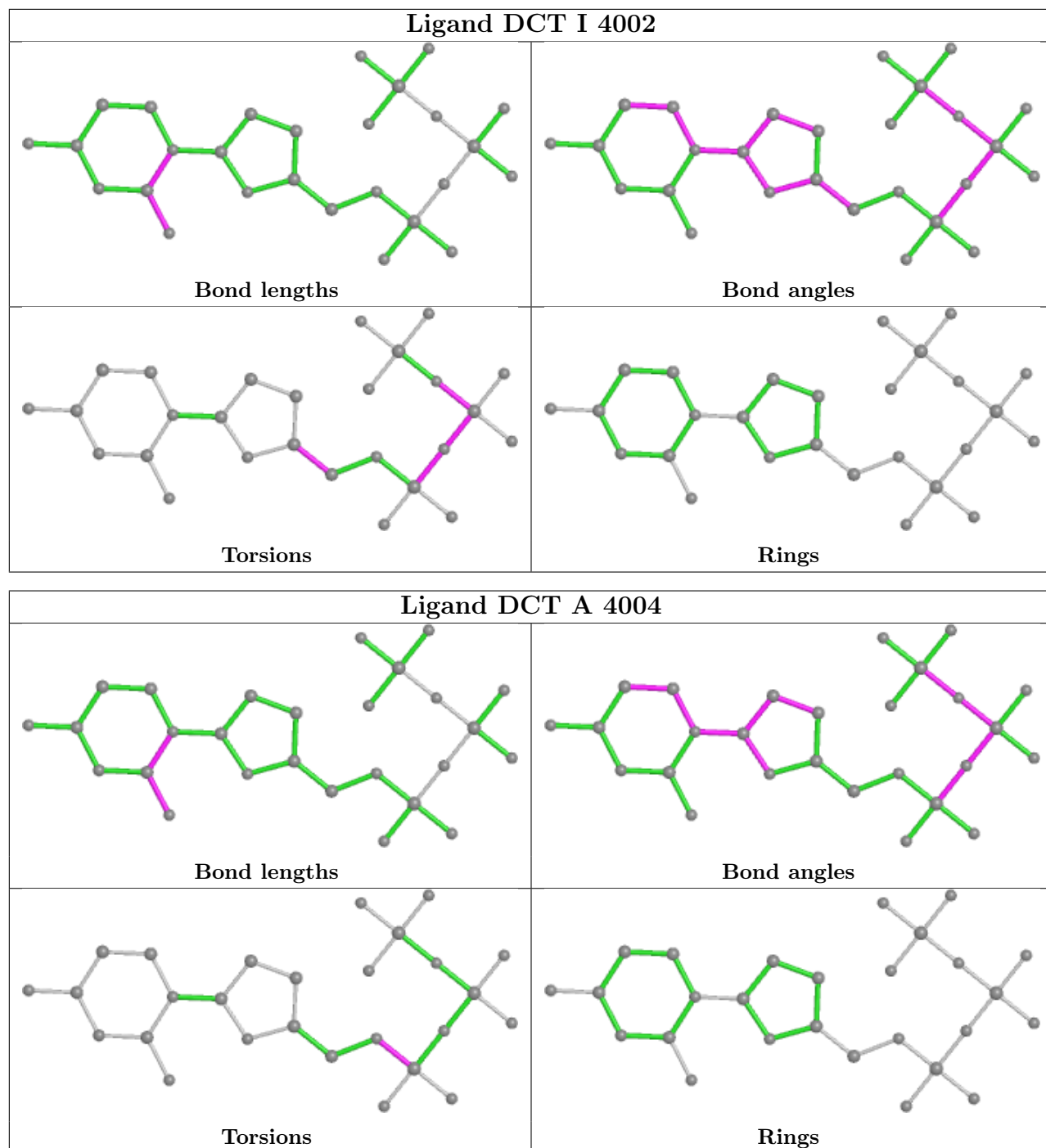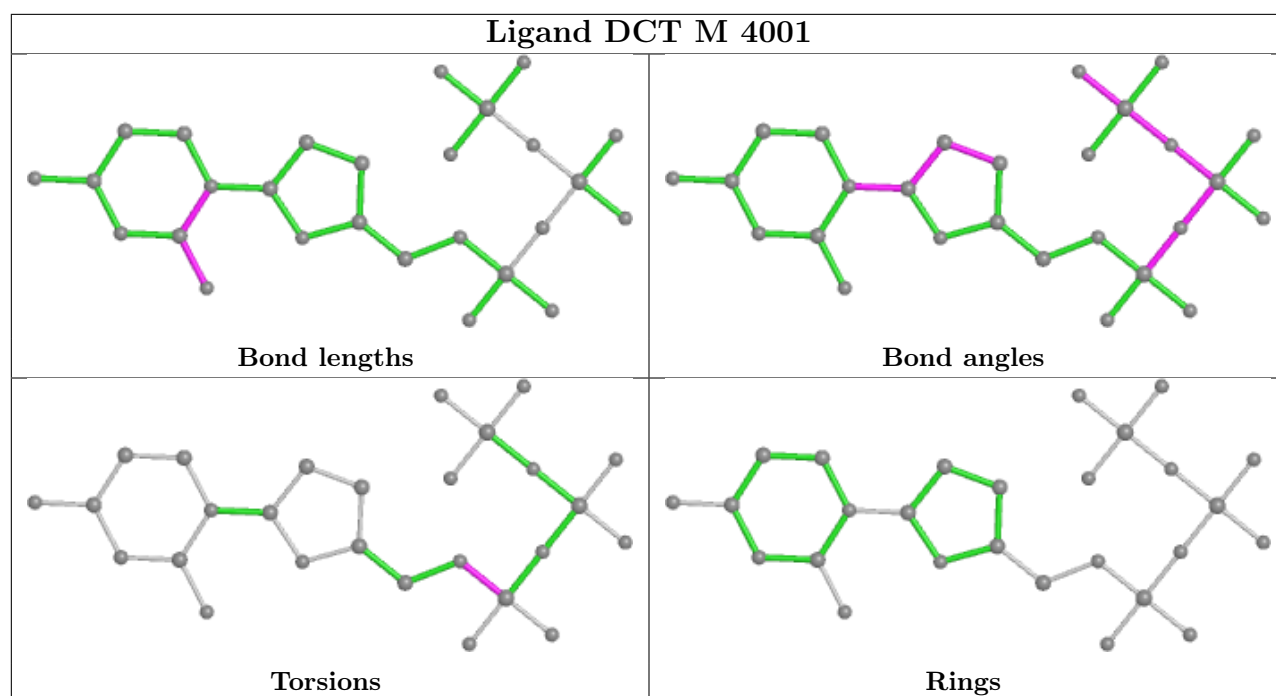
5.7 Other polymers (i)

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 ⓘ

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(Å²)	Q<0.9
1	A	461/471 (97%)	-0.28	9 (1%)	65	62	38, 57, 99, 130	0
1	E	461/471 (97%)	-0.32	8 (1%)	70	67	37, 56, 99, 130	0
1	I	461/471 (97%)	-0.34	7 (1%)	73	71	37, 57, 94, 131	0
1	M	461/471 (97%)	-0.31	11 (2%)	59	56	37, 57, 93, 131	0
2	B	18/26 (69%)	-0.91	0	100	100	47, 58, 140, 153	0
2	F	18/26 (69%)	-1.13	0	100	100	46, 57, 140, 153	0
2	J	19/26 (73%)	-0.67	1 (5%)	26	24	44, 62, 158, 162	0
2	N	19/26 (73%)	-1.03	0	100	100	45, 63, 158, 162	0
3	C	14/14 (100%)	-1.17	0	100	100	47, 55, 112, 119	0
3	G	14/14 (100%)	-1.06	0	100	100	47, 55, 111, 119	0
3	K	14/14 (100%)	-1.18	0	100	100	44, 58, 120, 121	0
3	O	14/14 (100%)	-1.05	0	100	100	44, 58, 120, 121	0
4	D	3/9 (33%)	0.14	0	100	100	134, 134, 137, 153	0
4	H	3/9 (33%)	0.65	1 (33%)	0	0	134, 134, 138, 154	0
4	L	4/9 (44%)	0.28	0	100	100	118, 121, 137, 168	0
4	P	4/9 (44%)	-0.04	0	100	100	118, 121, 137, 168	0
All	All	1988/2080 (95%)	-0.35	37 (1%)	66	64	37, 57, 102, 168	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	GLY	7.6
1	I	46	ASN	7.5
1	A	46	ASN	6.8
1	I	65	ASN	5.6
1	M	65	ASN	5.3

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
7	IPA	I	6026	4/4	0.78	0.18	49,72,82,97	0
5	ZN	A	2001	1/1	0.79	0.38	102,102,102,102	1
7	IPA	M	6025	4/4	0.81	0.19	76,79,96,118	0
7	IPA	O	6009	4/4	0.83	0.16	55,78,78,82	0
6	DCT	A	4004	27/27	0.84	0.17	35,86,154,172	27
7	IPA	E	6027	4/4	0.86	0.27	80,81,87,88	0
5	ZN	I	2003	1/1	0.87	0.05	96,96,96,96	1
6	DCT	M	4001	27/27	0.90	0.14	36,78,139,174	27
7	IPA	A	6008	4/4	0.90	0.32	48,67,69,80	0
6	DCT	I	4002	27/27	0.90	0.14	34,74,116,186	27
7	IPA	I	6023	4/4	0.91	0.27	68,97,99,114	0
7	IPA	M	6031	4/4	0.91	0.22	94,94,102,114	0
7	IPA	I	6015	4/4	0.91	0.23	63,80,80,88	0
5	ZN	M	2004	1/1	0.92	0.05	93,93,93,93	1
7	IPA	A	6032	4/4	0.92	0.14	57,78,78,86	0
6	DCT	E	4003	27/27	0.92	0.12	36,86,138,159	27
7	IPA	E	6028	4/4	0.93	0.13	67,76,82,84	0
7	IPA	E	6007	4/4	0.94	0.29	52,61,71,72	0
5	ZN	E	2002	1/1	0.96	0.30	116,116,116,116	1
7	IPA	E	6010	4/4	0.96	0.11	54,62,62,89	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 DCT A 4004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
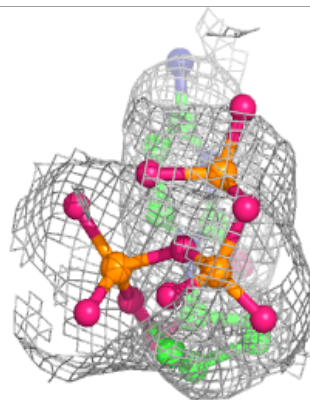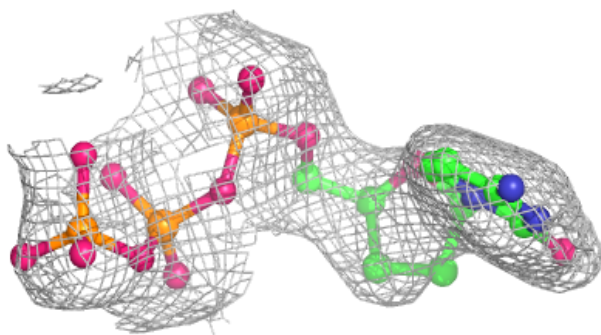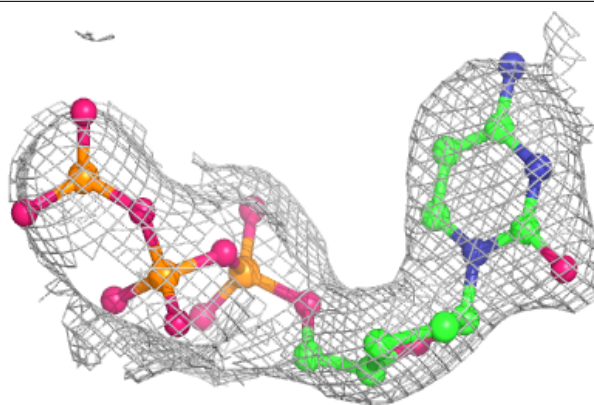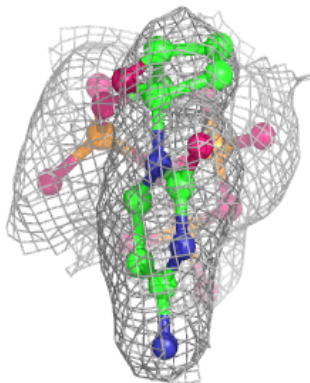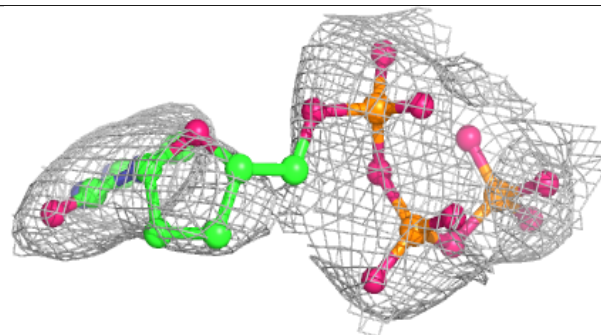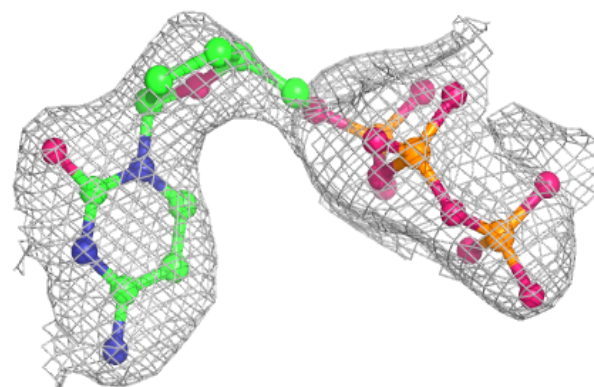mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
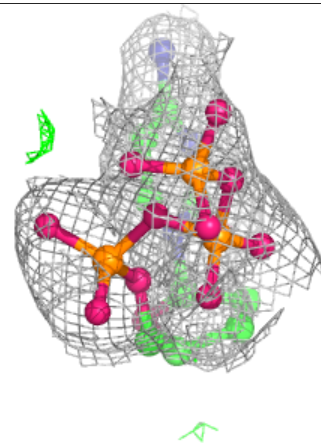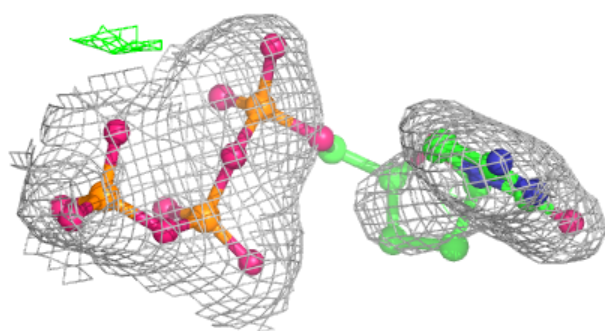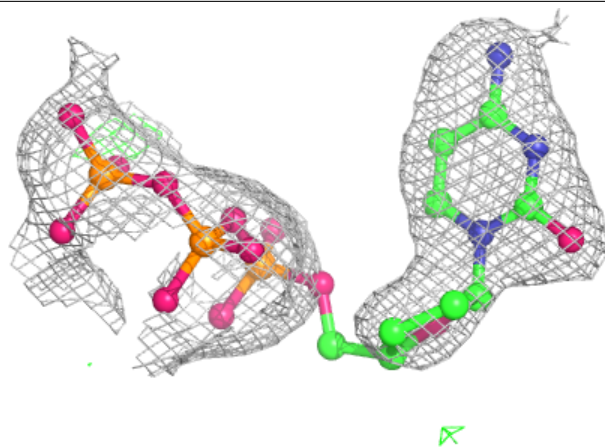
Electron density around DCT M 4001:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
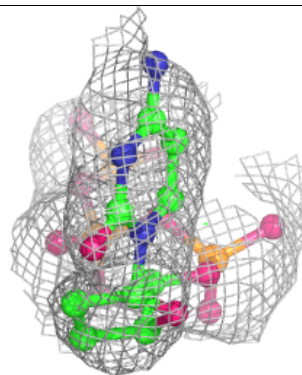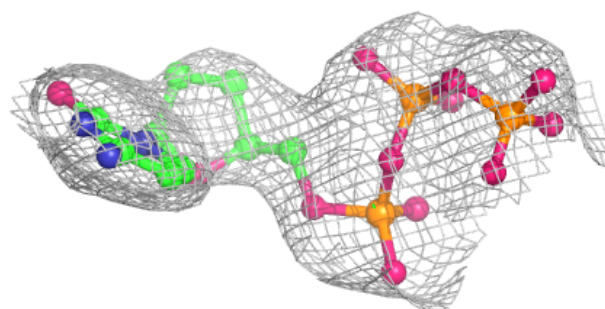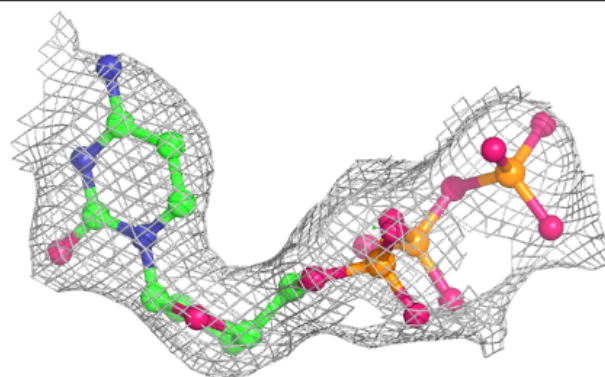
Electron density around DCT I 4002:

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

Electron density around DCT E 4003:

$2mF_o$-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.