



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:29 PM UTC

PDB ID : 2PPB / pdb_00002ppb
Title : Crystal structure of the T. thermophilus RNAP polymerase elongation complex with the ntp substrate analog and antibiotic streptolydigin
Authors : Vassylyev, D.G.; Vassylyeva, M.N.; Artsimovitch, I.; Landick, R.
Deposited on : 2007-04-28
Resolution : 3.00 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

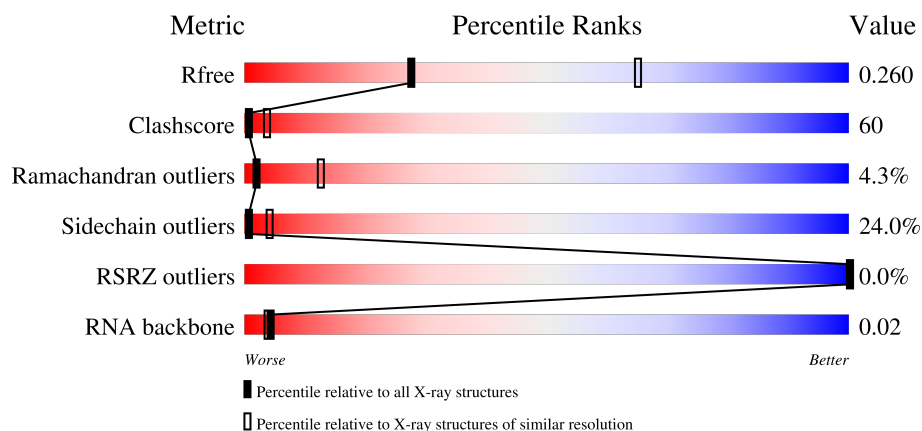
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.






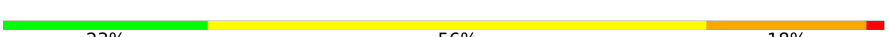

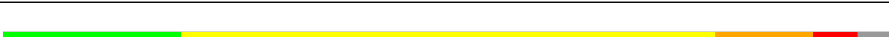
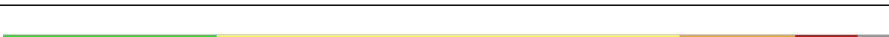
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	G	23	<div> <div>22%</div> <div>48%</div> <div>22%</div> <div>9%</div> </div>
1	X	23	<div> <div>17%</div> <div>52%</div> <div>17%</div> <div>13%</div> </div>
2	H	16	<div> <div>6%</div> <div>44%</div> <div>50%</div> </div>
2	Y	16	<div> <div>6%</div> <div>44%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	14	
3	Z	14	
4	A	315	
4	B	315	
4	K	315	
4	L	315	
5	C	1119	
5	M	1119	
6	D	1524	
6	N	1524	
7	E	99	
7	O	99	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 51962 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(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			
1	X	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			
2	Y	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			
3	Z	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 5 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
5	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

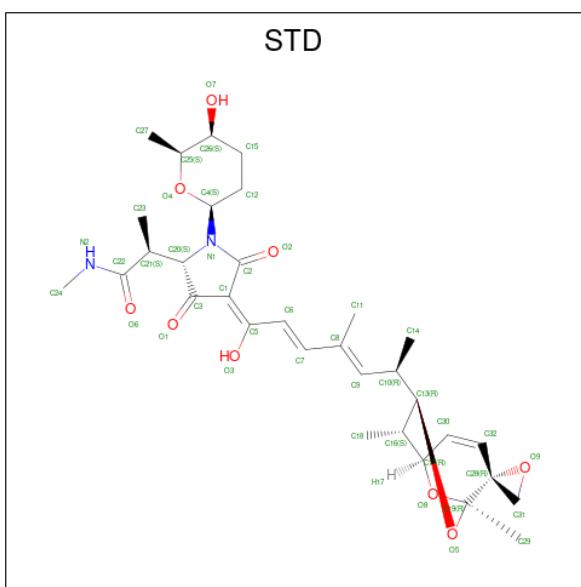
- Molecule 6 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	1314	Total	C	N	O	S	0	0	0
			10373	6565	1838	1937	33			
6	N	1314	Total	C	N	O	S	0	0	0
			10373	6565	1838	1937	33			

- Molecule 7 is a protein called DNA-directed RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
7	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

- Molecule 8 is STREPTOLYDIGIN (CCD ID: STD) (formula: C₃₂H₄₄N₂O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total 43	C 32	N 2	O 9	0	0
8	N	1	Total 43	C 32	N 2	O 9	0	0

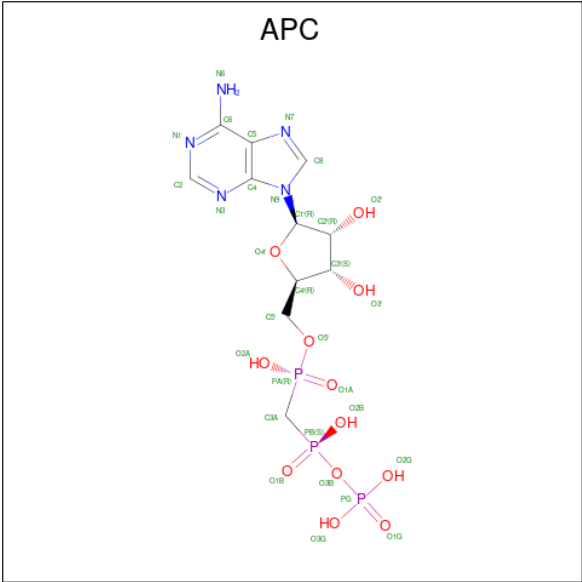
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total Zn 2 2	0	0
9	N	2	Total Zn 2 2	0	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Mg 2 2	0	0
10	N	2	Total Mg 2 2	0	0

- Molecule 11 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
11	M	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	G	39	Total	O	0	0
			39	39		
12	H	22	Total	O	0	0
			22	22		
12	I	31	Total	O	0	0
			31	31		
12	X	31	Total	O	0	0
			31	31		
12	Y	26	Total	O	0	0
			26	26		
12	Z	18	Total	O	0	0
			18	18		
12	A	78	Total	O	0	0
			78	78		
12	B	117	Total	O	0	0
			117	117		
12	C	408	Total	O	0	0
			408	408		
12	D	531	Total	O	0	0
			531	531		

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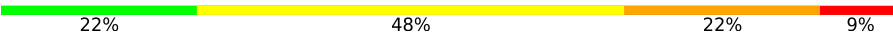
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	34	Total 34	O 34	0	0
12	K	81	Total 81	O 81	0	0
12	L	95	Total 95	O 95	0	0
12	M	396	Total 396	O 396	0	0
12	N	510	Total 510	O 510	0	0
12	O	53	Total 53	O 53	0	0

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 (5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3')

Chain G: 



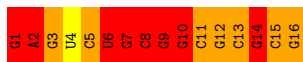
- Molecule 1: DNA (5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3')

Chain X: 



- Molecule 2: RNA (5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*GP*CP*G)-3')

Chain H: 

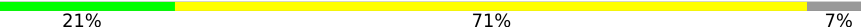


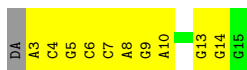
- Molecule 2: RNA (5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*GP*CP*G)-3')

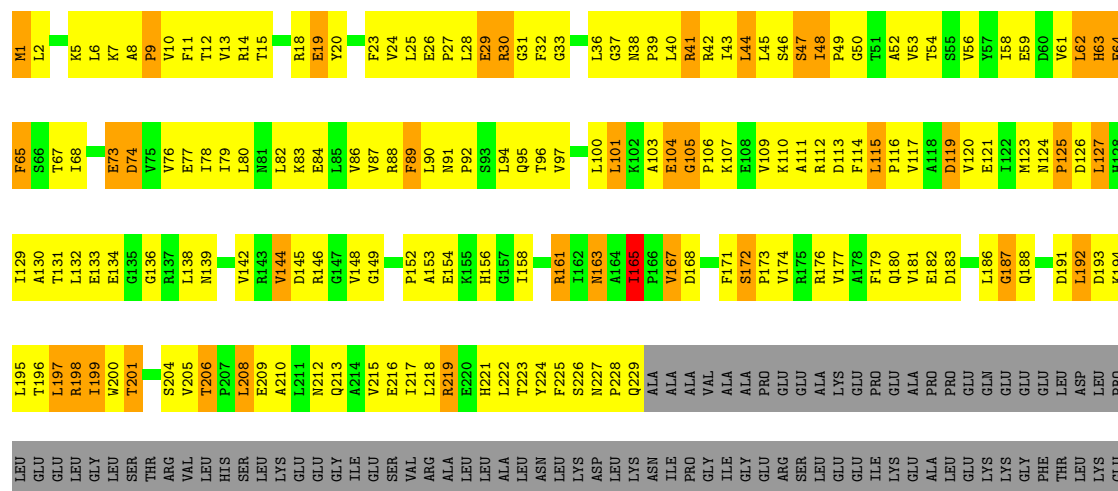
Chain Y: 



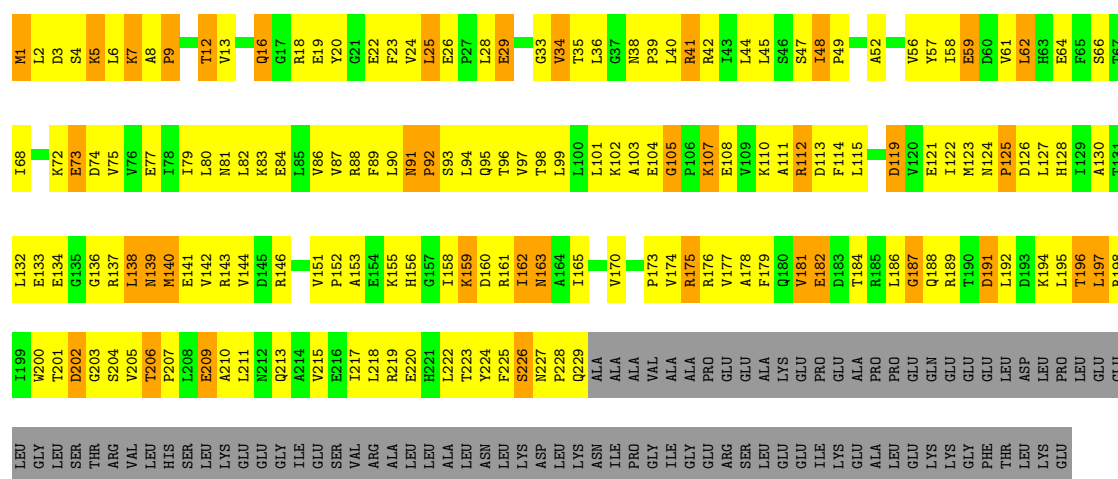
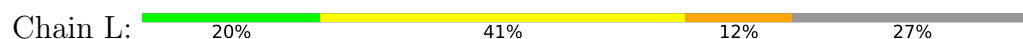
- Molecule 3: DNA (5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3')

Chain I: 

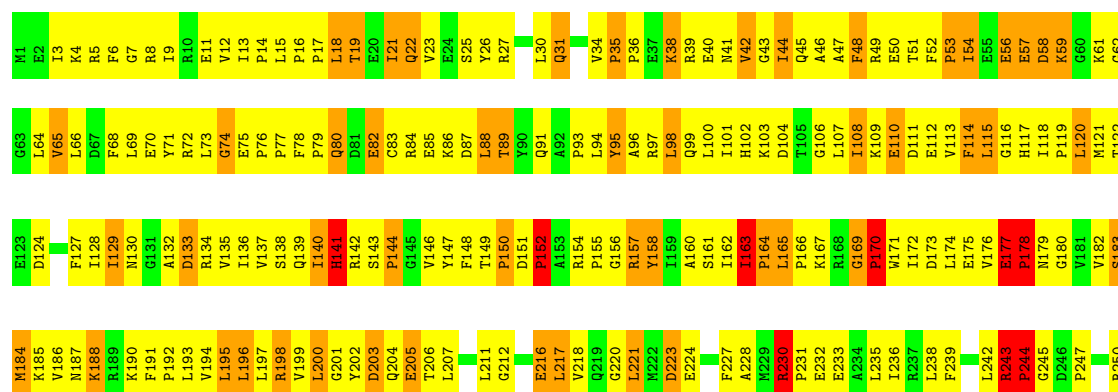


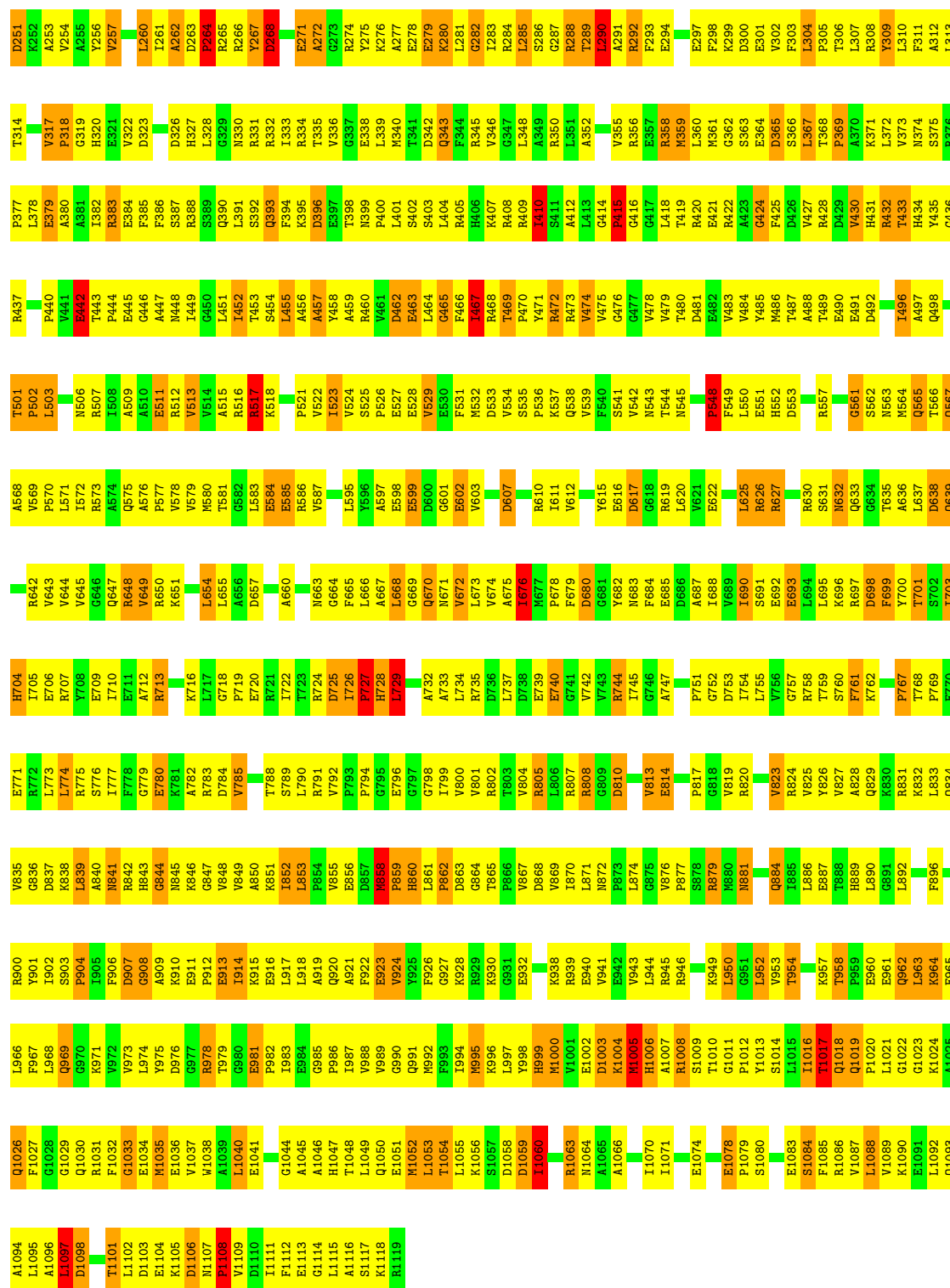


• Molecule 4: DNA-directed RNA polymerase alpha chain



• Molecule 5: DNA-directed RNA polymerase beta chain





- Molecule 5: DNA-directed RNA polymerase beta chain

Chain M:  21% 58% 19%

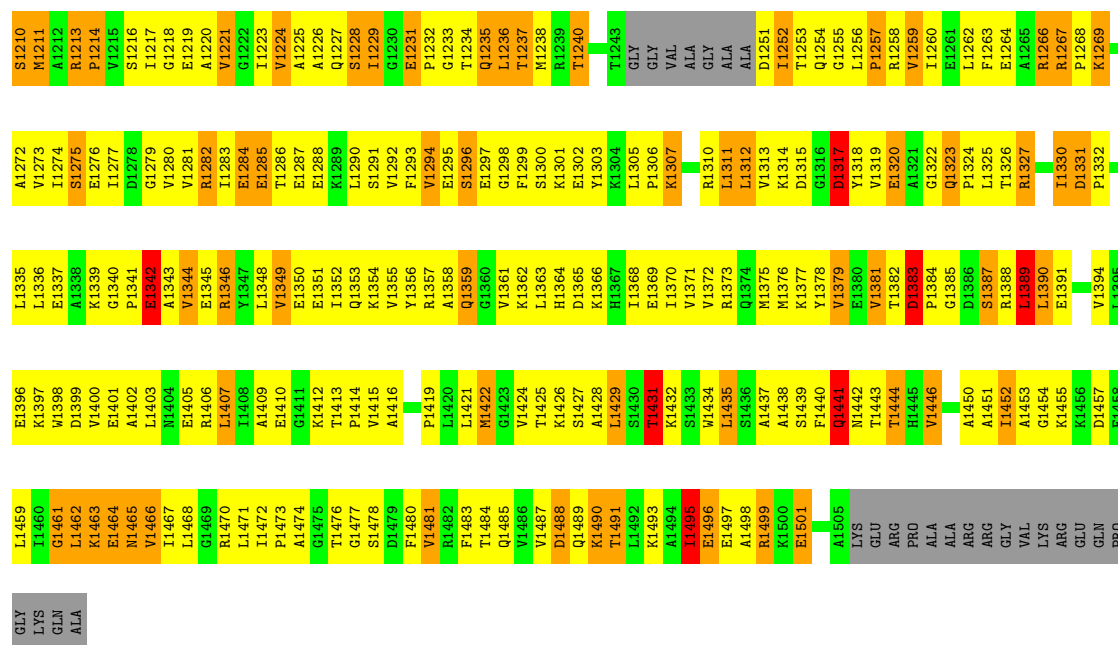




Chain D: 21% 49% 15% • 14%







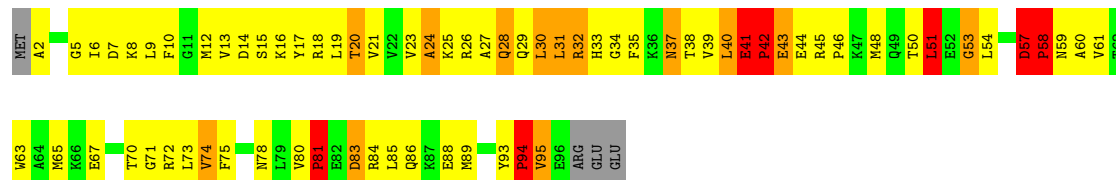
- Molecule 7: DNA-directed RNA polymerase omega chain

Chain E: 20% 60% 11% 5% .



- Molecule 7: DNA-directed RNA polymerase omega chain

Chain O: 24% 52% 13% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	155.38Å 155.38Å 496.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.8 (40.00-3.00) 82.1 (40.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.266 0.234 , 0.260	Depositor DCC
R_{free} test set	10938 reflections (5.70%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 122.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.147 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	51962	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: APC, STD, ZN, 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	G	0.52	0/520	1.10	4/798 (0.5%)
1	X	0.53	0/520	1.11	5/798 (0.6%)
2	H	1.06	2/387 (0.5%)	2.31	21/601 (3.5%)
2	Y	1.14	2/387 (0.5%)	2.28	22/601 (3.7%)
3	I	0.47	0/304	0.97	1/467 (0.2%)
3	Z	0.46	0/304	0.89	0/467
4	A	0.82	2/1838 (0.1%)	1.09	4/2498 (0.2%)
4	B	0.81	0/1838	1.06	8/2498 (0.3%)
4	K	0.81	1/1838 (0.1%)	1.11	8/2498 (0.3%)
4	L	0.84	0/1838	1.04	6/2498 (0.2%)
5	C	0.87	8/8997 (0.1%)	1.25	58/12164 (0.5%)
5	M	0.88	9/8997 (0.1%)	1.27	67/12164 (0.6%)
6	D	1.01	32/10547 (0.3%)	1.28	80/14245 (0.6%)
6	N	0.97	18/10547 (0.2%)	1.25	70/14245 (0.5%)
7	E	0.90	1/784 (0.1%)	1.53	13/1057 (1.2%)
7	O	0.98	2/784 (0.3%)	1.57	12/1057 (1.1%)
All	All	0.91	77/50430 (0.2%)	1.27	379/68656 (0.6%)

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	G	0	6
1	X	0	7
2	H	0	2
2	Y	0	1
6	D	0	1
All	All	0	17

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	133	ILE	N-CA	21.31	1.70	1.46
6	D	132	TYR	CA-C	18.98	1.78	1.52
6	N	132	TYR	CA-C	16.32	1.70	1.52
6	D	455	ARG	CA-C	14.46	1.72	1.52
6	N	133	ILE	N-CA	13.47	1.61	1.46

The worst 5 of 379 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	G	N9-C1'-C2'	21.66	146.50	114.00
7	O	94	PRO	N-CA-C	18.69	137.02	114.03
2	Y	1	G	N9-C1'-C2'	18.08	141.13	114.00
5	C	177	GLU	CA-C-N	17.47	141.68	119.84
5	C	177	GLU	C-N-CA	17.47	141.68	119.84

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1	DC	Sidechain
1	G	13	DT	Sidechain
1	G	15	DC	Sidechain
1	G	16	DG	Sidechain
1	G	17	DC	Sidechain

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	G	467	0	259	46	0
1	X	467	0	259	45	0
2	H	347	0	174	76	0
2	Y	347	0	174	61	0
3	I	270	0	144	18	0
3	Z	270	0	144	18	0
4	A	1806	0	1861	189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1806	0	1861	183	0
4	K	1806	0	1861	211	0
4	L	1806	0	1861	180	0
5	C	8829	0	8933	1115	0
5	M	8829	0	8933	1105	0
6	D	10373	0	10599	1507	0
6	N	10373	0	10599	1424	0
7	E	770	0	784	125	0
7	O	770	0	784	108	0
8	D	43	0	34	6	0
8	N	43	0	31	6	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	2	0	0	0	0
10	N	2	0	0	0	0
11	D	31	0	14	5	0
11	M	31	0	14	2	0
12	A	78	0	0	13	0
12	B	117	0	0	29	0
12	C	408	0	0	104	0
12	D	531	0	0	108	0
12	E	34	0	0	17	0
12	G	39	0	0	6	0
12	H	22	0	0	6	0
12	I	31	0	0	3	0
12	K	81	0	0	26	0
12	L	95	0	0	12	0
12	M	396	0	0	101	0
12	N	510	0	0	120	0
12	O	53	0	0	16	0
12	X	31	0	0	5	0
12	Y	26	0	0	3	0
12	Z	18	0	0	3	0
All	All	51962	0	49323	5902	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 60.

The worst 5 of 5902 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)
6:D:133:ILE:N	6:D:133:ILE:CA	1.70	1.55
6:D:132:TYR:C	6:D:132:TYR:CA	1.78	1.54
7:E:92:LEU:HD23	12:E:113:HOH:O	1.25	1.32
2:Y:2:A:OP2	6:N:671:LYS:NZ	1.72	1.21
6:D:87:ARG:HD3	6:D:524:LEU:HD11	1.30	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	
4	A	227/315 (72%)	208 (92%)	16 (7%)	3 (1%)	9	38
4	B	227/315 (72%)	208 (92%)	15 (7%)	4 (2%)	6	31
4	K	227/315 (72%)	208 (92%)	16 (7%)	3 (1%)	9	38
4	L	227/315 (72%)	206 (91%)	18 (8%)	3 (1%)	9	38
5	C	1117/1119 (100%)	922 (82%)	136 (12%)	59 (5%)	1	9
5	M	1117/1119 (100%)	919 (82%)	137 (12%)	61 (6%)	1	8
6	D	1308/1524 (86%)	1104 (84%)	145 (11%)	59 (4%)	2	12
6	N	1308/1524 (86%)	1099 (84%)	158 (12%)	51 (4%)	2	14
7	E	93/99 (94%)	73 (78%)	13 (14%)	7 (8%)	1	4
7	O	93/99 (94%)	73 (78%)	12 (13%)	8 (9%)	0	3
All	All	5944/6744 (88%)	5020 (84%)	666 (11%)	258 (4%)	2	12

5 of 258 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	29	GLU
4	B	29	GLU
4	B	187	GLY

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Mol	Chain	Res	Type
5	C	152	PRO
5	C	156	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	202/273 (74%)	158 (78%)	44 (22%)	1	6
4	B	202/273 (74%)	161 (80%)	41 (20%)	1	7
4	K	202/273 (74%)	157 (78%)	45 (22%)	1	5
4	L	202/273 (74%)	147 (73%)	55 (27%)	0	2
5	C	941/941 (100%)	707 (75%)	234 (25%)	0	4
5	M	941/941 (100%)	708 (75%)	233 (25%)	1	3
6	D	1111/1279 (87%)	855 (77%)	256 (23%)	1	5
6	N	1111/1279 (87%)	839 (76%)	272 (24%)	1	4
7	E	84/88 (96%)	66 (79%)	18 (21%)	1	6
7	O	84/88 (96%)	65 (77%)	19 (23%)	1	5
All	All	5080/5708 (89%)	3863 (76%)	1217 (24%)	1	4

5 of 1217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	N	3	LYS
6	N	1284	GLU
6	N	121	THR
5	M	1118	LYS
6	N	758	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
5	M	881	ASN

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Mol	Chain	Res	Type
6	N	861	GLN
5	M	1026	GLN
6	N	549	ASN
6	N	1046	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	H	16/16 (100%)	11 (68%)	6 (37%)
2	Y	16/16 (100%)	11 (68%)	7 (43%)
All	All	32/32 (100%)	22 (68%)	13 (40%)

5 of 22 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	2	A
2	H	3	G
2	H	6	U
2	H	7	G
2	H	8	C

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	Y	6	U
2	Y	7	G
2	Y	13	C
2	Y	9	G
2	Y	12	G

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

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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
8	STD	N	8001	-	41,47,47	7.04	24 (58%)	50,73,73	2.94	14 (28%)
11	APC	D	5999	10	29,33,33	1.22	3 (10%)	44,52,52	1.48	8 (18%)
8	STD	D	7001	-	41,47,47	7.18	25 (60%)	50,73,73	2.92	14 (28%)
11	APC	M	6999	10	29,33,33	1.11	3 (10%)	44,52,52	1.43	8 (18%)

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
8	STD	N	8001	-	-	11/31/101/101	0/6/5/5
11	APC	D	5999	10	-	4/19/38/38	0/3/3/3
8	STD	D	7001	-	-	11/31/101/101	0/6/5/5
11	APC	M	6999	10	-	4/19/38/38	0/3/3/3

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	7001	STD	O5-C19	-27.87	1.19	1.43
8	N	8001	STD	O5-C19	-27.19	1.19	1.43
8	D	7001	STD	C23-C21	-16.31	1.18	1.53
8	N	8001	STD	C23-C21	-15.64	1.20	1.53
8	N	8001	STD	C18-C16	-13.57	1.25	1.53

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	7001	STD	C20-N1-C2	-11.89	101.66	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	8001	STD	C20-N1-C2	-11.54	102.00	113.06
8	D	7001	STD	C19-O5-C13	9.43	122.53	112.81
8	N	8001	STD	C19-O5-C13	9.06	122.15	112.81
8	N	8001	STD	C2-C1-C3	-6.53	101.57	107.81

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

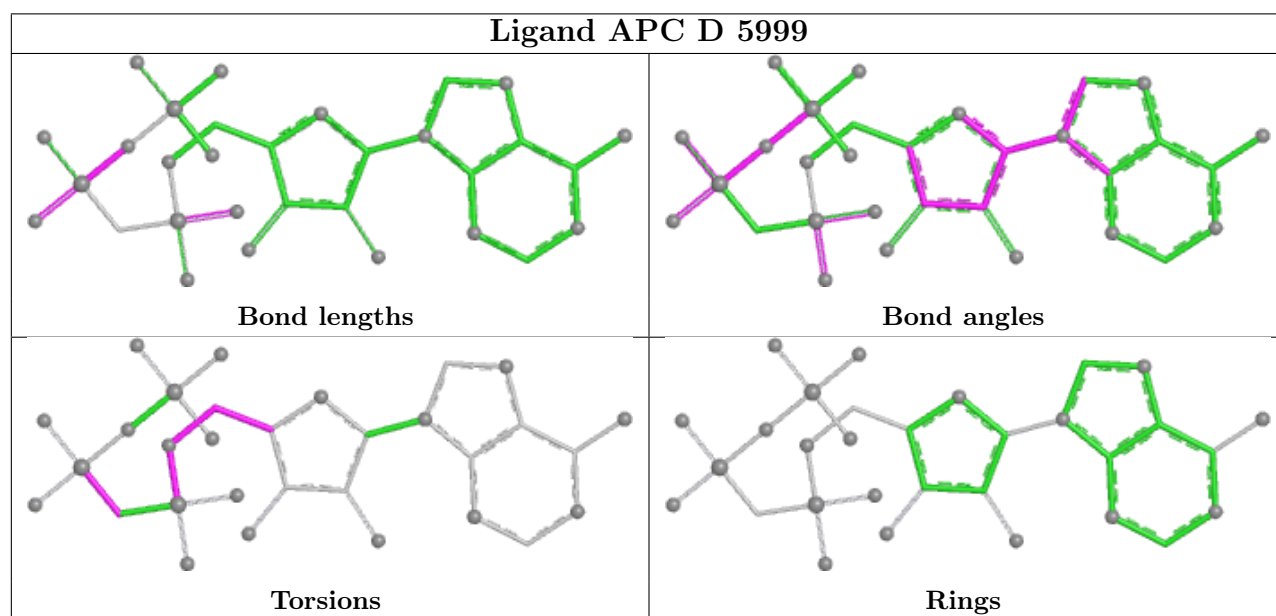
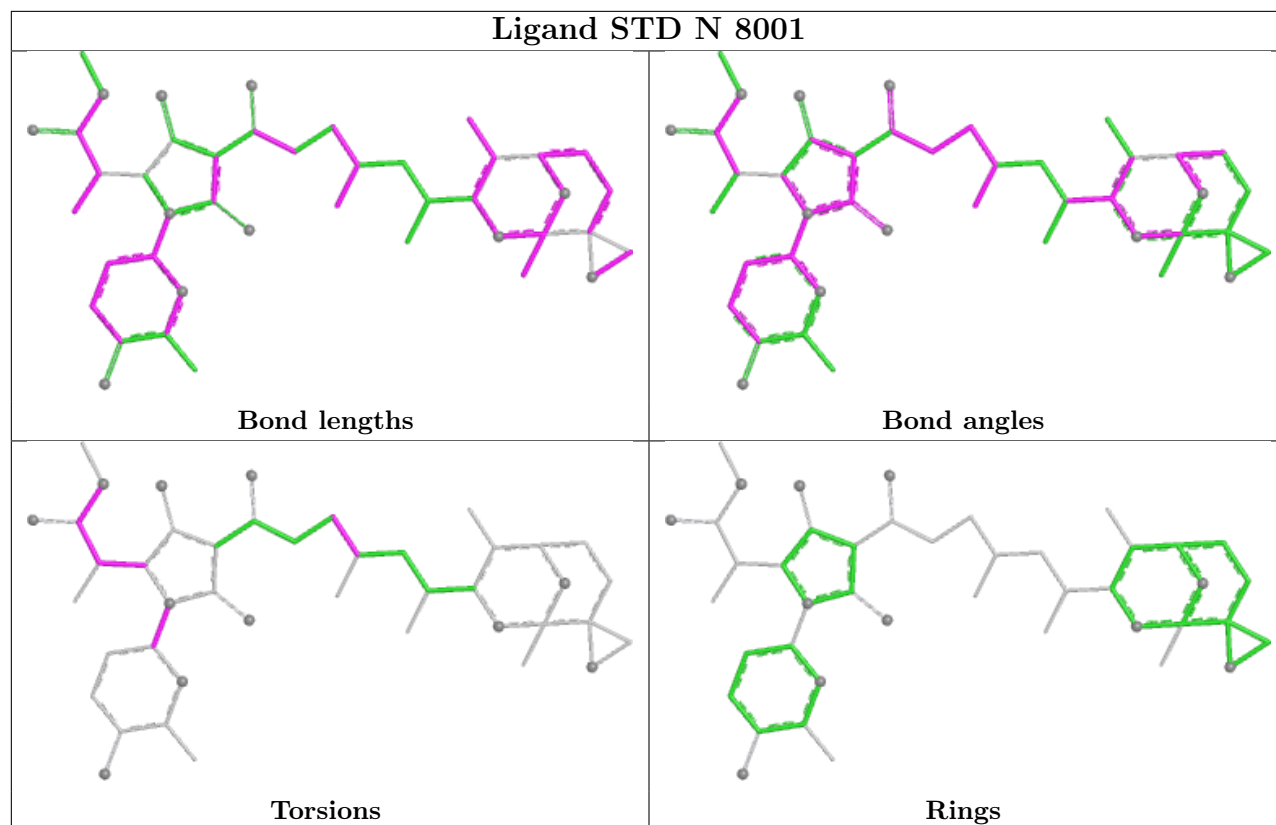
Mol	Chain	Res	Type	Atoms
8	D	7001	STD	O4-C4-N1-C20
8	D	7001	STD	C6-C7-C8-C9
8	D	7001	STD	C6-C7-C8-C11
8	D	7001	STD	N1-C20-C21-C23
8	D	7001	STD	C3-C20-C21-C22

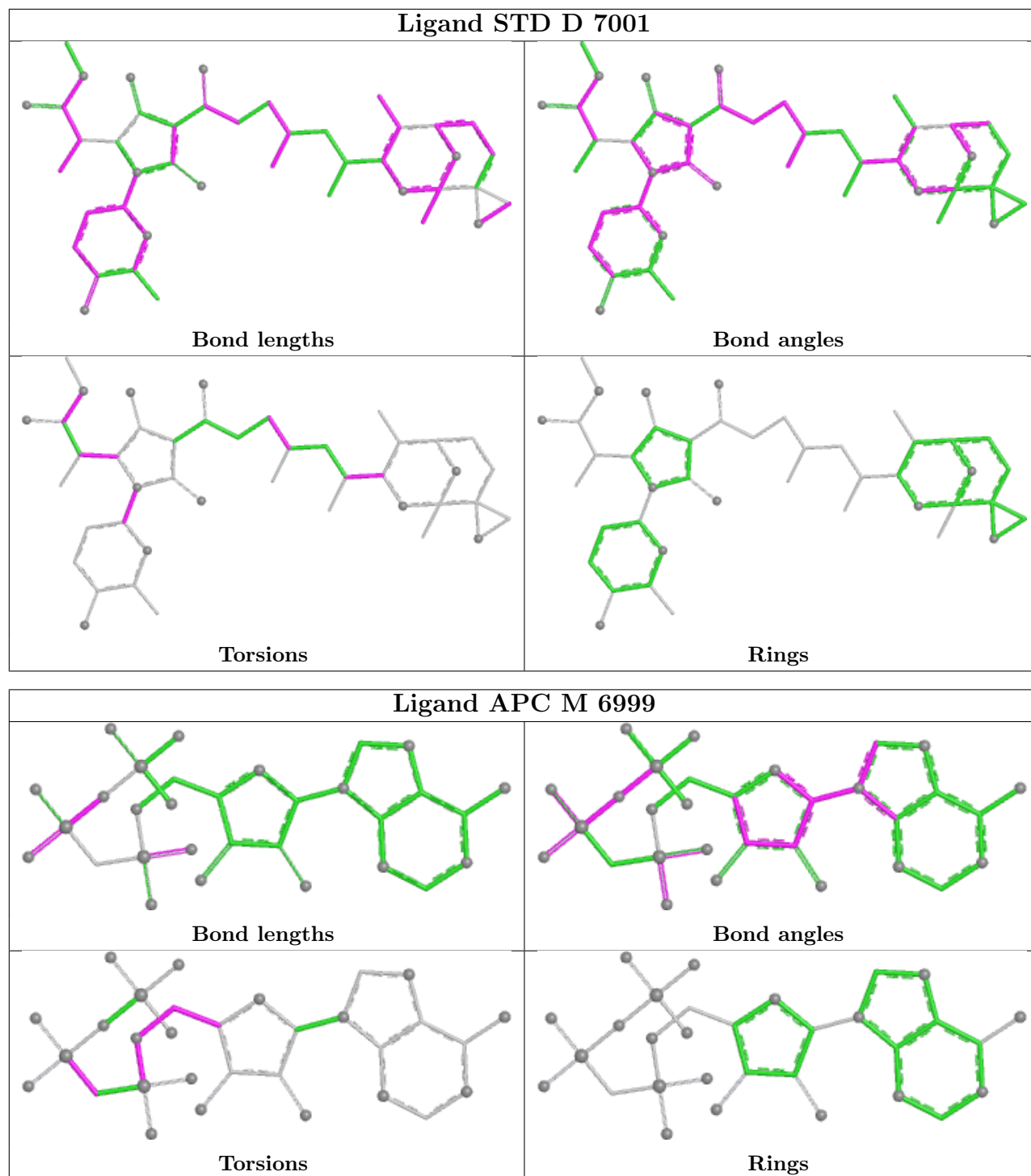
There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	8001	STD	6	0
11	D	5999	APC	5	0
8	D	7001	STD	6	0
11	M	6999	APC	2	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 ⓘ

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	G	23/23 (100%)	-1.77	0 100 100	23, 43, 66, 69	0
1	X	23/23 (100%)	-1.79	0 100 100	9, 37, 77, 92	0
2	H	16/16 (100%)	-1.90	0 100 100	24, 52, 92, 93	0
2	Y	16/16 (100%)	-1.98	0 100 100	25, 43, 96, 99	0
3	I	13/14 (92%)	-1.79	0 100 100	39, 55, 76, 77	0
3	Z	13/14 (92%)	-1.71	0 100 100	50, 61, 75, 79	0
4	A	229/315 (72%)	-1.54	0 100 100	31, 58, 73, 77	0
4	B	229/315 (72%)	-1.53	0 100 100	34, 62, 75, 82	0
4	K	229/315 (72%)	-1.56	0 100 100	30, 57, 71, 76	0
4	L	229/315 (72%)	-1.56	0 100 100	37, 62, 76, 87	0
5	C	1119/1119 (100%)	-1.55	0 100 100	7, 54, 77, 90	0
5	M	1119/1119 (100%)	-1.54	0 100 100	18, 54, 76, 90	0
6	D	1314/1524 (86%)	-1.51	1 (0%) 92 86	11, 56, 79, 89	0
6	N	1314/1524 (86%)	-1.51	0 100 100	8, 56, 76, 91	0
7	E	95/99 (95%)	-1.56	0 100 100	42, 58, 67, 71	0
7	O	95/99 (95%)	-1.53	0 100 100	33, 59, 75, 80	0
All	All	6076/6850 (88%)	-1.54	1 (0%) 100 100	7, 56, 77, 99	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	188	GLY	2.3

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

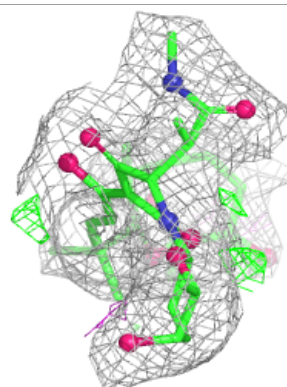
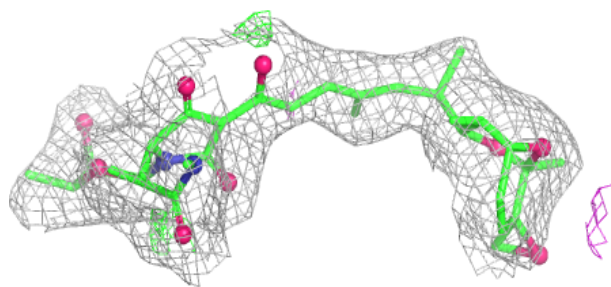
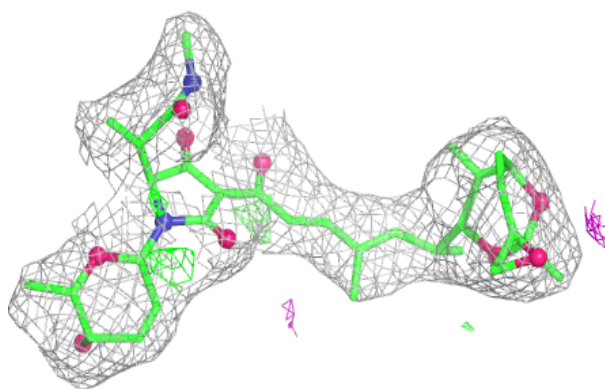
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	STD	N	8001	43/43	0.99	0.04	14,32,53,55	0
11	APC	D	5999	31/31	0.99	0.03	30,38,64,65	0
11	APC	M	6999	31/31	0.99	0.03	35,45,57,58	0
9	ZN	D	8112	1/1	1.00	0.02	58,58,58,58	0
9	ZN	N	7158	1/1	1.00	0.05	70,70,70,70	0
9	ZN	N	8212	1/1	1.00	0.02	54,54,54,54	0
10	MG	D	9001	1/1	1.00	0.01	22,22,22,22	0
10	MG	D	9002	1/1	1.00	0.01	25,25,25,25	0
10	MG	N	9003	1/1	1.00	0.01	21,21,21,21	0
10	MG	N	9004	1/1	1.00	0.01	27,27,27,27	0
8	STD	D	7001	43/43	1.00	0.03	11,24,27,28	0
9	ZN	D	7058	1/1	1.00	0.06	87,87,87,87	0

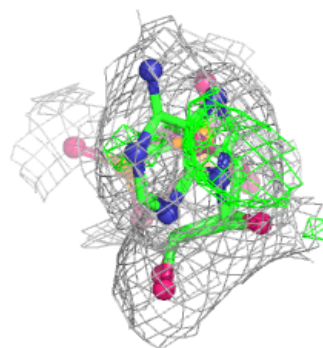
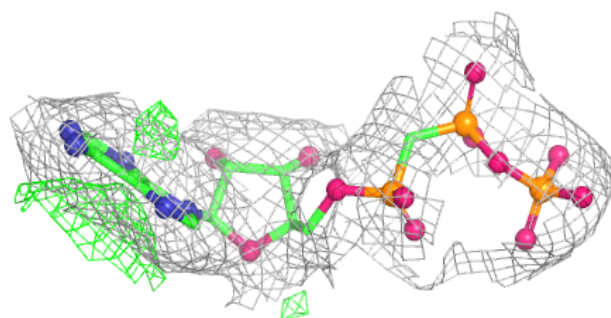
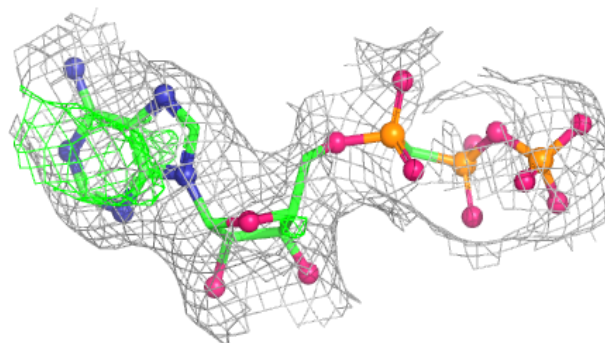
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STD N 8001:

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

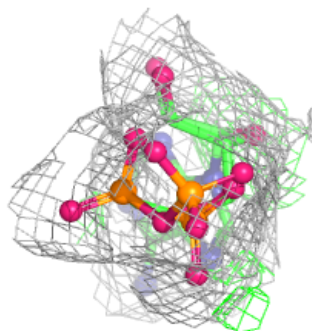
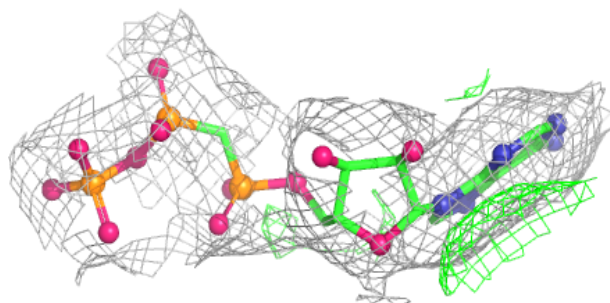
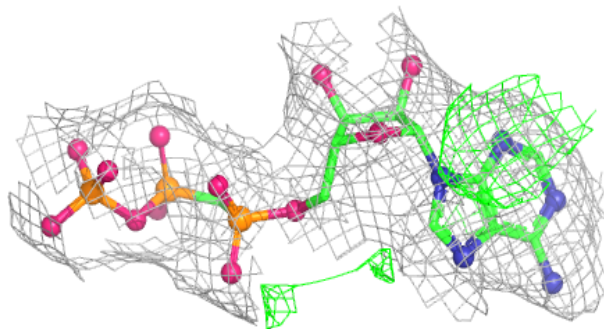
**Electron density around APC D 5999:**

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

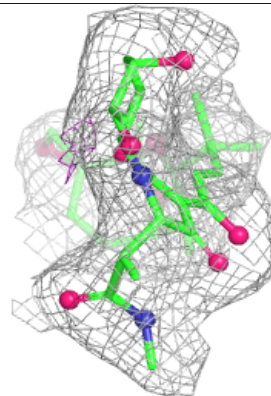
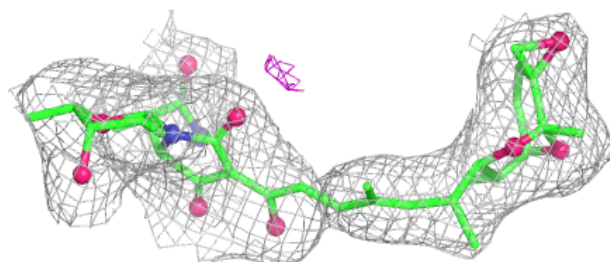
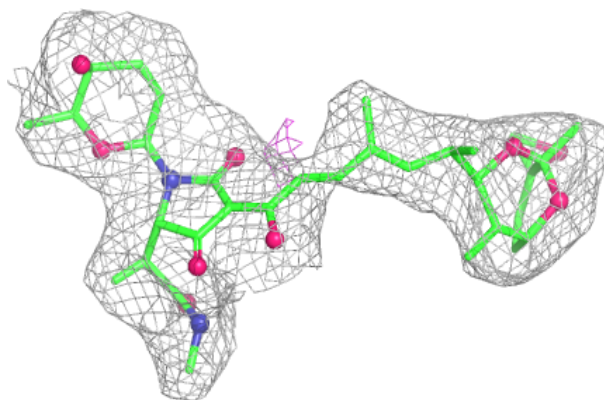


Electron density around APC M 6999:

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

**Electron density around STD D 7001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.