wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2024 – 06:48 PM EST

PDB ID	:	3U5Z
Title	:	Structure of T4 Bacteriophage clamp loader bound to the T4 clamp, primer-template DNA, and ATP analog
Authors	:	Kelch, B.A.; Makino, D.L.; O'Donnell, M.; Kuriyan, J.
Deposited on	:	2011-10-11
Resolution	:	3.50 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 (i) 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 (i)) were used in the production of this report:

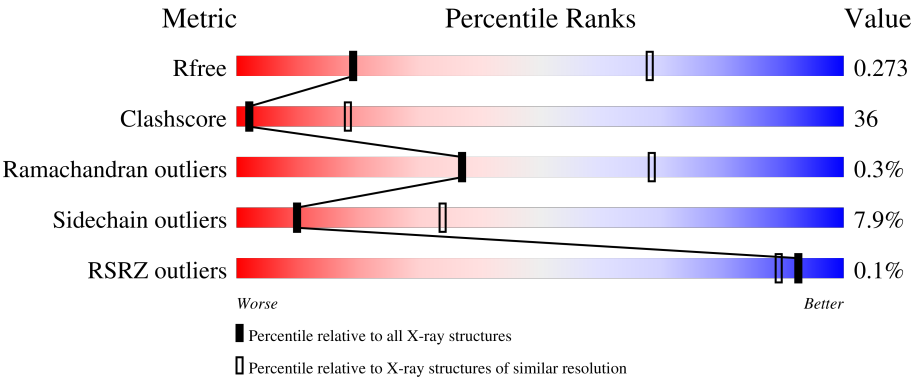
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	324	50% 45%
1	C	324	51% 44%
1	D	324	47% 49%
1	E	324	39% 51% 6%
1	L	324	53% 41% 5%

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Mol	Chain	Length	Quality of chain
1	M	324	49% 48%
1	N	324	51% 45%
1	O	324	41% 50% 6%
2	A	199	30% 53% 10% 7%
2	K	199	% 32% 50% 10% 7%
3	F	228	47% 47% 5%
3	G	228	52% 42% 6%
3	H	228	57% 38% 6%
3	P	228	39% 55% 6%
3	Q	228	42% 54% 5%
3	R	228	39% 58%
4	I	30	33% 40% 20%
4	S	30	10% 40% 30% 20%
5	J	20	5% 60% 40%
5	T	20	5% 90% 10%

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
6	08T	M	700	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 35424 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 accessory protein 44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	C	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	D	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	E	305	Total	C	N	O	S	0	0	0
			2408	1527	413	452	16			
1	L	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	M	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	N	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	O	305	Total	C	N	O	S	0	0	0
			2408	1527	413	452	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P04526
B	-3	PRO	-	expression tag	UNP P04526
B	-2	GLY	-	expression tag	UNP P04526
B	-1	GLY	-	expression tag	UNP P04526
B	0	SER	-	expression tag	UNP P04526
C	-4	GLY	-	expression tag	UNP P04526
C	-3	PRO	-	expression tag	UNP P04526
C	-2	GLY	-	expression tag	UNP P04526
C	-1	GLY	-	expression tag	UNP P04526
C	0	SER	-	expression tag	UNP P04526
D	-4	GLY	-	expression tag	UNP P04526
D	-3	PRO	-	expression tag	UNP P04526
D	-2	GLY	-	expression tag	UNP P04526

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P04526
D	0	SER	-	expression tag	UNP P04526
E	-4	GLY	-	expression tag	UNP P04526
E	-3	PRO	-	expression tag	UNP P04526
E	-2	GLY	-	expression tag	UNP P04526
E	-1	GLY	-	expression tag	UNP P04526
E	0	SER	-	expression tag	UNP P04526
L	-4	GLY	-	expression tag	UNP P04526
L	-3	PRO	-	expression tag	UNP P04526
L	-2	GLY	-	expression tag	UNP P04526
L	-1	GLY	-	expression tag	UNP P04526
L	0	SER	-	expression tag	UNP P04526
M	-4	GLY	-	expression tag	UNP P04526
M	-3	PRO	-	expression tag	UNP P04526
M	-2	GLY	-	expression tag	UNP P04526
M	-1	GLY	-	expression tag	UNP P04526
M	0	SER	-	expression tag	UNP P04526
N	-4	GLY	-	expression tag	UNP P04526
N	-3	PRO	-	expression tag	UNP P04526
N	-2	GLY	-	expression tag	UNP P04526
N	-1	GLY	-	expression tag	UNP P04526
N	0	SER	-	expression tag	UNP P04526
O	-4	GLY	-	expression tag	UNP P04526
O	-3	PRO	-	expression tag	UNP P04526
O	-2	GLY	-	expression tag	UNP P04526
O	-1	GLY	-	expression tag	UNP P04526
O	0	SER	-	expression tag	UNP P04526

- Molecule 2 is a protein called DNA polymerase accessory protein 62.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	186	Total	C	N	O	S	0	0	0
			1488	959	244	279	6			
2	K	186	Total	C	N	O	S	0	0	0
			1488	959	244	279	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	-	expression tag	UNP P04527
A	189	LEU	-	expression tag	UNP P04527
A	190	GLU	-	expression tag	UNP P04527

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Chain	Residue	Modelled	Actual	Comment	Reference
A	191	HIS	-	expression tag	UNP P04527
A	192	HIS	-	expression tag	UNP P04527
A	193	HIS	-	expression tag	UNP P04527
A	194	HIS	-	expression tag	UNP P04527
A	195	HIS	-	expression tag	UNP P04527
A	196	HIS	-	expression tag	UNP P04527
A	197	HIS	-	expression tag	UNP P04527
A	198	HIS	-	expression tag	UNP P04527
A	199	HIS	-	expression tag	UNP P04527
A	200	HIS	-	expression tag	UNP P04527
K	188	GLY	-	expression tag	UNP P04527
K	189	LEU	-	expression tag	UNP P04527
K	190	GLU	-	expression tag	UNP P04527
K	191	HIS	-	expression tag	UNP P04527
K	192	HIS	-	expression tag	UNP P04527
K	193	HIS	-	expression tag	UNP P04527
K	194	HIS	-	expression tag	UNP P04527
K	195	HIS	-	expression tag	UNP P04527
K	196	HIS	-	expression tag	UNP P04527
K	197	HIS	-	expression tag	UNP P04527
K	198	HIS	-	expression tag	UNP P04527
K	199	HIS	-	expression tag	UNP P04527
K	200	HIS	-	expression tag	UNP P04527

- Molecule 3 is a protein called DNA polymerase processivity component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	H	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	F	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	Q	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	R	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	P	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			

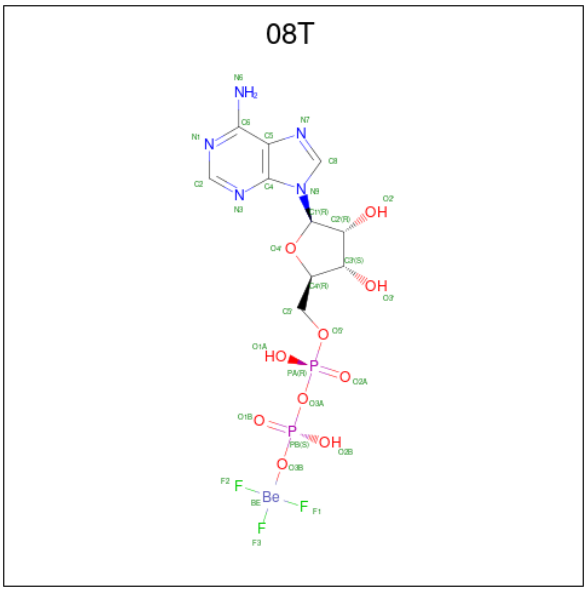
- Molecule 4 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			
4	S	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			

- Molecule 5 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	20	Total	C	N	O	P	0	0	0
			411	195	81	115	20			
5	T	20	Total	C	N	O	P	0	0	0
			411	195	81	115	20			

- Molecule 6 is [[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-tris(fluoranyl)beryllium (three-letter code: 08T) (formula: $C_{10}H_{14}BeF_3N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	B	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	C	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	D	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	L	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	M	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		

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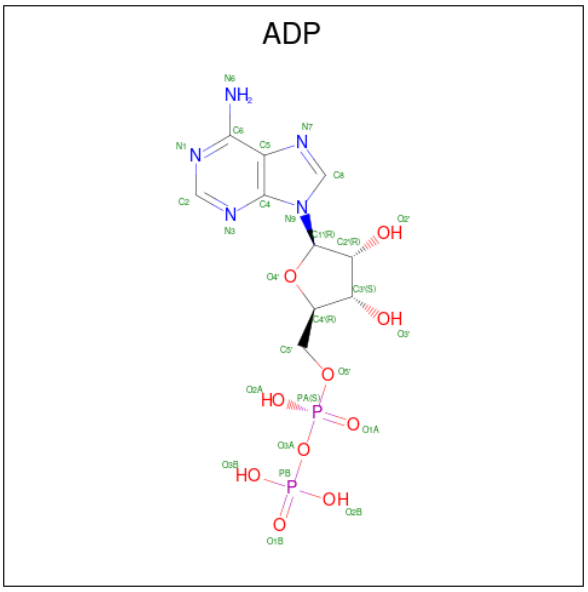
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	N	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	E	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		
7	M	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		
7	O	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



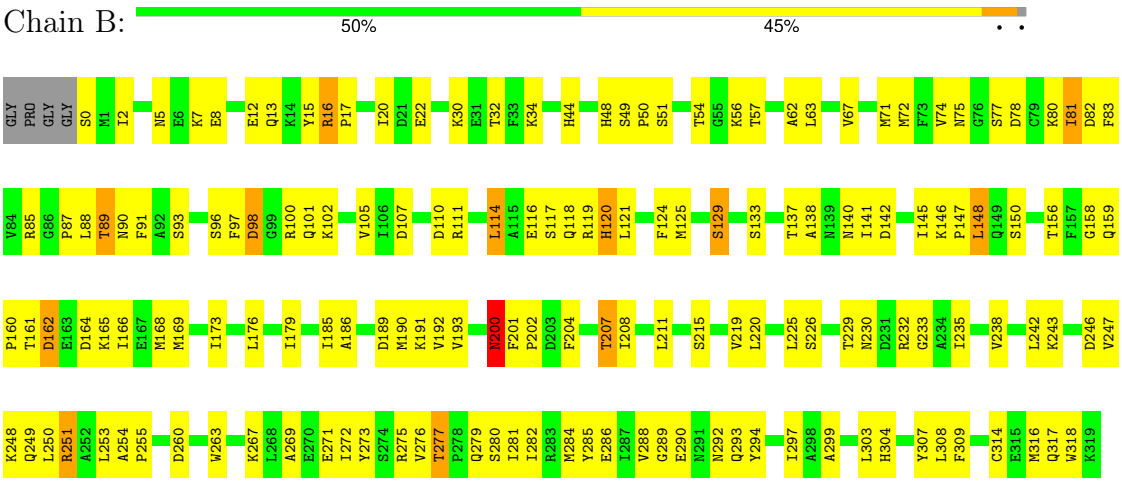
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

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.

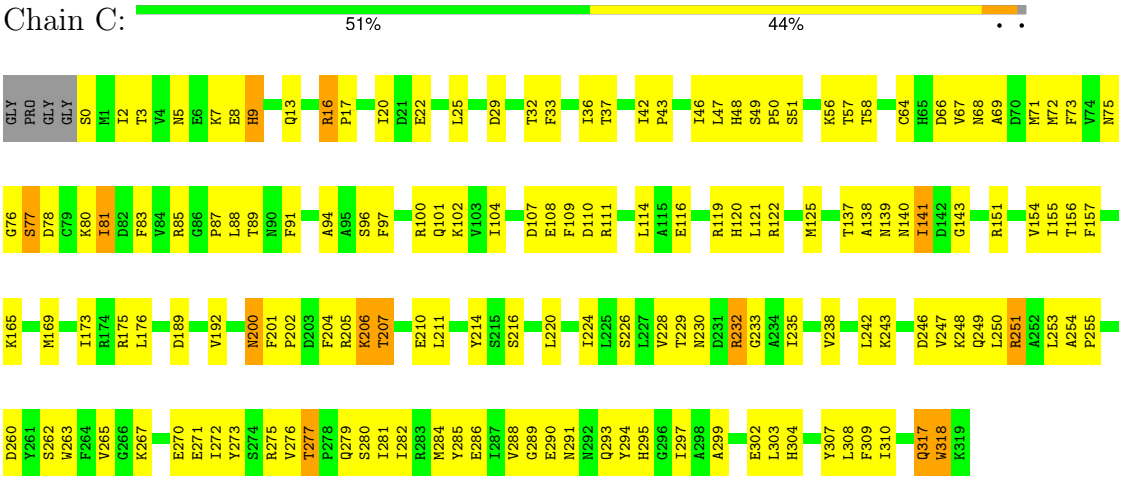
• Molecule 1: DNA polymerase accessory protein 44

Chain B:



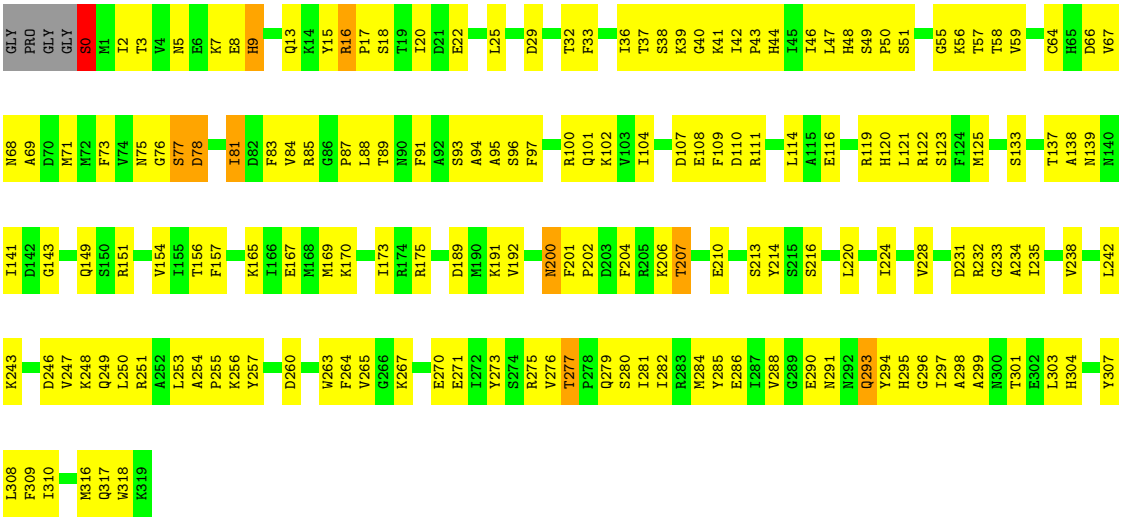
• Molecule 1: DNA polymerase accessory protein 44

Chain C:



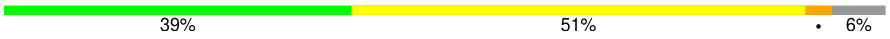
• Molecule 1: DNA polymerase accessory protein 44

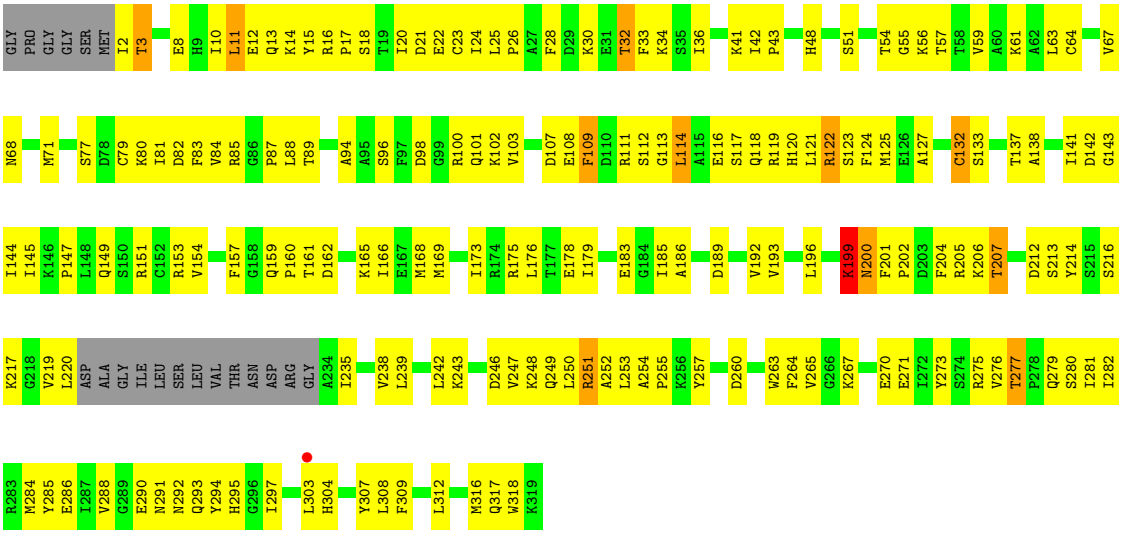
Chain D:



• Molecule 1: DNA polymerase accessory protein 44

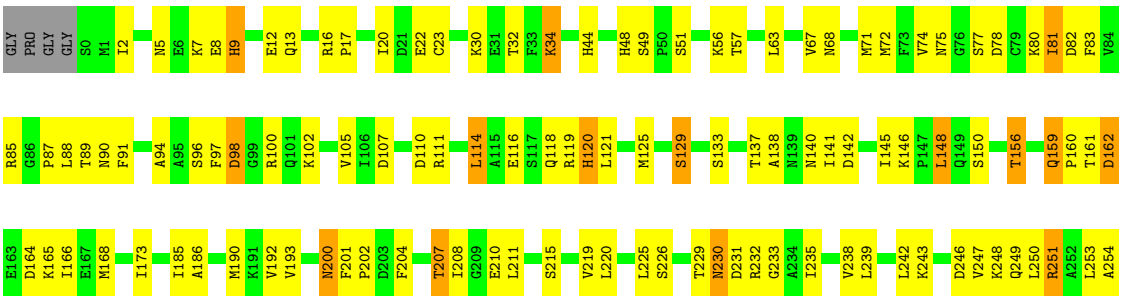
Chain E:

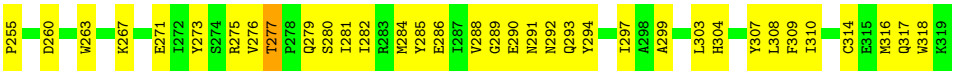




• Molecule 1: DNA polymerase accessory protein 44

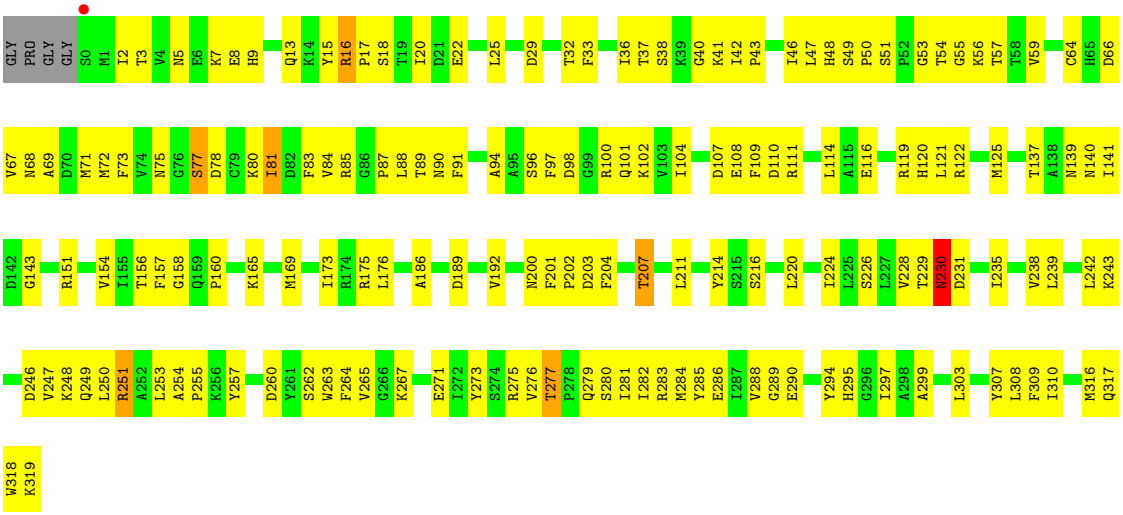
Chain L:





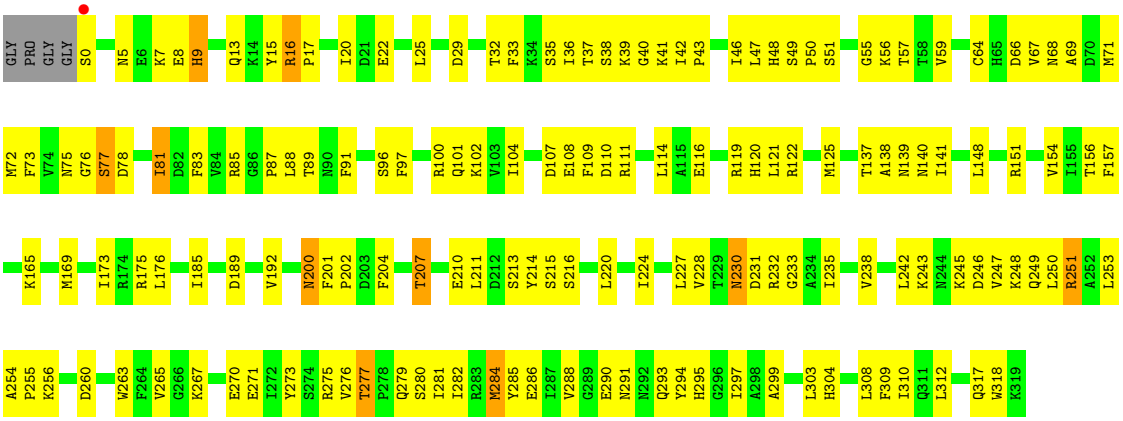
• Molecule 1: DNA polymerase accessory protein 44

Chain M:



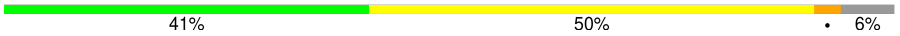
• Molecule 1: DNA polymerase accessory protein 44

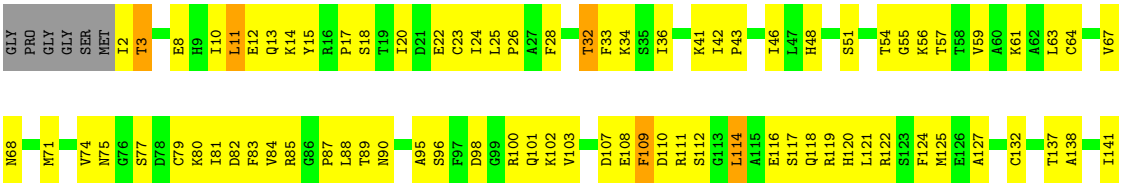
Chain N:

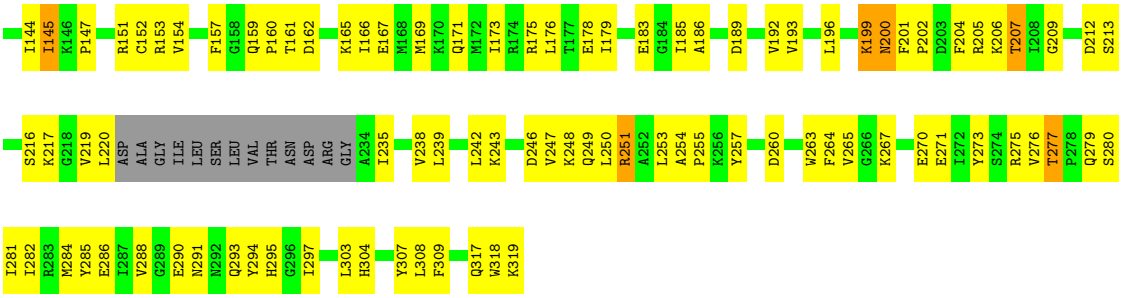


• Molecule 1: DNA polymerase accessory protein 44

Chain O:

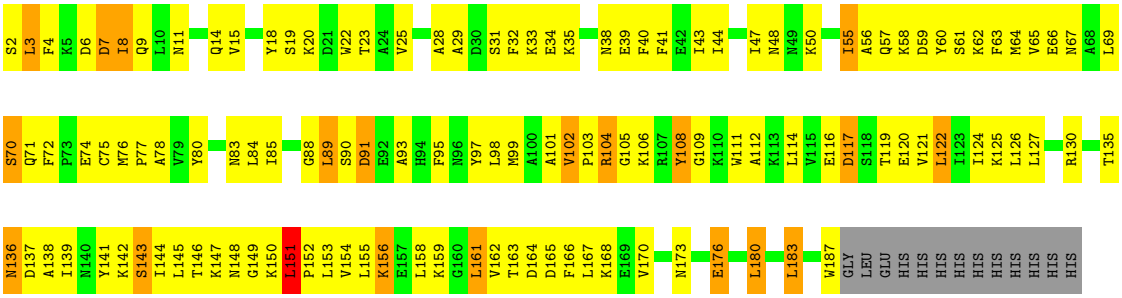






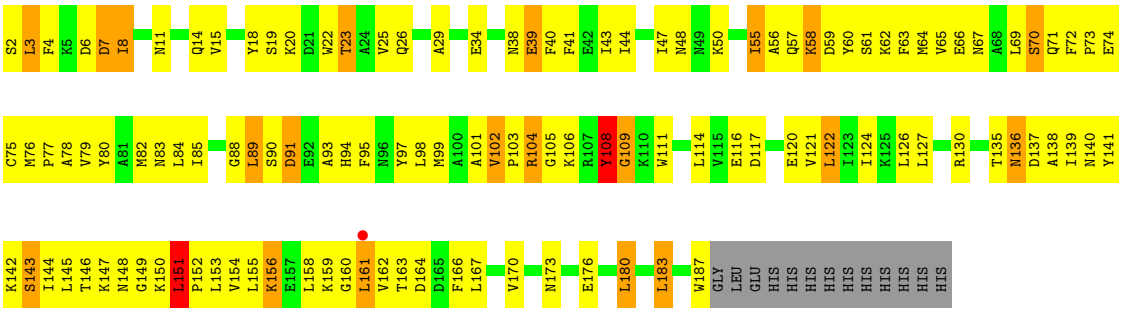
• Molecule 2: DNA polymerase accessory protein 62

Chain A:



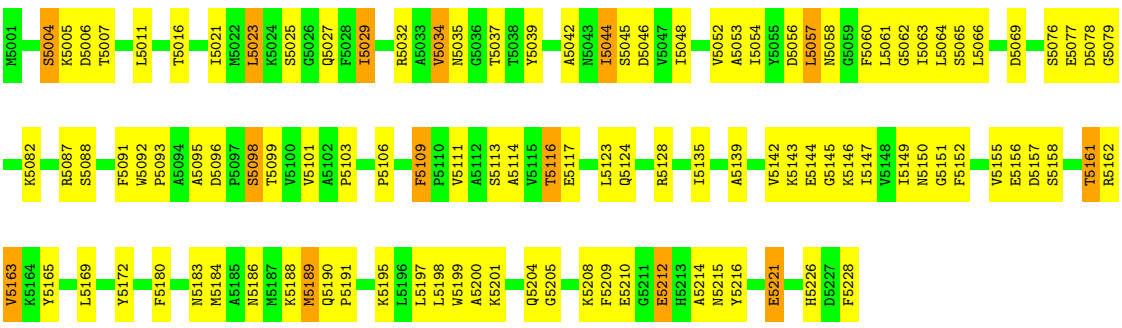
• Molecule 2: DNA polymerase accessory protein 62

Chain K:



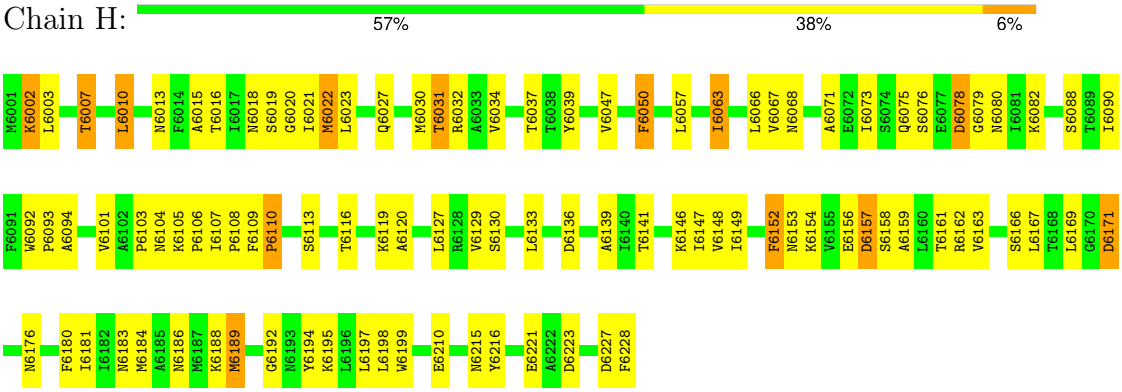
• Molecule 3: DNA polymerase processivity component

Chain G:



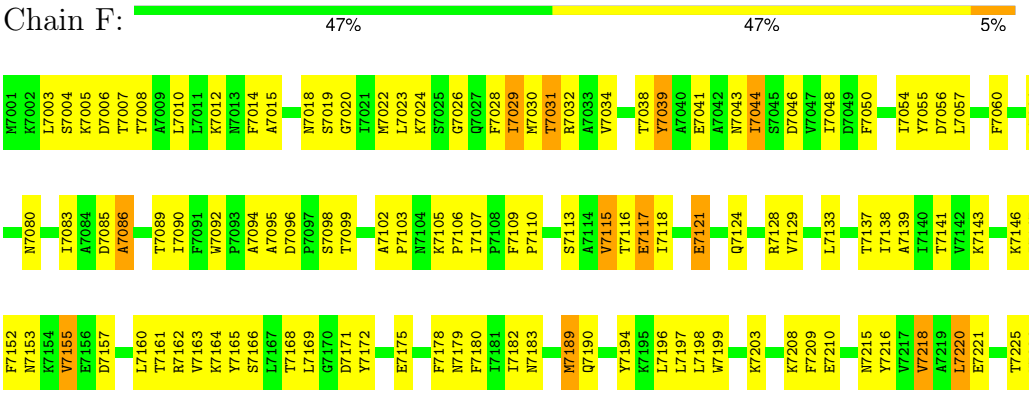
• Molecule 3: DNA polymerase processivity component

Chain H:



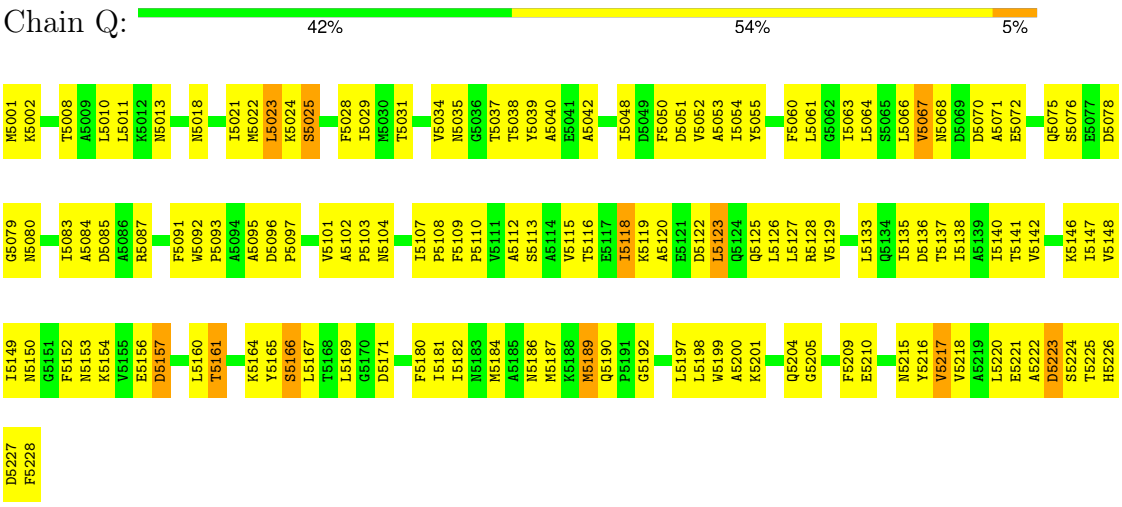
• Molecule 3: DNA polymerase processivity component

Chain F:



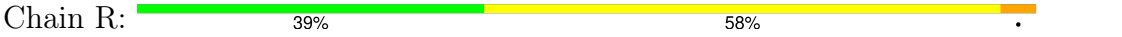
• Molecule 3: DNA polymerase processivity component

Chain Q:



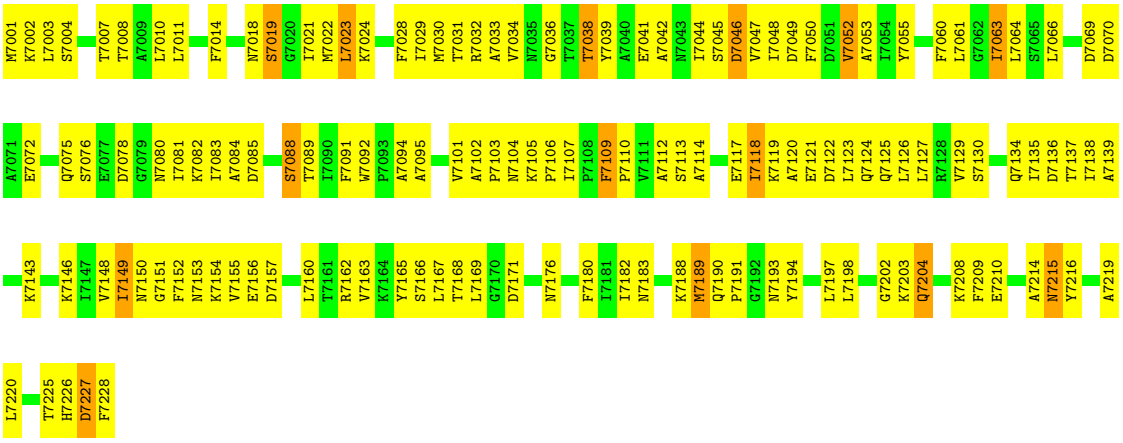
• Molecule 3: DNA polymerase processivity component

Chain R:



• Molecule 3: DNA polymerase processivity component

Chain P:

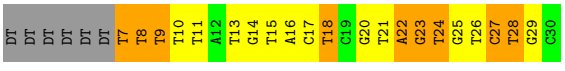


• Molecule 4: Template DNA strand

Chain I:

• Molecule 4: Template DNA strand

Chain S:

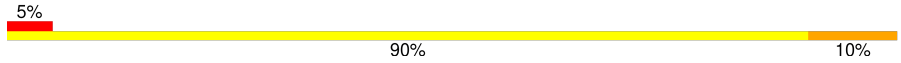


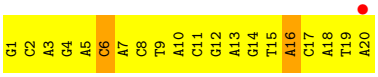
• Molecule 5: Primer DNA strand

Chain J:

• Molecule 5: Primer DNA strand

Chain T:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.70Å 239.18Å 247.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 3.50 49.19 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.19-3.50) 99.2 (49.19-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.231 , 0.279 0.223 , 0.273	Depositor DCC
R_{free} test set	1985 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	35424	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 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, 08T

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	0.63	1/2558 (0.0%)	0.77	0/3449
1	C	0.64	0/2558	0.77	4/3449 (0.1%)
1	D	0.64	1/2558 (0.0%)	0.75	0/3449
1	E	0.56	0/2451	0.71	0/3303
1	L	0.60	2/2558 (0.1%)	0.73	0/3449
1	M	0.64	0/2558	0.76	1/3449 (0.0%)
1	N	0.60	0/2558	0.75	0/3449
1	O	0.55	0/2451	0.71	0/3303
2	A	0.51	0/1516	0.74	1/2042 (0.0%)
2	K	0.48	0/1516	0.74	2/2042 (0.1%)
3	F	0.48	0/1774	0.71	0/2395
3	G	0.53	0/1774	0.73	0/2395
3	H	0.51	0/1774	0.70	0/2395
3	P	0.51	0/1774	0.75	0/2395
3	Q	0.56	0/1774	0.78	0/2395
3	R	0.59	0/1774	0.78	1/2395 (0.0%)
4	I	6.29	1/544 (0.2%)	3.85	28/838 (3.3%)
4	S	1.16	1/544 (0.2%)	1.91	19/838 (2.3%)
5	J	0.92	0/462	1.72	11/710 (1.5%)
5	T	0.90	0/462	1.53	2/710 (0.3%)
All	All	0.98	6/35938 (0.0%)	0.95	69/48850 (0.1%)

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
1	C	0	1
1	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
1	M	0	2
1	N	0	2
2	A	0	1
2	K	0	2
4	I	0	1
All	All	0	13

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	30	DC	C1'-N1	144.35	3.49	1.47
4	S	15	DT	N1-C2	6.50	1.43	1.38
1	B	159	GLN	CD-NE2	-6.26	1.17	1.32
1	L	159	GLN	CD-NE2	-6.05	1.17	1.32
1	D	293	GLN	CD-NE2	5.66	1.47	1.32

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	30	DC	O4'-C1'-N1	-87.18	46.97	108.00
4	I	30	DC	C2-N1-C1'	-30.76	84.97	118.80
4	I	30	DC	C6-N1-C1'	18.13	142.56	120.80
4	S	15	DT	N3-C2-O2	-9.38	116.67	122.30
5	J	16	DA	O4'-C1'-N9	9.33	114.53	108.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	7	ASP	Mainchain
1	B	200	ASN	Peptide
1	C	229	THR	Peptide
1	D	0	SER	Peptide
4	I	30	DC	Sidechain

5.2 Too-close contacts (i)

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	2514	0	2543	178	0
1	C	2514	0	2543	192	0
1	D	2514	0	2543	251	0
1	E	2408	0	2433	221	0
1	L	2514	0	2543	167	0
1	M	2514	0	2543	188	0
1	N	2514	0	2543	215	0
1	O	2408	0	2433	215	0
2	A	1488	0	1509	173	0
2	K	1488	0	1509	184	0
3	F	1750	0	1752	117	0
3	G	1750	0	1752	140	0
3	H	1750	0	1752	95	0
3	P	1750	0	1752	182	0
3	Q	1750	0	1752	138	0
3	R	1750	0	1752	164	0
4	I	489	0	277	43	0
4	S	489	0	277	37	0
5	J	411	0	224	31	0
5	T	411	0	224	27	0
6	B	31	0	13	8	0
6	C	31	0	13	8	0
6	D	31	0	13	6	0
6	L	31	0	13	6	0
6	M	31	0	13	9	0
6	N	31	0	13	7	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
8	E	27	0	12	5	0
8	O	27	0	12	4	0
All	All	35424	0	34758	2554	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 36.

The worst 5 of 2554 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:L:293:GLN:NE2	2:K:84:LEU:O	1.73	1.21
1:N:108:GLU:HB3	1:O:122:ARG:HH21	1.06	1.19
3:P:7109:PHE:HD1	3:P:7110:PRO:HD2	1.02	1.18
3:Q:5128:ARG:HG2	3:P:7066:LEU:HD13	1.24	1.13
3:F:7141:THR:HG22	3:F:7179:ASN:HA	1.26	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	B	318/324 (98%)	303 (95%)	15 (5%)	0	100	100
1	C	318/324 (98%)	296 (93%)	22 (7%)	0	100	100
1	D	318/324 (98%)	295 (93%)	23 (7%)	0	100	100
1	E	301/324 (93%)	277 (92%)	23 (8%)	1 (0%)	37	68
1	L	318/324 (98%)	301 (95%)	17 (5%)	0	100	100
1	M	318/324 (98%)	297 (93%)	21 (7%)	0	100	100
1	N	318/324 (98%)	294 (92%)	24 (8%)	0	100	100
1	O	301/324 (93%)	276 (92%)	25 (8%)	0	100	100
2	A	184/199 (92%)	155 (84%)	26 (14%)	3 (2%)	8	38
2	K	184/199 (92%)	153 (83%)	28 (15%)	3 (2%)	8	38
3	F	226/228 (99%)	211 (93%)	14 (6%)	1 (0%)	30	64
3	G	226/228 (99%)	209 (92%)	16 (7%)	1 (0%)	30	64
3	H	226/228 (99%)	211 (93%)	13 (6%)	2 (1%)	14	49
3	P	226/228 (99%)	203 (90%)	23 (10%)	0	100	100
3	Q	226/228 (99%)	211 (93%)	15 (7%)	0	100	100
3	R	226/228 (99%)	206 (91%)	18 (8%)	2 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4234/4358 (97%)	3898 (92%)	323 (8%)	13 (0%)	37 68

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	8	ILE
3	H	6079	GLY
3	R	6111	VAL
2	A	151	LEU
3	G	5057	LEU

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	B	278/279 (100%)	258 (93%)	20 (7%)	12 37
1	C	278/279 (100%)	263 (95%)	15 (5%)	18 46
1	D	278/279 (100%)	267 (96%)	11 (4%)	27 56
1	E	266/279 (95%)	245 (92%)	21 (8%)	10 34
1	L	278/279 (100%)	258 (93%)	20 (7%)	12 37
1	M	278/279 (100%)	266 (96%)	12 (4%)	25 54
1	N	278/279 (100%)	265 (95%)	13 (5%)	22 51
1	O	266/279 (95%)	246 (92%)	20 (8%)	11 35
2	A	161/174 (92%)	137 (85%)	24 (15%)	2 15
2	K	161/174 (92%)	138 (86%)	23 (14%)	2 16
3	F	189/183 (103%)	169 (89%)	20 (11%)	5 25
3	G	189/183 (103%)	169 (89%)	20 (11%)	5 25
3	H	189/183 (103%)	169 (89%)	20 (11%)	5 25
3	P	189/183 (103%)	171 (90%)	18 (10%)	7 28
3	Q	189/183 (103%)	173 (92%)	16 (8%)	8 32
3	R	189/183 (103%)	175 (93%)	14 (7%)	11 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3656/3678 (99%)	3369 (92%)	287 (8%)	10 34

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	135	THR
3	P	7227	ASP
2	K	183	LEU
3	R	6137	THR
3	G	5045	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	292	ASN
1	N	317	GLN
1	M	101	GLN
1	N	101	GLN
1	O	159	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	08T	D	700	-	27,33,33	2.82	11 (40%)	27,52,52	4.65	7 (25%)
8	ADP	E	700	7	24,29,29	0.94	0	29,45,45	1.36	4 (13%)
6	08T	N	700	-	27,33,33	2.79	11 (40%)	27,52,52	4.77	5 (18%)
6	08T	M	700	-	27,33,33	3.02	11 (40%)	27,52,52	4.65	9 (33%)
6	08T	L	700	7	27,33,33	2.85	12 (44%)	27,52,52	4.76	10 (37%)
6	08T	C	700	7	27,33,33	2.87	12 (44%)	27,52,52	4.21	10 (37%)
8	ADP	O	700	7	24,29,29	0.87	0	29,45,45	1.34	3 (10%)
6	08T	B	700	7	27,33,33	3.00	12 (44%)	27,52,52	4.72	7 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	08T	D	700	-	-	0/12/38/38	0/3/3/3
8	ADP	E	700	7	-	3/12/32/32	0/3/3/3
6	08T	N	700	-	-	3/12/38/38	0/3/3/3
6	08T	M	700	-	-	3/12/38/38	0/3/3/3
6	08T	L	700	7	-	2/12/38/38	0/3/3/3
6	08T	C	700	7	-	3/12/38/38	0/3/3/3
8	ADP	O	700	7	-	4/12/32/32	0/3/3/3
6	08T	B	700	7	-	5/12/38/38	0/3/3/3

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	700	08T	F1-BE	-7.45	1.37	1.54
6	M	700	08T	F1-BE	-7.16	1.37	1.54
6	C	700	08T	F1-BE	-7.08	1.38	1.54
6	L	700	08T	F1-BE	-6.99	1.38	1.54
6	M	700	08T	F3-BE	-6.78	1.38	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	700	08T	C1'-N9-C4	-23.29	85.72	126.64
6	B	700	08T	C1'-N9-C4	-22.63	86.88	126.64
6	D	700	08T	C1'-N9-C4	-22.39	87.31	126.64
6	L	700	08T	C1'-N9-C4	-22.11	87.80	126.64
6	M	700	08T	C1'-N9-C4	-21.19	89.42	126.64

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	700	08T	C5'-O5'-PA-O2A
6	B	700	08T	C5'-O5'-PA-O3A
6	C	700	08T	O4'-C4'-C5'-O5'
6	L	700	08T	O4'-C4'-C5'-O5'
6	M	700	08T	O4'-C4'-C5'-O5'

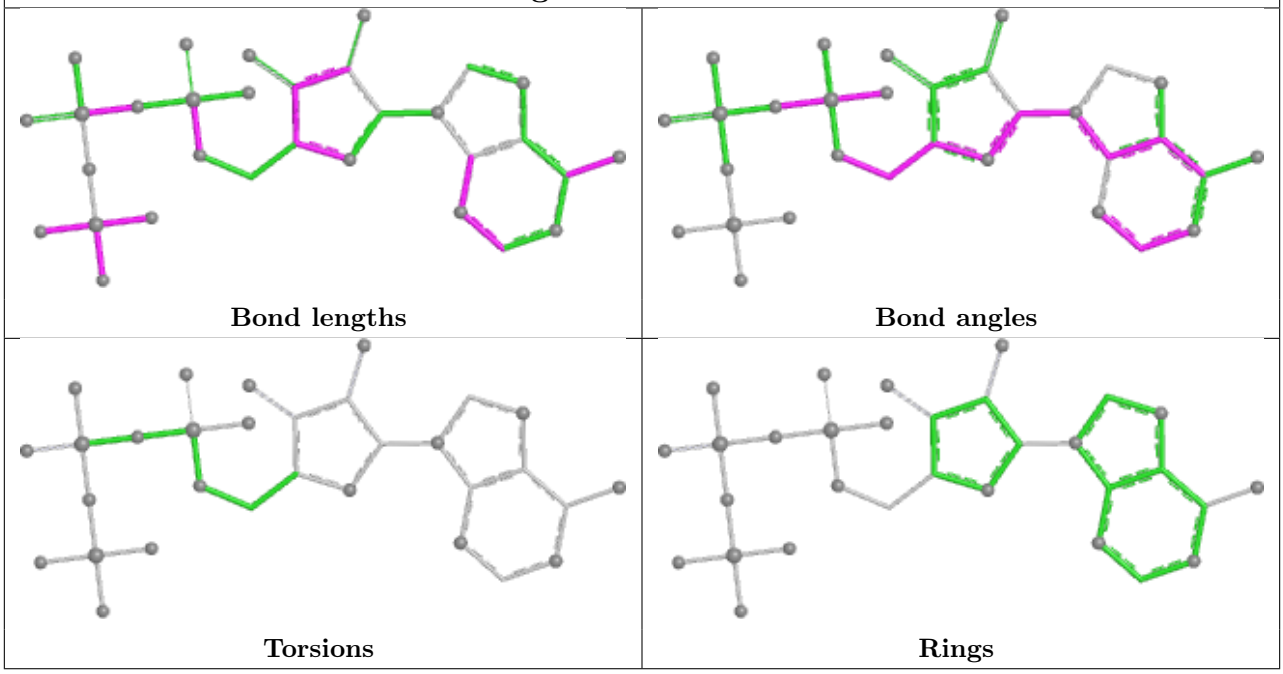
There are no ring outliers.

8 monomers are involved in 53 short contacts:

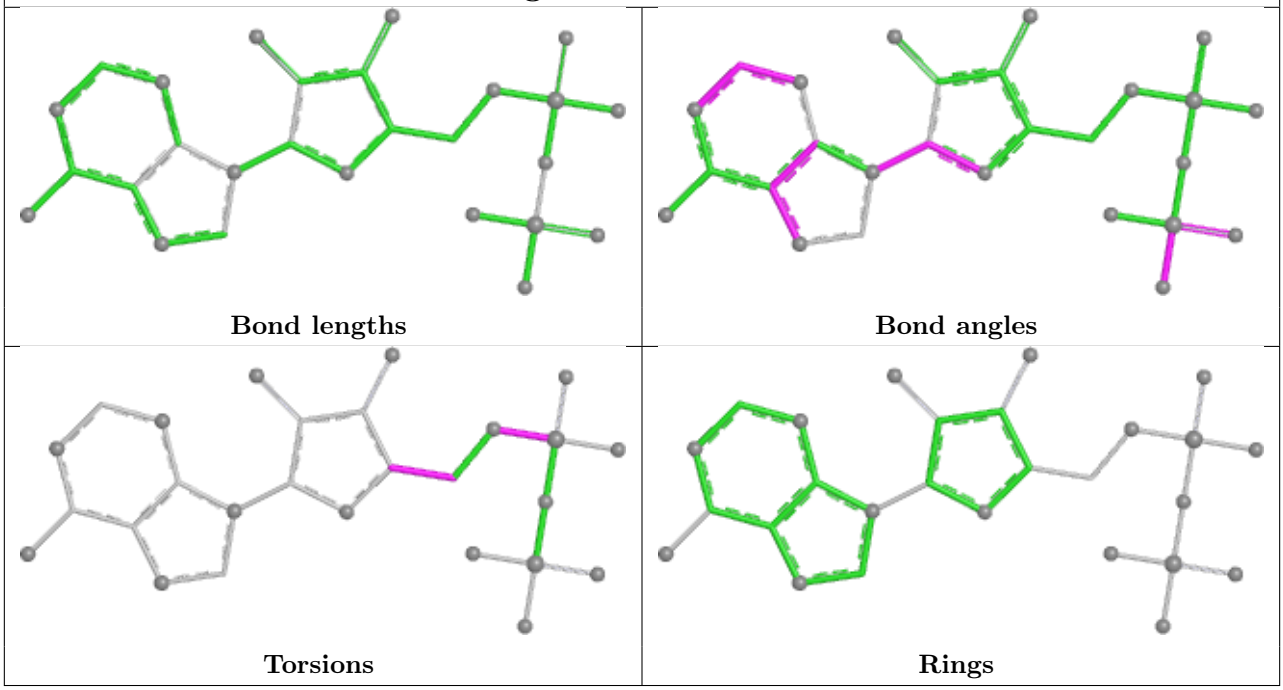
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	700	08T	6	0
8	E	700	ADP	5	0
6	N	700	08T	7	0
6	M	700	08T	9	0
6	L	700	08T	6	0
6	C	700	08T	8	0
8	O	700	ADP	4	0
6	B	700	08T	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

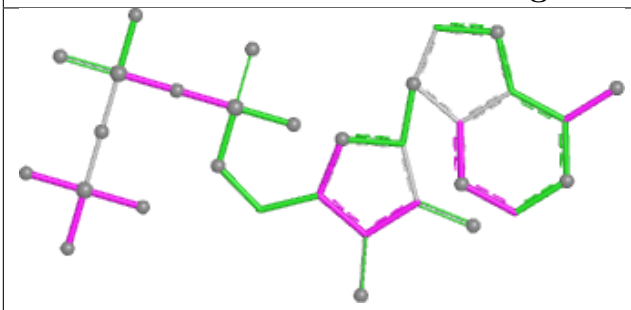
Ligand 08T D 700



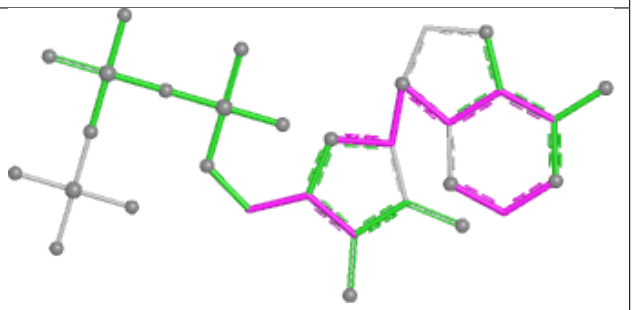
Ligand ADP E 700



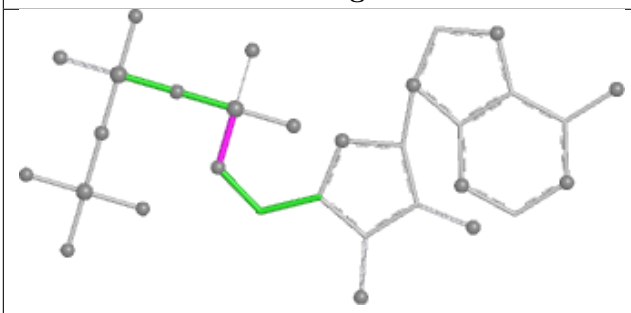
Ligand 08T N 700



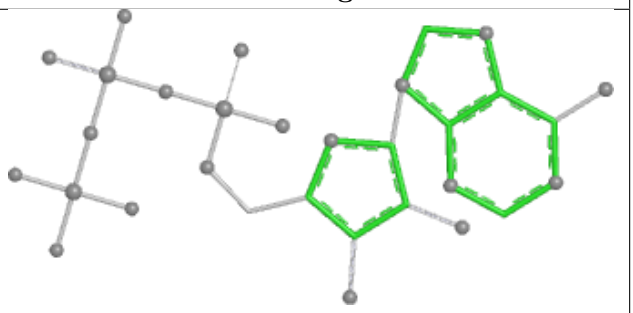
Bond lengths



Bond angles

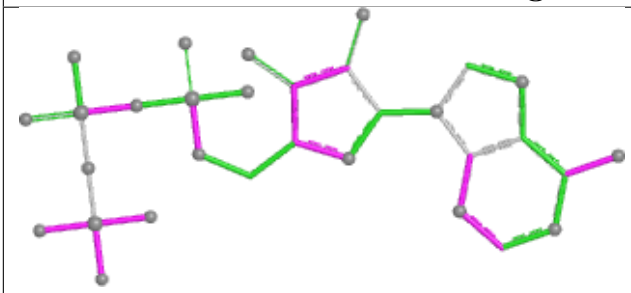


Torsions

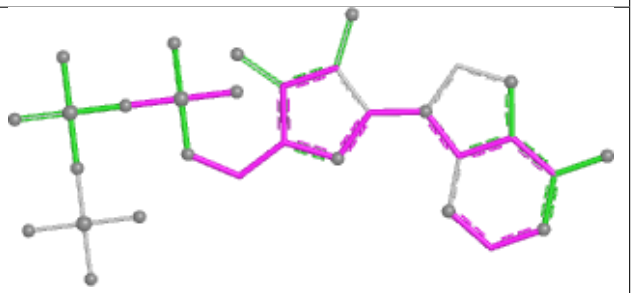


Rings

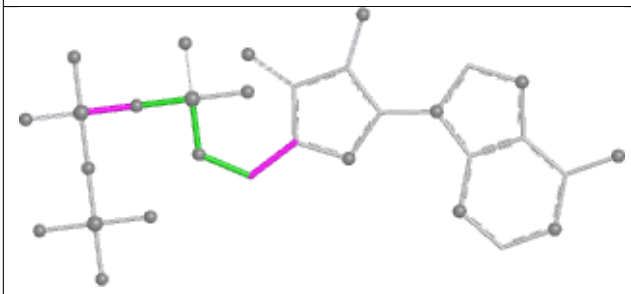
Ligand 08T M 700



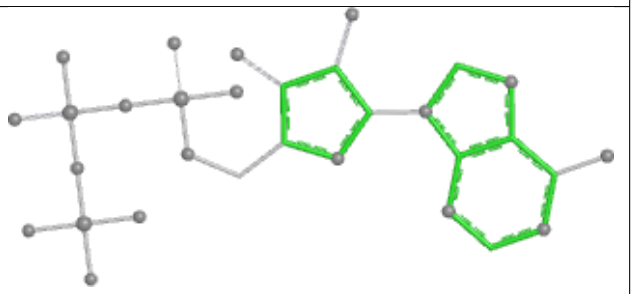
Bond lengths



Bond angles

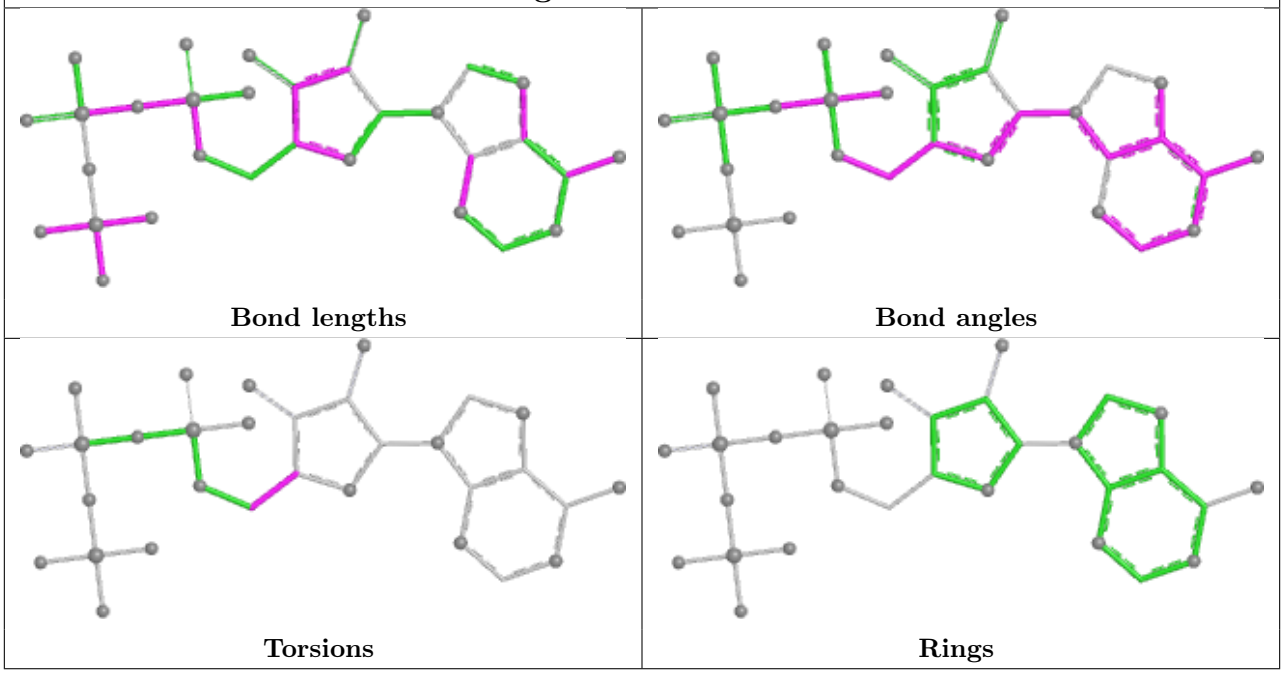


Torsions

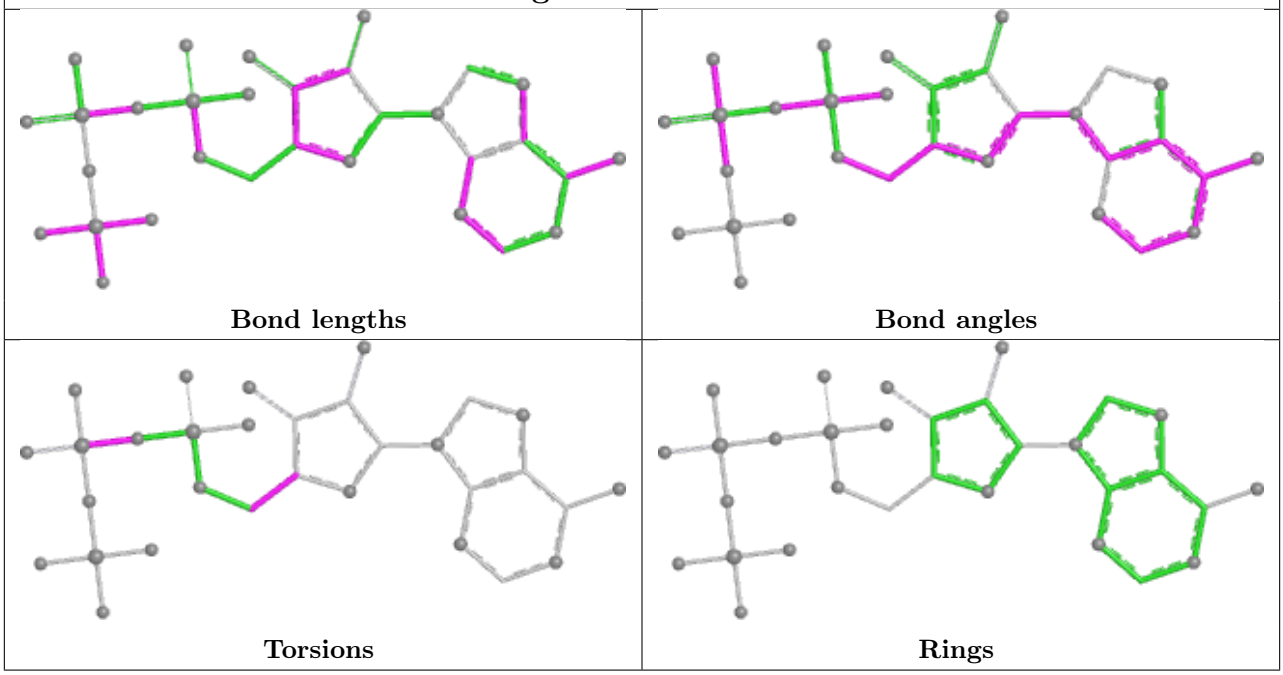


Rings

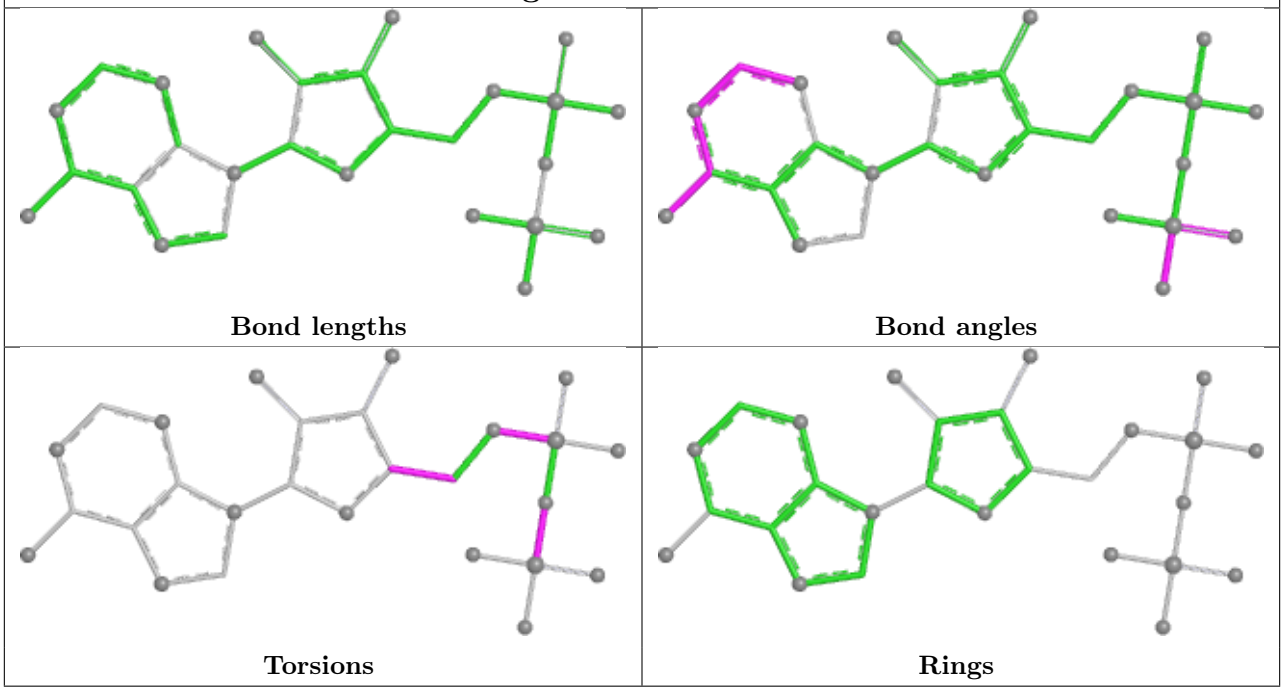
Ligand 08T L 700



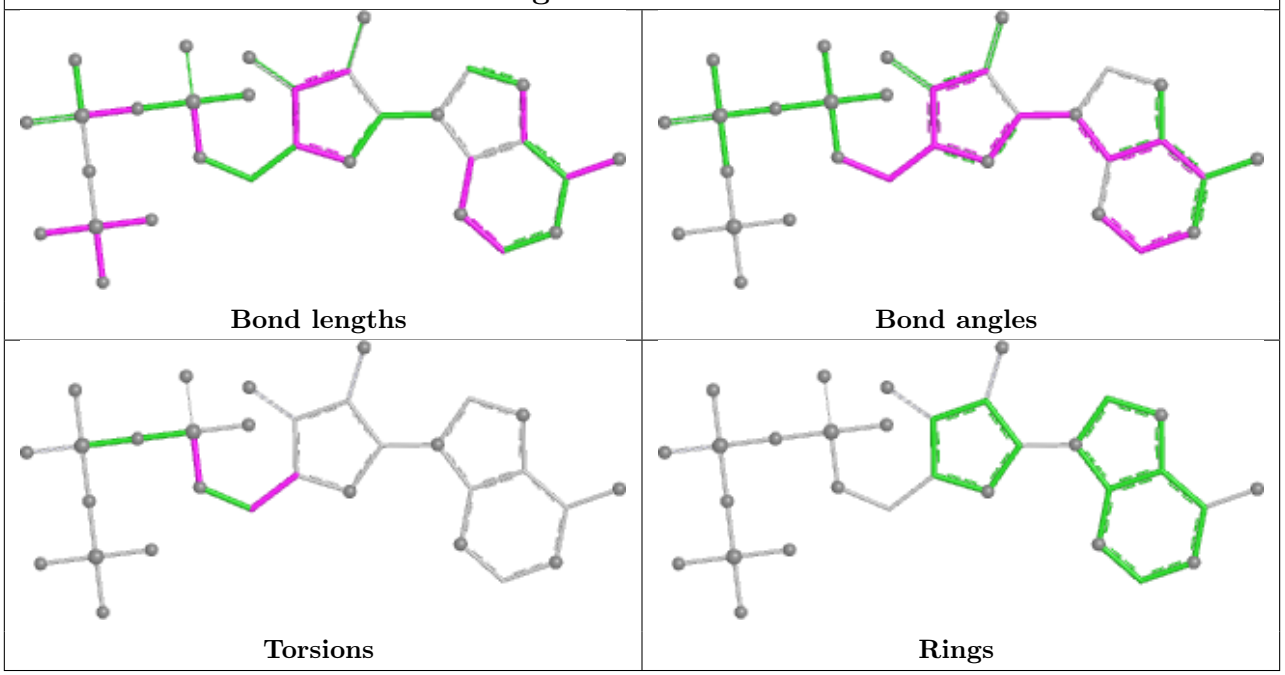
Ligand 08T C 700



Ligand ADP O 700



Ligand 08T B 700



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, 95^{th} 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	320/324 (98%)	-0.25	0 100 100	63, 76, 113, 193	0
1	C	320/324 (98%)	-0.20	0 100 100	59, 69, 118, 169	0
1	D	320/324 (98%)	-0.24	0 100 100	58, 68, 132, 172	0
1	E	305/324 (94%)	-0.16	1 (0%) 90 82	64, 89, 142, 194	0
1	L	320/324 (98%)	-0.17	0 100 100	68, 78, 141, 189	0
1	M	320/324 (98%)	-0.16	1 (0%) 90 82	60, 71, 139, 226	0
1	N	320/324 (98%)	-0.24	1 (0%) 90 82	58, 71, 134, 179	0
1	O	305/324 (94%)	-0.18	0 100 100	64, 92, 144, 179	0
2	A	186/199 (93%)	-0.16	0 100 100	69, 102, 165, 217	0
2	K	186/199 (93%)	-0.03	1 (0%) 87 75	78, 112, 163, 196	0
3	F	222/228 (97%)	-0.29	0 100 100	88, 112, 143, 182	0
3	G	222/228 (97%)	-0.40	0 100 100	69, 90, 127, 157	0
3	H	222/228 (97%)	-0.42	0 100 100	73, 102, 144, 166	0
3	P	222/228 (97%)	-0.21	0 100 100	83, 112, 163, 221	0
3	Q	222/228 (97%)	-0.41	0 100 100	64, 87, 124, 153	0
3	R	222/228 (97%)	-0.30	0 100 100	62, 99, 147, 211	0
4	I	24/30 (80%)	-0.33	0 100 100	67, 94, 150, 160	0
4	S	24/30 (80%)	-0.19	0 100 100	66, 100, 164, 171	0
5	J	20/20 (100%)	-0.04	1 (5%) 35 25	66, 122, 185, 190	0
5	T	20/20 (100%)	-0.09	1 (5%) 35 25	72, 104, 187, 196	0
All	All	4322/4458 (96%)	-0.23	6 (0%) 92 89	58, 89, 146, 226	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	0	SER	2.9
5	J	20	DA	2.8
5	T	20	DA	2.8
2	K	161	LEU	2.6
1	E	303	LEU	2.2

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 monosaccharides 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, 95^{th} 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.

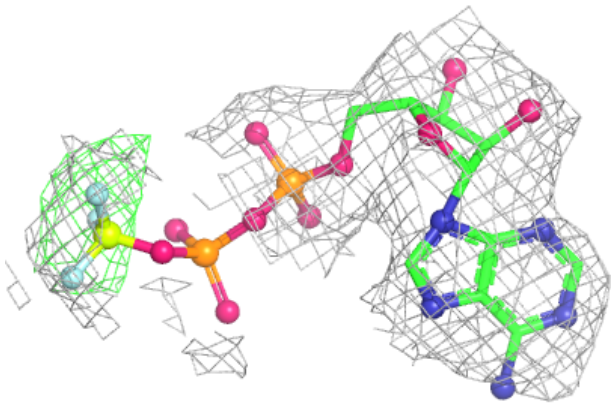
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	E	801	1/1	0.73	0.28	81,81,81,81	0
7	MG	O	801	1/1	0.77	0.25	83,83,83,83	0
7	MG	L	800	1/1	0.93	0.13	70,70,70,70	0
7	MG	B	800	1/1	0.94	0.15	71,71,71,71	0
7	MG	C	800	1/1	0.94	0.14	63,63,63,63	0
7	MG	D	800	1/1	0.94	0.15	63,63,63,63	0
7	MG	M	800	1/1	0.95	0.17	63,63,63,63	0
6	08T	N	700	31/31	0.95	0.08	65,66,67,67	0
8	ADP	E	700	27/27	0.95	0.08	80,85,87,88	0
7	MG	N	800	1/1	0.96	0.16	65,65,65,65	0
6	08T	M	700	31/31	0.96	0.07	64,65,66,66	0
6	08T	C	700	31/31	0.96	0.07	62,64,64,64	0
8	ADP	O	700	27/27	0.96	0.07	84,89,90,91	0
6	08T	B	700	31/31	0.97	0.07	71,73,74,74	0
6	08T	D	700	31/31	0.97	0.06	62,64,64,65	0
6	08T	L	700	31/31	0.97	0.08	71,73,74,75	0

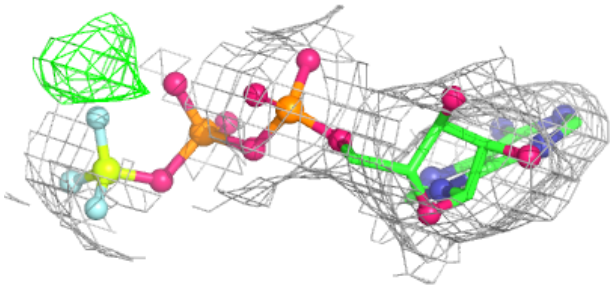
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

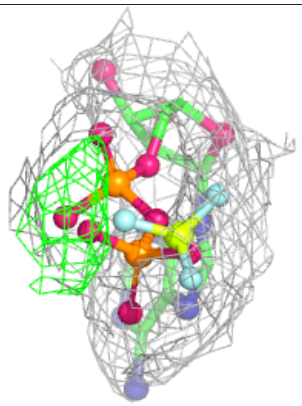
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 08T N 700:

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

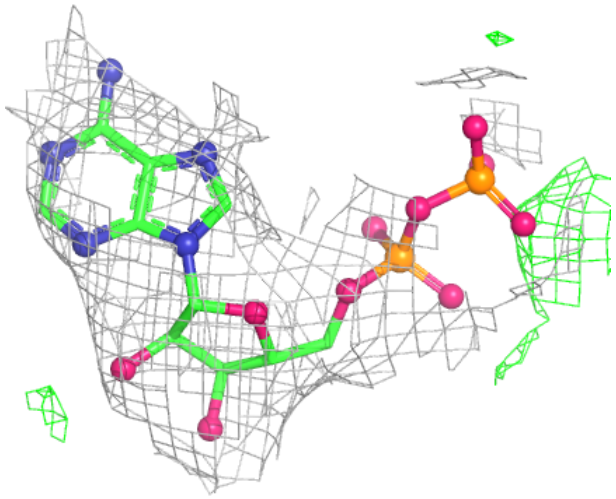


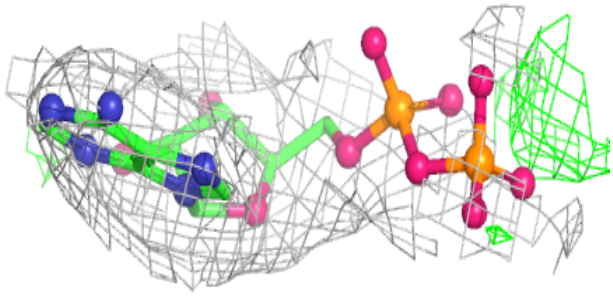


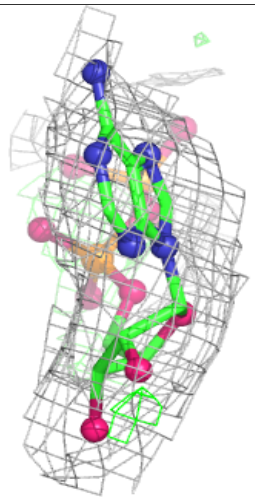


Electron density around ADP E 700:

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

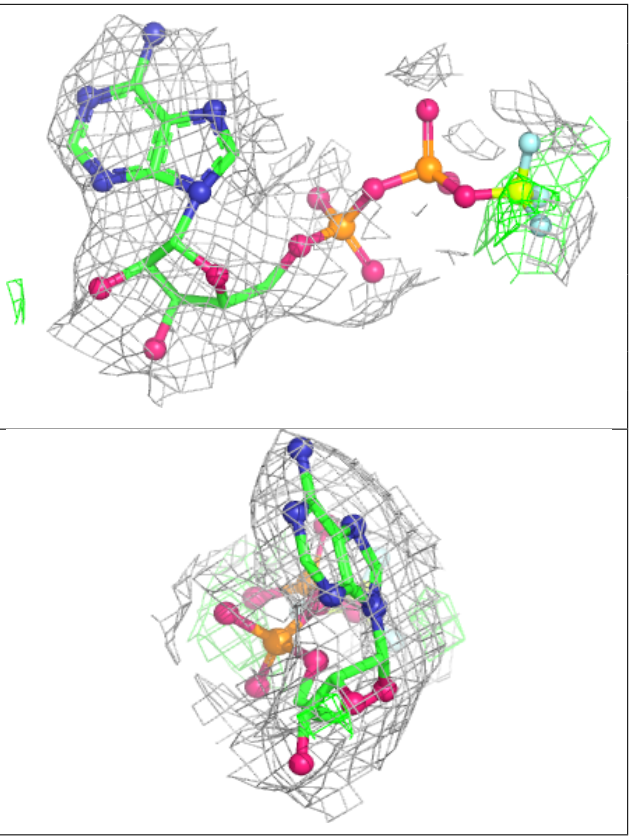






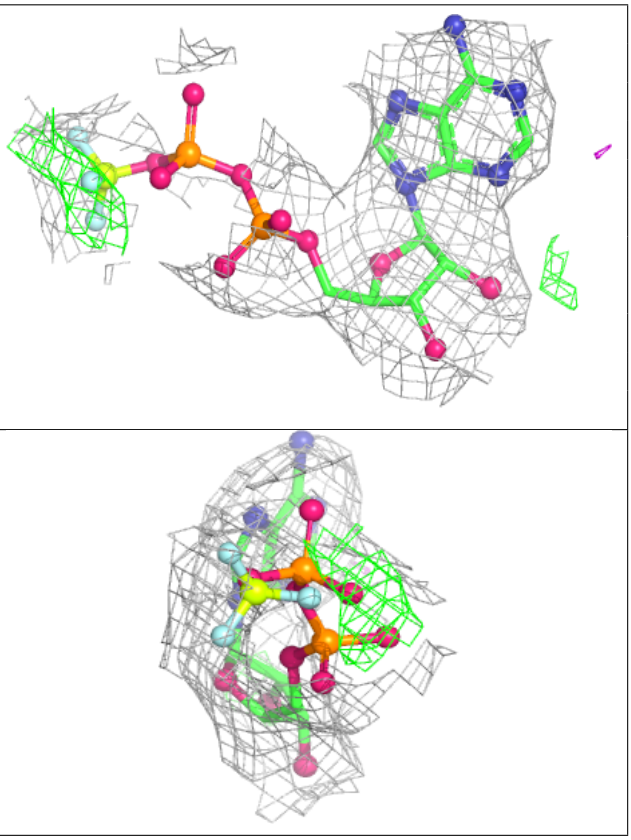
Electron density around 08T M 700:

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



Electron density around 08T C 700:

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



Electron density around ADP O 700:

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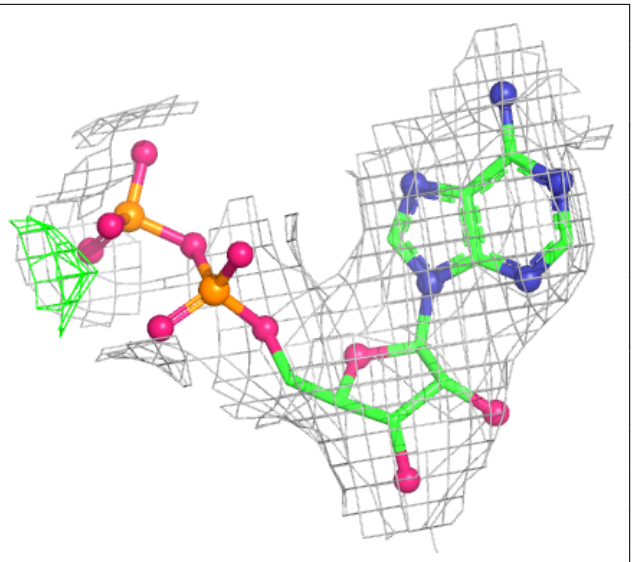
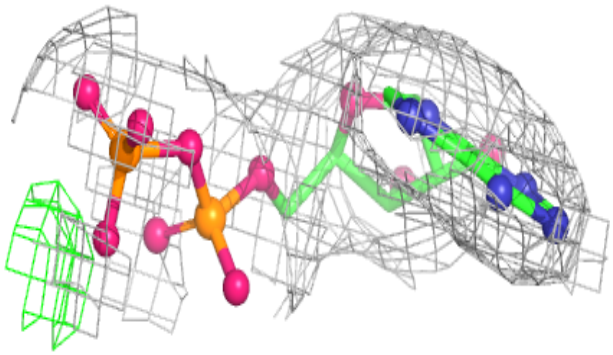
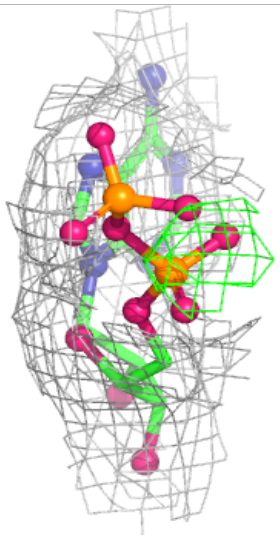
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

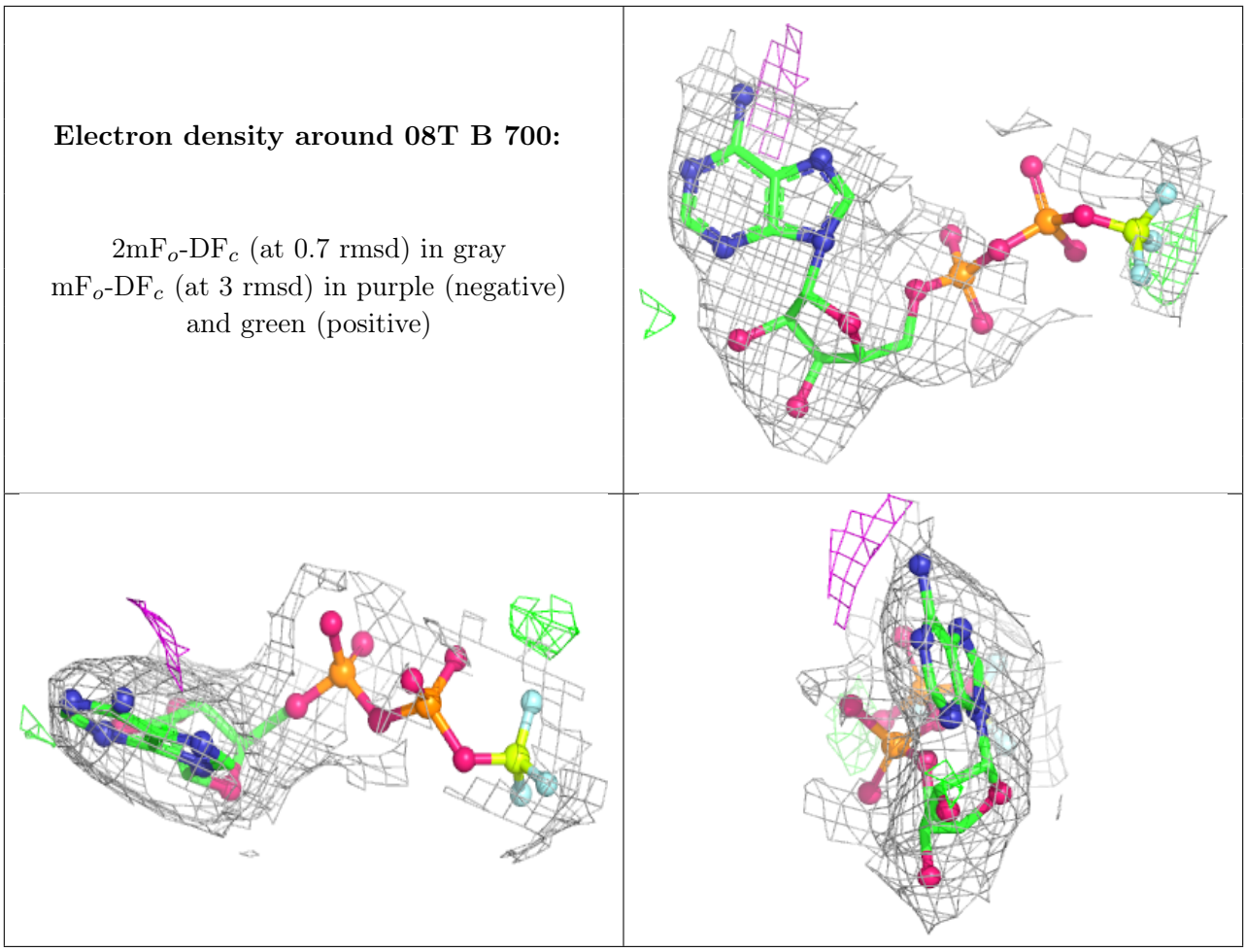






Electron density around 08T B 700:

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



Electron density around 08T D 700:

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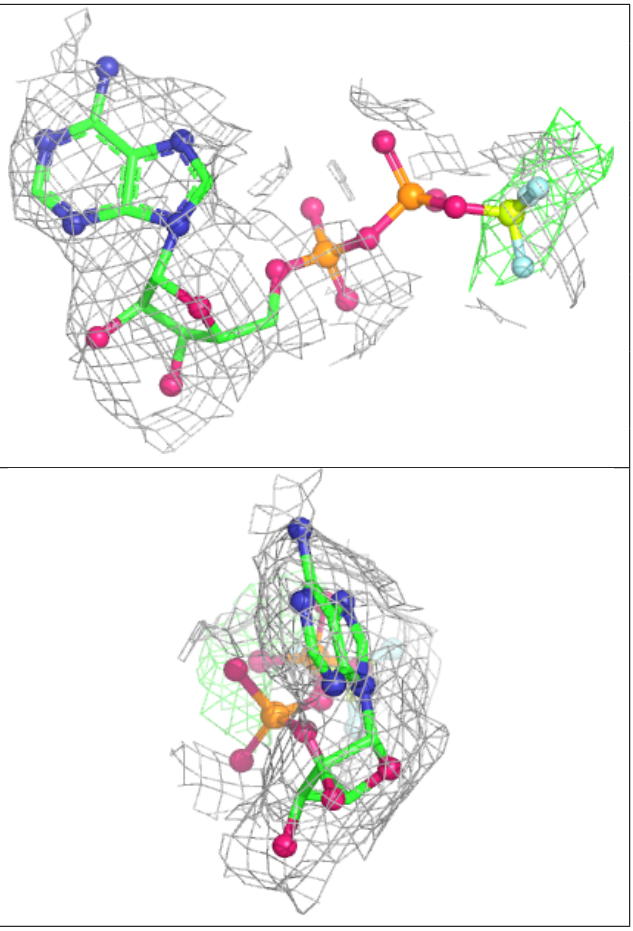
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 08T L 700:

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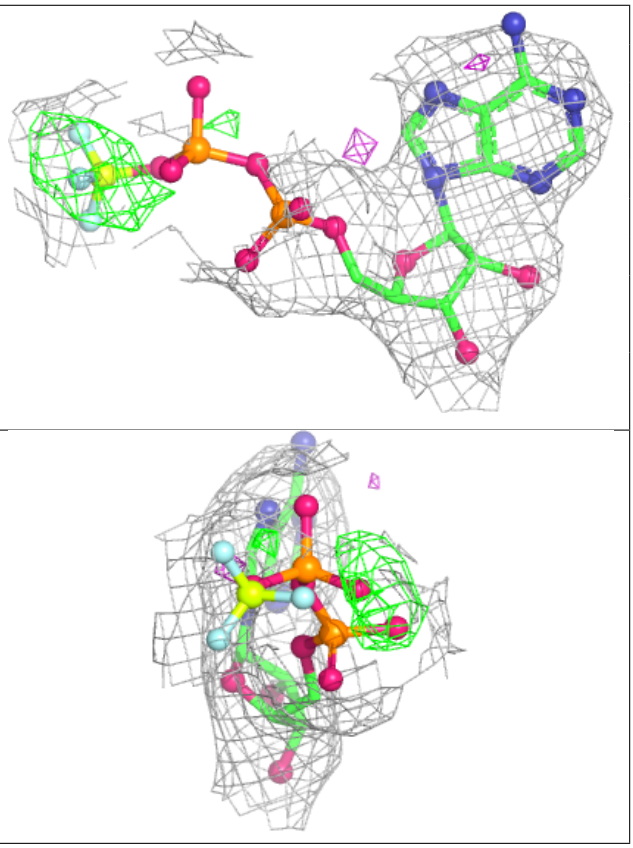
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.