WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 25, 2024 – 02:38 AM EST

PDB ID	:	4ZTZ
Title	:	Structural basis for processivity and antiviral drug toxicity in human mito-chondrial DNA replicase
Authors	:	Szymanski, M.R.; Yin, Y.W.
Deposited on	:	2015-05-15
Resolution	:	3.44 Å(reported)

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

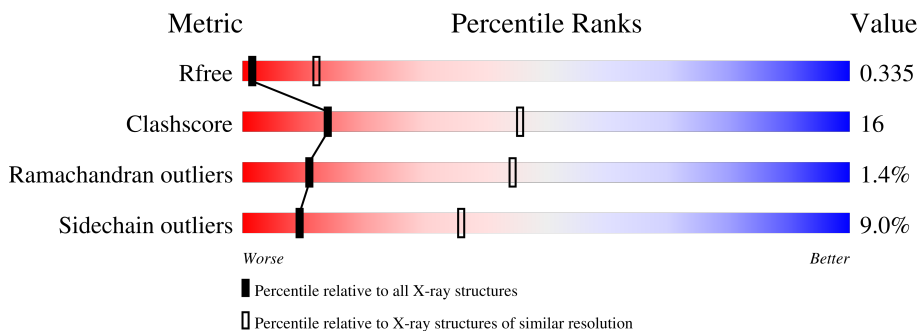|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.44 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		0.335
Clashscore		16
Ramachandran outliers		1.4%
Sidechain outliers		9.0%

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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)

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%

Mol	Chain	Length	Quality of chain
1	A	1222	53% 23% • 20%
2	B	472	58% 17% • 23%
2	C	472	55% 17% • 24%
3	T	27	52% 41% 7%
4	P	24	54% 38% 8%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 14651 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 polymerase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	983	Total 7823	C 4983	N 1371	O 1419	S 50	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	expression tag	UNP P54098
A	198	ALA	ASP	conflict	UNP P54098
A	200	ALA	GLU	conflict	UNP P54098
A	1240	ALA	-	expression tag	UNP P54098
A	1241	ALA	-	expression tag	UNP P54098
A	1242	ALA	-	expression tag	UNP P54098
A	1243	LEU	-	expression tag	UNP P54098
A	1244	GLU	-	expression tag	UNP P54098
A	1245	HIS	-	expression tag	UNP P54098
A	1246	HIS	-	expression tag	UNP P54098
A	1247	HIS	-	expression tag	UNP P54098
A	1248	HIS	-	expression tag	UNP P54098
A	1249	HIS	-	expression tag	UNP P54098
A	1250	HIS	-	expression tag	UNP P54098

- Molecule 2 is a protein called DNA polymerase subunit gamma-2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total 2942	C 1885	N 520	O 521	S 16	0	0	0
2	C	358	Total 2893	C 1857	N 509	O 511	S 16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	MET	-	expression tag	UNP Q9UHN1
B	486	ALA	-	expression tag	UNP Q9UHN1
B	487	ALA	-	expression tag	UNP Q9UHN1
B	488	ALA	-	expression tag	UNP Q9UHN1
B	489	LEU	-	expression tag	UNP Q9UHN1
B	490	GLU	-	expression tag	UNP Q9UHN1
B	491	HIS	-	expression tag	UNP Q9UHN1
B	492	HIS	-	expression tag	UNP Q9UHN1
B	493	HIS	-	expression tag	UNP Q9UHN1
B	494	HIS	-	expression tag	UNP Q9UHN1
B	495	HIS	-	expression tag	UNP Q9UHN1
B	496	HIS	-	expression tag	UNP Q9UHN1
C	25	MET	-	expression tag	UNP Q9UHN1
C	486	ALA	-	expression tag	UNP Q9UHN1
C	487	ALA	-	expression tag	UNP Q9UHN1
C	488	ALA	-	expression tag	UNP Q9UHN1
C	489	LEU	-	expression tag	UNP Q9UHN1
C	490	GLU	-	expression tag	UNP Q9UHN1
C	491	HIS	-	expression tag	UNP Q9UHN1
C	492	HIS	-	expression tag	UNP Q9UHN1
C	493	HIS	-	expression tag	UNP Q9UHN1
C	494	HIS	-	expression tag	UNP Q9UHN1
C	495	HIS	-	expression tag	UNP Q9UHN1
C	496	HIS	-	expression tag	UNP Q9UHN1

- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	25	Total 508	C 241	N 89	O 153	P 25	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(P*AP*AP*GP*AP*CP*GP*AP*GP*GP*G P*CP*CP*AP*GP*TP*GP*CP*CP*GP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	22	Total 455	C 214	N 92	O 127	P 22	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Mg 2	0	0

- Molecule 6 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).
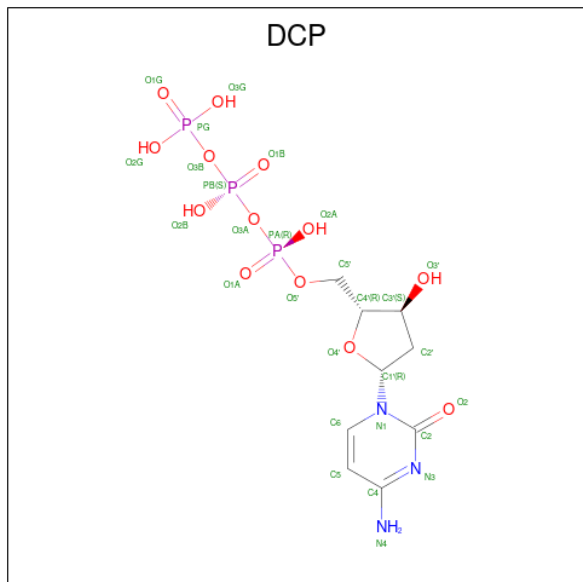
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	28	9	3	13	3	0	0

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. 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. 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 polymerase subunit gamma-1

Chain A:

E1084 P1085 V1088 Q1089 E1090 R1096 V1097 N1098 W1099 V1100 V1101 Y1108 A1115 W1118 L1119 F1120 A1124 F1129 C1130 I1133 H1134 D1135 E1136 L1140 V1141 E1142 E1143 E1144 R1148 Q1154 I1155 T1156 N1157 R1161 C1162 M1163 Y1166 K1167 D1172 L1173 P1174 V1177 A1178 V1183

D1184 I1185 D1186 R1187 R1190 K1191 C1197 K1198 T1199 P1200 S1201 N1202 E1207 R1208 R1209 Y1210 Q1214 G1215 L1218 K1228 GLY SER LEU GLU LYS ARG SER GLN PRO GLY PRO ALA ALA LEU GLU HIS HIS HIS HIS HIS

- Molecule 2: DNA polymerase subunit gamma-2, mitochondrial

Chain B: 58% 17% • 23%

MET ASP ALA GLY GLN PRO GLU LEU LEU THR GLU ARG SER SER PRO LYS GLY HIS VAL LYS SER HIS ALA GLU LEU GLU GLU ASN GLY GLU HIS PRO GLU ALA PRO GLY SER GLY GLY SER GLU A68 L69 L70 R75 R76 H77 F78 L79 K83 Q84 Q85 P101 L102 G103

V104 R107 S117 R122 H133 G136 PRO LEU LEU PRO GLY ASP SER ALA PHE ARG LEU VAL SER ALA GLU LEU GLU THR LEU ARG GLU GLU ILE LEU GLN ASP LYS GLU LEU SER LYS GLU GLN VAL ALA PHE LEU GLU ASN VAL LEU LYS THR SER G179 K180 L181 L185 L186

Y193 L197 V200 N201 K202 R203 V213 F219 D220 T221 LYS GLN ILE ARG ASN GLY VAL K229 S230 I231 T235 W241 P244 P245 L252 W262 W263 R264 K265 F266 C278 K288 L303 K329 P333 L336 S337 V338 Q355 LEU THR GLU ASN SER

PHE T362 R363 K364 K365 N366 L367 H368 L372 H375 K382 V383 A384 L385 G388 L393 E394 L395 R396 L402 F403 N404 L407 E408 S412 L418 E419 T420 M421 Q422 S423 S424 L428 K431 E434 M435 S436 I437 L438 F439 T440 V441 L442 V443 T444 E445 T446 T447

N450 G451 L452 I453 H454 L455 R456 S457 T460 T461 H467 I468 S469 K470 V485 ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS

- Molecule 2: DNA polymerase subunit gamma-2, mitochondrial

Chain C: 55% 17% • 24%

MET ASP ALA GLY GLN PRO GLU LEU LEU THR GLU ARG SER SER PRO LYS GLY HIS VAL LYS SER HIS ALA GLU LEU GLU GLU ASN GLY GLU HIS PRO GLU ALA PRO GLY SER GLY GLY SER GLU E67 I72 R75 K83 Q84 Q85 L86 S87 R88 L91 H96 P97 G98

P101 L102 G103 V104 E105 L106 N109 W115 V120 F121 R122 F126 H132 H133 K134 P135 G136 P137 LEU LEU PRO GLY ASP SER ALA PHE ARG LEU VAL SER ALA GLU THR LEU ARG GLU ILE LEU GLN ASP LYS GLU LEU SER LYS GLU GLN VAL ALA PHE LEU GLU ASN

VAL LEU LYS THR SER GLY K180 L181 N184 L185 L186 L197 D198 L199 V200 N201 K202 R203 L204 P205 A209 V213 F219 ASP THR LYS GLN ILE ARG ASN G227 V228 K229 E233 K234 T235 L239 T243 P244 P245 R246 W251 L252 L256 R257 W262 W263 R264 K265

P270 C278 E281 E282 G283 R284 K288 N292 F293 P294 W295 I300 L303 W304 N305 P316 G317 N318 V319 L322 D326 V338 D343 L347 Q355 LEU THR GLU ASN SER PHE THR ARG LYS LYS ASN LEU H368 P380 I381 L385 D386 R389

G390 P391 L395 L402 W414 P415 E419 T420 S424 Q427 T440 V441 L442 V443 T444 E445 I453 H454 L455 R456 K472 V485 ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS

- Molecule 3: DNA (25-MER)

Chain T: 52% 41% 7%

G2 C3 G4 A5 T6 A7 C8 G9 G10 T14 G15 G16 C21 T26 DT DT

• Molecule 4: DNA (5'-D(P*AP*AP*GP*AP*CP*GP*AP*GP*GP*GP*CP*CP*AP*GP*TP*G P*CP*CP*GP*TP*AP*C)-3')

Chain P:

54%   38%   8%

DA DA A3 G8 G12 C13 C14 A15 C20 G21 T22 A23 C24

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	217.60Å 217.60Å 165.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.50 – 3.44 49.25 – 3.45	Depositor EDS
% Data completeness (in resolution range)	91.6 (45.50-3.44) 95.2 (49.25-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.280 , 0.320 0.350 , 0.335	Depositor DCC
R_{free} test set	2000 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å^2)	140.7	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 20.0	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	14651	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: DOC, DCP, MG

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	0.26	1/8025 (0.0%)	0.48	6/10886 (0.1%)
2	B	0.21	0/3015	0.39	0/4074
2	C	0.23	0/2966	0.45	2/4009 (0.0%)
3	T	0.47	0/567	0.88	0/872
4	P	0.49	0/492	0.77	0/758
All	All	0.27	1/15065 (0.0%)	0.50	8/20599 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	611	PRO	N-CD	-10.82	1.32	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	611	PRO	N-CA-CB	-11.49	89.52	103.30
2	C	135	PRO	CA-N-CD	-8.60	99.46	111.50
2	C	96	HIS	C-N-CD	-8.37	102.18	120.60
1	A	611	PRO	N-CD-CG	-6.82	92.97	103.20
1	A	752	LEU	C-N-CD	-6.27	106.81	120.60

There are no chirality outliers.

There are no planarity outliers.

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	7823	0	7729	293	0
2	B	2942	0	2939	58	0
2	C	2893	0	2880	97	0
3	T	508	0	282	15	0
4	P	455	0	245	8	0
5	A	2	0	0	0	0
6	A	28	0	12	4	0
All	All	14651	0	14087	452	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 16.

The worst 5 of 452 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:610:PHE:CE1	1:A:652:ILE:HD13	1.26	1.70
1:A:610:PHE:CD1	1:A:611:PRO:HG3	1.19	1.67
1:A:610:PHE:CE1	1:A:611:PRO:HG3	1.12	1.64
1:A:610:PHE:CG	1:A:611:PRO:HD3	1.29	1.59
1:A:610:PHE:CD1	1:A:611:PRO:CG	1.80	1.58

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	969/1222 (79%)	846 (87%)	106 (11%)	17 (2%)	8	39
2	B	355/472 (75%)	326 (92%)	27 (8%)	2 (1%)	25	62
2	C	350/472 (74%)	327 (93%)	18 (5%)	5 (1%)	11	44
All	All	1674/2166 (77%)	1499 (90%)	151 (9%)	24 (1%)	11	44

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	LEU
1	A	1070	PRO
2	C	97	PRO
1	A	648	PRO
1	A	767	ALA

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	830/1029 (81%)	737 (89%)	93 (11%)	6	26
2	B	325/415 (78%)	308 (95%)	17 (5%)	23	55
2	C	318/415 (77%)	295 (93%)	23 (7%)	14	46
All	All	1473/1859 (79%)	1340 (91%)	133 (9%)	9	36

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

Mol	Chain	Res	Type
2	C	186	LEU
2	C	243	THR
2	C	402	LEU
1	A	761	ASN
1	A	752	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	354	ASN
1	A	497	GLN
1	A	1134	HIS
2	C	427	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	DOC	P	24	4,3	16,19,20	0.43	0	20,26,29	0.44	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
4	DOC	P	24	4,3	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 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	$\#|Z| > 2$
6	DCP	A	4003	5	25,29,29	1.67	6 (24%)	37,45,45	1.32	5 (13%)

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	DCP	A	4003	5	-	0/22/34/34	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4003	DCP	C4-N4	3.69	1.42	1.33
6	A	4003	DCP	C2-N1	-3.51	1.32	1.40
6	A	4003	DCP	C1'-N1	-3.02	1.40	1.48
6	A	4003	DCP	C6-C5	2.57	1.41	1.35
6	A	4003	DCP	PB-O1B	2.23	1.58	1.50

All (5) bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4003	DCP	PB-O3A-PA	-2.94	122.72	132.83
6	A	4003	DCP	PB-O3B-PG	-2.80	123.20	132.83
6	A	4003	DCP	O3'-C3'-C4'	2.68	120.36	110.10
6	A	4003	DCP	O3'-C3'-C2'	2.68	120.47	110.90
6	A	4003	DCP	O2-C2-N3	-2.27	118.64	122.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4003	DCP	4	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 DCP A 4003

Bond lengths

Bond angles

Torsions

Rings
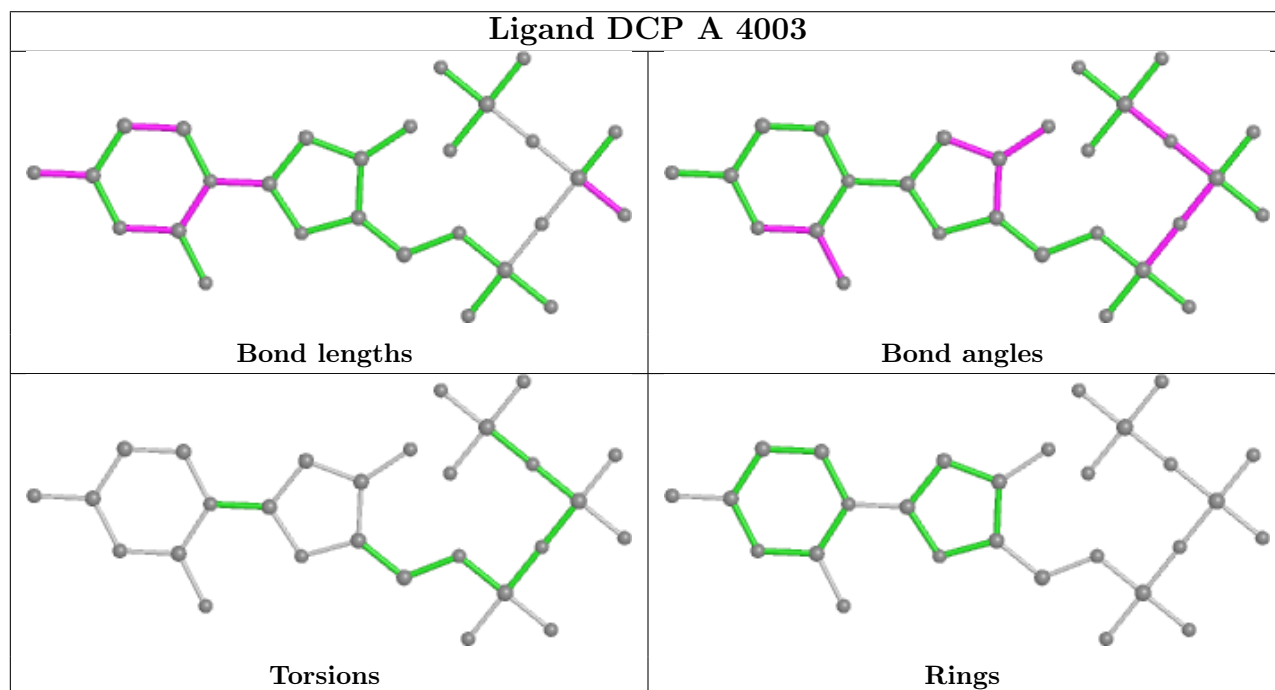
5.7 Other polymers ⓘ

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 ⓘ

6.1   Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

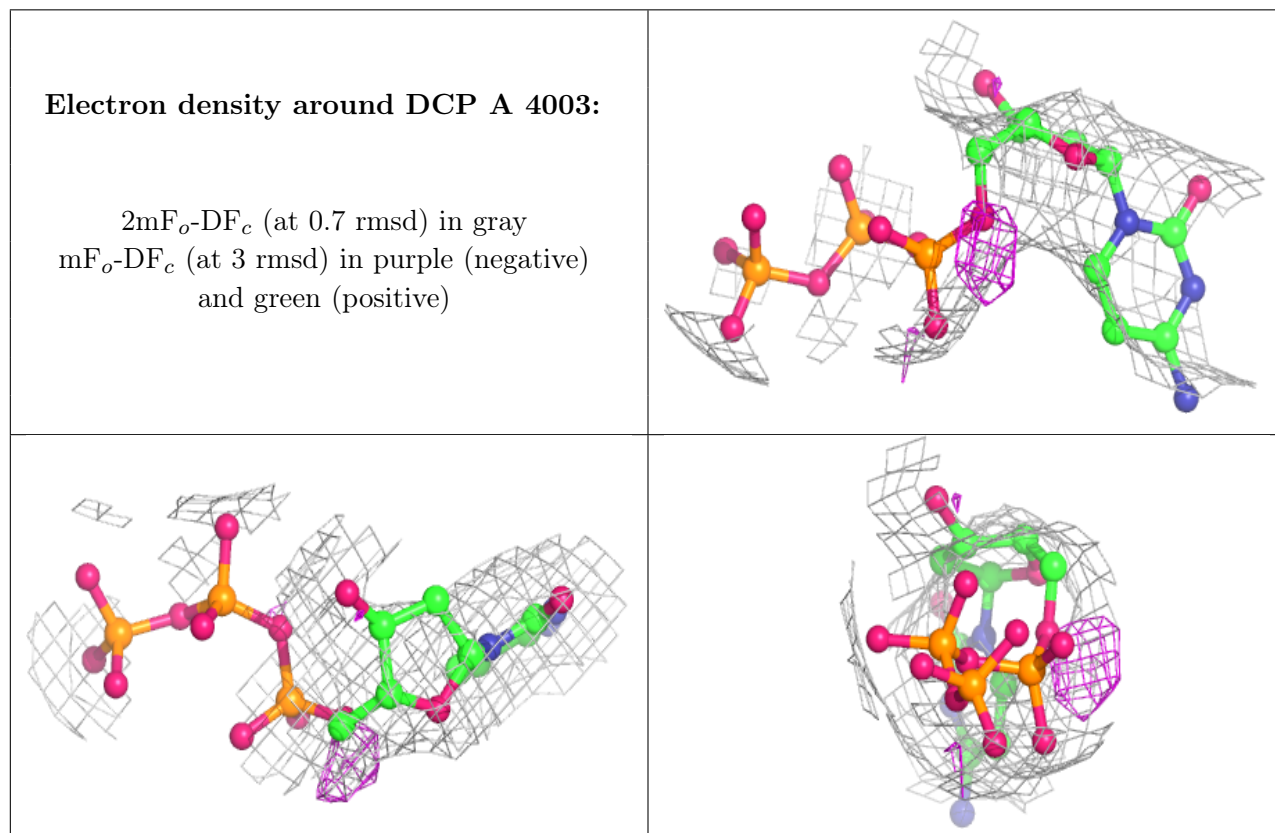Unable to reproduce the depositors R factor - this section is therefore empty.

6.3   Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4   Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 DCP A 4003:

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

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.