



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 09:13 AM UTC

PDB ID : 6WOX / pdb_00006wox
Title : Thermus thermophilus RNA polymerase initially transcribing complex with 2'dCTP
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2020-04-26
Resolution : 3.14 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

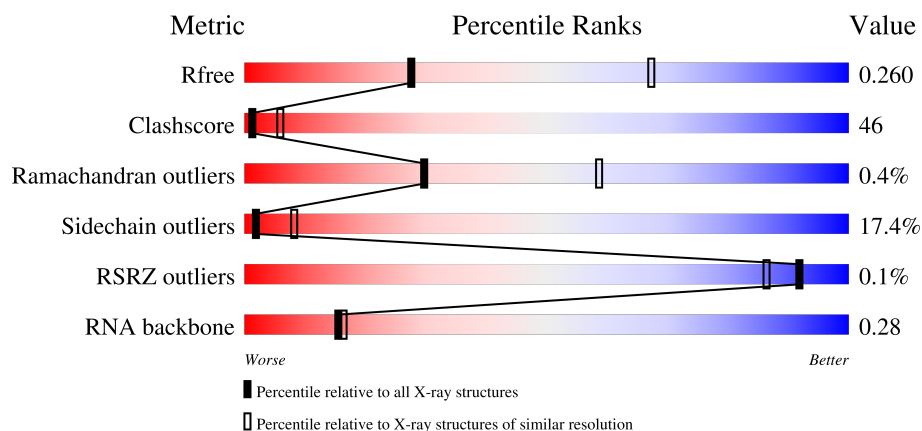
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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.



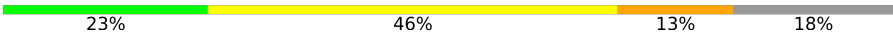
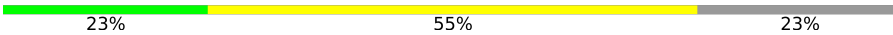
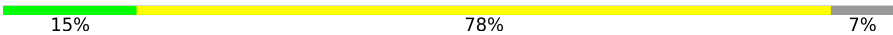
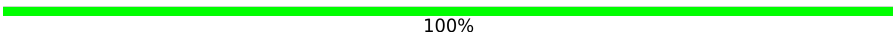
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)
RNA backbone	3983	1040 (3.38-2.90)

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	315	15% 46% 10% 28%
1	B	315	21% 41% 9% 29%
2	C	1119	34% 55% 10% .
3	D	1505	37% 52% 10% .

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Mol	Chain	Length	Quality of chain
4	E	99	 32% 56% 7% 5%
5	F	423	 23% 46% 13% 18%
6	G	22	 23% 55% 23%
7	H	27	 15% 78% 7%
8	I	3	 100%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28581 atoms, of which 12 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1485	Total	C	N	O	S	0	0	0
			11721	7431	2063	2192	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	86	LYS	ARG	conflict	UNP Q8RQE8

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			351	166	65	103	17			

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

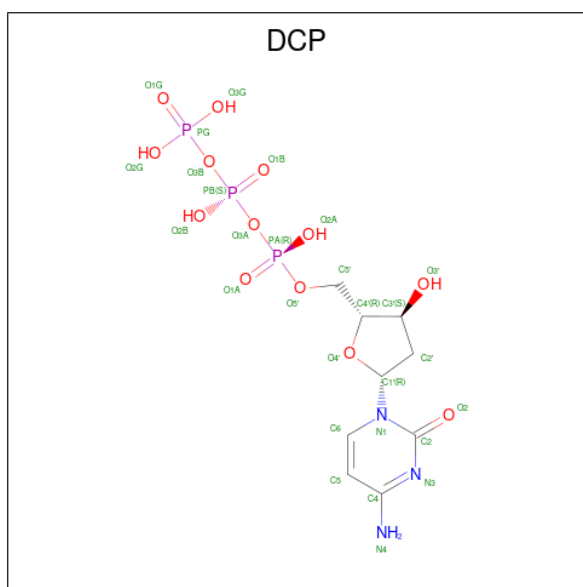
- Molecule 8 is a RNA chain called RNA (5'-R(*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			62	29	13	18	2			

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Na	0	0
			1	1		

- Molecule 10 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	D	1	Total	C	H	N	O	P	0	0
			40	9	12	3	13	3		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total Mg 1 1	0	0

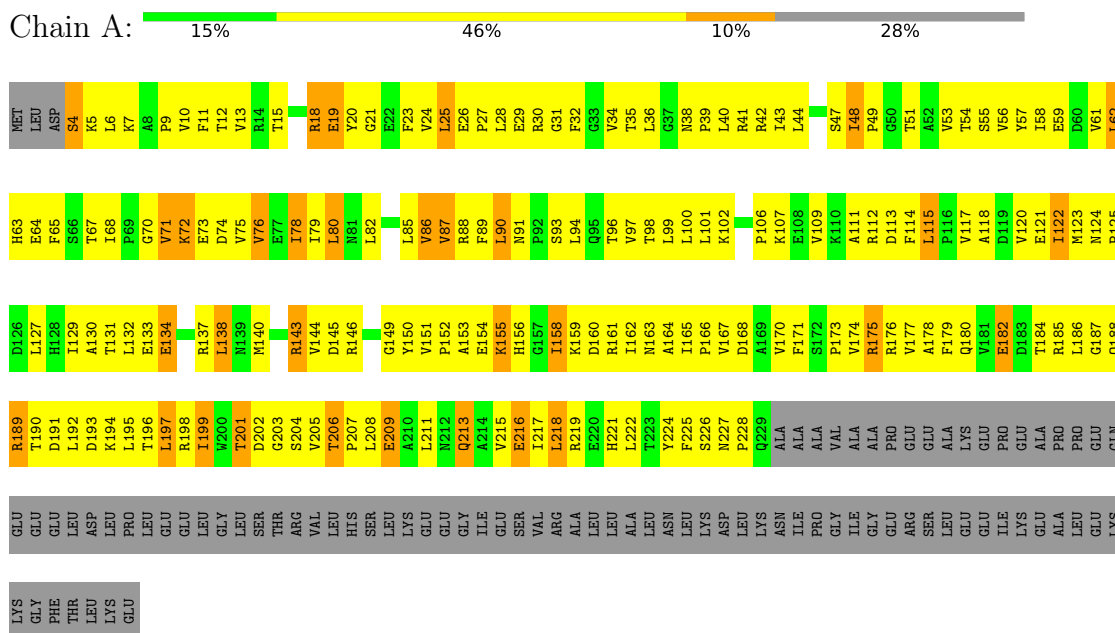
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	D	2	Total Zn 2 2	0	0

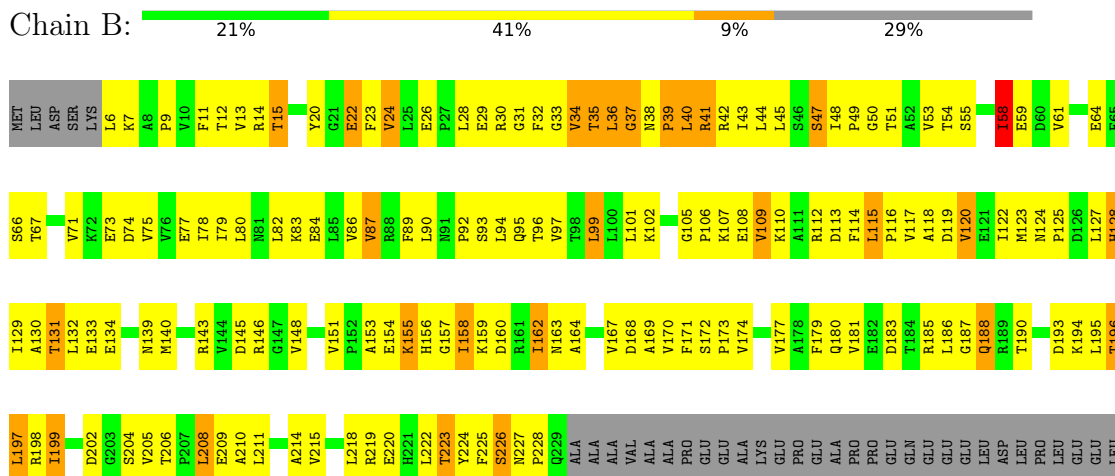
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



GLY	LEU	SER	THR	ARG	VAL	LEU	HIS	SER	LYS	GLU	GLY	ILE	GLU	SER	VAL	ARG	ALA	LEU	LEU	ALA	LEU	ASN	ILE	PRO	GLY	ILE	R39	GLY	GLY	ARG	SER	LEU	GLU	GLY	LYS	GLY	LYS	GLY	THR	LEU	LYS	GLY	GLY
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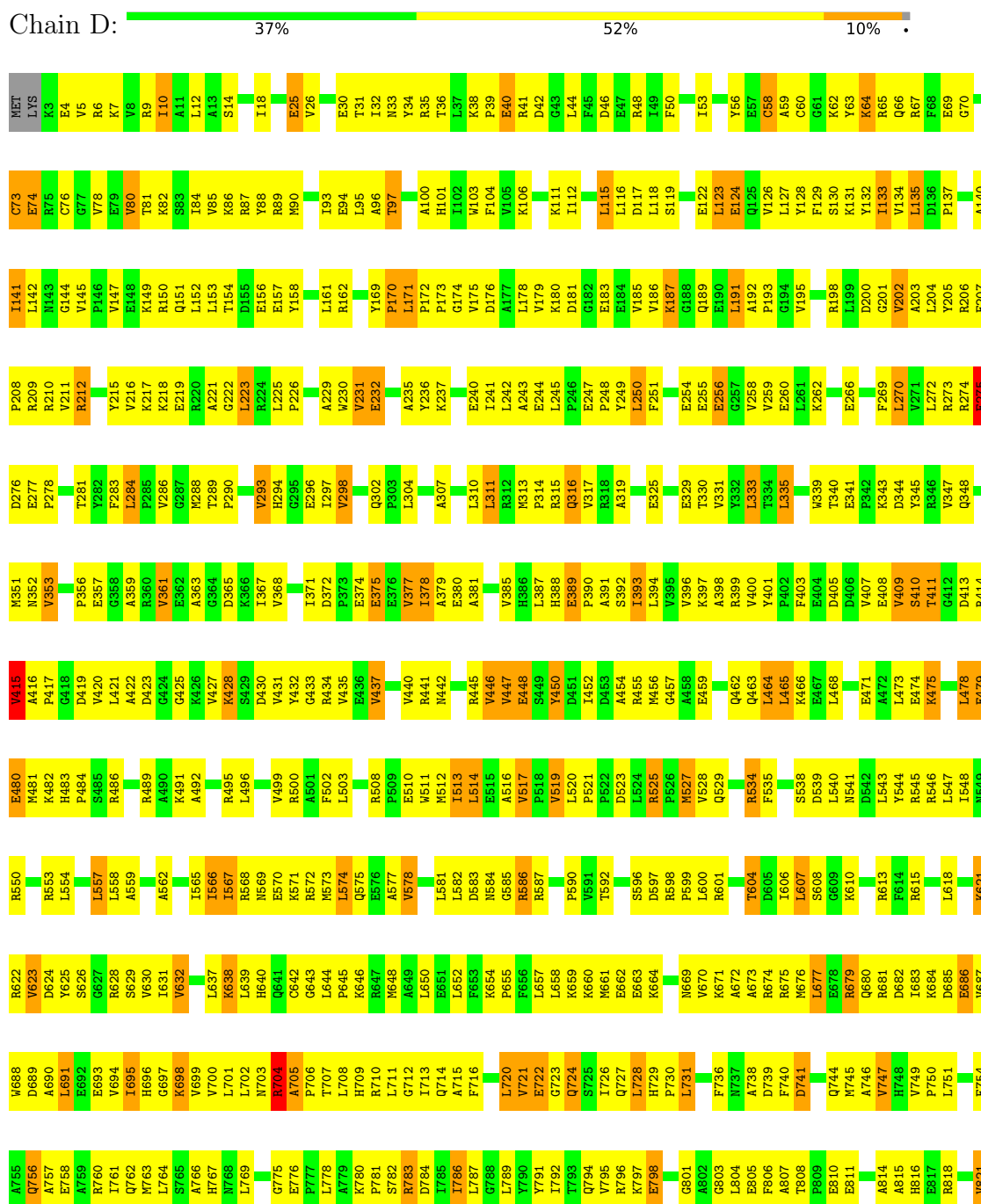
● Molecule 2: DNA-directed RNA polymerase subunit beta

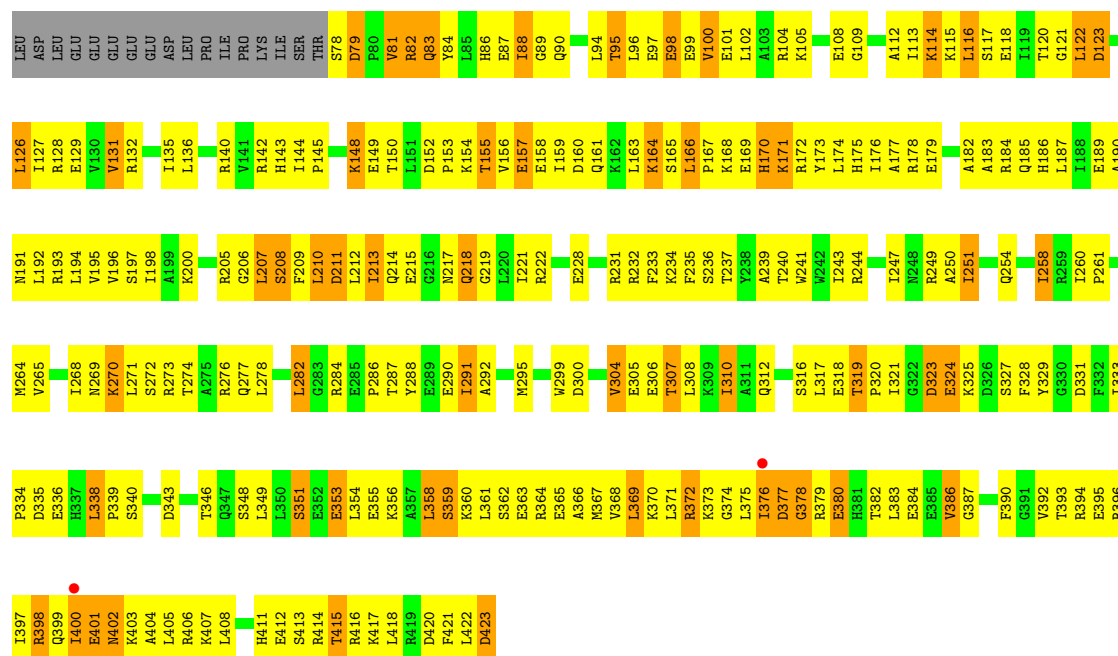
Chain C:  34% 55% 10%

P904	D837	R772	E706	Q567	A497	G424	M359	I283	G215	I140	D67	M1
R906	K838	L773	R707	A568	Q498	F425	M359	R284	E216	I140	D67	E2
F906	L839	L774	T708	A499	Q499	D426	M361	L285	L217	S143	Y71	I3
G908	R841	D907	E709	P570	N500	V427	M361	L290	Q219	F148	L73	F6
A909	R842	S776	T710	L571	T501	R428	M362	L290	G220	T149	G74	G7
K910	H843	I777	E711	L572	P502	D429	S363	R292	L221	P150	E75	R8
E911			A712	V644	L503		E364	R292	M222		P76	
P912	W848	E780	T715	P577	E504	R432	D365	F293		R154		R10
E913	R849	K781	K716	V578		T433	S366	F293	D223			E11
K914	A850	A782	V649	V578	I508	H434	L367	E297	E224	R157	R84	V12
E915	R851	R783	L717	N580	A509	Y435	T368	F298	S225		E85	
E916	L852	D784	G718	T581	A510	G436	P369	K299	V226	A160	K86	L15
	L852	W785	P719	G582	E511	R437	A370	D300	F227		D87	
Q920	L853	K786	E720	L583	R512	I438	K371	E301	A228	S161	L88	
A921	P854	D787	A656	E584	V513	C439	L372		M229	I162		L18
F922	W855	T788	R723	E585	V514		V373	P305	R230	I163		T19
		S789	R724	R586		E442	N374		E233	P164		E20
F926	N858	L790	D725	V587	B517	T443	S375	Y309	E233	K167	L94	I21
G927	P859	R791	I726	V587	K518	P444	R376	L310	A234		P93	Q22
K928	H860	W792	R736	N588	Q519	E445	P377	F311	L235	R168	Y95	V23
R929	L861	P793	D737	V588	G519	A446	L378	A312	I236	G169	A96	E24
G930	P862		H728	D590	V524	A447	E379	L313	R237	P170	R97	
K931	D863	E796	S730	L592		R448		T314	L238	W171	Y26	
E932	C864	G797		A593	E528	I449	R383		F239	I172	L100	R27
	T865	G798	L734	A594	V529	G450	E384	V317	T240	D173	I101	R28
F936	P866	I799	R735	L595	E530	L451	F385	G319	L241	L174	H102	A29
G937	R867	V800	D736	L596	F531	L452	F386	P318	R243	E175	K103	L30
K938	L868	R802	L737	A597	N532	T453	R387	H320	R243	V176	D104	Q31
F936	R869	H801	D738	E598	D533	S454	R388	E321		E177	T105	A32
D937	L870	T803	E739	E599	V634		S389	V322	D246	P178	G106	D33
	L871	W804	E740		S535	A459	Q390	D323	P247	H179	L107	
R939	N872	R805	G741	E602	P536	R460	L391		R248	G180	I108	P36
E940	L873		V742	V603	K537	V461	S392	D326	K249	V181	E37	
F941	R874	R808	V743	A604	Q538	D462		H327	R250	V182	K109	E37
E942	G875		R744	K605	V539	E463	K395	L328		S183	D111	R39
K943	R876		I745	V606	F540	L464	D396		A253	M184	E112	E40
L944	P877	P811		D607	S541		E397	R331	V254	K185	V113	M41
R945	L877	G812	E748	G681	V542	L467	T398	R332			F114	
E946	R879	V813	P751	N609	N543	R468	P399	I333	V257	K190	L115	T44
A947	N880	R815	G752	R610	T544		P400	R334	G258			Q45
E948	L881	K816	G752	T611	N545	R472	L401	T335	D259	L193	I118	A46
K949	L882		D753	V612	L546	R473	S402	V336	L260	V194	P119	
L950	G883	V819	L754	R613	P547	V475	S403	G337	I261	L195	M121	R49
Q951	Q884	R820	L755	V614	P548	V475	L404	E338	A262	L196	L120	E50
L952	L885	E821	V756	Y615	F548	G477	R405	L339	R405	L197		T51
V953	L886	V822	G757	E616	L550	V476	H406	P264	P264		D124	F52
T954	E887	W823	R758	D617	E551	V478	K407	T341	R265	L200		P53
	R887	R824	T759	G618			R408	Q342	R266		F127	I54
R889	R889	W825	T760	R619	D554	E482	R409	Q343	Y267		I128	E55
F957	L890	R825	L759	G618			R409	D342	L268	D203	I128	E55
P959	G891	Y826	F761	L695			R410	F344	L269	Q204	I129	E56
E960	L892		K762	K696	V621	Y485	S411	R345	L269	E205	N130	GLU
	L892		G763	R697	A568	M486	A412	R345	G270	T206	G131	ASP
E961		Q829	E764	D698	L559	T487	L413	L348	E271	L207	A132	LYS
Q962	L897	W830	S765	F699	R626	R627	G414		A272	A208	D133	GLY
L963	Q898	R831	E766	Y700	F628			L351	E278	R209	R134	LYS
	R899	W832	P767	T701	Y629	S562	L418	A352		E210	V135	GLY
L966	Q900	N901	T768	S702	R630	R493	T419	R353	E279	G212	I136	GLY
F967	L901	Q834	P769	I703	S631	Y564	Y494	G354	K260	G212	V137	GLY
L968	L902	V835	E770	H704	N632	O565	T495	V355	L261	A213	L261	V65
E969	L903	Q926	E771	T705	E633	W566	A423	R422	G292	E144	O149	



● Molecule 3: DNA-directed RNA polymerase subunit beta'





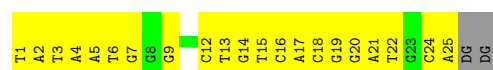
- Molecule 6: DNA (5'-D(P*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*A P*G)-3')

Chain G: 23% 55% 23%



- Molecule 7: DNA (25-MER)

Chain H: 15% 78% 7%



- Molecule 8: RNA (5'-R(*GP*CP*A)-3')

Chain I: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.44Å 102.65Å 295.38Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	29.93 – 3.14 29.93 – 3.14	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.93-3.14) 93.5 (29.93-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.196 , 0.261 0.197 , 0.260	Depositor DCC
R_{free} test set	2004 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28581	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, ZN, DCP

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	0.47	0/1814	0.68	0/2466
1	B	0.47	0/1799	0.68	0/2447
2	C	0.47	1/8937 (0.0%)	0.69	1/12087 (0.0%)
3	D	0.48	2/11927 (0.0%)	0.72	8/16127 (0.0%)
4	E	0.44	0/775	0.63	0/1045
5	F	0.44	0/2852	0.66	0/3837
6	G	0.57	0/393	0.64	0/605
7	H	0.52	0/580	0.65	0/895
8	I	0.42	0/69	0.74	0/106
All	All	0.47	3/29146 (0.0%)	0.70	9/39615 (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
1	B	0	1
2	C	0	1
3	D	0	5
5	F	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	135	LEU	C-N	5.89	1.38	1.33
3	D	1114	THR	CB-CG2	5.33	1.70	1.52
2	C	682	TYR	CA-C	5.18	1.59	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	135	LEU	CA-C-N	6.78	129.32	122.00
3	D	135	LEU	C-N-CA	6.78	129.32	122.00
2	C	682	TYR	O-C-N	-6.77	113.59	122.59
3	D	170	PRO	CA-C-N	-5.82	105.08	122.71
3	D	170	PRO	C-N-CA	-5.82	105.08	122.71

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	ILE	Peptide
2	C	362	GLY	Peptide
3	D	275	GLU	Peptide
3	D	64	LYS	Peptide
3	D	704	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	226	0
1	B	1767	0	1816	222	0
2	C	8770	0	8874	850	0
3	D	11721	0	11941	1167	0
4	E	761	0	778	89	0
5	F	2807	0	2882	300	0
6	G	351	0	192	17	0
7	H	516	0	283	41	0
8	I	62	0	34	0	0
9	C	1	0	0	0	0
10	D	28	12	12	3	0
11	D	1	0	0	0	0
12	D	2	0	0	0	0
All	All	28569	12	28646	2656	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 46.

The worst 5 of 2656 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)
3:D:203:ALA:HB1	3:D:393:ILE:HD11	1.17	1.15
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.21	1.14
3:D:1234:THR:HB	3:D:1235:GLN:HB2	1.31	1.13
3:D:767:HIS:HA	3:D:924:MET:HE3	1.28	1.12
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	1.21	1.12

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	224/315 (71%)	192 (86%)	32 (14%)	0	100	100
1	B	222/315 (70%)	192 (86%)	28 (13%)	2 (1%)	14	41
2	C	1107/1119 (99%)	960 (87%)	146 (13%)	1 (0%)	48	76
3	D	1481/1505 (98%)	1255 (85%)	218 (15%)	8 (0%)	24	54
4	E	92/99 (93%)	83 (90%)	9 (10%)	0	100	100
5	F	344/423 (81%)	291 (85%)	51 (15%)	2 (1%)	21	50
All	All	3470/3776 (92%)	2973 (86%)	484 (14%)	13 (0%)	30	59

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	GLY
3	D	276	ASP
1	B	154	GLU
5	F	168	LYS
2	C	212	GLY

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	
1	A	199/273 (73%)	153 (77%)	46 (23%)	1	3
1	B	197/273 (72%)	162 (82%)	35 (18%)	2	8
2	C	936/941 (100%)	776 (83%)	160 (17%)	2	9
3	D	1249/1265 (99%)	1052 (84%)	197 (16%)	2	10
4	E	83/88 (94%)	72 (87%)	11 (13%)	4	15
5	F	301/371 (81%)	233 (77%)	68 (23%)	1	4
All	All	2965/3211 (92%)	2448 (83%)	517 (17%)	2	8

5 of 517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	131	VAL
5	F	207	LEU
5	F	126	LEU
2	C	785	VAL
2	C	730	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	680	GLN
3	D	909	ASN
5	F	399	GLN
3	D	1489	GLN
3	D	709	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	2/3 (66%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	$\# Z > 2$
10	DCP	D	1601	9	28,29,29	4.27	14 (50%)	41,45,45	1.69	10 (24%)

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
10	DCP	D	1601	9	-	9/22/34/34	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1601	DCP	C2'-C1'	-10.54	1.23	1.52
10	D	1601	DCP	O4'-C4'	-8.64	1.25	1.45
10	D	1601	DCP	O4'-C1'	8.38	1.61	1.42
10	D	1601	DCP	PB-O3B	6.84	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1601	DCP	PA-O3A	6.66	1.66	1.59

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1601	DCP	C1'-N1-C2	4.33	125.27	117.83
10	D	1601	DCP	O3G-PG-O3B	3.93	117.81	104.64
10	D	1601	DCP	C4-N3-C2	3.57	125.89	120.26
10	D	1601	DCP	C1'-N1-C6	-2.96	115.71	121.53
10	D	1601	DCP	O4'-C4'-C3'	-2.94	98.95	105.65

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

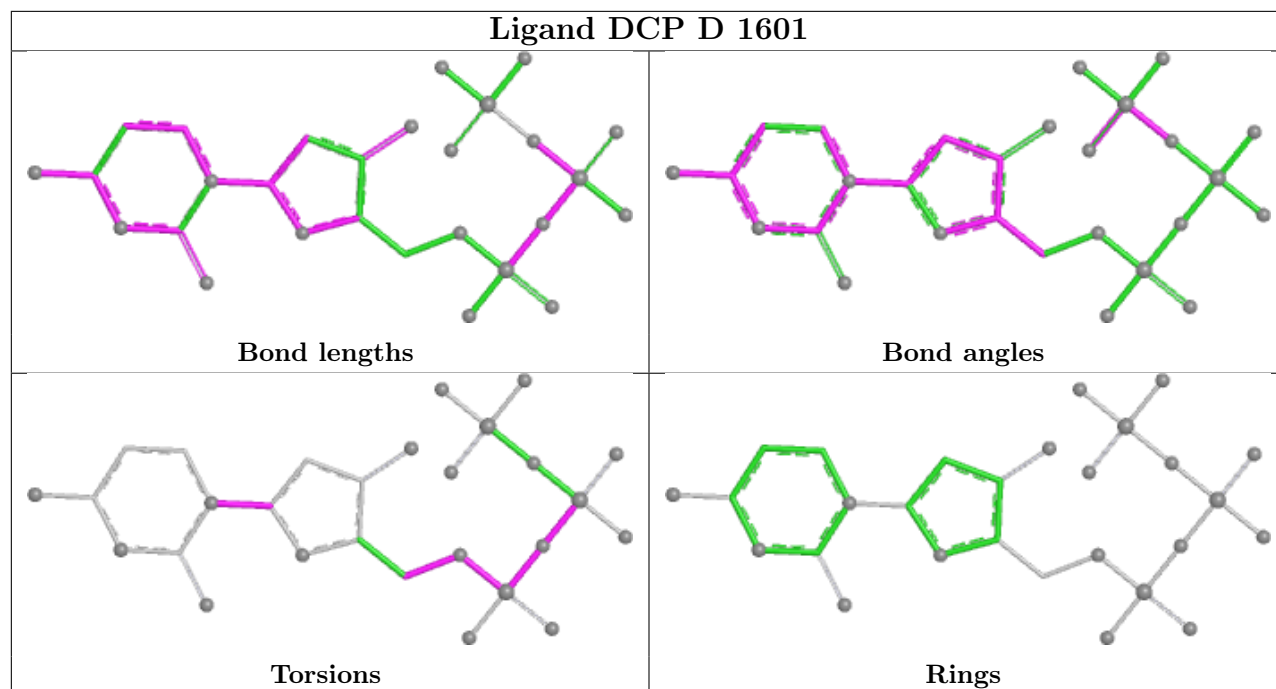
Mol	Chain	Res	Type	Atoms
10	D	1601	DCP	C5'-O5'-PA-O1A
10	D	1601	DCP	C5'-O5'-PA-O3A
10	D	1601	DCP	C2'-C1'-N1-C6
10	D	1601	DCP	PB-O3A-PA-O5'
10	D	1601	DCP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1601	DCP	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	226/315 (71%)	-0.49	0	100	100	73, 91, 110, 124	0
1	B	224/315 (71%)	-0.53	0	100	100	66, 96, 121, 133	0
2	C	1111/1119 (99%)	-0.55	0	100	100	56, 91, 138, 160	0
3	D	1485/1505 (98%)	-0.55	1 (0%)	92	86	50, 85, 138, 160	0
4	E	94/99 (94%)	-0.51	0	100	100	64, 101, 132, 139	0
5	F	346/423 (81%)	-0.44	2 (0%)	85	70	64, 101, 153, 163	0
6	G	17/22 (77%)	-0.53	0	100	100	69, 95, 169, 171	0
7	H	25/27 (92%)	-0.36	0	100	100	90, 121, 169, 179	0
8	I	3/3 (100%)	-1.05	0	100	100	73, 73, 76, 87	0
All	All	3531/3828 (92%)	-0.54	3 (0%)	92	86	50, 91, 142, 179	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	376	ILE	2.2
3	D	1313	VAL	2.1
5	F	400	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

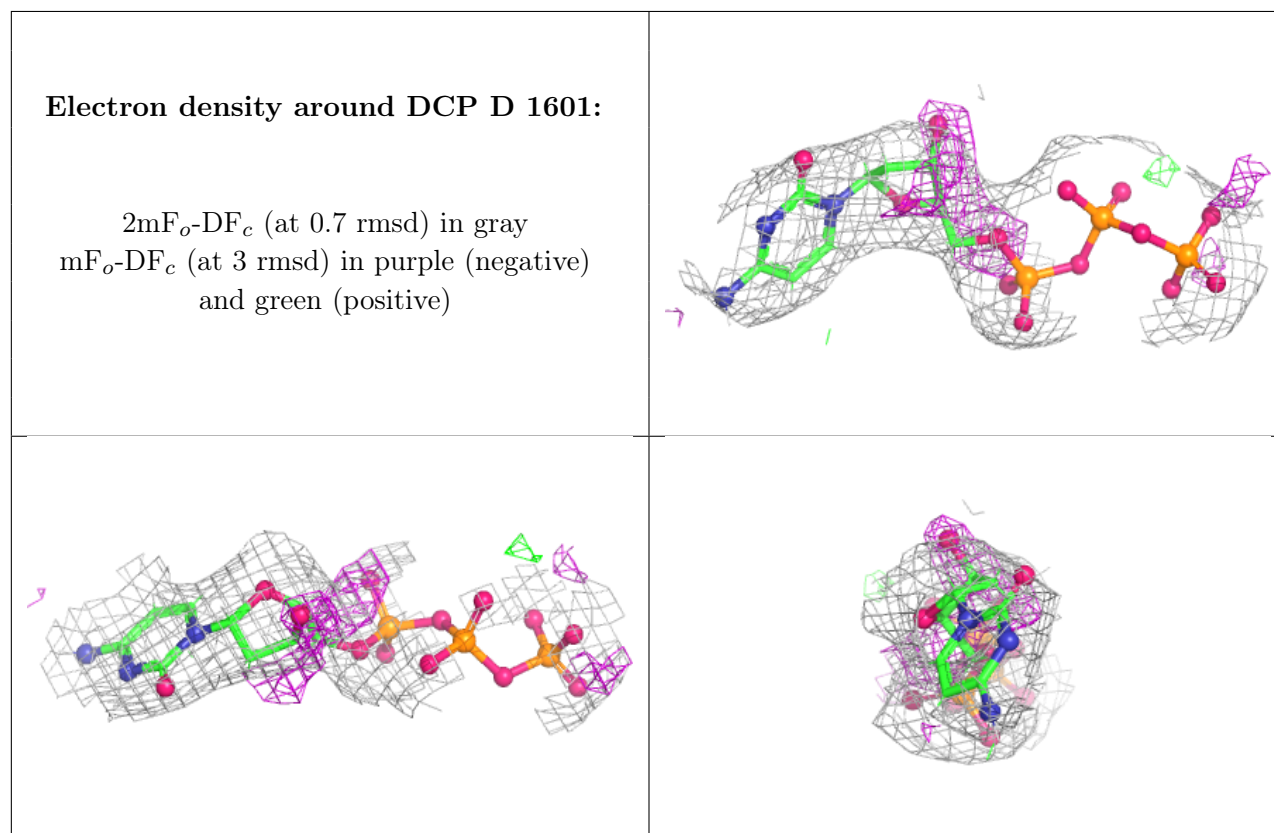
There are no oligosaccharides in this entry.

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
9	NA	C	1201	1/1	0.79	0.10	70,70,70,70	0
12	ZN	D	1604	1/1	0.90	0.09	120,120,120,120	0
10	DCP	D	1601	28/28	0.92	0.06	80,93,112,115	0
12	ZN	D	1603	1/1	0.98	0.04	125,125,125,125	0
11	MG	D	1602	1/1	0.98	0.05	67,67,67,67	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 [i](#)

There are no such residues in this entry.