



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 09:50 PM UTC

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

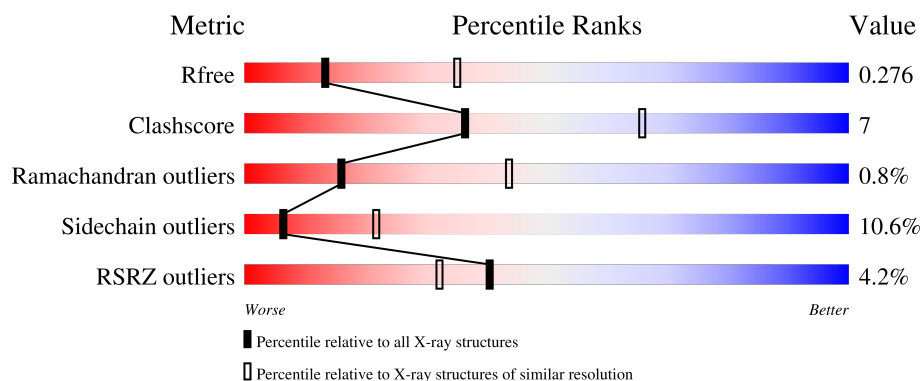
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 $\leq 5\%$. 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	B	15	
1	D	15	
2	A	1706	
2	C	1706	

2 Entry composition

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*DT)*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3').

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

- Molecule 2 is a protein called Protein recA.

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

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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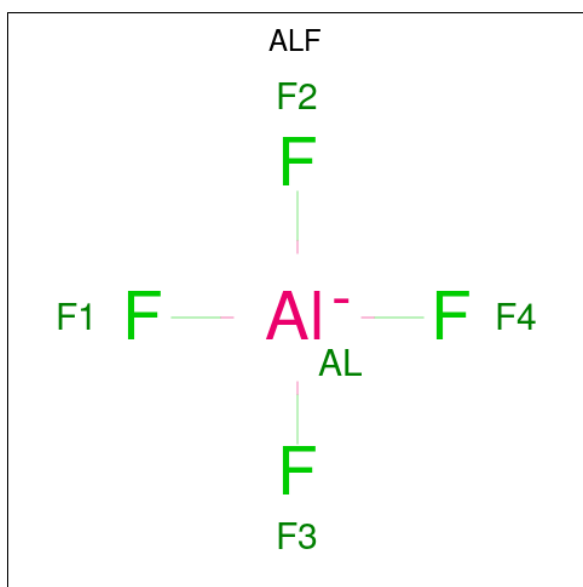
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Chain	Residue	Modelled	Actual	Comment	Reference
C	2985	THR	-	linker	UNP P0A7G6
C	2986	GLY	-	linker	UNP P0A7G6
C	2987	SER	-	linker	UNP P0A7G6
C	2988	THR	-	linker	UNP P0A7G6
C	2989	GLY	-	linker	UNP P0A7G6
C	2990	SER	-	linker	UNP P0A7G6
C	2991	ALA	-	linker	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).

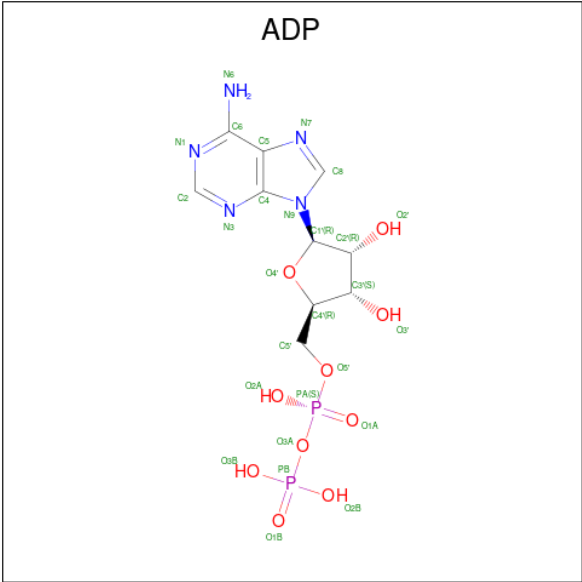
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Mg 5 5	0	0
3	C	5	Total Mg 5 5	0	0

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



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

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

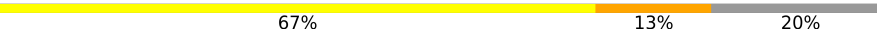


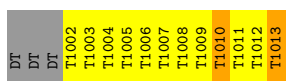
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C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

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.

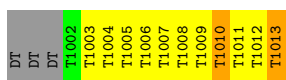
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

Chain B: 



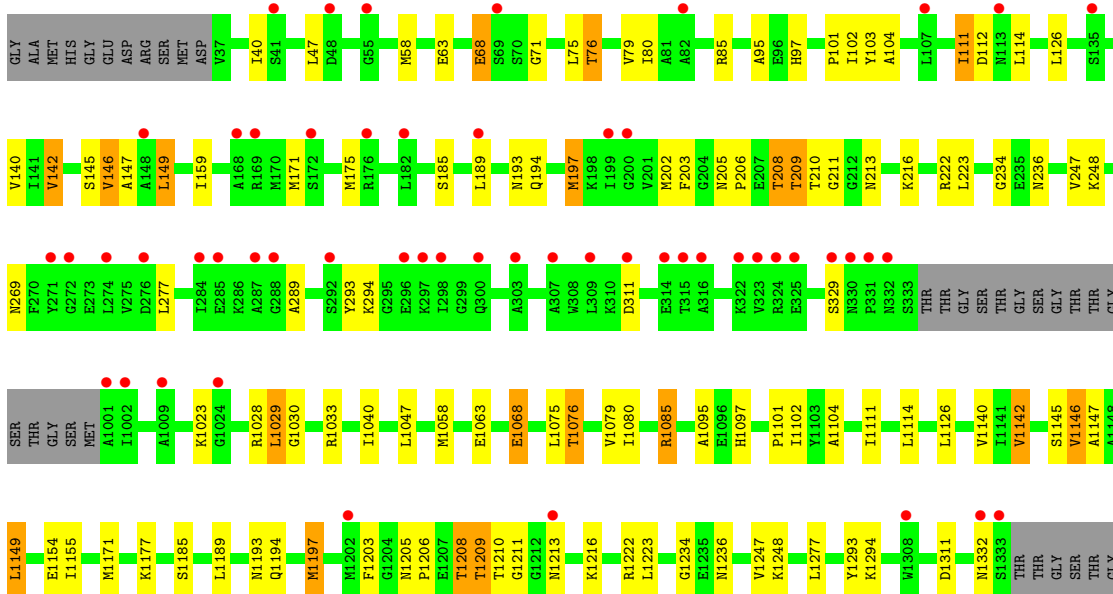
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

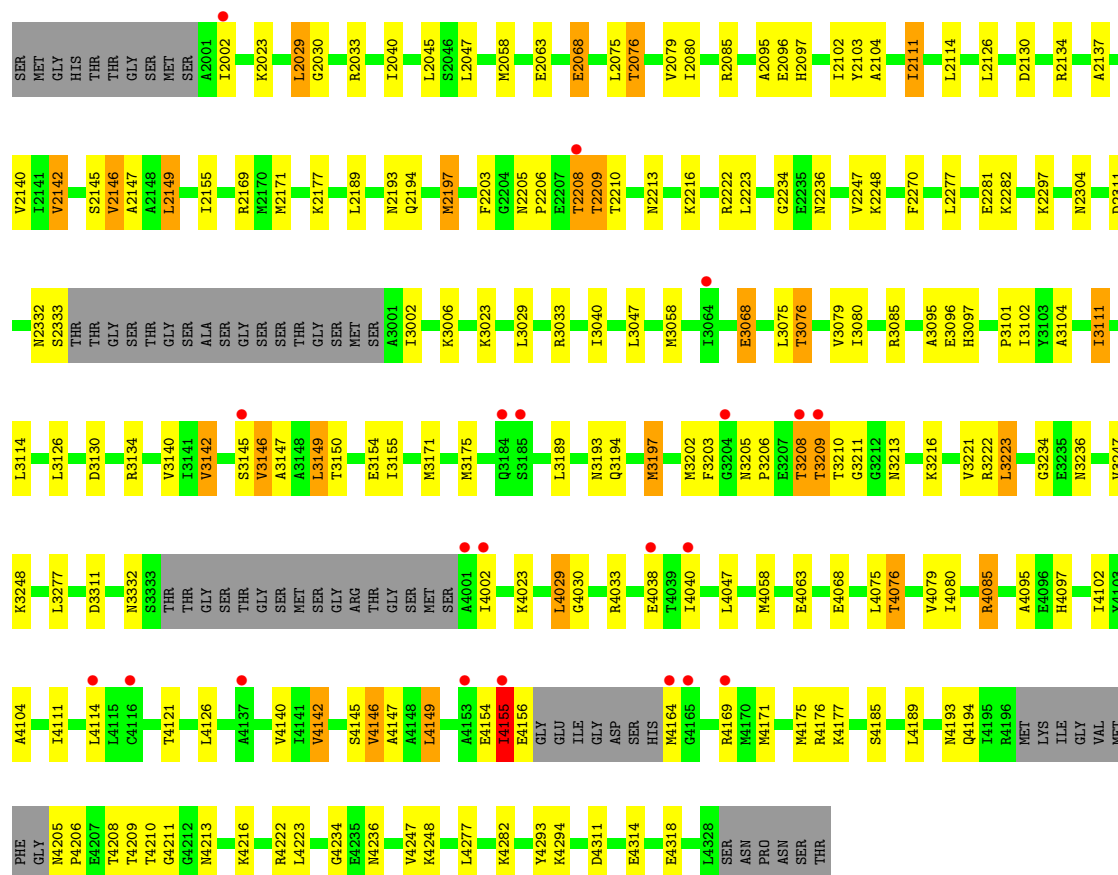
Chain D: 



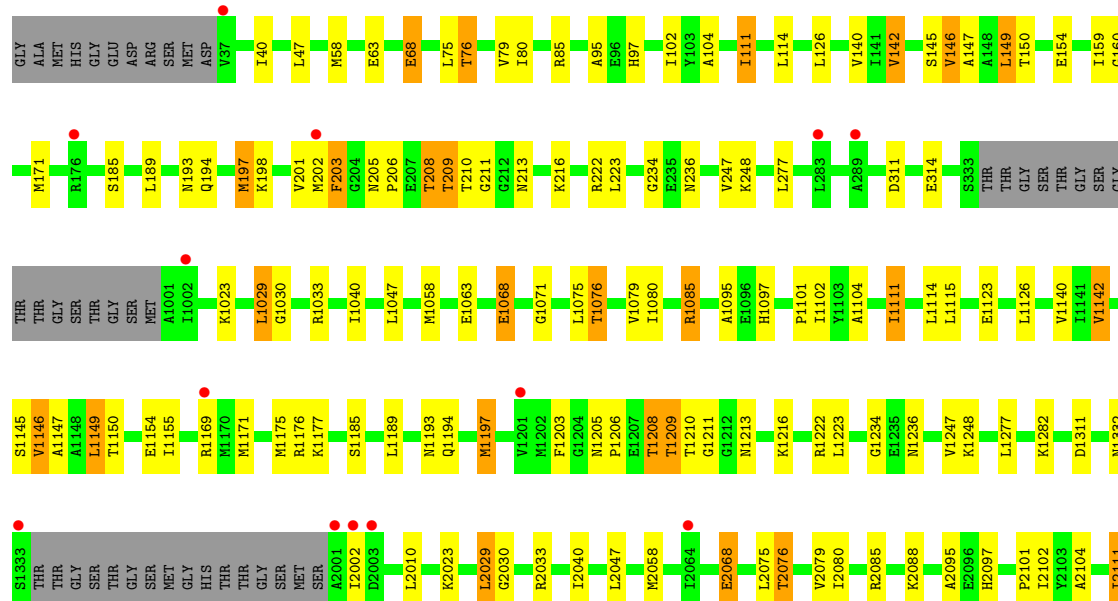
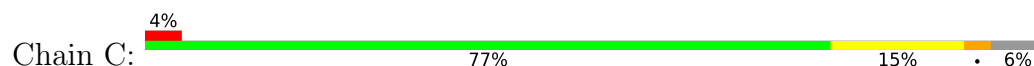
- Molecule 2: Protein recA

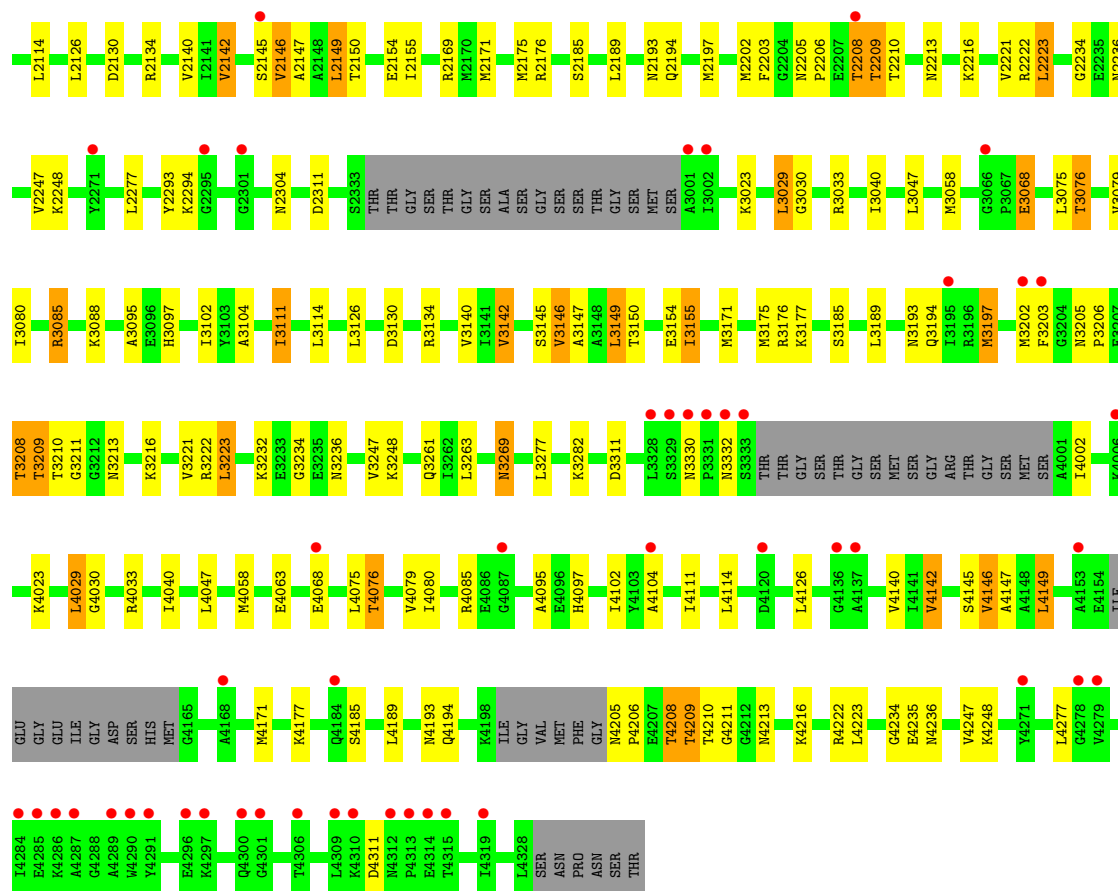
Chain A: 





• Molecule 2: Protein recA





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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 ⓘ

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

Continued on next page...

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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	C	1502	3	28,29,29	1.54	6 (21%)	43,45,45	1.94	11 (25%)
4	ALF	A	1501	-	4,4,4	1.28	0	-		
5	ADP	A	502	3	28,29,29	1.56	5 (17%)	43,45,45	1.87	10 (23%)
4	ALF	A	501	-	4,4,4	1.34	0	-		
5	ADP	C	502	3	28,29,29	1.58	7 (25%)	43,45,45	1.83	10 (23%)
5	ADP	A	1502	3	28,29,29	1.47	5 (17%)	43,45,45	1.92	14 (32%)
4	ALF	C	1501	-	4,4,4	1.31	0	-		
4	ALF	A	4501	-	4,4,4	1.49	0	-		
5	ADP	C	4502	3	28,29,29	1.56	6 (21%)	43,45,45	1.84	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ALF	C	4501	-	4,4,4	1.50	0	-		
4	ALF	C	2501	-	4,4,4	1.26	0	-		
5	ADP	A	4502	3	28,29,29	1.60	6 (21%)	43,45,45	1.57	8 (18%)
4	ALF	C	3501	-	4,4,4	1.29	0	-		
5	ADP	A	2502	3	28,29,29	1.50	6 (21%)	43,45,45	1.84	11 (25%)
5	ADP	A	3502	3	28,29,29	1.47	4 (14%)	43,45,45	2.02	12 (27%)
5	ADP	C	2502	3	28,29,29	1.57	6 (21%)	43,45,45	1.82	12 (27%)
4	ALF	A	2501	-	4,4,4	1.24	0	-		
4	ALF	C	501	-	4,4,4	1.22	0	-		
5	ADP	C	3502	3	28,29,29	1.48	4 (14%)	43,45,45	1.88	10 (23%)
4	ALF	A	3501	-	4,4,4	1.23	0	-		

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	C	2502	3	-	1/16/32/32	0/3/3/3
5	ADP	C	502	3	-	1/16/32/32	0/3/3/3
5	ADP	C	1502	3	-	1/16/32/32	0/3/3/3
5	ADP	A	1502	3	-	1/16/32/32	0/3/3/3
5	ADP	A	4502	3	-	1/16/32/32	0/3/3/3
5	ADP	C	4502	3	-	1/16/32/32	0/3/3/3
5	ADP	C	3502	3	-	1/16/32/32	0/3/3/3
5	ADP	A	2502	3	-	3/16/32/32	0/3/3/3
5	ADP	A	502	3	-	1/16/32/32	0/3/3/3
5	ADP	A	3502	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(°)	Ideal(°)
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:

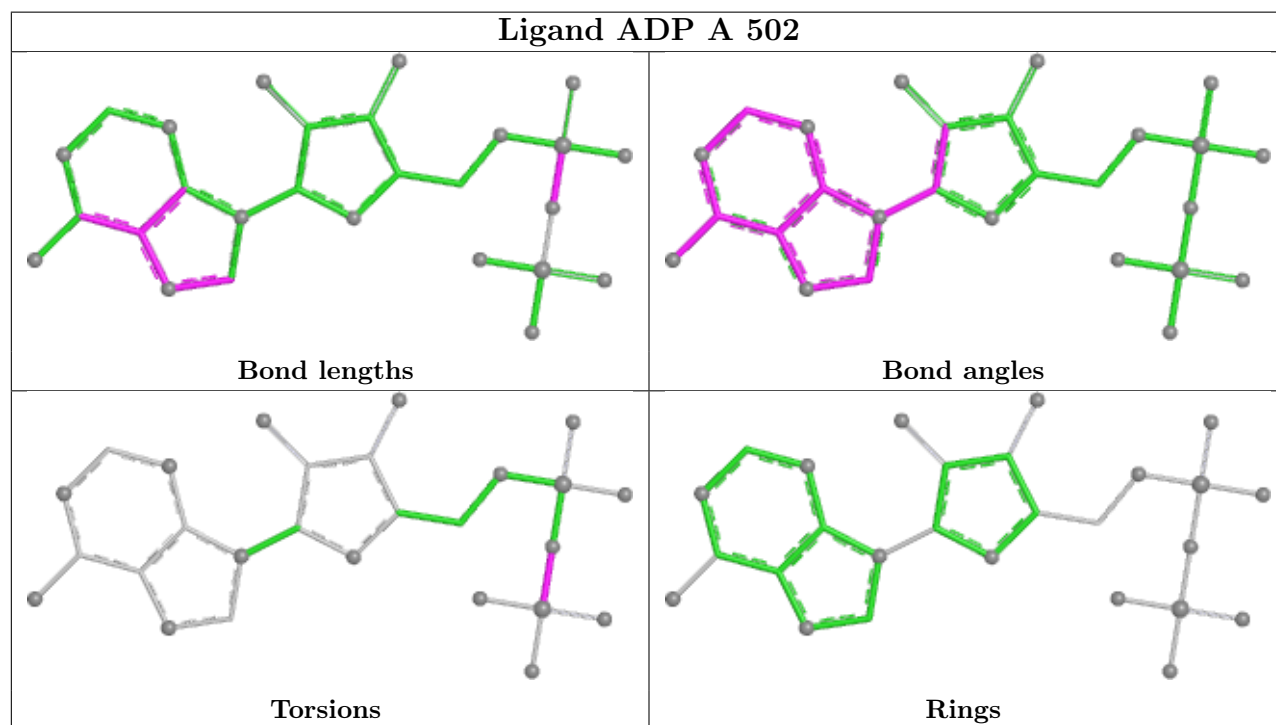
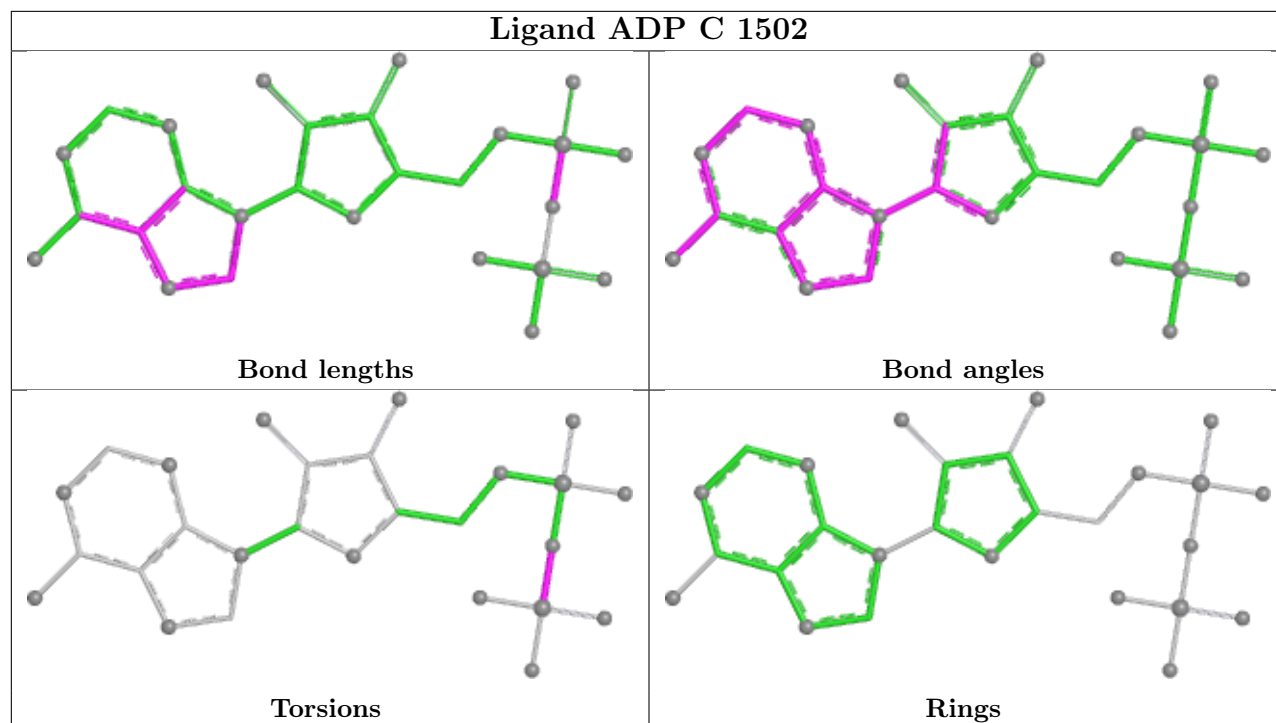
Mol	Chain	Res	Type	Atoms
5	A	502	ADP	PA-O3A-PB-O2B
5	A	4502	ADP	PA-O3A-PB-O2B
5	C	502	ADP	PA-O3A-PB-O2B
5	C	1502	ADP	PA-O3A-PB-O2B
5	A	1502	ADP	PA-O3A-PB-O2B

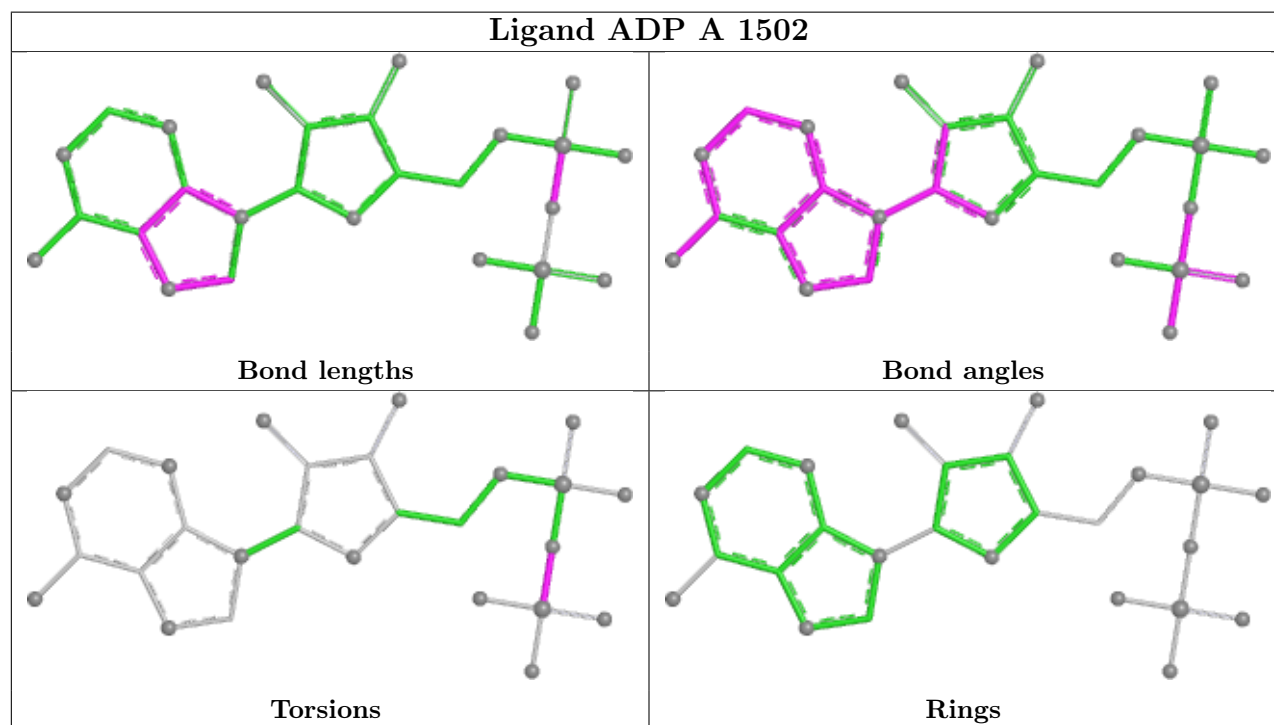
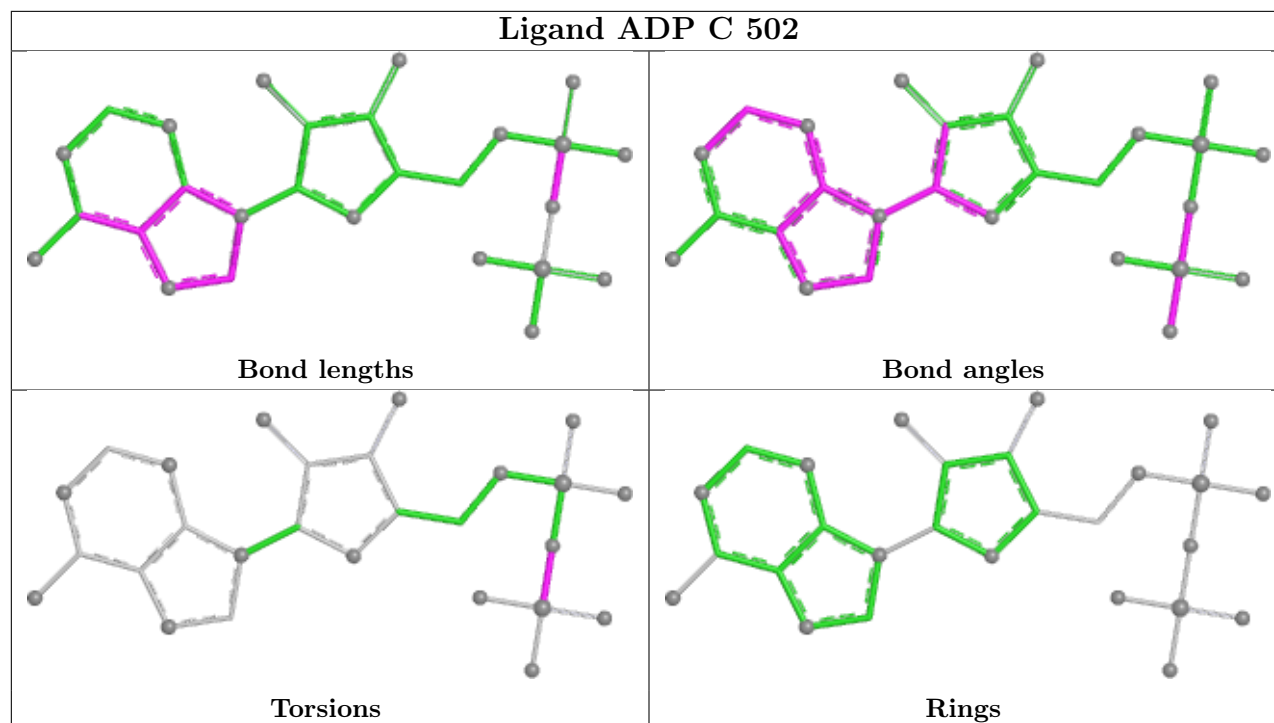
There are no ring outliers.

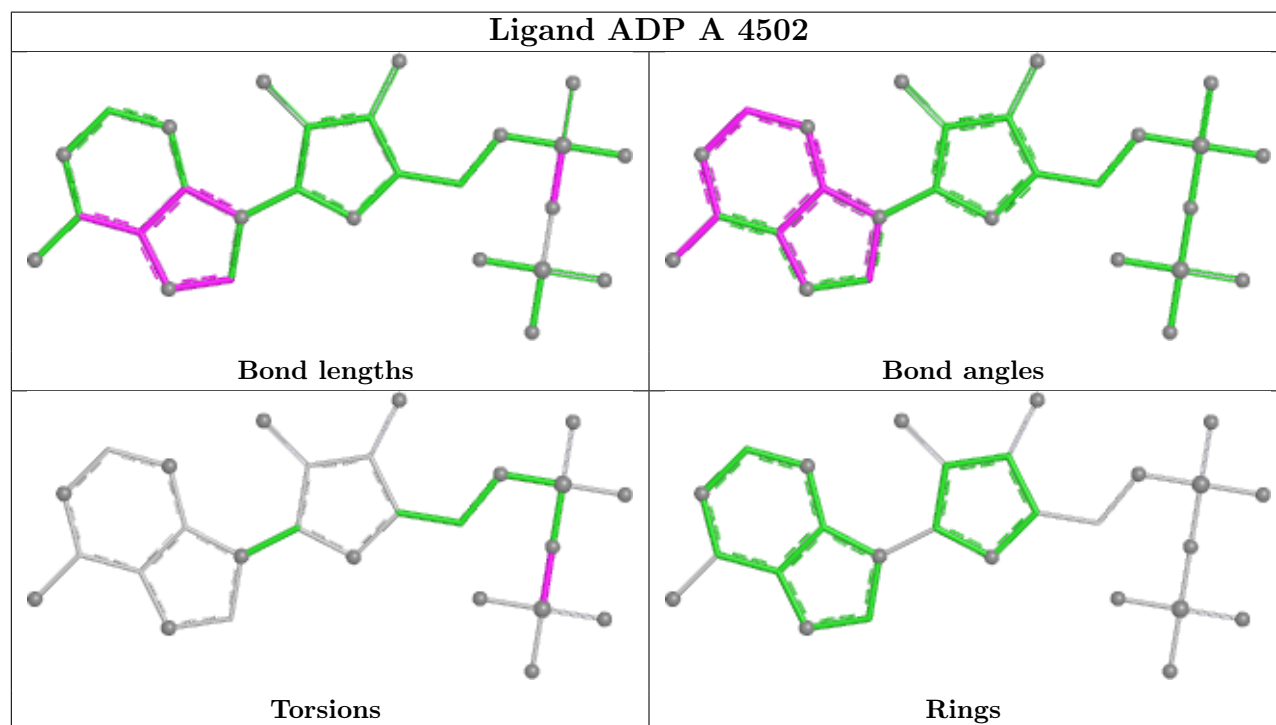
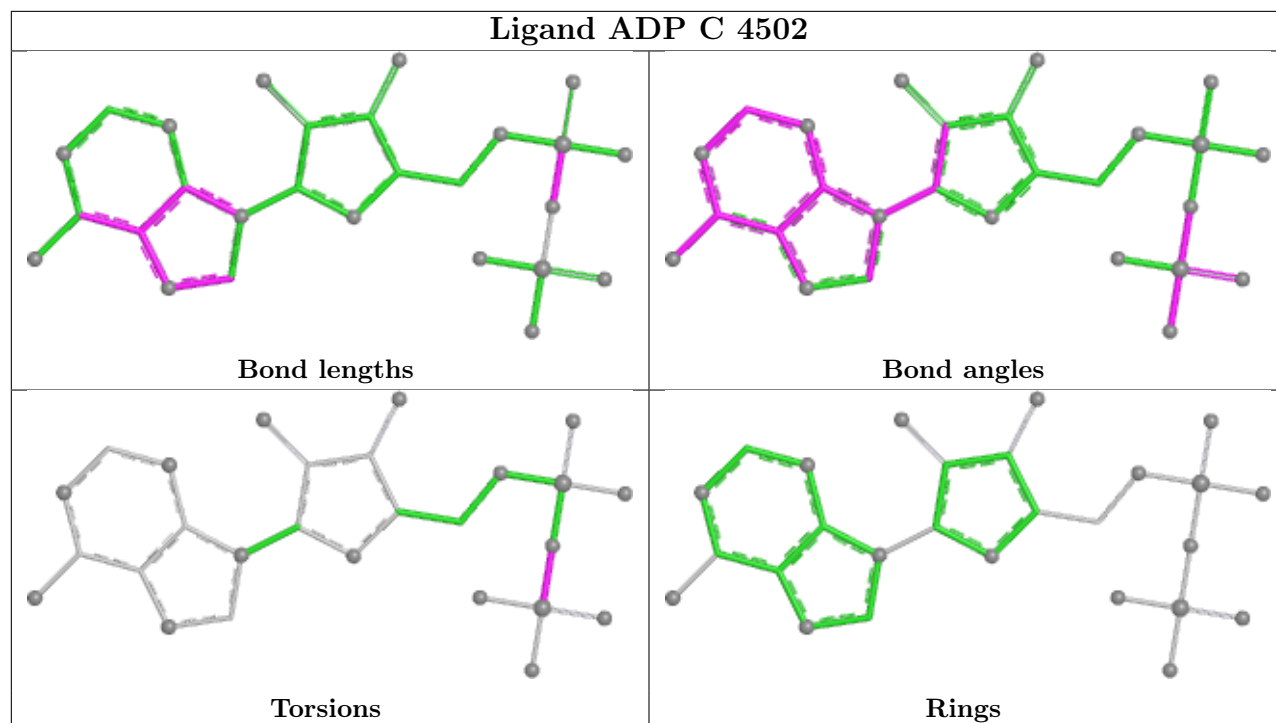
3 monomers are involved in 4 short contacts:

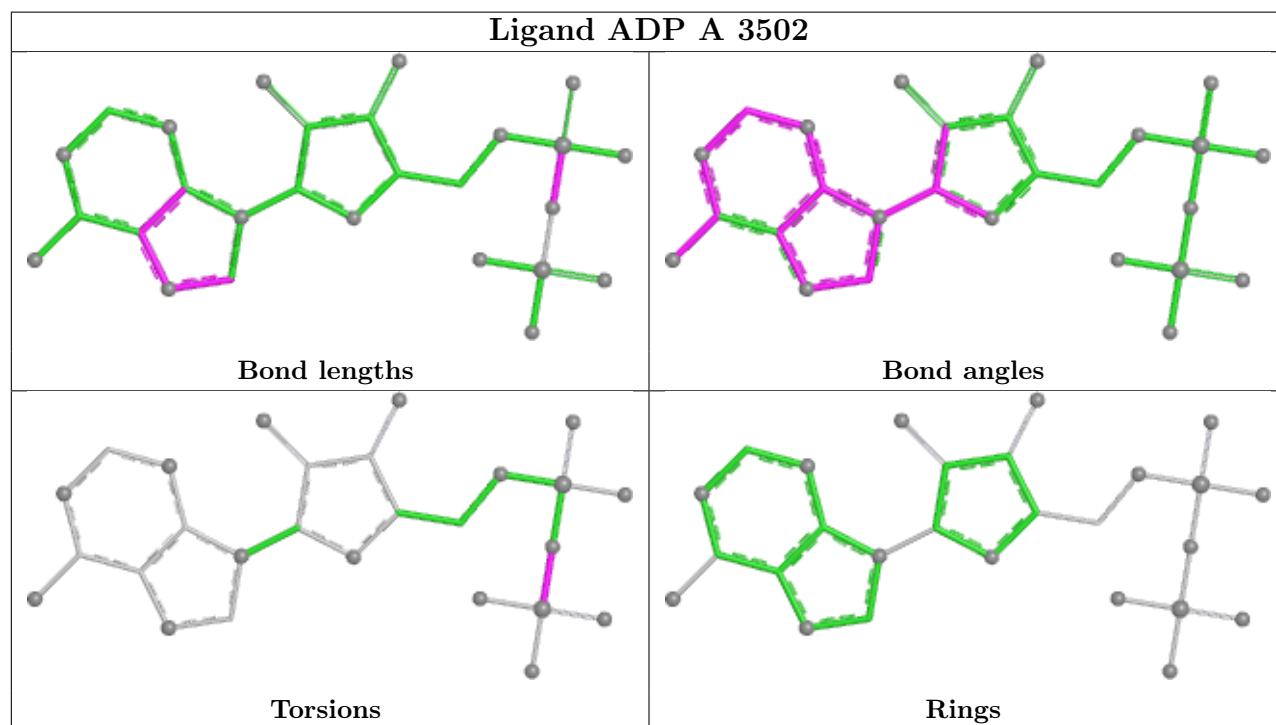
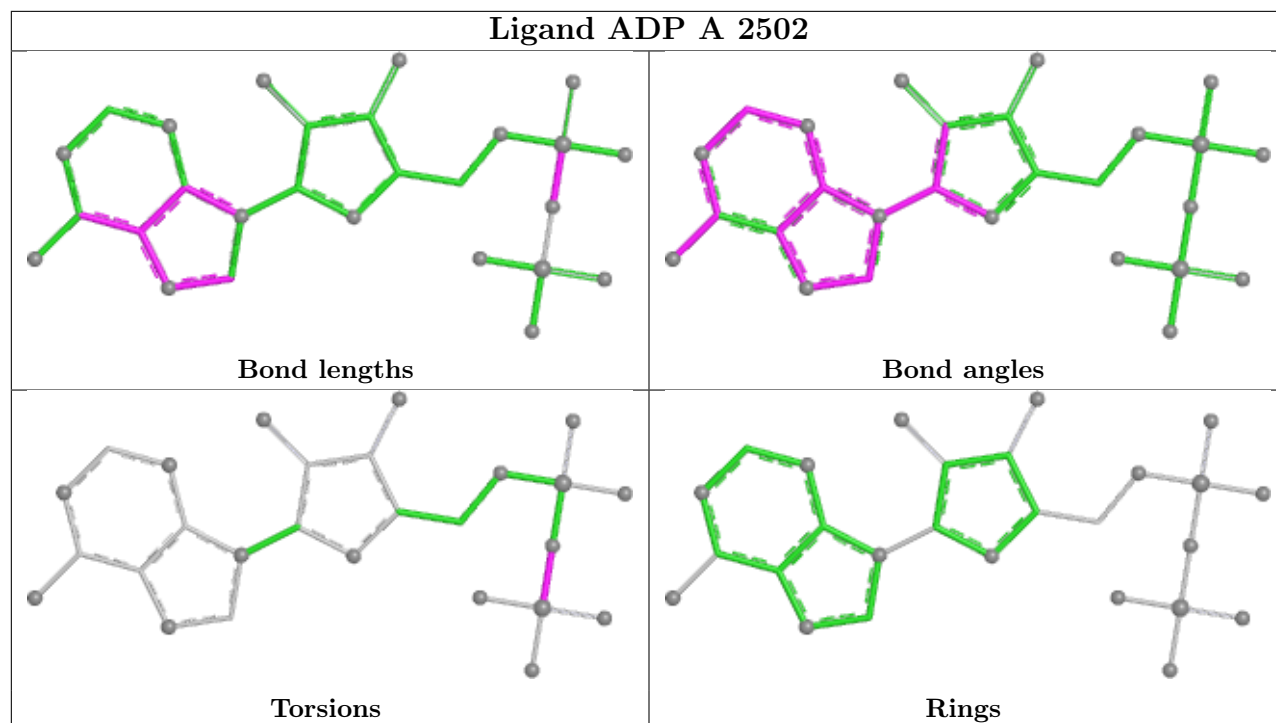
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1502	ADP	1	0
5	A	502	ADP	2	0
5	A	2502	ADP	1	0

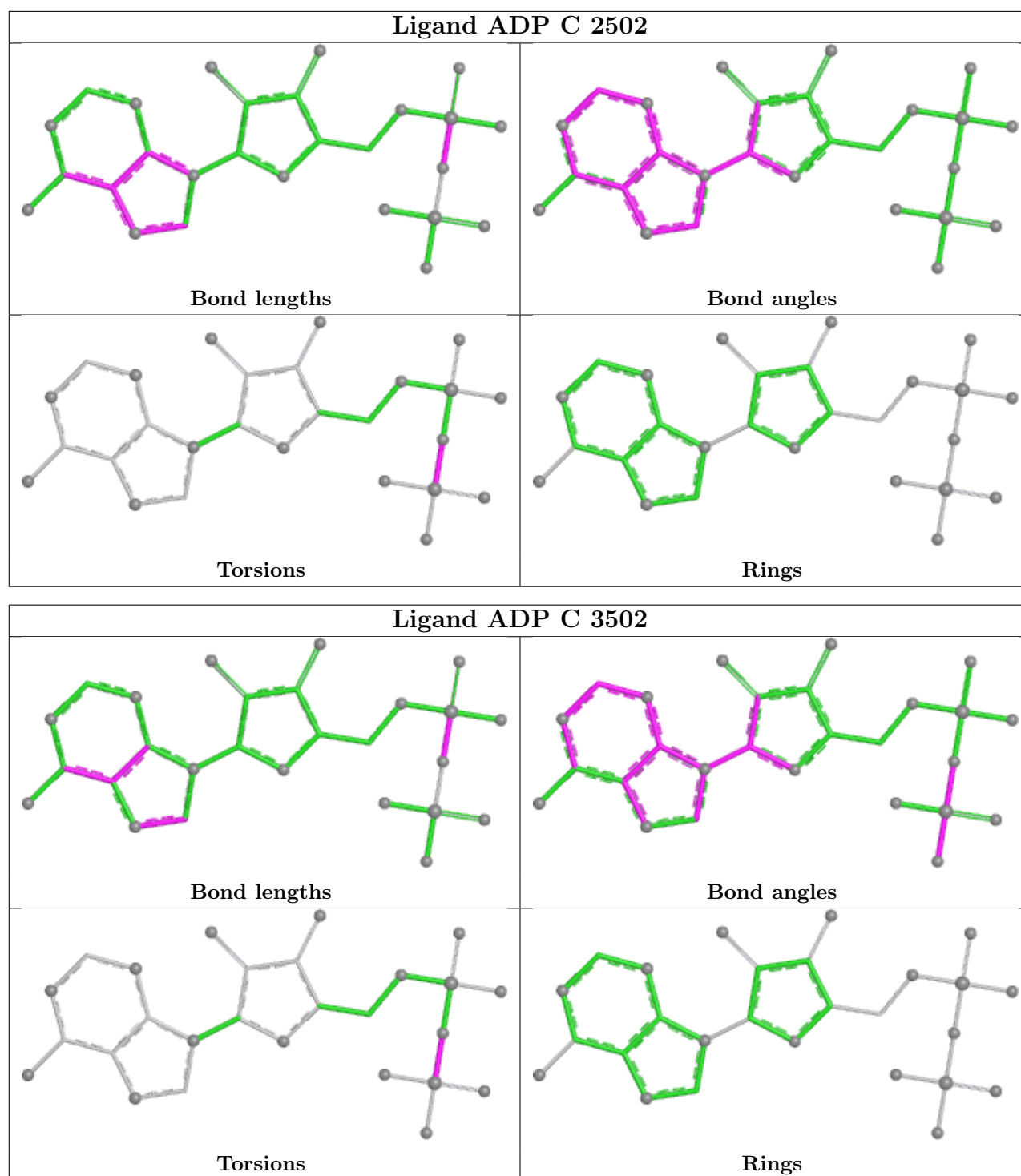
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	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](#)

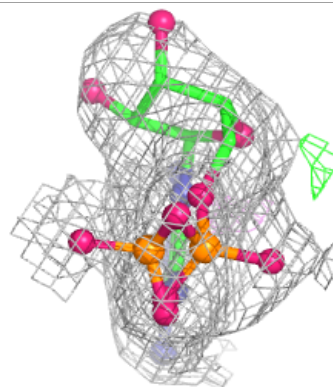
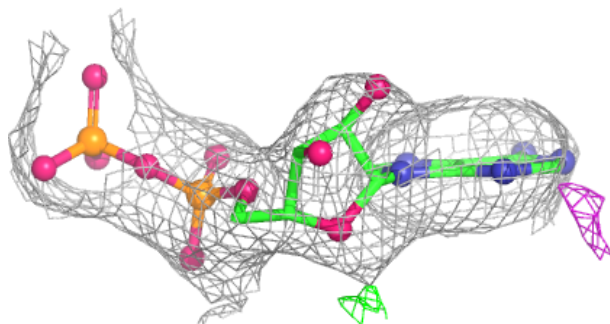
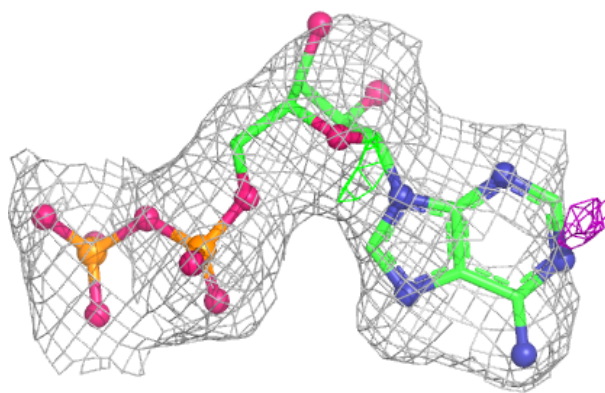
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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.

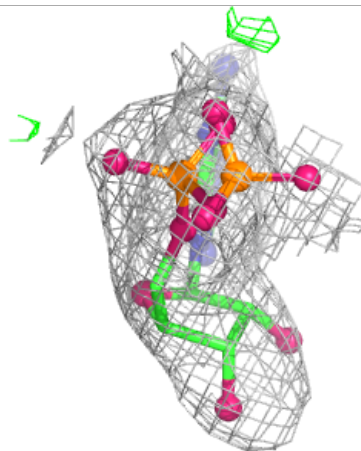
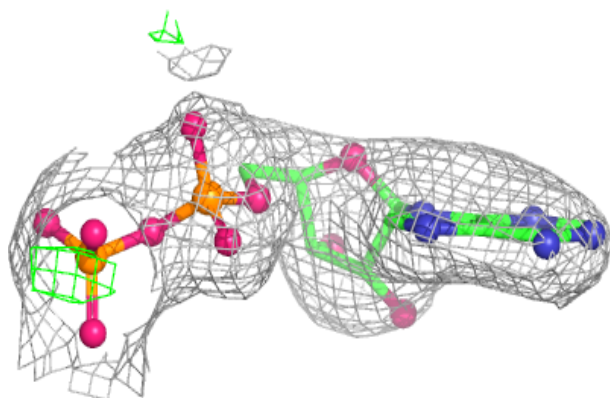
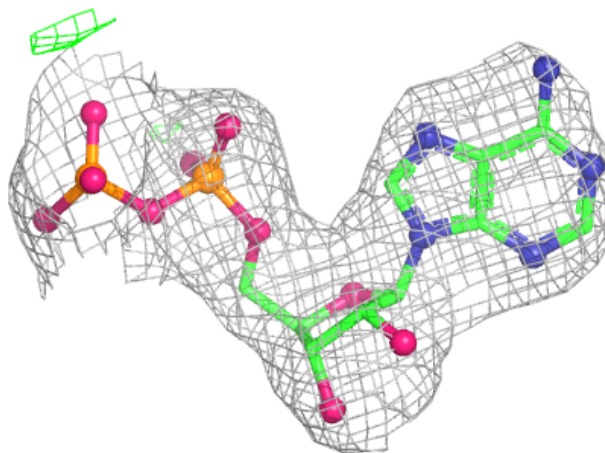
Electron density around ADP A 4502:

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



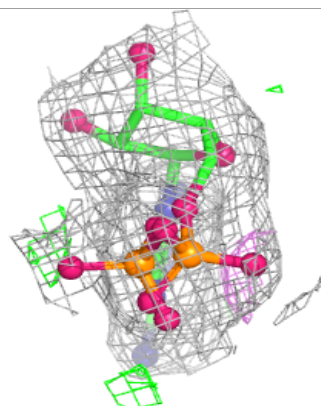
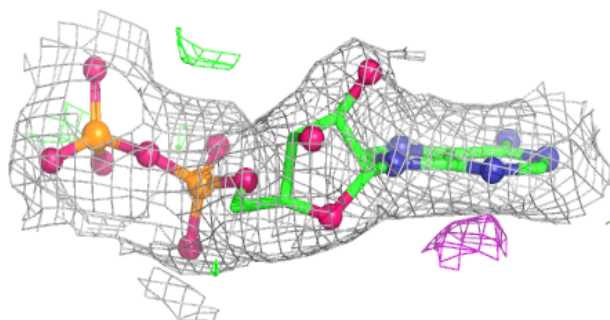
Electron density around ADP C 4502:

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

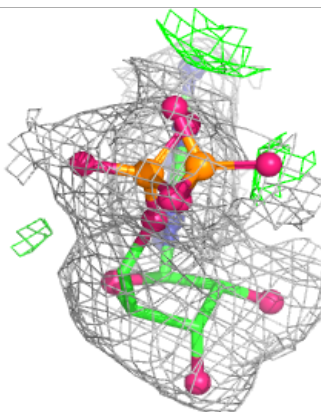
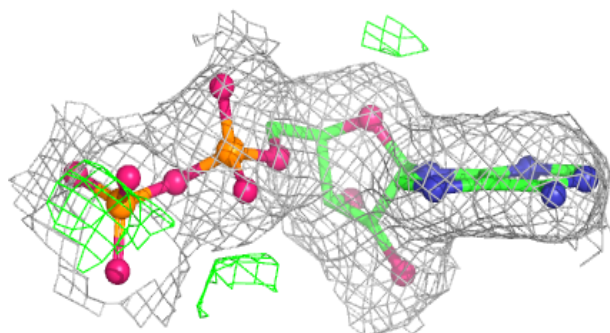
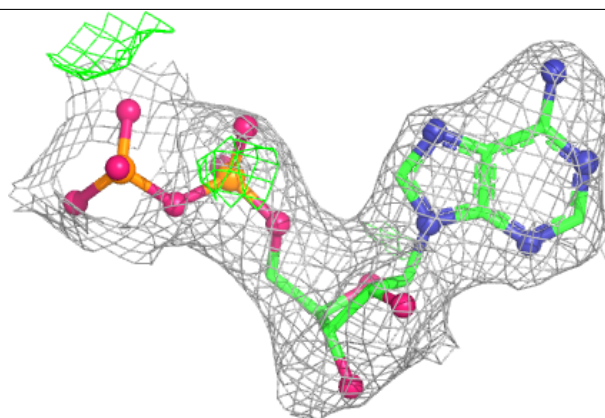


Electron density around ADP A 502:

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and green (positive)

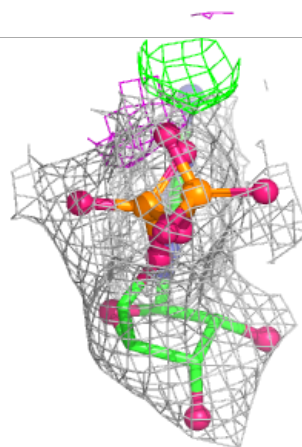
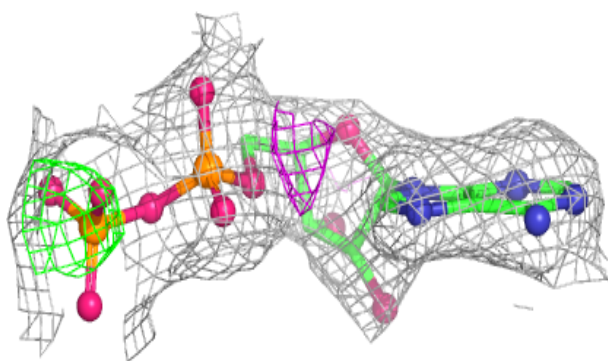
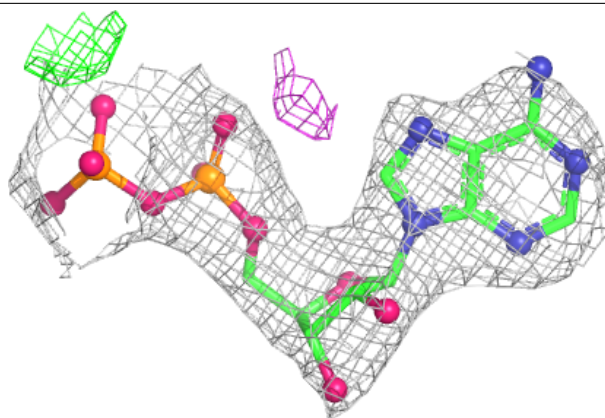
**Electron density around ADP C 2502:**

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



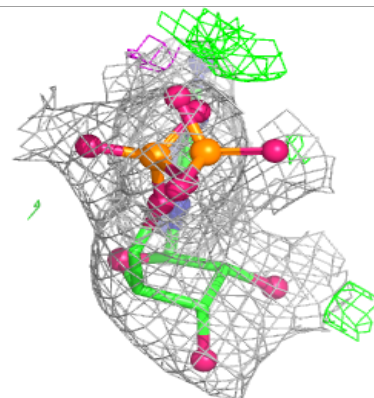
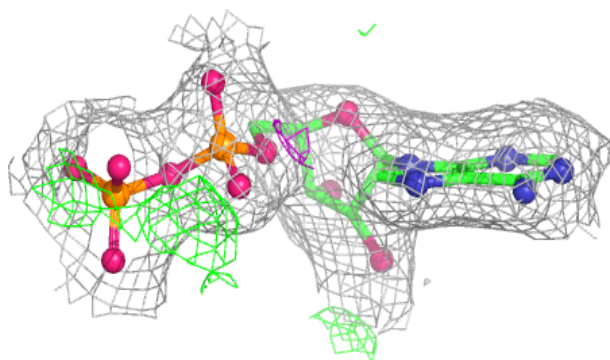
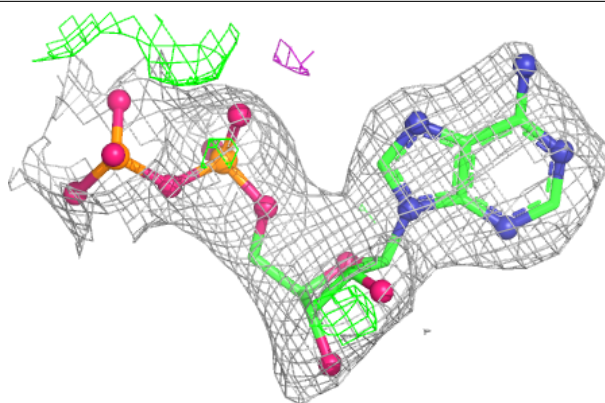
Electron density around ADP C 3502:

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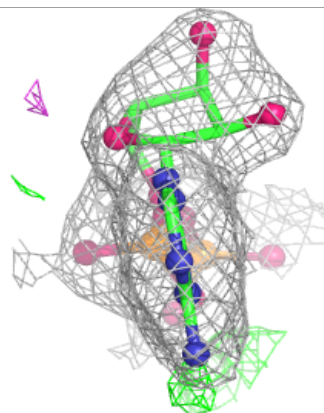
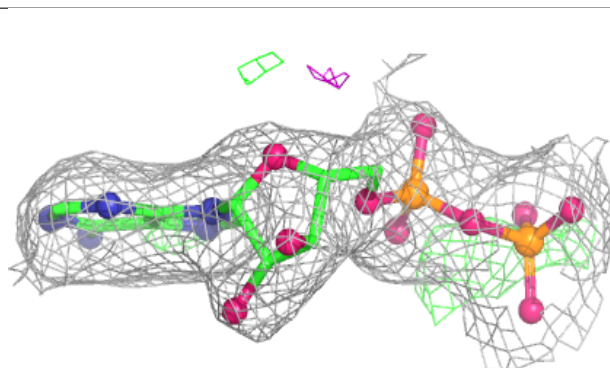
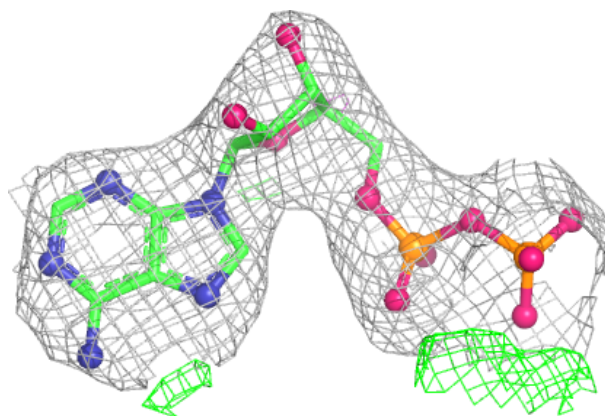


Electron density around ADP C 1502:

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and green (positive)

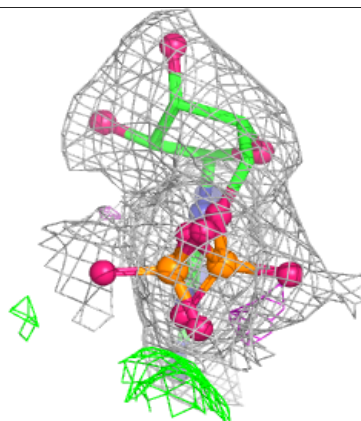
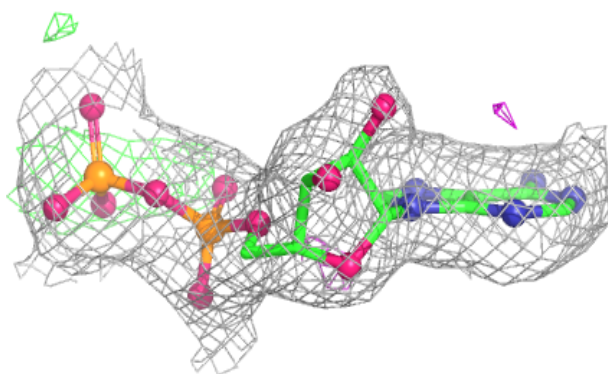
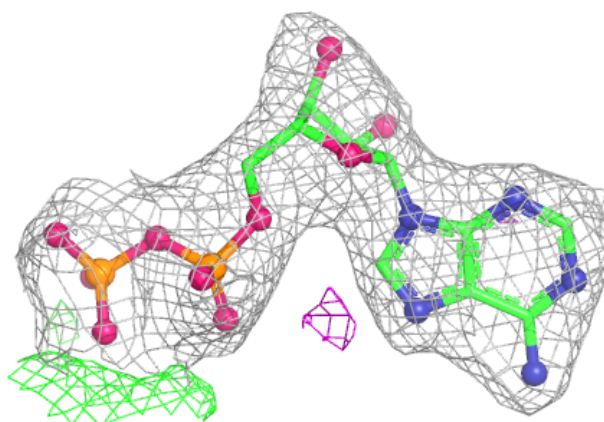
**Electron density around ADP A 1502:**

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



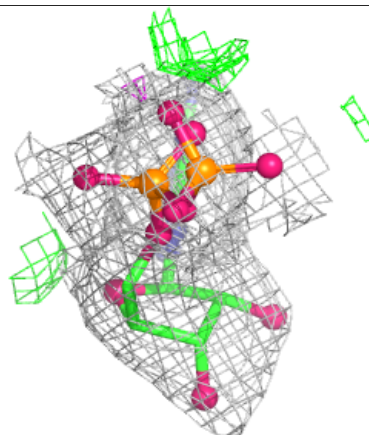
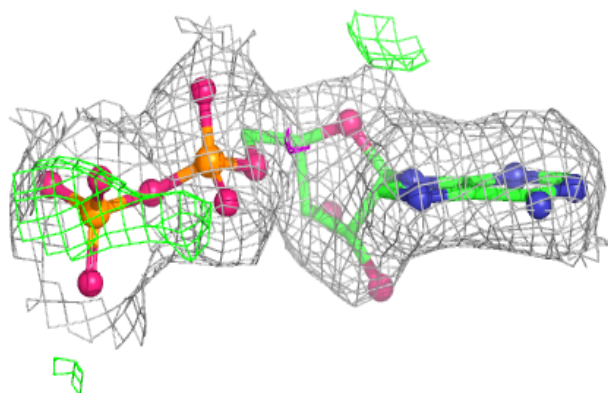
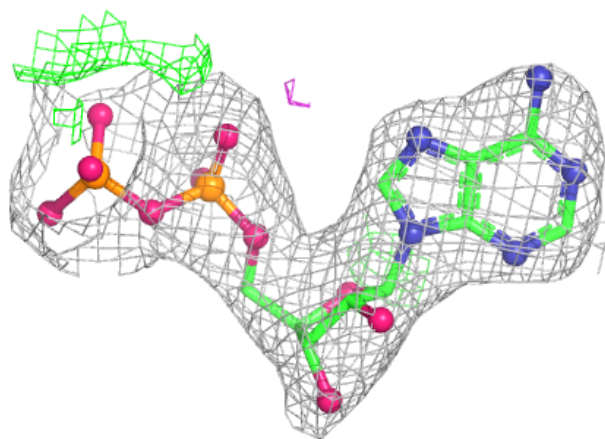
Electron density around ADP A 2502:

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

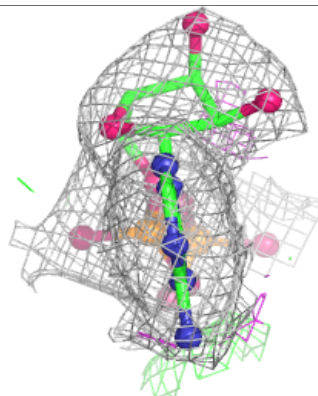
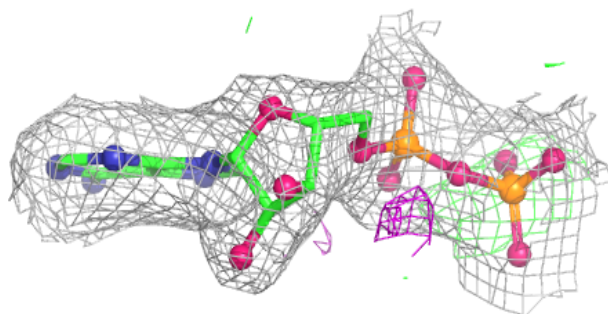
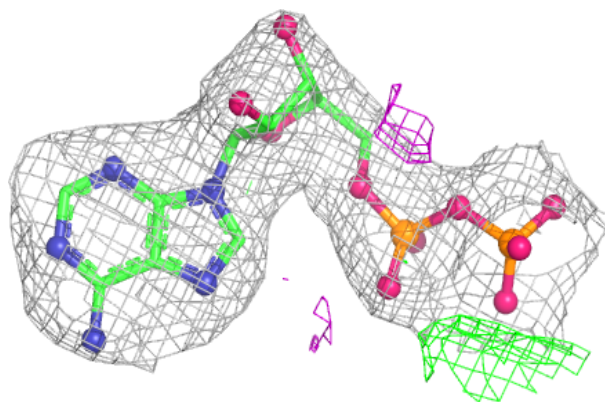


Electron density around ADP C 502:

$2mF_o-DF_c$ (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.