



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:55 PM EDT

PDB ID : 3LZJ / pdb_00003lzh
Title : RB69 DNA Polymerase (Y567A) ternary complex with dCTP Opposite 7,8-Dihydro-8-oxoguanine
Authors : Wang, M.; Beckman, J.; Blaha, G.; Wang, J.; Konigsberg, W.H.
Deposited on : 2010-03-01
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

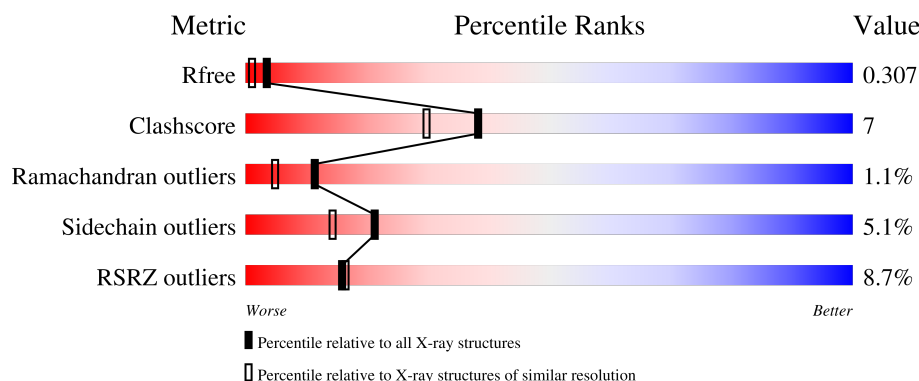
1 Overall quality at a glance

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	A	903	9% 86% 12% .
2	T	18	11% 72% 17% 11%
3	P	13	46% 54%

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
2	8OG	T	4	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8619 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	2	0
			7385	4742	1232	1378	33			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
A	567	ALA	TYR	engineered mutation	UNP Q38087

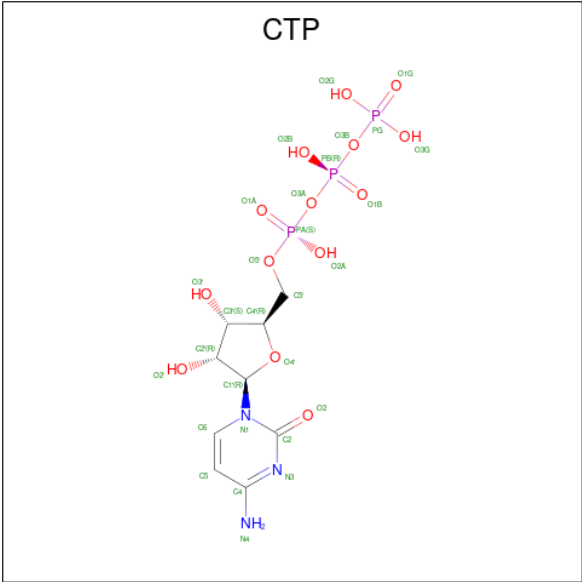
- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*CP*AP*(8OG)P*GP*TP*AP*AP*G P*CP*AP*GP*TP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	18	Total	C	N	O	P	0	0	0
			372	175	71	108	18			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			262	126	48	76	12			

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: C₉H₁₆N₃O₁₄P₃).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Ca	0	0
			4	4		

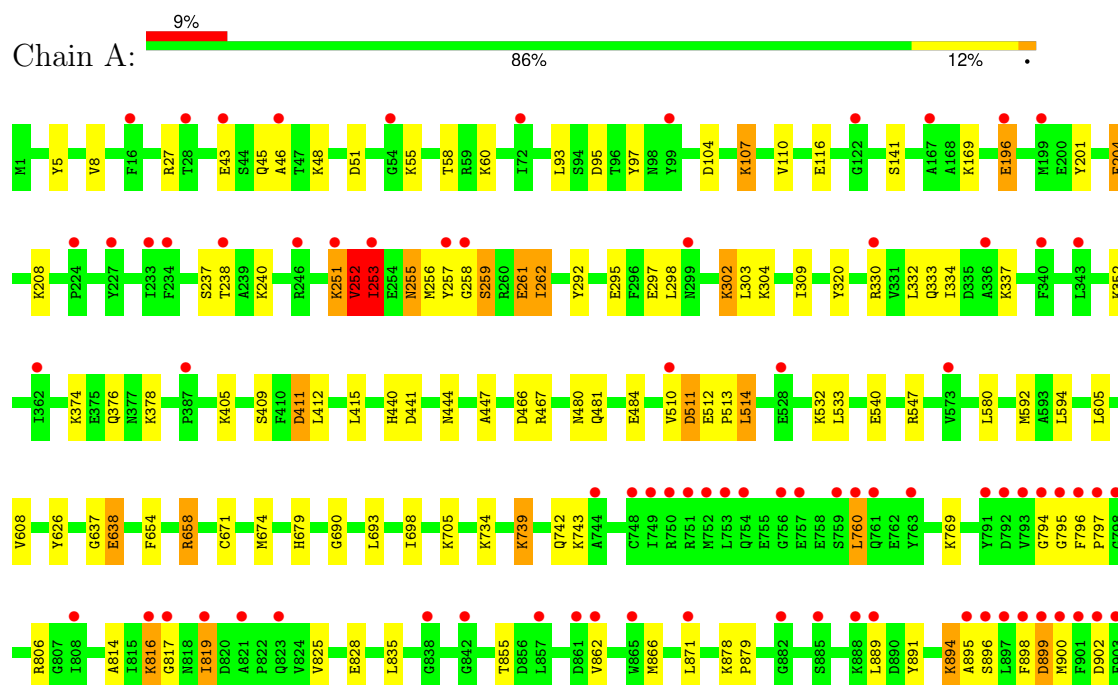
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	514	Total	O	0	0
			514	514		
6	T	38	Total	O	0	0
			38	38		
6	P	16	Total	O	0	0
			16	16		

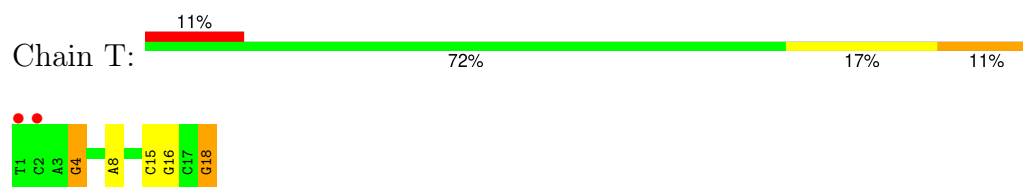
3 Residue-property plots

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.

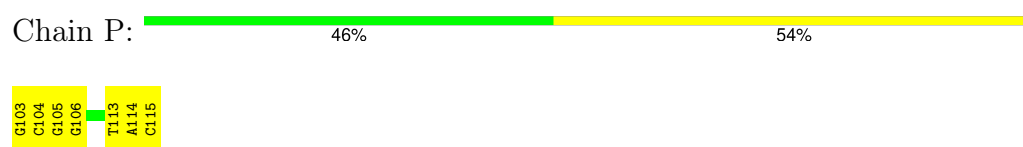
• Molecule 1: DNA polymerase



• Molecule 2: DNA (5'-D(P*TP*CP*AP*(8OG)P*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*C P*GP*CP*G)-3')



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.39Å 121.09Å 122.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 2.05 38.81 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.8 (38.81-2.05) 90.8 (38.81-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.205 , 0.251 0.265 , 0.307	Depositor DCC
R_{free} test set	3317 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	1.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8619	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: CA, 8OG, CTP, DOC

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	0.58	0/7569	0.83	0/10227
2	T	0.34	0/390	1.03	1/597 (0.2%)
3	P	0.32	0/273	0.92	0/420
All	All	0.56	0/8232	0.84	1/11244 (0.0%)

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
2	T	2	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	18	DG	O5'-C5'-C4'	5.08	118.43	110.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	4	8OG	C3',C4'

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	7385	0	7282	102	0
2	T	372	0	200	3	0
3	P	262	0	148	5	0
4	A	28	0	10	0	0
5	A	4	0	0	0	0
6	A	514	0	0	11	0
6	P	16	0	0	0	0
6	T	38	0	0	0	0
All	All	8619	0	7640	108	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 7.

All (108) 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:251:LYS:HB3	1:A:252:VAL:HA	1.16	1.15
1:A:898:PHE:HA	1:A:899:ASP:HB3	1.29	1.15
1:A:510:VAL:HA	1:A:511:ASP:CB	1.95	0.97
1:A:251:LYS:HB3	1:A:252:VAL:CA	1.96	0.95
1:A:258:GLY:HA3	1:A:259:SER:HB2	1.46	0.94
1:A:794:GLY:HA3	1:A:796:PHE:H	1.31	0.94
1:A:895:ALA:HB3	1:A:896:SER:HA	1.47	0.94
1:A:794:GLY:HA3	1:A:796:PHE:N	1.82	0.92
1:A:894:LYS:HD3	1:A:896:SER:HB3	1.53	0.90
1:A:330[B]:ARG:HH11	1:A:333:GLN:HE22	1.23	0.86
1:A:898:PHE:HA	1:A:899:ASP:CB	2.06	0.85
1:A:794:GLY:CA	1:A:796:PHE:H	1.92	0.82
1:A:510:VAL:HA	1:A:511:ASP:HB2	1.65	0.78
1:A:251:LYS:CB	1:A:252:VAL:HA	2.07	0.78
1:A:510:VAL:CA	1:A:511:ASP:HB2	2.16	0.76
1:A:201:TYR:O	6:A:1079:HOH:O	2.04	0.75
1:A:510:VAL:HA	1:A:511:ASP:HB3	1.67	0.73
1:A:895:ALA:CB	1:A:896:SER:HA	2.21	0.71
1:A:252:VAL:HG21	1:A:262:ILE:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLY:CA	1:A:259:SER:HB2	2.22	0.68
1:A:512:GLU:HG3	1:A:513:PRO:HD2	1.73	0.68
1:A:480:ASN:O	1:A:484:GLU:HG2	1.94	0.67
1:A:898:PHE:HB3	1:A:900:MET:H	1.58	0.67
1:A:201:TYR:C	6:A:1079:HOH:O	2.38	0.67
1:A:251:LYS:CB	1:A:252:VAL:CA	2.70	0.66
1:A:898:PHE:CA	1:A:899:ASP:HB3	2.18	0.65
1:A:252:VAL:HG11	1:A:261:GLU:HA	1.79	0.65
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.79	0.64
1:A:739:LYS:HE2	1:A:742:GLN:OE1	1.98	0.64
1:A:895:ALA:HB3	1:A:896:SER:CA	2.23	0.64
1:A:196:GLU:HG2	6:A:1405:HOH:O	1.97	0.63
1:A:825:VAL:HB	1:A:828:GLU:HG3	1.81	0.63
1:A:894:LYS:CD	1:A:896:SER:HB3	2.26	0.61
1:A:894:LYS:HD3	1:A:896:SER:CB	2.30	0.61
1:A:816:LYS:HG2	1:A:817:GLY:N	2.16	0.61
1:A:376:GLN:HB2	1:A:378:LYS:HG3	1.84	0.60
1:A:330[B]:ARG:HH11	1:A:333:GLN:NE2	1.98	0.60
1:A:794:GLY:N	1:A:796:PHE:H	2.00	0.59
1:A:60:LYS:HD3	6:A:1559:HOH:O	2.02	0.58
1:A:510:VAL:CA	1:A:511:ASP:CB	2.70	0.56
1:A:637:GLY:O	1:A:638:GLU:CB	2.53	0.56
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.90	0.54
1:A:292:TYR:OH	1:A:739:LYS:NZ	2.40	0.54
1:A:256:MET:HB3	1:A:257:TYR:HB2	1.89	0.54
1:A:698:ILE:HG21	1:A:889:LEU:HD11	1.89	0.54
1:A:411:ASP:OD1	1:A:411:ASP:C	2.50	0.53
1:A:894:LYS:CD	1:A:896:SER:CB	2.87	0.53
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.44	0.53
1:A:240:LYS:HG3	6:A:1546:HOH:O	2.09	0.53
1:A:252:VAL:CG1	1:A:261:GLU:HA	2.39	0.52
1:A:251:LYS:HB2	1:A:252:VAL:HB	1.91	0.52
1:A:816:LYS:HG2	1:A:817:GLY:H	1.75	0.51
1:A:898:PHE:HB3	1:A:900:MET:N	2.24	0.51
1:A:330[B]:ARG:NH1	1:A:333:GLN:HE22	2.02	0.51
1:A:605:LEU:HA	1:A:608:VAL:HG22	1.93	0.51
1:A:97:TYR:O	1:A:352:LYS:HE2	2.11	0.51
1:A:878:LYS:HB3	1:A:879:PRO:HD3	1.94	0.50
1:A:251:LYS:CB	1:A:252:VAL:HB	2.43	0.49
1:A:252:VAL:O	1:A:253:ILE:C	2.56	0.49
1:A:794:GLY:H	1:A:796:PHE:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:VAL:HG21	1:A:262:ILE:H	1.78	0.49
2:T:15:DC:H2''	2:T:16:DG:C8	2.47	0.49
1:A:8:VAL:HG11	1:A:93:LEU:HD11	1.95	0.48
1:A:256:MET:HB3	1:A:257:TYR:CB	2.44	0.47
1:A:797:PRO:HG2	1:A:806:ARG:NH1	2.29	0.47
1:A:862:VAL:O	1:A:866:MET:HG3	2.15	0.47
1:A:510:VAL:N	1:A:511:ASP:HB2	2.30	0.47
1:A:898:PHE:HD1	1:A:899:ASP:HB3	1.80	0.47
1:A:679:HIS:HE1	6:A:1562:HOH:O	1.98	0.46
1:A:252:VAL:HG11	1:A:261:GLU:HG3	1.97	0.46
3:P:105:DG:H4'	3:P:106:DG:OP1	2.16	0.45
1:A:5:TYR:HB3	1:A:97:TYR:CE1	2.52	0.45
1:A:104:ASP:HB3	1:A:107:LYS:HG3	1.97	0.45
3:P:113:DT:H2''	3:P:114:DA:H5'	1.99	0.45
1:A:237:SER:N	6:A:1546:HOH:O	2.49	0.45
1:A:592:MET:HE1	1:A:674:MET:HG3	1.98	0.45
1:A:252:VAL:HG11	1:A:262:ILE:H	1.83	0.44
1:A:255:ASN:HB2	1:A:256:MET:HA	1.99	0.44
1:A:734:LYS:HG2	3:P:113:DT:H5'	1.99	0.44
1:A:760:LEU:HD13	1:A:891:TYR:HA	1.99	0.44
1:A:895:ALA:CB	1:A:896:SER:CA	2.91	0.44
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.18	0.44
1:A:654:PHE:O	1:A:658:ARG:HB2	2.19	0.43
1:A:705:LYS:HD3	2:T:8:DA:H5''	2.00	0.43
1:A:440[A]:HIS:CE1	1:A:444:ASN:HD21	2.36	0.43
1:A:794:GLY:CA	1:A:796:PHE:N	2.59	0.43
3:P:104:DC:H2''	3:P:105:DG:C8	2.53	0.43
1:A:297:GLU:O	1:A:337:LYS:NZ	2.47	0.43
3:P:103:DG:H2''	3:P:104:DC:C6	2.54	0.42
1:A:169:LYS:HG2	6:A:1284:HOH:O	2.19	0.42
1:A:819:ILE:H	1:A:819:ILE:HG13	1.56	0.42
2:T:18:DG:H3'	2:T:18:DG:OP1	2.19	0.42
1:A:51:ASP:HB2	6:A:1047:HOH:O	2.19	0.42
1:A:409:SER:HB3	1:A:626:TYR:CD2	2.55	0.42
1:A:298:LEU:HD11	1:A:334:ILE:HG13	2.01	0.41
1:A:481:GLN:HG2	6:A:1169:HOH:O	2.19	0.41
1:A:816:LYS:HD2	1:A:816:LYS:H	1.85	0.41
1:A:302:LYS:HG2	1:A:304:LYS:HG3	2.02	0.41
1:A:110:VAL:HB	1:A:141:SER:HB3	2.03	0.41
1:A:671:CYS:SG	6:A:1560:HOH:O	2.33	0.41
1:A:258:GLY:HA3	1:A:259:SER:CB	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LYS:O	1:A:690:GLY:HA2	2.21	0.41
1:A:547:ARG:HD3	1:A:547:ARG:HA	1.90	0.40
1:A:898:PHE:CB	1:A:900:MET:H	2.32	0.40
1:A:95:ASP:OD2	1:A:374:LYS:HE3	2.22	0.40
1:A:256:MET:HB3	1:A:257:TYR:CA	2.51	0.40
1:A:637:GLY:O	1:A:638:GLU:HB2	2.21	0.40
1:A:514:LEU:HD22	1:A:533:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	903/903 (100%)	855 (95%)	38 (4%)	10 (1%)	11 5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ILE
1	A	259	SER
1	A	511	ASP
1	A	638	GLU
1	A	251	LYS
1	A	252	VAL
1	A	795	GLY
1	A	814	ALA
1	A	899	ASP
1	A	46	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	801/799 (100%)	760 (95%)	41 (5%)	21	14

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	43	GLU
1	A	45	GLN
1	A	48	LYS
1	A	55	LYS
1	A	58	THR
1	A	107	LYS
1	A	196	GLU
1	A	204	PHE
1	A	238	THR
1	A	252	VAL
1	A	253	ILE
1	A	255	ASN
1	A	261	GLU
1	A	262	ILE
1	A	295	GLU
1	A	302	LYS
1	A	303	LEU
1	A	309	ILE
1	A	332	LEU
1	A	411	ASP
1	A	466	ASP
1	A	467	ARG
1	A	514	LEU
1	A	532	LYS
1	A	540	GLU
1	A	580	LEU
1	A	594	LEU
1	A	658	ARG
1	A	693	LEU

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Mol	Chain	Res	Type
1	A	739	LYS
1	A	743	LYS
1	A	760	LEU
1	A	769	LYS
1	A	816	LYS
1	A	819	ILE
1	A	835	LEU
1	A	855	THR
1	A	871	LEU
1	A	894	LYS
1	A	902	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	112	ASN
1	A	131	HIS
1	A	173	GLN
1	A	333	GLN
1	A	339	GLN
1	A	376	GLN
1	A	444	ASN
1	A	539	ASN
1	A	546	GLN
1	A	564	ASN
1	A	679	HIS
1	A	733	GLN
1	A	761	GLN
1	A	773	GLN
1	A	823	GLN
1	A	839	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$
3	DOC	P	115	3,2	16,19,20	0.91	0	20,26,29	1.96	4 (20%)
2	8OG	T	4	2	22,25,26	4.25	8 (36%)	26,37,40	2.98	14 (53%)

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
3	DOC	P	115	3,2	-	1/7/18/19	0/2/2/2
2	8OG	T	4	2	2/2/4/4	5/7/21/22	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	4	8OG	O8-C8	13.79	1.47	1.23
2	T	4	8OG	C3'-C4'	-7.53	1.33	1.53
2	T	4	8OG	O6-C6	6.63	1.36	1.23
2	T	4	8OG	C5'-C4'	-6.18	1.33	1.51
2	T	4	8OG	O3'-C3'	-4.85	1.33	1.43
2	T	4	8OG	C8-N9	-4.24	1.33	1.40
2	T	4	8OG	C4-N9	-3.01	1.33	1.39
2	T	4	8OG	C5-C4	2.02	1.40	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4	8OG	N7-C8-N9	7.33	114.76	106.61
3	P	115	DOC	C4'-O4'-C1'	-6.35	103.81	109.81
2	T	4	8OG	C5-N7-C8	-4.56	103.19	109.47
2	T	4	8OG	C2-N3-C4	4.31	119.72	112.30
2	T	4	8OG	N9-C4-N3	4.11	131.26	126.13
2	T	4	8OG	O3'-C3'-C4'	4.04	125.38	110.07
2	T	4	8OG	O3'-C3'-C2'	3.84	124.23	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4	8OG	C2'-C3'-C4'	3.70	110.32	102.80
3	P	115	DOC	O4'-C1'-N1	3.63	114.30	107.86
2	T	4	8OG	O4'-C4'-C5'	3.61	120.91	109.33
2	T	4	8OG	O6-C6-C5	-3.16	119.65	127.26
2	T	4	8OG	O4'-C4'-C3'	3.06	112.62	105.65
3	P	115	DOC	O4'-C4'-C5'	2.96	114.68	109.34
2	T	4	8OG	O8-C8-N7	-2.76	121.29	126.47
2	T	4	8OG	C2-N1-C6	-2.64	120.33	125.11
2	T	4	8OG	C5-C6-N1	2.63	119.35	112.13
2	T	4	8OG	C5'-C4'-C3'	2.12	126.47	114.64
3	P	115	DOC	C2'-C1'-N1	-2.06	108.49	112.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	4	8OG	C3'
2	T	4	8OG	C4'

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	4	8OG	O4'-C4'-C5'-O5'
2	T	4	8OG	O4'-C1'-N9-C8
2	T	4	8OG	O4'-C1'-N9-C4
2	T	4	8OG	C2'-C1'-N9-C4
3	P	115	DOC	C3'-C4'-C5'-O5'
2	T	4	8OG	C2'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

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
4	CTP	A	904	5	28,29,30	1.28	3 (10%)	41,45,47	1.45	5 (12%)

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	CTP	A	904	5	-	5/22/34/38	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	CTP	PB-O3B	3.55	1.63	1.59
4	A	904	CTP	PA-O3A	3.48	1.63	1.59
4	A	904	CTP	C6-C5	2.33	1.40	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	CTP	O2B-PB-O3A	5.21	121.34	107.27
4	A	904	CTP	O4'-C1'-N1	3.43	113.95	107.86
4	A	904	CTP	O2-C2-N3	-2.79	117.94	122.33
4	A	904	CTP	O3A-PB-O1B	-2.37	103.58	110.70
4	A	904	CTP	O3A-PA-O1A	-2.11	104.36	110.70

There are no chirality outliers.

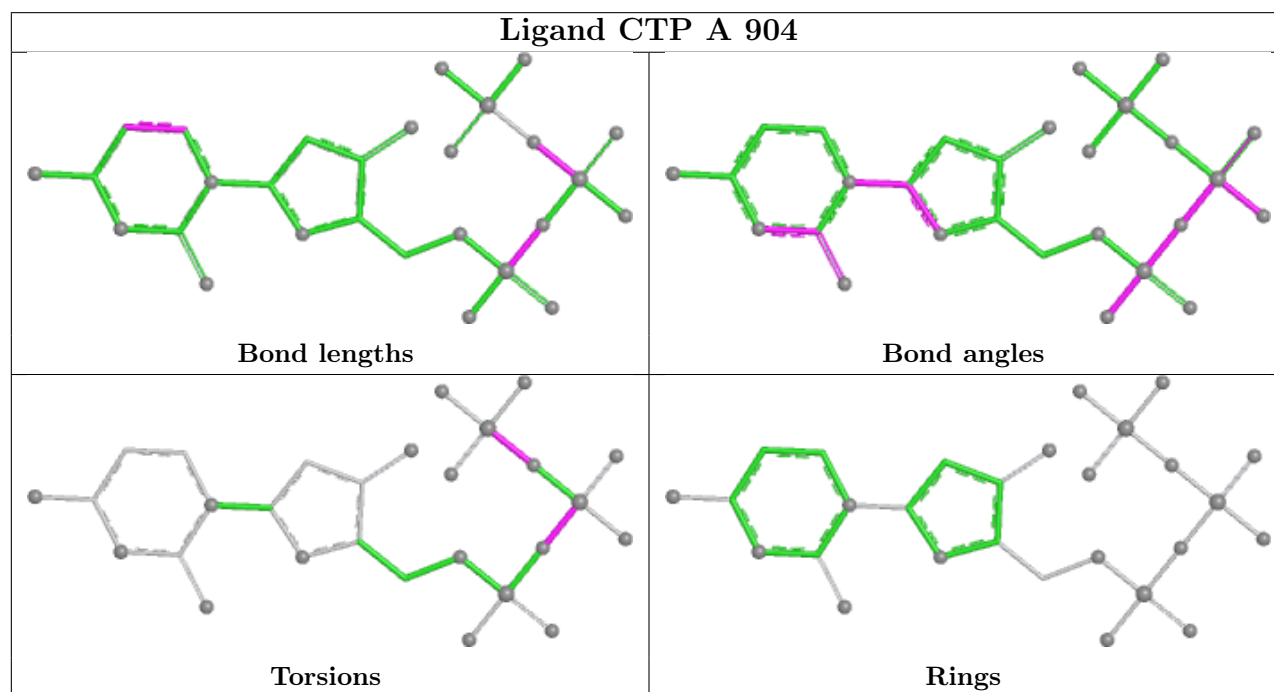
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	904	CTP	PA-O3A-PB-O2B
4	A	904	CTP	PB-O3B-PG-O1G
4	A	904	CTP	PB-O3B-PG-O2G
4	A	904	CTP	PB-O3B-PG-O3G
4	A	904	CTP	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	A	903/903 (100%)	0.55	79 (8%) 16 16	1, 7, 27, 125	2 (0%)
2	T	17/18 (94%)	0.50	2 (11%) 9 8	2, 5, 83, 105	0
3	P	12/13 (92%)	-0.02	0 100 100	2, 8, 33, 38	0
All	All	932/934 (99%)	0.54	81 (8%) 16 16	1, 7, 28, 125	2 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	901	PHE	6.2
1	A	753	LEU	5.9
1	A	897	LEU	5.3
1	A	749	ILE	5.2
1	A	898	PHE	4.8
1	A	900	MET	4.7
1	A	817	GLY	4.1
1	A	861	ASP	4.1
1	A	387	PRO	4.1
1	A	794	GLY	4.0
1	A	253	ILE	3.9
1	A	792	ASP	3.7
1	A	857	LEU	3.7
1	A	838	GLY	3.6
1	A	251	LYS	3.4
1	A	899	ASP	3.4
1	A	257	TYR	3.4
1	A	842	GLY	3.4
1	A	903	PHE	3.4
1	A	573	VAL	3.3
1	A	510	VAL	3.3
1	A	199	MET	3.2
1	A	752	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	896	SER	3.1
1	A	902	ASP	3.1
1	A	16	PHE	3.1
1	A	756	GLY	3.1
1	A	795	GLY	3.1
1	A	793	VAL	3.1
1	A	816	LYS	3.0
1	A	43	GLU	2.9
1	A	750	ARG	2.9
1	A	28	THR	2.8
1	A	238	THR	2.8
1	A	336	ALA	2.8
1	A	760	LEU	2.8
2	T	2	DC	2.8
1	A	821	ALA	2.7
1	A	791	TYR	2.7
1	A	895	ALA	2.7
1	A	233	ILE	2.7
2	T	1	DT	2.7
1	A	258	GLY	2.7
1	A	798	GLY	2.7
1	A	871	LEU	2.6
1	A	99	TYR	2.6
1	A	234	PHE	2.6
1	A	796	PHE	2.5
1	A	808	ILE	2.5
1	A	763	TYR	2.5
1	A	823	GLN	2.5
1	A	196	GLU	2.5
1	A	72	ILE	2.5
1	A	819	ILE	2.5
1	A	797	PRO	2.4
1	A	888	LYS	2.4
1	A	299	ASN	2.4
1	A	362	ILE	2.4
1	A	340	PHE	2.4
1	A	46	ALA	2.3
1	A	885	SER	2.3
1	A	167	ALA	2.3
1	A	343	LEU	2.3
1	A	54	GLY	2.3
1	A	865	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	862	VAL	2.2
1	A	330[A]	ARG	2.2
1	A	751	ARG	2.2
1	A	744	ALA	2.2
1	A	528	GLU	2.2
1	A	748	CYS	2.2
1	A	754	GLN	2.2
1	A	882	GLY	2.2
1	A	761	GLN	2.2
1	A	889	LEU	2.2
1	A	227	TYR	2.2
1	A	759	SER	2.1
1	A	224	PRO	2.1
1	A	122	GLY	2.1
1	A	757	GLU	2.0
1	A	246	ARG	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
3	DOC	P	115	18/19	0.88	0.15	2,2,7,8	0
2	8OG	T	4	23/24	0.91	0.10	2,2,4,4	0

6.3 Carbohydrates [i](#)

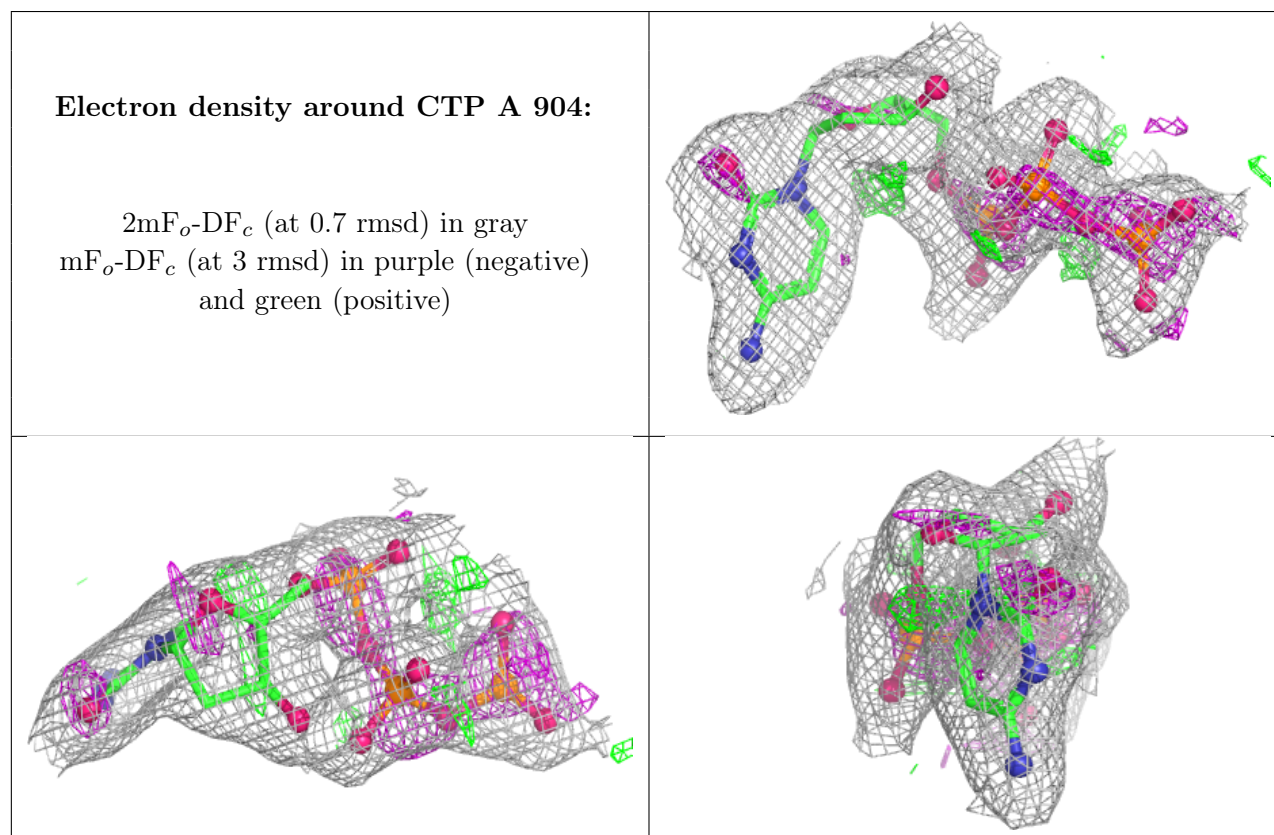
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
5	CA	A	907	1/1	0.86	0.14	69,69,69,69	0
5	CA	A	906	1/1	0.89	0.10	54,54,54,54	0
5	CA	A	908	1/1	0.89	0.08	59,59,59,59	0
5	CA	A	905	1/1	0.95	0.07	31,31,31,31	0
4	CTP	A	904	28/29	0.95	0.07	2,2,2,4	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.