



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 04:17 am BST

PDB ID : 3CMX
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors : Pavletich, N.P.
Deposited on : 2008-03-24
Resolution : 3.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

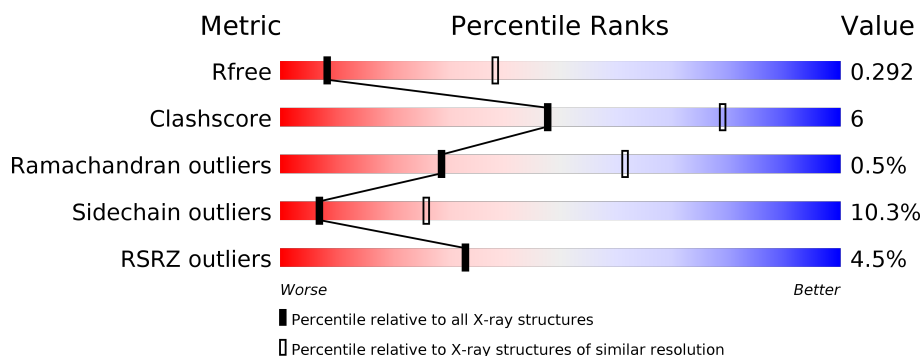
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on 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	<div> <div>20%</div> <div>40%</div> <div>27%</div> <div>13%</div> </div>
1	E	15	<div> <div>20%</div> <div>33%</div> <div>33%</div> <div>13%</div> </div>
2	C	12	<div> <div>42%</div> <div>75%</div> <div>17%</div> <div>8%</div> </div>
2	F	12	<div> <div>92%</div> <div>92%</div> <div>8%</div> </div>
3	A	1706	<div> <div>4%</div> <div>78%</div> <div>14%</div> <div>6%</div> </div>
3	D	1706	<div> <div>3%</div> <div>78%</div> <div>13%</div> <div>6%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25459 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	13	Total	C	N	O	P	0	0	0
			260	130	26	91	13			
1	E	13	Total	C	N	O	P	0	0	0
			260	130	26	91	13			

- Molecule 2 is a DNA chain called DNA (5'-D(*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			211	100	50	51	10			
2	F	12	Total	C	N	O	P	0	0	0
			232	110	55	56	11			

- Molecule 3 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1603	Total	C	N	O	S	0	0	0
			12083	7595	2094	2339	55			
3	D	1603	Total	C	N	O	S	0	0	0
			12083	7595	2094	2339	55			

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
D	26	GLY	-	linker	UNP P0A7G6
D	27	ALA	-	linker	UNP P0A7G6
D	28	MET	-	linker	UNP P0A7G6
D	29	HIS	-	linker	UNP P0A7G6
D	986	THR	-	linker	UNP P0A7G6
D	987	GLY	-	linker	UNP P0A7G6
D	988	SER	-	linker	UNP P0A7G6
D	989	THR	-	linker	UNP P0A7G6
D	990	GLY	-	linker	UNP P0A7G6
D	991	SER	-	linker	UNP P0A7G6
D	992	GLY	-	linker	UNP P0A7G6
D	993	THR	-	linker	UNP P0A7G6
D	994	THR	-	linker	UNP P0A7G6
D	995	GLY	-	linker	UNP P0A7G6
D	996	SER	-	linker	UNP P0A7G6
D	997	THR	-	linker	UNP P0A7G6
D	998	GLY	-	linker	UNP P0A7G6
D	999	SER	-	linker	UNP P0A7G6
D	1000	MET	-	linker	UNP P0A7G6
D	1986	THR	-	linker	UNP P0A7G6
D	1987	GLY	-	linker	UNP P0A7G6
D	1988	SER	-	linker	UNP P0A7G6
D	1989	THR	-	linker	UNP P0A7G6
D	1990	GLY	-	linker	UNP P0A7G6
D	1991	SER	-	linker	UNP P0A7G6

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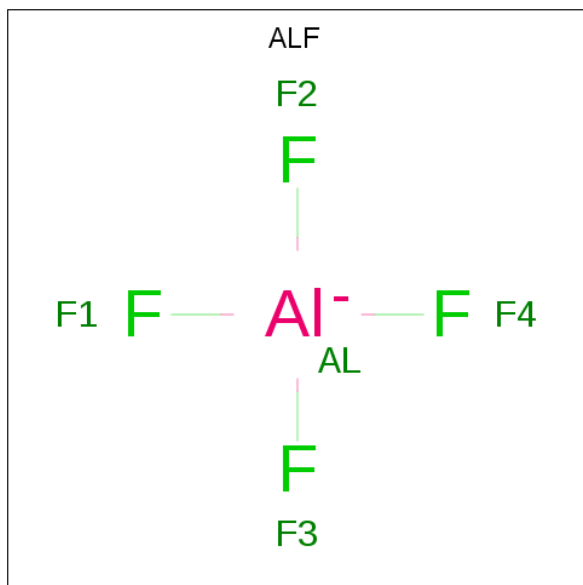
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1992	MET	-	linker	UNP P0A7G6
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker	UNP P0A7G6
D	2000	SER	-	linker	UNP P0A7G6
D	2985	THR	-	linker	UNP P0A7G6
D	2986	GLY	-	linker	UNP P0A7G6
D	2987	SER	-	linker	UNP P0A7G6
D	2988	THR	-	linker	UNP P0A7G6
D	2989	GLY	-	linker	UNP P0A7G6
D	2990	SER	-	linker	UNP P0A7G6
D	2991	ALA	-	linker	UNP P0A7G6
D	2992	SER	-	linker	UNP P0A7G6
D	2993	GLY	-	linker	UNP P0A7G6
D	2994	SER	-	linker	UNP P0A7G6
D	2995	SER	-	linker	UNP P0A7G6
D	2996	THR	-	linker	UNP P0A7G6
D	2997	GLY	-	linker	UNP P0A7G6
D	2998	SER	-	linker	UNP P0A7G6
D	2999	MET	-	linker	UNP P0A7G6
D	3000	SER	-	linker	UNP P0A7G6
D	3986	THR	-	linker	UNP P0A7G6
D	3987	GLY	-	linker	UNP P0A7G6
D	3988	SER	-	linker	UNP P0A7G6
D	3989	THR	-	linker	UNP P0A7G6
D	3990	GLY	-	linker	UNP P0A7G6
D	3991	SER	-	linker	UNP P0A7G6
D	3992	MET	-	linker	UNP P0A7G6
D	3993	SER	-	linker	UNP P0A7G6
D	3994	GLY	-	linker	UNP P0A7G6
D	3995	ARG	-	linker	UNP P0A7G6
D	3996	THR	-	linker	UNP P0A7G6
D	3997	GLY	-	linker	UNP P0A7G6
D	3998	SER	-	linker	UNP P0A7G6
D	3999	MET	-	linker	UNP P0A7G6
D	4000	SER	-	linker	UNP P0A7G6

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

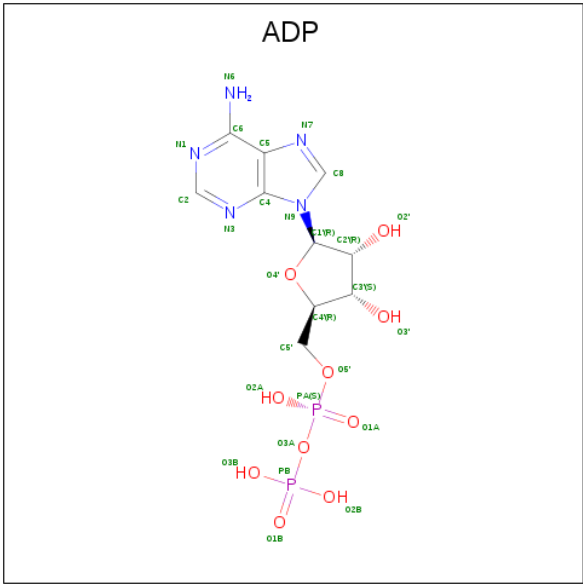
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	D	5	Total	Mg	0	0
			5	5		

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

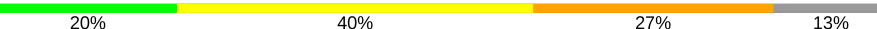


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	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 and DNA 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)*DTP*DTP*DT)-3')

Chain B: 




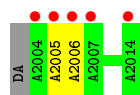
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)*DTP*DTP*DT)-3')

Chain E: 



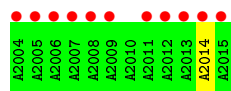
- Molecule 2: DNA (5'-D(*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DA)-3')

Chain C: 




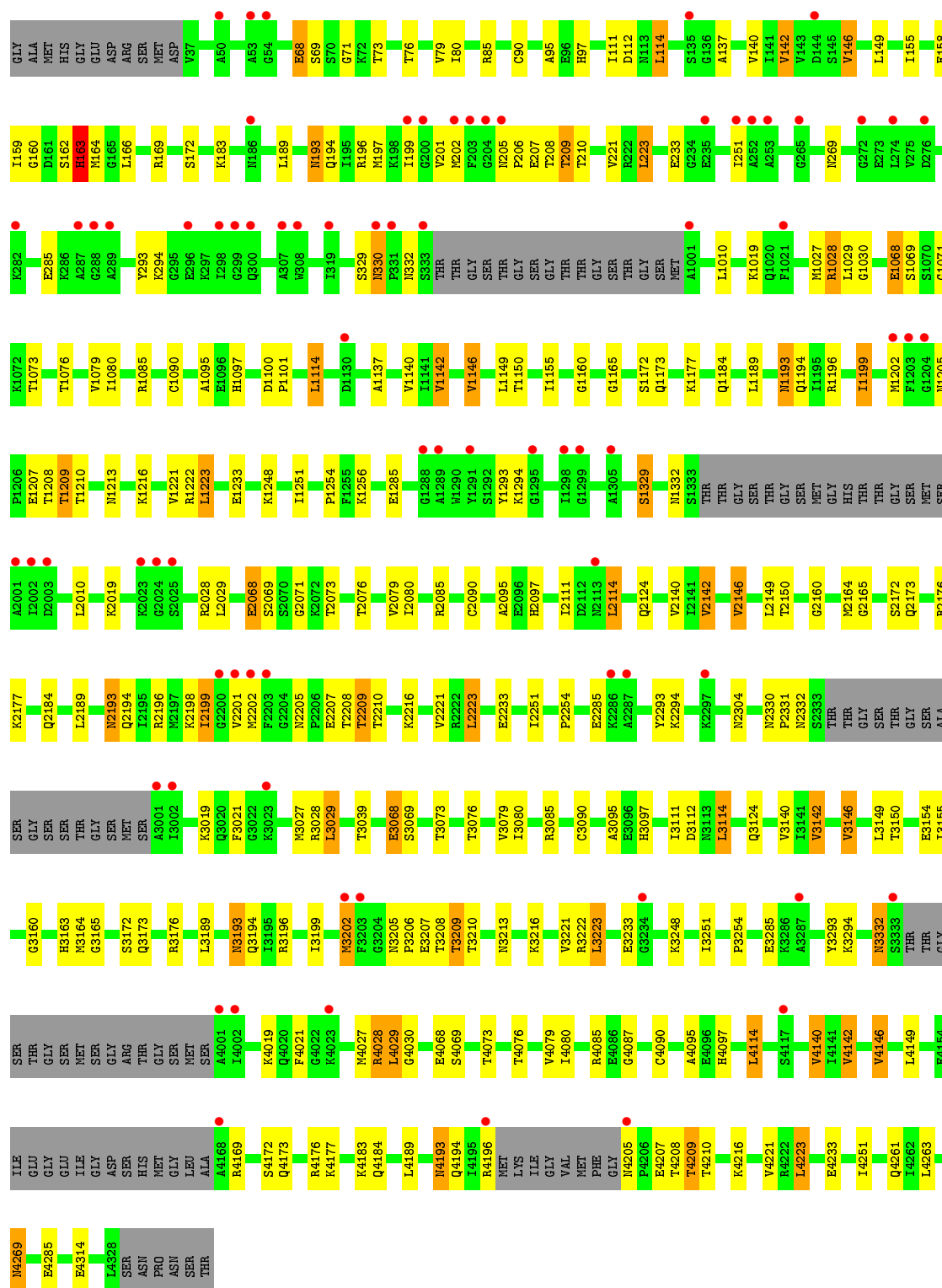
- Molecule 2: DNA (5'-D(*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DA)-3')

Chain F: 

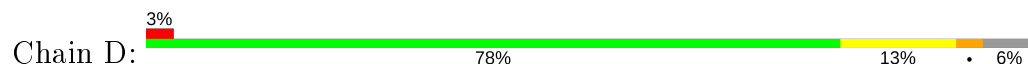


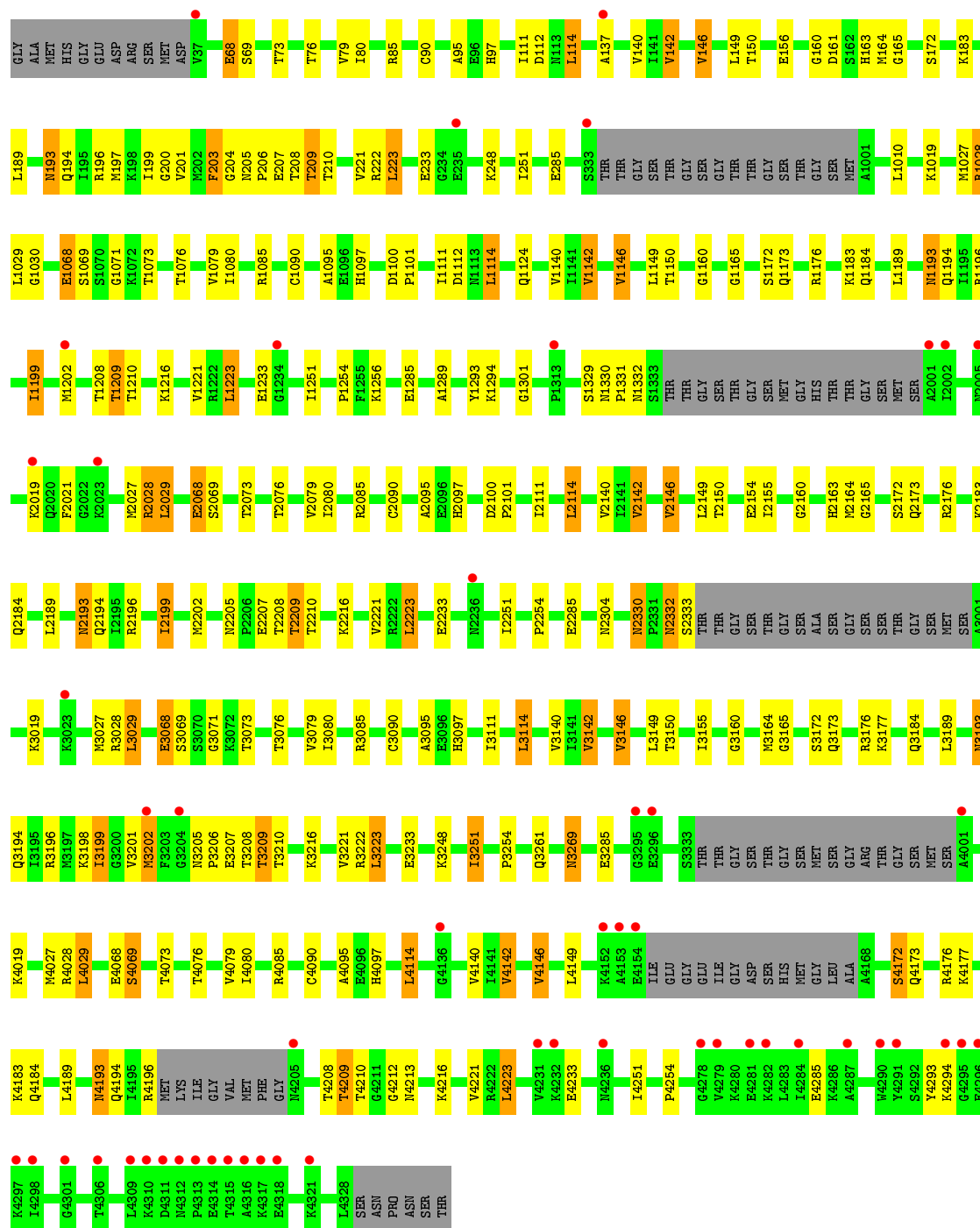
- Molecule 3: Protein recA

Chain A: 



• Molecule 3: 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	159.00 Å 300.50 Å 80.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 39.75 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (40.00-3.40) 94.7 (39.75-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.40 Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.238 , 0.256 0.279 , 0.292	Depositor DCC
R_{free} test set	1623 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	83.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 4.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	25459	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: ALF, MG, ADP

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	1.18	0/285	1.85	10/438 (2.3%)
1	E	1.19	1/285 (0.4%)	1.87	13/438 (3.0%)
2	C	0.68	0/240	1.33	1/369 (0.3%)
2	F	0.72	0/264	1.49	3/406 (0.7%)
3	A	0.43	0/12222	0.56	0/16447
3	D	0.43	0/12222	0.57	0/16447
All	All	0.47	1/25518 (0.0%)	0.66	27/34545 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1006	DT	O3'-P	-5.02	1.55	1.61

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1012	DT	C4-C5-C7	8.48	124.09	119.00
1	E	1009	DT	C4-C5-C7	8.41	124.05	119.00
1	B	1006	DT	C4-C5-C7	8.17	123.90	119.00
1	B	1009	DT	C4-C5-C7	8.03	123.82	119.00
2	F	2014	DA	C1'-O4'-C4'	-7.97	102.13	110.10

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	260	0	157	7	0
1	E	260	0	157	13	0
2	C	211	0	111	1	0
2	F	232	0	122	0	0
3	A	12083	0	12406	158	1
3	D	12083	0	12406	162	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	25	0	0	1	0
5	D	25	0	0	0	0
6	A	135	0	60	7	0
6	D	135	0	60	7	0
All	All	25459	0	25479	313	1

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 6.

The worst 5 of 313 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:76:THR:HG21	3:D:142:VAL:HG21	1.46	0.95
3:A:4076:THR:HG21	3:A:4142:VAL:HG21	1.48	0.95
3:D:68:GLU:HG2	3:D:1216:LYS:HB3	1.47	0.95
3:D:2076:THR:HG21	3:D:2142:VAL:HG21	1.49	0.94
3:A:2076:THR:HG21	3:A:2142:VAL:HG21	1.51	0.93

All (1) 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)
3:A:4087:GLY:O	3:A:4314:GLU:OE2[2_555]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	
3	A	1589/1706 (93%)	1494 (94%)	87 (6%)	8 (0%)	29	61
3	D	1589/1706 (93%)	1501 (94%)	81 (5%)	7 (0%)	34	67
All	All	3178/3412 (93%)	2995 (94%)	168 (5%)	15 (0%)	29	61

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1332	ASN
3	A	4269	ASN
3	D	164	MET
3	D	1332	ASN
3	D	2332	ASN

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	
3	A	1263/1339 (94%)	1133 (90%)	130 (10%)	7	26
3	D	1263/1339 (94%)	1133 (90%)	130 (10%)	7	26
All	All	2526/2678 (94%)	2266 (90%)	260 (10%)	7	26

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	4146	VAL

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Mol	Chain	Res	Type
3	D	197	MET
3	D	4069	SER
3	A	4189	LEU
3	D	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	4173	GLN
3	D	181	ASN
3	D	4173	GLN
3	A	4181	ASN
3	A	4300	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 carbohydrates 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	ALF	A	4501	-	0,4,4	0.00	-	-		
6	ADP	D	3502	4	24,29,29	1.14	2 (8%)	29,45,45	1.41	5 (17%)
6	ADP	D	2502	4	24,29,29	1.14	2 (8%)	29,45,45	1.39	5 (17%)
5	ALF	D	4501	-	0,4,4	0.00	-	-		
6	ADP	A	1502	4	24,29,29	0.96	1 (4%)	29,45,45	1.42	5 (17%)
6	ADP	D	4502	4	24,29,29	1.15	3 (12%)	29,45,45	1.28	3 (10%)
5	ALF	A	1501	-	0,4,4	0.00	-	-		
5	ALF	A	501	-	0,4,4	0.00	-	-		
5	ALF	A	3501	-	0,4,4	0.00	-	-		
5	ALF	D	2501	-	0,4,4	0.00	-	-		
5	ALF	D	1501	-	0,4,4	0.00	-	-		
6	ADP	A	4502	-	24,29,29	0.99	1 (4%)	29,45,45	1.37	4 (13%)
6	ADP	A	2502	4	24,29,29	1.02	1 (4%)	29,45,45	1.39	5 (17%)
6	ADP	A	502	4	24,29,29	1.16	3 (12%)	29,45,45	1.49	3 (10%)
6	ADP	D	1502	4	24,29,29	1.04	2 (8%)	29,45,45	1.28	4 (13%)
5	ALF	D	501	-	0,4,4	0.00	-	-		
6	ADP	D	502	4	24,29,29	1.09	2 (8%)	29,45,45	1.31	5 (17%)
6	ADP	A	3502	4	24,29,29	1.01	1 (4%)	29,45,45	1.33	4 (13%)
5	ALF	D	3501	-	0,4,4	0.00	-	-		
5	ALF	A	2501	-	0,4,4	0.00	-	-		

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	ADP	D	3502	4	-	2/12/32/32	0/3/3/3
6	ADP	D	2502	4	-	3/12/32/32	0/3/3/3
6	ADP	D	4502	4	-	5/12/32/32	0/3/3/3
6	ADP	A	2502	4	-	1/12/32/32	0/3/3/3
6	ADP	A	4502	-	-	5/12/32/32	0/3/3/3
6	ADP	D	1502	4	-	2/12/32/32	0/3/3/3
6	ADP	A	502	4	-	3/12/32/32	0/3/3/3
6	ADP	D	502	4	-	1/12/32/32	0/3/3/3
6	ADP	A	3502	4	-	3/12/32/32	0/3/3/3
6	ADP	A	1502	4	-	1/12/32/32	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3502	ADP	C5-C4	3.04	1.49	1.40
6	D	2502	ADP	C5-C4	3.03	1.48	1.40
6	D	4502	ADP	C5-C4	2.92	1.48	1.40
6	D	502	ADP	C5-C4	2.91	1.48	1.40
6	A	502	ADP	C5-C4	2.79	1.48	1.40

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	502	ADP	N3-C2-N1	-4.32	121.93	128.68
6	A	502	ADP	PA-O3A-PB	-3.58	120.53	132.83
6	A	2502	ADP	N3-C2-N1	-3.51	123.19	128.68
6	A	4502	ADP	N3-C2-N1	-3.45	123.29	128.68
6	A	1502	ADP	N3-C2-N1	-3.39	123.38	128.68

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	502	ADP	PA-O3A-PB-O2B
6	D	4502	ADP	O4'-C4'-C5'-O5'
6	D	4502	ADP	PA-O3A-PB-O1B
6	A	4502	ADP	PA-O3A-PB-O2B
6	A	1502	ADP	PA-O3A-PB-O2B

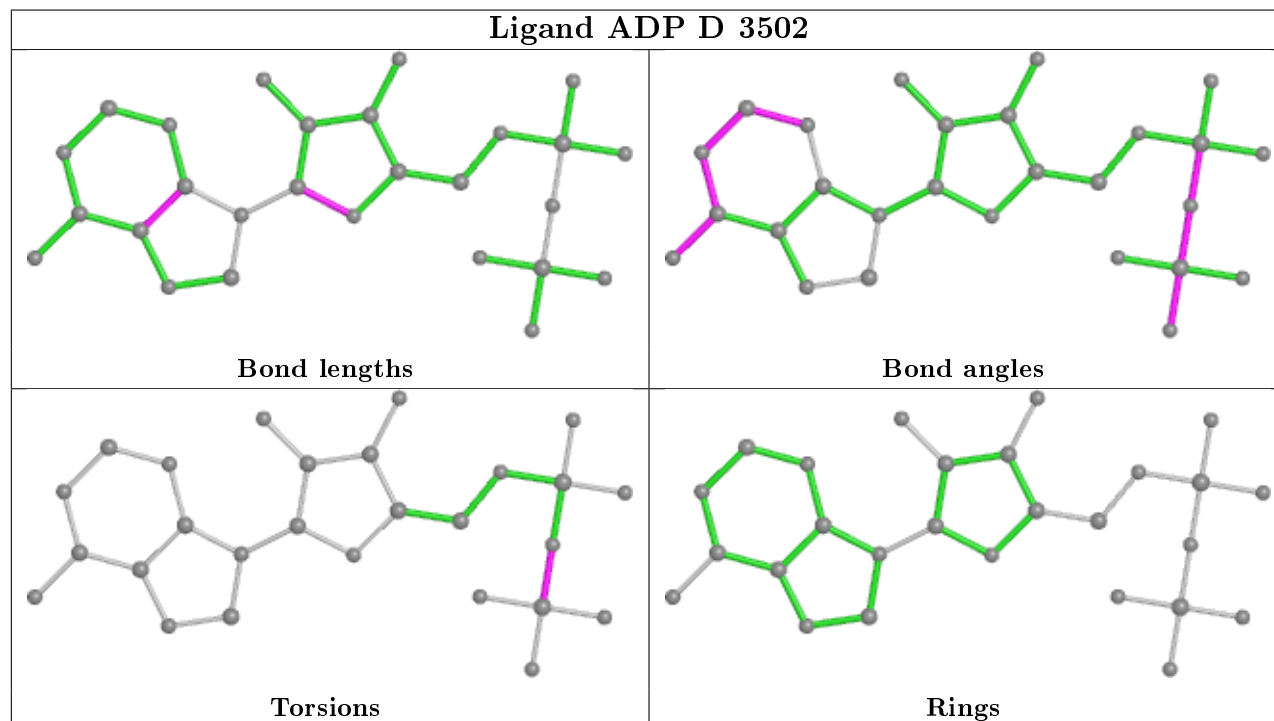
There are no ring outliers.

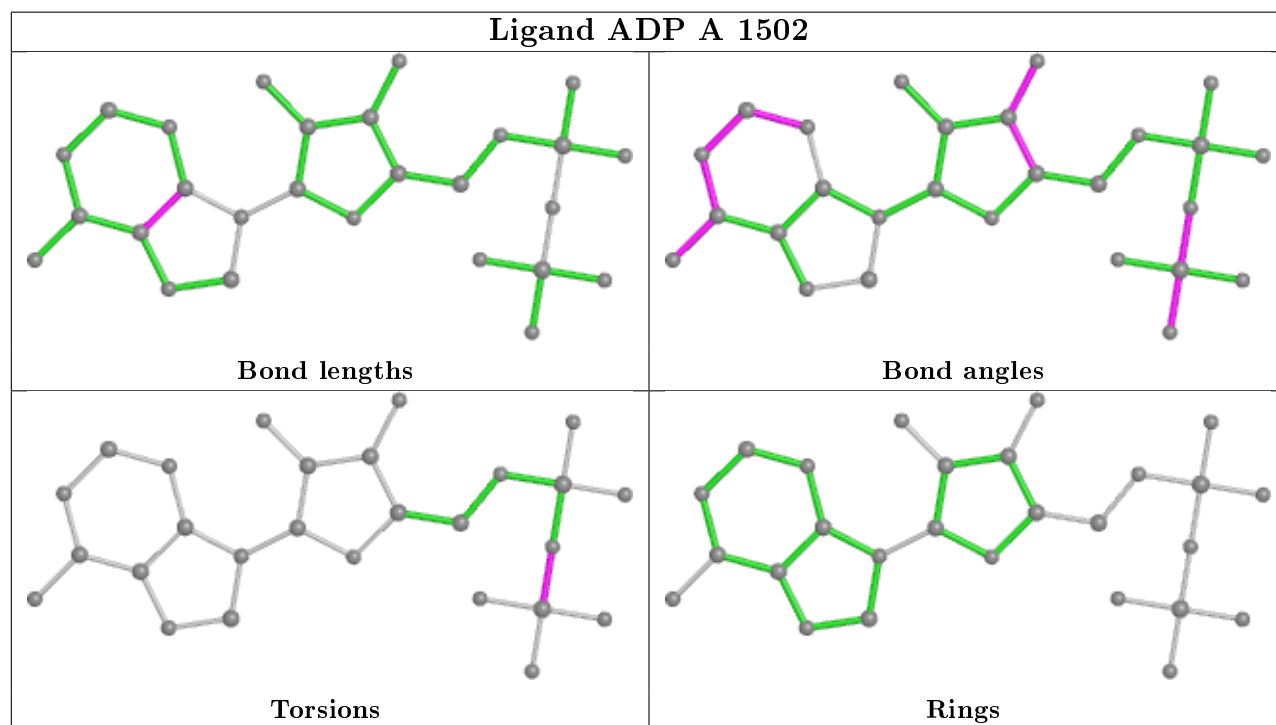
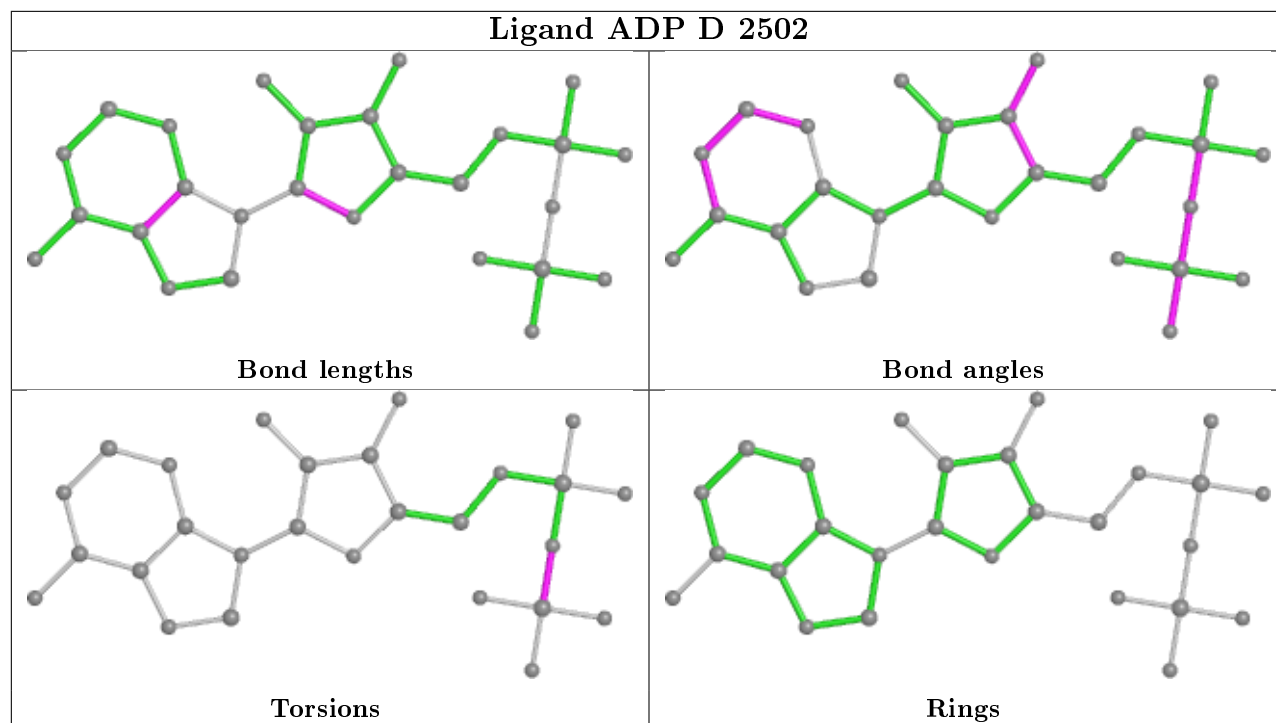
10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4501	ALF	1	0
6	D	3502	ADP	2	0
6	D	2502	ADP	1	0
6	A	1502	ADP	2	0
6	D	4502	ADP	1	0
6	A	4502	ADP	1	0
6	A	2502	ADP	2	0
6	A	502	ADP	2	0
6	D	1502	ADP	2	0
6	D	502	ADP	1	0

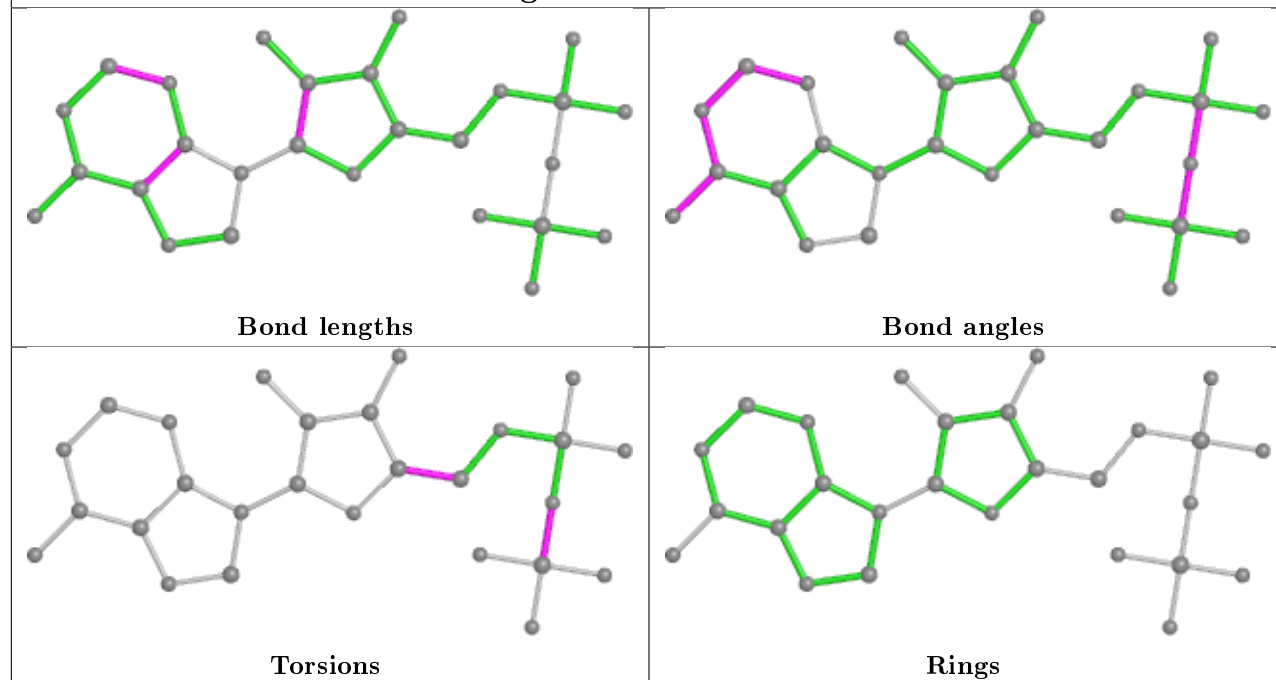
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

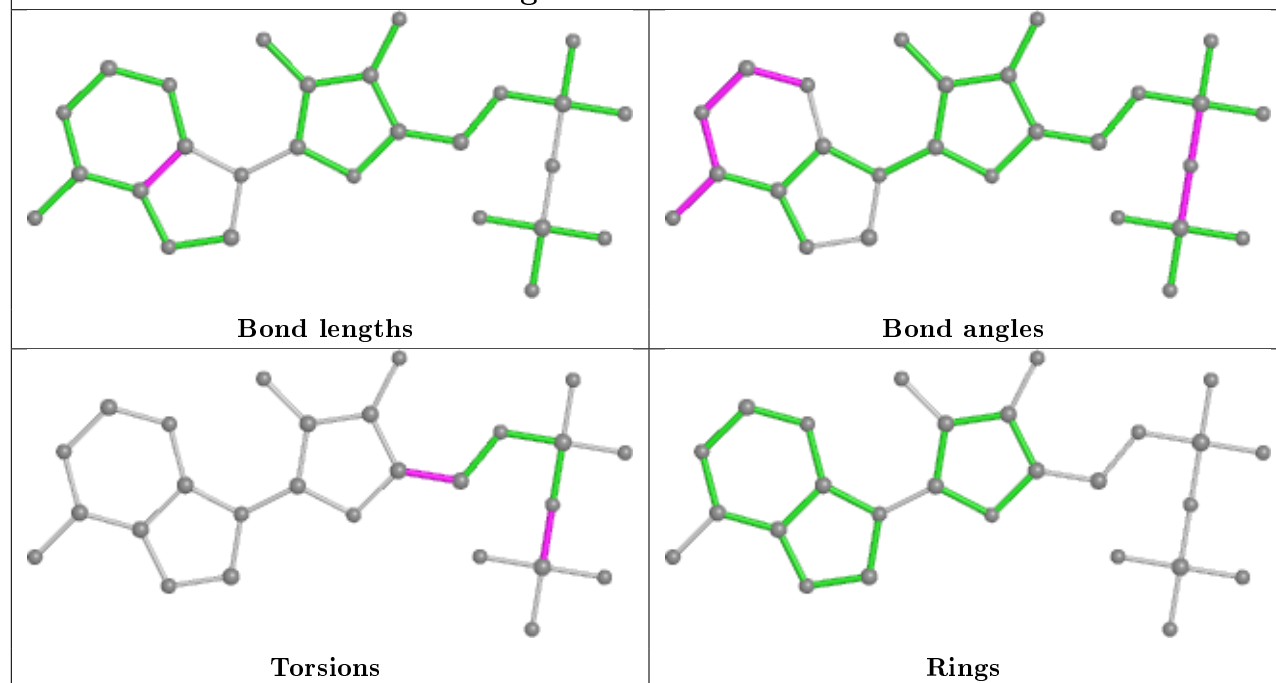




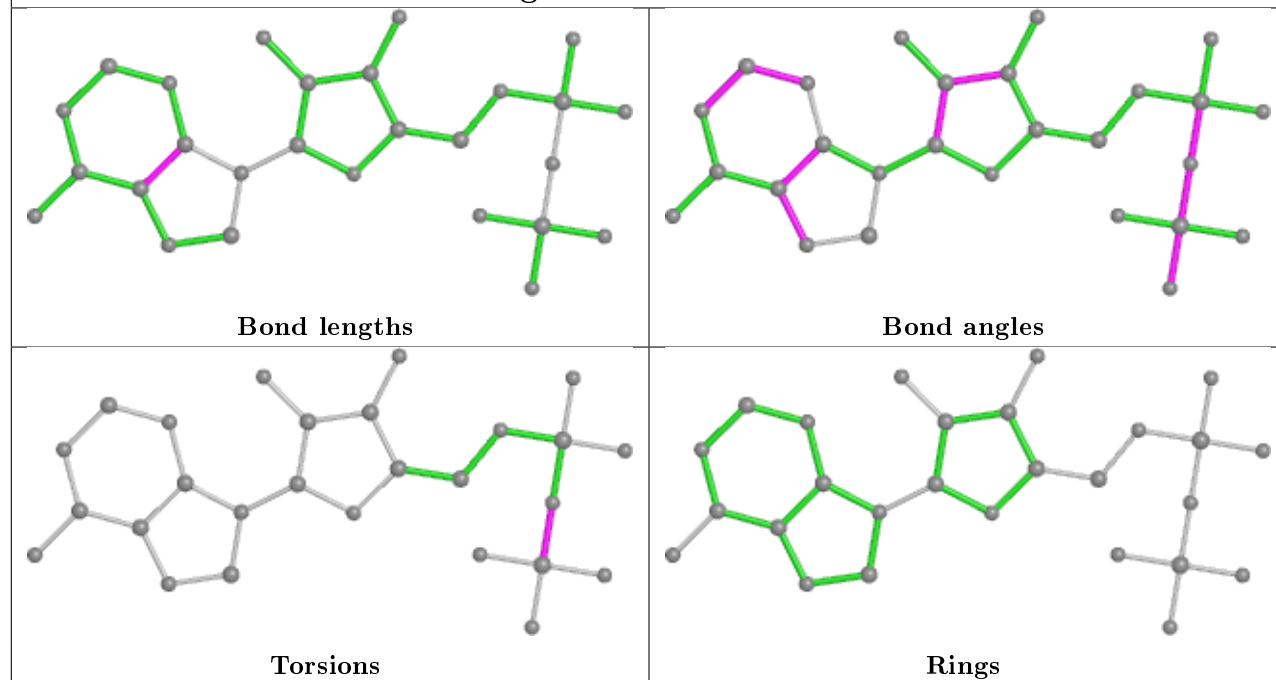
Ligand ADP D 4502



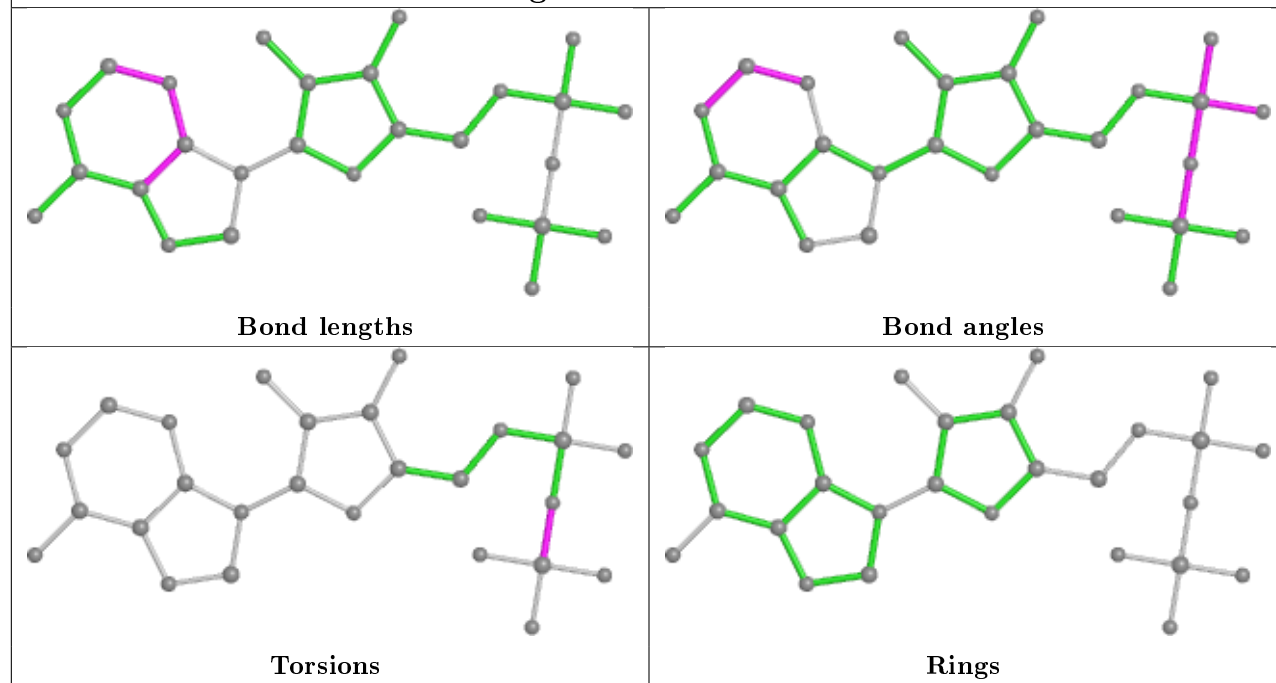
Ligand ADP A 4502



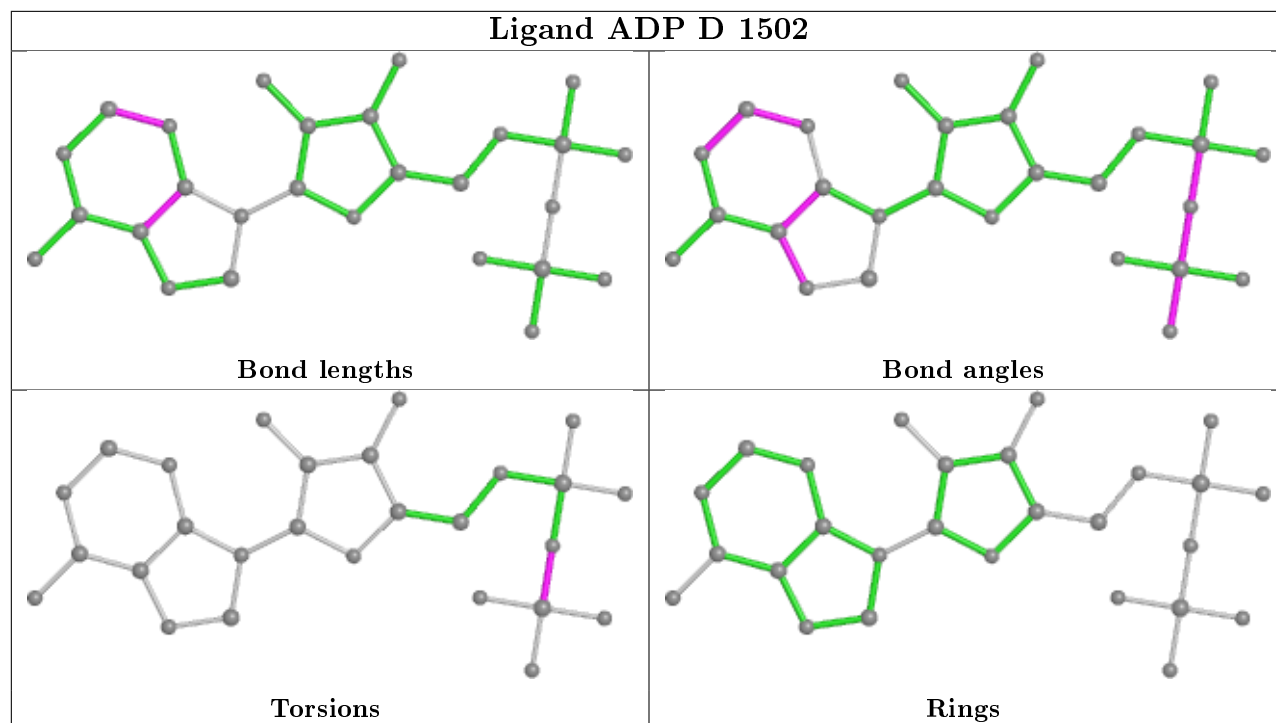
Ligand ADP A 2502



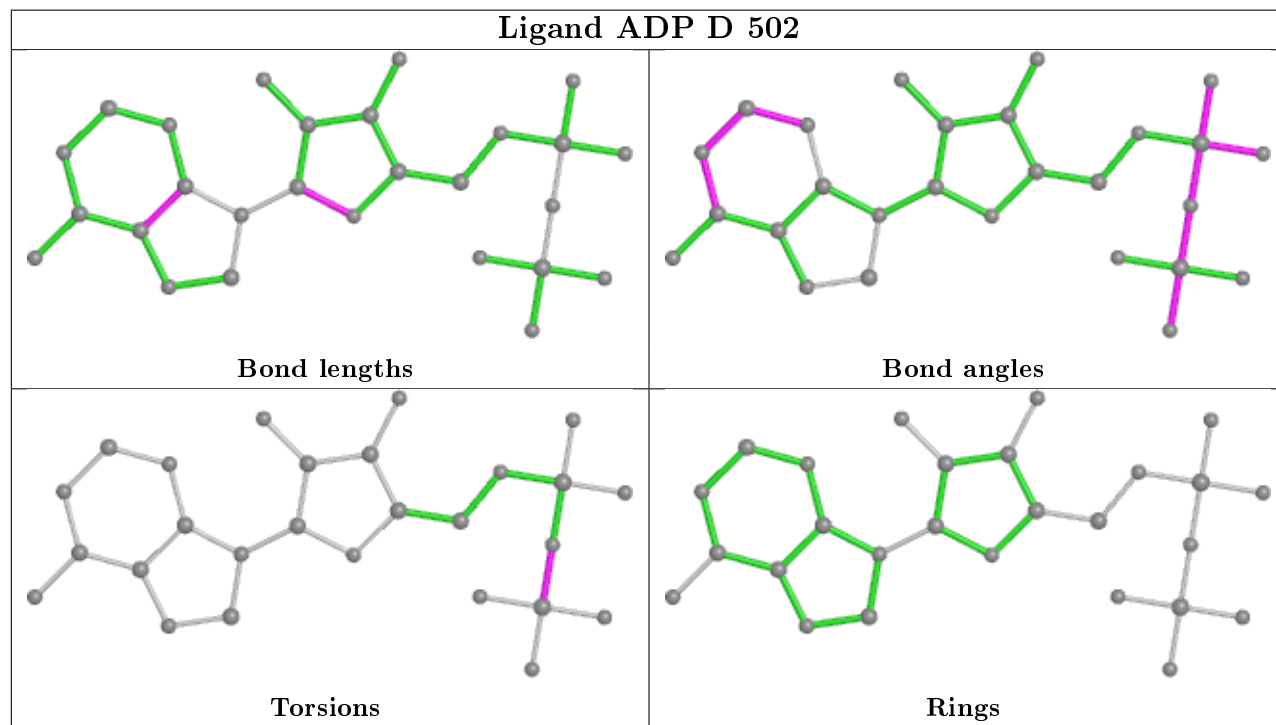
Ligand ADP A 502

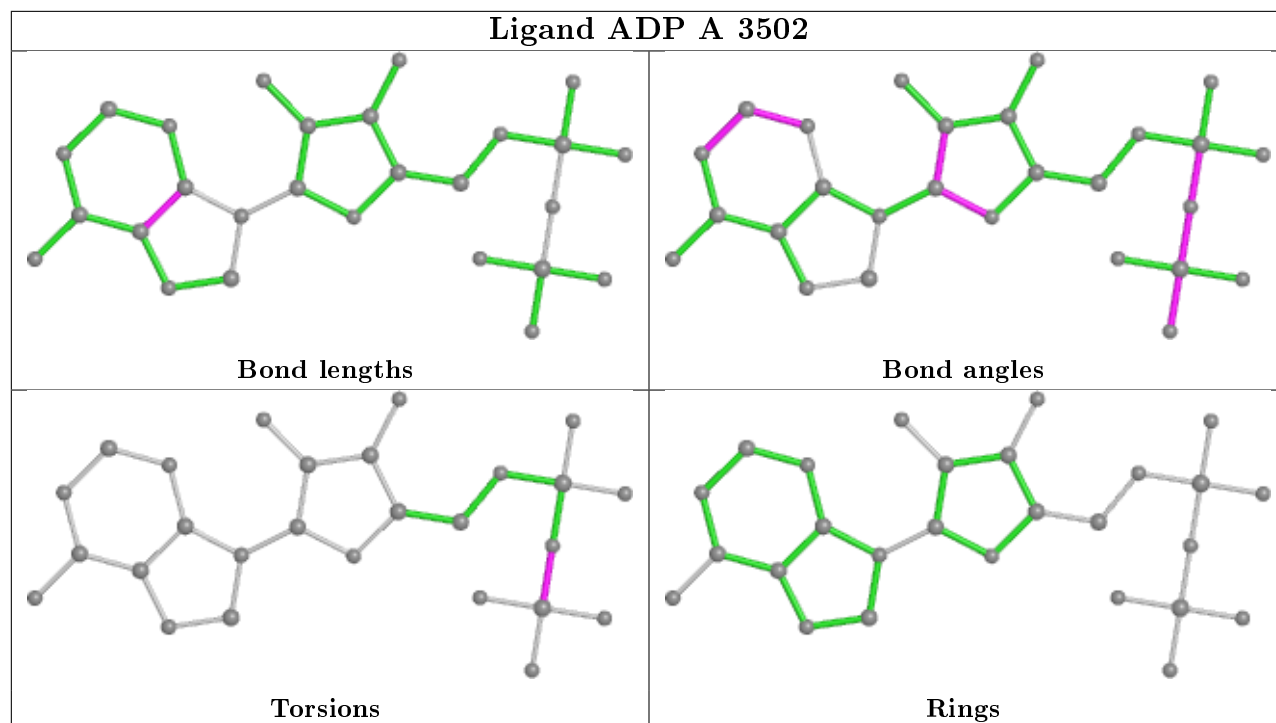


Ligand ADP D 1502



Ligand ADP D 502





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, 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(Å²)	Q<0.9
1	B	13/15 (86%)	0.37	0	100100	14, 20, 22, 24	0
1	E	13/15 (86%)	0.14	0	100100	11, 19, 23, 28	0
2	C	11/12 (91%)	2.44	5 (45%)	00	46, 49, 51, 56	0
2	F	12/12 (100%)	3.35	11 (91%)	00	47, 49, 51, 51	0
3	A	1603/1706 (93%)	0.30	76 (4%)	3131	19, 30, 45, 76	0
3	D	1603/1706 (93%)	0.21	53 (3%)	4645	18, 30, 45, 75	0
All	All	3255/3466 (93%)	0.28	145 (4%)	3333	11, 30, 48, 76	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	4316	ALA	6.1
2	F	2012	DA	6.0
3	D	4291	TYR	6.0
3	A	3001	ALA	5.6
2	F	2004	DA	5.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

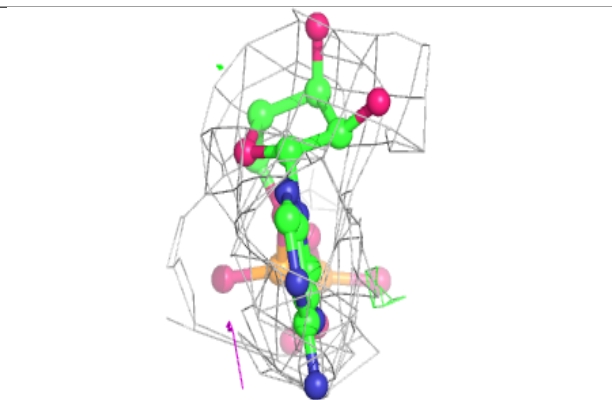
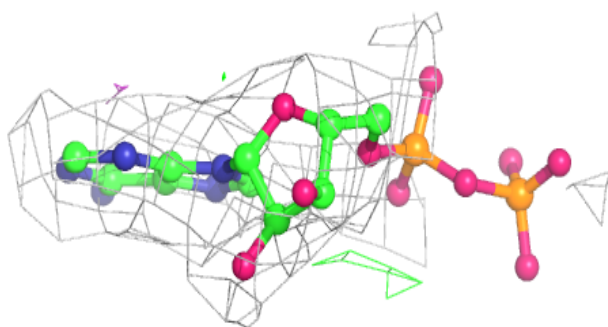
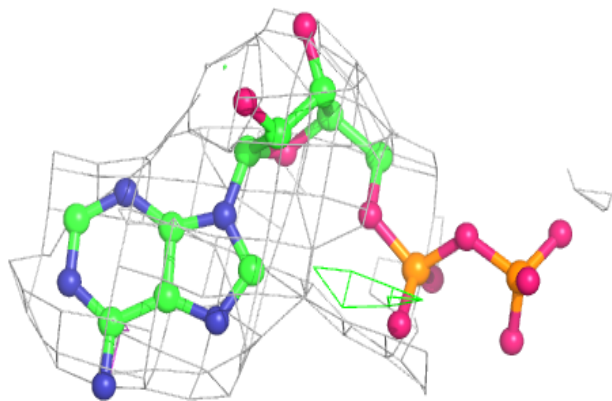
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ALF	D	4501	5/5	0.81	0.20	26,30,32,32	0
4	MG	D	4500	1/1	0.88	0.22	17,17,17,17	0
4	MG	A	4500	1/1	0.89	0.12	2,2,2,2	0
6	ADP	A	502	27/27	0.92	0.26	18,21,27,29	0
5	ALF	A	4501	5/5	0.92	0.15	36,38,40,40	0
6	ADP	A	4502	27/27	0.93	0.13	11,19,23,23	0
4	MG	D	1500	1/1	0.94	0.36	2,2,2,2	0
4	MG	A	1500	1/1	0.94	0.33	3,3,3,3	0
5	ALF	A	2501	5/5	0.95	0.27	2,2,2,2	0
6	ADP	D	4502	27/27	0.95	0.13	17,19,21,24	0
6	ADP	D	3502	27/27	0.95	0.18	2,4,9,9	0
6	ADP	A	2502	27/27	0.95	0.21	2,2,2,5	0
6	ADP	A	1502	27/27	0.96	0.23	2,2,3,5	0
6	ADP	D	2502	27/27	0.96	0.19	2,5,6,7	0
4	MG	A	500	1/1	0.96	0.56	24,24,24,24	0
6	ADP	A	3502	27/27	0.96	0.18	2,2,2,2	0
4	MG	A	2500	1/1	0.96	0.36	2,2,2,2	0
5	ALF	D	3501	5/5	0.96	0.21	2,2,3,6	0
4	MG	D	2500	1/1	0.97	0.35	2,2,2,2	0
6	ADP	D	1502	27/27	0.97	0.20	2,2,3,5	0
6	ADP	D	502	27/27	0.97	0.20	2,2,4,5	0
5	ALF	A	3501	5/5	0.97	0.26	2,2,2,2	0
5	ALF	D	1501	5/5	0.97	0.27	2,2,2,2	0
5	ALF	A	501	5/5	0.97	0.34	17,21,22,23	0
4	MG	D	3500	1/1	0.98	0.28	6,6,6,6	0
5	ALF	D	2501	5/5	0.98	0.33	2,2,2,2	0
4	MG	A	3500	1/1	0.98	0.37	2,2,2,2	0
5	ALF	A	1501	5/5	0.98	0.29	2,2,4,5	0
5	ALF	D	501	5/5	0.98	0.29	2,2,2,2	0
4	MG	D	500	1/1	0.99	0.23	5,5,5,5	0

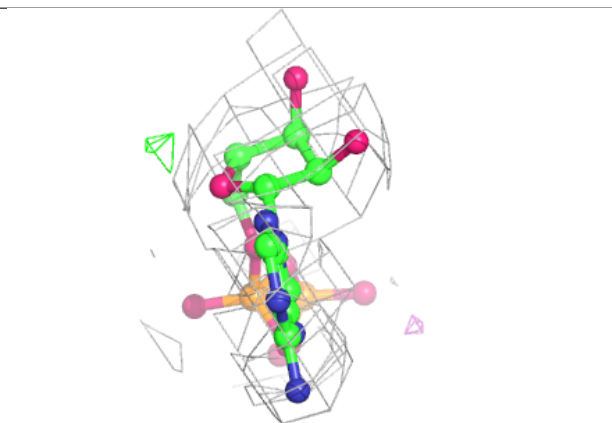
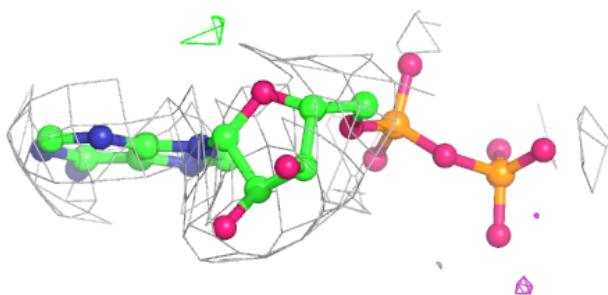
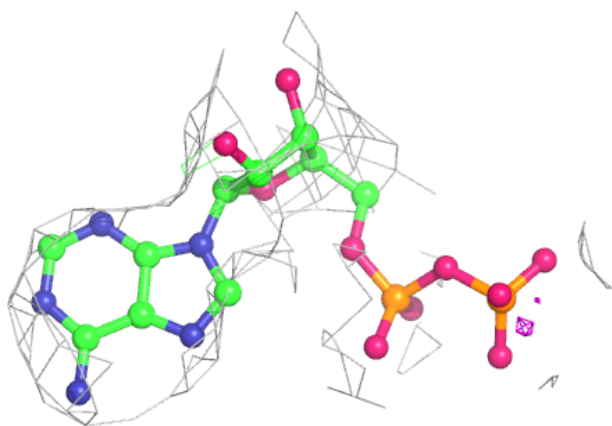
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 502:

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

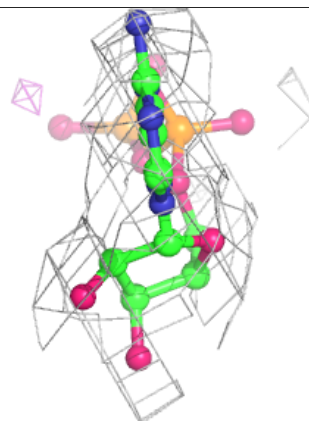
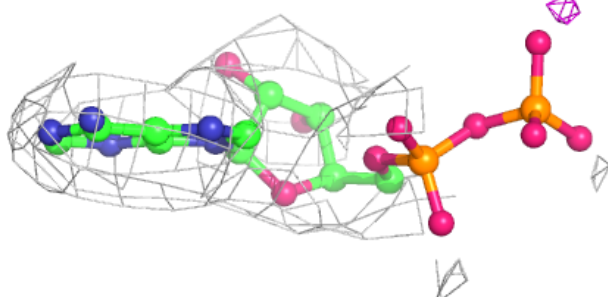
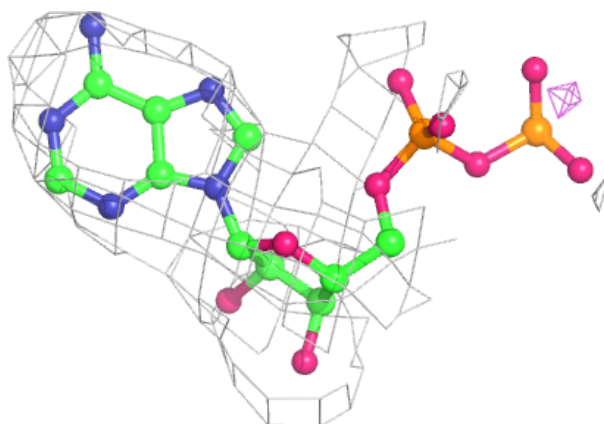
**Electron density around ADP A 4502:**

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

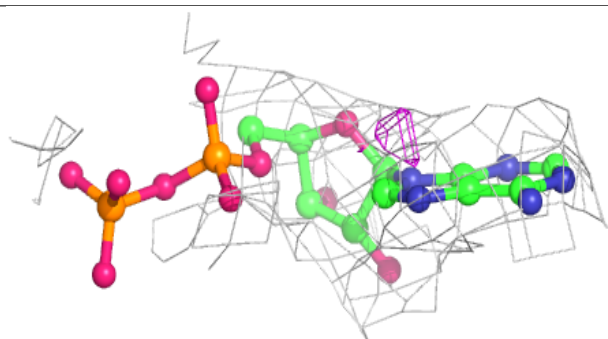
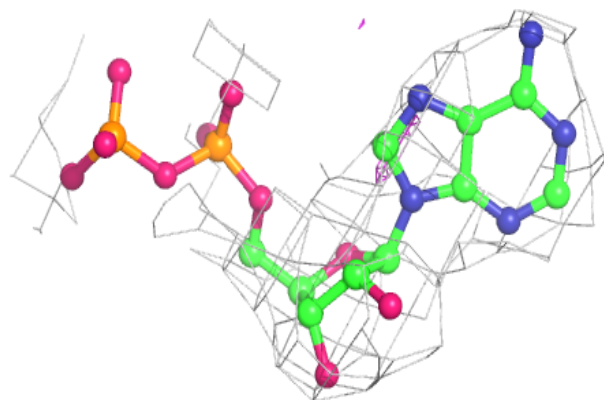


Electron density around ADP D 4502:

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

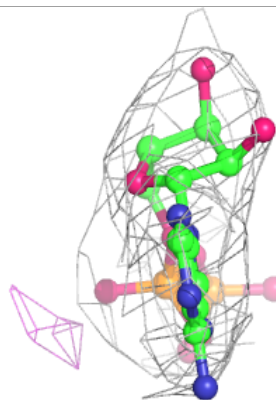
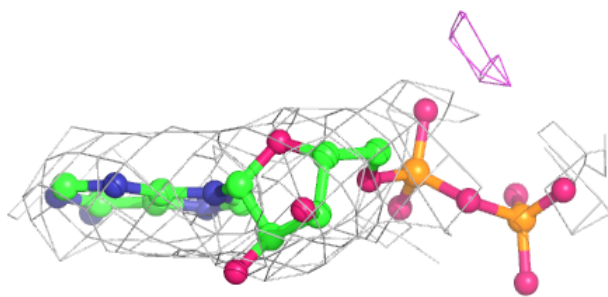
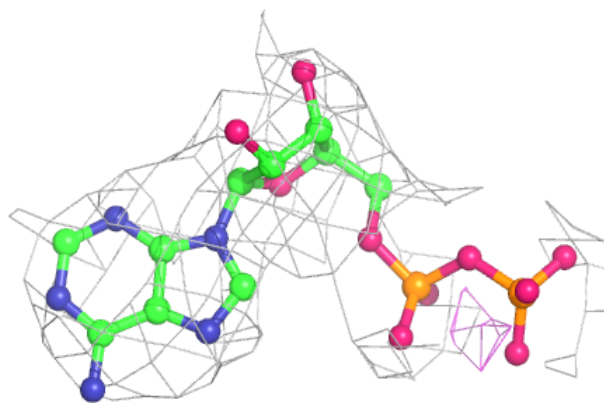
**Electron density around ADP D 3502:**

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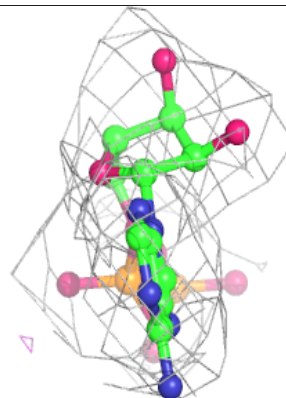
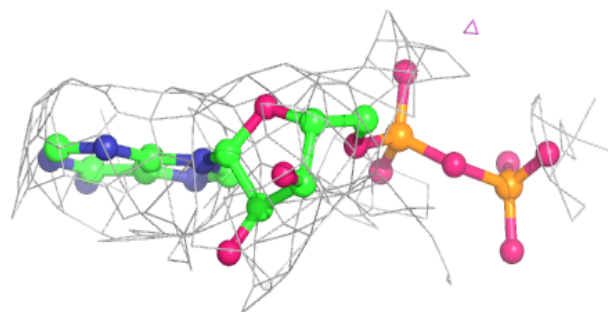
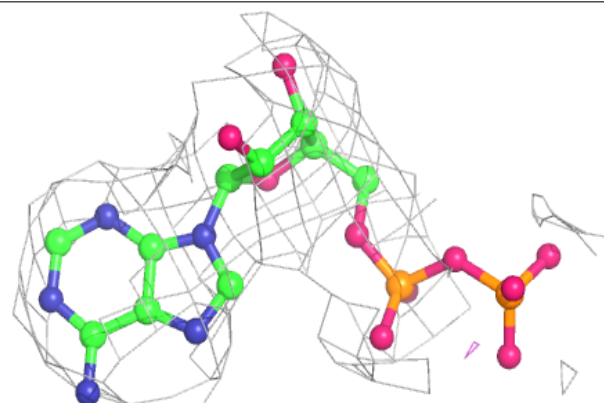


Electron density around ADP A 2502:

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and green (positive)

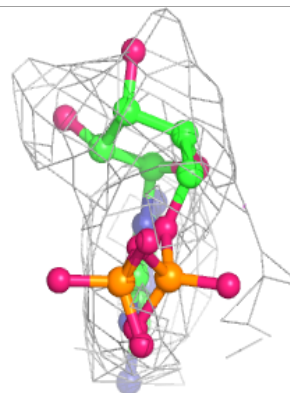
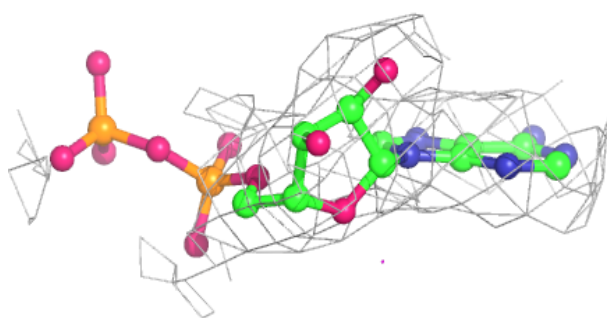
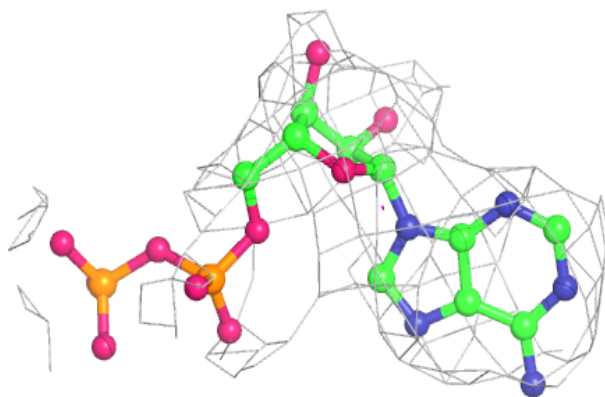
**Electron density around ADP A 1502:**

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

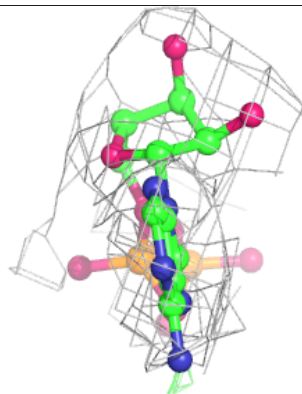
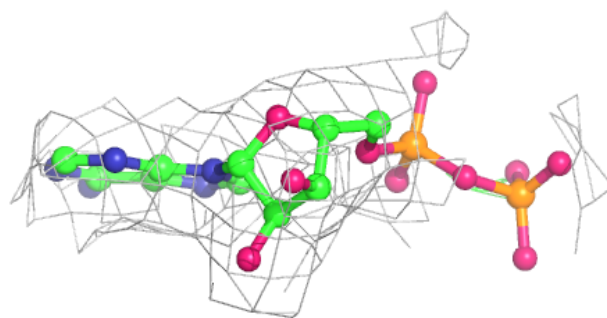
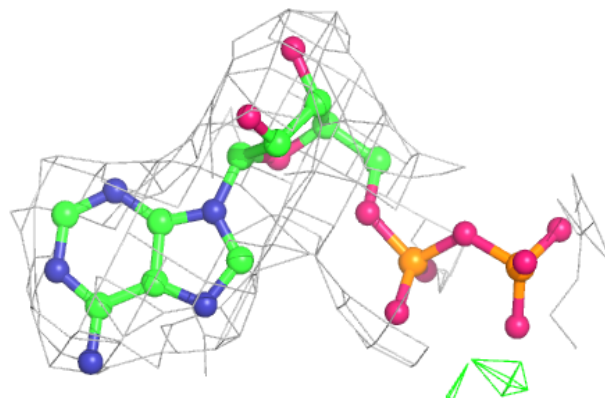


Electron density around ADP D 2502:

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

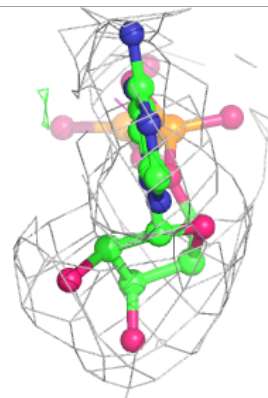
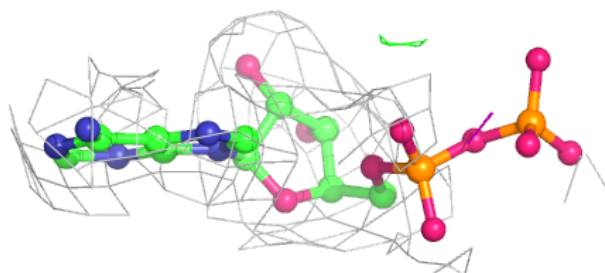
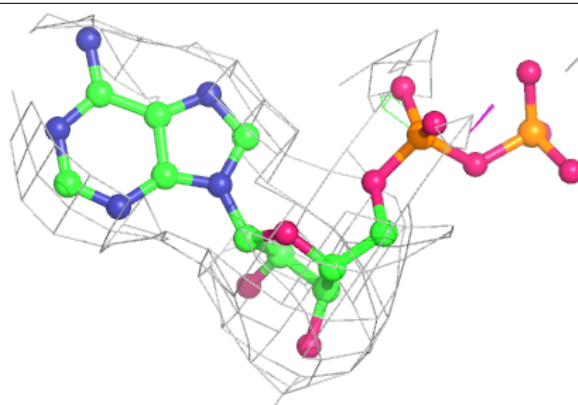
**Electron density around ADP A 3502:**

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

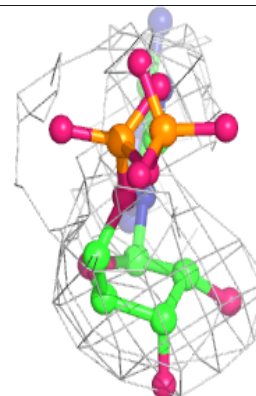
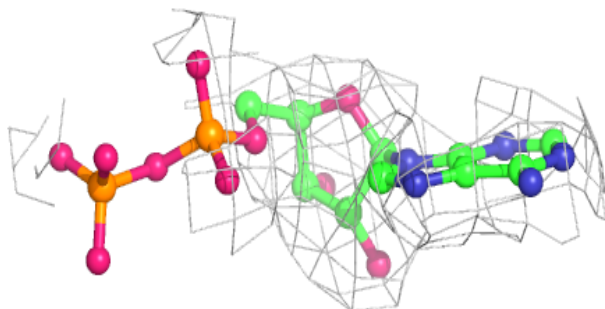
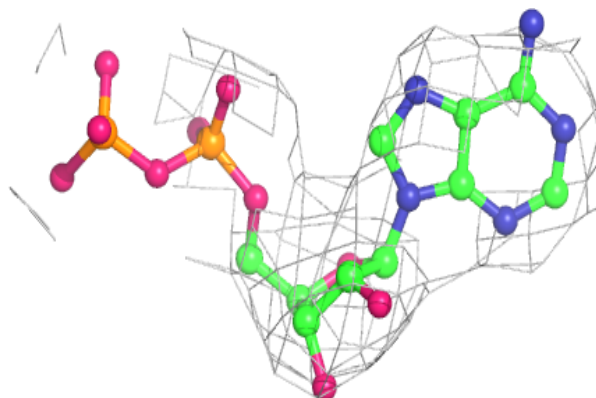


Electron density around ADP D 1502:

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

**Electron density around ADP D 502:**

$2mF_o-DF_c$ (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.