



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:25 PM UTC

PDB ID : 4FS2 / pdb_00004fs2
Title : Base pairing mechanism of N2,3-ethenoguanine with dCTP by human polymerase iota
Authors : Zhao, L.
Deposited on : 2012-06-26
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

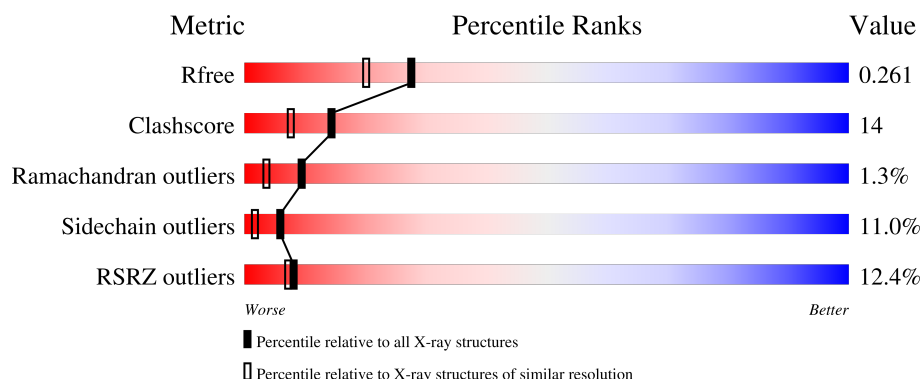
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 $\leq 5\%$. 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	B	18	
1	C	18	
2	A	420	

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
3	MG	A	505	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3422 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 DNA chain called DNA (5'-D(*TP*CP*TP*(EFG)P*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	7	Total	C	N	O	P	0	0	0
			142	67	29	39	7			
1	C	8	Total	C	F	N	O	P	0	0
			169	80	1	30	50	8		

- Molecule 2 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	383	Total	C	N	O	S	0	0	0
			2900	1828	511	540	21			

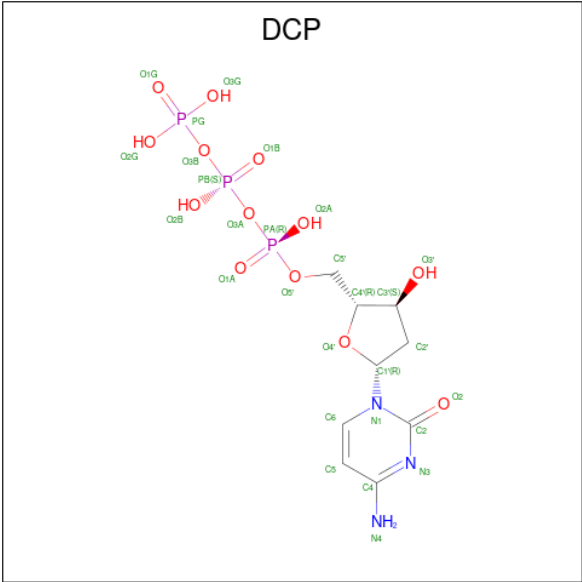
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 6 is water.

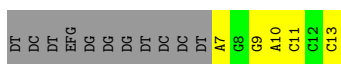
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	8	Total	O	0	0
			8	8		
6	C	22	Total	O	0	0
			22	22		
6	A	149	Total	O	0	0
			149	149		

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.

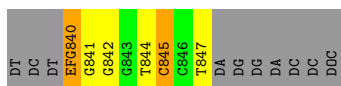
- Molecule 1: DNA (5'-D(*TP*CP*TP*(EFG)P*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*(DOC))-3')

Chain B: 



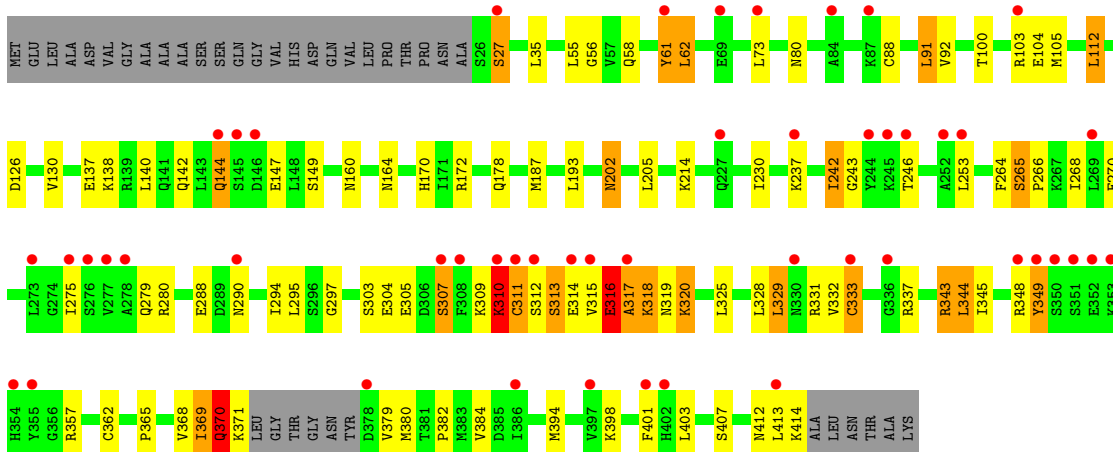
- Molecule 1: DNA (5'-D(*TP*CP*TP*(EFG)P*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*(DOC))-3')

Chain C: 



- Molecule 2: DNA polymerase iota

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.30Å 97.30Å 202.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.26 – 2.05 84.26 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (84.26-2.05) 99.7 (84.26-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.261 0.218 , 0.261	Depositor DCC
R_{free} test set	1822 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3422	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DOC, EFG, 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	B	0.41	0/139	0.90	0/212
1	C	1.03	1/160 (0.6%)	0.91	1/245 (0.4%)
2	A	1.23	5/2940 (0.2%)	1.23	7/3982 (0.2%)
All	All	1.20	6/3239 (0.2%)	1.20	8/4439 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	130	VAL	C-O	6.50	1.30	1.24
2	A	288	GLU	CA-C	-6.38	1.44	1.52
2	A	92	VAL	CA-C	5.88	1.59	1.52
2	A	242	ILE	C-O	5.70	1.30	1.24
2	A	297	GLY	N-CA	5.67	1.52	1.44
1	C	842	DG	O3'-P	-5.33	1.53	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	316	GLU	N-CA-C	-9.16	102.49	114.31
2	A	337	ARG	N-CA-C	-7.61	99.25	110.52
2	A	370	GLN	N-CA-C	6.46	118.01	107.23
2	A	403	LEU	N-CA-C	5.97	118.68	109.07
2	A	349	TYR	N-CA-C	5.44	118.80	110.20
2	A	362	CYS	N-CA-C	-5.39	103.28	108.13
1	C	845	DC	P-O3'-C3'	5.24	128.06	120.20
2	A	27	SER	N-CA-C	5.15	117.94	109.76

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	B	142	0	78	3	2
1	C	169	0	90	5	2
2	A	2900	0	2897	83	0
3	A	3	0	0	0	0
4	A	1	0	0	0	0
5	A	28	0	12	0	0
6	A	149	0	0	6	0
6	B	8	0	0	0	0
6	C	22	0	0	0	0
All	All	3422	0	3077	89	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 14.

All (89) 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:A:310:LYS:HE2	2:A:349:TYR:CB	1.74	1.18
2:A:237:LYS:HE2	6:A:746:HOH:O	1.42	1.16
2:A:35:LEU:HD21	2:A:187:MET:HE1	1.20	1.11
2:A:137:GLU:HG2	2:A:172:ARG:NH2	1.75	1.01
2:A:310:LYS:CE	2:A:349:TYR:CB	2.43	0.96
1:B:11:DC:OP1	2:A:246:THR:HG22	1.67	0.95
2:A:275:ILE:HD11	2:A:279:GLN:HE21	1.31	0.93
2:A:275:ILE:HD11	2:A:279:GLN:NE2	1.84	0.92
2:A:35:LEU:CD2	2:A:187:MET:HE1	2.01	0.90
2:A:35:LEU:HD21	2:A:187:MET:CE	2.02	0.90
2:A:164:ASN:H	2:A:170:HIS:HD2	1.19	0.89
2:A:137:GLU:CG	2:A:172:ARG:HH21	1.89	0.86
2:A:137:GLU:HG2	2:A:172:ARG:HH21	1.36	0.85
2:A:103:ARG:CZ	2:A:331:ARG:HD3	2.08	0.84
1:C:844:DT:H2''	1:C:845:DC:H5'	1.59	0.82
2:A:144:GLN:H	2:A:144:GLN:CD	1.91	0.78
2:A:275:ILE:CD1	2:A:279:GLN:HE21	1.97	0.77
1:C:841:DG:OP2	2:A:307:SER:HB2	1.86	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:331:ARG:HD2	6:A:747:HOH:O	1.85	0.76
2:A:266:PRO:O	2:A:270:GLU:HG3	1.93	0.68
2:A:112:LEU:C	2:A:112:LEU:HD23	2.18	0.68
2:A:164:ASN:H	2:A:170:HIS:CD2	2.09	0.67
2:A:314:GLU:O	2:A:316:GLU:N	2.31	0.64
2:A:318:LYS:HE3	2:A:384:VAL:HG11	1.81	0.63
1:C:840:EFG:O4'	1:C:840:EFG:H10	1.99	0.61
2:A:345:ILE:HB	2:A:407:SER:HB3	1.82	0.61
2:A:144:GLN:CD	2:A:144:GLN:N	2.57	0.60
2:A:243:GLY:H	2:A:246:THR:CG2	2.14	0.60
2:A:368:VAL:O	2:A:368:VAL:HG12	2.00	0.60
2:A:343:ARG:HD3	2:A:345:ILE:HD11	1.84	0.58
2:A:369:ILE:O	2:A:369:ILE:HG22	2.02	0.58
2:A:304:GLU:HG2	2:A:331:ARG:HH21	1.67	0.58
2:A:100:THR:O	2:A:104:GLU:HG3	2.05	0.57
2:A:103:ARG:NH2	2:A:331:ARG:HD3	2.20	0.56
2:A:164:ASN:N	2:A:170:HIS:HD2	1.98	0.55
1:C:844:DT:H2''	1:C:845:DC:C5'	2.35	0.55
2:A:303:SER:O	2:A:331:ARG:NH2	2.40	0.54
2:A:348:ARG:NH1	2:A:394:MET:O	2.36	0.54
2:A:368:VAL:O	2:A:370:GLN:N	2.40	0.54
2:A:379:VAL:O	2:A:382:PRO:HD2	2.09	0.53
2:A:144:GLN:OE1	2:A:147:GLU:CB	2.58	0.52
2:A:242:ILE:HA	2:A:246:THR:HG21	1.90	0.52
2:A:178:GLN:HG2	6:A:717:HOH:O	2.11	0.51
2:A:243:GLY:N	2:A:246:THR:CG2	2.73	0.51
2:A:320:LYS:HE3	2:A:320:LYS:HA	1.91	0.51
2:A:320:LYS:HE3	2:A:320:LYS:CA	2.40	0.51
2:A:202:ASN:ND2	2:A:205:LEU:H	2.08	0.50
2:A:214:LYS:NZ	6:A:637:HOH:O	2.36	0.50
2:A:309:LYS:O	2:A:311:CYS:N	2.44	0.50
2:A:325:LEU:CD1	2:A:329:LEU:HD22	2.42	0.50
2:A:304:GLU:HG3	2:A:328:LEU:HG	1.92	0.50
2:A:412:ASN:HD21	2:A:414:LYS:HE3	1.76	0.50
2:A:202:ASN:HD22	2:A:202:ASN:C	2.20	0.50
2:A:316:GLU:O	2:A:319:ASN:N	2.45	0.50
2:A:371:LYS:N	2:A:371:LYS:HD2	2.27	0.50
1:B:9:DG:H2''	1:B:10:DA:C8	2.47	0.49
2:A:103:ARG:NH1	2:A:331:ARG:HD3	2.27	0.48
2:A:325:LEU:HD12	2:A:380:MET:SD	2.52	0.48
2:A:88:CYS:O	2:A:91:LEU:HB2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:379:VAL:C	2:A:382:PRO:HD2	2.39	0.48
2:A:412:ASN:ND2	2:A:414:LYS:HE3	2.29	0.47
2:A:331:ARG:CD	6:A:747:HOH:O	2.52	0.47
2:A:316:GLU:HG2	2:A:317:ALA:N	2.23	0.47
2:A:265:SER:OG	2:A:268:ILE:HG13	2.15	0.47
2:A:325:LEU:C	2:A:325:LEU:HD13	2.40	0.47
1:B:10:DA:H2'	1:B:11:DC:C6	2.49	0.47
2:A:138:LYS:O	2:A:142:GLN:HG2	2.14	0.47
2:A:112:LEU:C	2:A:112:LEU:CD2	2.88	0.46
2:A:343:ARG:HG2	2:A:344:LEU:N	2.30	0.46
1:C:844:DT:H2'	1:C:845:DC:C6	2.51	0.45
2:A:304:GLU:HG2	2:A:331:ARG:NH2	2.32	0.45
2:A:380:MET:O	2:A:384:VAL:HG23	2.17	0.45
2:A:243:GLY:H	2:A:246:THR:HG22	1.82	0.45
2:A:325:LEU:HD13	2:A:325:LEU:O	2.16	0.45
2:A:62:LEU:HA	2:A:62:LEU:HD22	1.73	0.44
2:A:313:SER:OG	2:A:401:PHE:CB	2.65	0.44
2:A:316:GLU:C	2:A:318:LYS:N	2.74	0.44
2:A:61:TYR:O	2:A:61:TYR:CG	2.70	0.43
2:A:105:MET:CG	2:A:193:LEU:HD11	2.49	0.43
2:A:253:LEU:HD22	2:A:264:PHE:CZ	2.54	0.42
2:A:105:MET:HE1	6:A:741:HOH:O	2.20	0.41
2:A:140:LEU:HD23	2:A:140:LEU:HA	1.89	0.41
2:A:253:LEU:HD22	2:A:264:PHE:HZ	1.85	0.41
2:A:365:PRO:HB2	2:A:368:VAL:HG23	2.02	0.41
2:A:310:LYS:HA	2:A:310:LYS:HD3	1.80	0.41
2:A:61:TYR:CD1	2:A:62:LEU:HD23	2.55	0.41
2:A:329:LEU:O	2:A:333:CYS:HB2	2.20	0.40
2:A:55:LEU:HG	2:A:56:GLY:N	2.37	0.40
2:A:58:GLN:HA	2:A:62:LEU:O	2.22	0.40

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)
1:B:7:DA:P	1:C:847:DT:O3'[10_445]	1.35	0.85
1:B:7:DA:O5'	1:C:847:DT:O3'[10_445]	2.15	0.05

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
2	A	379/420 (90%)	358 (94%)	16 (4%)	5 (1%)	9 3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	310	LYS
2	A	315	VAL
2	A	317	ALA
2	A	73	LEU
2	A	369	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	318/376 (85%)	283 (89%)	35 (11%)	6 2

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	27	SER
2	A	61	TYR
2	A	62	LEU
2	A	80	ASN
2	A	91	LEU
2	A	112	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	126	ASP
2	A	144	GLN
2	A	149	SER
2	A	160	ASN
2	A	202	ASN
2	A	230	ILE
2	A	265	SER
2	A	280	ARG
2	A	290	ASN
2	A	294	ILE
2	A	295	LEU
2	A	305	GLU
2	A	307	SER
2	A	310	LYS
2	A	311	CYS
2	A	312	SER
2	A	313	SER
2	A	316	GLU
2	A	318	LYS
2	A	320	LYS
2	A	329	LEU
2	A	332	VAL
2	A	333	CYS
2	A	343	ARG
2	A	344	LEU
2	A	357	ARG
2	A	370	GLN
2	A	398	LYS
2	A	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	58	GLN
2	A	80	ASN
2	A	170	HIS
2	A	202	ASN
2	A	235	HIS
2	A	262	GLN
2	A	279	GLN
2	A	330	ASN
2	A	340	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	367	HIS
2	A	370	GLN
2	A	412	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	EFG	C	840	-	24,28,29	2.59	13 (54%)	31,42,45	2.12	12 (38%)
1	DOC	B	13	1	16,19,20	0.95	1 (6%)	20,26,29	1.31	3 (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
1	EFG	C	840	-	-	4/7/25/26	0/4/4/4
1	DOC	B	13	1	-	0/7/18/19	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	840	EFG	C9-N3	-5.92	1.29	1.39
1	C	840	EFG	C5-N7	-4.85	1.29	1.39
1	C	840	EFG	C10-N2	-3.71	1.31	1.38
1	C	840	EFG	C4-N3	-3.39	1.30	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	840	EFG	C5-C6	-3.28	1.32	1.44
1	C	840	EFG	C8-N9	-3.12	1.30	1.37
1	C	840	EFG	O3'-C3'	-3.12	1.35	1.43
1	C	840	EFG	C4-N9	-2.64	1.30	1.38
1	C	840	EFG	C2'-C3'	-2.43	1.49	1.52
1	B	13	DOC	C6-N1	-2.28	1.32	1.38
1	C	840	EFG	C2-N2	-2.15	1.30	1.33
1	C	840	EFG	C9-C10	-2.13	1.30	1.35
1	C	840	EFG	C6-N1	-2.12	1.34	1.38
1	C	840	EFG	C5-C4	-2.00	1.33	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	840	EFG	N3-C2-N2	-6.63	108.17	113.33
1	C	840	EFG	F-C2'-C3'	-3.20	102.82	109.14
1	C	840	EFG	O4'-C1'-C2'	-3.07	102.60	105.84
1	C	840	EFG	C10-N2-C2	3.07	107.08	103.26
1	B	13	DOC	O4'-C4'-C3'	2.66	109.18	104.81
1	C	840	EFG	O3'-C3'-C4'	-2.63	103.54	111.08
1	C	840	EFG	C6-C5-C4	2.56	123.09	119.47
1	C	840	EFG	N1-C2-N3	2.50	121.12	119.21
1	C	840	EFG	O4'-C4'-C5'	2.43	117.12	109.33
1	C	840	EFG	C4'-O4'-C1'	-2.33	104.31	109.47
1	B	13	DOC	O4'-C1'-N1	2.14	111.66	107.86
1	B	13	DOC	C3'-C2'-C1'	2.14	105.34	102.87
1	C	840	EFG	C10-C9-N3	2.11	107.31	105.02
1	C	840	EFG	C8-N7-C5	2.11	108.02	104.26
1	C	840	EFG	C5'-C4'-C3'	-2.04	107.87	115.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	840	EFG	O4'-C4'-C5'-O5'
1	C	840	EFG	C3'-C4'-C5'-O5'
1	C	840	EFG	O4'-C1'-N9-C4
1	C	840	EFG	O4'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	840	EFG	1	0

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
5	DCP	A	503	3	28,29,29	1.76	5 (17%)	41,45,45	1.24	4 (9%)

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
5	DCP	A	503	3	-	3/22/34/34	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	DCP	PA-O3A	5.08	1.65	1.59
5	A	503	DCP	PB-O3B	3.13	1.62	1.59
5	A	503	DCP	C5-C4	-3.13	1.35	1.42
5	A	503	DCP	PB-O3A	2.87	1.62	1.59
5	A	503	DCP	O2-C2	2.59	1.28	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	DCP	O3G-PG-O2G	2.93	118.79	107.80
5	A	503	DCP	O2A-PA-O1A	2.81	125.50	112.44
5	A	503	DCP	O2A-PA-O3A	-2.76	99.82	107.27
5	A	503	DCP	C4-N3-C2	2.37	124.00	120.26

There are no chirality outliers.

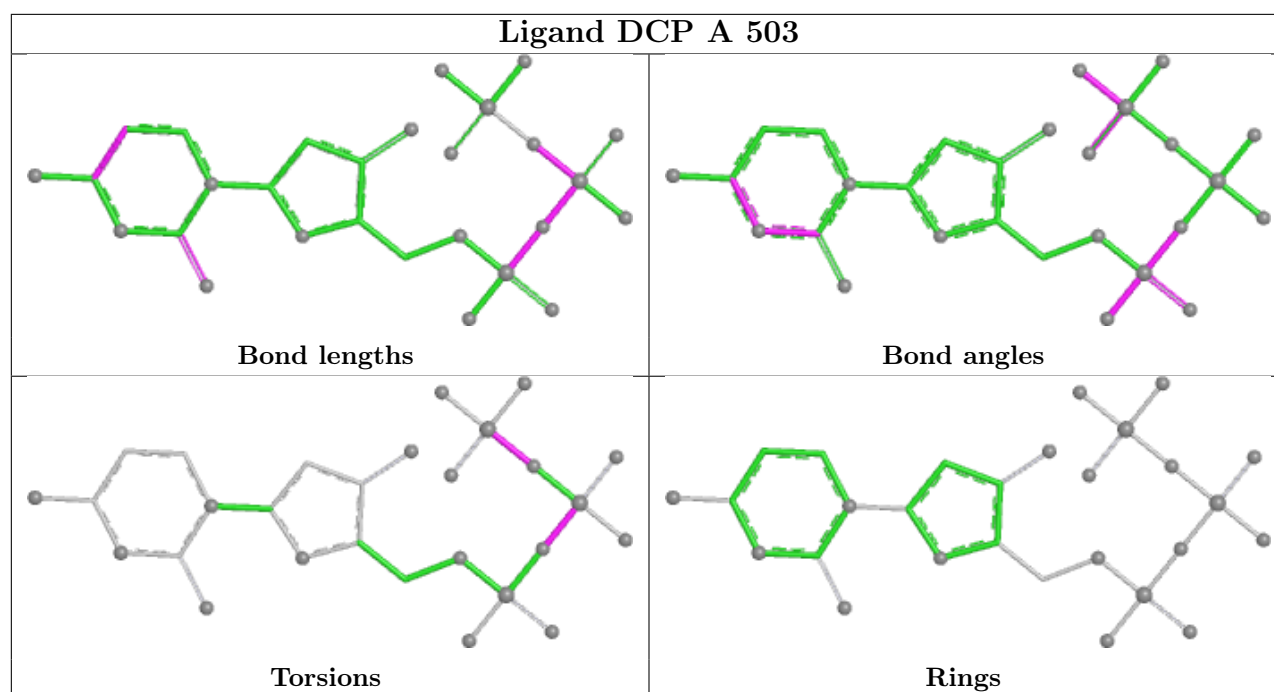
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	DCP	PA-O3A-PB-O2B
5	A	503	DCP	PB-O3B-PG-O3G
5	A	503	DCP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	B	6/18 (33%)	0.22	0	100 100	42, 56, 59, 63	0
1	C	7/18 (38%)	-0.54	0	100 100	36, 39, 48, 49	0
2	A	383/420 (91%)	0.63	49 (12%)	7 7	28, 50, 94, 176	1 (0%)
All	All	396/456 (86%)	0.60	49 (12%)	8 7	28, 50, 94, 176	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	311	CYS	7.7
2	A	61	TYR	7.2
2	A	401	PHE	4.9
2	A	145	SER	4.5
2	A	350	SER	4.4
2	A	353	LYS	4.3
2	A	146	ASP	4.1
2	A	273	LEU	4.1
2	A	355	TYR	4.0
2	A	315	VAL	3.8
2	A	336	GLY	3.8
2	A	354	HIS	3.5
2	A	317	ALA	3.3
2	A	349	TYR	3.2
2	A	252	ALA	3.2
2	A	73	LEU	3.1
2	A	227	GLN	2.8
2	A	290	ASN	2.7
2	A	314	GLU	2.7
2	A	84	ALA	2.6
2	A	351	SER	2.6
2	A	402	HIS	2.5
2	A	330	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	144	GLN	2.5
2	A	245	LYS	2.5
2	A	69	GLU	2.5
2	A	276	SER	2.5
2	A	103	ARG	2.4
2	A	237	LYS	2.3
2	A	310	LYS	2.3
2	A	275	ILE	2.3
2	A	277	VAL	2.3
2	A	312	SER	2.3
2	A	386	ILE	2.3
2	A	87	LYS	2.3
2	A	308	PHE	2.3
2	A	333	CYS	2.3
2	A	397	VAL	2.2
2	A	413	LEU	2.2
2	A	269	LEU	2.2
2	A	244	TYR	2.1
2	A	246	THR	2.1
2	A	348	ARG	2.1
2	A	278	ALA	2.1
2	A	27	SER	2.1
2	A	352	GLU	2.0
2	A	378	ASP	2.0
2	A	307	SER	2.0
2	A	253	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	EFG	C	840	25/26	0.94	0.09	40,48,67,71	0
1	DOC	B	13	18/19	0.97	0.07	40,44,48,48	0

6.3 Carbohydrates [i](#)

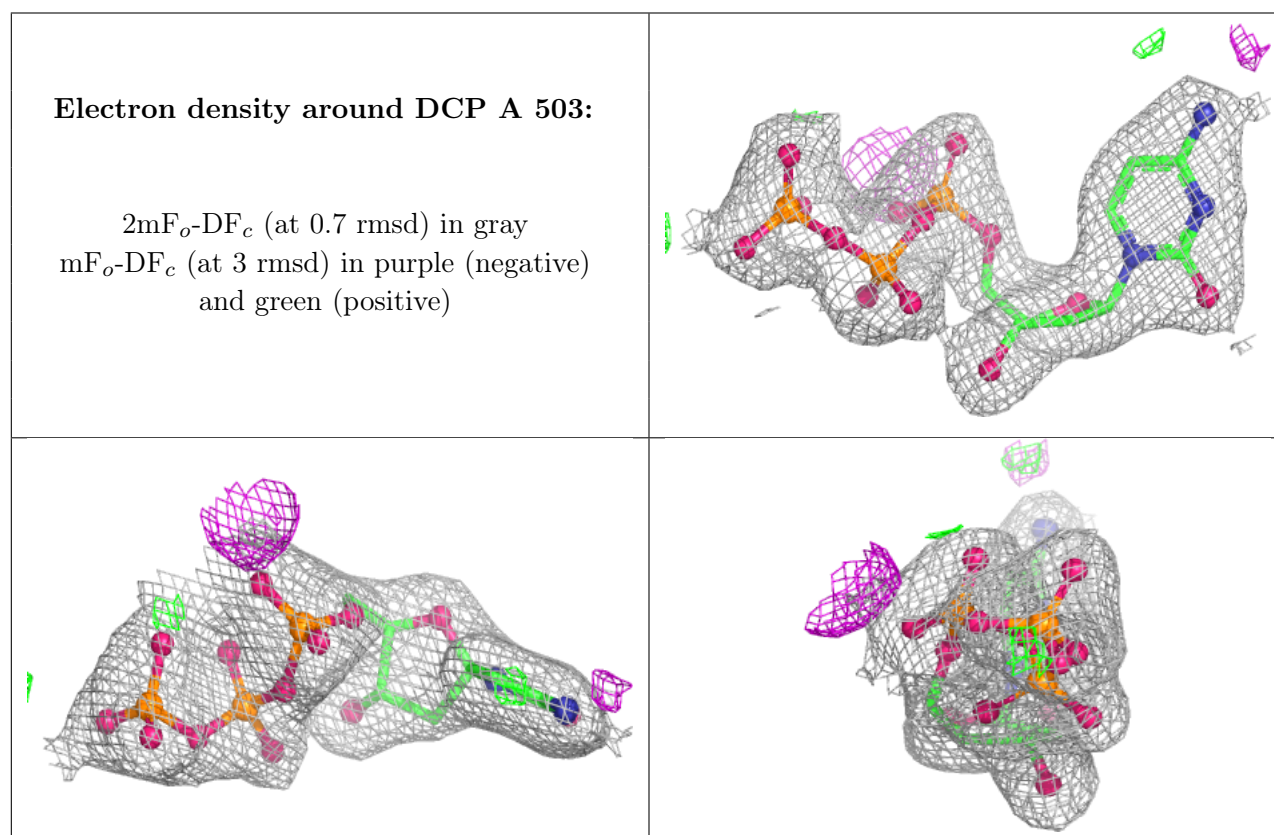
There are no oligosaccharides in this entry.

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
3	MG	A	505	1/1	0.73	0.59	30,30,30,30	0
4	NA	A	502	1/1	0.92	0.06	38,38,38,38	0
3	MG	A	504	1/1	0.95	0.08	41,41,41,41	0
5	DCP	A	503	28/28	0.97	0.06	29,38,42,44	0
3	MG	A	501	1/1	0.98	0.10	15,15,15,15	1

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 [i](#)

There are no such residues in this entry.