wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 09:43 AM EDT

PDB ID	:	3CMW / pdb_00003cmw
Title	:	Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors	:	Pavletich, N.P.
Deposited on	:	2008-03-24
Resolution	:	2.80 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:

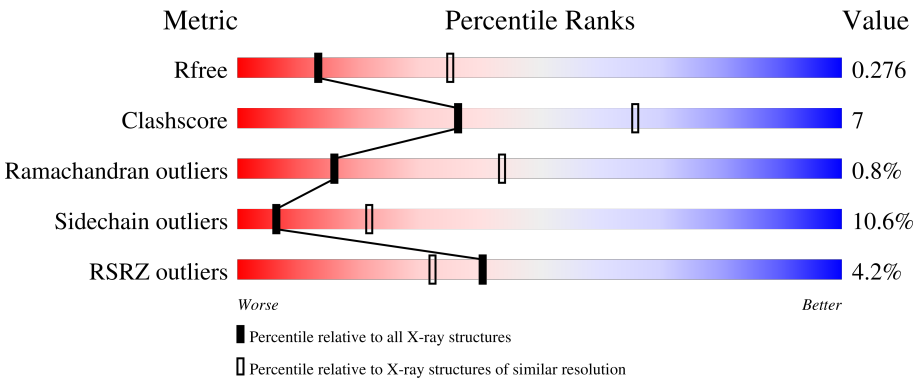
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 <=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	15	67% 13% 20%
1	D	15	7% 60% 13% 20%
2	A	1706	4% 76% 15% • 6%
2	C	1706	4% 77% 15% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25046 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(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	12	237	120	24	82	11	0	0	0
1	D	12	237	120	24	82	11	0	0	0

- Molecule 2 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	1609	12125	7622	2100	2347	56	0	0	0
2	C	1608	12117	7617	2100	2344	56	0	0	0

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP P0A7G6
A	27	ALA	-	linker	UNP P0A7G6
A	28	MET	-	linker	UNP P0A7G6
A	29	HIS	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6
A	988	SER	-	linker	UNP P0A7G6
A	989	THR	-	linker	UNP P0A7G6
A	990	GLY	-	linker	UNP P0A7G6
A	991	SER	-	linker	UNP P0A7G6
A	992	GLY	-	linker	UNP P0A7G6
A	993	THR	-	linker	UNP P0A7G6
A	994	THR	-	linker	UNP P0A7G6
A	995	GLY	-	linker	UNP P0A7G6
A	996	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	997	THR	-	linker	UNP P0A7G6
A	998	GLY	-	linker	UNP P0A7G6
A	999	SER	-	linker	UNP P0A7G6
A	1000	MET	-	linker	UNP P0A7G6
A	1986	THR	-	linker	UNP P0A7G6
A	1987	GLY	-	linker	UNP P0A7G6
A	1988	SER	-	linker	UNP P0A7G6
A	1989	THR	-	linker	UNP P0A7G6
A	1990	GLY	-	linker	UNP P0A7G6
A	1991	SER	-	linker	UNP P0A7G6
A	1992	MET	-	linker	UNP P0A7G6
A	1993	GLY	-	linker	UNP P0A7G6
A	1994	HIS	-	linker	UNP P0A7G6
A	1995	THR	-	linker	UNP P0A7G6
A	1996	THR	-	linker	UNP P0A7G6
A	1997	GLY	-	linker	UNP P0A7G6
A	1998	SER	-	linker	UNP P0A7G6
A	1999	MET	-	linker	UNP P0A7G6
A	2000	SER	-	linker	UNP P0A7G6
A	2985	THR	-	linker	UNP P0A7G6
A	2986	GLY	-	linker	UNP P0A7G6
A	2987	SER	-	linker	UNP P0A7G6
A	2988	THR	-	linker	UNP P0A7G6
A	2989	GLY	-	linker	UNP P0A7G6
A	2990	SER	-	linker	UNP P0A7G6
A	2991	ALA	-	linker	UNP P0A7G6
A	2992	SER	-	linker	UNP P0A7G6
A	2993	GLY	-	linker	UNP P0A7G6
A	2994	SER	-	linker	UNP P0A7G6
A	2995	SER	-	linker	UNP P0A7G6
A	2996	THR	-	linker	UNP P0A7G6
A	2997	GLY	-	linker	UNP P0A7G6
A	2998	SER	-	linker	UNP P0A7G6
A	2999	MET	-	linker	UNP P0A7G6
A	3000	SER	-	linker	UNP P0A7G6
A	3986	THR	-	linker	UNP P0A7G6
A	3987	GLY	-	linker	UNP P0A7G6
A	3988	SER	-	linker	UNP P0A7G6
A	3989	THR	-	linker	UNP P0A7G6
A	3990	GLY	-	linker	UNP P0A7G6
A	3991	SER	-	linker	UNP P0A7G6
A	3992	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3993	SER	-	linker	UNP P0A7G6
A	3994	GLY	-	linker	UNP P0A7G6
A	3995	ARG	-	linker	UNP P0A7G6
A	3996	THR	-	linker	UNP P0A7G6
A	3997	GLY	-	linker	UNP P0A7G6
A	3998	SER	-	linker	UNP P0A7G6
A	3999	MET	-	linker	UNP P0A7G6
A	4000	SER	-	linker	UNP P0A7G6
C	26	GLY	-	linker	UNP P0A7G6
C	27	ALA	-	linker	UNP P0A7G6
C	28	MET	-	linker	UNP P0A7G6
C	29	HIS	-	linker	UNP P0A7G6
C	986	THR	-	linker	UNP P0A7G6
C	987	GLY	-	linker	UNP P0A7G6
C	988	SER	-	linker	UNP P0A7G6
C	989	THR	-	linker	UNP P0A7G6
C	990	GLY	-	linker	UNP P0A7G6
C	991	SER	-	linker	UNP P0A7G6
C	992	GLY	-	linker	UNP P0A7G6
C	993	THR	-	linker	UNP P0A7G6
C	994	THR	-	linker	UNP P0A7G6
C	995	GLY	-	linker	UNP P0A7G6
C	996	SER	-	linker	UNP P0A7G6
C	997	THR	-	linker	UNP P0A7G6
C	998	GLY	-	linker	UNP P0A7G6
C	999	SER	-	linker	UNP P0A7G6
C	1000	MET	-	linker	UNP P0A7G6
C	1986	THR	-	linker	UNP P0A7G6
C	1987	GLY	-	linker	UNP P0A7G6
C	1988	SER	-	linker	UNP P0A7G6
C	1989	THR	-	linker	UNP P0A7G6
C	1990	GLY	-	linker	UNP P0A7G6
C	1991	SER	-	linker	UNP P0A7G6
C	1992	MET	-	linker	UNP P0A7G6
C	1993	GLY	-	linker	UNP P0A7G6
C	1994	HIS	-	linker	UNP P0A7G6
C	1995	THR	-	linker	UNP P0A7G6
C	1996	THR	-	linker	UNP P0A7G6
C	1997	GLY	-	linker	UNP P0A7G6
C	1998	SER	-	linker	UNP P0A7G6
C	1999	MET	-	linker	UNP P0A7G6
C	2000	SER	-	linker	UNP P0A7G6

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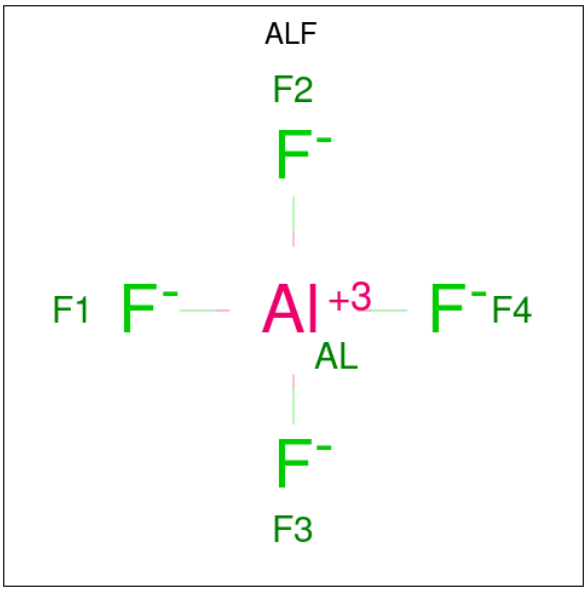
Chain	Residue	Modelled	Actual	Comment	Reference
C	2985	THR	-	linker	UNP P0A7G6
C	2986	GLY	-	linker	UNP P0A7G6
C	2987	SER	-	linker	UNP P0A7G6
C	2988	THR	-	linker	UNP P0A7G6
C	2989	GLY	-	linker	UNP P0A7G6
C	2990	SER	-	linker	UNP P0A7G6
C	2991	ALA	-	linker	UNP P0A7G6
C	2992	SER	-	linker	UNP P0A7G6
C	2993	GLY	-	linker	UNP P0A7G6
C	2994	SER	-	linker	UNP P0A7G6
C	2995	SER	-	linker	UNP P0A7G6
C	2996	THR	-	linker	UNP P0A7G6
C	2997	GLY	-	linker	UNP P0A7G6
C	2998	SER	-	linker	UNP P0A7G6
C	2999	MET	-	linker	UNP P0A7G6
C	3000	SER	-	linker	UNP P0A7G6
C	3986	THR	-	linker	UNP P0A7G6
C	3987	GLY	-	linker	UNP P0A7G6
C	3988	SER	-	linker	UNP P0A7G6
C	3989	THR	-	linker	UNP P0A7G6
C	3990	GLY	-	linker	UNP P0A7G6
C	3991	SER	-	linker	UNP P0A7G6
C	3992	MET	-	linker	UNP P0A7G6
C	3993	SER	-	linker	UNP P0A7G6
C	3994	GLY	-	linker	UNP P0A7G6
C	3995	ARG	-	linker	UNP P0A7G6
C	3996	THR	-	linker	UNP P0A7G6
C	3997	GLY	-	linker	UNP P0A7G6
C	3998	SER	-	linker	UNP P0A7G6
C	3999	MET	-	linker	UNP P0A7G6
C	4000	SER	-	linker	UNP P0A7G6

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

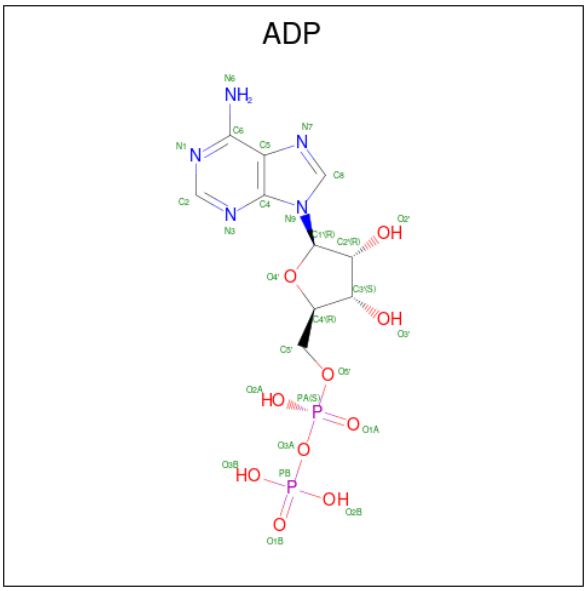
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	5	5	5	0	0
3	C	5	5	5	0	0

- Molecule 4 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
4	A	1	5	1	4	0	0
4	A	1	5	1	4	0	0
4	A	1	5	1	4	0	0
4	A	1	5	1	4	0	0
4	A	1	5	1	4	0	0
4	C	1	5	1	4	0	0
4	C	1	5	1	4	0	0
4	C	1	5	1	4	0	0
4	C	1	5	1	4	0	0
4	C	1	5	1	4	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



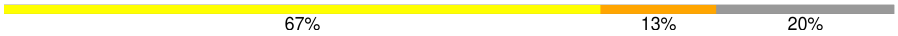
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C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

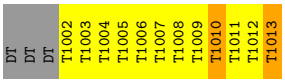
3 Residue-property plots (i)

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 (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

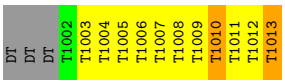
Chain B:





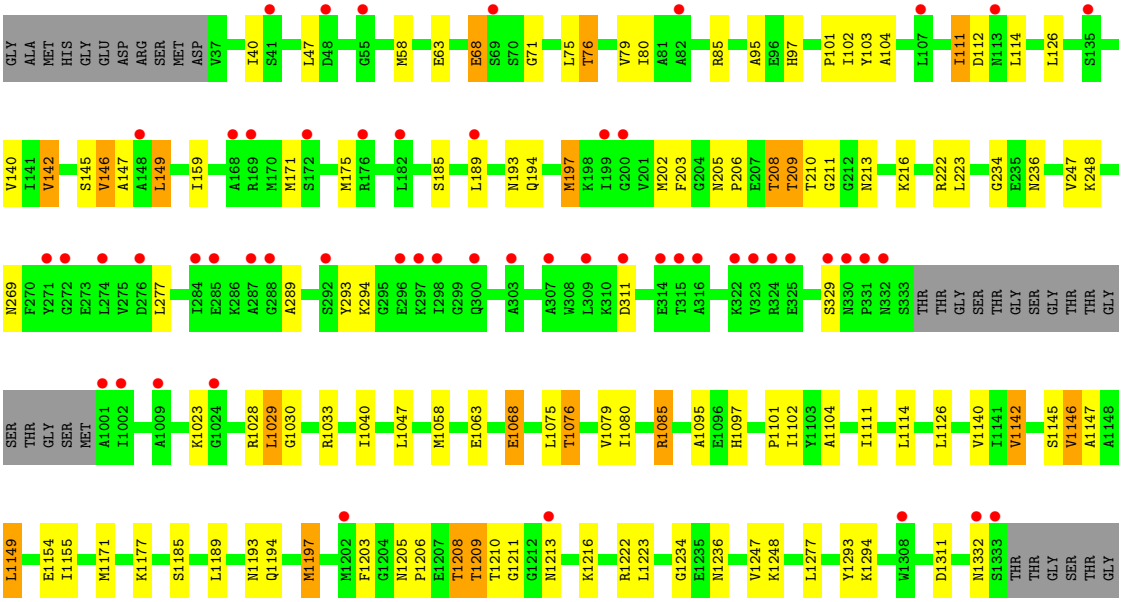
• Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

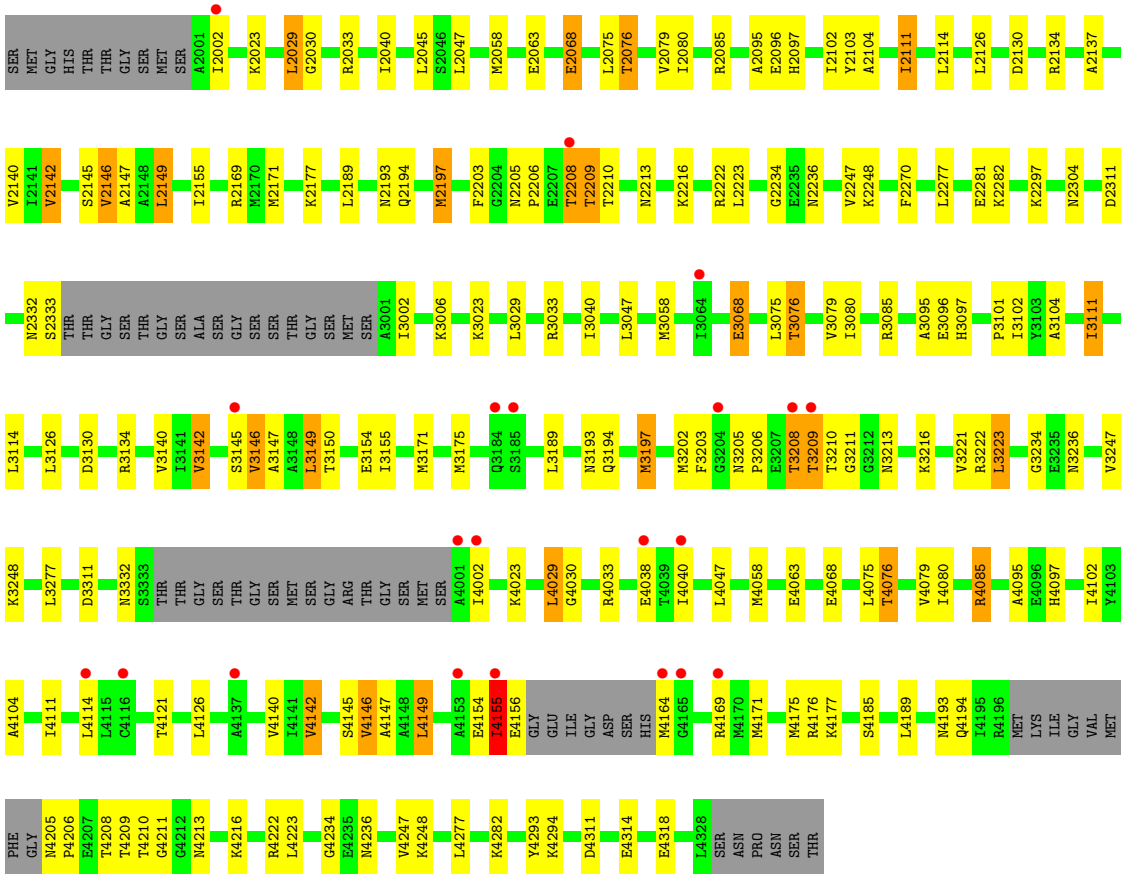
Chain D:



• Molecule 2: Protein recA

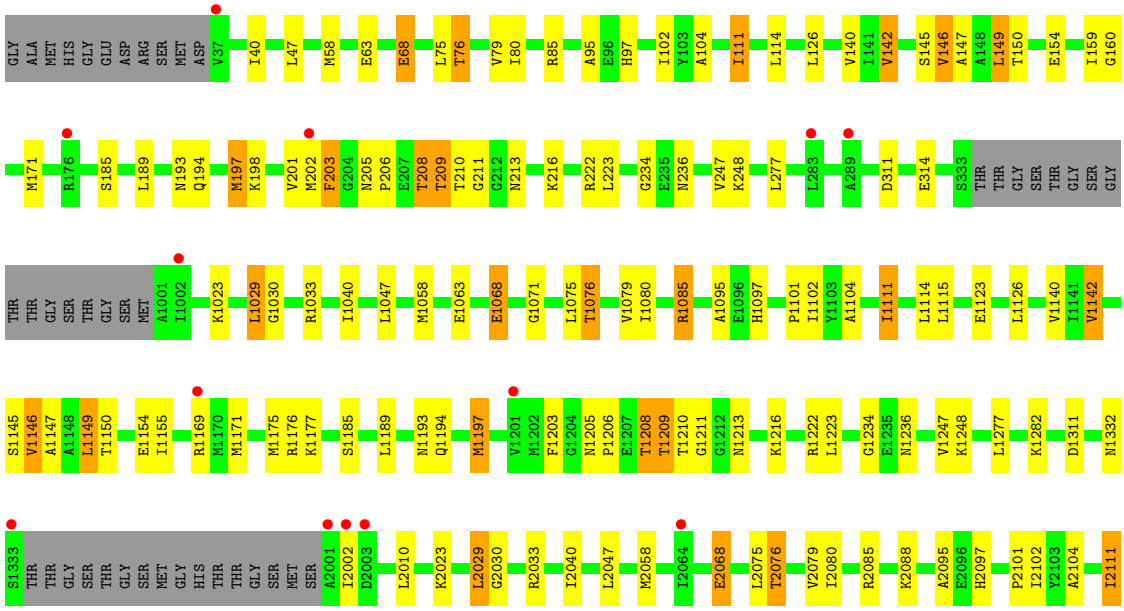
Chain A:

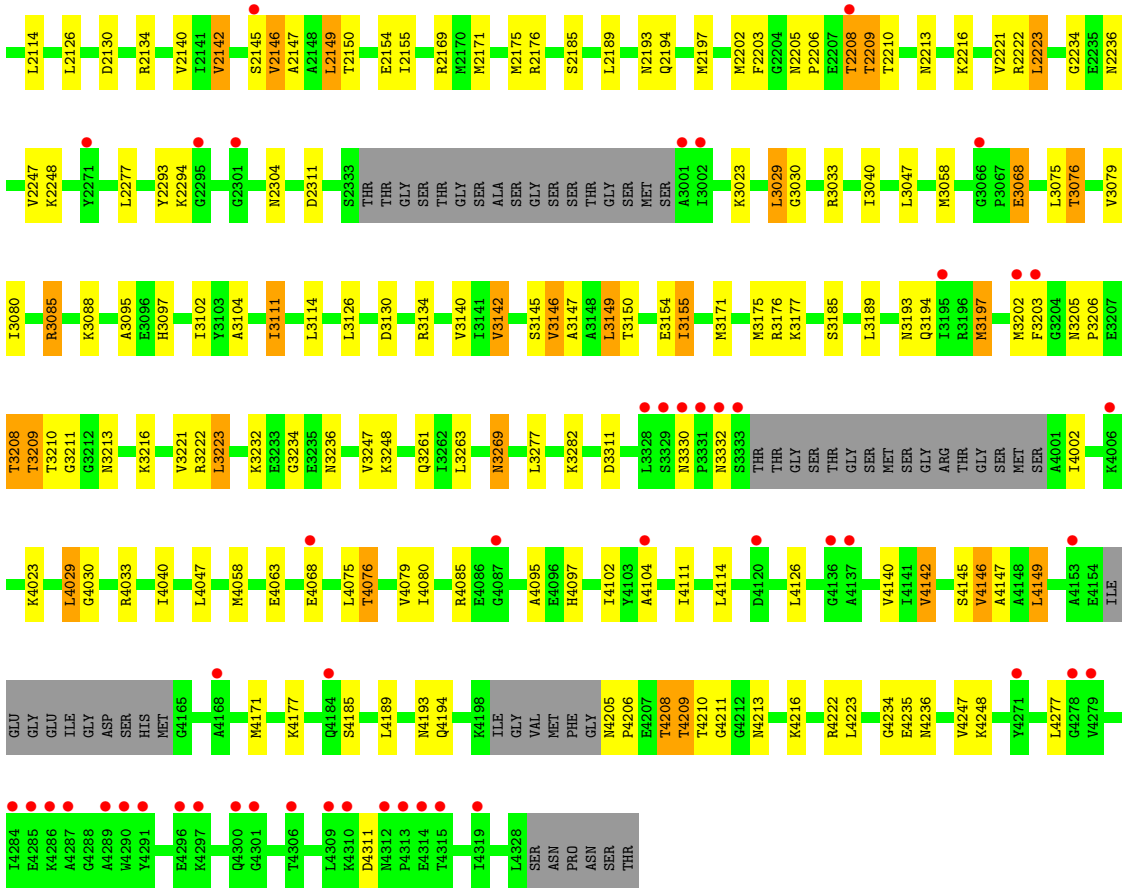




- Molecule 2: Protein recA

Chain C:




L2114 L2126 D2130 R2134 V2140 I2141 V2142 S2145 V2146 A2147 A2148 L2149 T2150 E2154 I2155 R2169 M2170 M2171 M2175 R2176 S2185 L2189 N2193 Q2194 M2197 M2202 F2203 G2204 N2205 P2206 E2207 T2208 T2209 T2210 N2213 K2216 V2221 R2222 L2223 G2234 E2235 N2236
V2247 K2248 Y2271 L2277 Y2293 K2294 G2295 G2301 N2304 D2311 S2333 THR THR GLY SER THR GLY SER ALA SER GLY SER SER THR GLY SER MET SER A3001 I3002 K3023 L3029 G3030 R3033 I3040 L3047 M3058 G3066 P3067 E3068 L3075 T3076 V3079
I3080 R3085 K3088 A3095 E3096 H3097 I3102 Y3103 A3104 I3111 L3114 L3126 D3130 R3134 V3140 I3141 V3142 S3145 V3146 A3147 A3148 L3149 T3150 E3154 I3155 M3171 M3175 R3176 K3177 S3185 L3189 N3193 Q3194 I3195 R3196 M3197 M3202 F3203 G3204 N3205 P3206 E3207
T3208 T3209 T3210 G3211 G3212 N3213 K3216 V3221 R3222 L3223 K3232 E3233 G3234 E3235 N3236 V3247 K3248 Q3261 I3262 L3263 N3269 L3277 K3282 D3311 L3328 S3329 N3330 P3331 N3332 S3333 THR THR GLY SER THR GLY SER MET SER GLY ARG THR GLY SER MET SER A4001 I4002 K4006
K4023 L4029 G4030 R4033 I4040 L4047 M4058 E4063 E4068 L4075 T4076 V4079 I4080 R4085 E4086 G4087 A4095 E4096 H4097 I4102 Y4103 A4104 I4111 L4114 D4120 L4126 G4136 A4137 V4140 I4141 V4142 S4145 V4146 A4147 A4148 L4149 A4153 E4154 ILE
GLU GLY GLU ILE GLY ASP SER HIS MET G4165 A4168 M4171 K4177 Q4184 S4185 L4189 N4193 Q4194 K4198 ILE GLY VAL MET PHE GLY N4205 P4206 E4207 T4208 T4209 T4210 G4211 G4212 N4213 K4216 R4222 L4223 G4234 E4235 N4236 V4247 K4248 Y4271 L4277 G4278 V4279
I4284 E4285 K4286 A4287 G4288 A4289 W4290 Y4291 E4296 K4297 Q4300 G4301 T4306 L4309 K4310 D4311 N4312 P4313 E4314 T4315 I4319 L4328 SER ASN PRO ASN SER THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.00Å 300.50Å 80.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.0 (20.00-2.80) 87.6 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.214 , 0.236 0.266 , 0.276	Depositor DCC
R_{free} test set	1749 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25046	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: MG, ADP, ALF

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	0.76	0/260	1.65	4/400 (1.0%)
1	D	0.69	0/260	1.42	2/400 (0.5%)
2	A	0.57	0/12264	0.86	0/16503
2	C	0.57	0/12256	0.86	1/16491 (0.0%)
All	All	0.57	0/25040	0.88	7/33794 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1013	DT	C1'-O4'-C4'	-8.33	97.21	109.70
1	B	1013	DT	N1-C1'-C2'	7.08	124.11	113.50
1	B	1010	DT	P-O3'-C3'	-6.62	110.27	120.20
1	B	1002	DT	P-O3'-C3'	5.97	129.16	120.20
1	D	1013	DT	C1'-O4'-C4'	-5.97	100.75	109.70

There are no chirality outliers.

There are no planarity outliers.

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	237	0	146	12	0
1	D	237	0	146	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12125	0	12452	181	2
2	C	12117	0	12447	177	1
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	25	0	0	0	0
4	C	25	0	0	0	0
5	A	135	0	60	3	0
5	C	135	0	60	1	0
All	All	25046	0	25311	360	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 360 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:D:1013:DT:O4	2:A:3202:MET:HG2	1.49	1.10
2:A:2068:GLU:HG2	2:A:3216:LYS:HB3	1.33	1.08
2:A:68:GLU:HG2	2:A:1216:LYS:HB3	1.24	1.07
2:C:68:GLU:HG2	2:C:1216:LYS:HB3	1.42	0.99
2:A:3068:GLU:HG2	2:A:4216:LYS:HB3	1.48	0.95

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4038:GLU:OE1	2:A:4318:GLU:OE2[2_555]	1.97	0.23
2:A:2297:LYS:NZ	2:C:4097:HIS:O[1_554]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	1595/1706 (94%)	1545 (97%)	37 (2%)	13 (1%)	16	44
2	C	1594/1706 (93%)	1550 (97%)	33 (2%)	11 (1%)	18	47
All	All	3189/3412 (94%)	3095 (97%)	70 (2%)	24 (1%)	16	44

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1023	LYS
2	A	2023	LYS
2	A	3023	LYS
2	A	3332	ASN
2	A	4023	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	1267/1339 (95%)	1131 (89%)	136 (11%)	6	21
2	C	1266/1339 (94%)	1133 (90%)	133 (10%)	6	22
All	All	2533/2678 (95%)	2264 (89%)	269 (11%)	6	22

5 of 269 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	3146	VAL
2	C	3208	THR
2	C	4185	SER
2	A	3149	LEU
2	A	3142	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	2020	GLN

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Mol	Chain	Res	Type
2	C	3304	ASN
2	C	2181	ASN
2	C	3097	HIS
2	C	4181	ASN

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 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	A	1502	4,3	28,29,29	1.47	5 (17%)	43,45,45	1.92	14 (32%)
4	ALF	A	1501	5	4,4,4	1.28	0	-		
5	ADP	A	4502	4,3	28,29,29	1.60	6 (21%)	43,45,45	1.57	8 (18%)
5	ADP	A	3502	4,3	28,29,29	1.47	4 (14%)	43,45,45	2.02	12 (27%)
4	ALF	C	1501	5	4,4,4	1.31	0	-		
5	ADP	C	502	4,3	28,29,29	1.58	7 (25%)	43,45,45	1.83	10 (23%)
4	ALF	A	3501	5	4,4,4	1.23	0	-		
4	ALF	A	501	5	4,4,4	1.34	0	-		
5	ADP	A	502	4,3	28,29,29	1.56	5 (17%)	43,45,45	1.87	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ALF	C	2501	5	4,4,4	1.26	0	-		
5	ADP	A	2502	4,3	28,29,29	1.50	6 (21%)	43,45,45	1.84	11 (25%)
4	ALF	A	2501	5	4,4,4	1.24	0	-		
5	ADP	C	4502	4,3	28,29,29	1.56	6 (21%)	43,45,45	1.84	12 (27%)
5	ADP	C	1502	4,3	28,29,29	1.54	6 (21%)	43,45,45	1.94	11 (25%)
4	ALF	C	501	5	4,4,4	1.22	0	-		
4	ALF	C	4501	5	4,4,4	1.50	0	-		
4	ALF	A	4501	5	4,4,4	1.49	0	-		
5	ADP	C	2502	4,3	28,29,29	1.57	6 (21%)	43,45,45	1.82	12 (27%)
4	ALF	C	3501	5	4,4,4	1.29	0	-		
5	ADP	C	3502	4,3	28,29,29	1.48	4 (14%)	43,45,45	1.88	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	1502	4,3	-	1/16/32/32	0/3/3/3
5	ADP	A	502	4,3	-	1/16/32/32	0/3/3/3
5	ADP	A	4502	4,3	-	1/16/32/32	0/3/3/3
5	ADP	C	4502	4,3	-	1/16/32/32	0/3/3/3
5	ADP	A	2502	4,3	-	3/16/32/32	0/3/3/3
5	ADP	C	2502	4,3	-	1/16/32/32	0/3/3/3
5	ADP	C	1502	4,3	-	1/16/32/32	0/3/3/3
5	ADP	A	3502	4,3	-	1/16/32/32	0/3/3/3
5	ADP	C	502	4,3	-	1/16/32/32	0/3/3/3
5	ADP	C	3502	4,3	-	1/16/32/32	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)
5	A	4502	ADP	C5-C4	5.57	1.49	1.39
5	C	4502	ADP	C5-C4	5.26	1.48	1.39
5	A	502	ADP	C5-C4	4.80	1.47	1.39
5	C	3502	ADP	C5-C4	4.73	1.47	1.39
5	A	2502	ADP	C5-C4	4.60	1.47	1.39

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	502	ADP	C5-C4-N3	-5.79	118.74	126.72
5	C	1502	ADP	C5-C4-N3	-5.75	118.79	126.72
5	C	502	ADP	C5-C4-N3	-5.49	119.16	126.72
5	A	2502	ADP	C5-C4-N3	-5.17	119.60	126.72
5	A	502	ADP	N3-C4-N9	5.05	135.76	127.17

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	ADP	PA-O3A-PB-O2B
5	A	4502	ADP	PA-O3A-PB-O2B
5	C	502	ADP	PA-O3A-PB-O2B
5	C	1502	ADP	PA-O3A-PB-O2B
5	A	1502	ADP	PA-O3A-PB-O2B

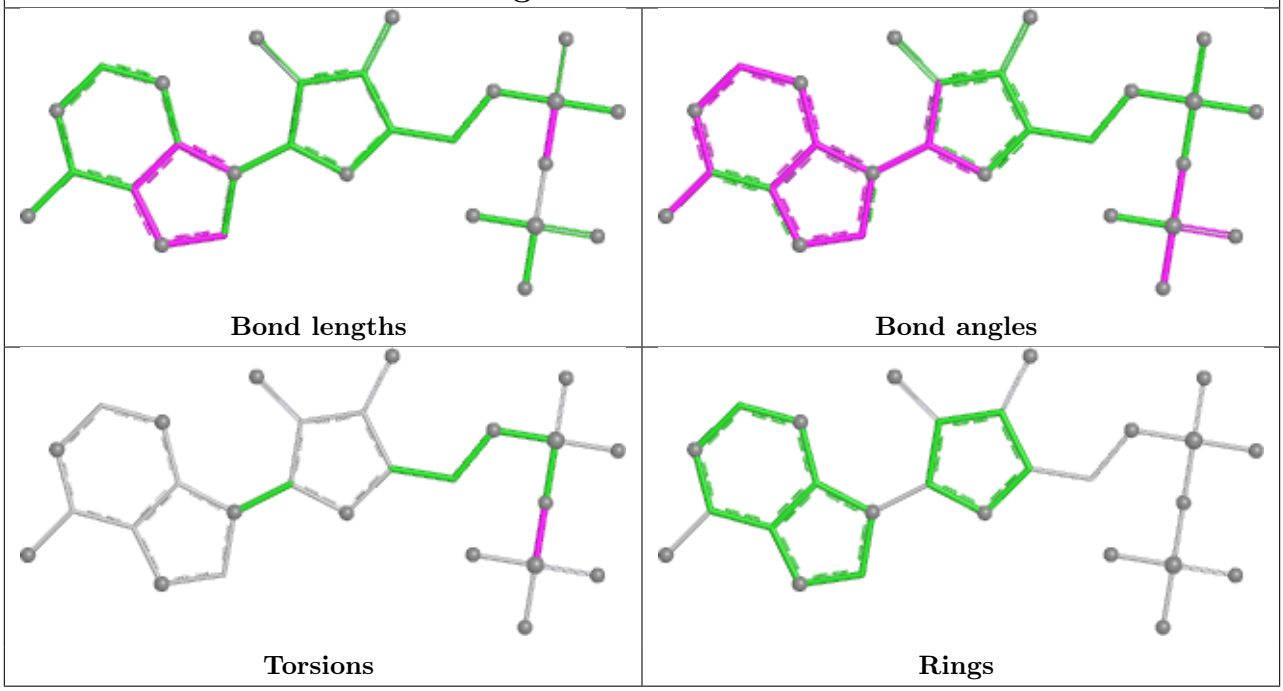
There are no ring outliers.

3 monomers are involved in 4 short contacts:

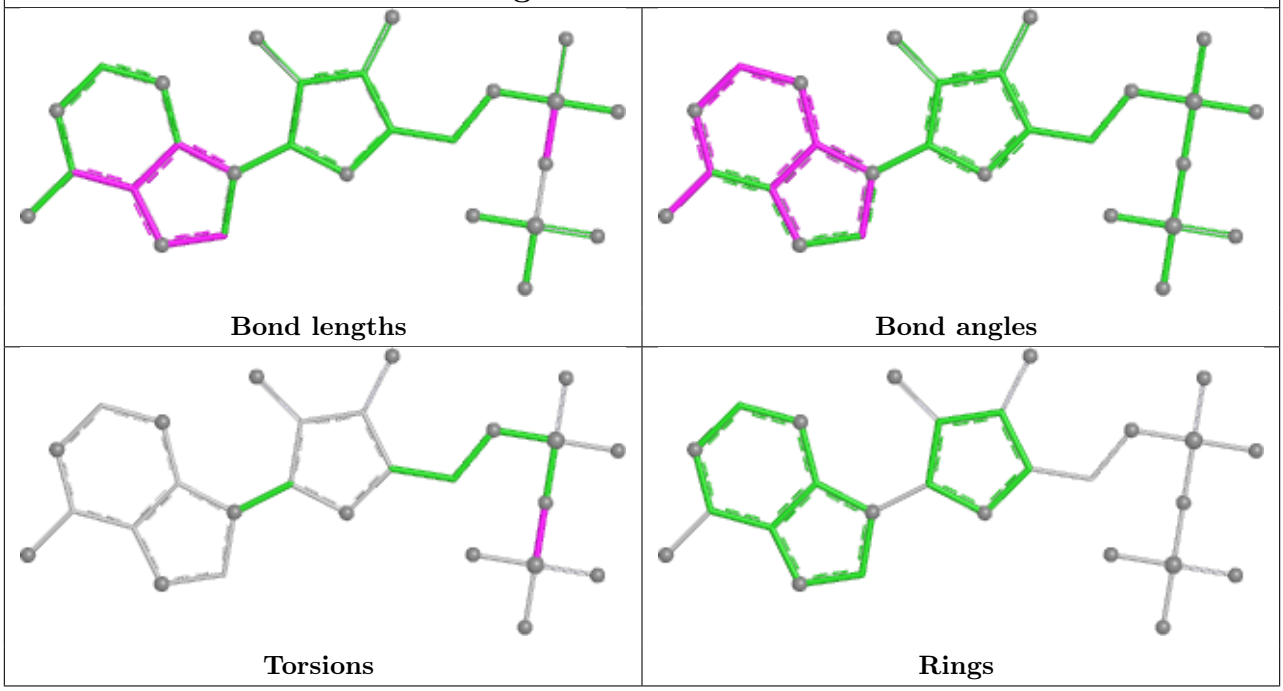
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	ADP	2	0
5	A	2502	ADP	1	0
5	C	1502	ADP	1	0

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.

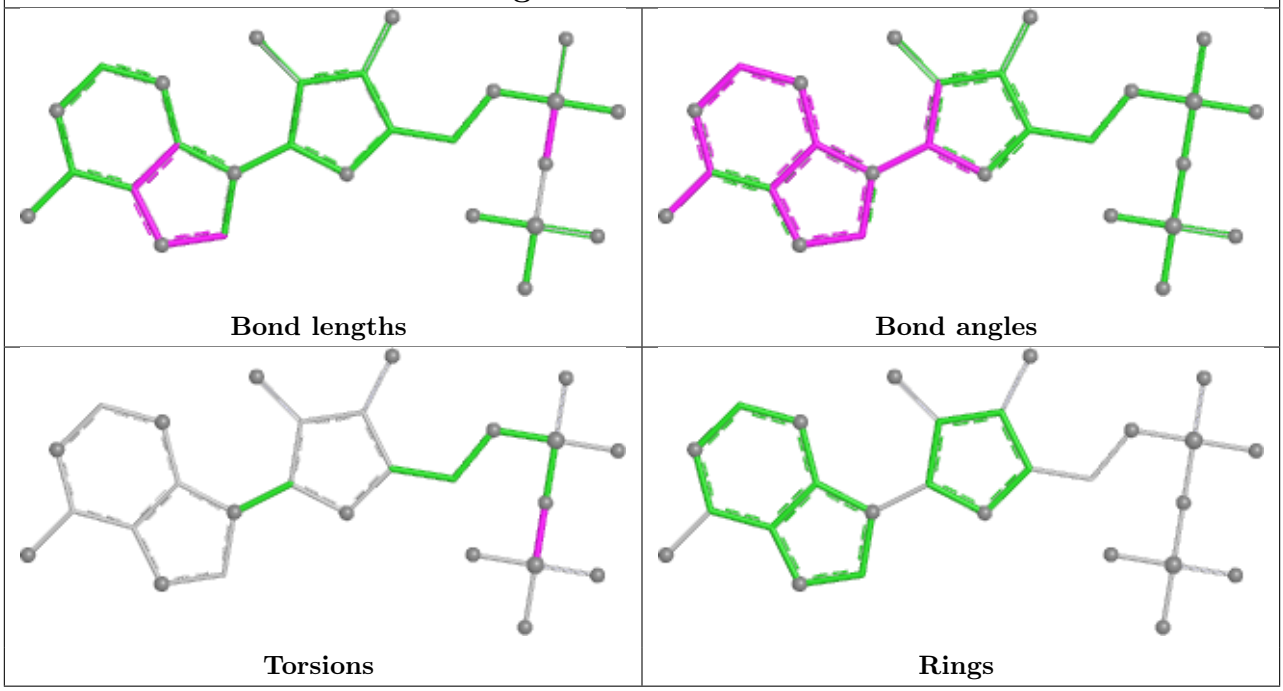
Ligand ADP A 1502



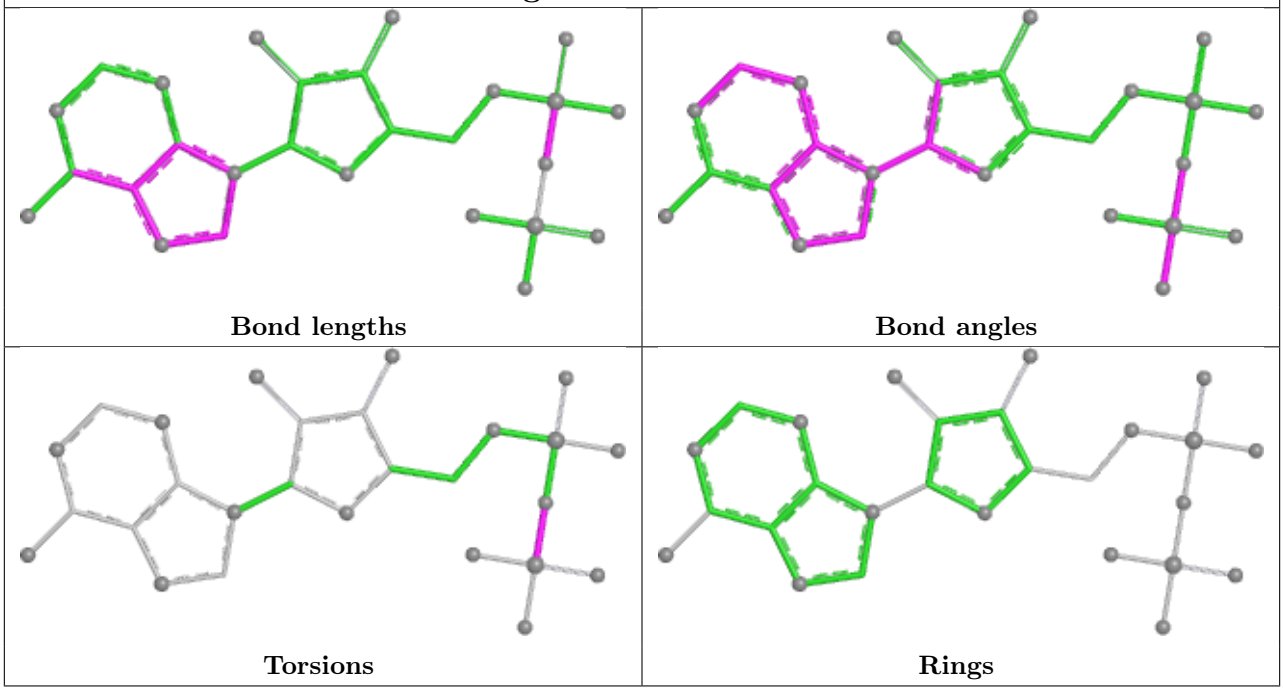
Ligand ADP A 4502



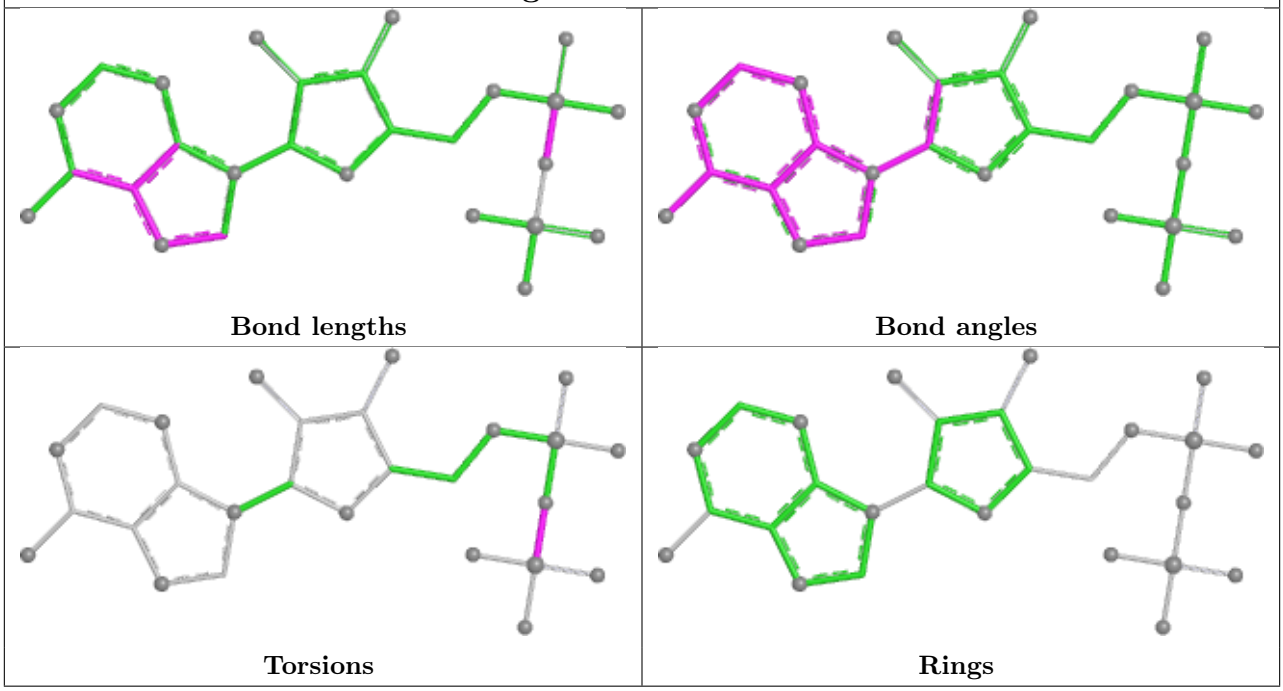
Ligand ADP A 3502



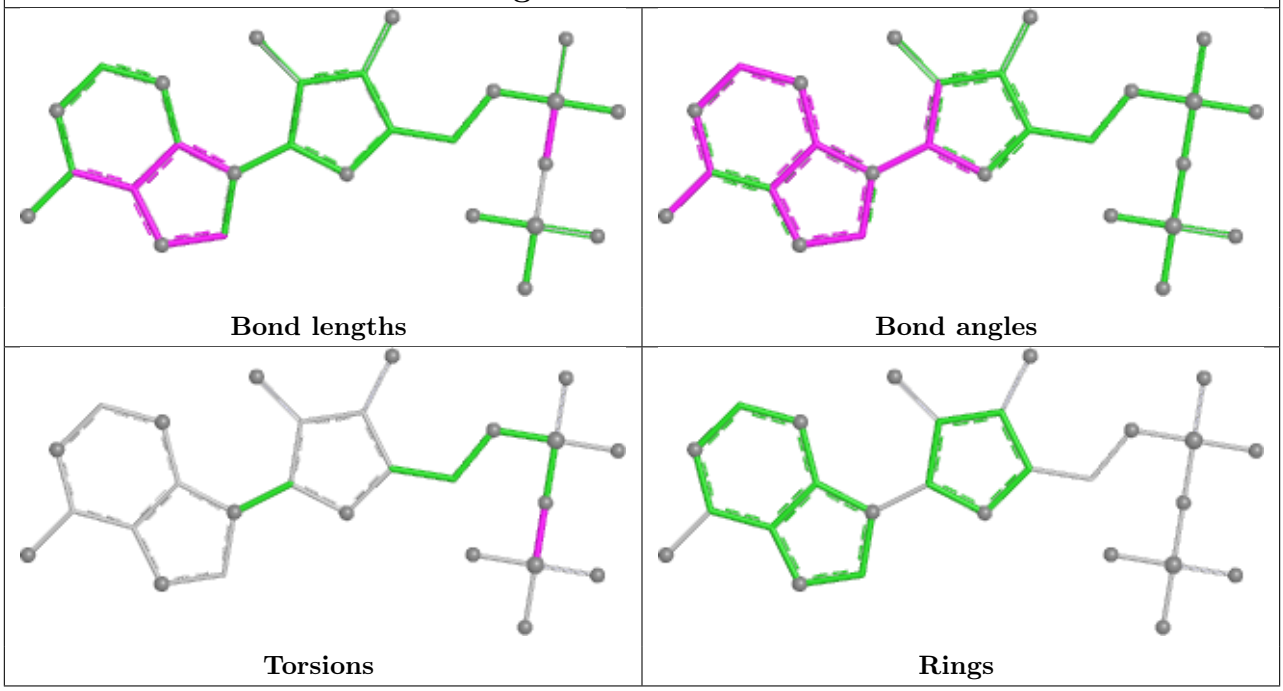
Ligand ADP C 502



Ligand ADP A 502



Ligand ADP A 2502



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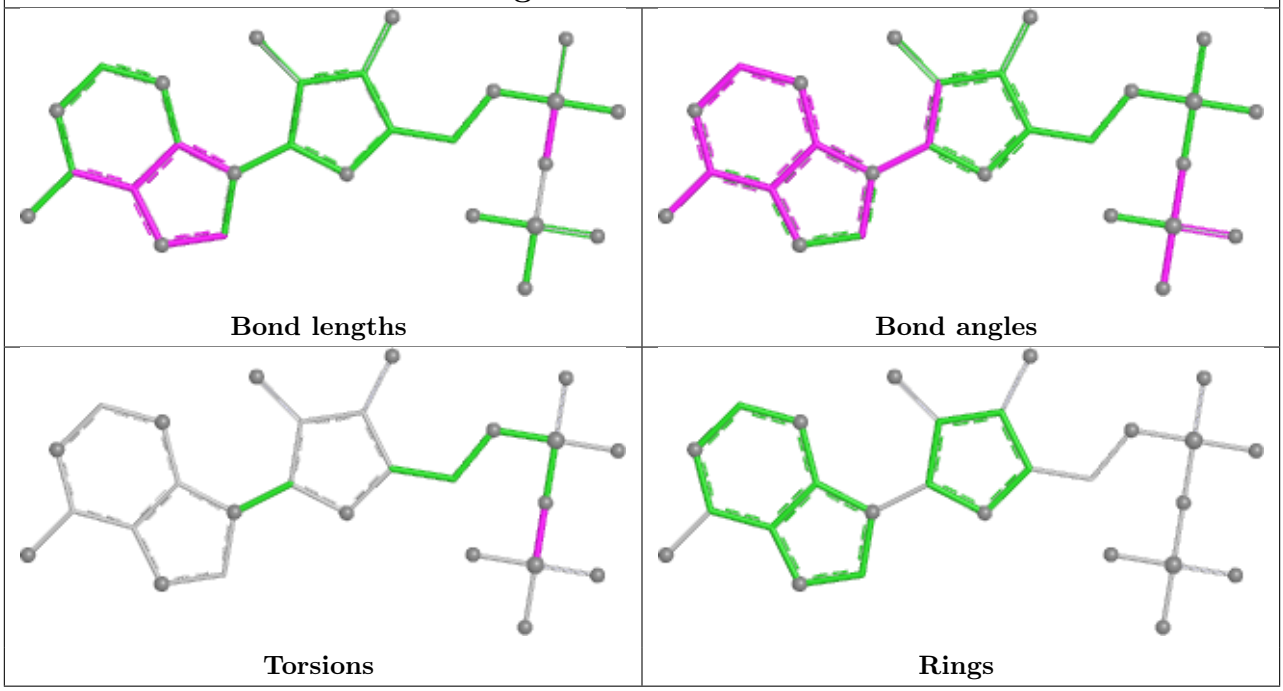

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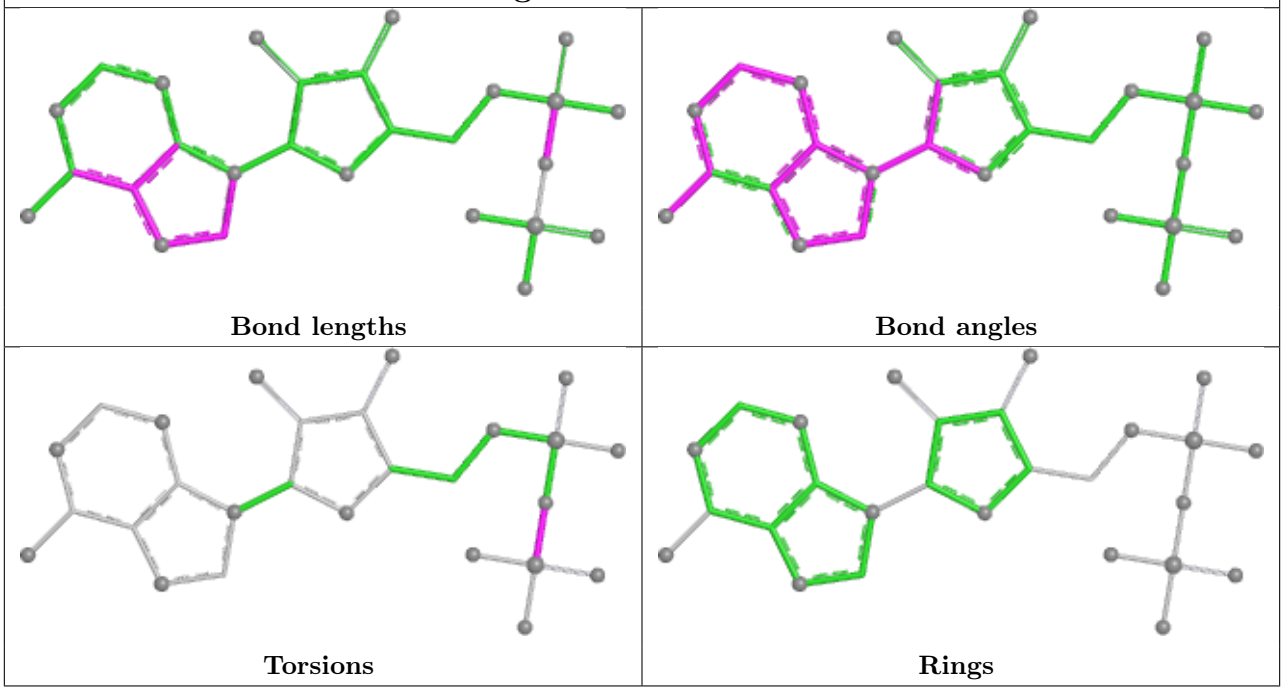

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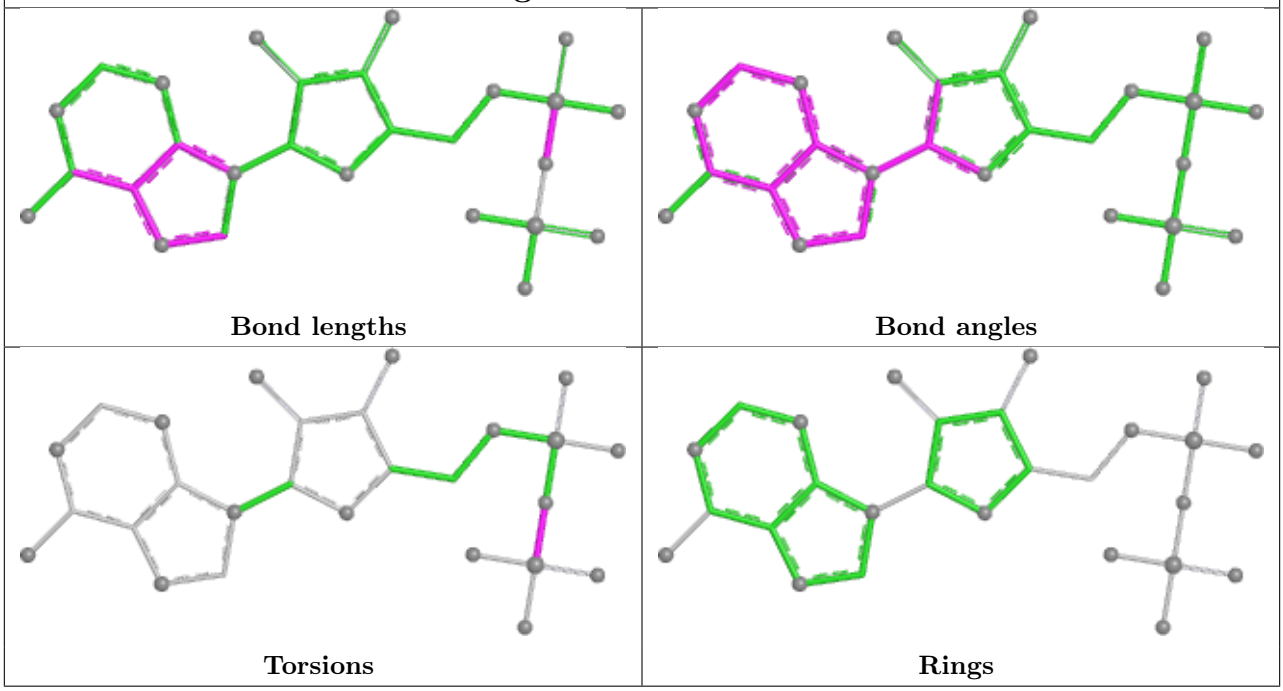
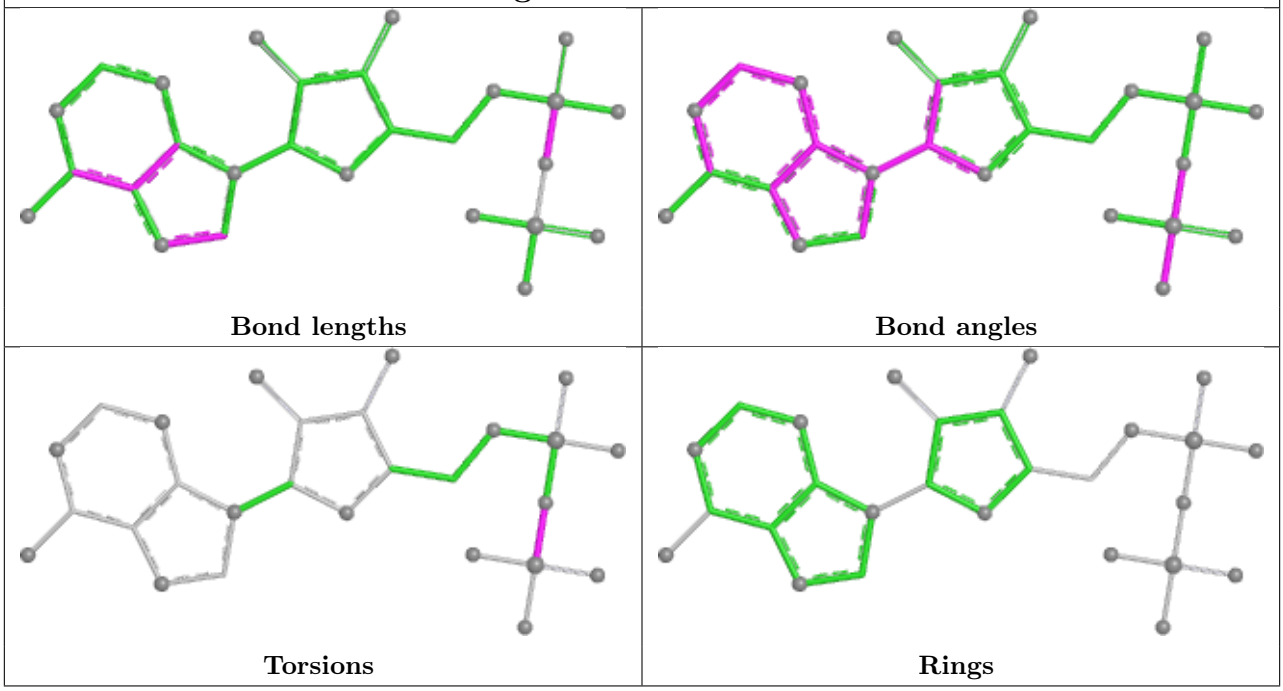


Ligand ADP C 3502



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	B	12/15 (80%)	0.67	0	100	100	29, 56, 64, 65	0
1	D	12/15 (80%)	0.66	0	100	100	22, 52, 61, 61	0
2	A	1609/1706 (94%)	0.51	75 (4%)	36	29	52, 62, 78, 107	0
2	C	1608/1706 (94%)	0.42	62 (3%)	43	34	50, 62, 79, 108	0
All	All	3241/3442 (94%)	0.47	137 (4%)	40	32	22, 62, 79, 108	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	4291	TYR	6.4
2	A	331	PRO	5.8
2	A	1001	ALA	5.5
2	C	4306	THR	5.3
2	C	4314	GLU	5.1

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)

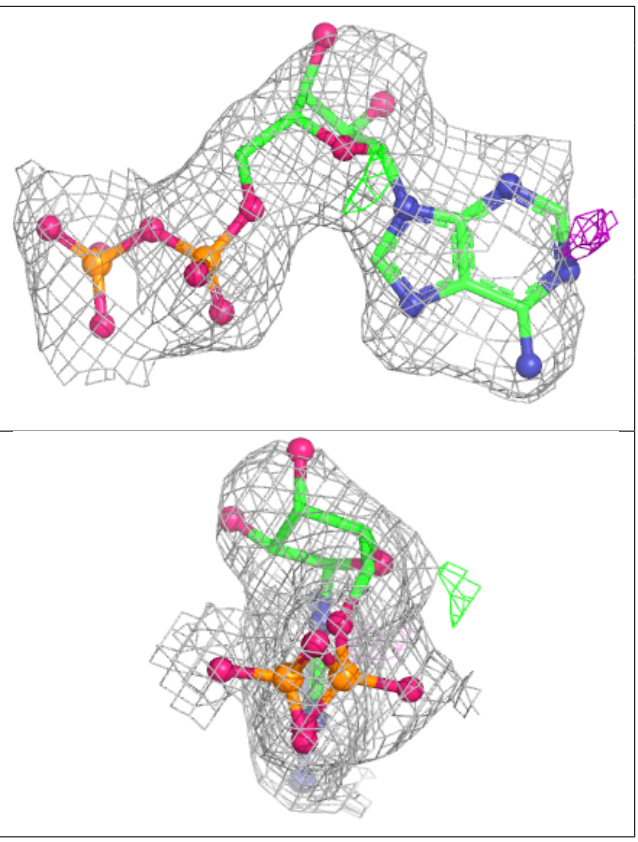
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ALF	A	4501	5/5	0.65	0.16	78,79,81,82	0
4	ALF	C	4501	5/5	0.68	0.14	67,71,73,75	0
3	MG	C	4500	1/1	0.74	0.22	56,56,56,56	0
3	MG	A	4500	1/1	0.76	0.19	60,60,60,60	0
3	MG	A	2500	1/1	0.78	0.24	42,42,42,42	0
3	MG	A	500	1/1	0.78	0.21	57,57,57,57	0
3	MG	C	500	1/1	0.78	0.25	50,50,50,50	0
3	MG	C	1500	1/1	0.79	0.23	45,45,45,45	0
3	MG	C	2500	1/1	0.84	0.22	48,48,48,48	0
3	MG	A	3500	1/1	0.84	0.27	46,46,46,46	0
3	MG	A	1500	1/1	0.86	0.21	47,47,47,47	0
3	MG	C	3500	1/1	0.87	0.20	45,45,45,45	0
4	ALF	C	3501	5/5	0.90	0.12	47,49,52,53	0
5	ADP	A	4502	27/27	0.90	0.09	47,62,63,68	0
4	ALF	A	501	5/5	0.91	0.11	60,60,63,64	0
5	ADP	C	4502	27/27	0.92	0.08	54,56,61,63	0
4	ALF	A	1501	5/5	0.93	0.09	45,47,50,53	0
5	ADP	A	502	27/27	0.93	0.08	50,53,57,60	0
4	ALF	C	2501	5/5	0.95	0.10	45,47,50,50	0
5	ADP	C	2502	27/27	0.95	0.07	41,46,49,49	0
5	ADP	C	3502	27/27	0.95	0.08	40,50,52,53	0
4	ALF	A	3501	5/5	0.95	0.10	42,46,49,51	0
4	ALF	A	2501	5/5	0.96	0.11	40,44,45,47	0
5	ADP	C	1502	27/27	0.96	0.07	32,36,39,41	0
4	ALF	C	501	5/5	0.96	0.10	44,49,49,52	0
5	ADP	A	1502	27/27	0.96	0.07	33,40,44,46	0
5	ADP	A	2502	27/27	0.96	0.07	37,42,45,47	0
4	ALF	C	1501	5/5	0.97	0.10	40,42,46,47	0
5	ADP	C	502	27/27	0.97	0.05	37,40,43,47	0
5	ADP	A	3502	27/27	0.97	0.06	28,35,39,40	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.

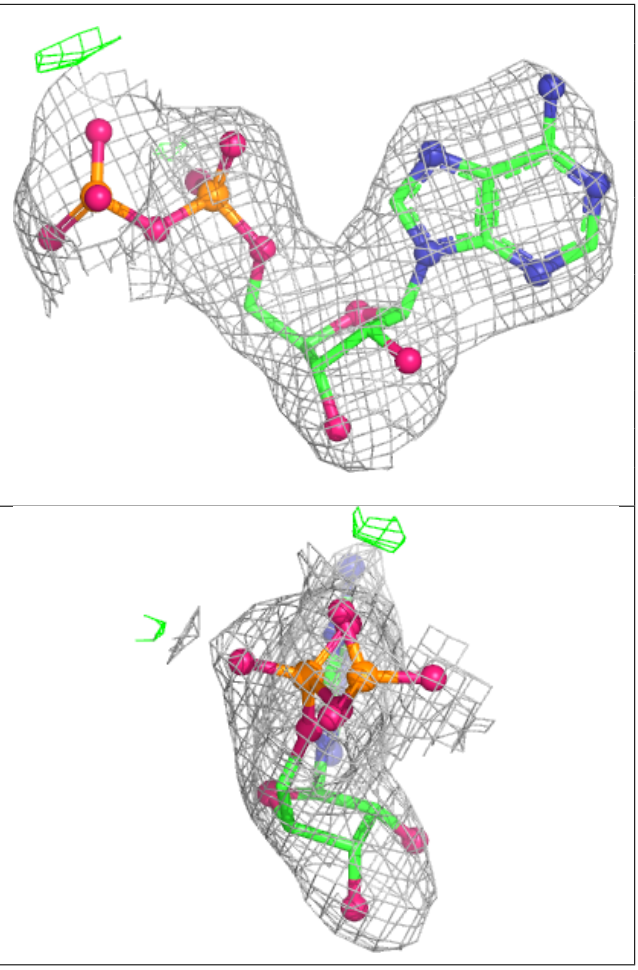
Electron density around ADP A 4502:

$2mF_o$-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 C 4502:

$2mF_o$-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 A 502:

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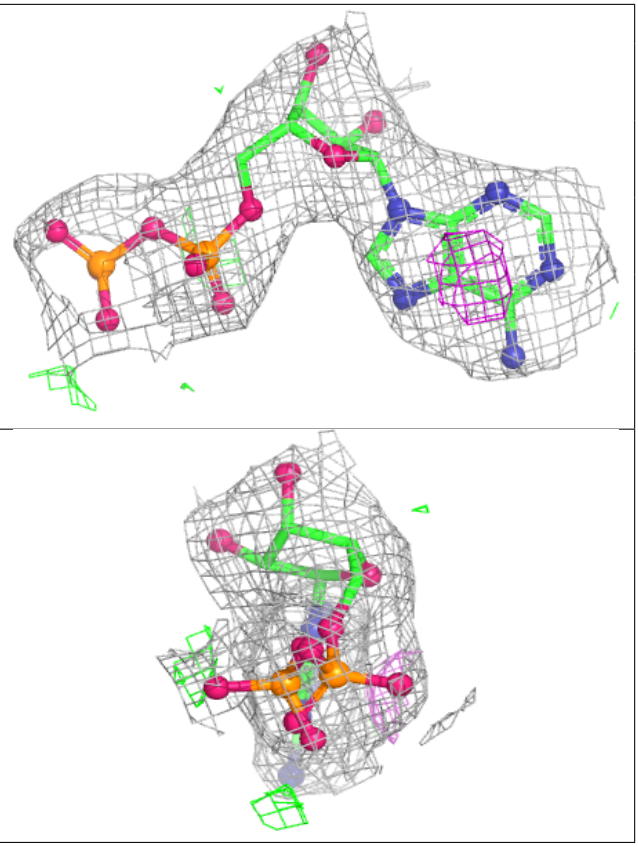
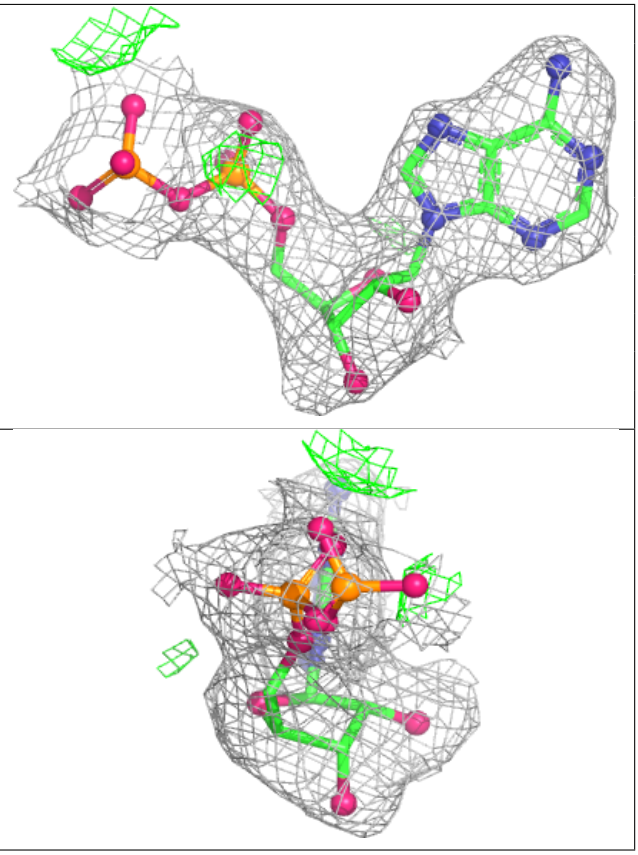
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



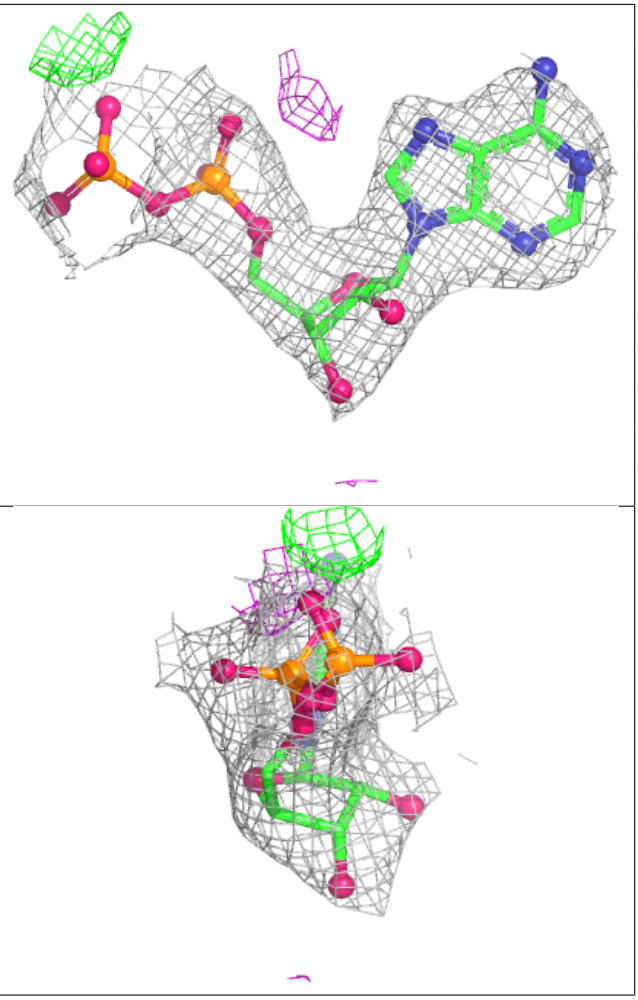
Electron density around ADP C 2502:

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



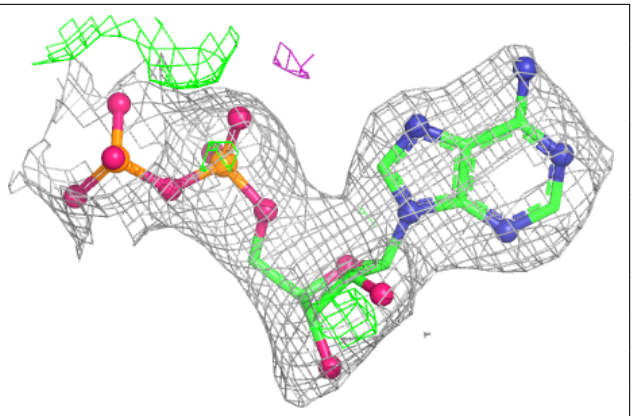
Electron density around ADP C 3502:

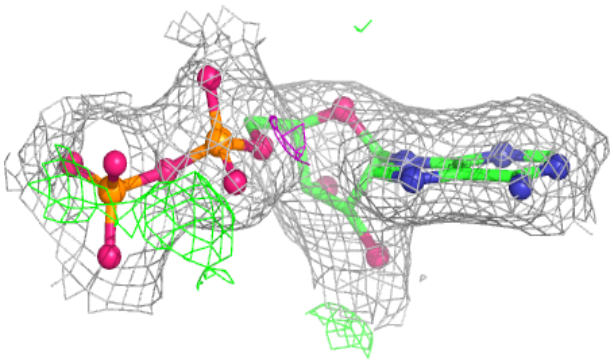
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

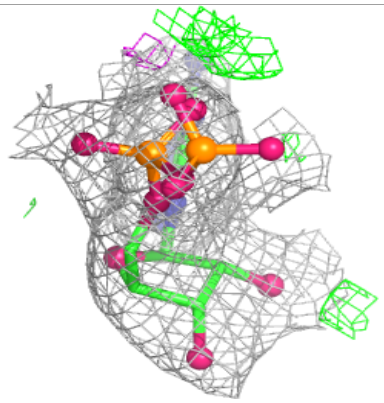


Electron density around ADP C 1502:

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

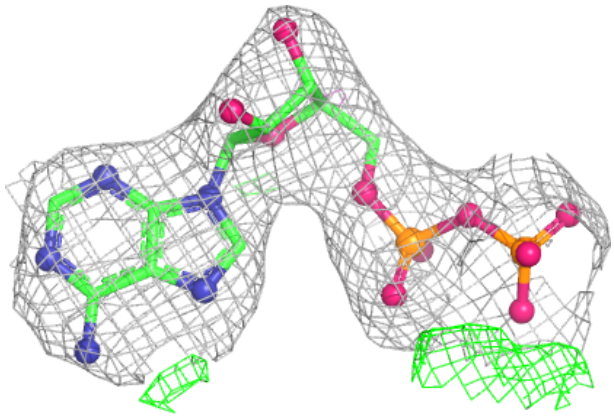


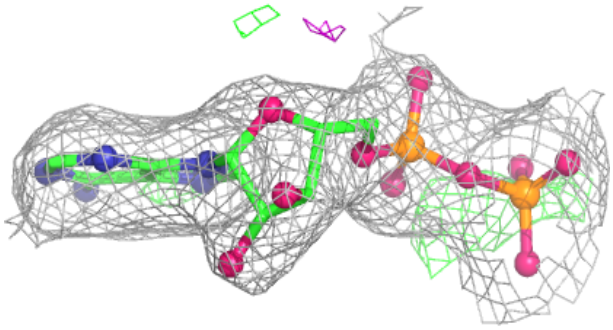


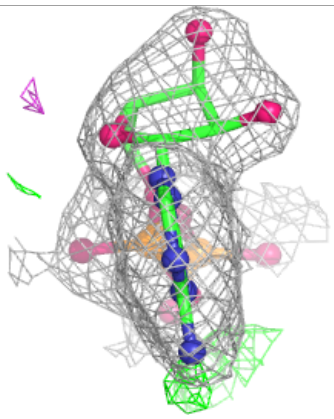


Electron density around ADP A 1502:

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

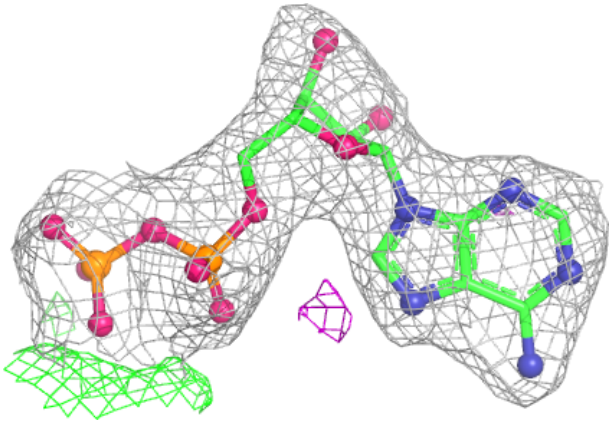


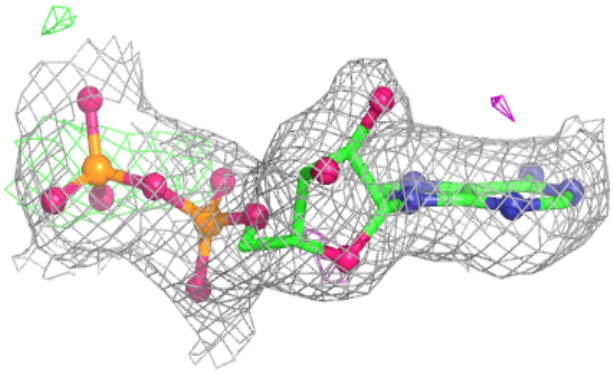


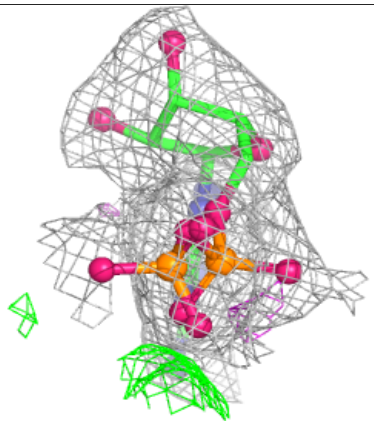


Electron density around ADP A 2502:

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

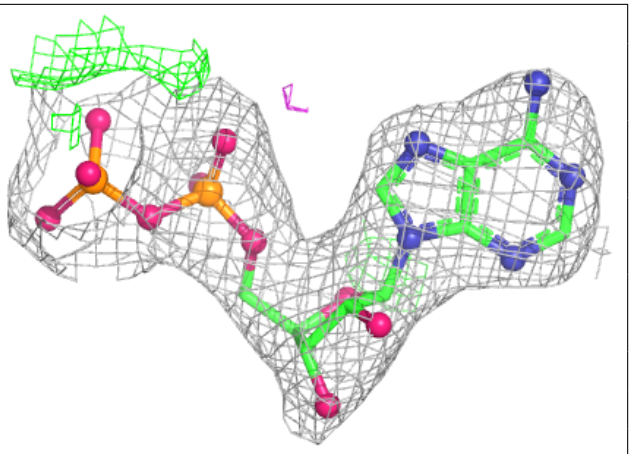


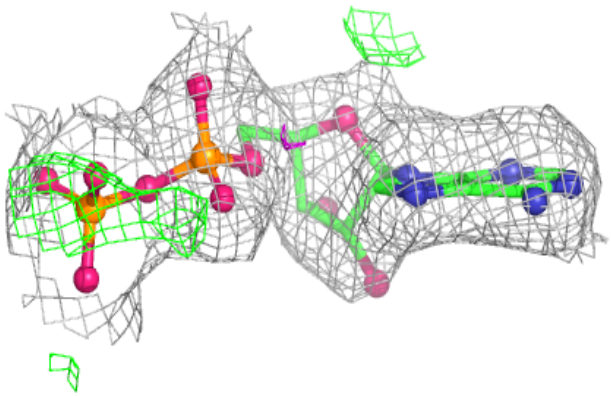


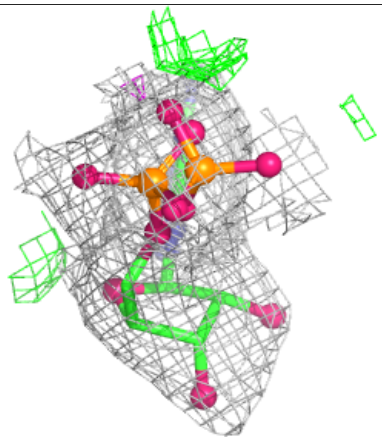


Electron density around ADP C 502:

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

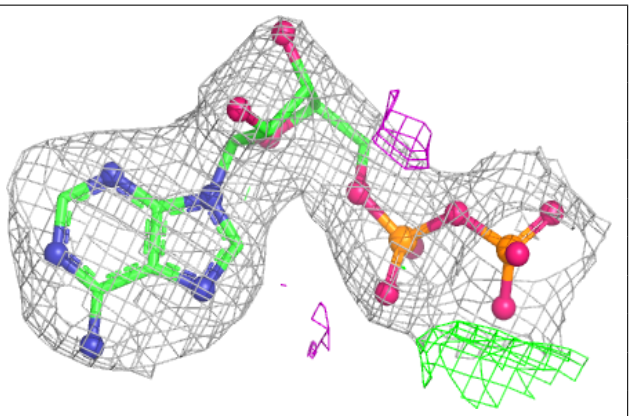


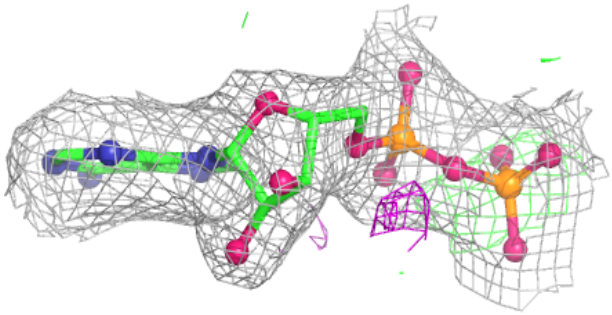


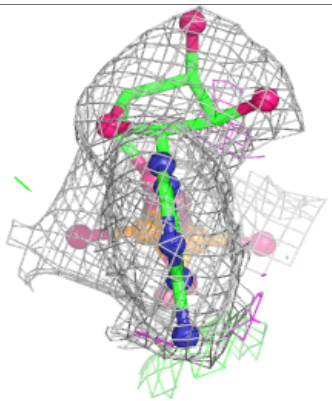


Electron density around ADP A 3502:

$2mF_o$-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.