



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 11:37 PM UTC

PDB ID : 3CMX / pdb_00003cmx
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 types of validation reports are described at

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

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

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

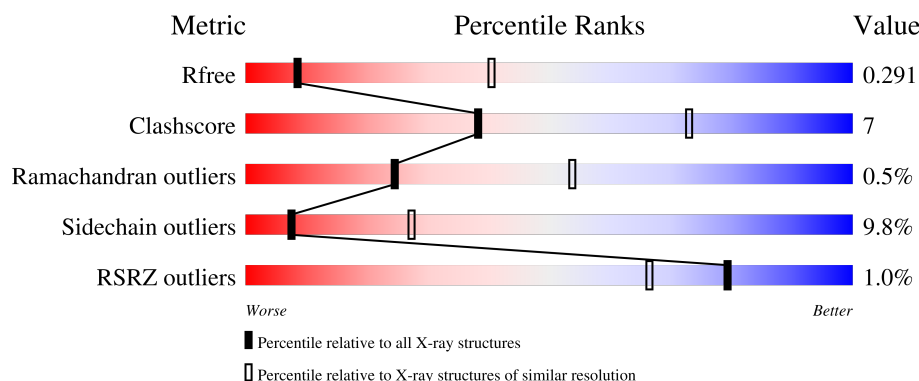
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	E	15	
2	C	12	
2	F	12	
3	A	1706	

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Mol	Chain	Length	Quality of chain
3	D	1706	% 78% 13% • 6%

2 Entry composition [i](#)

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*TP*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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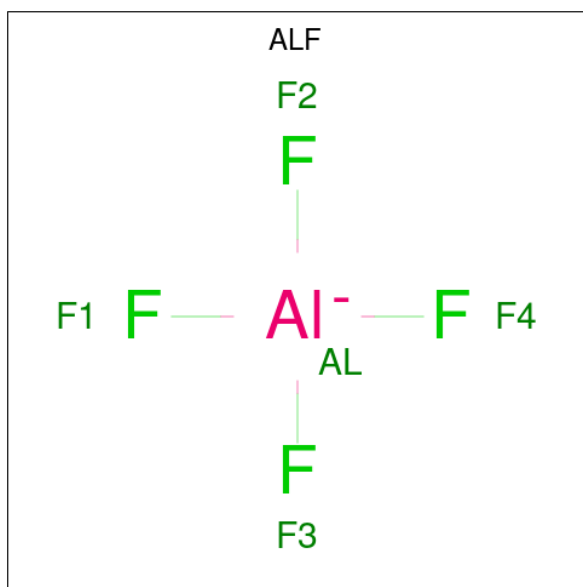
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1992	MET	-	linker	UNP P0A7G6
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6
D	1998	SER	-	linker	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 (CCD ID: MG) (formula: Mg).

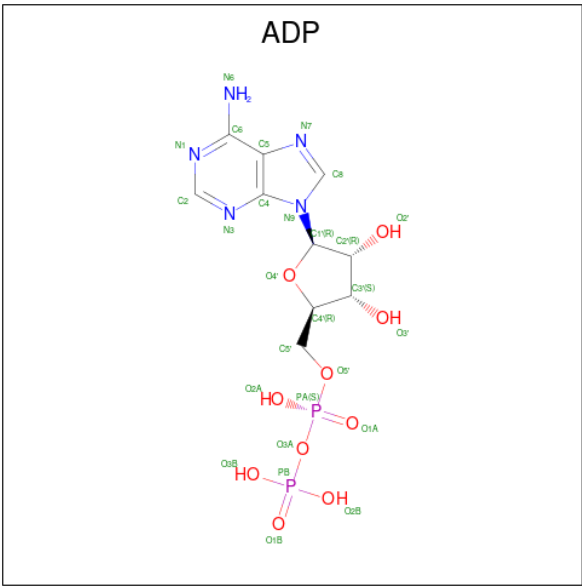
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	D	5	Total	Mg	0	0
			5	5		

- Molecule 5 is TETRAFLUOROALUMINATE ION (CCD ID: 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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

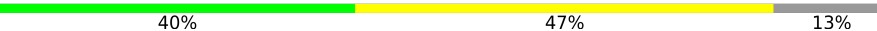


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	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](#)

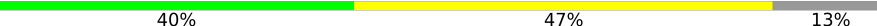
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

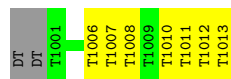
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

Chain B: 



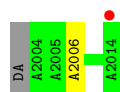
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

Chain E: 



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

Chain C: 



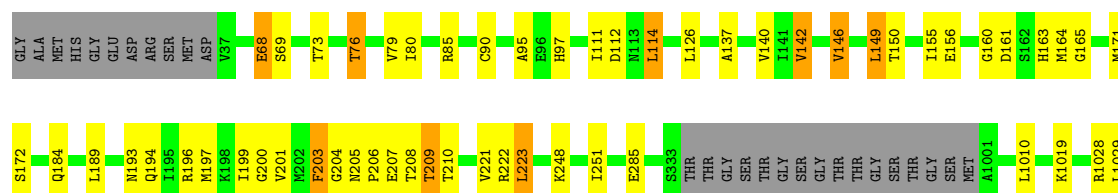
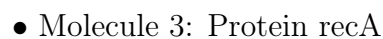
- Molecule 2: DNA (5'-D(*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*A)-3')

Chain F: 



- Molecule 3: Protein recA

Chain A: 



ASN	Q4194	M4035	I3195	M3085	M2197	R2028	R1196	G1030
PRO	I4196	E4068	R3196	M3085	K2196	L2028	M1197	R1196
ASN	R4196	S4069	M3197	E3088	G2199	E2068	K1198	E1068
SER	MET	S4069	K3198	S3069	G2200	S2069	I1199	S1069
THR	LYS	T4073	I3199	S3070	V2201	T2073	G1201	S1070
	ILE	T4073	G3200	G3071	M2202	T2073	V1201	G1071
	GLY	T4076	V3201	G3072	N2205	T2076	K1072	K1072
	VAL	T4076	M3202	T3073	P2206	T2076	T1107	T1107
	MET	V4079	N3205	T3076	E2207	T2079	T1209	T1076
	PHE	I4080	P3206	T3076	T2208	V2079	T1210	T1076
	GLY	R4085	E3207	V3079	T2209	I2080	V1079	V1079
	N4205	R4085	T3208	I3080	T2210	I2080	I1080	I1080
	T4208	C4090	T3209	R3085	N2213	R2085	V1221	R1085
	T4209	A4095	T3210	R3085	K2216	C2090	R1222	C1090
	T4210	A4095	N3213	C3090	V2221	A2095	L1223	C1090
	G4211	A4096	K3216	A3095	K2222	E2096	I1251	A1095
	G4212	H4097	V3221	E3096	K2222	H2097	P1254	E1096
	N4213	L4114	R3222	H3097	L2223	D2100	F1255	H1097
	K4216	G4136	L3223	I3111	H2236	P2101	K1256	D1100
	V4221	V4140	K3248	L3114	I2251	I2111	E1285	P1101
	R4222	I4141	I3251	L3115	P2254	L2114	A1289	T1111
	L4223	V4142	P3254	C3116	E2285	V2140	N1113	D1112
	T4251	V4146	Q3261	L3126	N2304	I2141	L1114	L1114
	P4254	L4149	N3269	V3140	K2330	V2142	Q1124	Q1124
	F4270	E4154	E3285	I3141	P2331	V2146	A1125	A1125
	G4278	ILE	N3285	V3142	N2332	L2149	L1126	L1126
	V4279	GLU	E3285	V3146	S2333	T2150	V1140	V1140
	I4284	GLU	N3332	V3146	THR	E2154	I1141	I1141
	E4285	ILE	S3333	L3149	THR	I2155	V1142	V1142
	Y4291	GLY	THR	T3150	GLY	G2160	V1146	V1146
	S4292	ASP	THR	I3155	SER	C2160	L1149	L1149
	Y4293	SER	GLY	I3155	THR	G2160	T1150	T1150
	K4294	HIS	SER	G3160	THR	H2163	G1160	G1160
	K4294	MET	THR	M3164	ALA	N2164	G1165	G1165
	G4301	GLY	GLY	G3165	SER	G2165	M1171	M1171
	T4306	LEU	SER	M3164	GLY	M2171	S1172	S1172
	L4309	ALA	GLY	G3165	SER	S2172	Q1173	Q1173
	K4310	M4171	ARG	M3171	SER	Q2173	GLY	GLY
	D4311	S4172	THR	S3172	THR	R2176	SER	SER
	N4312	Q4173	GLY	Q3173	GLY	Q2184	MET	MET
	N4312	R4176	THR	R3176	SER	Q2184	A2001	A2001
	P4313	K4177	GLY	K3177	SER	L2189	K2019	K2019
	E4314	K4177	MET	Q3184	A3001	N2193	Q2020	Q2020
	T4315	Q4184	SER	L3189	K3019	Q2194	F2021	F2021
	A4316	L4184	ALA	N3193	L3029	I2195	I1195	I1195
	T4319	L4189	K4019	Q3194	D3032	R2196		
	L4328	N4193	L4029					
	SER							

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)	40.00 – 3.40 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (40.00-3.40) 94.6 (40.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.238 , 0.256 0.278 , 0.291	Depositor DCC
R_{free} test set	1623 reflections (3.01%)	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)	0.28 , 0.4	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	0.87	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	0.53	0/285	1.11	0/438
1	E	0.60	0/285	1.19	0/438
2	C	0.28	0/240	0.82	0/369
2	F	0.30	0/264	0.93	1/406 (0.2%)
3	A	0.55	0/12222	0.87	1/16447 (0.0%)
3	D	0.54	0/12222	0.87	2/16447 (0.0%)
All	All	0.54	0/25518	0.88	4/34545 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	155	ILE	N-CA-C	7.74	118.32	110.82
3	A	166	LEU	N-CA-C	-6.15	105.54	113.16
3	D	1332	ASN	N-CA-C	5.39	122.29	110.80
2	F	2014	DA	C1'-O4'-C4'	-5.04	102.13	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	260	0	157	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	179	1
3	D	12083	0	12406	180	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	8	0
6	D	135	0	60	7	0
All	All	25459	0	25479	352	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 7.

The worst 5 of 352 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 [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	
3	A	1589/1706 (93%)	1494 (94%)	87 (6%)	8 (0%)	24	54
3	D	1589/1706 (93%)	1501 (94%)	81 (5%)	7 (0%)	30	59
All	All	3178/3412 (93%)	2995 (94%)	168 (5%)	15 (0%)	24	54

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%)	1135 (90%)	128 (10%)	7	25
3	D	1263/1339 (94%)	1143 (90%)	120 (10%)	8	29
All	All	2526/2678 (94%)	2278 (90%)	248 (10%)	7	27

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	4140	VAL
3	D	3210	THR
3	D	189	LEU
3	D	3208	THR
3	D	4146	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1194	GLN
3	D	3173	GLN
3	D	1300	GLN
3	D	2193	ASN
3	D	3205	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	$\# Z > 2$
6	ADP	A	502	4	28,29,29	1.49	4 (14%)	43,45,45	2.05	11 (25%)
6	ADP	A	2502	4	28,29,29	1.42	4 (14%)	43,45,45	1.79	8 (18%)
5	ALF	D	501	-	4,4,4	1.42	0	-		
5	ALF	A	4501	-	4,4,4	1.49	0	-		
6	ADP	A	1502	4	28,29,29	1.60	5 (17%)	43,45,45	1.78	9 (20%)
5	ALF	A	3501	-	4,4,4	1.31	0	-		
5	ALF	D	1501	-	4,4,4	1.29	0	-		
6	ADP	A	4502	-	28,29,29	1.46	4 (14%)	43,45,45	1.72	10 (23%)
5	ALF	A	2501	-	4,4,4	1.37	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	D	1502	4	28,29,29	1.62	4 (14%)	43,45,45	1.94	10 (23%)
6	ADP	A	3502	4	28,29,29	1.51	6 (21%)	43,45,45	1.71	8 (18%)
5	ALF	D	4501	-	4,4,4	1.55	0	-	-	-
5	ALF	A	1501	-	4,4,4	1.35	0	-	-	-
5	ALF	D	3501	-	4,4,4	1.31	0	-	-	-
6	ADP	D	4502	4	28,29,29	1.56	6 (21%)	43,45,45	1.67	7 (16%)
5	ALF	A	501	-	4,4,4	1.41	0	-	-	-
5	ALF	D	2501	-	4,4,4	1.32	0	-	-	-
6	ADP	D	502	4	28,29,29	1.54	5 (17%)	43,45,45	1.64	11 (25%)
6	ADP	D	3502	4	28,29,29	1.53	4 (14%)	43,45,45	1.74	9 (20%)
6	ADP	D	2502	4	28,29,29	1.63	5 (17%)	43,45,45	1.74	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
6	ADP	A	502	4	-	3/16/32/32	0/3/3/3
6	ADP	A	2502	4	-	1/16/32/32	0/3/3/3
6	ADP	D	4502	4	-	5/16/32/32	0/3/3/3
6	ADP	D	502	4	-	1/16/32/32	0/3/3/3
6	ADP	A	4502	-	-	4/16/32/32	0/3/3/3
6	ADP	D	3502	4	-	2/16/32/32	0/3/3/3
6	ADP	D	1502	4	-	2/16/32/32	0/3/3/3
6	ADP	D	2502	4	-	4/16/32/32	0/3/3/3
6	ADP	A	3502	4	-	4/16/32/32	0/3/3/3
6	ADP	A	1502	4	-	1/16/32/32	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3502	ADP	C5-C4	5.54	1.49	1.39
6	D	2502	ADP	C5-C4	5.53	1.48	1.39
6	D	4502	ADP	C5-C4	5.36	1.48	1.39
6	D	502	ADP	C5-C4	5.35	1.48	1.39
6	A	502	ADP	C5-C4	5.17	1.48	1.39

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1502	ADP	C5-C4-N3	-6.57	117.67	126.72
6	A	2502	ADP	C5-C4-N3	-5.79	118.74	126.72
6	A	502	ADP	C5-C4-N3	-5.65	118.93	126.72
6	A	3502	ADP	C5-C4-N3	-5.58	119.03	126.72
6	A	1502	ADP	C5-C4-N3	-5.28	119.45	126.72

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

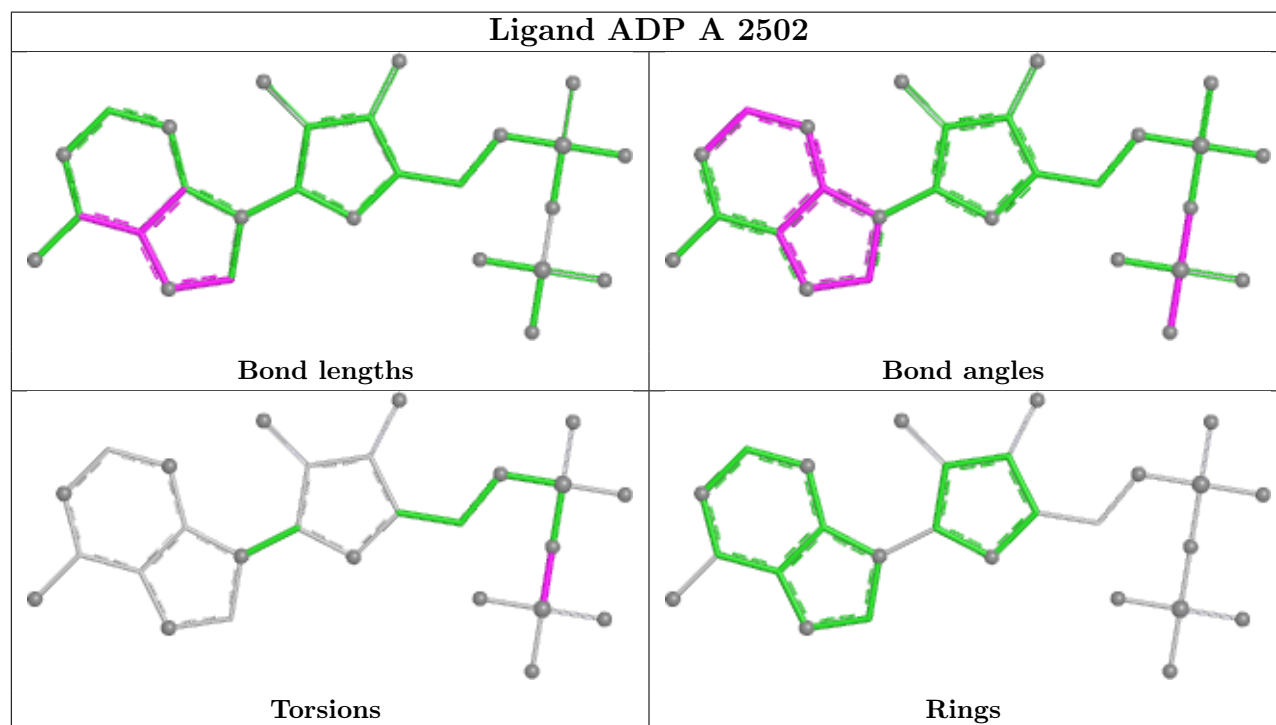
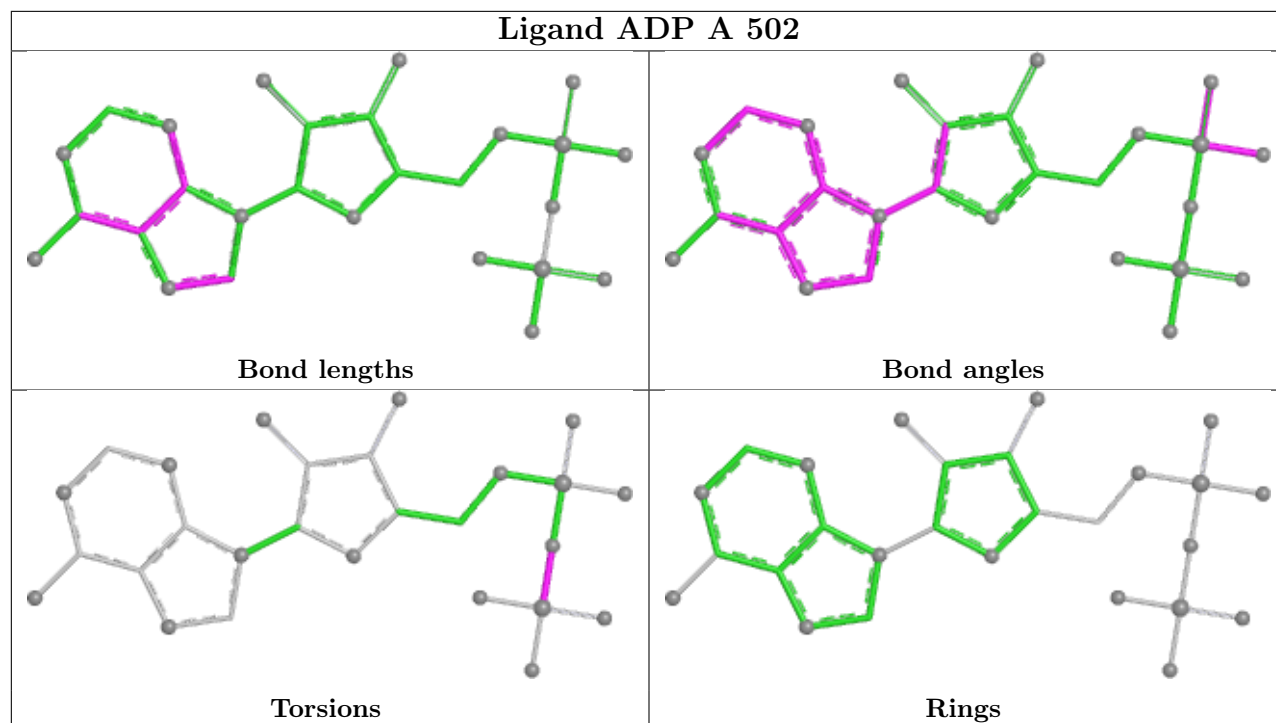
Mol	Chain	Res	Type	Atoms
6	D	502	ADP	PA-O3A-PB-O2B
6	D	4502	ADP	O4'-C4'-C5'-O5'
6	D	4502	ADP	PA-O3A-PB-O1B
6	A	1502	ADP	PA-O3A-PB-O2B
6	A	2502	ADP	PA-O3A-PB-O2B

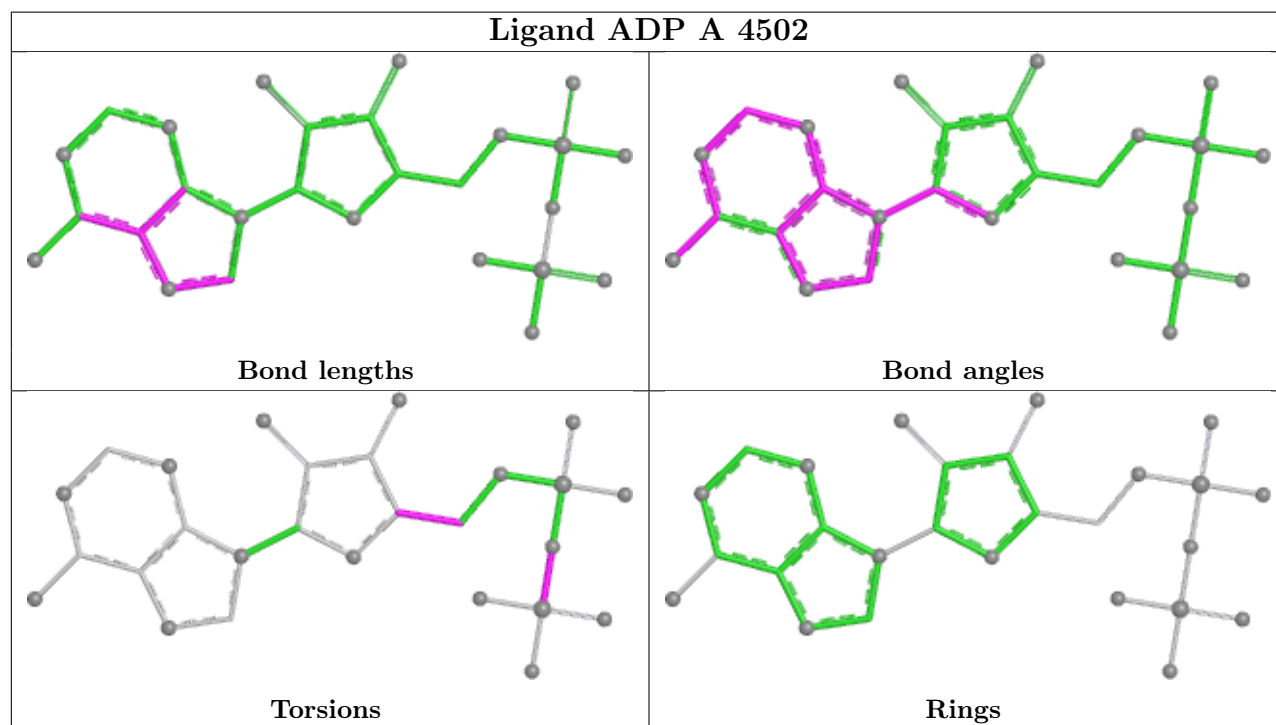
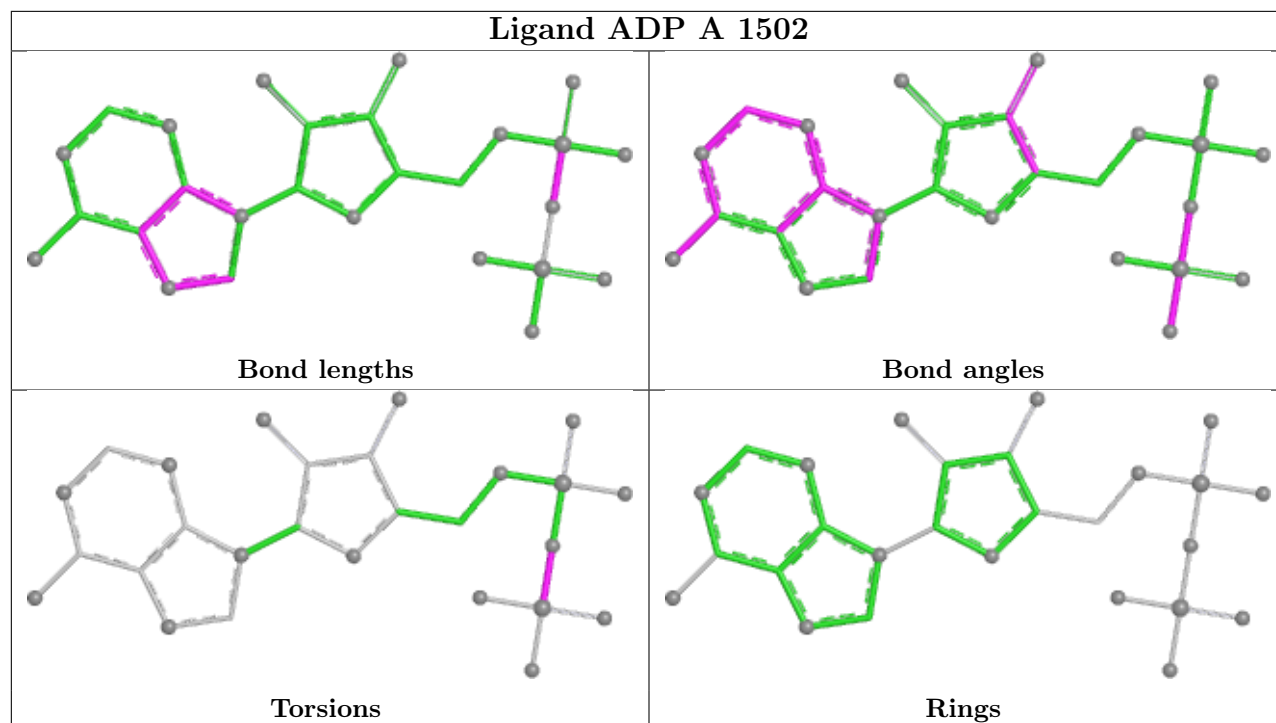
There are no ring outliers.

10 monomers are involved in 15 short contacts:

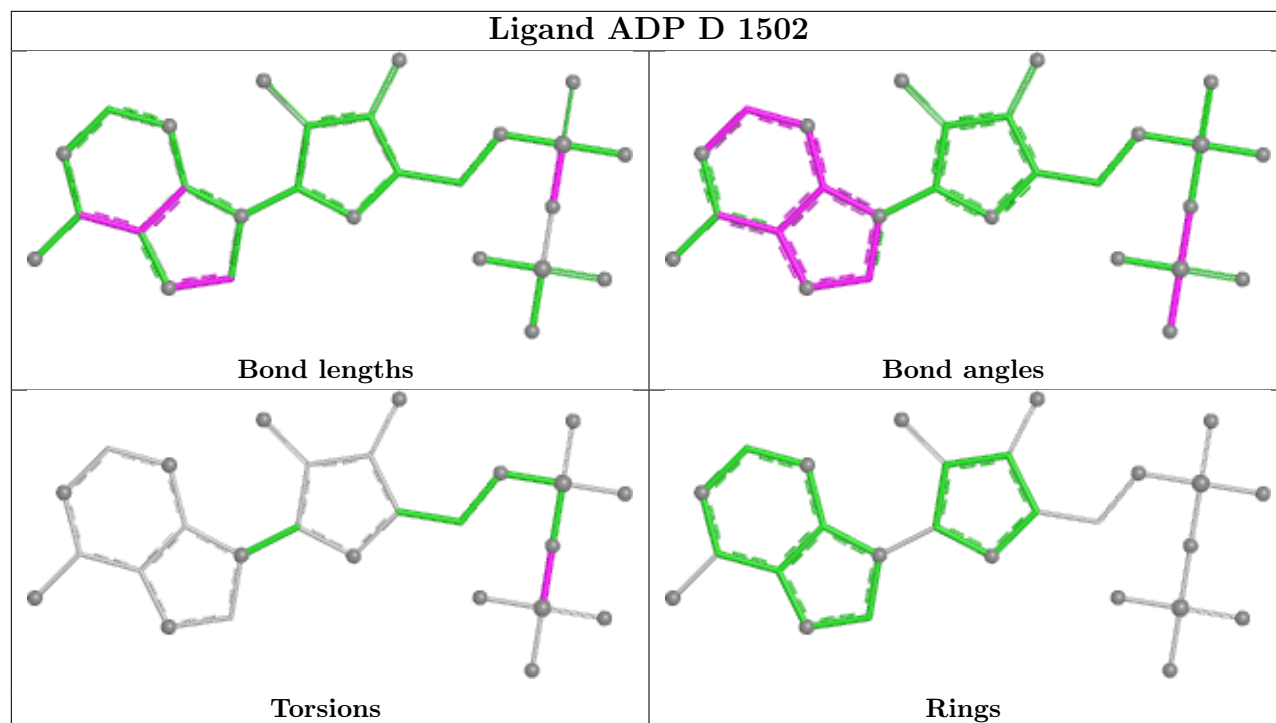
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502	ADP	2	0
6	A	2502	ADP	3	0
5	A	4501	ALF	1	0
6	A	1502	ADP	2	0
6	A	4502	ADP	1	0
6	D	1502	ADP	2	0
6	D	4502	ADP	1	0
6	D	502	ADP	1	0
6	D	3502	ADP	2	0
6	D	2502	ADP	1	0

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.

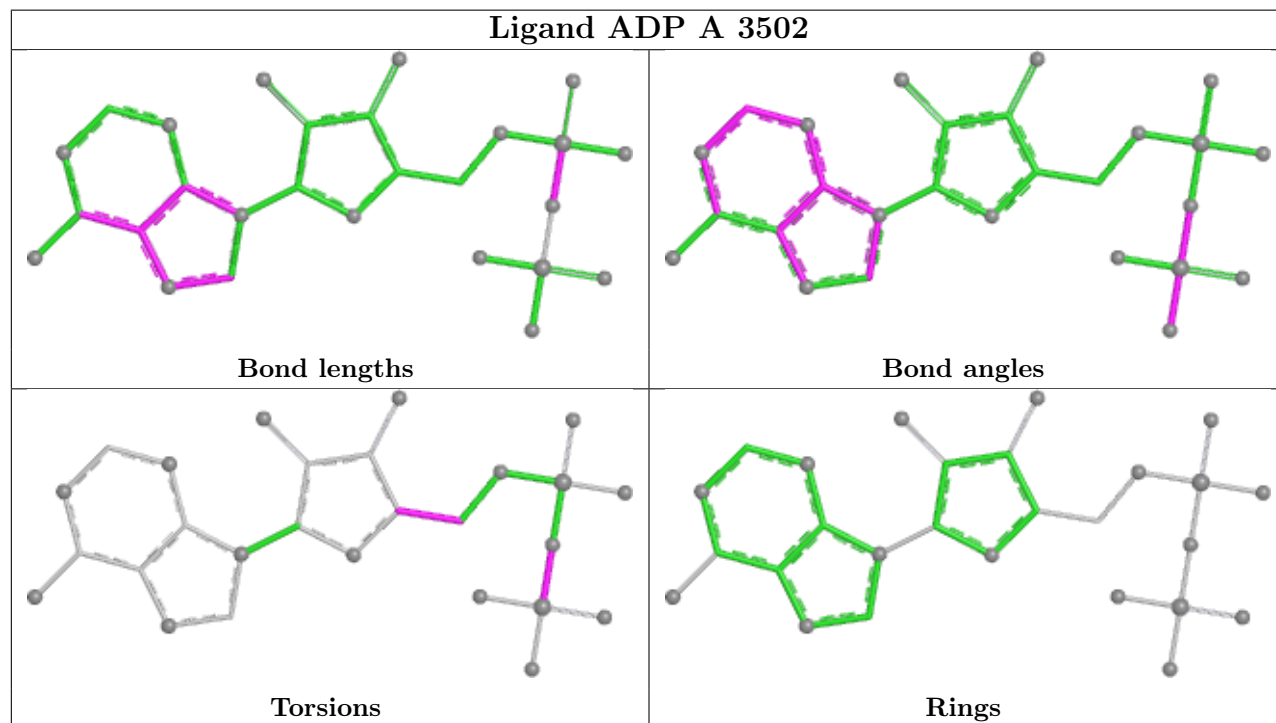


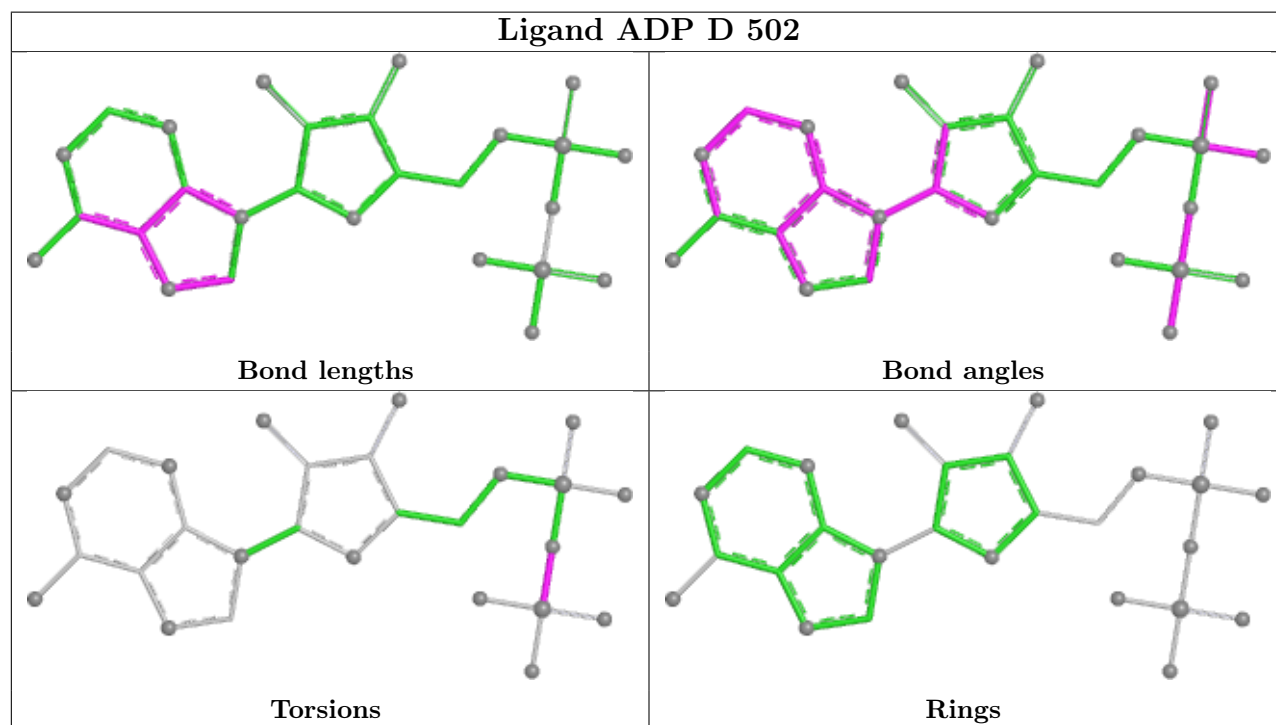
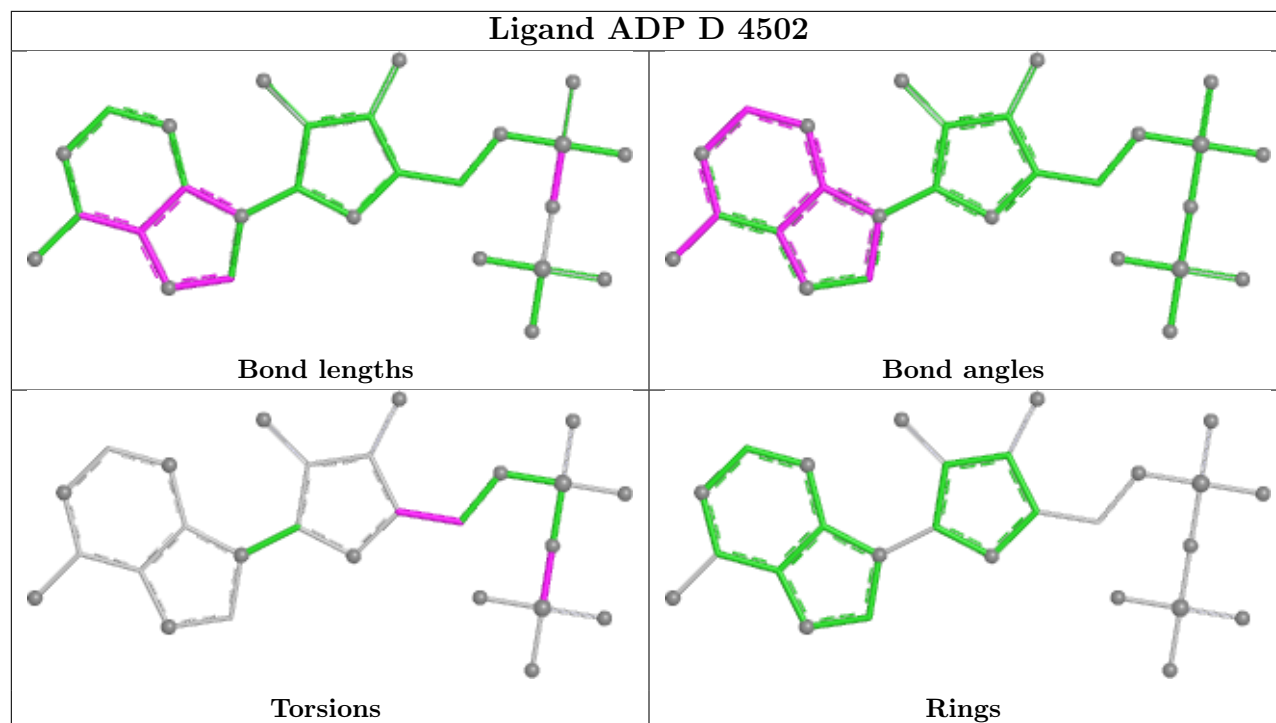


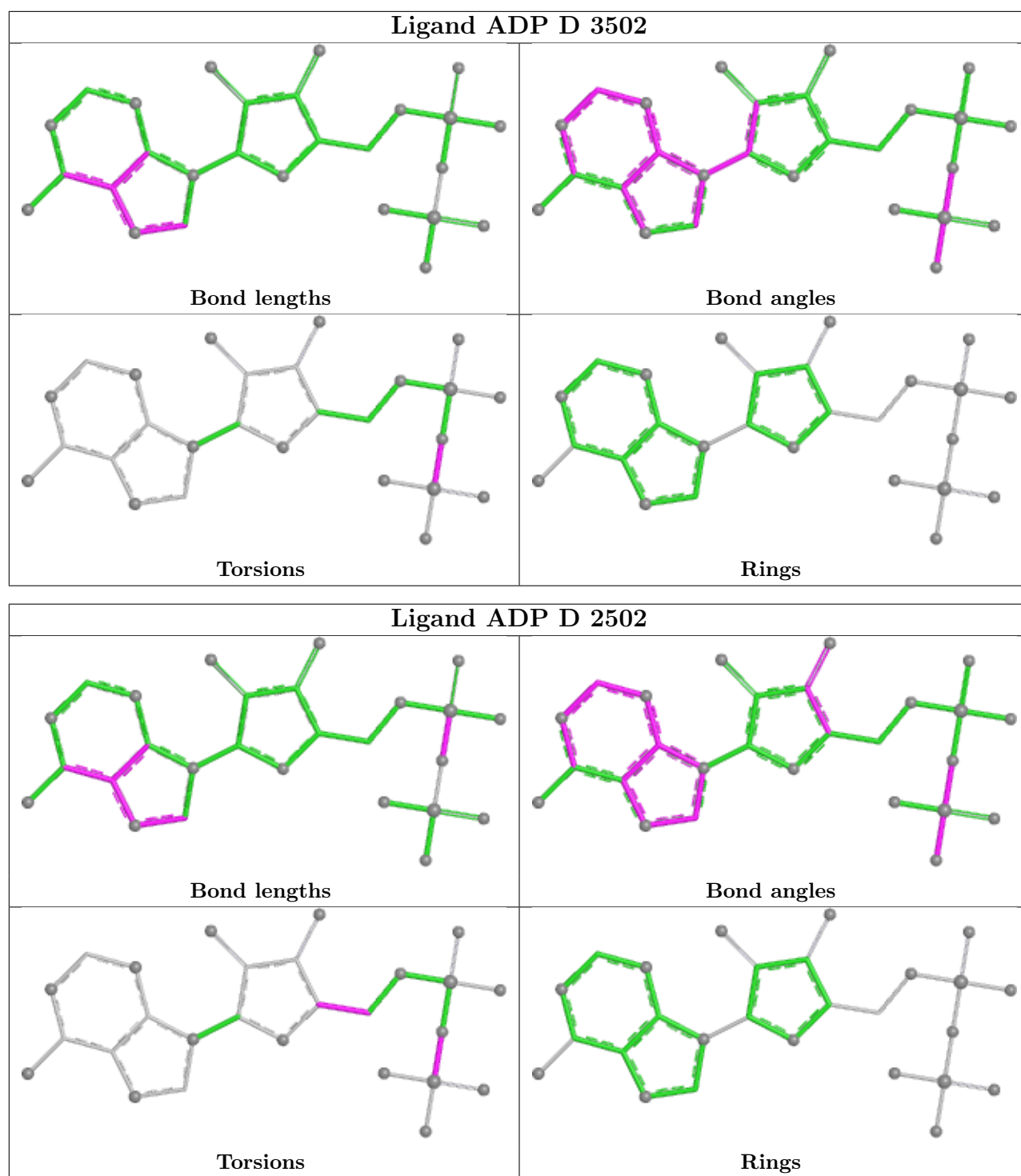
Ligand ADP D 1502



Ligand ADP A 3502







5.7 Other polymers ⓘ

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	13/15 (86%)	-0.18	0 100 100	14, 20, 22, 24	0
1	E	13/15 (86%)	-0.32	0 100 100	11, 19, 23, 28	0
2	C	11/12 (91%)	0.11	1 (9%) 15 14	46, 49, 51, 56	0
2	F	12/12 (100%)	-0.02	0 100 100	47, 49, 51, 51	0
3	A	1603/1706 (93%)	-0.04	14 (0%) 81 68	19, 30, 45, 76	0
3	D	1603/1706 (93%)	-0.14	16 (0%) 79 66	18, 30, 45, 75	0
All	All	3255/3466 (93%)	-0.09	31 (0%) 79 66	11, 30, 48, 76	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	4316	ALA	4.6
3	D	4311	ASP	3.6
3	D	4309	LEU	3.5
3	D	4291	TYR	3.4
3	D	4313	PRO	3.4

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

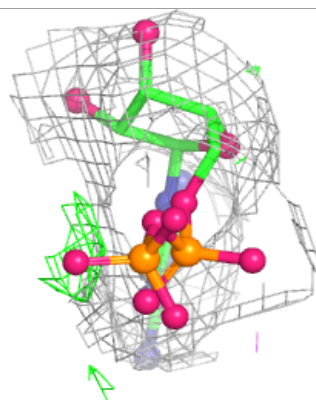
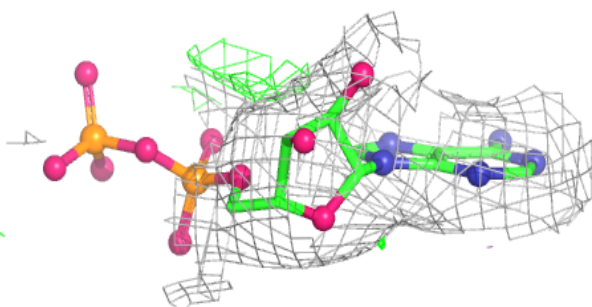
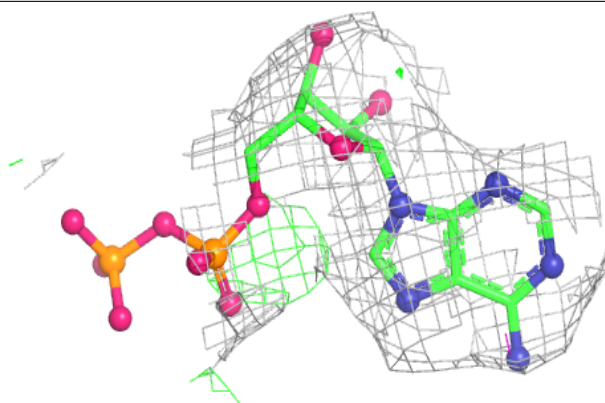
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
5	ALF	D	4501	5/5	0.73	0.14	26,30,32,32	0
4	MG	A	500	1/1	0.90	0.17	24,24,24,24	0
5	ALF	A	4501	5/5	0.92	0.07	36,38,40,40	0
4	MG	D	4500	1/1	0.92	0.15	17,17,17,17	0
6	ADP	A	502	27/27	0.93	0.07	18,21,27,29	0
5	ALF	A	501	5/5	0.94	0.08	17,21,22,23	0
4	MG	D	1500	1/1	0.94	0.16	2,2,2,2	0
5	ALF	A	2501	5/5	0.95	0.07	2,2,2,2	0
6	ADP	A	4502	27/27	0.95	0.07	11,19,23,23	0
5	ALF	D	501	5/5	0.97	0.07	2,2,2,2	0
5	ALF	D	1501	5/5	0.97	0.08	2,2,2,2	0
5	ALF	D	3501	5/5	0.97	0.05	2,2,3,6	0
5	ALF	A	1501	5/5	0.97	0.08	2,2,4,5	0
4	MG	D	500	1/1	0.97	0.05	5,5,5,5	0
6	ADP	A	1502	27/27	0.97	0.06	2,2,3,5	0
6	ADP	A	2502	27/27	0.97	0.06	2,2,2,5	0
6	ADP	A	3502	27/27	0.97	0.06	2,2,2,2	0
4	MG	A	2500	1/1	0.97	0.09	2,2,2,2	0
6	ADP	D	3502	27/27	0.97	0.06	2,4,9,9	0
6	ADP	D	4502	27/27	0.97	0.05	17,19,21,24	0
5	ALF	A	3501	5/5	0.98	0.08	2,2,2,2	0
6	ADP	D	1502	27/27	0.98	0.04	2,2,3,5	0
6	ADP	D	2502	27/27	0.98	0.05	2,5,6,7	0
4	MG	D	2500	1/1	0.98	0.12	2,2,2,2	0
5	ALF	D	2501	5/5	0.98	0.09	2,2,2,2	0
4	MG	A	1500	1/1	0.99	0.08	3,3,3,3	0
4	MG	D	3500	1/1	0.99	0.06	6,6,6,6	0
4	MG	A	3500	1/1	0.99	0.14	2,2,2,2	0
6	ADP	D	502	27/27	0.99	0.04	2,2,4,5	0
4	MG	A	4500	1/1	1.00	0.02	2,2,2,2	0

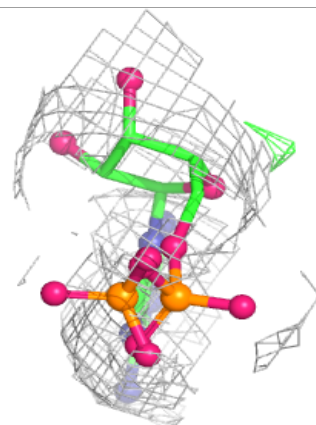
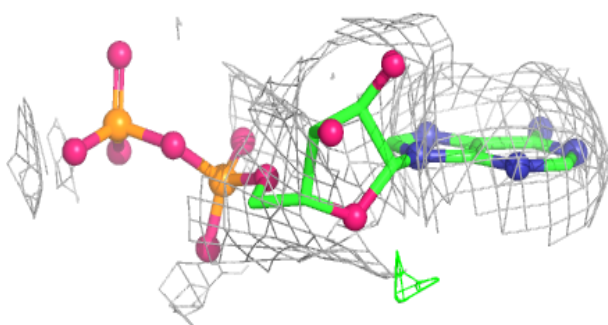
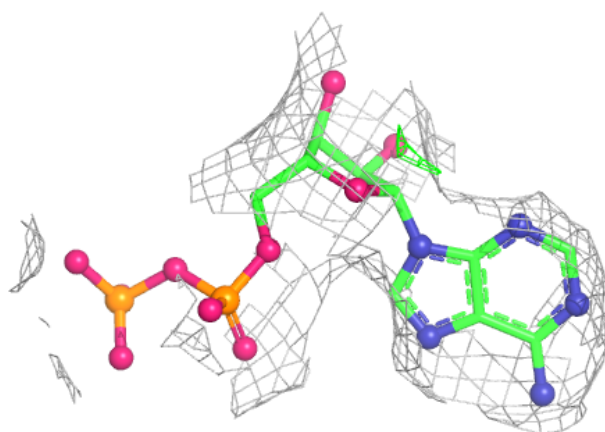
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

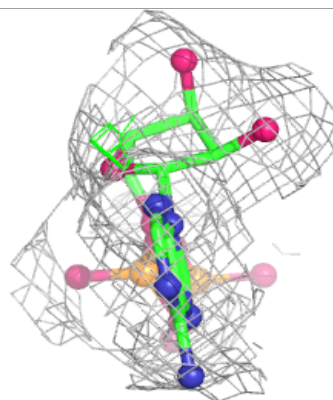
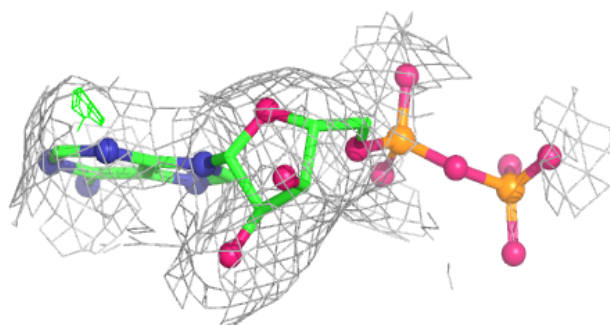
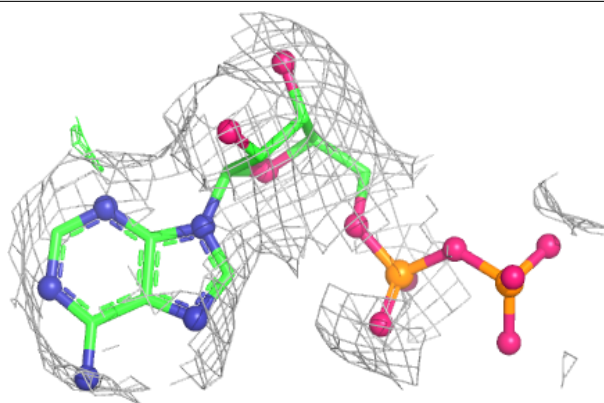
**Electron density around ADP A 4502:**

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

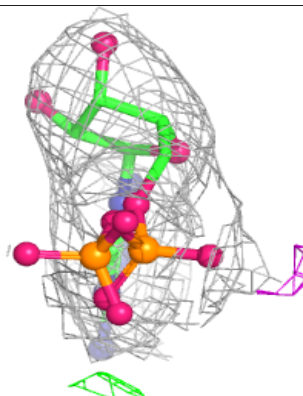
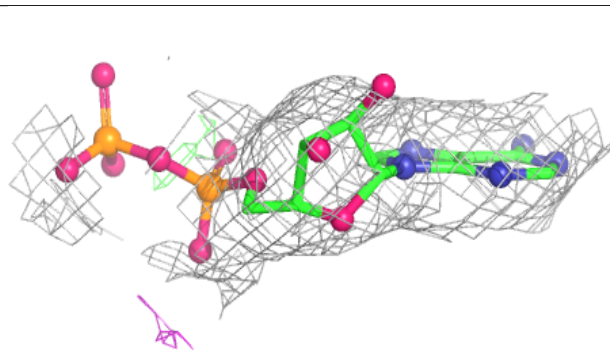
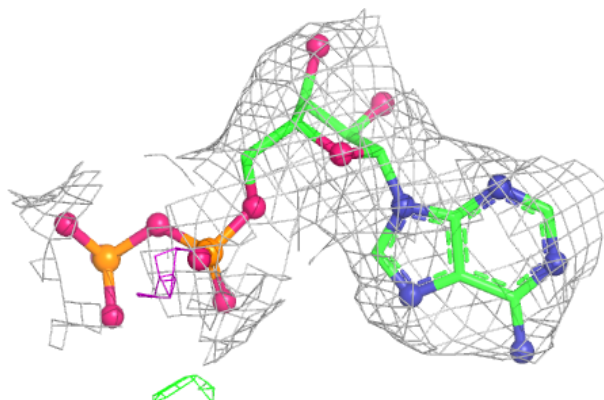


Electron density around ADP A 1502:

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

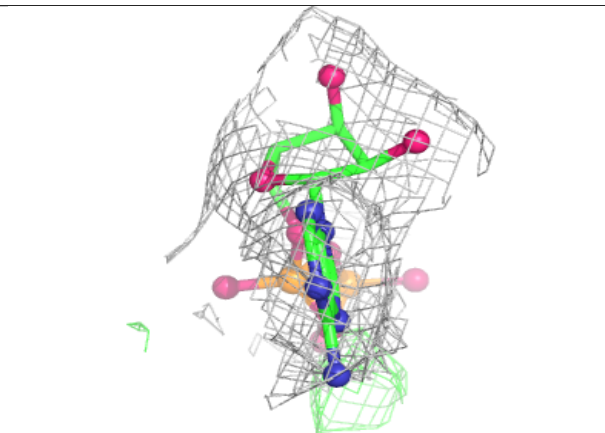
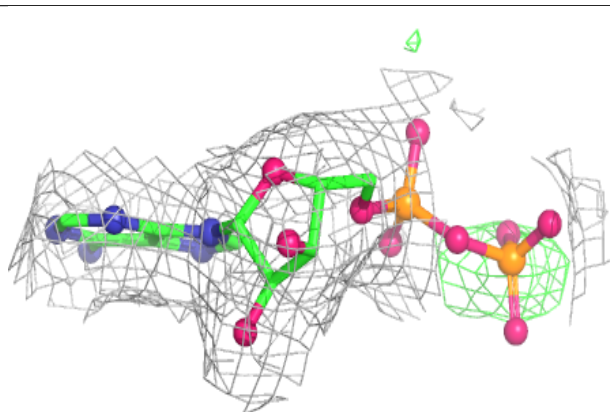
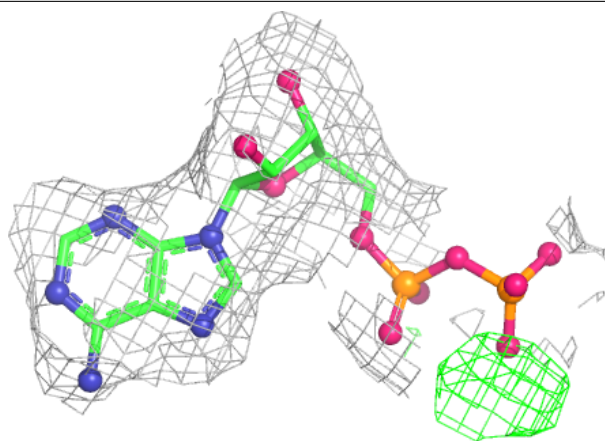
**Electron density around ADP A 2502:**

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

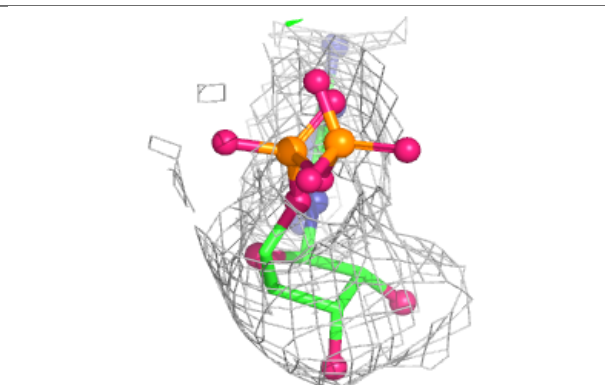
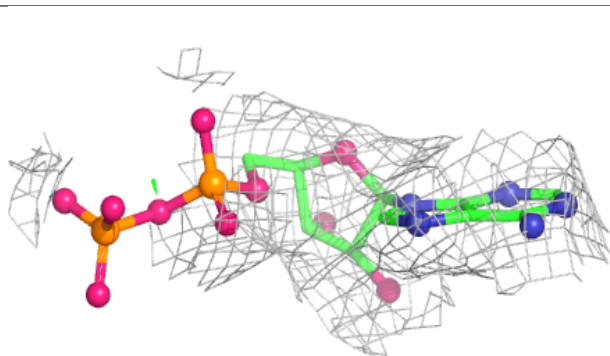
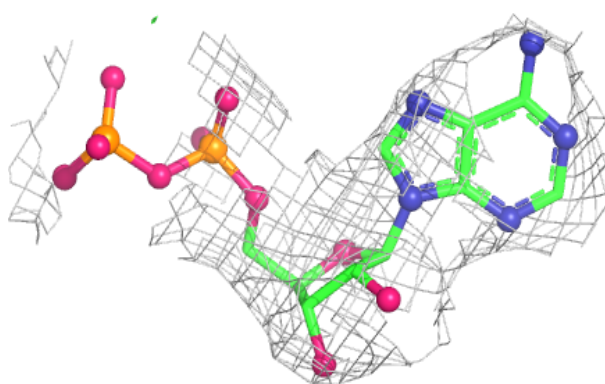


Electron density around ADP A 3502:

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

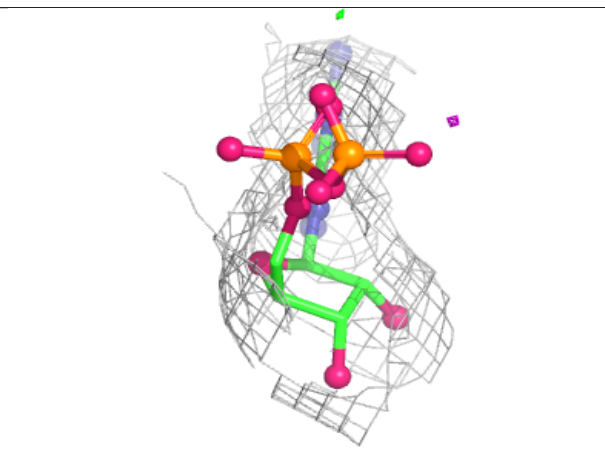
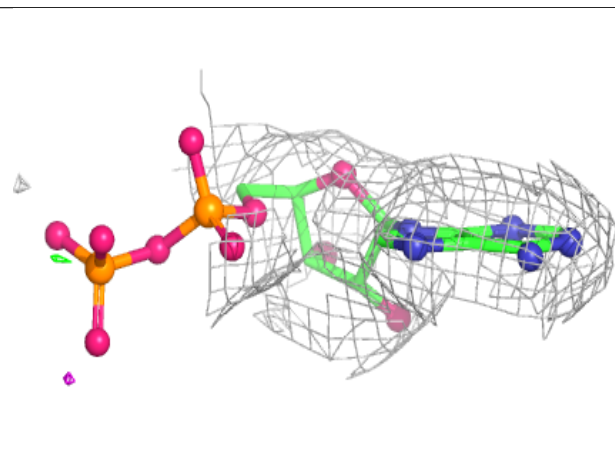
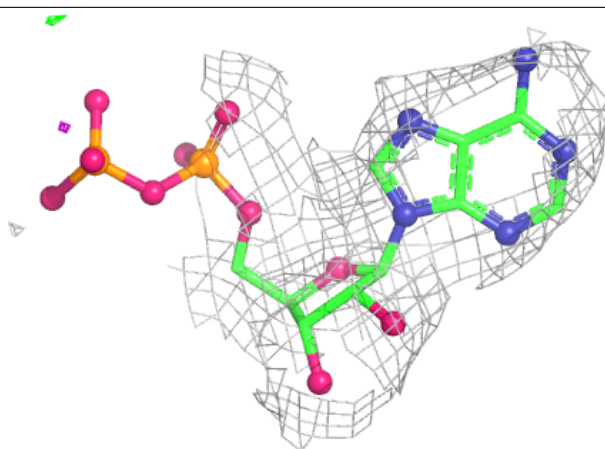
**Electron density around ADP D 3502:**

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

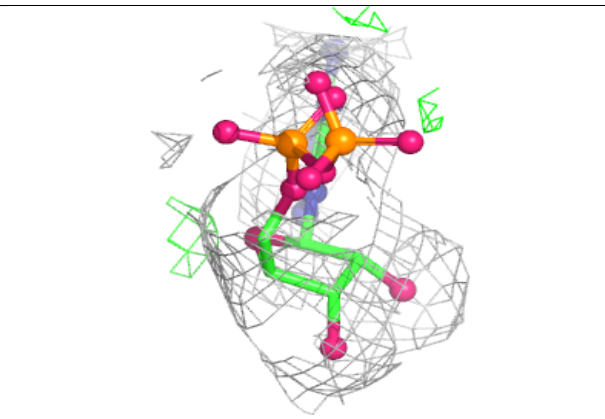
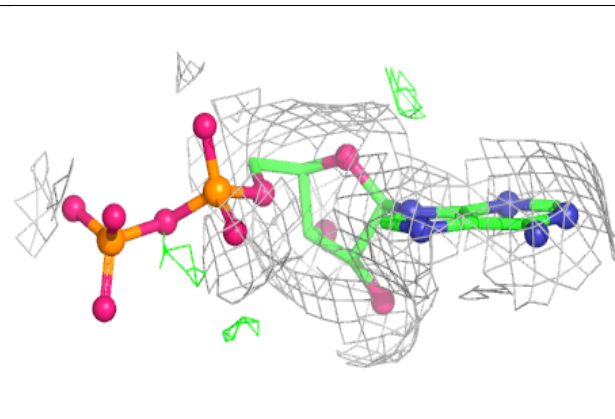
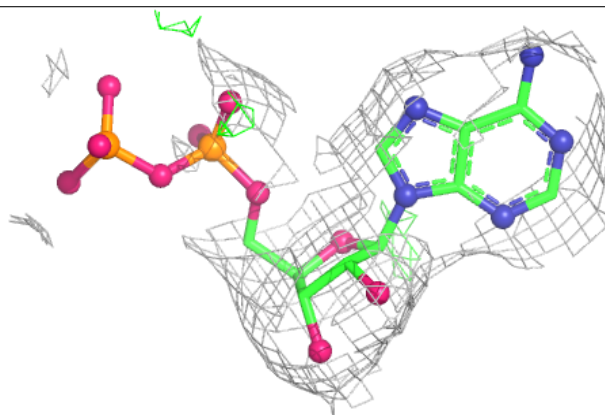


Electron density around ADP D 4502:

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

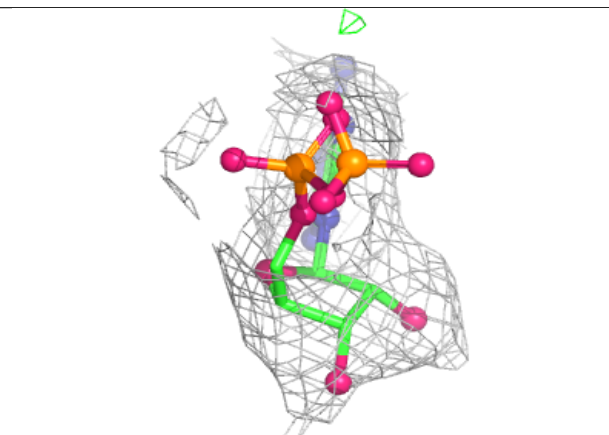
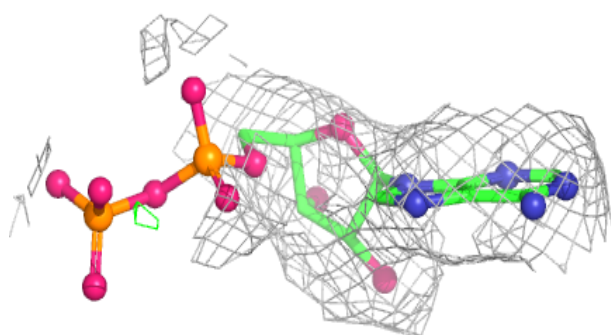
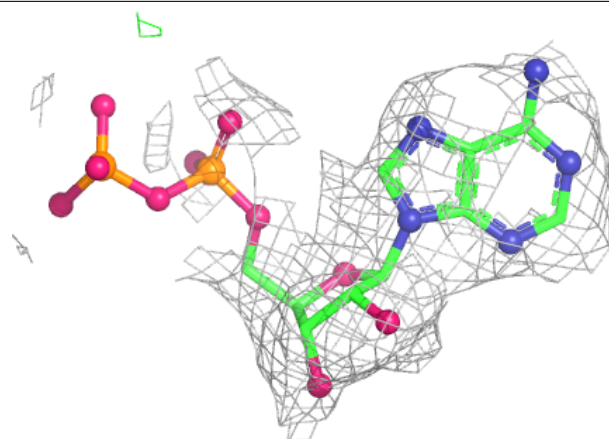
**Electron density around ADP D 1502:**

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

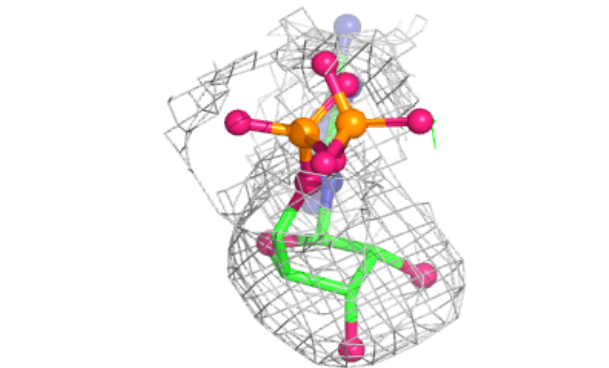
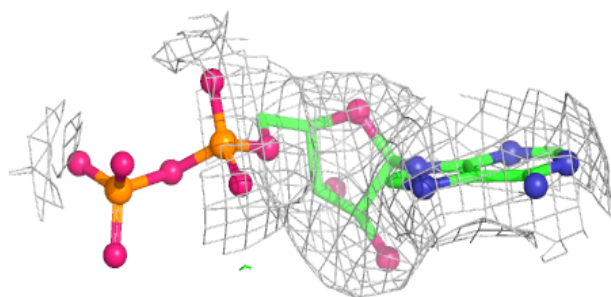
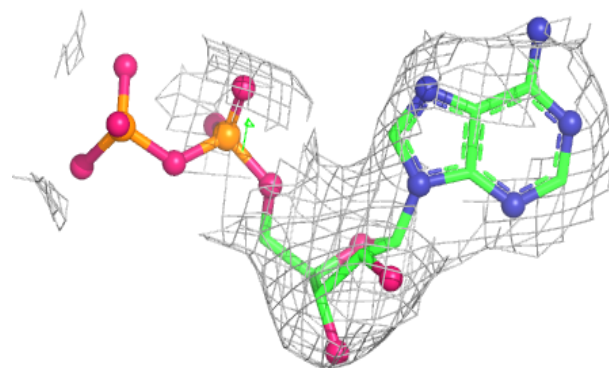


Electron density around ADP D 2502:

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

**Electron density around ADP 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.